Full wwPDB EM Validation Report ⓘ

Sep 11, 2026 – 03:49 AM JST

PDB ID	:	7Y5E / pdb_00007y5e
EMDB ID	:	EMD-33618
Title	:	In situ single-PBS-PSII-PSI-LHCs megacomplex.
Authors	:	You, X.; Zhang, X.; Cheng, J.; Xiao, Y.N.; Sui, S.F.
Deposited on	:	2022-06-17
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

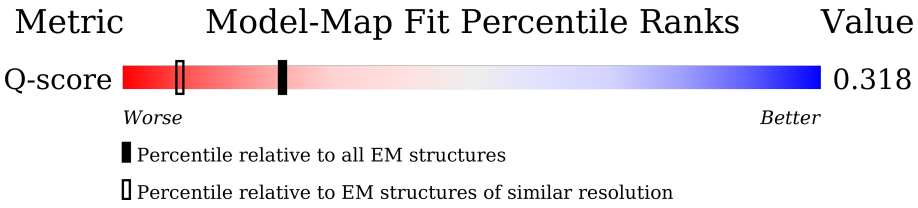
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	15087 (2.80 - 3.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	MEN	B3	71	-	X	-	-
69	MEN	D3	71	-	X	-	-
69	MEN	F3	71	-	X	-	-
69	MEN	H3	71	-	X	-	-
69	MEN	I3	71	-	X	-	-
69	MEN	L3	71	-	X	-	-
69	MEN	M3	71	-	X	-	-
69	MEN	Q3	71	-	X	-	-
69	MEN	S3	71	-	X	-	-
69	MEN	U3	71	-	X	-	-
69	MEN	d3	71	-	X	-	-
69	MEN	f3	71	-	X	-	-
69	MEN	h3	71	-	X	-	-
69	MEN	j3	71	-	X	-	-
69	MEN	k3	71	-	X	-	-
69	MEN	n3	71	-	X	-	-
69	MEN	o3	71	-	X	-	-
69	MEN	q3	71	-	X	-	-
69	MEN	s3	71	-	X	-	-
69	MEN	u3	71	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	MEN	w3	71	-	X	-	-

2 Entry composition (i)

There are 104 unique types of molecules in this entry. The entry contains 1264616 atoms, of which 2032 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	BD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	DD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	FD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	LD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ND	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	II	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	NI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UJ	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
1	WJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	YJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	QM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UM	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
1	WM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YM	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
1	OO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	UP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WP	164	Total	C	N	O	S	0	0
			1246	777	219	243	7		
1	BQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	DQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	FQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	HQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	LQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	NQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	h1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	h4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	I5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	N5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	P5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	X5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	M7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	z8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	p8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	r8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	t8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	v8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	x8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	N9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	P9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	X9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	zC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	pC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	rC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	tC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	vC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	xC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bE	164	Total	C	N	O	S	0	0
			1243	773	219	244	7		
1	dE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	eF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	kF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	qF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	sF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	uF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bG	164	Total	C	N	O	S	0	0
			1243	773	219	244	7		
1	dG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	fG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lG	164	Total	C	N	O	S	0	0
			1246	777	219	243	7		
1	fH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	eK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	kK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	qK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	sK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	uK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 2 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	FA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HA	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	JA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	NA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	RA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	TA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	VA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	XA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	BB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	CB	177	Total	C	N	O	S	0	0
			1291	799	225	255	12		
2	DB	146	Total	C	N	O	S	0	0
			1065	654	187	213	11		
2	FB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	GB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HB	174	Total	C	N	O	S	0	0
			1270	785	222	252	11		
2	IB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LB	177	Total	C	N	O	S	0	0
			1290	797	224	257	12		
2	MB	177	Total	C	N	O	S	0	0
			1284	793	225	254	12		
2	NB	146	Total	C	N	O	S	0	0
			1062	651	187	213	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	OB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	PB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QB	174	Total	C	N	O	S	0	0
			1270	785	222	252	11		
2	RB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SB	177	Total	C	N	O	S	0	0
			1287	794	225	256	12		
2	VB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	XB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	ZB	152	Total	C	N	O	S	0	0
			1111	687	194	219	11		
2	CD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	ED	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	GD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	ID	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	KD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	MD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UD	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	WD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	PE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	VE	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	YE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	BF	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	DF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	HF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	LF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	RF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	TF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	VF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	XF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	ZF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	VG	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	YG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	PH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TH	177	Total	C	N	O	S	0	0
			1288	797	222	257	12		
2	VH	177	Total	C	N	O	S	1	0
			1278	789	225	252	12		
2	YH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	BI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	DI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	FI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HI	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	JI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UI	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	WI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	DJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	HJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	LJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RJ	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	TJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	VJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	XJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	ZJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	BK	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	DK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	HK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	LK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	RK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	TK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	VK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	XK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	ZK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	DM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	HM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JM	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	LM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PM	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RM	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	TM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	VM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	XM	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	ZM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	VO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	BP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	DP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	FP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HP	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	JP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	NP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	PP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TP	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	VP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	XP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	CQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	EQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	GQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	IQ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	KQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	MQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UQ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	WQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	YQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	P1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	R1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	T1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	V1	177	Total	C	N	O	S	2	0
			1291	797	225	257	12		
2	Y1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	g1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	i1	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	k1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	m1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	a1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	c1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	e1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	P4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	R4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	T4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	V4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	i4	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	k4	177	Total	C	N	O	S	0	0
			1288	794	225	257	12		
2	m4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	a4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	c4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	e4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	g4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	B5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	D5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H5	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	J5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	L5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	O5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Q5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	S5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	U5	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	W5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	B7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	D7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H7	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	J7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	N7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	P7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	R7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	T7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	V7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	X7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	y8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	18	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	q8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	s8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	u8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	w8	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	B9	177	Total	C	N	O	S	0	0
			1291	799	224	256	12		
2	D9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H9	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	J9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	L9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	O9	177	Total	C	N	O	S	0	0
			1291	799	224	256	12		
2	Q9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	S9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	U9	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	W9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	aB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	bB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	dB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gB	152	Total	C	N	O	S	0	0
			1101	679	194	217	11		
2	yC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	1C	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	qC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	sC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	uC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	wC	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	aE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	iE	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	kE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	mE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	bF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	dF	177	Total	C	N	O	S	2	0
			1296	802	225	257	12		
2	fF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	hF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	jF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	lF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	nF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	pF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	rF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	tF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	vF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	aG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eG	177	Total	C	N	O	S	0	0
			1290	797	224	257	12		
2	gG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	iG	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	kG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	mG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	iH	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	kH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	mH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	aH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	eJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	gJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	iJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	kJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	mJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	bK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	dK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	fK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	hK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	jK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	lK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	nK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	pK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	rK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	tK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	vK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	cM	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	eM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	gM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	iM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	kM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	mM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	iO	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	kO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	mO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	aO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

- Molecule 3 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	YA	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
3	AD	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
3	AE	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	AG	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	AH	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AO	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	AQ	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
3	A1	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	A4	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	Y7	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		

- Molecule 4 is a protein called Linker4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AB	103	Total	C	N	O	S	0	0
			781	497	130	150	4		
4	EB	103	Total	C	N	O	S	0	0
			777	492	130	150	5		

- Molecule 5 is a protein called CaRSPs1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	KB	226	Total	C	N	O	S	0	0
			1721	1085	305	322	9		
5	UB	226	Total	C	N	O	S	0	0
			1723	1086	305	323	9		

- Molecule 6 is a protein called CaRSP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	WB	134	Total	C	N	O	S	0	0
			1032	655	176	198	3		
6	cB	139	Total	C	N	O	S	0	0
			1068	675	181	210	2		

- Molecule 7 is a protein called LRH.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AC	150	Total	C	N	O	0	0
			750	450	150	150		
7	A8	150	Total	C	N	O	0	0
			750	450	150	150		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	a8	87	Total 435	C 261	N 87	O 87	0	0
7	aC	87	Total 435	C 261	N 87	O 87	0	0

- Molecule 8 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BE	231	Total 1897	C 1212	N 332	O 349	S 4	0	0
8	BG	231	Total 1897	C 1212	N 332	O 349	S 4	0	0
8	BH	227	Total 1874	C 1197	N 328	O 345	S 4	0	0
8	BO	230	Total 1889	C 1206	N 331	O 348	S 4	0	0
8	B1	227	Total 1874	C 1197	N 328	O 345	S 4	0	0
8	B4	230	Total 1889	C 1206	N 331	O 348	S 4	0	0

- Molecule 9 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	EE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	GE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	IE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	KE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	ME	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	CG	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	EG	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	GG	162	Total 1228	C 773	N 209	O 240	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	IG	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KG	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MG	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	CH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	EH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	GH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	IH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	CO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	EO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	GO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	IO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	M1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	C1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	E1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	G1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	I1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	K1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	G4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	I4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	K4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	M4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	C4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	E4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

- Molecule 10 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JG	172	Total	C	N	O	S	0	0
			1269	785	224	251	9		
10	LG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	FH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HH	172	Total	C	N	O	S	0	0
			1262	781	221	251	9		
10	JH	172	Total	C	N	O	S	0	0
			1268	784	224	251	9		
10	LH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	N4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

- Molecule 11 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	XE	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	XG	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	XH	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	XO	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	X1	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	X4	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XE	275	ALA	SER	conflict	UNP A0A5J4YM59
XG	275	ALA	SER	conflict	UNP A0A5J4YM59
XH	275	ALA	SER	conflict	UNP A0A5J4YM59
XO	275	ALA	SER	conflict	UNP A0A5J4YM59
X1	275	ALA	SER	conflict	UNP A0A5J4YM59
X4	275	ALA	SER	conflict	UNP A0A5J4YM59

- Molecule 12 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	MI	265	Total	C	N	O	S	0	0
			2079	1309	364	396	10		
12	ZI	265	Total	C	N	O	S	0	0
			2085	1313	364	398	10		

- Molecule 13 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	AM	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	wF	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	xF	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	wK	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	xK	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		

- Molecule 14 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	BM	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	yF	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	yK	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		

- Molecule 15 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	334	Total	C	N	O	S	0	0
			2571	1683	420	455	13		
15	A6	334	Total	C	N	O	S	0	0
			2565	1678	420	454	13		
15	a6	334	Total	C	N	O	S	0	0
			2565	1678	420	454	13		
15	aL	334	Total	C	N	O	S	0	0
			2571	1683	420	455	13		

- Molecule 16 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	506	Total	C	N	O	S	0	0
			3928	2571	657	688	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	B6	506	Total	C	N	O	S	0	0
			3928	2571	657	688	12		
16	b6	506	Total	C	N	O	S	0	0
			3928	2571	657	688	12		
16	bL	506	Total	C	N	O	S	0	0
			3934	2574	660	688	12		

- Molecule 17 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CL	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		
17	C6	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		
17	c6	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		
17	cL	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		

- Molecule 18 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DL	341	Total	C	N	O	S	0	0
			2699	1785	438	464	12		
18	D6	341	Total	C	N	O	S	0	0
			2699	1785	438	464	12		
18	d6	342	Total	C	N	O	S	0	0
			2703	1787	439	465	12		
18	dL	342	Total	C	N	O	S	0	0
			2703	1787	439	465	12		

- Molecule 19 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	EL	78	Total	C	N	O	0	0
			616	402	104	110		
19	E6	78	Total	C	N	O	0	0
			616	402	104	110		
19	e6	79	Total	C	N	O	0	0
			622	404	105	113		
19	eL	79	Total	C	N	O	0	0
			622	404	105	113		

- Molecule 20 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	FL	41	Total	C	N	O	S	0	0
			318	215	51	51	1		
20	F6	41	Total	C	N	O	S	0	0
			318	215	51	51	1		
20	f6	41	Total	C	N	O	S	0	0
			324	218	54	51	1		
20	fL	41	Total	C	N	O	S	0	0
			324	218	54	51	1		

- Molecule 21 is a protein called PSII_Pbs31 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	GL	152	Total	C	N	O	S	0	0
			1161	738	197	224	2		
21	G6	152	Total	C	N	O	S	0	0
			1161	738	197	224	2		
21	g6	145	Total	C	N	O	S	0	0
			1106	702	189	213	2		
21	gL	145	Total	C	N	O	S	0	0
			1106	702	189	213	2		

- Molecule 22 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	HL	66	Total	C	N	O	S	0	0
			508	340	78	88	2		
22	H6	66	Total	C	N	O	S	0	0
			508	340	78	88	2		
22	h6	65	Total	C	N	O	S	0	0
			500	336	76	86	2		
22	hL	65	Total	C	N	O	S	0	0
			500	336	76	86	2		

- Molecule 23 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	IL	35	Total	C	N	O	S	0	0
			295	201	46	47	1		
23	I6	35	Total	C	N	O	S	0	0
			295	201	46	47	1		
23	i6	35	Total	C	N	O	S	0	0
			295	201	46	47	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
23	iL	35	Total	C	N	O	S	0	0
			295	201	46	47	1		

- Molecule 24 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	JL	36	Total	C	N	O	0	0
			255	173	40	42		
24	J6	36	Total	C	N	O	0	0
			255	173	40	42		
24	j6	36	Total	C	N	O	0	0
			255	173	40	42		
24	jL	36	Total	C	N	O	0	0
			255	173	40	42		

- Molecule 25 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	KL	37	Total	C	N	O	0	0
			294	209	43	42		
25	K6	37	Total	C	N	O	0	0
			294	209	43	42		
25	k6	37	Total	C	N	O	0	0
			294	209	43	42		
25	kL	37	Total	C	N	O	0	0
			294	209	43	42		

- Molecule 26 is a protein called PsbL.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	LL	37	Total	C	N	O	0	0
			302	204	48	50		
26	L6	37	Total	C	N	O	0	0
			302	204	48	50		
26	l6	37	Total	C	N	O	0	0
			302	204	48	50		
26	lL	37	Total	C	N	O	0	0
			302	204	48	50		

- Molecule 27 is a protein called PsbM.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	ML	42	Total	C	N	O	S	0	0
			306	203	48	54	1		
27	M6	42	Total	C	N	O	S	0	0
			306	203	48	54	1		
27	m6	42	Total	C	N	O	S	0	0
			306	203	48	54	1		
27	mL	42	Total	C	N	O	S	0	0
			306	203	48	54	1		

- Molecule 28 is a protein called Psb34.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	NL	29	Total	C	N	O	0	0
			145	87	29	29		
28	N6	29	Total	C	N	O	0	0
			145	87	29	29		
28	n6	27	Total	C	N	O	0	0
			135	81	27	27		
28	nL	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 29 is a protein called Oxygen-evolving enhancer protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	OL	254	Total	C	N	O	S	0	0
			1857	1167	305	376	9		
29	O6	254	Total	C	N	O	S	0	0
			1857	1167	305	376	9		
29	o6	254	Total	C	N	O	S	0	0
			1859	1168	305	377	9		
29	oL	254	Total	C	N	O	S	0	0
			1859	1168	305	377	9		

- Molecule 30 is a protein called PsbQ'.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	QL	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		
30	Q6	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		
30	q6	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
30	qL	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		

- Molecule 31 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	RL	33	Total	C	N	O	0	0
			263	175	47	41		
31	R6	33	Total	C	N	O	0	0
			263	175	47	41		
31	r6	33	Total	C	N	O	0	0
			263	175	47	41		
31	rL	33	Total	C	N	O	0	0
			263	175	47	41		

- Molecule 32 is a protein called LPP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	SL	119	Total	C	N	O	0	0
			595	357	119	119		
32	S6	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 33 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	TL	31	Total	C	N	O	S	0	0
			252	177	36	37	2		
33	T6	31	Total	C	N	O	S	0	0
			252	177	36	37	2		
33	t6	31	Total	C	N	O	S	0	0
			252	177	36	37	2		
33	tL	31	Total	C	N	O	S	0	0
			252	177	36	37	2		

- Molecule 34 is a protein called PS II complex 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	UL	93	Total	C	N	O	S	0	0
			726	460	120	143	3		
34	U6	93	Total	C	N	O	S	0	0
			726	460	120	143	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	u6	93	Total	C	N	O	S	0	0
			735	466	121	145	3		
34	uL	93	Total	C	N	O	S	0	0
			735	466	121	145	3		

- Molecule 35 is a protein called Cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	VL	134	Total	C	N	O	S	0	0
			980	615	168	193	4		
35	V6	134	Total	C	N	O	S	0	0
			980	615	168	193	4		
35	v6	134	Total	C	N	O	S	0	0
			980	615	168	193	4		
35	vL	134	Total	C	N	O	S	0	0
			980	615	168	193	4		

- Molecule 36 is a protein called PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	WL	46	Total	C	N	O	0	0
			230	138	46	46		
36	W6	46	Total	C	N	O	0	0
			230	138	46	46		
36	w6	46	Total	C	N	O	0	0
			230	138	46	46		
36	wL	46	Total	C	N	O	0	0
			230	138	46	46		

- Molecule 37 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	XL	39	Total	C	N	O	S	0	0
			268	177	40	50	1		
37	X6	39	Total	C	N	O	S	0	0
			268	177	40	50	1		
37	x6	39	Total	C	N	O	S	0	0
			278	183	44	50	1		
37	xL	39	Total	C	N	O	S	0	0
			278	183	44	50	1		

- Molecule 38 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	YL	33	Total	C	N	O	S	0	0
			251	172	40	38	1		
38	Y6	33	Total	C	N	O	S	0	0
			251	172	40	38	1		
38	y6	33	Total	C	N	O	S	0	0
			251	172	40	38	1		
38	yL	33	Total	C	N	O	S	0	0
			251	172	40	38	1		

- Molecule 39 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	ZL	59	Total	C	N	O		0	0
			438	294	67	77			
39	Z6	60	Total	C	N	O	S	0	0
			446	299	68	78	1		
39	z6	60	Total	C	N	O	S	0	0
			446	299	68	78	1		
39	zL	59	Total	C	N	O		0	0
			438	294	67	77			

- Molecule 40 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AN	745	Total	C	N	O	S	0	0
			5843	3819	1000	997	27		
40	A2	745	Total	C	N	O	S	0	0
			5843	3819	1000	997	27		

- Molecule 41 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BN	732	Total	C	N	O	S	0	0
			5828	3834	980	996	18		
41	B2	732	Total	C	N	O	S	0	0
			5828	3834	980	996	18		

- Molecule 42 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	CN	80	Total	C	N	O	S	0	0
			595	368	104	114	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	C2	80	Total 595	C 368	N 104	O 114	S 9	0	0

- Molecule 43 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	DN	130	Total 989	C 627	N 170	O 189	S 3	0	0
43	D2	130	Total 989	C 627	N 170	O 189	S 3	0	0

- Molecule 44 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	EN	58	Total 466	C 295	N 82	O 89	0	0
44	E2	58	Total 466	C 295	N 82	O 89	0	0

- Molecule 45 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	FN	158	Total 1245	C 813	N 207	O 222	S 3	0	0
45	F2	158	Total 1245	C 813	N 207	O 222	S 3	0	0

- Molecule 46 is a protein called Cytochrome c6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	GN	84	Total 620	C 378	N 110	O 127	S 5	0	0
46	G2	84	Total 620	C 378	N 110	O 127	S 5	0	0

- Molecule 47 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	IN	31	Total 239	C 168	N 32	O 38	S 1	0	0
47	I2	31	Total 239	C 168	N 32	O 38	S 1	0	0

- Molecule 48 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	JN	38	Total	C	N	O	S	0	0
			308	211	45	50	2		
48	J2	38	Total	C	N	O	S	0	0
			308	211	45	50	2		

- Molecule 49 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	KN	70	Total	C	N	O	S	0	0
			489	315	82	89	3		
49	K2	70	Total	C	N	O	S	0	0
			489	315	82	89	3		

- Molecule 50 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LN	140	Total	C	N	O	S	0	0
			1055	689	166	198	2		
50	L2	140	Total	C	N	O	S	0	0
			1055	689	166	198	2		

- Molecule 51 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	MN	30	Total	C	N	O	S	0	0
			223	146	35	41	1		
51	M2	30	Total	C	N	O	S	0	0
			223	146	35	41	1		

- Molecule 52 is a protein called Ferredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	NN	99	Total	C	N	O	S	0	0
			737	451	114	165	7		
52	N2	99	Total	C	N	O	S	0	0
			737	451	114	165	7		

- Molecule 53 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ON	92	Total	C	N	O	S	0	0
			699	462	112	123	2		
53	O2	92	Total	C	N	O	S	0	0
			699	462	112	123	2		

- Molecule 54 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	RN	78	Total	C	N	O	S	0	0
			582	380	93	108	1		
54	R2	78	Total	C	N	O	S	0	0
			582	380	93	108	1		

- Molecule 55 is a protein called LPS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	ZN	66	Total	C	N	O	0	0
			330	198	66	66		
55	Z2	66	Total	C	N	O	0	0
			330	198	66	66		

- Molecule 56 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	YP	372	Total	C	N	O	S	0	0
			2832	1780	483	557	12		
56	bP	372	Total	C	N	O	S	0	0
			2826	1777	480	557	12		

- Molecule 57 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	12	174	Total	C	N	O	S	0	0
			1330	876	208	236	10		
57	1N	174	Total	C	N	O	S	0	0
			1330	876	208	236	10		

- Molecule 58 is a protein called Chlorophyll a-b binding protein of LHCII type III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	22	166	Total	C	N	O	S	0	0
			1229	811	192	223	3		
58	2N	166	Total	C	N	O	S	0	0
			1229	811	192	223	3		

- Molecule 59 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	32	169	Total	C	N	O	S	0	0
			1256	818	203	225	10		
59	3N	169	Total	C	N	O	S	0	0
			1256	818	203	225	10		

- Molecule 60 is a protein called Chlorophyll a-b binding protein 1B-21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	42	172	Total	C	N	O	S	0	0
			1332	879	208	233	12		
60	4N	172	Total	C	N	O	S	0	0
			1332	879	208	233	12		

- Molecule 61 is a protein called Chlorophyll a-b binding protein 1B-21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	52	174	Total	C	N	O	S	0	0
			1328	860	222	236	10		
61	5N	174	Total	C	N	O	S	0	0
			1328	860	222	236	10		

- Molecule 62 is a protein called Chlorophyll a-b binding protein 1B-21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	62	169	Total	C	N	O	S	0	0
			1314	857	216	233	8		
62	6N	169	Total	C	N	O	S	0	0
			1314	857	216	233	8		

- Molecule 63 is a protein called Fucoxanthin-chlorophyll a-c binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	72	164	Total	C	N	O	S	0	0
			1270	828	209	227	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
63	7N	164	Total	C	N	O	S	0	0
			1270	828	209	227	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
72	?	-	LYS	deletion	UNP A0A5J4YKR2
72	?	-	THR	deletion	UNP A0A5J4YKR2
7N	?	-	LYS	deletion	UNP A0A5J4YKR2
7N	?	-	THR	deletion	UNP A0A5J4YKR2

- Molecule 64 is a protein called RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	82	180	Total	C	N	O	S	0	0
			1378	896	232	243	7		
64	8N	180	Total	C	N	O	S	0	0
			1378	896	232	243	7		

- Molecule 65 is a protein called Lrc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	23	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		
65	Z3	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		

- Molecule 66 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	33	253	Total	C	N	O	S	0	0
			1889	1186	325	371	7		
66	a3	253	Total	C	N	O	S	0	0
			1894	1189	325	373	7		

- Molecule 67 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	43	206	Total	C	N	O	S	0	0
			1528	980	259	284	5		
67	b3	206	Total	C	N	O	S	0	0
			1532	982	259	286	5		

- Molecule 68 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	C3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	E3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	G3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	J3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	K3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	N3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	P3	160	Total	C	N	O	S	0	0
			1221	766	211	237	7		
68	R3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	T3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	c3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	e3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	g3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	i3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	l3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	m3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	p3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	r3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	t3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	v3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		

- Molecule 69 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	B3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	D3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	F3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	H3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	I3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	L3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	M3	161	Total	C	N	O	S	0	0
			1216	764	205	240	7		
69	O3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	Q3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	S3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	U3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	d3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	f3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	h3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	j3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	k3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	n3	161	Total	C	N	O	S	0	0
			1217	766	206	238	7		
69	o3	161	Total	C	N	O	S	0	0
			1216	764	205	240	7		
69	q3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	s3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	u3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	w3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 70 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V3	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
70	x3	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 71 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	W3	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		
71	y3	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

- Molecule 72 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	X3	92	Total	C	N	O	S	0	0
			720	453	127	135	5		
72	z3	92	Total	C	N	O	S	0	0
			720	453	127	135	5		

- Molecule 73 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	63	868	Total	C	N	O	S	0	0
			6933	4434	1198	1286	15		
73	73	865	Total	C	N	O	S	0	0
			6907	4421	1194	1277	15		

- Molecule 74 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	M5	238	Total	C	N	O	S	0	0
			1851	1140	348	348	15		
74	Z5	238	Total	C	N	O	S	0	0
			1851	1140	348	348	15		
74	Z9	275	Total	C	N	O	S	0	0
			2148	1327	404	401	16		
74	M9	275	Total	C	N	O	S	0	0
			2142	1324	401	401	16		

- Molecule 75 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	e7	248	Total	C	N	O	S	0	0
			1932	1217	336	369	10		
75	eA	248	Total	C	N	O	S	0	0
			1932	1217	336	369	10		

- Molecule 76 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	fB	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		
76	hB	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		

- Molecule 77 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	dD	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		
77	dQ	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		

- Molecule 78 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	zF	462	Total	C	N	O	S	0	0
			3610	2280	636	679	15		
78	zK	463	Total	C	N	O	S	0	0
			3622	2288	637	682	15		

- Molecule 79 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	bJ	407	Total	C	N	O	S	0	0
			3083	1946	535	590	12		
79	bM	405	Total	C	N	O	S	0	0
			3082	1943	536	588	15		

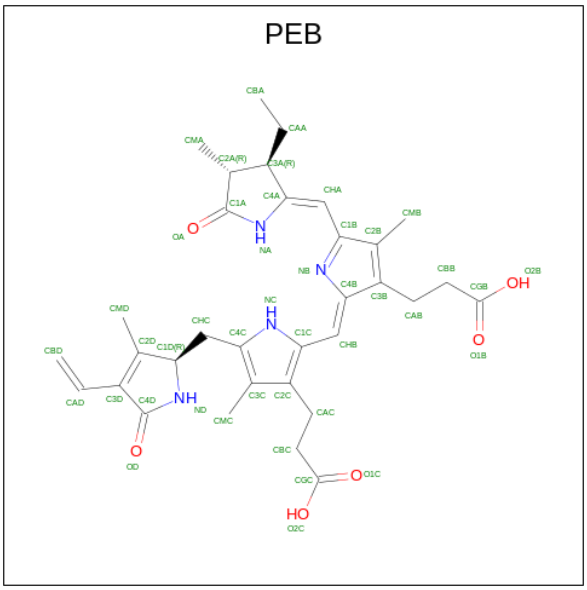
- Molecule 80 is a protein called LPP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Y3	61	Total	C	N	O	S	0	0
			415	256	77	79	3		
80	53	57	Total	C	N	O	S	0	0
			369	230	70	66	3		

- Molecule 81 is a protein called CNT.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	46	118	Total	C	N	O	0	0
			590	354	118	118		
81	16	118	Total	C	N	O	0	0
			590	354	118	118		
81	4L	118	Total	C	N	O	0	0
			590	354	118	118		
81	1L	118	Total	C	N	O	0	0
			590	354	118	118		

- Molecule 82 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
82	AA	1	Total	C	N	O	0
			43	33	4	6	
82	AA	1	Total	C	N	O	0
			43	33	4	6	
82	BA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	BA	1	Total	C	N	O	0
			43	33	4	6	
82	BA	1	Total	C	N	O	0
			43	33	4	6	
82	CA	1	Total	C	N	O	0
			43	33	4	6	
82	CA	1	Total	C	N	O	0
			43	33	4	6	
82	DA	1	Total	C	N	O	0
			43	33	4	6	
82	DA	1	Total	C	N	O	0
			43	33	4	6	
82	DA	1	Total	C	N	O	0
			43	33	4	6	
82	EA	1	Total	C	N	O	0
			43	33	4	6	
82	EA	1	Total	C	N	O	0
			43	33	4	6	
82	FA	1	Total	C	N	O	0
			43	33	4	6	
82	FA	1	Total	C	N	O	0
			43	33	4	6	
82	FA	1	Total	C	N	O	0
			43	33	4	6	
82	GA	1	Total	C	N	O	0
			43	33	4	6	
82	GA	1	Total	C	N	O	0
			43	33	4	6	
82	HA	1	Total	C	N	O	0
			43	33	4	6	
82	HA	1	Total	C	N	O	0
			43	33	4	6	
82	HA	1	Total	C	N	O	0
			43	33	4	6	
82	IA	1	Total	C	N	O	0
			43	33	4	6	
82	IA	1	Total	C	N	O	0
			43	33	4	6	
82	JA	1	Total	C	N	O	0
			43	33	4	6	
82	JA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	JA	1	Total	C	N	O	0
			43	33	4	6	
82	KA	1	Total	C	N	O	0
			43	33	4	6	
82	KA	1	Total	C	N	O	0
			43	33	4	6	
82	LA	1	Total	C	N	O	0
			43	33	4	6	
82	LA	1	Total	C	N	O	0
			43	33	4	6	
82	LA	1	Total	C	N	O	0
			43	33	4	6	
82	MA	1	Total	C	N	O	0
			43	33	4	6	
82	MA	1	Total	C	N	O	0
			43	33	4	6	
82	NA	1	Total	C	N	O	0
			43	33	4	6	
82	NA	1	Total	C	N	O	0
			43	33	4	6	
82	NA	1	Total	C	N	O	0
			43	33	4	6	
82	OA	1	Total	C	N	O	0
			43	33	4	6	
82	OA	1	Total	C	N	O	0
			43	33	4	6	
82	PA	1	Total	C	N	O	0
			43	33	4	6	
82	PA	1	Total	C	N	O	0
			43	33	4	6	
82	PA	1	Total	C	N	O	0
			43	33	4	6	
82	QA	1	Total	C	N	O	0
			43	33	4	6	
82	QA	1	Total	C	N	O	0
			43	33	4	6	
82	RA	1	Total	C	N	O	0
			43	33	4	6	
82	RA	1	Total	C	N	O	0
			43	33	4	6	
82	RA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	SA	1	Total	C	N	O	0
			43	33	4	6	
82	SA	1	Total	C	N	O	0
			43	33	4	6	
82	TA	1	Total	C	N	O	0
			43	33	4	6	
82	TA	1	Total	C	N	O	0
			43	33	4	6	
82	TA	1	Total	C	N	O	0
			43	33	4	6	
82	UA	1	Total	C	N	O	0
			43	33	4	6	
82	UA	1	Total	C	N	O	0
			43	33	4	6	
82	VA	1	Total	C	N	O	0
			43	33	4	6	
82	VA	1	Total	C	N	O	0
			43	33	4	6	
82	VA	1	Total	C	N	O	0
			43	33	4	6	
82	WA	1	Total	C	N	O	0
			43	33	4	6	
82	WA	1	Total	C	N	O	0
			43	33	4	6	
82	XA	1	Total	C	N	O	0
			43	33	4	6	
82	XA	1	Total	C	N	O	0
			43	33	4	6	
82	XA	1	Total	C	N	O	0
			43	33	4	6	
82	YA	1	Total	C	N	O	0
			43	33	4	6	
82	YA	1	Total	C	N	O	0
			43	33	4	6	
82	YA	1	Total	C	N	O	0
			43	33	4	6	
82	AB	1	Total	C	N	O	0
			43	33	4	6	
82	BB	1	Total	C	N	O	0
			43	33	4	6	
82	BB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	BB	1	Total	C	N	O	0
			43	33	4	6	
82	CB	1	Total	C	N	O	0
			43	33	4	6	
82	CB	1	Total	C	N	O	0
			43	33	4	6	
82	DB	1	Total	C	N	O	0
			43	33	4	6	
82	DB	1	Total	C	N	O	0
			43	33	4	6	
82	DB	1	Total	C	N	O	0
			43	33	4	6	
82	EB	1	Total	C	N	O	0
			43	33	4	6	
82	FB	1	Total	C	N	O	0
			43	33	4	6	
82	GB	1	Total	C	N	O	0
			43	33	4	6	
82	GB	1	Total	C	N	O	0
			43	33	4	6	
82	GB	1	Total	C	N	O	0
			43	33	4	6	
82	HB	1	Total	C	N	O	0
			43	33	4	6	
82	HB	1	Total	C	N	O	0
			43	33	4	6	
82	HB	1	Total	C	N	O	0
			43	33	4	6	
82	IB	1	Total	C	N	O	0
			43	33	4	6	
82	IB	1	Total	C	N	O	0
			43	33	4	6	
82	IB	1	Total	C	N	O	0
			43	33	4	6	
82	JB	1	Total	C	N	O	0
			43	33	4	6	
82	JB	1	Total	C	N	O	0
			43	33	4	6	
82	KB	1	Total	C	N	O	0
			43	33	4	6	
82	KB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	KB	1	Total	C	N	O	0
			43	33	4	6	
82	KB	1	Total	C	N	O	0
			43	33	4	6	
82	LB	1	Total	C	N	O	0
			43	33	4	6	
82	MB	1	Total	C	N	O	0
			43	33	4	6	
82	MB	1	Total	C	N	O	0
			43	33	4	6	
82	NB	1	Total	C	N	O	0
			43	33	4	6	
82	NB	1	Total	C	N	O	0
			43	33	4	6	
82	NB	1	Total	C	N	O	0
			43	33	4	6	
82	OB	1	Total	C	N	O	0
			43	33	4	6	
82	PB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	RB	1	Total	C	N	O	0
			43	33	4	6	
82	RB	1	Total	C	N	O	0
			43	33	4	6	
82	SB	1	Total	C	N	O	0
			43	33	4	6	
82	SB	1	Total	C	N	O	0
			43	33	4	6	
82	SB	1	Total	C	N	O	0
			43	33	4	6	
82	TB	1	Total	C	N	O	0
			43	33	4	6	
82	TB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UB	1	Total	C	N	O	0
			43	33	4	6	
82	UB	1	Total	C	N	O	0
			43	33	4	6	
82	UB	1	Total	C	N	O	0
			43	33	4	6	
82	VB	1	Total	C	N	O	0
			43	33	4	6	
82	VB	1	Total	C	N	O	0
			43	33	4	6	
82	WB	1	Total	C	N	O	0
			43	33	4	6	
82	WB	1	Total	C	N	O	0
			43	33	4	6	
82	XB	1	Total	C	N	O	0
			43	33	4	6	
82	XB	1	Total	C	N	O	0
			43	33	4	6	
82	YB	1	Total	C	N	O	0
			43	33	4	6	
82	YB	1	Total	C	N	O	0
			43	33	4	6	
82	ZB	1	Total	C	N	O	0
			43	33	4	6	
82	ZB	1	Total	C	N	O	0
			43	33	4	6	
82	ZB	1	Total	C	N	O	0
			43	33	4	6	
82	AD	1	Total	C	N	O	0
			43	33	4	6	
82	AD	1	Total	C	N	O	0
			43	33	4	6	
82	AD	1	Total	C	N	O	0
			43	33	4	6	
82	BD	1	Total	C	N	O	0
			43	33	4	6	
82	BD	1	Total	C	N	O	0
			43	33	4	6	
82	BD	1	Total	C	N	O	0
			43	33	4	6	
82	CD	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	CD	1	Total	C	N	O	0
			43	33	4	6	
82	DD	1	Total	C	N	O	0
			43	33	4	6	
82	DD	1	Total	C	N	O	0
			43	33	4	6	
82	DD	1	Total	C	N	O	0
			43	33	4	6	
82	ED	1	Total	C	N	O	0
			43	33	4	6	
82	ED	1	Total	C	N	O	0
			43	33	4	6	
82	FD	1	Total	C	N	O	0
			43	33	4	6	
82	FD	1	Total	C	N	O	0
			43	33	4	6	
82	FD	1	Total	C	N	O	0
			43	33	4	6	
82	GD	1	Total	C	N	O	0
			43	33	4	6	
82	GD	1	Total	C	N	O	0
			43	33	4	6	
82	HD	1	Total	C	N	O	0
			43	33	4	6	
82	HD	1	Total	C	N	O	0
			43	33	4	6	
82	HD	1	Total	C	N	O	0
			43	33	4	6	
82	ID	1	Total	C	N	O	0
			43	33	4	6	
82	ID	1	Total	C	N	O	0
			43	33	4	6	
82	JD	1	Total	C	N	O	0
			43	33	4	6	
82	JD	1	Total	C	N	O	0
			43	33	4	6	
82	JD	1	Total	C	N	O	0
			43	33	4	6	
82	KD	1	Total	C	N	O	0
			43	33	4	6	
82	KD	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	LD	1	Total	C	N	O	0
			43	33	4	6	
82	LD	1	Total	C	N	O	0
			43	33	4	6	
82	LD	1	Total	C	N	O	0
			43	33	4	6	
82	MD	1	Total	C	N	O	0
			43	33	4	6	
82	MD	1	Total	C	N	O	0
			43	33	4	6	
82	ND	1	Total	C	N	O	0
			43	33	4	6	
82	ND	1	Total	C	N	O	0
			43	33	4	6	
82	ND	1	Total	C	N	O	0
			43	33	4	6	
82	OD	1	Total	C	N	O	0
			43	33	4	6	
82	OD	1	Total	C	N	O	0
			43	33	4	6	
82	PD	1	Total	C	N	O	0
			43	33	4	6	
82	PD	1	Total	C	N	O	0
			43	33	4	6	
82	PD	1	Total	C	N	O	0
			43	33	4	6	
82	QD	1	Total	C	N	O	0
			43	33	4	6	
82	QD	1	Total	C	N	O	0
			43	33	4	6	
82	RD	1	Total	C	N	O	0
			43	33	4	6	
82	RD	1	Total	C	N	O	0
			43	33	4	6	
82	RD	1	Total	C	N	O	0
			43	33	4	6	
82	SD	1	Total	C	N	O	0
			43	33	4	6	
82	SD	1	Total	C	N	O	0
			43	33	4	6	
82	TD	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	TD	1	Total	C	N	O	0
			43	33	4	6	
82	TD	1	Total	C	N	O	0
			43	33	4	6	
82	UD	1	Total	C	N	O	0
			43	33	4	6	
82	UD	1	Total	C	N	O	0
			43	33	4	6	
82	VD	1	Total	C	N	O	0
			43	33	4	6	
82	VD	1	Total	C	N	O	0
			43	33	4	6	
82	VD	1	Total	C	N	O	0
			43	33	4	6	
82	WD	1	Total	C	N	O	0
			43	33	4	6	
82	WD	1	Total	C	N	O	0
			43	33	4	6	
82	XD	1	Total	C	N	O	0
			43	33	4	6	
82	XD	1	Total	C	N	O	0
			43	33	4	6	
82	XD	1	Total	C	N	O	0
			43	33	4	6	
82	YD	1	Total	C	N	O	0
			43	33	4	6	
82	YD	1	Total	C	N	O	0
			43	33	4	6	
82	AE	1	Total	C	N	O	0
			43	33	4	6	
82	AE	1	Total	C	N	O	0
			43	33	4	6	
82	DE	1	Total	C	N	O	0
			43	33	4	6	
82	GE	1	Total	C	N	O	0
			43	33	4	6	
82	HE	1	Total	C	N	O	0
			43	33	4	6	
82	KE	1	Total	C	N	O	0
			43	33	4	6	
82	LE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	NE	1	Total	C	N	O	0
			43	33	4	6	
82	OE	1	Total	C	N	O	0
			43	33	4	6	
82	OE	1	Total	C	N	O	0
			43	33	4	6	
82	OE	1	Total	C	N	O	0
			43	33	4	6	
82	PE	1	Total	C	N	O	0
			43	33	4	6	
82	PE	1	Total	C	N	O	0
			43	33	4	6	
82	QE	1	Total	C	N	O	0
			43	33	4	6	
82	QE	1	Total	C	N	O	0
			43	33	4	6	
82	QE	1	Total	C	N	O	0
			43	33	4	6	
82	RE	1	Total	C	N	O	0
			43	33	4	6	
82	RE	1	Total	C	N	O	0
			43	33	4	6	
82	SE	1	Total	C	N	O	0
			43	33	4	6	
82	SE	1	Total	C	N	O	0
			43	33	4	6	
82	TE	1	Total	C	N	O	0
			43	33	4	6	
82	UE	1	Total	C	N	O	0
			43	33	4	6	
82	UE	1	Total	C	N	O	0
			43	33	4	6	
82	UE	1	Total	C	N	O	0
			43	33	4	6	
82	VE	1	Total	C	N	O	0
			43	33	4	6	
82	VE	1	Total	C	N	O	0
			43	33	4	6	
82	WE	1	Total	C	N	O	0
			43	33	4	6	
82	WE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	WE	1	Total	C	N	O	0
			43	33	4	6	
82	YE	1	Total	C	N	O	0
			43	33	4	6	
82	YE	1	Total	C	N	O	0
			43	33	4	6	
82	ZE	1	Total	C	N	O	0
			43	33	4	6	
82	ZE	1	Total	C	N	O	0
			43	33	4	6	
82	ZE	1	Total	C	N	O	0
			43	33	4	6	
82	AF	1	Total	C	N	O	0
			43	33	4	6	
82	AF	1	Total	C	N	O	0
			43	33	4	6	
82	BF	1	Total	C	N	O	0
			43	33	4	6	
82	BF	1	Total	C	N	O	0
			43	33	4	6	
82	CF	1	Total	C	N	O	0
			43	33	4	6	
82	CF	1	Total	C	N	O	0
			43	33	4	6	
82	CF	1	Total	C	N	O	0
			43	33	4	6	
82	DF	1	Total	C	N	O	0
			43	33	4	6	
82	DF	1	Total	C	N	O	0
			43	33	4	6	
82	DF	1	Total	C	N	O	0
			43	33	4	6	
82	EF	1	Total	C	N	O	0
			43	33	4	6	
82	EF	1	Total	C	N	O	0
			43	33	4	6	
82	FF	1	Total	C	N	O	0
			43	33	4	6	
82	FF	1	Total	C	N	O	0
			43	33	4	6	
82	GF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	GF	1	Total	C	N	O	0
			43	33	4	6	
82	GF	1	Total	C	N	O	0
			43	33	4	6	
82	HF	1	Total	C	N	O	0
			43	33	4	6	
82	HF	1	Total	C	N	O	0
			43	33	4	6	
82	IF	1	Total	C	N	O	0
			43	33	4	6	
82	IF	1	Total	C	N	O	0
			43	33	4	6	
82	IF	1	Total	C	N	O	0
			43	33	4	6	
82	JF	1	Total	C	N	O	0
			43	33	4	6	
82	JF	1	Total	C	N	O	0
			43	33	4	6	
82	KF	1	Total	C	N	O	0
			43	33	4	6	
82	KF	1	Total	C	N	O	0
			43	33	4	6	
82	KF	1	Total	C	N	O	0
			43	33	4	6	
82	LF	1	Total	C	N	O	0
			43	33	4	6	
82	LF	1	Total	C	N	O	0
			43	33	4	6	
82	MF	1	Total	C	N	O	0
			43	33	4	6	
82	MF	1	Total	C	N	O	0
			43	33	4	6	
82	MF	1	Total	C	N	O	0
			43	33	4	6	
82	NF	1	Total	C	N	O	0
			43	33	4	6	
82	NF	1	Total	C	N	O	0
			43	33	4	6	
82	OF	1	Total	C	N	O	0
			43	33	4	6	
82	OF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	OF	1	Total	C	N	O	0
			43	33	4	6	
82	PF	1	Total	C	N	O	0
			43	33	4	6	
82	PF	1	Total	C	N	O	0
			43	33	4	6	
82	QF	1	Total	C	N	O	0
			43	33	4	6	
82	QF	1	Total	C	N	O	0
			43	33	4	6	
82	QF	1	Total	C	N	O	0
			43	33	4	6	
82	RF	1	Total	C	N	O	0
			43	33	4	6	
82	RF	1	Total	C	N	O	0
			43	33	4	6	
82	SF	1	Total	C	N	O	0
			43	33	4	6	
82	SF	1	Total	C	N	O	0
			43	33	4	6	
82	SF	1	Total	C	N	O	0
			43	33	4	6	
82	TF	1	Total	C	N	O	0
			43	33	4	6	
82	TF	1	Total	C	N	O	0
			43	33	4	6	
82	UF	1	Total	C	N	O	0
			43	33	4	6	
82	UF	1	Total	C	N	O	0
			43	33	4	6	
82	VF	1	Total	C	N	O	0
			43	33	4	6	
82	VF	1	Total	C	N	O	0
			43	33	4	6	
82	WF	1	Total	C	N	O	0
			43	33	4	6	
82	WF	1	Total	C	N	O	0
			43	33	4	6	
82	WF	1	Total	C	N	O	0
			43	33	4	6	
82	XF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	XF	1	Total	C	N	O	0
			43	33	4	6	
82	XF	1	Total	C	N	O	0
			43	33	4	6	
82	YF	1	Total	C	N	O	0
			43	33	4	6	
82	YF	1	Total	C	N	O	0
			43	33	4	6	
82	YF	1	Total	C	N	O	0
			43	33	4	6	
82	ZF	1	Total	C	N	O	0
			43	33	4	6	
82	ZF	1	Total	C	N	O	0
			43	33	4	6	
82	AG	1	Total	C	N	O	0
			43	33	4	6	
82	AG	1	Total	C	N	O	0
			43	33	4	6	
82	DG	1	Total	C	N	O	0
			43	33	4	6	
82	GG	1	Total	C	N	O	0
			43	33	4	6	
82	HG	1	Total	C	N	O	0
			43	33	4	6	
82	KG	1	Total	C	N	O	0
			43	33	4	6	
82	LG	1	Total	C	N	O	0
			43	33	4	6	
82	NG	1	Total	C	N	O	0
			43	33	4	6	
82	OG	1	Total	C	N	O	0
			43	33	4	6	
82	OG	1	Total	C	N	O	0
			43	33	4	6	
82	OG	1	Total	C	N	O	0
			43	33	4	6	
82	PG	1	Total	C	N	O	0
			43	33	4	6	
82	PG	1	Total	C	N	O	0
			43	33	4	6	
82	QG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	QG	1	Total	C	N	O	0
			43	33	4	6	
82	QG	1	Total	C	N	O	0
			43	33	4	6	
82	RG	1	Total	C	N	O	0
			43	33	4	6	
82	RG	1	Total	C	N	O	0
			43	33	4	6	
82	SG	1	Total	C	N	O	0
			43	33	4	6	
82	SG	1	Total	C	N	O	0
			43	33	4	6	
82	SG	1	Total	C	N	O	0
			43	33	4	6	
82	TG	1	Total	C	N	O	0
			43	33	4	6	
82	UG	1	Total	C	N	O	0
			43	33	4	6	
82	UG	1	Total	C	N	O	0
			43	33	4	6	
82	UG	1	Total	C	N	O	0
			43	33	4	6	
82	VG	1	Total	C	N	O	0
			43	33	4	6	
82	VG	1	Total	C	N	O	0
			43	33	4	6	
82	WG	1	Total	C	N	O	0
			43	33	4	6	
82	WG	1	Total	C	N	O	0
			43	33	4	6	
82	WG	1	Total	C	N	O	0
			43	33	4	6	
82	YG	1	Total	C	N	O	0
			43	33	4	6	
82	YG	1	Total	C	N	O	0
			43	33	4	6	
82	ZG	1	Total	C	N	O	0
			43	33	4	6	
82	ZG	1	Total	C	N	O	0
			43	33	4	6	
82	ZG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	AH	1	Total	C	N	O	0
			43	33	4	6	
82	AH	1	Total	C	N	O	0
			43	33	4	6	
82	AH	1	Total	C	N	O	0
			43	33	4	6	
82	DH	1	Total	C	N	O	0
			43	33	4	6	
82	FH	1	Total	C	N	O	0
			43	33	4	6	
82	HH	1	Total	C	N	O	0
			43	33	4	6	
82	JH	1	Total	C	N	O	0
			43	33	4	6	
82	LH	1	Total	C	N	O	0
			43	33	4	6	
82	NH	1	Total	C	N	O	0
			43	33	4	6	
82	OH	1	Total	C	N	O	0
			43	33	4	6	
82	OH	1	Total	C	N	O	0
			43	33	4	6	
82	OH	1	Total	C	N	O	0
			43	33	4	6	
82	PH	1	Total	C	N	O	0
			43	33	4	6	
82	PH	1	Total	C	N	O	0
			43	33	4	6	
82	QH	1	Total	C	N	O	0
			43	33	4	6	
82	QH	1	Total	C	N	O	0
			43	33	4	6	
82	QH	1	Total	C	N	O	0
			43	33	4	6	
82	RH	1	Total	C	N	O	0
			43	33	4	6	
82	RH	1	Total	C	N	O	0
			43	33	4	6	
82	SH	1	Total	C	N	O	0
			43	33	4	6	
82	SH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	SH	1	Total	C	N	O	0
			43	33	4	6	
82	TH	1	Total	C	N	O	0
			43	33	4	6	
82	TH	1	Total	C	N	O	0
			43	33	4	6	
82	UH	1	Total	C	N	O	0
			43	33	4	6	
82	UH	1	Total	C	N	O	0
			43	33	4	6	
82	UH	1	Total	C	N	O	0
			43	33	4	6	
82	VH	1	Total	C	N	O	0
			43	33	4	6	
82	VH	1	Total	C	N	O	0
			43	33	4	6	
82	WH	1	Total	C	N	O	0
			43	33	4	6	
82	WH	1	Total	C	N	O	0
			43	33	4	6	
82	WH	1	Total	C	N	O	0
			43	33	4	6	
82	YH	1	Total	C	N	O	0
			43	33	4	6	
82	YH	1	Total	C	N	O	0
			43	33	4	6	
82	ZH	1	Total	C	N	O	0
			43	33	4	6	
82	ZH	1	Total	C	N	O	0
			43	33	4	6	
82	ZH	1	Total	C	N	O	0
			43	33	4	6	
82	AI	1	Total	C	N	O	0
			43	33	4	6	
82	AI	1	Total	C	N	O	0
			43	33	4	6	
82	AI	1	Total	C	N	O	0
			43	33	4	6	
82	BI	1	Total	C	N	O	0
			43	33	4	6	
82	BI	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	BI	1	Total	C	N	O	0
			43	33	4	6	
82	CI	1	Total	C	N	O	0
			43	33	4	6	
82	CI	1	Total	C	N	O	0
			43	33	4	6	
82	DI	1	Total	C	N	O	0
			43	33	4	6	
82	DI	1	Total	C	N	O	0
			43	33	4	6	
82	EI	1	Total	C	N	O	0
			43	33	4	6	
82	EI	1	Total	C	N	O	0
			43	33	4	6	
82	FI	1	Total	C	N	O	0
			43	33	4	6	
82	FI	1	Total	C	N	O	0
			43	33	4	6	
82	GI	1	Total	C	N	O	0
			43	33	4	6	
82	GI	1	Total	C	N	O	0
			43	33	4	6	
82	GI	1	Total	C	N	O	0
			43	33	4	6	
82	HI	1	Total	C	N	O	0
			43	33	4	6	
82	HI	1	Total	C	N	O	0
			43	33	4	6	
82	HI	1	Total	C	N	O	0
			43	33	4	6	
82	II	1	Total	C	N	O	0
			43	33	4	6	
82	II	1	Total	C	N	O	0
			43	33	4	6	
82	II	1	Total	C	N	O	0
			43	33	4	6	
82	JI	1	Total	C	N	O	0
			43	33	4	6	
82	JI	1	Total	C	N	O	0
			43	33	4	6	
82	KI	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	KI	1	Total	C	N	O	0
			43	33	4	6	
82	KI	1	Total	C	N	O	0
			43	33	4	6	
82	LI	1	Total	C	N	O	0
			43	33	4	6	
82	LI	1	Total	C	N	O	0
			43	33	4	6	
82	MI	1	Total	C	N	O	0
			43	33	4	6	
82	NI	1	Total	C	N	O	0
			43	33	4	6	
82	NI	1	Total	C	N	O	0
			43	33	4	6	
82	NI	1	Total	C	N	O	0
			43	33	4	6	
82	OI	1	Total	C	N	O	0
			43	33	4	6	
82	OI	1	Total	C	N	O	0
			43	33	4	6	
82	OI	1	Total	C	N	O	0
			43	33	4	6	
82	PI	1	Total	C	N	O	0
			43	33	4	6	
82	PI	1	Total	C	N	O	0
			43	33	4	6	
82	QI	1	Total	C	N	O	0
			43	33	4	6	
82	RI	1	Total	C	N	O	0
			43	33	4	6	
82	RI	1	Total	C	N	O	0
			43	33	4	6	
82	RI	1	Total	C	N	O	0
			43	33	4	6	
82	SI	1	Total	C	N	O	0
			43	33	4	6	
82	SI	1	Total	C	N	O	0
			43	33	4	6	
82	TI	1	Total	C	N	O	0
			43	33	4	6	
82	TI	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	TI	1	Total	C	N	O	0
			43	33	4	6	
82	UI	1	Total	C	N	O	0
			43	33	4	6	
82	UI	1	Total	C	N	O	0
			43	33	4	6	
82	VI	1	Total	C	N	O	0
			43	33	4	6	
82	VI	1	Total	C	N	O	0
			43	33	4	6	
82	VI	1	Total	C	N	O	0
			43	33	4	6	
82	WI	1	Total	C	N	O	0
			43	33	4	6	
82	WI	1	Total	C	N	O	0
			43	33	4	6	
82	WI	1	Total	C	N	O	0
			43	33	4	6	
82	XI	1	Total	C	N	O	0
			43	33	4	6	
82	XI	1	Total	C	N	O	0
			43	33	4	6	
82	YI	1	Total	C	N	O	0
			43	33	4	6	
82	YI	1	Total	C	N	O	0
			43	33	4	6	
82	ZI	1	Total	C	N	O	0
			43	33	4	6	
82	AJ	1	Total	C	N	O	0
			43	33	4	6	
82	AJ	1	Total	C	N	O	0
			43	33	4	6	
82	BJ	1	Total	C	N	O	0
			43	33	4	6	
82	CJ	1	Total	C	N	O	0
			43	33	4	6	
82	CJ	1	Total	C	N	O	0
			43	33	4	6	
82	CJ	1	Total	C	N	O	0
			43	33	4	6	
82	DJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	DJ	1	Total	C	N	O	0
			43	33	4	6	
82	EJ	1	Total	C	N	O	0
			43	33	4	6	
82	EJ	1	Total	C	N	O	0
			43	33	4	6	
82	EJ	1	Total	C	N	O	0
			43	33	4	6	
82	FJ	1	Total	C	N	O	0
			43	33	4	6	
82	FJ	1	Total	C	N	O	0
			43	33	4	6	
82	GJ	1	Total	C	N	O	0
			43	33	4	6	
82	GJ	1	Total	C	N	O	0
			43	33	4	6	
82	GJ	1	Total	C	N	O	0
			43	33	4	6	
82	HJ	1	Total	C	N	O	0
			43	33	4	6	
82	HJ	1	Total	C	N	O	0
			43	33	4	6	
82	IJ	1	Total	C	N	O	0
			43	33	4	6	
82	IJ	1	Total	C	N	O	0
			43	33	4	6	
82	IJ	1	Total	C	N	O	0
			43	33	4	6	
82	JJ	1	Total	C	N	O	0
			43	33	4	6	
82	JJ	1	Total	C	N	O	0
			43	33	4	6	
82	KJ	1	Total	C	N	O	0
			43	33	4	6	
82	KJ	1	Total	C	N	O	0
			43	33	4	6	
82	KJ	1	Total	C	N	O	0
			43	33	4	6	
82	LJ	1	Total	C	N	O	0
			43	33	4	6	
82	LJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	MJ	1	Total	C	N	O	0
			43	33	4	6	
82	MJ	1	Total	C	N	O	0
			43	33	4	6	
82	MJ	1	Total	C	N	O	0
			43	33	4	6	
82	NJ	1	Total	C	N	O	0
			43	33	4	6	
82	NJ	1	Total	C	N	O	0
			43	33	4	6	
82	OJ	1	Total	C	N	O	0
			43	33	4	6	
82	OJ	1	Total	C	N	O	0
			43	33	4	6	
82	OJ	1	Total	C	N	O	0
			43	33	4	6	
82	PJ	1	Total	C	N	O	0
			43	33	4	6	
82	PJ	1	Total	C	N	O	0
			43	33	4	6	
82	QJ	1	Total	C	N	O	0
			43	33	4	6	
82	QJ	1	Total	C	N	O	0
			43	33	4	6	
82	QJ	1	Total	C	N	O	0
			43	33	4	6	
82	RJ	1	Total	C	N	O	0
			43	33	4	6	
82	RJ	1	Total	C	N	O	0
			43	33	4	6	
82	SJ	1	Total	C	N	O	0
			43	33	4	6	
82	SJ	1	Total	C	N	O	0
			43	33	4	6	
82	SJ	1	Total	C	N	O	0
			43	33	4	6	
82	TJ	1	Total	C	N	O	0
			43	33	4	6	
82	TJ	1	Total	C	N	O	0
			43	33	4	6	
82	UJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UJ	1	Total	C	N	O	0
			43	33	4	6	
82	UJ	1	Total	C	N	O	0
			43	33	4	6	
82	VJ	1	Total	C	N	O	0
			43	33	4	6	
82	VJ	1	Total	C	N	O	0
			43	33	4	6	
82	WJ	1	Total	C	N	O	0
			43	33	4	6	
82	WJ	1	Total	C	N	O	0
			43	33	4	6	
82	WJ	1	Total	C	N	O	0
			43	33	4	6	
82	XJ	1	Total	C	N	O	0
			43	33	4	6	
82	XJ	1	Total	C	N	O	0
			43	33	4	6	
82	YJ	1	Total	C	N	O	0
			43	33	4	6	
82	YJ	1	Total	C	N	O	0
			43	33	4	6	
82	YJ	1	Total	C	N	O	0
			43	33	4	6	
82	ZJ	1	Total	C	N	O	0
			43	33	4	6	
82	ZJ	1	Total	C	N	O	0
			43	33	4	6	
82	AK	1	Total	C	N	O	0
			43	33	4	6	
82	AK	1	Total	C	N	O	0
			43	33	4	6	
82	BK	1	Total	C	N	O	0
			43	33	4	6	
82	BK	1	Total	C	N	O	0
			43	33	4	6	
82	CK	1	Total	C	N	O	0
			43	33	4	6	
82	CK	1	Total	C	N	O	0
			43	33	4	6	
82	CK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	DK	1	Total	C	N	O	0
			43	33	4	6	
82	DK	1	Total	C	N	O	0
			43	33	4	6	
82	DK	1	Total	C	N	O	0
			43	33	4	6	
82	EK	1	Total	C	N	O	0
			43	33	4	6	
82	EK	1	Total	C	N	O	0
			43	33	4	6	
82	FK	1	Total	C	N	O	0
			43	33	4	6	
82	FK	1	Total	C	N	O	0
			43	33	4	6	
82	GK	1	Total	C	N	O	0
			43	33	4	6	
82	GK	1	Total	C	N	O	0
			43	33	4	6	
82	GK	1	Total	C	N	O	0
			43	33	4	6	
82	HK	1	Total	C	N	O	0
			43	33	4	6	
82	HK	1	Total	C	N	O	0
			43	33	4	6	
82	IK	1	Total	C	N	O	0
			43	33	4	6	
82	IK	1	Total	C	N	O	0
			43	33	4	6	
82	IK	1	Total	C	N	O	0
			43	33	4	6	
82	JK	1	Total	C	N	O	0
			43	33	4	6	
82	JK	1	Total	C	N	O	0
			43	33	4	6	
82	KK	1	Total	C	N	O	0
			43	33	4	6	
82	KK	1	Total	C	N	O	0
			43	33	4	6	
82	KK	1	Total	C	N	O	0
			43	33	4	6	
82	LK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	LK	1	Total	C	N	O	0
			43	33	4	6	
82	MK	1	Total	C	N	O	0
			43	33	4	6	
82	MK	1	Total	C	N	O	0
			43	33	4	6	
82	MK	1	Total	C	N	O	0
			43	33	4	6	
82	NK	1	Total	C	N	O	0
			43	33	4	6	
82	NK	1	Total	C	N	O	0
			43	33	4	6	
82	OK	1	Total	C	N	O	0
			43	33	4	6	
82	OK	1	Total	C	N	O	0
			43	33	4	6	
82	OK	1	Total	C	N	O	0
			43	33	4	6	
82	PK	1	Total	C	N	O	0
			43	33	4	6	
82	PK	1	Total	C	N	O	0
			43	33	4	6	
82	QK	1	Total	C	N	O	0
			43	33	4	6	
82	QK	1	Total	C	N	O	0
			43	33	4	6	
82	QK	1	Total	C	N	O	0
			43	33	4	6	
82	RK	1	Total	C	N	O	0
			43	33	4	6	
82	RK	1	Total	C	N	O	0
			43	33	4	6	
82	SK	1	Total	C	N	O	0
			43	33	4	6	
82	SK	1	Total	C	N	O	0
			43	33	4	6	
82	SK	1	Total	C	N	O	0
			43	33	4	6	
82	TK	1	Total	C	N	O	0
			43	33	4	6	
82	TK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UK	1	Total	C	N	O	0
			43	33	4	6	
82	UK	1	Total	C	N	O	0
			43	33	4	6	
82	VK	1	Total	C	N	O	0
			43	33	4	6	
82	VK	1	Total	C	N	O	0
			43	33	4	6	
82	WK	1	Total	C	N	O	0
			43	33	4	6	
82	WK	1	Total	C	N	O	0
			43	33	4	6	
82	WK	1	Total	C	N	O	0
			43	33	4	6	
82	XK	1	Total	C	N	O	0
			43	33	4	6	
82	XK	1	Total	C	N	O	0
			43	33	4	6	
82	XK	1	Total	C	N	O	0
			43	33	4	6	
82	YK	1	Total	C	N	O	0
			43	33	4	6	
82	YK	1	Total	C	N	O	0
			43	33	4	6	
82	YK	1	Total	C	N	O	0
			43	33	4	6	
82	ZK	1	Total	C	N	O	0
			43	33	4	6	
82	ZK	1	Total	C	N	O	0
			43	33	4	6	
82	AM	1	Total	C	N	O	0
			43	33	4	6	
82	AM	1	Total	C	N	O	0
			43	33	4	6	
82	BM	1	Total	C	N	O	0
			43	33	4	6	
82	CM	1	Total	C	N	O	0
			43	33	4	6	
82	CM	1	Total	C	N	O	0
			43	33	4	6	
82	CM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	DM	1	Total	C	N	O	0
			43	33	4	6	
82	DM	1	Total	C	N	O	0
			43	33	4	6	
82	EM	1	Total	C	N	O	0
			43	33	4	6	
82	EM	1	Total	C	N	O	0
			43	33	4	6	
82	EM	1	Total	C	N	O	0
			43	33	4	6	
82	FM	1	Total	C	N	O	0
			43	33	4	6	
82	FM	1	Total	C	N	O	0
			43	33	4	6	
82	GM	1	Total	C	N	O	0
			43	33	4	6	
82	GM	1	Total	C	N	O	0
			43	33	4	6	
82	GM	1	Total	C	N	O	0
			43	33	4	6	
82	HM	1	Total	C	N	O	0
			43	33	4	6	
82	HM	1	Total	C	N	O	0
			43	33	4	6	
82	IM	1	Total	C	N	O	0
			43	33	4	6	
82	IM	1	Total	C	N	O	0
			43	33	4	6	
82	IM	1	Total	C	N	O	0
			43	33	4	6	
82	JM	1	Total	C	N	O	0
			43	33	4	6	
82	JM	1	Total	C	N	O	0
			43	33	4	6	
82	KM	1	Total	C	N	O	0
			43	33	4	6	
82	KM	1	Total	C	N	O	0
			43	33	4	6	
82	KM	1	Total	C	N	O	0
			43	33	4	6	
82	LM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	LM	1	Total	C	N	O	0
			43	33	4	6	
82	MM	1	Total	C	N	O	0
			43	33	4	6	
82	MM	1	Total	C	N	O	0
			43	33	4	6	
82	MM	1	Total	C	N	O	0
			43	33	4	6	
82	NM	1	Total	C	N	O	0
			43	33	4	6	
82	NM	1	Total	C	N	O	0
			43	33	4	6	
82	OM	1	Total	C	N	O	0
			43	33	4	6	
82	OM	1	Total	C	N	O	0
			43	33	4	6	
82	OM	1	Total	C	N	O	0
			43	33	4	6	
82	PM	1	Total	C	N	O	0
			43	33	4	6	
82	PM	1	Total	C	N	O	0
			43	33	4	6	
82	QM	1	Total	C	N	O	0
			43	33	4	6	
82	QM	1	Total	C	N	O	0
			43	33	4	6	
82	QM	1	Total	C	N	O	0
			43	33	4	6	
82	RM	1	Total	C	N	O	0
			43	33	4	6	
82	RM	1	Total	C	N	O	0
			43	33	4	6	
82	SM	1	Total	C	N	O	0
			43	33	4	6	
82	SM	1	Total	C	N	O	0
			43	33	4	6	
82	SM	1	Total	C	N	O	0
			43	33	4	6	
82	TM	1	Total	C	N	O	0
			43	33	4	6	
82	TM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UM	1	Total	C	N	O	0
			43	33	4	6	
82	UM	1	Total	C	N	O	0
			43	33	4	6	
82	UM	1	Total	C	N	O	0
			43	33	4	6	
82	VM	1	Total	C	N	O	0
			43	33	4	6	
82	VM	1	Total	C	N	O	0
			43	33	4	6	
82	WM	1	Total	C	N	O	0
			43	33	4	6	
82	WM	1	Total	C	N	O	0
			43	33	4	6	
82	WM	1	Total	C	N	O	0
			43	33	4	6	
82	XM	1	Total	C	N	O	0
			43	33	4	6	
82	XM	1	Total	C	N	O	0
			43	33	4	6	
82	YM	1	Total	C	N	O	0
			43	33	4	6	
82	YM	1	Total	C	N	O	0
			43	33	4	6	
82	YM	1	Total	C	N	O	0
			43	33	4	6	
82	ZM	1	Total	C	N	O	0
			43	33	4	6	
82	ZM	1	Total	C	N	O	0
			43	33	4	6	
82	AO	1	Total	C	N	O	0
			43	33	4	6	
82	AO	1	Total	C	N	O	0
			43	33	4	6	
82	AO	1	Total	C	N	O	0
			43	33	4	6	
82	DO	1	Total	C	N	O	0
			43	33	4	6	
82	FO	1	Total	C	N	O	0
			43	33	4	6	
82	HO	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	JO	1	Total	C	N	O	0
			43	33	4	6	
82	LO	1	Total	C	N	O	0
			43	33	4	6	
82	NO	1	Total	C	N	O	0
			43	33	4	6	
82	OO	1	Total	C	N	O	0
			43	33	4	6	
82	OO	1	Total	C	N	O	0
			43	33	4	6	
82	PO	1	Total	C	N	O	0
			43	33	4	6	
82	PO	1	Total	C	N	O	0
			43	33	4	6	
82	PO	1	Total	C	N	O	0
			43	33	4	6	
82	QO	1	Total	C	N	O	0
			43	33	4	6	
82	QO	1	Total	C	N	O	0
			43	33	4	6	
82	RO	1	Total	C	N	O	0
			43	33	4	6	
82	RO	1	Total	C	N	O	0
			43	33	4	6	
82	RO	1	Total	C	N	O	0
			43	33	4	6	
82	SO	1	Total	C	N	O	0
			43	33	4	6	
82	SO	1	Total	C	N	O	0
			43	33	4	6	
82	TO	1	Total	C	N	O	0
			43	33	4	6	
82	TO	1	Total	C	N	O	0
			43	33	4	6	
82	TO	1	Total	C	N	O	0
			43	33	4	6	
82	UO	1	Total	C	N	O	0
			43	33	4	6	
82	UO	1	Total	C	N	O	0
			43	33	4	6	
82	VO	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	VO	1	Total	C	N	O	0
			43	33	4	6	
82	WO	1	Total	C	N	O	0
			43	33	4	6	
82	YO	1	Total	C	N	O	0
			43	33	4	6	
82	YO	1	Total	C	N	O	0
			43	33	4	6	
82	YO	1	Total	C	N	O	0
			43	33	4	6	
82	ZO	1	Total	C	N	O	0
			43	33	4	6	
82	ZO	1	Total	C	N	O	0
			43	33	4	6	
82	AP	1	Total	C	N	O	0
			43	33	4	6	
82	AP	1	Total	C	N	O	0
			43	33	4	6	
82	AP	1	Total	C	N	O	0
			43	33	4	6	
82	BP	1	Total	C	N	O	0
			43	33	4	6	
82	BP	1	Total	C	N	O	0
			43	33	4	6	
82	CP	1	Total	C	N	O	0
			43	33	4	6	
82	CP	1	Total	C	N	O	0
			43	33	4	6	
82	CP	1	Total	C	N	O	0
			43	33	4	6	
82	DP	1	Total	C	N	O	0
			43	33	4	6	
82	DP	1	Total	C	N	O	0
			43	33	4	6	
82	EP	1	Total	C	N	O	0
			43	33	4	6	
82	EP	1	Total	C	N	O	0
			43	33	4	6	
82	EP	1	Total	C	N	O	0
			43	33	4	6	
82	FP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	FP	1	Total	C	N	O	0
			43	33	4	6	
82	GP	1	Total	C	N	O	0
			43	33	4	6	
82	GP	1	Total	C	N	O	0
			43	33	4	6	
82	GP	1	Total	C	N	O	0
			43	33	4	6	
82	HP	1	Total	C	N	O	0
			43	33	4	6	
82	HP	1	Total	C	N	O	0
			43	33	4	6	
82	IP	1	Total	C	N	O	0
			43	33	4	6	
82	IP	1	Total	C	N	O	0
			43	33	4	6	
82	IP	1	Total	C	N	O	0
			43	33	4	6	
82	JP	1	Total	C	N	O	0
			43	33	4	6	
82	JP	1	Total	C	N	O	0
			43	33	4	6	
82	KP	1	Total	C	N	O	0
			43	33	4	6	
82	KP	1	Total	C	N	O	0
			43	33	4	6	
82	LP	1	Total	C	N	O	0
			43	33	4	6	
82	LP	1	Total	C	N	O	0
			43	33	4	6	
82	MP	1	Total	C	N	O	0
			43	33	4	6	
82	MP	1	Total	C	N	O	0
			43	33	4	6	
82	MP	1	Total	C	N	O	0
			43	33	4	6	
82	NP	1	Total	C	N	O	0
			43	33	4	6	
82	NP	1	Total	C	N	O	0
			43	33	4	6	
82	OP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	OP	1	Total	C	N	O	0
			43	33	4	6	
82	OP	1	Total	C	N	O	0
			43	33	4	6	
82	PP	1	Total	C	N	O	0
			43	33	4	6	
82	PP	1	Total	C	N	O	0
			43	33	4	6	
82	QP	1	Total	C	N	O	0
			43	33	4	6	
82	QP	1	Total	C	N	O	0
			43	33	4	6	
82	QP	1	Total	C	N	O	0
			43	33	4	6	
82	RP	1	Total	C	N	O	0
			43	33	4	6	
82	RP	1	Total	C	N	O	0
			43	33	4	6	
82	SP	1	Total	C	N	O	0
			43	33	4	6	
82	SP	1	Total	C	N	O	0
			43	33	4	6	
82	SP	1	Total	C	N	O	0
			43	33	4	6	
82	TP	1	Total	C	N	O	0
			43	33	4	6	
82	TP	1	Total	C	N	O	0
			43	33	4	6	
82	UP	1	Total	C	N	O	0
			43	33	4	6	
82	UP	1	Total	C	N	O	0
			43	33	4	6	
82	UP	1	Total	C	N	O	0
			43	33	4	6	
82	VP	1	Total	C	N	O	0
			43	33	4	6	
82	VP	1	Total	C	N	O	0
			43	33	4	6	
82	WP	1	Total	C	N	O	0
			43	33	4	6	
82	WP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	XP	1	Total	C	N	O	0
			43	33	4	6	
82	XP	1	Total	C	N	O	0
			43	33	4	6	
82	YP	1	Total	C	N	O	0
			43	33	4	6	
82	YP	1	Total	C	N	O	0
			43	33	4	6	
82	YP	1	Total	C	N	O	0
			43	33	4	6	
82	AQ	1	Total	C	N	O	0
			43	33	4	6	
82	AQ	1	Total	C	N	O	0
			43	33	4	6	
82	AQ	1	Total	C	N	O	0
			43	33	4	6	
82	BQ	1	Total	C	N	O	0
			43	33	4	6	
82	BQ	1	Total	C	N	O	0
			43	33	4	6	
82	BQ	1	Total	C	N	O	0
			43	33	4	6	
82	CQ	1	Total	C	N	O	0
			43	33	4	6	
82	CQ	1	Total	C	N	O	0
			43	33	4	6	
82	DQ	1	Total	C	N	O	0
			43	33	4	6	
82	DQ	1	Total	C	N	O	0
			43	33	4	6	
82	DQ	1	Total	C	N	O	0
			43	33	4	6	
82	EQ	1	Total	C	N	O	0
			43	33	4	6	
82	EQ	1	Total	C	N	O	0
			43	33	4	6	
82	FQ	1	Total	C	N	O	0
			43	33	4	6	
82	FQ	1	Total	C	N	O	0
			43	33	4	6	
82	FQ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	GQ	1	Total	C	N	O	0
			43	33	4	6	
82	GQ	1	Total	C	N	O	0
			43	33	4	6	
82	HQ	1	Total	C	N	O	0
			43	33	4	6	
82	HQ	1	Total	C	N	O	0
			43	33	4	6	
82	HQ	1	Total	C	N	O	0
			43	33	4	6	
82	IQ	1	Total	C	N	O	0
			43	33	4	6	
82	IQ	1	Total	C	N	O	0
			43	33	4	6	
82	JQ	1	Total	C	N	O	0
			43	33	4	6	
82	JQ	1	Total	C	N	O	0
			43	33	4	6	
82	JQ	1	Total	C	N	O	0
			43	33	4	6	
82	KQ	1	Total	C	N	O	0
			43	33	4	6	
82	KQ	1	Total	C	N	O	0
			43	33	4	6	
82	LQ	1	Total	C	N	O	0
			43	33	4	6	
82	LQ	1	Total	C	N	O	0
			43	33	4	6	
82	LQ	1	Total	C	N	O	0
			43	33	4	6	
82	MQ	1	Total	C	N	O	0
			43	33	4	6	
82	MQ	1	Total	C	N	O	0
			43	33	4	6	
82	NQ	1	Total	C	N	O	0
			43	33	4	6	
82	NQ	1	Total	C	N	O	0
			43	33	4	6	
82	NQ	1	Total	C	N	O	0
			43	33	4	6	
82	OQ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	OQ	1	Total	C	N	O	0
			43	33	4	6	
82	PQ	1	Total	C	N	O	0
			43	33	4	6	
82	PQ	1	Total	C	N	O	0
			43	33	4	6	
82	PQ	1	Total	C	N	O	0
			43	33	4	6	
82	QQ	1	Total	C	N	O	0
			43	33	4	6	
82	QQ	1	Total	C	N	O	0
			43	33	4	6	
82	RQ	1	Total	C	N	O	0
			43	33	4	6	
82	RQ	1	Total	C	N	O	0
			43	33	4	6	
82	RQ	1	Total	C	N	O	0
			43	33	4	6	
82	SQ	1	Total	C	N	O	0
			43	33	4	6	
82	SQ	1	Total	C	N	O	0
			43	33	4	6	
82	TQ	1	Total	C	N	O	0
			43	33	4	6	
82	TQ	1	Total	C	N	O	0
			43	33	4	6	
82	TQ	1	Total	C	N	O	0
			43	33	4	6	
82	UQ	1	Total	C	N	O	0
			43	33	4	6	
82	UQ	1	Total	C	N	O	0
			43	33	4	6	
82	VQ	1	Total	C	N	O	0
			43	33	4	6	
82	VQ	1	Total	C	N	O	0
			43	33	4	6	
82	VQ	1	Total	C	N	O	0
			43	33	4	6	
82	WQ	1	Total	C	N	O	0
			43	33	4	6	
82	WQ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	XQ	1	Total	C	N	O	0
			43	33	4	6	
82	XQ	1	Total	C	N	O	0
			43	33	4	6	
82	XQ	1	Total	C	N	O	0
			43	33	4	6	
82	YQ	1	Total	C	N	O	0
			43	33	4	6	
82	YQ	1	Total	C	N	O	0
			43	33	4	6	
82	L1	1	Total	C	N	O	0
			43	33	4	6	
82	N1	1	Total	C	N	O	0
			43	33	4	6	
82	O1	1	Total	C	N	O	0
			43	33	4	6	
82	O1	1	Total	C	N	O	0
			43	33	4	6	
82	O1	1	Total	C	N	O	0
			43	33	4	6	
82	P1	1	Total	C	N	O	0
			43	33	4	6	
82	P1	1	Total	C	N	O	0
			43	33	4	6	
82	Q1	1	Total	C	N	O	0
			43	33	4	6	
82	Q1	1	Total	C	N	O	0
			43	33	4	6	
82	Q1	1	Total	C	N	O	0
			43	33	4	6	
82	R1	1	Total	C	N	O	0
			43	33	4	6	
82	R1	1	Total	C	N	O	0
			43	33	4	6	
82	S1	1	Total	C	N	O	0
			43	33	4	6	
82	S1	1	Total	C	N	O	0
			43	33	4	6	
82	T1	1	Total	C	N	O	0
			43	33	4	6	
82	T1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	U1	1	Total	C	N	O	0
			43	33	4	6	
82	U1	1	Total	C	N	O	0
			43	33	4	6	
82	U1	1	Total	C	N	O	0
			43	33	4	6	
82	A1	1	Total	C	N	O	0
			43	33	4	6	
82	A1	1	Total	C	N	O	0
			43	33	4	6	
82	A1	1	Total	C	N	O	0
			43	33	4	6	
82	D1	1	Total	C	N	O	0
			43	33	4	6	
82	F1	1	Total	C	N	O	0
			43	33	4	6	
82	H1	1	Total	C	N	O	0
			43	33	4	6	
82	J1	1	Total	C	N	O	0
			43	33	4	6	
82	V1	1	Total	C	N	O	0
			43	33	4	6	
82	V1	1	Total	C	N	O	0
			43	33	4	6	
82	V1	1	Total	C	N	O	0
			43	33	4	6	
82	W1	1	Total	C	N	O	0
			43	33	4	6	
82	W1	1	Total	C	N	O	0
			43	33	4	6	
82	W1	1	Total	C	N	O	0
			43	33	4	6	
82	Y1	1	Total	C	N	O	0
			43	33	4	6	
82	Y1	1	Total	C	N	O	0
			43	33	4	6	
82	Z1	1	Total	C	N	O	0
			43	33	4	6	
82	Z1	1	Total	C	N	O	0
			43	33	4	6	
82	Z1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	f1	1	Total	C	N	O	0
			43	33	4	6	
82	f1	1	Total	C	N	O	0
			43	33	4	6	
82	f1	1	Total	C	N	O	0
			43	33	4	6	
82	g1	1	Total	C	N	O	0
			43	33	4	6	
82	g1	1	Total	C	N	O	0
			43	33	4	6	
82	h1	1	Total	C	N	O	0
			43	33	4	6	
82	h1	1	Total	C	N	O	0
			43	33	4	6	
82	h1	1	Total	C	N	O	0
			43	33	4	6	
82	i1	1	Total	C	N	O	0
			43	33	4	6	
82	i1	1	Total	C	N	O	0
			43	33	4	6	
82	j1	1	Total	C	N	O	0
			43	33	4	6	
82	j1	1	Total	C	N	O	0
			43	33	4	6	
82	j1	1	Total	C	N	O	0
			43	33	4	6	
82	k1	1	Total	C	N	O	0
			43	33	4	6	
82	k1	1	Total	C	N	O	0
			43	33	4	6	
82	l1	1	Total	C	N	O	0
			43	33	4	6	
82	l1	1	Total	C	N	O	0
			43	33	4	6	
82	l1	1	Total	C	N	O	0
			43	33	4	6	
82	m1	1	Total	C	N	O	0
			43	33	4	6	
82	m1	1	Total	C	N	O	0
			43	33	4	6	
82	a1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	a1	1	Total	C	N	O	0
			43	33	4	6	
82	b1	1	Total	C	N	O	0
			43	33	4	6	
82	b1	1	Total	C	N	O	0
			43	33	4	6	
82	b1	1	Total	C	N	O	0
			43	33	4	6	
82	c1	1	Total	C	N	O	0
			43	33	4	6	
82	c1	1	Total	C	N	O	0
			43	33	4	6	
82	d1	1	Total	C	N	O	0
			43	33	4	6	
82	d1	1	Total	C	N	O	0
			43	33	4	6	
82	d1	1	Total	C	N	O	0
			43	33	4	6	
82	e1	1	Total	C	N	O	0
			43	33	4	6	
82	e1	1	Total	C	N	O	0
			43	33	4	6	
82	F4	1	Total	C	N	O	0
			43	33	4	6	
82	H4	1	Total	C	N	O	0
			43	33	4	6	
82	J4	1	Total	C	N	O	0
			43	33	4	6	
82	L4	1	Total	C	N	O	0
			43	33	4	6	
82	N4	1	Total	C	N	O	0
			43	33	4	6	
82	O4	1	Total	C	N	O	0
			43	33	4	6	
82	O4	1	Total	C	N	O	0
			43	33	4	6	
82	A4	1	Total	C	N	O	0
			43	33	4	6	
82	A4	1	Total	C	N	O	0
			43	33	4	6	
82	A4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	D4	1	Total	C	N	O	0
			43	33	4	6	
82	P4	1	Total	C	N	O	0
			43	33	4	6	
82	P4	1	Total	C	N	O	0
			43	33	4	6	
82	Q4	1	Total	C	N	O	0
			43	33	4	6	
82	Q4	1	Total	C	N	O	0
			43	33	4	6	
82	R4	1	Total	C	N	O	0
			43	33	4	6	
82	R4	1	Total	C	N	O	0
			43	33	4	6	
82	R4	1	Total	C	N	O	0
			43	33	4	6	
82	S4	1	Total	C	N	O	0
			43	33	4	6	
82	S4	1	Total	C	N	O	0
			43	33	4	6	
82	T4	1	Total	C	N	O	0
			43	33	4	6	
82	T4	1	Total	C	N	O	0
			43	33	4	6	
82	T4	1	Total	C	N	O	0
			43	33	4	6	
82	U4	1	Total	C	N	O	0
			43	33	4	6	
82	U4	1	Total	C	N	O	0
			43	33	4	6	
82	V4	1	Total	C	N	O	0
			43	33	4	6	
82	V4	1	Total	C	N	O	0
			43	33	4	6	
82	W4	1	Total	C	N	O	0
			43	33	4	6	
82	Y4	1	Total	C	N	O	0
			43	33	4	6	
82	Y4	1	Total	C	N	O	0
			43	33	4	6	
82	Y4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	Z4	1	Total	C	N	O	0
			43	33	4	6	
82	Z4	1	Total	C	N	O	0
			43	33	4	6	
82	i4	1	Total	C	N	O	0
			43	33	4	6	
82	i4	1	Total	C	N	O	0
			43	33	4	6	
82	i4	1	Total	C	N	O	0
			43	33	4	6	
82	j4	1	Total	C	N	O	0
			43	33	4	6	
82	j4	1	Total	C	N	O	0
			43	33	4	6	
82	j4	1	Total	C	N	O	0
			43	33	4	6	
82	k4	1	Total	C	N	O	0
			43	33	4	6	
82	k4	1	Total	C	N	O	0
			43	33	4	6	
82	l4	1	Total	C	N	O	0
			43	33	4	6	
82	l4	1	Total	C	N	O	0
			43	33	4	6	
82	m4	1	Total	C	N	O	0
			43	33	4	6	
82	m4	1	Total	C	N	O	0
			43	33	4	6	
82	m4	1	Total	C	N	O	0
			43	33	4	6	
82	a4	1	Total	C	N	O	0
			43	33	4	6	
82	a4	1	Total	C	N	O	0
			43	33	4	6	
82	a4	1	Total	C	N	O	0
			43	33	4	6	
82	b4	1	Total	C	N	O	0
			43	33	4	6	
82	b4	1	Total	C	N	O	0
			43	33	4	6	
82	c4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	c4	1	Total	C	N	O	0
			43	33	4	6	
82	c4	1	Total	C	N	O	0
			43	33	4	6	
82	d4	1	Total	C	N	O	0
			43	33	4	6	
82	d4	1	Total	C	N	O	0
			43	33	4	6	
82	e4	1	Total	C	N	O	0
			43	33	4	6	
82	e4	1	Total	C	N	O	0
			43	33	4	6	
82	e4	1	Total	C	N	O	0
			43	33	4	6	
82	f4	1	Total	C	N	O	0
			43	33	4	6	
82	f4	1	Total	C	N	O	0
			43	33	4	6	
82	g4	1	Total	C	N	O	0
			43	33	4	6	
82	g4	1	Total	C	N	O	0
			43	33	4	6	
82	g4	1	Total	C	N	O	0
			43	33	4	6	
82	h4	1	Total	C	N	O	0
			43	33	4	6	
82	h4	1	Total	C	N	O	0
			43	33	4	6	
82	A5	1	Total	C	N	O	0
			43	33	4	6	
82	A5	1	Total	C	N	O	0
			43	33	4	6	
82	B5	1	Total	C	N	O	0
			43	33	4	6	
82	B5	1	Total	C	N	O	0
			43	33	4	6	
82	B5	1	Total	C	N	O	0
			43	33	4	6	
82	C5	1	Total	C	N	O	0
			43	33	4	6	
82	C5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	D5	1	Total	C	N	O	0
			43	33	4	6	
82	D5	1	Total	C	N	O	0
			43	33	4	6	
82	D5	1	Total	C	N	O	0
			43	33	4	6	
82	E5	1	Total	C	N	O	0
			43	33	4	6	
82	E5	1	Total	C	N	O	0
			43	33	4	6	
82	F5	1	Total	C	N	O	0
			43	33	4	6	
82	F5	1	Total	C	N	O	0
			43	33	4	6	
82	F5	1	Total	C	N	O	0
			43	33	4	6	
82	G5	1	Total	C	N	O	0
			43	33	4	6	
82	G5	1	Total	C	N	O	0
			43	33	4	6	
82	H5	1	Total	C	N	O	0
			43	33	4	6	
82	H5	1	Total	C	N	O	0
			43	33	4	6	
82	H5	1	Total	C	N	O	0
			43	33	4	6	
82	I5	1	Total	C	N	O	0
			43	33	4	6	
82	I5	1	Total	C	N	O	0
			43	33	4	6	
82	J5	1	Total	C	N	O	0
			43	33	4	6	
82	J5	1	Total	C	N	O	0
			43	33	4	6	
82	J5	1	Total	C	N	O	0
			43	33	4	6	
82	K5	1	Total	C	N	O	0
			43	33	4	6	
82	K5	1	Total	C	N	O	0
			43	33	4	6	
82	L5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	L5	1	Total	C	N	O	0
			43	33	4	6	
82	L5	1	Total	C	N	O	0
			43	33	4	6	
82	M5	1	Total	C	N	O	0
			43	33	4	6	
82	M5	1	Total	C	N	O	0
			43	33	4	6	
82	M5	1	Total	C	N	O	0
			43	33	4	6	
82	N5	1	Total	C	N	O	0
			43	33	4	6	
82	N5	1	Total	C	N	O	0
			43	33	4	6	
82	O5	1	Total	C	N	O	0
			43	33	4	6	
82	O5	1	Total	C	N	O	0
			43	33	4	6	
82	O5	1	Total	C	N	O	0
			43	33	4	6	
82	P5	1	Total	C	N	O	0
			43	33	4	6	
82	P5	1	Total	C	N	O	0
			43	33	4	6	
82	Q5	1	Total	C	N	O	0
			43	33	4	6	
82	Q5	1	Total	C	N	O	0
			43	33	4	6	
82	Q5	1	Total	C	N	O	0
			43	33	4	6	
82	R5	1	Total	C	N	O	0
			43	33	4	6	
82	R5	1	Total	C	N	O	0
			43	33	4	6	
82	S5	1	Total	C	N	O	0
			43	33	4	6	
82	S5	1	Total	C	N	O	0
			43	33	4	6	
82	S5	1	Total	C	N	O	0
			43	33	4	6	
82	T5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	T5	1	Total	C	N	O	0
			43	33	4	6	
82	U5	1	Total	C	N	O	0
			43	33	4	6	
82	U5	1	Total	C	N	O	0
			43	33	4	6	
82	U5	1	Total	C	N	O	0
			43	33	4	6	
82	V5	1	Total	C	N	O	0
			43	33	4	6	
82	V5	1	Total	C	N	O	0
			43	33	4	6	
82	W5	1	Total	C	N	O	0
			43	33	4	6	
82	W5	1	Total	C	N	O	0
			43	33	4	6	
82	W5	1	Total	C	N	O	0
			43	33	4	6	
82	X5	1	Total	C	N	O	0
			43	33	4	6	
82	X5	1	Total	C	N	O	0
			43	33	4	6	
82	Y5	1	Total	C	N	O	0
			43	33	4	6	
82	Y5	1	Total	C	N	O	0
			43	33	4	6	
82	Y5	1	Total	C	N	O	0
			43	33	4	6	
82	Z5	1	Total	C	N	O	0
			43	33	4	6	
82	Z5	1	Total	C	N	O	0
			43	33	4	6	
82	Z5	1	Total	C	N	O	0
			43	33	4	6	
82	A7	1	Total	C	N	O	0
			43	33	4	6	
82	A7	1	Total	C	N	O	0
			43	33	4	6	
82	B7	1	Total	C	N	O	0
			43	33	4	6	
82	B7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	B7	1	Total	C	N	O	0
			43	33	4	6	
82	C7	1	Total	C	N	O	0
			43	33	4	6	
82	C7	1	Total	C	N	O	0
			43	33	4	6	
82	D7	1	Total	C	N	O	0
			43	33	4	6	
82	D7	1	Total	C	N	O	0
			43	33	4	6	
82	D7	1	Total	C	N	O	0
			43	33	4	6	
82	E7	1	Total	C	N	O	0
			43	33	4	6	
82	E7	1	Total	C	N	O	0
			43	33	4	6	
82	F7	1	Total	C	N	O	0
			43	33	4	6	
82	F7	1	Total	C	N	O	0
			43	33	4	6	
82	F7	1	Total	C	N	O	0
			43	33	4	6	
82	G7	1	Total	C	N	O	0
			43	33	4	6	
82	G7	1	Total	C	N	O	0
			43	33	4	6	
82	H7	1	Total	C	N	O	0
			43	33	4	6	
82	H7	1	Total	C	N	O	0
			43	33	4	6	
82	H7	1	Total	C	N	O	0
			43	33	4	6	
82	I7	1	Total	C	N	O	0
			43	33	4	6	
82	I7	1	Total	C	N	O	0
			43	33	4	6	
82	J7	1	Total	C	N	O	0
			43	33	4	6	
82	J7	1	Total	C	N	O	0
			43	33	4	6	
82	J7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	K7	1	Total	C	N	O	0
			43	33	4	6	
82	K7	1	Total	C	N	O	0
			43	33	4	6	
82	L7	1	Total	C	N	O	0
			43	33	4	6	
82	L7	1	Total	C	N	O	0
			43	33	4	6	
82	L7	1	Total	C	N	O	0
			43	33	4	6	
82	M7	1	Total	C	N	O	0
			43	33	4	6	
82	M7	1	Total	C	N	O	0
			43	33	4	6	
82	N7	1	Total	C	N	O	0
			43	33	4	6	
82	N7	1	Total	C	N	O	0
			43	33	4	6	
82	N7	1	Total	C	N	O	0
			43	33	4	6	
82	O7	1	Total	C	N	O	0
			43	33	4	6	
82	O7	1	Total	C	N	O	0
			43	33	4	6	
82	P7	1	Total	C	N	O	0
			43	33	4	6	
82	P7	1	Total	C	N	O	0
			43	33	4	6	
82	P7	1	Total	C	N	O	0
			43	33	4	6	
82	Q7	1	Total	C	N	O	0
			43	33	4	6	
82	Q7	1	Total	C	N	O	0
			43	33	4	6	
82	R7	1	Total	C	N	O	0
			43	33	4	6	
82	R7	1	Total	C	N	O	0
			43	33	4	6	
82	R7	1	Total	C	N	O	0
			43	33	4	6	
82	S7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	S7	1	Total	C	N	O	0
			43	33	4	6	
82	T7	1	Total	C	N	O	0
			43	33	4	6	
82	T7	1	Total	C	N	O	0
			43	33	4	6	
82	T7	1	Total	C	N	O	0
			43	33	4	6	
82	U7	1	Total	C	N	O	0
			43	33	4	6	
82	U7	1	Total	C	N	O	0
			43	33	4	6	
82	V7	1	Total	C	N	O	0
			43	33	4	6	
82	V7	1	Total	C	N	O	0
			43	33	4	6	
82	V7	1	Total	C	N	O	0
			43	33	4	6	
82	W7	1	Total	C	N	O	0
			43	33	4	6	
82	W7	1	Total	C	N	O	0
			43	33	4	6	
82	X7	1	Total	C	N	O	0
			43	33	4	6	
82	X7	1	Total	C	N	O	0
			43	33	4	6	
82	X7	1	Total	C	N	O	0
			43	33	4	6	
82	Y7	1	Total	C	N	O	0
			43	33	4	6	
82	Y7	1	Total	C	N	O	0
			43	33	4	6	
82	Y7	1	Total	C	N	O	0
			43	33	4	6	
82	e7	1	Total	C	N	O	0
			43	33	4	6	
82	y8	1	Total	C	N	O	0
			43	33	4	6	
82	y8	1	Total	C	N	O	0
			43	33	4	6	
82	y8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	z8	1	Total	C	N	O	0
			43	33	4	6	
82	z8	1	Total	C	N	O	0
			43	33	4	6	
82	18	1	Total	C	N	O	0
			43	33	4	6	
82	18	1	Total	C	N	O	0
			43	33	4	6	
82	18	1	Total	C	N	O	0
			43	33	4	6	
82	p8	1	Total	C	N	O	0
			43	33	4	6	
82	p8	1	Total	C	N	O	0
			43	33	4	6	
82	q8	1	Total	C	N	O	0
			43	33	4	6	
82	q8	1	Total	C	N	O	0
			43	33	4	6	
82	q8	1	Total	C	N	O	0
			43	33	4	6	
82	r8	1	Total	C	N	O	0
			43	33	4	6	
82	r8	1	Total	C	N	O	0
			43	33	4	6	
82	s8	1	Total	C	N	O	0
			43	33	4	6	
82	s8	1	Total	C	N	O	0
			43	33	4	6	
82	s8	1	Total	C	N	O	0
			43	33	4	6	
82	t8	1	Total	C	N	O	0
			43	33	4	6	
82	t8	1	Total	C	N	O	0
			43	33	4	6	
82	u8	1	Total	C	N	O	0
			43	33	4	6	
82	u8	1	Total	C	N	O	0
			43	33	4	6	
82	u8	1	Total	C	N	O	0
			43	33	4	6	
82	v8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	v8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	x8	1	Total	C	N	O	0
			43	33	4	6	
82	x8	1	Total	C	N	O	0
			43	33	4	6	
82	A9	1	Total	C	N	O	0
			43	33	4	6	
82	A9	1	Total	C	N	O	0
			43	33	4	6	
82	B9	1	Total	C	N	O	0
			43	33	4	6	
82	B9	1	Total	C	N	O	0
			43	33	4	6	
82	B9	1	Total	C	N	O	0
			43	33	4	6	
82	C9	1	Total	C	N	O	0
			43	33	4	6	
82	C9	1	Total	C	N	O	0
			43	33	4	6	
82	D9	1	Total	C	N	O	0
			43	33	4	6	
82	D9	1	Total	C	N	O	0
			43	33	4	6	
82	D9	1	Total	C	N	O	0
			43	33	4	6	
82	E9	1	Total	C	N	O	0
			43	33	4	6	
82	E9	1	Total	C	N	O	0
			43	33	4	6	
82	F9	1	Total	C	N	O	0
			43	33	4	6	
82	F9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	F9	1	Total	C	N	O	0
			43	33	4	6	
82	G9	1	Total	C	N	O	0
			43	33	4	6	
82	G9	1	Total	C	N	O	0
			43	33	4	6	
82	H9	1	Total	C	N	O	0
			43	33	4	6	
82	H9	1	Total	C	N	O	0
			43	33	4	6	
82	H9	1	Total	C	N	O	0
			43	33	4	6	
82	I9	1	Total	C	N	O	0
			43	33	4	6	
82	I9	1	Total	C	N	O	0
			43	33	4	6	
82	J9	1	Total	C	N	O	0
			43	33	4	6	
82	J9	1	Total	C	N	O	0
			43	33	4	6	
82	J9	1	Total	C	N	O	0
			43	33	4	6	
82	K9	1	Total	C	N	O	0
			43	33	4	6	
82	K9	1	Total	C	N	O	0
			43	33	4	6	
82	L9	1	Total	C	N	O	0
			43	33	4	6	
82	L9	1	Total	C	N	O	0
			43	33	4	6	
82	L9	1	Total	C	N	O	0
			43	33	4	6	
82	N9	1	Total	C	N	O	0
			43	33	4	6	
82	N9	1	Total	C	N	O	0
			43	33	4	6	
82	O9	1	Total	C	N	O	0
			43	33	4	6	
82	O9	1	Total	C	N	O	0
			43	33	4	6	
82	O9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	P9	1	Total	C	N	O	0
			43	33	4	6	
82	P9	1	Total	C	N	O	0
			43	33	4	6	
82	Q9	1	Total	C	N	O	0
			43	33	4	6	
82	Q9	1	Total	C	N	O	0
			43	33	4	6	
82	Q9	1	Total	C	N	O	0
			43	33	4	6	
82	R9	1	Total	C	N	O	0
			43	33	4	6	
82	R9	1	Total	C	N	O	0
			43	33	4	6	
82	S9	1	Total	C	N	O	0
			43	33	4	6	
82	S9	1	Total	C	N	O	0
			43	33	4	6	
82	S9	1	Total	C	N	O	0
			43	33	4	6	
82	T9	1	Total	C	N	O	0
			43	33	4	6	
82	T9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	V9	1	Total	C	N	O	0
			43	33	4	6	
82	V9	1	Total	C	N	O	0
			43	33	4	6	
82	W9	1	Total	C	N	O	0
			43	33	4	6	
82	W9	1	Total	C	N	O	0
			43	33	4	6	
82	W9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	X9	1	Total	C	N	O	0
			43	33	4	6	
82	X9	1	Total	C	N	O	0
			43	33	4	6	
82	Y9	1	Total	C	N	O	0
			43	33	4	6	
82	Y9	1	Total	C	N	O	0
			43	33	4	6	
82	Y9	1	Total	C	N	O	0
			43	33	4	6	
82	eA	1	Total	C	N	O	0
			43	33	4	6	
82	fB	1	Total	C	N	O	0
			43	33	4	6	
82	aB	1	Total	C	N	O	0
			43	33	4	6	
82	aB	1	Total	C	N	O	0
			43	33	4	6	
82	bB	1	Total	C	N	O	0
			43	33	4	6	
82	cB	1	Total	C	N	O	0
			43	33	4	6	
82	cB	1	Total	C	N	O	0
			43	33	4	6	
82	cB	1	Total	C	N	O	0
			43	33	4	6	
82	dB	1	Total	C	N	O	0
			43	33	4	6	
82	dB	1	Total	C	N	O	0
			43	33	4	6	
82	eB	1	Total	C	N	O	0
			43	33	4	6	
82	eB	1	Total	C	N	O	0
			43	33	4	6	
82	gB	1	Total	C	N	O	0
			43	33	4	6	
82	gB	1	Total	C	N	O	0
			43	33	4	6	
82	gB	1	Total	C	N	O	0
			43	33	4	6	
82	hB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	yC	1	Total	C	N	O	0
			43	33	4	6	
82	yC	1	Total	C	N	O	0
			43	33	4	6	
82	yC	1	Total	C	N	O	0
			43	33	4	6	
82	zC	1	Total	C	N	O	0
			43	33	4	6	
82	zC	1	Total	C	N	O	0
			43	33	4	6	
82	1C	1	Total	C	N	O	0
			43	33	4	6	
82	1C	1	Total	C	N	O	0
			43	33	4	6	
82	1C	1	Total	C	N	O	0
			43	33	4	6	
82	pC	1	Total	C	N	O	0
			43	33	4	6	
82	pC	1	Total	C	N	O	0
			43	33	4	6	
82	qC	1	Total	C	N	O	0
			43	33	4	6	
82	qC	1	Total	C	N	O	0
			43	33	4	6	
82	qC	1	Total	C	N	O	0
			43	33	4	6	
82	rC	1	Total	C	N	O	0
			43	33	4	6	
82	rC	1	Total	C	N	O	0
			43	33	4	6	
82	sC	1	Total	C	N	O	0
			43	33	4	6	
82	sC	1	Total	C	N	O	0
			43	33	4	6	
82	sC	1	Total	C	N	O	0
			43	33	4	6	
82	tC	1	Total	C	N	O	0
			43	33	4	6	
82	tC	1	Total	C	N	O	0
			43	33	4	6	
82	uC	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	uC	1	Total	C	N	O	0
			43	33	4	6	
82	uC	1	Total	C	N	O	0
			43	33	4	6	
82	vC	1	Total	C	N	O	0
			43	33	4	6	
82	vC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	xC	1	Total	C	N	O	0
			43	33	4	6	
82	xC	1	Total	C	N	O	0
			43	33	4	6	
82	dD	1	Total	C	N	O	0
			43	33	4	6	
82	aE	1	Total	C	N	O	0
			43	33	4	6	
82	aE	1	Total	C	N	O	0
			43	33	4	6	
82	bE	1	Total	C	N	O	0
			43	33	4	6	
82	bE	1	Total	C	N	O	0
			43	33	4	6	
82	cE	1	Total	C	N	O	0
			43	33	4	6	
82	cE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	eE	1	Total	C	N	O	0
			43	33	4	6	
82	eE	1	Total	C	N	O	0
			43	33	4	6	
82	eE	1	Total	C	N	O	0
			43	33	4	6	
82	fE	1	Total	C	N	O	0
			43	33	4	6	
82	fE	1	Total	C	N	O	0
			43	33	4	6	
82	fE	1	Total	C	N	O	0
			43	33	4	6	
82	gE	1	Total	C	N	O	0
			43	33	4	6	
82	gE	1	Total	C	N	O	0
			43	33	4	6	
82	hE	1	Total	C	N	O	0
			43	33	4	6	
82	hE	1	Total	C	N	O	0
			43	33	4	6	
82	hE	1	Total	C	N	O	0
			43	33	4	6	
82	iE	1	Total	C	N	O	0
			43	33	4	6	
82	iE	1	Total	C	N	O	0
			43	33	4	6	
82	jE	1	Total	C	N	O	0
			43	33	4	6	
82	jE	1	Total	C	N	O	0
			43	33	4	6	
82	kE	1	Total	C	N	O	0
			43	33	4	6	
82	kE	1	Total	C	N	O	0
			43	33	4	6	
82	lE	1	Total	C	N	O	0
			43	33	4	6	
82	lE	1	Total	C	N	O	0
			43	33	4	6	
82	lE	1	Total	C	N	O	0
			43	33	4	6	
82	mE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	mE	1	Total	C	N	O	0
			43	33	4	6	
82	mE	1	Total	C	N	O	0
			43	33	4	6	
82	aF	1	Total	C	N	O	0
			43	33	4	6	
82	aF	1	Total	C	N	O	0
			43	33	4	6	
82	aF	1	Total	C	N	O	0
			43	33	4	6	
82	bF	1	Total	C	N	O	0
			43	33	4	6	
82	bF	1	Total	C	N	O	0
			43	33	4	6	
82	cF	1	Total	C	N	O	0
			43	33	4	6	
82	cF	1	Total	C	N	O	0
			43	33	4	6	
82	cF	1	Total	C	N	O	0
			43	33	4	6	
82	dF	1	Total	C	N	O	0
			43	33	4	6	
82	dF	1	Total	C	N	O	0
			43	33	4	6	
82	eF	1	Total	C	N	O	0
			43	33	4	6	
82	eF	1	Total	C	N	O	0
			43	33	4	6	
82	eF	1	Total	C	N	O	0
			43	33	4	6	
82	fF	1	Total	C	N	O	0
			43	33	4	6	
82	fF	1	Total	C	N	O	0
			43	33	4	6	
82	gF	1	Total	C	N	O	0
			43	33	4	6	
82	gF	1	Total	C	N	O	0
			43	33	4	6	
82	gF	1	Total	C	N	O	0
			43	33	4	6	
82	hF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	hF	1	Total	C	N	O	0
			43	33	4	6	
82	iF	1	Total	C	N	O	0
			43	33	4	6	
82	iF	1	Total	C	N	O	0
			43	33	4	6	
82	iF	1	Total	C	N	O	0
			43	33	4	6	
82	jF	1	Total	C	N	O	0
			43	33	4	6	
82	jF	1	Total	C	N	O	0
			43	33	4	6	
82	kF	1	Total	C	N	O	0
			43	33	4	6	
82	kF	1	Total	C	N	O	0
			43	33	4	6	
82	kF	1	Total	C	N	O	0
			43	33	4	6	
82	lF	1	Total	C	N	O	0
			43	33	4	6	
82	lF	1	Total	C	N	O	0
			43	33	4	6	
82	lF	1	Total	C	N	O	0
			43	33	4	6	
82	mF	1	Total	C	N	O	0
			43	33	4	6	
82	mF	1	Total	C	N	O	0
			43	33	4	6	
82	nF	1	Total	C	N	O	0
			43	33	4	6	
82	nF	1	Total	C	N	O	0
			43	33	4	6	
82	oF	1	Total	C	N	O	0
			43	33	4	6	
82	oF	1	Total	C	N	O	0
			43	33	4	6	
82	oF	1	Total	C	N	O	0
			43	33	4	6	
82	pF	1	Total	C	N	O	0
			43	33	4	6	
82	pF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	qF	1	Total	C	N	O	0
			43	33	4	6	
82	qF	1	Total	C	N	O	0
			43	33	4	6	
82	qF	1	Total	C	N	O	0
			43	33	4	6	
82	rF	1	Total	C	N	O	0
			43	33	4	6	
82	rF	1	Total	C	N	O	0
			43	33	4	6	
82	sF	1	Total	C	N	O	0
			43	33	4	6	
82	sF	1	Total	C	N	O	0
			43	33	4	6	
82	sF	1	Total	C	N	O	0
			43	33	4	6	
82	tF	1	Total	C	N	O	0
			43	33	4	6	
82	tF	1	Total	C	N	O	0
			43	33	4	6	
82	uF	1	Total	C	N	O	0
			43	33	4	6	
82	uF	1	Total	C	N	O	0
			43	33	4	6	
82	uF	1	Total	C	N	O	0
			43	33	4	6	
82	vF	1	Total	C	N	O	0
			43	33	4	6	
82	vF	1	Total	C	N	O	0
			43	33	4	6	
82	wF	1	Total	C	N	O	0
			43	33	4	6	
82	wF	1	Total	C	N	O	0
			43	33	4	6	
82	wF	1	Total	C	N	O	0
			43	33	4	6	
82	xF	1	Total	C	N	O	0
			43	33	4	6	
82	xF	1	Total	C	N	O	0
			43	33	4	6	
82	xF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	yF	1	Total	C	N	O	0
			43	33	4	6	
82	zF	1	Total	C	N	O	0
			43	33	4	6	
82	aG	1	Total	C	N	O	0
			43	33	4	6	
82	aG	1	Total	C	N	O	0
			43	33	4	6	
82	bG	1	Total	C	N	O	0
			43	33	4	6	
82	cG	1	Total	C	N	O	0
			43	33	4	6	
82	cG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	eG	1	Total	C	N	O	0
			43	33	4	6	
82	eG	1	Total	C	N	O	0
			43	33	4	6	
82	eG	1	Total	C	N	O	0
			43	33	4	6	
82	fG	1	Total	C	N	O	0
			43	33	4	6	
82	fG	1	Total	C	N	O	0
			43	33	4	6	
82	fG	1	Total	C	N	O	0
			43	33	4	6	
82	gG	1	Total	C	N	O	0
			43	33	4	6	
82	gG	1	Total	C	N	O	0
			43	33	4	6	
82	hG	1	Total	C	N	O	0
			43	33	4	6	
82	hG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	hG	1	Total	C	N	O	0
			43	33	4	6	
82	iG	1	Total	C	N	O	0
			43	33	4	6	
82	iG	1	Total	C	N	O	0
			43	33	4	6	
82	jG	1	Total	C	N	O	0
			43	33	4	6	
82	jG	1	Total	C	N	O	0
			43	33	4	6	
82	kG	1	Total	C	N	O	0
			43	33	4	6	
82	kG	1	Total	C	N	O	0
			43	33	4	6	
82	lG	1	Total	C	N	O	0
			43	33	4	6	
82	lG	1	Total	C	N	O	0
			43	33	4	6	
82	lG	1	Total	C	N	O	0
			43	33	4	6	
82	mG	1	Total	C	N	O	0
			43	33	4	6	
82	mG	1	Total	C	N	O	0
			43	33	4	6	
82	mG	1	Total	C	N	O	0
			43	33	4	6	
82	fH	1	Total	C	N	O	0
			43	33	4	6	
82	fH	1	Total	C	N	O	0
			43	33	4	6	
82	fH	1	Total	C	N	O	0
			43	33	4	6	
82	gH	1	Total	C	N	O	0
			43	33	4	6	
82	gH	1	Total	C	N	O	0
			43	33	4	6	
82	gH	1	Total	C	N	O	0
			43	33	4	6	
82	hH	1	Total	C	N	O	0
			43	33	4	6	
82	hH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	iH	1	Total	C	N	O	0
			43	33	4	6	
82	iH	1	Total	C	N	O	0
			43	33	4	6	
82	jH	1	Total	C	N	O	0
			43	33	4	6	
82	jH	1	Total	C	N	O	0
			43	33	4	6	
82	jH	1	Total	C	N	O	0
			43	33	4	6	
82	kH	1	Total	C	N	O	0
			43	33	4	6	
82	kH	1	Total	C	N	O	0
			43	33	4	6	
82	kH	1	Total	C	N	O	0
			43	33	4	6	
82	lH	1	Total	C	N	O	0
			43	33	4	6	
82	lH	1	Total	C	N	O	0
			43	33	4	6	
82	mH	1	Total	C	N	O	0
			43	33	4	6	
82	mH	1	Total	C	N	O	0
			43	33	4	6	
82	aH	1	Total	C	N	O	0
			43	33	4	6	
82	aH	1	Total	C	N	O	0
			43	33	4	6	
82	bH	1	Total	C	N	O	0
			43	33	4	6	
82	bH	1	Total	C	N	O	0
			43	33	4	6	
82	cH	1	Total	C	N	O	0
			43	33	4	6	
82	cH	1	Total	C	N	O	0
			43	33	4	6	
82	dH	1	Total	C	N	O	0
			43	33	4	6	
82	dH	1	Total	C	N	O	0
			43	33	4	6	
82	dH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	eH	1	Total	C	N	O	0
			43	33	4	6	
82	eH	1	Total	C	N	O	0
			43	33	4	6	
82	eH	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	cJ	1	Total	C	N	O	0
			43	33	4	6	
82	cJ	1	Total	C	N	O	0
			43	33	4	6	
82	dJ	1	Total	C	N	O	0
			43	33	4	6	
82	dJ	1	Total	C	N	O	0
			43	33	4	6	
82	eJ	1	Total	C	N	O	0
			43	33	4	6	
82	eJ	1	Total	C	N	O	0
			43	33	4	6	
82	fJ	1	Total	C	N	O	0
			43	33	4	6	
82	fJ	1	Total	C	N	O	0
			43	33	4	6	
82	fJ	1	Total	C	N	O	0
			43	33	4	6	
82	gJ	1	Total	C	N	O	0
			43	33	4	6	
82	gJ	1	Total	C	N	O	0
			43	33	4	6	
82	hJ	1	Total	C	N	O	0
			43	33	4	6	
82	hJ	1	Total	C	N	O	0
			43	33	4	6	
82	hJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	iJ	1	Total	C	N	O	0
			43	33	4	6	
82	iJ	1	Total	C	N	O	0
			43	33	4	6	
82	jJ	1	Total	C	N	O	0
			43	33	4	6	
82	jJ	1	Total	C	N	O	0
			43	33	4	6	
82	jJ	1	Total	C	N	O	0
			43	33	4	6	
82	kJ	1	Total	C	N	O	0
			43	33	4	6	
82	kJ	1	Total	C	N	O	0
			43	33	4	6	
82	lJ	1	Total	C	N	O	0
			43	33	4	6	
82	lJ	1	Total	C	N	O	0
			43	33	4	6	
82	lJ	1	Total	C	N	O	0
			43	33	4	6	
82	mJ	1	Total	C	N	O	0
			43	33	4	6	
82	mJ	1	Total	C	N	O	0
			43	33	4	6	
82	aK	1	Total	C	N	O	0
			43	33	4	6	
82	aK	1	Total	C	N	O	0
			43	33	4	6	
82	aK	1	Total	C	N	O	0
			43	33	4	6	
82	bK	1	Total	C	N	O	0
			43	33	4	6	
82	bK	1	Total	C	N	O	0
			43	33	4	6	
82	cK	1	Total	C	N	O	0
			43	33	4	6	
82	cK	1	Total	C	N	O	0
			43	33	4	6	
82	cK	1	Total	C	N	O	0
			43	33	4	6	
82	dK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	dK	1	Total	C	N	O	0
			43	33	4	6	
82	eK	1	Total	C	N	O	0
			43	33	4	6	
82	eK	1	Total	C	N	O	0
			43	33	4	6	
82	eK	1	Total	C	N	O	0
			43	33	4	6	
82	fK	1	Total	C	N	O	0
			43	33	4	6	
82	fK	1	Total	C	N	O	0
			43	33	4	6	
82	gK	1	Total	C	N	O	0
			43	33	4	6	
82	gK	1	Total	C	N	O	0
			43	33	4	6	
82	gK	1	Total	C	N	O	0
			43	33	4	6	
82	hK	1	Total	C	N	O	0
			43	33	4	6	
82	hK	1	Total	C	N	O	0
			43	33	4	6	
82	iK	1	Total	C	N	O	0
			43	33	4	6	
82	iK	1	Total	C	N	O	0
			43	33	4	6	
82	iK	1	Total	C	N	O	0
			43	33	4	6	
82	jK	1	Total	C	N	O	0
			43	33	4	6	
82	jK	1	Total	C	N	O	0
			43	33	4	6	
82	kK	1	Total	C	N	O	0
			43	33	4	6	
82	kK	1	Total	C	N	O	0
			43	33	4	6	
82	kK	1	Total	C	N	O	0
			43	33	4	6	
82	lK	1	Total	C	N	O	0
			43	33	4	6	
82	lK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	lK	1	Total	C	N	O	0
			43	33	4	6	
82	mK	1	Total	C	N	O	0
			43	33	4	6	
82	mK	1	Total	C	N	O	0
			43	33	4	6	
82	nK	1	Total	C	N	O	0
			43	33	4	6	
82	nK	1	Total	C	N	O	0
			43	33	4	6	
82	oK	1	Total	C	N	O	0
			43	33	4	6	
82	oK	1	Total	C	N	O	0
			43	33	4	6	
82	oK	1	Total	C	N	O	0
			43	33	4	6	
82	pK	1	Total	C	N	O	0
			43	33	4	6	
82	pK	1	Total	C	N	O	0
			43	33	4	6	
82	qK	1	Total	C	N	O	0
			43	33	4	6	
82	qK	1	Total	C	N	O	0
			43	33	4	6	
82	qK	1	Total	C	N	O	0
			43	33	4	6	
82	rK	1	Total	C	N	O	0
			43	33	4	6	
82	rK	1	Total	C	N	O	0
			43	33	4	6	
82	sK	1	Total	C	N	O	0
			43	33	4	6	
82	sK	1	Total	C	N	O	0
			43	33	4	6	
82	sK	1	Total	C	N	O	0
			43	33	4	6	
82	tK	1	Total	C	N	O	0
			43	33	4	6	
82	tK	1	Total	C	N	O	0
			43	33	4	6	
82	tK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	uK	1	Total	C	N	O	0
			43	33	4	6	
82	uK	1	Total	C	N	O	0
			43	33	4	6	
82	vK	1	Total	C	N	O	0
			43	33	4	6	
82	vK	1	Total	C	N	O	0
			43	33	4	6	
82	wK	1	Total	C	N	O	0
			43	33	4	6	
82	wK	1	Total	C	N	O	0
			43	33	4	6	
82	wK	1	Total	C	N	O	0
			43	33	4	6	
82	xK	1	Total	C	N	O	0
			43	33	4	6	
82	xK	1	Total	C	N	O	0
			43	33	4	6	
82	xK	1	Total	C	N	O	0
			43	33	4	6	
82	yK	1	Total	C	N	O	0
			43	33	4	6	
82	zK	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	cM	1	Total	C	N	O	0
			43	33	4	6	
82	cM	1	Total	C	N	O	0
			43	33	4	6	
82	dM	1	Total	C	N	O	0
			43	33	4	6	
82	dM	1	Total	C	N	O	0
			43	33	4	6	
82	dM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	eM	1	Total	C	N	O	0
			43	33	4	6	
82	eM	1	Total	C	N	O	0
			43	33	4	6	
82	fM	1	Total	C	N	O	0
			43	33	4	6	
82	fM	1	Total	C	N	O	0
			43	33	4	6	
82	fM	1	Total	C	N	O	0
			43	33	4	6	
82	gM	1	Total	C	N	O	0
			43	33	4	6	
82	gM	1	Total	C	N	O	0
			43	33	4	6	
82	hM	1	Total	C	N	O	0
			43	33	4	6	
82	hM	1	Total	C	N	O	0
			43	33	4	6	
82	hM	1	Total	C	N	O	0
			43	33	4	6	
82	iM	1	Total	C	N	O	0
			43	33	4	6	
82	iM	1	Total	C	N	O	0
			43	33	4	6	
82	jM	1	Total	C	N	O	0
			43	33	4	6	
82	jM	1	Total	C	N	O	0
			43	33	4	6	
82	jM	1	Total	C	N	O	0
			43	33	4	6	
82	kM	1	Total	C	N	O	0
			43	33	4	6	
82	kM	1	Total	C	N	O	0
			43	33	4	6	
82	lM	1	Total	C	N	O	0
			43	33	4	6	
82	lM	1	Total	C	N	O	0
			43	33	4	6	
82	lM	1	Total	C	N	O	0
			43	33	4	6	
82	mM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	mM	1	Total	C	N	O	0
			43	33	4	6	
82	iO	1	Total	C	N	O	0
			43	33	4	6	
82	iO	1	Total	C	N	O	0
			43	33	4	6	
82	iO	1	Total	C	N	O	0
			43	33	4	6	
82	jO	1	Total	C	N	O	0
			43	33	4	6	
82	jO	1	Total	C	N	O	0
			43	33	4	6	
82	kO	1	Total	C	N	O	0
			43	33	4	6	
82	kO	1	Total	C	N	O	0
			43	33	4	6	
82	kO	1	Total	C	N	O	0
			43	33	4	6	
82	lO	1	Total	C	N	O	0
			43	33	4	6	
82	lO	1	Total	C	N	O	0
			43	33	4	6	
82	mO	1	Total	C	N	O	0
			43	33	4	6	
82	mO	1	Total	C	N	O	0
			43	33	4	6	
82	mO	1	Total	C	N	O	0
			43	33	4	6	
82	aO	1	Total	C	N	O	0
			43	33	4	6	
82	aO	1	Total	C	N	O	0
			43	33	4	6	
82	aO	1	Total	C	N	O	0
			43	33	4	6	
82	bO	1	Total	C	N	O	0
			43	33	4	6	
82	bO	1	Total	C	N	O	0
			43	33	4	6	
82	cO	1	Total	C	N	O	0
			43	33	4	6	
82	cO	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	cO	1	Total	C	N	O	0
			43	33	4	6	
82	dO	1	Total	C	N	O	0
			43	33	4	6	
82	dO	1	Total	C	N	O	0
			43	33	4	6	
82	eO	1	Total	C	N	O	0
			43	33	4	6	
82	eO	1	Total	C	N	O	0
			43	33	4	6	
82	eO	1	Total	C	N	O	0
			43	33	4	6	
82	fO	1	Total	C	N	O	0
			43	33	4	6	
82	fO	1	Total	C	N	O	0
			43	33	4	6	
82	gO	1	Total	C	N	O	0
			43	33	4	6	
82	gO	1	Total	C	N	O	0
			43	33	4	6	
82	gO	1	Total	C	N	O	0
			43	33	4	6	
82	hO	1	Total	C	N	O	0
			43	33	4	6	
82	hO	1	Total	C	N	O	0
			43	33	4	6	
82	bP	1	Total	C	N	O	0
			43	33	4	6	
82	bP	1	Total	C	N	O	0
			43	33	4	6	
82	dQ	1	Total	C	N	O	0
			43	33	4	6	
82	Z9	1	Total	C	N	O	0
			43	33	4	6	
82	Z9	1	Total	C	N	O	0
			43	33	4	6	
82	Z9	1	Total	C	N	O	0
			43	33	4	6	
82	M9	1	Total	C	N	O	0
			43	33	4	6	
82	M9	1	Total	C	N	O	0
			43	33	4	6	

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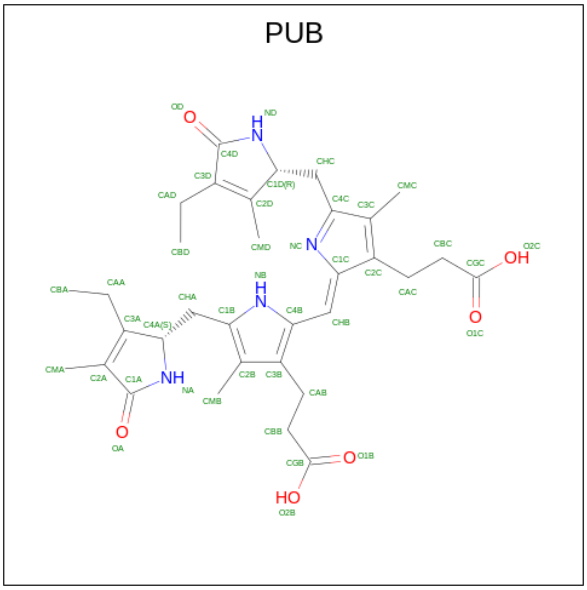
Mol	Chain	Residues	Atoms				AltConf
82	M9	1	Total	C	N	O	0
			43	33	4	6	
82	M9	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 83 is PHYCOUROBILIN (CCD ID: PUB) (formula: $C_{33}H_{42}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
83	KA	1	Total	C	N	O	0
			43	33	4	6	
83	YA	1	Total	C	N	O	0
			43	33	4	6	
83	AD	1	Total	C	N	O	0
			43	33	4	6	
83	ND	1	Total	C	N	O	0
			43	33	4	6	
83	AE	1	Total	C	N	O	0
			43	33	4	6	
83	AE	1	Total	C	N	O	0
			43	33	4	6	
83	AG	1	Total	C	N	O	0
			43	33	4	6	
83	AG	1	Total	C	N	O	0
			43	33	4	6	
83	AH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
83	AH	1	Total	C	N	O	0
			43	33	4	6	
83	AJ	1	Total	C	N	O	0
			43	33	4	6	
83	AJ	1	Total	C	N	O	0
			43	33	4	6	
83	BJ	1	Total	C	N	O	0
			43	33	4	6	
83	QJ	1	Total	C	N	O	0
			43	33	4	6	
83	AM	1	Total	C	N	O	0
			43	33	4	6	
83	AM	1	Total	C	N	O	0
			43	33	4	6	
83	BM	1	Total	C	N	O	0
			43	33	4	6	
83	QM	1	Total	C	N	O	0
			43	33	4	6	
83	AO	1	Total	C	N	O	0
			43	33	4	6	
83	AO	1	Total	C	N	O	0
			43	33	4	6	
83	AQ	1	Total	C	N	O	0
			43	33	4	6	
83	NQ	1	Total	C	N	O	0
			43	33	4	6	
83	A1	1	Total	C	N	O	0
			43	33	4	6	
83	A1	1	Total	C	N	O	0
			43	33	4	6	
83	A4	1	Total	C	N	O	0
			43	33	4	6	
83	A4	1	Total	C	N	O	0
			43	33	4	6	
83	M5	1	Total	C	N	O	0
			43	33	4	6	
83	M5	1	Total	C	N	O	0
			43	33	4	6	
83	Z5	1	Total	C	N	O	0
			43	33	4	6	
83	Z5	1	Total	C	N	O	0
			43	33	4	6	

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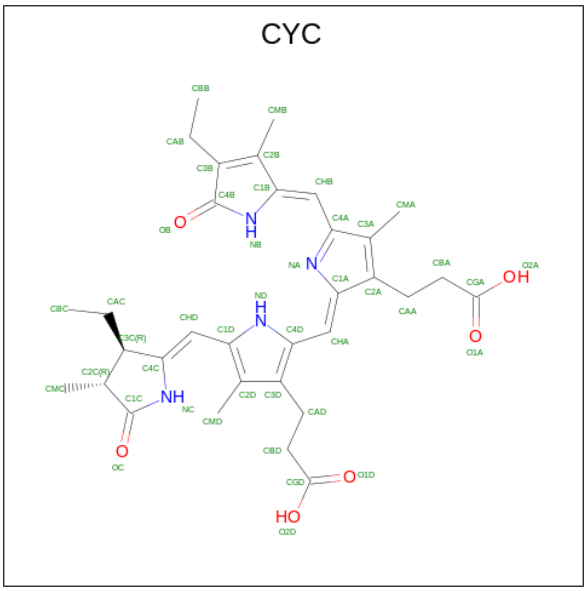
Mol	Chain	Residues	Atoms				AltConf
83	K7	1	Total	C	N	O	0
			43	33	4	6	
83	Y7	1	Total	C	N	O	0
			43	33	4	6	
83	wF	1	Total	C	N	O	0
			43	33	4	6	
83	xF	1	Total	C	N	O	0
			43	33	4	6	
83	xF	1	Total	C	N	O	0
			43	33	4	6	
83	xF	1	Total	C	N	O	0
			43	33	4	6	
83	yF	1	Total	C	N	O	0
			43	33	4	6	
83	yF	1	Total	C	N	O	0
			43	33	4	6	
83	wK	1	Total	C	N	O	0
			43	33	4	6	
83	xK	1	Total	C	N	O	0
			43	33	4	6	
83	xK	1	Total	C	N	O	0
			43	33	4	6	
83	xK	1	Total	C	N	O	0
			43	33	4	6	
83	yK	1	Total	C	N	O	0
			43	33	4	6	
83	yK	1	Total	C	N	O	0
			43	33	4	6	
83	Z9	1	Total	C	N	O	0
			43	33	4	6	
83	Z9	1	Total	C	N	O	0
			43	33	4	6	
83	M9	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 84 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
84	BE	1	Total	C	N	O	0
			43	33	4	6	
84	BE	1	Total	C	N	O	0
			43	33	4	6	
84	DE	1	Total	C	N	O	0
			43	33	4	6	
84	EE	1	Total	C	N	O	0
			43	33	4	6	
84	FE	1	Total	C	N	O	0
			43	33	4	6	
84	FE	1	Total	C	N	O	0
			43	33	4	6	
84	GE	1	Total	C	N	O	0
			43	33	4	6	
84	HE	1	Total	C	N	O	0
			43	33	4	6	
84	IE	1	Total	C	N	O	0
			43	33	4	6	
84	LE	1	Total	C	N	O	0
			43	33	4	6	
84	ME	1	Total	C	N	O	0
			43	33	4	6	
84	NE	1	Total	C	N	O	0
			43	33	4	6	
84	BG	1	Total	C	N	O	0
			43	33	4	6	
84	BG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
84	CG	1	Total	C	N	O	0
			43	33	4	6	
84	DG	1	Total	C	N	O	0
			43	33	4	6	
84	EG	1	Total	C	N	O	0
			43	33	4	6	
84	FG	1	Total	C	N	O	0
			43	33	4	6	
84	GG	1	Total	C	N	O	0
			43	33	4	6	
84	HG	1	Total	C	N	O	0
			43	33	4	6	
84	IG	1	Total	C	N	O	0
			43	33	4	6	
84	KG	1	Total	C	N	O	0
			43	33	4	6	
84	LG	1	Total	C	N	O	0
			43	33	4	6	
84	MG	1	Total	C	N	O	0
			43	33	4	6	
84	CH	1	Total	C	N	O	0
			43	33	4	6	
84	DH	1	Total	C	N	O	0
			43	33	4	6	
84	DH	1	Total	C	N	O	0
			43	33	4	6	
84	EH	1	Total	C	N	O	0
			43	33	4	6	
84	FH	1	Total	C	N	O	0
			43	33	4	6	
84	HH	1	Total	C	N	O	0
			43	33	4	6	
84	JH	1	Total	C	N	O	0
			43	33	4	6	
84	JH	1	Total	C	N	O	0
			43	33	4	6	
84	KH	1	Total	C	N	O	0
			43	33	4	6	
84	LH	1	Total	C	N	O	0
			43	33	4	6	
84	LH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
84	NH	1	Total	C	N	O	0
			43	33	4	6	
84	CO	1	Total	C	N	O	0
			43	33	4	6	
84	DO	1	Total	C	N	O	0
			43	33	4	6	
84	EO	1	Total	C	N	O	0
			43	33	4	6	
84	FO	1	Total	C	N	O	0
			43	33	4	6	
84	GO	1	Total	C	N	O	0
			43	33	4	6	
84	HO	1	Total	C	N	O	0
			43	33	4	6	
84	IO	1	Total	C	N	O	0
			43	33	4	6	
84	JO	1	Total	C	N	O	0
			43	33	4	6	
84	KO	1	Total	C	N	O	0
			43	33	4	6	
84	LO	1	Total	C	N	O	0
			43	33	4	6	
84	MO	1	Total	C	N	O	0
			43	33	4	6	
84	NO	1	Total	C	N	O	0
			43	33	4	6	
84	L1	1	Total	C	N	O	0
			43	33	4	6	
84	M1	1	Total	C	N	O	0
			43	33	4	6	
84	N1	1	Total	C	N	O	0
			43	33	4	6	
84	C1	1	Total	C	N	O	0
			43	33	4	6	
84	D1	1	Total	C	N	O	0
			43	33	4	6	
84	D1	1	Total	C	N	O	0
			43	33	4	6	
84	E1	1	Total	C	N	O	0
			43	33	4	6	
84	F1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms					AltConf
84	H1	1	Total	C	N	O		0
			43	33	4	6		
84	I1	1	Total	C	N	O		0
			43	33	4	6		
84	J1	1	Total	C	N	O		0
			43	33	4	6		
84	K1	1	Total	C	N	O		0
			43	33	4	6		
84	A3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	B3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	C3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	D3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	E3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	F3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	G3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	H3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	I3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	J3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	K3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	L3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	M3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	N3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	O3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	P3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	Q3	1	Total	C	H	N	O	0
			81	33	38	4	6	

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Mol	Chain	Residues	Atoms					AltConf
84	R3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	S3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	T3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	U3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	V3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	W3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	c3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	d3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	e3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	f3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	g3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	h3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	i3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	j3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	k3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	l3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	m3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	n3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	o3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	p3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	q3	1	Total	C	H	N	O	0
			81	33	38	4	6	

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Mol	Chain	Residues	Atoms					AltConf
84	r3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	t3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	u3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	v3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	w3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	x3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	y3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	63	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	73	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	73	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	F4	1	Total	C	N	O		0
			43	33	4	6		
84	G4	1	Total	C	N	O		0
			43	33	4	6		
84	H4	1	Total	C	N	O		0
			43	33	4	6		
84	I4	1	Total	C	N	O		0
			43	33	4	6		
84	J4	1	Total	C	N	O		0
			43	33	4	6		
84	K4	1	Total	C	N	O		0
			43	33	4	6		
84	L4	1	Total	C	N	O		0
			43	33	4	6		
84	M4	1	Total	C	N	O		0
			43	33	4	6		
84	N4	1	Total	C	N	O		0
			43	33	4	6		
84	C4	1	Total	C	N	O		0
			43	33	4	6		
84	D4	1	Total	C	N	O		0
			43	33	4	6		

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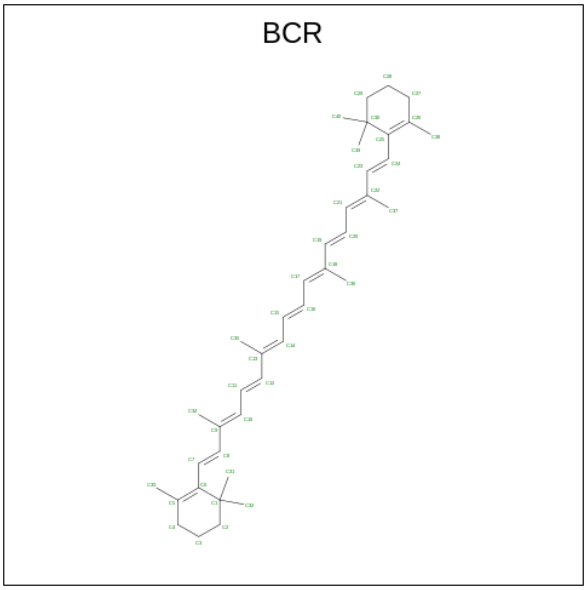
Mol	Chain	Residues	Atoms	AltConf
84	E4	1	Total C N O 43 33 4 6	0

- Molecule 85 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
85	AL	1	Total C 40 40	0
85	BL	1	Total C 40 40	0
85	BL	1	Total C 40 40	0
85	BL	1	Total C 40 40	0
85	CL	1	Total C 40 40	0
85	CL	1	Total C 40 40	0
85	CL	1	Total C 40 40	0
85	FL	1	Total C 40 40	0
85	HL	1	Total C 40 40	0
85	KL	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	FN	1	Total C 40 40	0
85	FN	1	Total C 40 40	0
85	IN	1	Total C 40 40	0
85	JN	1	Total C 40 40	0
85	JN	1	Total C 40 40	0
85	KN	1	Total C 40 40	0
85	KN	1	Total C 40 40	0
85	LN	1	Total C 40 40	0
85	LN	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	F2	1	Total C 40 40	0
85	F2	1	Total C 40 40	0
85	I2	1	Total C 40 40	0
85	J2	1	Total C 40 40	0
85	J2	1	Total C 40 40	0
85	K2	1	Total C 40 40	0
85	K2	1	Total C 40 40	0
85	L2	1	Total C 40 40	0
85	L2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
85	A6	1	Total C 40 40	0
85	B6	1	Total C 40 40	0
85	B6	1	Total C 40 40	0
85	B6	1	Total C 40 40	0
85	C6	1	Total C 40 40	0
85	C6	1	Total C 40 40	0
85	F6	1	Total C 40 40	0
85	H6	1	Total C 40 40	0
85	K6	1	Total C 40 40	0
85	Z6	1	Total C 40 40	0
85	a6	1	Total C 40 40	0
85	b6	1	Total C 40 40	0
85	b6	1	Total C 40 40	0
85	b6	1	Total C 40 40	0
85	c6	1	Total C 40 40	0
85	c6	1	Total C 40 40	0
85	c6	1	Total C 40 40	0
85	d6	1	Total C 40 40	0
85	h6	1	Total C 40 40	0
85	k6	1	Total C 40 40	0
85	aL	1	Total C 40 40	0

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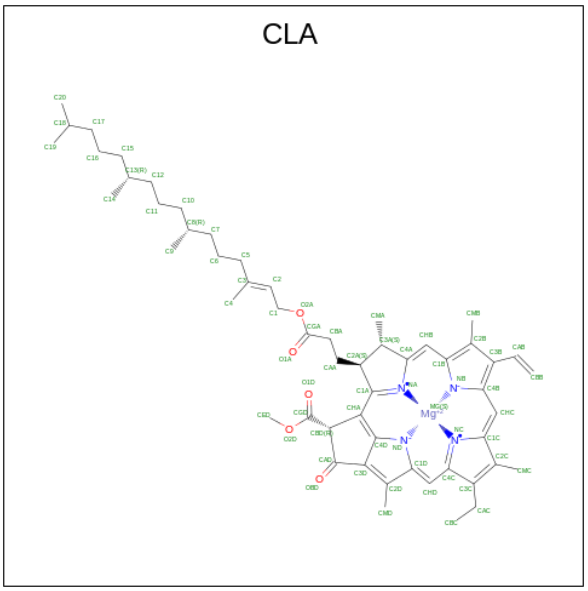
Mol	Chain	Residues	Atoms	AltConf
85	bL	1	Total C 40 40	0
85	bL	1	Total C 40 40	0
85	bL	1	Total C 40 40	0
85	cL	1	Total C 40 40	0
85	cL	1	Total C 40 40	0
85	cL	1	Total C 40 40	0
85	fL	1	Total C 40 40	0
85	hL	1	Total C 40 40	0
85	kL	1	Total C 40 40	0

- Molecule 86 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
86	AL	1	Total Cl 1 1	0
86	C6	1	Total Cl 1 1	0
86	a6	1	Total Cl 1 1	0
86	aL	1	Total Cl 1 1	0

- Molecule 87 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
87	AL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	AL	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	DL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	DL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	DL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	HL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	HL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	AN	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	BN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	BN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	FN	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	FN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	FN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	IN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	IN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	JN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	KN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	KN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	KN	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
87	MN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	ON	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	ON	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	ON	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	12	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	12	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	22	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	22	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	32	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	32	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	42	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	52	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	62	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	72	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	36	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
87	A2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	B2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
87	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	F2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	F2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	F2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	I2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	I2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	J2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	K2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	K2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	K2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	K2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
87	M2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	O2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	O2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	O2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	D6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	D6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	D6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	H6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	H6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	K6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	a6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	a6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	d6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	d6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	d6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	aL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	nL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	1N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	2N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	3N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	4N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	5N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	6N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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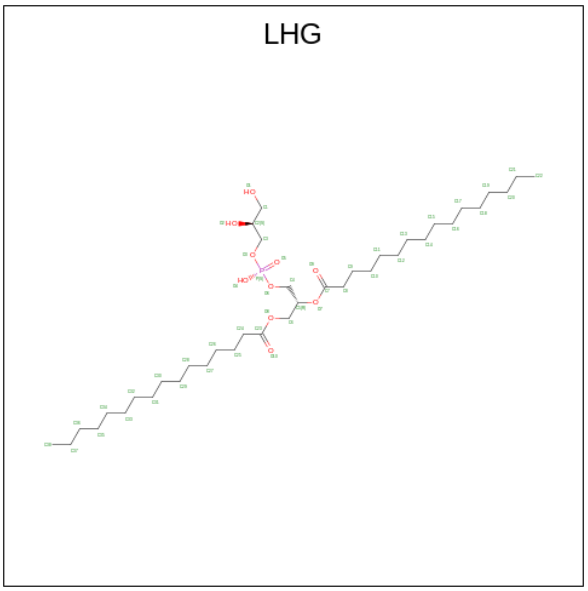
Mol	Chain	Residues	Atoms					AltConf
87	7N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	7N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 88 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
88	AL	1	Total	C	O	P	0
			49	38	10	1	
88	AL	1	Total	C	O	P	0
			43	32	10	1	
88	BL	1	Total	C	O	P	0
			49	38	10	1	
88	BL	1	Total	C	O	P	0
			41	30	10	1	
88	CL	1	Total	C	O	P	0
			37	26	10	1	
88	CL	1	Total	C	O	P	0
			32	21	10	1	
88	DL	1	Total	C	O	P	0
			49	38	10	1	
88	ML	1	Total	C	O	P	0
			39	28	10	1	
88	AN	1	Total	C	O	P	0
			49	38	10	1	
88	AN	1	Total	C	O	P	0
			40	29	10	1	
88	A2	1	Total	C	O	P	0
			49	38	10	1	
88	A2	1	Total	C	O	P	0
			40	29	10	1	
88	B6	1	Total	C	O	P	0
			49	38	10	1	
88	C6	1	Total	C	O	P	0
			37	26	10	1	

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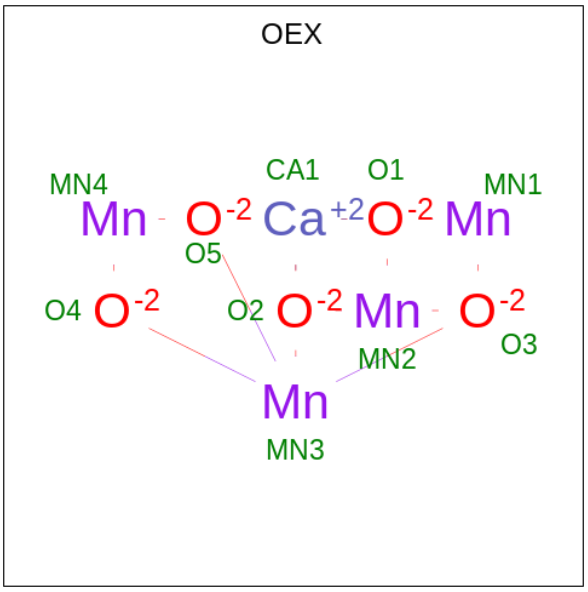
Mol	Chain	Residues	Atoms	AltConf
88	C6	1	Total C O P 32 21 10 1	0
88	D6	1	Total C O P 43 32 10 1	0
88	D6	1	Total C O P 49 38 10 1	0
88	I6	1	Total C H O P 123 38 74 10 1	0
88	L6	1	Total C O P 49 38 10 1	0
88	M6	1	Total C O P 39 28 10 1	0
88	a6	1	Total C O P 43 32 10 1	0
88	c6	1	Total C O P 32 21 10 1	0
88	d6	1	Total C O P 46 35 10 1	0
88	d6	1	Total C O P 49 38 10 1	0
88	i6	1	Total C H O P 123 38 74 10 1	0
88	l6	1	Total C O P 49 38 10 1	0
88	m6	1	Total C O P 39 28 10 1	0
88	aL	1	Total C O P 43 32 10 1	0
88	bL	1	Total C O P 49 38 10 1	0
88	cL	1	Total C O P 32 21 10 1	0
88	dL	1	Total C O P 49 38 10 1	0
88	dL	1	Total C O P 46 35 10 1	0
88	iL	1	Total C O P 49 38 10 1	0
88	mL	1	Total C O P 39 28 10 1	0

- Molecule 89 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

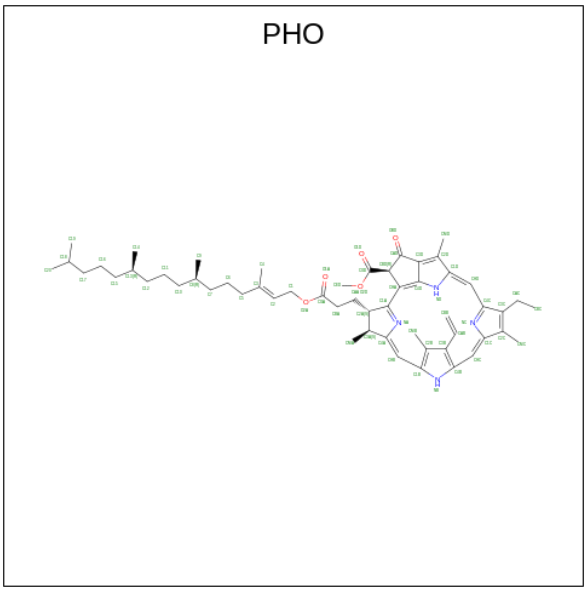


Mol	Chain	Residues	Atoms				AltConf
89	AL	1	Total	Ca	Mn	O	0
			10	1	4	5	
89	A6	1	Total	Ca	Mn	O	0
			10	1	4	5	
89	a6	1	Total	Ca	Mn	O	0
			10	1	4	5	
89	aL	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 90 is FE (III) ION (CCD ID: FE) (formula: Fe).

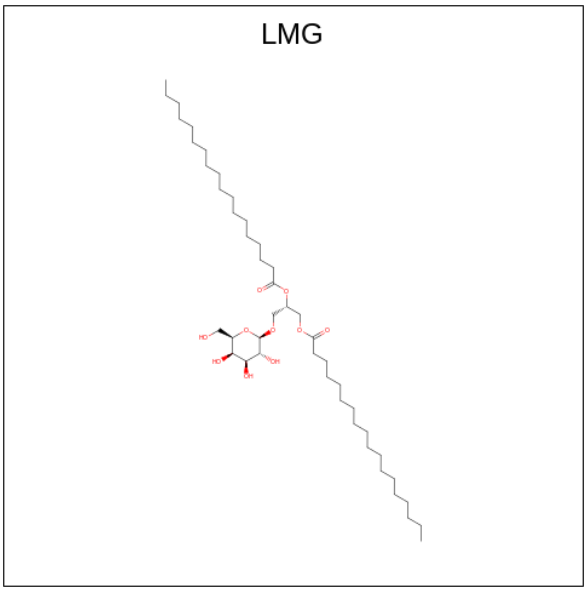
Mol	Chain	Residues	Atoms		AltConf
90	AL	1	Total	Fe	0
			1	1	
90	A6	1	Total	Fe	0
			1	1	
90	a6	1	Total	Fe	0
			1	1	
90	aL	1	Total	Fe	0
			1	1	

- Molecule 91 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
91	AL	1	Total	C	N	O	0
			64	55	4	5	
91	DL	1	Total	C	N	O	0
			64	55	4	5	
91	A6	1	Total	C	N	O	0
			64	55	4	5	
91	D6	1	Total	C	N	O	0
			64	55	4	5	
91	a6	1	Total	C	N	O	0
			64	55	4	5	
91	d6	1	Total	C	N	O	0
			64	55	4	5	
91	aL	1	Total	C	N	O	0
			64	55	4	5	
91	dL	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 92 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
92	AL	1	Total C O 51 41 10	0
92	BL	1	Total C O 40 30 10	0
92	BL	1	Total C O 39 29 10	0
92	CL	1	Total C O 55 45 10	0
92	DL	1	Total C O 54 44 10	0
92	JL	1	Total C O 43 33 10	0
92	JL	1	Total C O 33 23 10	0
92	ML	1	Total C O 41 31 10	0
92	XL	1	Total C O 50 40 10	0
92	A6	1	Total C O 51 41 10	0
92	B6	1	Total C O 40 30 10	0
92	B6	1	Total C O 39 29 10	0
92	B6	1	Total C O 50 40 10	0
92	C6	1	Total C O 55 45 10	0

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Mol	Chain	Residues	Atoms	AltConf
92	D6	1	Total C O 33 23 10	0
92	D6	1	Total C O 54 44 10	0
92	J6	1	Total C O 43 33 10	0
92	a6	1	Total C O 42 32 10	0
92	b6	1	Total C O 41 31 10	0
92	b6	1	Total C O 39 29 10	0
92	b6	1	Total C O 41 31 10	0
92	b6	1	Total C O 36 26 10	0
92	d6	1	Total C O 54 44 10	0
92	j6	1	Total C O 43 33 10	0
92	j6	1	Total C O 33 23 10	0
92	k6	1	Total C O 55 45 10	0
92	m6	1	Total C O 41 31 10	0
92	m6	1	Total C O 41 31 10	0
92	x6	1	Total C O 50 40 10	0
92	aL	1	Total C O 42 32 10	0
92	bL	1	Total C O 41 31 10	0
92	bL	1	Total C O 41 31 10	0
92	bL	1	Total C O 50 40 10	0
92	bL	1	Total C O 41 31 10	0
92	bL	1	Total C O 39 29 10	0

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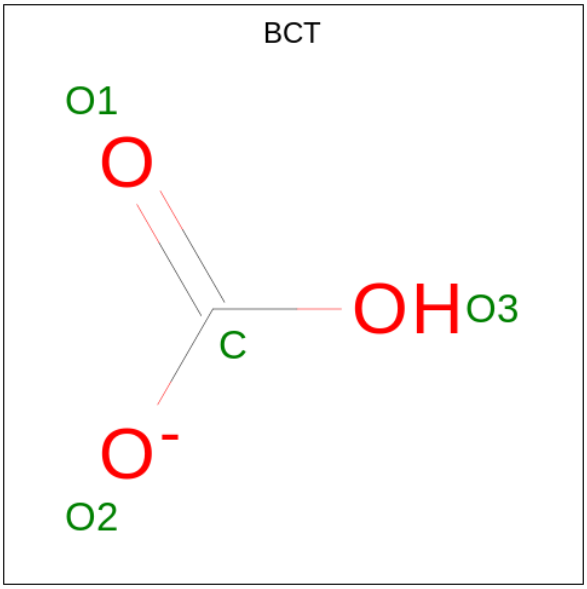
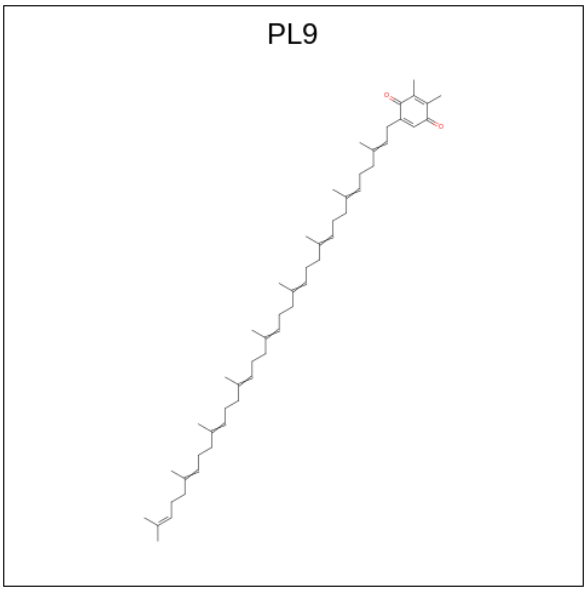
Mol	Chain	Residues	Atoms	AltConf
92	dL	1	Total C O 54 44 10	0
92	jL	1	Total C O 33 23 10	0
92	mL	1	Total C O 41 31 10	0
92	qL	1	Total C O 43 33 10	0
92	yL	1	Total C O 55 45 10	0

- Molecule 93 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



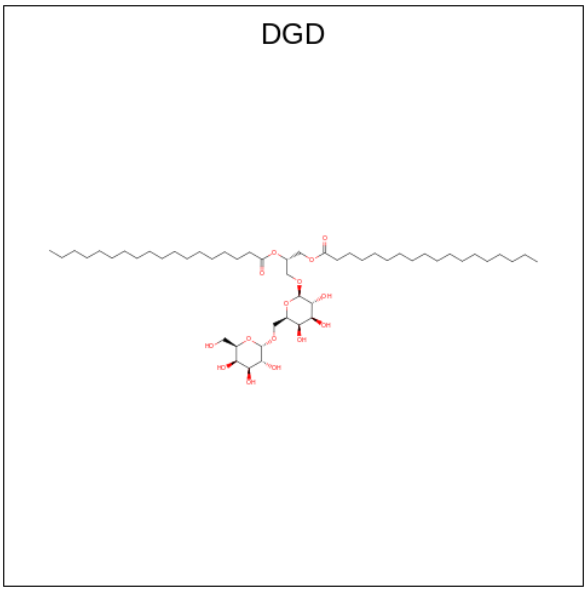
Mol	Chain	Residues	Atoms	AltConf
93	AL	1	Total C O 4 1 3	0
93	A6	1	Total C O 4 1 3	0
93	d6	1	Total C O 4 1 3	0
93	aL	1	Total C O 4 1 3	0

- Molecule 94 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	AltConf
94	AL	1	Total C O 55 53 2	0
94	DL	1	Total C O 55 53 2	0
94	A6	1	Total C O 55 53 2	0
94	D6	1	Total C O 55 53 2	0
94	a6	1	Total C O 55 53 2	0
94	d6	1	Total C O 55 53 2	0
94	aL	1	Total C O 55 53 2	0
94	dL	1	Total C O 55 53 2	0

- Molecule 95 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
95	AL	1	Total C O 62 47 15	0
95	AL	1	Total C O 40 25 15	0
95	AL	1	Total C O 40 25 15	0
95	BL	1	Total C O 40 25 15	0
95	BL	1	Total C O 40 25 15	0
95	BL	1	Total C O 58 43 15	0
95	CL	1	Total C O 62 47 15	0
95	CL	1	Total C O 42 27 15	0
95	CL	1	Total C O 48 33 15	0
95	DL	1	Total C O 62 47 15	0
95	JL	1	Total C O 62 47 15	0
95	BN	1	Total C O 66 51 15	0
95	B2	1	Total C O 66 51 15	0
95	B6	1	Total C O 58 43 15	0

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Mol	Chain	Residues	Atoms	AltConf
95	C6	1	Total C O 62 47 15	0
95	C6	1	Total C O 42 27 15	0
95	C6	1	Total C O 42 27 15	0
95	C6	1	Total C O 62 47 15	0
95	C6	1	Total C O 48 33 15	0
95	D6	1	Total C O 62 47 15	0
95	J6	1	Total C O 62 47 15	0
95	L6	1	Total C O 58 43 15	0
95	O6	1	Total C O 40 25 15	0
95	a6	1	Total C O 40 25 15	0
95	a6	1	Total C O 40 25 15	0
95	a6	1	Total C O 53 38 15	0
95	b6	1	Total C O 40 25 15	0
95	b6	1	Total C O 42 27 15	0
95	c6	1	Total C O 62 47 15	0
95	c6	1	Total C O 62 47 15	0
95	c6	1	Total C O 48 33 15	0
95	h6	1	Total C O 62 47 15	0
95	aL	1	Total C O 53 38 15	0
95	cL	1	Total C O 62 47 15	0
95	cL	1	Total C O 62 47 15	0

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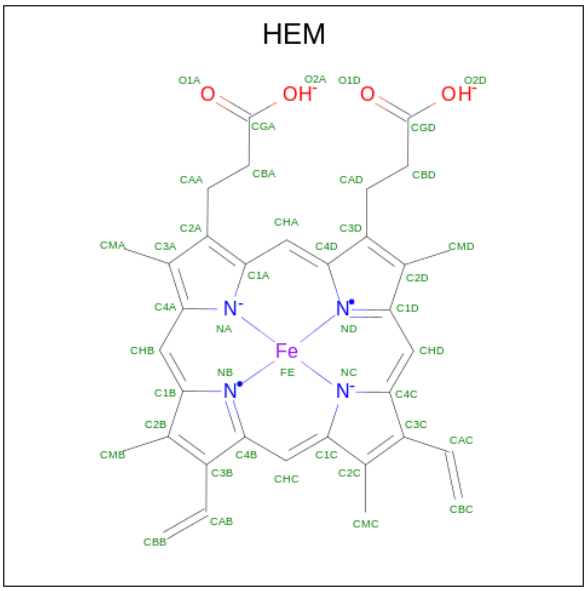
Mol	Chain	Residues	Atoms	AltConf
95	cL	1	Total C O 48 33 15	0
95	hL	1	Total C O 62 47 15	0
95	lL	1	Total C O 58 43 15	0

- Molecule 96 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	AltConf
96	FL	1	Total C Fe N O 43 34 1 4 4	0
96	VL	1	Total C Fe N O 43 34 1 4 4	0
96	GN	1	Total C Fe N O 43 34 1 4 4	0
96	G2	1	Total C Fe N O 43 34 1 4 4	0
96	E6	1	Total C Fe H N O 73 34 1 30 4 4	0
96	V6	1	Total C Fe N O 43 34 1 4 4	0
96	f6	1	Total C Fe H N O 73 34 1 30 4 4	0
96	v6	1	Total C Fe N O 43 34 1 4 4	0

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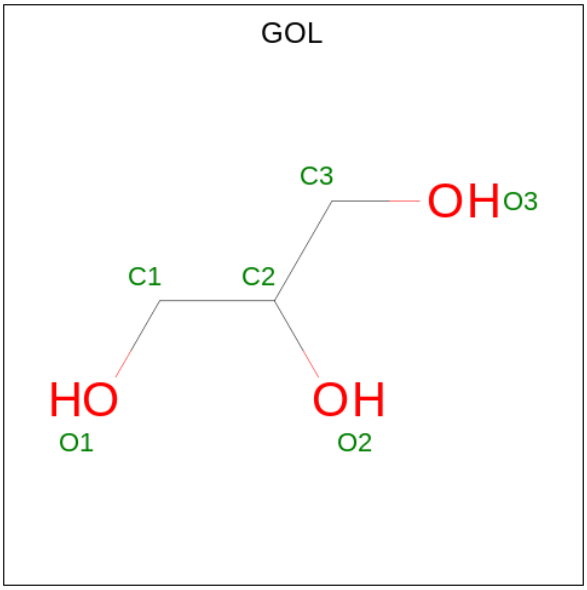
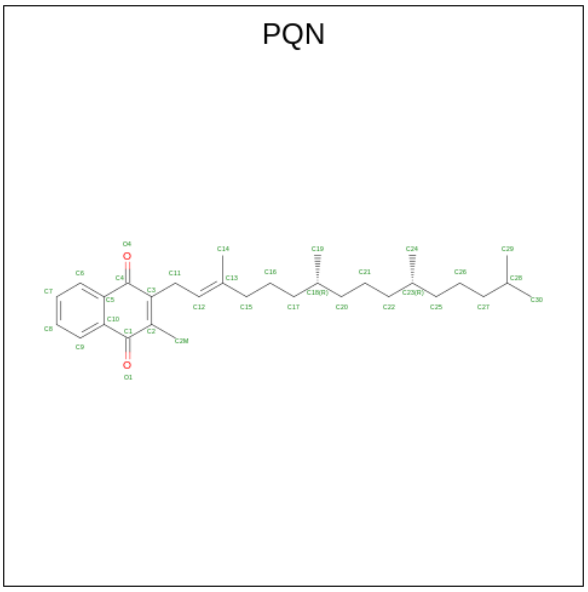
Mol	Chain	Residues	Atoms					AltConf
96	fL	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
96	vL	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 97 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



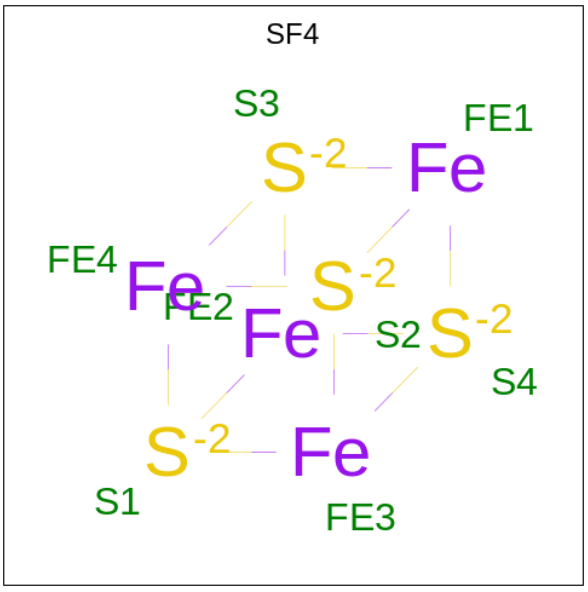
Mol	Chain	Residues	Atoms			AltConf
97	WL	1	Total	C	O	0
			6	3	3	
97	I6	1	Total	C	O	0
			6	3	3	
97	i6	1	Total	C	O	0
			6	3	3	
97	wL	1	Total	C	O	0
			6	3	3	

- Molecule 98 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



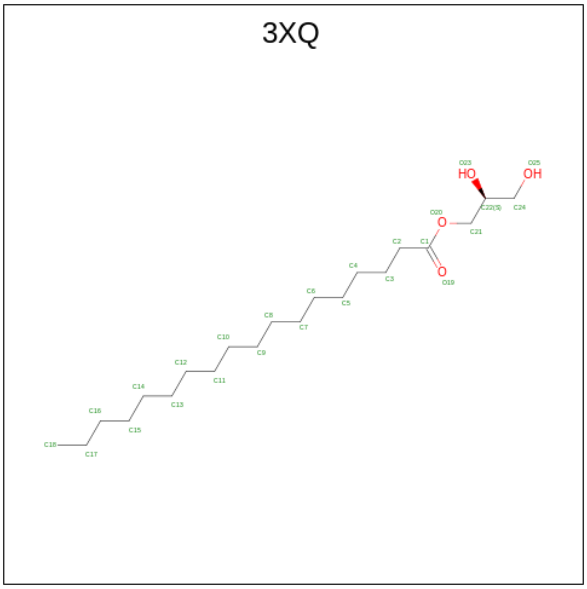
Mol	Chain	Residues	Atoms	AltConf
98	AN	1	Total C O 33 31 2	0
98	BN	1	Total C O 33 31 2	0
98	A2	1	Total C O 33 31 2	0
98	B2	1	Total C O 33 31 2	0

- Molecule 99 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



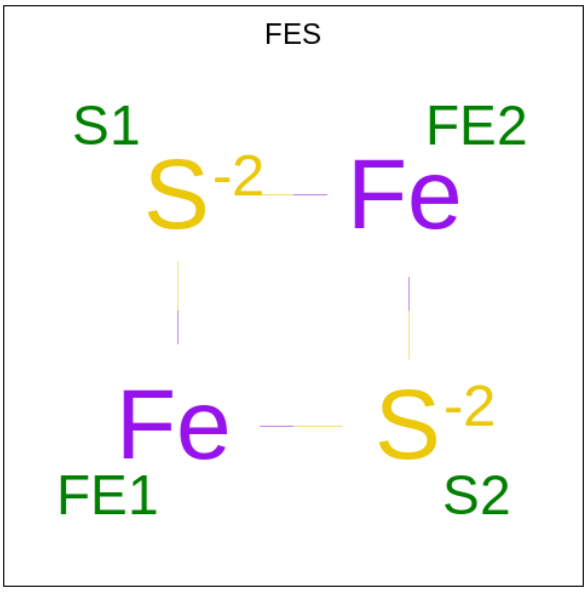
Mol	Chain	Residues	Atoms	AltConf
99	BN	1	Total Fe S 8 4 4	0
99	CN	1	Total Fe S 8 4 4	0
99	CN	1	Total Fe S 8 4 4	0
99	B2	1	Total Fe S 8 4 4	0
99	C2	1	Total Fe S 8 4 4	0
99	C2	1	Total Fe S 8 4 4	0

- Molecule 100 is (2S)-2,3-dihydroxypropyl octadecanoate (CCD ID: 3XQ) (formula: $C_{21}H_{42}O_4$) (labeled as "Ligand of Interest" by depositor).



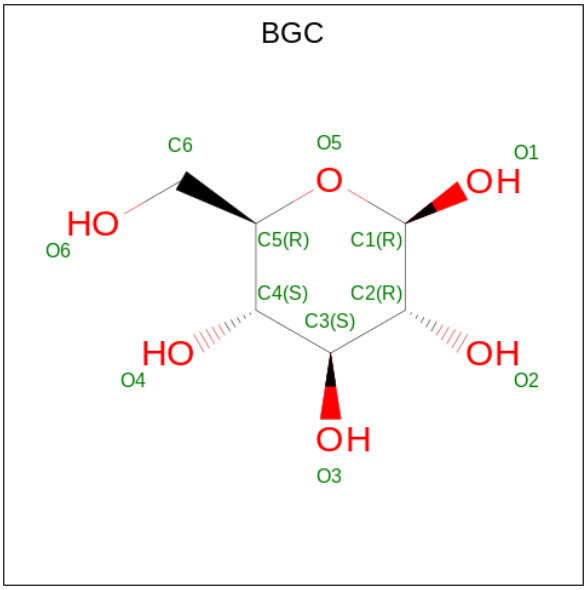
Mol	Chain	Residues	Atoms	AltConf
100	JN	1	Total C O 25 21 4	0
100	J2	1	Total C O 25 21 4	0

- Molecule 101 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



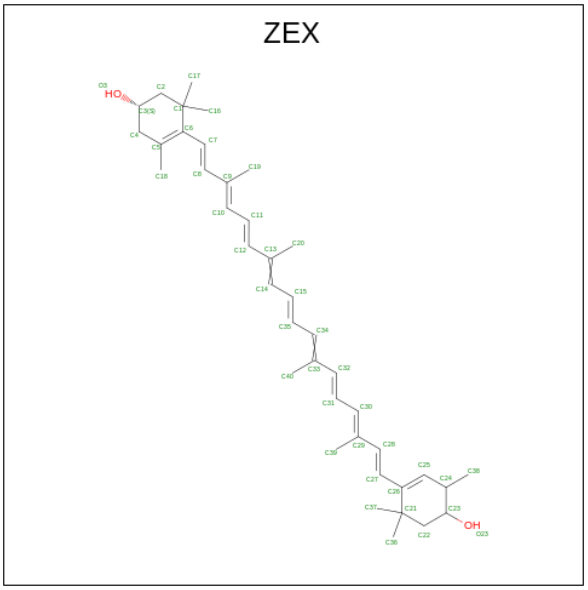
Mol	Chain	Residues	Atoms	AltConf
101	NN	1	Total Fe S 4 2 2	0
101	N2	1	Total Fe S 4 2 2	0

- Molecule 102 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	AltConf
102	32	1	Total C O 11 6 5	0
102	3N	1	Total C O 11 6 5	0

- Molecule 103 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
103	82	1	Total C O 42 40 2	0
103	82	1	Total C O 42 40 2	0
103	8N	1	Total C O 42 40 2	0
103	8N	1	Total C O 42 40 2	0

- Molecule 104 is water.

Mol	Chain	Residues	Atoms	AltConf
104	a6	2	Total O 2 2	0
104	aL	2	Total O 2 2	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.570	Depositor
Minimum map value	-4.947	Depositor
Average map value	0.045	Depositor
Map value standard deviation	0.418	Depositor
Recommended contour level	1	Depositor
Map size (Å)	626.688, 626.688, 626.688	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.632, 1.632, 1.632	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

346 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MEN	RB	72	2	7,8,9	0.79	0	6,9,11	1.08	1 (16%)
2	MEN	kG	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
10	MEN	D1	72	10	7,8,9	0.86	0	6,9,11	1.58	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	B9	72	2	7,8,9	1.15	0	6,9,11	1.95	2 (33%)
2	MEN	u8	72	2	7,8,9	0.90	0	6,9,11	1.24	1 (16%)
2	MEN	fF	72	2,82	7,8,9	1.31	1 (14%)	6,9,11	2.30	2 (33%)
2	MEN	XB	72	2	7,8,9	0.66	0	6,9,11	1.14	1 (16%)
2	MEN	YO	72	2	7,8,9	0.83	0	6,9,11	1.46	1 (16%)
2	MEN	dB	72	2	7,8,9	0.69	0	6,9,11	0.88	0
2	MEN	JP	72	2	7,8,9	0.85	0	6,9,11	1.58	1 (16%)
2	MEN	V1	72	2	7,8,9	0.85	0	6,9,11	1.62	2 (33%)
2	MEN	m1	72	2	7,8,9	0.86	0	6,9,11	1.32	1 (16%)
2	MEN	X7	72	2	7,8,9	0.93	0	6,9,11	1.61	2 (33%)
2	MEN	OQ	72	2	7,8,9	0.92	0	6,9,11	1.29	2 (33%)
2	MEN	hK	72	2,82	7,8,9	1.18	1 (14%)	6,9,11	0.88	0
2	MEN	R7	72	2	7,8,9	0.92	0	6,9,11	1.19	0
2	MEN	q8	72	2	7,8,9	0.92	0	6,9,11	1.66	1 (16%)
2	MEN	F7	72	2	7,8,9	1.01	0	6,9,11	1.62	2 (33%)
2	MEN	rK	72	2,82	7,8,9	1.23	1 (14%)	6,9,11	1.00	1 (16%)
2	MEN	VM	72	2	7,8,9	0.86	0	6,9,11	1.65	1 (16%)
10	MEN	LO	72	10	7,8,9	0.85	0	6,9,11	1.84	2 (33%)
2	MEN	W9	72	2	7,8,9	0.92	0	6,9,11	1.32	1 (16%)
2	MEN	J9	72	2	7,8,9	0.96	0	6,9,11	1.26	1 (16%)
2	MEN	iJ	72	2	7,8,9	0.86	0	6,9,11	1.38	1 (16%)
2	MEN	IB	72	2	7,8,9	0.78	0	6,9,11	1.08	1 (16%)
2	MEN	g4	72	2	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	eE	72	2	7,8,9	0.84	0	6,9,11	1.48	1 (16%)
2	MEN	RG	72	2	7,8,9	0.91	0	6,9,11	1.46	1 (16%)
2	MEN	lF	72	2,82	7,8,9	1.04	0	6,9,11	1.70	2 (33%)
2	MEN	DJ	72	2	7,8,9	0.89	0	6,9,11	1.18	0
2	MEN	IQ	72	2	7,8,9	0.87	0	6,9,11	1.67	1 (16%)
2	MEN	HM	72	2	7,8,9	0.87	0	6,9,11	1.62	1 (16%)
10	MEN	HO	72	10	7,8,9	0.87	0	6,9,11	1.66	1 (16%)
69	MEN	S3	71	69	7,8,9	27.44	6 (85%)	6,9,11	17.30	6 (100%)
2	MEN	KQ	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
2	MEN	VF	72	2,82	7,8,9	1.38	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	RP	72	2	7,8,9	0.85	0	6,9,11	1.86	2 (33%)
69	MEN	h3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	VH	72	2	7,8,9	0.86	0	6,9,11	1.63	2 (33%)
2	MEN	aE	72	2	7,8,9	0.86	0	6,9,11	1.68	2 (33%)
2	MEN	k1	72	2	7,8,9	0.91	0	6,9,11	1.08	1 (16%)
2	MEN	dK	72	2,82	7,8,9	1.43	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	w8	72	2	7,8,9	0.93	0	6,9,11	0.94	0
2	MEN	DA	72	2	7,8,9	0.89	0	6,9,11	1.08	1 (16%)
2	MEN	cM	72	2	7,8,9	0.91	0	6,9,11	1.39	1 (16%)
69	MEN	d3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	k4	72	2	7,8,9	0.90	0	6,9,11	1.49	1 (16%)
2	MEN	QD	72	2	7,8,9	0.82	0	6,9,11	1.70	2 (33%)
2	MEN	YH	72	2	7,8,9	0.95	0	6,9,11	1.30	1 (16%)
2	MEN	WD	72	2	7,8,9	0.89	0	6,9,11	1.43	1 (16%)
2	MEN	PE	72	2	7,8,9	0.83	0	6,9,11	1.59	1 (16%)
69	MEN	F3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	QB	72	2	7,8,9	0.83	0	6,9,11	0.86	0
2	MEN	MB	72	2	7,8,9	0.69	0	6,9,11	0.97	0
2	MEN	DF	72	2,82	7,8,9	1.58	1 (14%)	6,9,11	2.43	2 (33%)
2	MEN	JI	72	2	7,8,9	0.89	0	6,9,11	1.61	2 (33%)
2	MEN	VG	72	2	7,8,9	0.82	0	6,9,11	1.51	2 (33%)
2	MEN	R4	72	2	7,8,9	0.88	0	6,9,11	1.43	2 (33%)
10	MEN	DG	72	11,10	7,8,9	0.88	0	6,9,11	1.60	2 (33%)
2	MEN	OB	72	2	7,8,9	0.82	0	6,9,11	1.13	1 (16%)
69	MEN	D3	71	69	7,8,9	13.87	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	LB	72	2	7,8,9	0.74	0	6,9,11	1.14	1 (16%)
10	MEN	LH	72	10	7,8,9	0.91	0	6,9,11	2.59	2 (33%)
10	MEN	N1	72	10	7,8,9	0.98	0	6,9,11	1.12	0
2	MEN	g1	72	2	7,8,9	0.91	0	6,9,11	1.62	2 (33%)
2	MEN	cE	72	2	7,8,9	0.88	0	6,9,11	1.08	1 (16%)
2	MEN	bF	72	2	7,8,9	0.92	0	6,9,11	1.29	1 (16%)
2	MEN	XA	72	2	7,8,9	0.90	0	6,9,11	1.59	2 (33%)
10	MEN	JH	72	10	7,8,9	0.83	0	6,9,11	1.65	1 (16%)
2	MEN	P1	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
69	MEN	j3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	FB	72	2	7,8,9	0.76	0	6,9,11	0.98	0
2	MEN	SQ	72	2	7,8,9	0.95	0	6,9,11	1.34	1 (16%)
2	MEN	TP	72	2	7,8,9	0.88	0	6,9,11	1.46	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	gM	72	2	7,8,9	0.85	0	6,9,11	1.67	2 (33%)
10	MEN	LG	72	10	7,8,9	0.95	0	6,9,11	1.62	2 (33%)
2	MEN	eG	72	2	7,8,9	0.83	0	6,9,11	1.48	1 (16%)
2	MEN	Q5	72	2	7,8,9	0.92	0	6,9,11	1.68	1 (16%)
10	MEN	N4	72	10	7,8,9	0.93	0	6,9,11	1.40	2 (33%)
2	MEN	RA	72	2	7,8,9	0.91	0	6,9,11	1.19	0
2	MEN	YQ	72	2	7,8,9	0.88	0	6,9,11	1.63	1 (16%)
2	MEN	VJ	72	2	7,8,9	0.87	0	6,9,11	1.53	1 (16%)
2	MEN	gE	72	2	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	FM	72	2	7,8,9	0.87	0	6,9,11	1.53	1 (16%)
2	MEN	BF	72	2,82	7,8,9	1.62	1 (14%)	6,9,11	3.01	1 (16%)
2	MEN	D5	72	2	7,8,9	0.86	0	6,9,11	1.50	1 (16%)
2	MEN	H9	72	2	7,8,9	0.92	0	6,9,11	1.49	2 (33%)
69	MEN	M3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	NJ	72	2	7,8,9	0.94	0	6,9,11	1.54	2 (33%)
2	MEN	nF	72	2,82	7,8,9	1.41	1 (14%)	6,9,11	1.45	1 (16%)
10	MEN	DO	72	10	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
2	MEN	TH	72	2	7,8,9	0.92	0	6,9,11	1.79	2 (33%)
2	MEN	L9	72	2	7,8,9	1.07	0	6,9,11	1.89	2 (33%)
2	MEN	MD	72	2	7,8,9	0.85	0	6,9,11	1.73	2 (33%)
2	MEN	fK	72	2,82	7,8,9	1.28	1 (14%)	6,9,11	2.31	2 (33%)
2	MEN	TE	72	2	7,8,9	0.95	0	6,9,11	1.41	1 (16%)
10	MEN	JO	72	10	7,8,9	0.84	0	6,9,11	1.85	2 (33%)
2	MEN	UI	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	Y9	72	2	7,8,9	0.96	0	6,9,11	1.26	1 (16%)
2	MEN	jF	72	2,82	7,8,9	1.32	1 (14%)	6,9,11	1.79	2 (33%)
2	MEN	uC	72	2	7,8,9	0.93	0	6,9,11	1.24	1 (16%)
2	MEN	tF	72	2,82	7,8,9	1.18	1 (14%)	6,9,11	1.41	1 (16%)
2	MEN	e1	72	2	7,8,9	0.91	0	6,9,11	1.27	1 (16%)
2	MEN	ZK	72	2	7,8,9	0.91	0	6,9,11	1.41	1 (16%)
2	MEN	GQ	72	2	7,8,9	0.88	0	6,9,11	1.79	2 (33%)
2	MEN	mG	72	2	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	U9	72	2	7,8,9	0.94	0	6,9,11	1.29	2 (33%)
2	MEN	iO	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
2	MEN	iM	72	2	7,8,9	0.83	0	6,9,11	1.44	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	ZJ	72	2	7,8,9	0.91	0	6,9,11	1.30	1 (16%)
2	MEN	RF	72	2,82	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	HI	72	2	7,8,9	0.89	0	6,9,11	1.37	1 (16%)
2	MEN	wC	72	2	7,8,9	0.94	0	6,9,11	0.94	0
2	MEN	LA	72	2	7,8,9	0.89	0	6,9,11	1.18	0
69	MEN	H3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	1C	72	2	7,8,9	0.90	0	6,9,11	1.46	2 (33%)
2	MEN	cJ	72	2	7,8,9	0.88	0	6,9,11	1.25	1 (16%)
2	MEN	FK	72	2,82	7,8,9	1.91	1 (14%)	6,9,11	3.71	3 (50%)
2	MEN	JM	72	2	7,8,9	0.88	0	6,9,11	1.67	2 (33%)
2	MEN	BK	72	2,82	7,8,9	1.61	1 (14%)	6,9,11	3.01	1 (16%)
2	MEN	s8	72	2	7,8,9	0.88	0	6,9,11	1.41	2 (33%)
2	MEN	NP	72	2	7,8,9	0.89	0	6,9,11	1.53	1 (16%)
2	MEN	FJ	72	2	7,8,9	0.88	0	6,9,11	1.67	1 (16%)
2	MEN	PF	72	2,82	7,8,9	1.54	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	V4	72	2	7,8,9	0.89	0	6,9,11	1.32	2 (33%)
2	MEN	XK	72	2,82	7,8,9	1.93	1 (14%)	6,9,11	3.18	2 (33%)
2	MEN	T7	72	2,75	7,8,9	0.86	0	6,9,11	3.08	2 (33%)
2	MEN	dF	72	2,82	7,8,9	1.42	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	BB	72	2	7,8,9	0.80	0	6,9,11	1.25	1 (16%)
69	MEN	L3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	RO	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	S5	72	2	7,8,9	0.92	0	6,9,11	1.79	1 (16%)
10	MEN	J4	72	10	7,8,9	0.87	0	6,9,11	1.85	2 (33%)
2	MEN	O9	72	2	7,8,9	0.99	0	6,9,11	1.72	2 (33%)
10	MEN	FH	72	10	7,8,9	0.89	0	6,9,11	1.40	1 (16%)
2	MEN	Y5	72	2	7,8,9	0.86	0	6,9,11	1.86	1 (16%)
2	MEN	D9	72	2	7,8,9	0.96	0	6,9,11	1.31	1 (16%)
10	MEN	NG	72	10	7,8,9	0.86	0	6,9,11	1.51	2 (33%)
2	MEN	T1	72	2	7,8,9	0.95	0	6,9,11	1.81	2 (33%)
69	MEN	f3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	eJ	72	2	7,8,9	0.91	0	6,9,11	1.50	2 (33%)
2	MEN	bB	72	2	7,8,9	0.68	0	6,9,11	0.75	0
2	MEN	ID	72	2	7,8,9	0.83	0	6,9,11	1.63	1 (16%)
2	MEN	TM	72	2	7,8,9	0.87	0	6,9,11	1.24	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	rF	72	2,82	7,8,9	1.28	1 (14%)	6,9,11	0.98	1 (16%)
2	MEN	UQ	72	2	7,8,9	0.96	0	6,9,11	1.65	1 (16%)
10	MEN	J1	72	10	7,8,9	0.84	0	6,9,11	1.68	1 (16%)
2	MEN	aH	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
10	MEN	HH	72	10	7,8,9	0.85	0	6,9,11	1.53	1 (16%)
10	MEN	L1	72	10	7,8,9	0.86	0	6,9,11	2.62	2 (33%)
2	MEN	gJ	72	2	7,8,9	0.87	0	6,9,11	1.46	1 (16%)
2	MEN	FF	72	2,82	7,8,9	1.95	1 (14%)	6,9,11	3.67	3 (50%)
10	MEN	JG	72	10	7,8,9	0.88	0	6,9,11	1.53	1 (16%)
2	MEN	TJ	72	2	7,8,9	0.87	0	6,9,11	1.34	1 (16%)
2	MEN	iG	72	2	7,8,9	0.93	0	6,9,11	1.19	1 (16%)
2	MEN	NB	72	2	7,8,9	0.81	0	6,9,11	0.44	0
2	MEN	KD	72	2	7,8,9	0.88	0	6,9,11	1.44	1 (16%)
10	MEN	H4	72	10	7,8,9	0.87	0	6,9,11	1.69	2 (33%)
2	MEN	DM	72	2	7,8,9	0.90	0	6,9,11	1.27	1 (16%)
2	MEN	hF	72	2,82	7,8,9	1.22	1 (14%)	6,9,11	0.85	0
2	MEN	qC	72	2	7,8,9	0.91	0	6,9,11	1.65	1 (16%)
69	MEN	I3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	c1	72	2	7,8,9	0.83	0	6,9,11	1.84	1 (16%)
2	MEN	HJ	72	2	7,8,9	0.87	0	6,9,11	1.88	1 (16%)
2	MEN	WI	72	2	7,8,9	0.88	0	6,9,11	1.42	1 (16%)
2	MEN	aB	72	2	7,8,9	0.82	0	6,9,11	0.78	0
2	MEN	LF	72	2,82	7,8,9	1.80	1 (14%)	6,9,11	3.80	3 (50%)
2	MEN	DI	72	2	7,8,9	0.97	0	6,9,11	1.24	1 (16%)
2	MEN	CQ	72	2	7,8,9	0.85	0	6,9,11	1.47	2 (33%)
69	MEN	n3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	FI	72	2	7,8,9	0.93	0	6,9,11	1.52	1 (16%)
2	MEN	gH	72	2	7,8,9	0.91	0	6,9,11	1.63	2 (33%)
2	MEN	kO	72	2	7,8,9	0.85	0	6,9,11	1.50	1 (16%)
2	MEN	TG	72	2	7,8,9	0.95	0	6,9,11	1.44	1 (16%)
69	MEN	O3	71	69	7,8,9	0.68	0	6,9,11	0.78	0
2	MEN	CD	72	2	7,8,9	0.84	0	6,9,11	1.48	2 (33%)
2	MEN	GB	72	2	7,8,9	0.79	0	6,9,11	1.29	1 (16%)
2	MEN	J5	72	2	7,8,9	0.87	0	6,9,11	1.59	2 (33%)
2	MEN	kJ	72	2	7,8,9	0.83	0	6,9,11	1.41	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	mH	72	2	7,8,9	0.84	0	6,9,11	1.31	1 (16%)
2	MEN	L7	72	2	7,8,9	0.88	0	6,9,11	1.20	0
2	MEN	PJ	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
69	MEN	B3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	B5	72	2	7,8,9	0.81	0	6,9,11	1.89	1 (16%)
2	MEN	B7	72	2	7,8,9	0.95	0	6,9,11	1.13	1 (16%)
2	MEN	RM	72	2	7,8,9	0.88	0	6,9,11	1.29	1 (16%)
2	MEN	YD	72	2	7,8,9	0.91	0	6,9,11	1.66	1 (16%)
2	MEN	WQ	72	2	7,8,9	0.91	0	6,9,11	1.42	1 (16%)
2	MEN	cO	72	2	7,8,9	0.91	0	6,9,11	1.29	1 (16%)
2	MEN	lK	72	2,82	7,8,9	1.02	0	6,9,11	1.69	2 (33%)
2	MEN	FP	72	2	7,8,9	0.88	0	6,9,11	1.70	1 (16%)
2	MEN	PM	72	2	7,8,9	0.88	0	6,9,11	1.56	2 (33%)
10	MEN	NH	72	10	7,8,9	0.97	0	6,9,11	1.13	0
2	MEN	LK	72	2,82	7,8,9	1.80	1 (14%)	6,9,11	3.80	3 (50%)
2	MEN	VO	72	2	7,8,9	0.94	0	6,9,11	1.36	2 (33%)
2	MEN	LP	72	2	7,8,9	0.86	0	6,9,11	1.56	1 (16%)
69	MEN	U3	71	69	7,8,9	27.43	6 (85%)	6,9,11	17.30	6 (100%)
10	MEN	FG	72	10	7,8,9	0.91	0	6,9,11	1.57	1 (16%)
2	MEN	H7	72	2	7,8,9	0.91	0	6,9,11	1.77	1 (16%)
69	MEN	q3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	mM	72	2	7,8,9	0.87	0	6,9,11	1.65	1 (16%)
2	MEN	VB	72	2	7,8,9	0.77	0	6,9,11	0.90	1 (16%)
2	MEN	CB	72	2	7,8,9	0.71	0	6,9,11	1.14	1 (16%)
2	MEN	HF	72	2,82	7,8,9	1.58	1 (14%)	6,9,11	2.45	2 (33%)
2	MEN	Y1	72	2	7,8,9	0.94	0	6,9,11	1.28	1 (16%)
2	MEN	QI	72	2	7,8,9	1.01	0	6,9,11	1.18	1 (16%)
10	MEN	NO	72	10	7,8,9	0.90	0	6,9,11	1.40	2 (33%)
2	MEN	nK	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	1.50	1 (16%)
2	MEN	YG	72	2	7,8,9	0.94	0	6,9,11	1.32	1 (16%)
2	MEN	Y4	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
2	MEN	vF	72	2,82	7,8,9	1.40	1 (14%)	6,9,11	1.17	1 (16%)
2	MEN	pK	72	2,82	7,8,9	1.11	0	6,9,11	1.35	1 (16%)
2	MEN	HA	72	2	7,8,9	0.90	0	6,9,11	1.76	1 (16%)
2	MEN	T4	72	2	7,8,9	0.81	0	6,9,11	1.62	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	kM	72	2	7,8,9	0.88	0	6,9,11	1.45	1 (16%)
69	MEN	o3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	yC	72	2	7,8,9	0.99	0	6,9,11	1.22	1 (16%)
2	MEN	pF	72	2,82	7,8,9	1.11	0	6,9,11	1.34	1 (16%)
2	MEN	H5	72	2	7,8,9	0.85	0	6,9,11	1.78	2 (33%)
2	MEN	PA	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
2	MEN	SD	72	2	7,8,9	0.95	0	6,9,11	1.35	1 (16%)
2	MEN	eH	72	2	7,8,9	0.92	0	6,9,11	1.28	1 (16%)
2	MEN	bK	72	2	7,8,9	0.92	0	6,9,11	1.31	1 (16%)
2	MEN	N7	72	2	7,8,9	0.92	0	6,9,11	1.45	1 (16%)
2	MEN	P7	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
69	MEN	u3	71	69	7,8,9	27.42	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	VP	72	2	7,8,9	0.88	0	6,9,11	1.50	1 (16%)
2	MEN	O5	72	2	7,8,9	0.84	0	6,9,11	1.71	1 (16%)
2	MEN	PG	72	2	7,8,9	0.85	0	6,9,11	1.62	1 (16%)
2	MEN	LJ	72	2	7,8,9	0.92	0	6,9,11	1.38	2 (33%)
10	MEN	JE	72	10	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
2	MEN	mE	72	2	7,8,9	0.89	0	6,9,11	1.41	1 (16%)
2	MEN	i4	72	2	7,8,9	0.85	0	6,9,11	1.47	1 (16%)
2	MEN	eB	72	2	7,8,9	0.68	0	6,9,11	1.23	1 (16%)
2	MEN	TO	72	2	7,8,9	0.81	0	6,9,11	1.63	2 (33%)
2	MEN	VA	72	2	7,8,9	0.87	0	6,9,11	1.40	1 (16%)
2	MEN	e4	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	U5	72	2	7,8,9	0.90	0	6,9,11	1.72	1 (16%)
2	MEN	NA	72	2	7,8,9	0.93	0	6,9,11	1.47	1 (16%)
2	MEN	SB	72	2	7,8,9	0.78	0	6,9,11	0.98	0
2	MEN	c4	72	2	7,8,9	0.87	0	6,9,11	1.29	1 (16%)
2	MEN	F9	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
2	MEN	gB	72	2	7,8,9	0.65	0	6,9,11	0.75	0
10	MEN	F1	72	10	7,8,9	0.92	0	6,9,11	1.39	1 (16%)
2	MEN	PK	72	2,82	7,8,9	1.57	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	V7	72	2	7,8,9	0.85	0	6,9,11	1.39	1 (16%)
2	MEN	jK	72	2,82	7,8,9	1.29	1 (14%)	6,9,11	1.81	1 (16%)
10	MEN	D4	72	10	7,8,9	0.87	0	6,9,11	1.34	2 (33%)
2	MEN	y8	72	2	7,8,9	0.99	0	6,9,11	1.24	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	MEN	k3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	NM	72	2	7,8,9	0.87	0	6,9,11	1.42	2 (33%)
2	MEN	BI	72	2	7,8,9	0.87	0	6,9,11	1.49	1 (16%)
2	MEN	P4	72	2	7,8,9	0.89	0	6,9,11	1.25	0
2	MEN	J7	72	2	7,8,9	0.85	0	6,9,11	1.41	1 (16%)
2	MEN	RE	72	2	7,8,9	0.92	0	6,9,11	1.47	1 (16%)
2	MEN	HK	72	2,82	7,8,9	1.57	1 (14%)	6,9,11	2.47	2 (33%)
2	MEN	R1	72	2	7,8,9	0.83	0	6,9,11	1.14	1 (16%)
2	MEN	XP	72	2	7,8,9	0.87	0	6,9,11	1.69	1 (16%)
2	MEN	aG	72	2	7,8,9	0.87	0	6,9,11	1.70	2 (33%)
2	MEN	YB	72	2	7,8,9	0.84	0	6,9,11	1.38	1 (16%)
2	MEN	JA	72	2	7,8,9	0.86	0	6,9,11	1.43	1 (16%)
2	MEN	HB	72	2	7,8,9	0.83	0	6,9,11	1.20	1 (16%)
2	MEN	m4	72	2	7,8,9	0.91	0	6,9,11	1.56	2 (33%)
2	MEN	iE	72	2	7,8,9	0.93	0	6,9,11	1.20	1 (16%)
2	MEN	vK	72	2,82	7,8,9	1.42	1 (14%)	6,9,11	1.13	0
2	MEN	18	72	2	7,8,9	0.90	0	6,9,11	1.46	2 (33%)
2	MEN	F5	72	2	7,8,9	0.87	0	6,9,11	1.70	1 (16%)
2	MEN	gO	72	2	7,8,9	0.90	0	6,9,11	1.39	1 (16%)
2	MEN	PH	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
2	MEN	DB	72	2	7,8,9	0.83	0	6,9,11	1.23	0
2	MEN	RH	72	2	7,8,9	0.82	0	6,9,11	1.14	1 (16%)
2	MEN	FA	72	2	7,8,9	1.01	0	6,9,11	1.63	2 (33%)
2	MEN	RK	72	2,82	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	eO	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	DP	72	2	7,8,9	0.88	0	6,9,11	1.60	1 (16%)
2	MEN	kH	72	2	7,8,9	0.93	0	6,9,11	1.11	1 (16%)
2	MEN	SI	72	2	7,8,9	0.88	0	6,9,11	1.54	1 (16%)
2	MEN	YE	72	2	7,8,9	0.93	0	6,9,11	1.31	1 (16%)
10	MEN	H1	72	10	7,8,9	0.85	0	6,9,11	1.53	1 (16%)
2	MEN	mO	72	2	7,8,9	0.88	0	6,9,11	1.54	2 (33%)
2	MEN	eM	72	2	7,8,9	0.86	0	6,9,11	1.57	1 (16%)
69	MEN	w3	71	69	7,8,9	27.42	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	NF	72	2,82	7,8,9	1.50	1 (14%)	6,9,11	2.71	2 (33%)
2	MEN	D7	72	2	7,8,9	0.87	0	6,9,11	1.08	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	YI	72	2	7,8,9	0.97	0	6,9,11	1.38	2 (33%)
2	MEN	EQ	72	2	7,8,9	0.88	0	6,9,11	1.45	1 (16%)
2	MEN	GD	72	2	7,8,9	0.83	0	6,9,11	1.76	2 (33%)
2	MEN	OI	72	2	7,8,9	0.92	0	6,9,11	1.35	1 (16%)
2	MEN	NK	72	2,82	7,8,9	1.52	1 (14%)	6,9,11	2.76	3 (50%)
2	MEN	VE	72	2	7,8,9	0.81	0	6,9,11	1.52	2 (33%)
2	MEN	ZB	72	2	7,8,9	0.65	0	6,9,11	0.55	0
2	MEN	UD	72	2	7,8,9	0.94	0	6,9,11	1.66	1 (16%)
2	MEN	TA	72	2,75	7,8,9	0.86	0	6,9,11	3.06	2 (33%)
2	MEN	LM	72	2	7,8,9	0.86	0	6,9,11	1.44	1 (16%)
2	MEN	cG	72	2	7,8,9	0.90	0	6,9,11	1.10	1 (16%)
2	MEN	tK	72	2,82	7,8,9	1.19	1 (14%)	6,9,11	1.45	1 (16%)
2	MEN	BA	72	2	7,8,9	0.93	0	6,9,11	1.12	1 (16%)
69	MEN	Q3	71	69	7,8,9	27.43	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	PP	72	2	7,8,9	0.90	0	6,9,11	1.50	1 (16%)
2	MEN	XM	72	2	7,8,9	0.87	0	6,9,11	1.56	2 (33%)
2	MEN	ZM	72	2	7,8,9	0.87	0	6,9,11	1.60	1 (16%)
10	MEN	FE	72	10	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
10	MEN	DH	72	10	7,8,9	0.86	0	6,9,11	1.59	2 (33%)
2	MEN	L5	72	2	7,8,9	0.90	0	6,9,11	1.94	1 (16%)
2	MEN	TK	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	2.25	2 (33%)
69	MEN	s3	71	69	7,8,9	27.44	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	DK	72	2,82	7,8,9	1.57	1 (14%)	6,9,11	2.45	2 (33%)
10	MEN	FO	72	10	7,8,9	0.89	0	6,9,11	1.55	1 (16%)
2	MEN	ED	72	2	7,8,9	0.82	0	6,9,11	1.44	1 (16%)
2	MEN	mJ	72	2	7,8,9	0.90	0	6,9,11	1.41	1 (16%)
2	MEN	OD	72	2	7,8,9	0.92	0	6,9,11	1.29	2 (33%)
2	MEN	TF	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	2.24	2 (33%)
2	MEN	VK	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	BP	72	2	7,8,9	0.87	0	6,9,11	1.54	1 (16%)
10	MEN	HE	72	10	7,8,9	0.89	0	6,9,11	1.39	1 (16%)
2	MEN	RJ	72	2	7,8,9	0.91	0	6,9,11	1.57	1 (16%)
2	MEN	PB	72	2	7,8,9	0.79	0	6,9,11	0.93	0
2	MEN	aO	72	2	7,8,9	0.87	0	6,9,11	1.47	2 (33%)
2	MEN	W5	72	2	7,8,9	0.92	0	6,9,11	1.70	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	HP	72	2	7,8,9	0.87	0	6,9,11	1.50	1 (16%)
2	MEN	Q9	72	2	7,8,9	0.94	0	6,9,11	1.37	2 (33%)
2	MEN	iH	72	2	7,8,9	0.83	0	6,9,11	1.42	1 (16%)
10	MEN	L4	72	10	7,8,9	0.82	0	6,9,11	1.86	2 (33%)
2	MEN	JJ	72	2	7,8,9	0.87	0	6,9,11	1.61	2 (33%)
2	MEN	a1	72	2	7,8,9	0.92	0	6,9,11	1.33	1 (16%)
2	MEN	a4	72	2	7,8,9	0.86	0	6,9,11	1.45	2 (33%)
10	MEN	LE	72	10	7,8,9	0.96	0	6,9,11	1.65	2 (33%)
10	MEN	NE	72	10	7,8,9	0.85	0	6,9,11	1.52	2 (33%)
2	MEN	sC	72	2	7,8,9	0.87	0	6,9,11	1.42	2 (33%)
2	MEN	PO	72	2	7,8,9	0.93	0	6,9,11	1.22	0
2	MEN	ZF	72	2	7,8,9	0.89	0	6,9,11	1.35	1 (16%)
2	MEN	QQ	72	2	7,8,9	0.81	0	6,9,11	1.69	2 (33%)
2	MEN	i1	72	2	7,8,9	0.85	0	6,9,11	1.39	1 (16%)
2	MEN	S9	72	2	7,8,9	0.95	0	6,9,11	1.36	1 (16%)
2	MEN	JK	72	2,82	7,8,9	1.49	1 (14%)	6,9,11	2.15	2 (33%)
2	MEN	LI	72	2	7,8,9	0.97	0	6,9,11	1.68	2 (33%)
10	MEN	DE	72	11,10	7,8,9	0.86	0	6,9,11	1.60	2 (33%)
10	MEN	F4	72	10	7,8,9	0.90	0	6,9,11	1.52	1 (16%)
2	MEN	XF	72	2,82	7,8,9	1.93	1 (14%)	6,9,11	3.17	2 (33%)
2	MEN	XJ	72	2	7,8,9	0.89	0	6,9,11	1.64	2 (33%)
2	MEN	cH	72	2	7,8,9	0.82	0	6,9,11	1.85	1 (16%)
2	MEN	JF	72	2,82	7,8,9	1.46	1 (14%)	6,9,11	2.20	2 (33%)
2	MEN	gG	72	2	7,8,9	0.84	0	6,9,11	1.53	1 (16%)
2	MEN	kE	72	2	7,8,9	0.90	0	6,9,11	1.47	1 (16%)
10	MEN	HG	72	10	7,8,9	0.91	0	6,9,11	1.44	2 (33%)
2	MEN	MQ	72	2	7,8,9	0.89	0	6,9,11	1.74	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	RB	72	2	-	7/7/8/10	-
2	MEN	kG	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	D1	72	10	-	4/7/8/10	-
2	MEN	B9	72	2	-	4/7/8/10	-
2	MEN	u8	72	2	-	3/7/8/10	-
2	MEN	fF	72	2,82	-	2/7/8/10	-
2	MEN	XB	72	2	-	5/7/8/10	-
2	MEN	YO	72	2	-	4/7/8/10	-
2	MEN	dB	72	2	-	5/7/8/10	-
2	MEN	JP	72	2	-	4/7/8/10	-
2	MEN	V1	72	2	-	4/7/8/10	-
2	MEN	m1	72	2	-	4/7/8/10	-
2	MEN	X7	72	2	-	4/7/8/10	-
2	MEN	OQ	72	2	-	2/7/8/10	-
2	MEN	hK	72	2,82	-	2/7/8/10	-
2	MEN	R7	72	2	-	4/7/8/10	-
2	MEN	q8	72	2	-	3/7/8/10	-
2	MEN	F7	72	2	-	4/7/8/10	-
2	MEN	rK	72	2,82	-	3/7/8/10	-
2	MEN	VM	72	2	-	4/7/8/10	-
10	MEN	LO	72	10	-	4/7/8/10	-
2	MEN	W9	72	2	-	2/7/8/10	-
2	MEN	J9	72	2	-	2/7/8/10	-
2	MEN	iJ	72	2	-	4/7/8/10	-
2	MEN	IB	72	2	-	4/7/8/10	-
2	MEN	g4	72	2	-	4/7/8/10	-
2	MEN	eE	72	2	-	2/7/8/10	-
2	MEN	RG	72	2	-	3/7/8/10	-
2	MEN	lF	72	2,82	-	4/7/8/10	-
2	MEN	DJ	72	2	-	3/7/8/10	-
2	MEN	IQ	72	2	-	4/7/8/10	-
2	MEN	HM	72	2	-	4/7/8/10	-
10	MEN	HO	72	10	-	2/7/8/10	-
69	MEN	S3	71	69	-	6/7/8/10	-
2	MEN	KQ	72	2	-	4/7/8/10	-
2	MEN	VF	72	2,82	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	RP	72	2	-	4/7/8/10	-
69	MEN	h3	71	69	-	5/7/8/10	-
2	MEN	VH	72	2	-	4/7/8/10	-
2	MEN	aE	72	2	-	4/7/8/10	-
2	MEN	k1	72	2	-	4/7/8/10	-
2	MEN	dK	72	2,82	-	3/7/8/10	-
2	MEN	w8	72	2	-	2/7/8/10	-
2	MEN	DA	72	2	-	3/7/8/10	-
2	MEN	cM	72	2	-	4/7/8/10	-
69	MEN	d3	71	69	-	5/7/8/10	-
2	MEN	k4	72	2	-	5/7/8/10	-
2	MEN	QD	72	2	-	4/7/8/10	-
2	MEN	YH	72	2	-	4/7/8/10	-
2	MEN	WD	72	2	-	4/7/8/10	-
2	MEN	PE	72	2	-	3/7/8/10	-
69	MEN	F3	71	69	-	4/7/8/10	-
2	MEN	QB	72	2	-	6/7/8/10	-
2	MEN	MB	72	2	-	2/7/8/10	-
2	MEN	DF	72	2,82	-	2/7/8/10	-
2	MEN	JI	72	2	-	5/7/8/10	-
2	MEN	VG	72	2	-	4/7/8/10	-
2	MEN	R4	72	2	-	4/7/8/10	-
10	MEN	DG	72	11,10	-	4/7/8/10	-
2	MEN	OB	72	2	-	4/7/8/10	-
69	MEN	D3	71	69	-	5/7/8/10	-
2	MEN	LB	72	2	-	4/7/8/10	-
10	MEN	LH	72	10	-	2/7/8/10	-
10	MEN	N1	72	10	-	2/7/8/10	-
2	MEN	g1	72	2	-	3/7/8/10	-
2	MEN	cE	72	2	-	3/7/8/10	-
2	MEN	bF	72	2	-	4/7/8/10	-
2	MEN	XA	72	2	-	4/7/8/10	-
10	MEN	JH	72	10	-	1/7/8/10	-
2	MEN	P1	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	MEN	j3	71	69	-	4/7/8/10	-
2	MEN	FB	72	2	-	3/7/8/10	-
2	MEN	SQ	72	2	-	4/7/8/10	-
2	MEN	TP	72	2	-	4/7/8/10	-
2	MEN	gM	72	2	-	5/7/8/10	-
10	MEN	LG	72	10	-	4/7/8/10	-
2	MEN	eG	72	2	-	2/7/8/10	-
2	MEN	Q5	72	2	-	4/7/8/10	-
10	MEN	N4	72	10	-	3/7/8/10	-
2	MEN	RA	72	2	-	4/7/8/10	-
2	MEN	YQ	72	2	-	4/7/8/10	-
2	MEN	VJ	72	2	-	4/7/8/10	-
2	MEN	gE	72	2	-	4/7/8/10	-
2	MEN	FM	72	2	-	4/7/8/10	-
2	MEN	BF	72	2,82	-	2/7/8/10	-
2	MEN	D5	72	2	-	4/7/8/10	-
2	MEN	H9	72	2	-	2/7/8/10	-
69	MEN	M3	71	69	-	4/7/8/10	-
2	MEN	NJ	72	2	-	5/7/8/10	-
2	MEN	nF	72	2,82	-	3/7/8/10	-
10	MEN	DO	72	10	-	2/7/8/10	-
2	MEN	TH	72	2	-	5/7/8/10	-
2	MEN	L9	72	2	-	2/7/8/10	-
2	MEN	MD	72	2	-	2/7/8/10	-
2	MEN	fK	72	2,82	-	2/7/8/10	-
2	MEN	TE	72	2	-	3/7/8/10	-
10	MEN	JO	72	10	-	2/7/8/10	-
2	MEN	UI	72	2	-	4/7/8/10	-
2	MEN	Y9	72	2	-	2/7/8/10	-
2	MEN	jF	72	2,82	-	4/7/8/10	-
2	MEN	uC	72	2	-	3/7/8/10	-
2	MEN	tF	72	2,82	-	4/7/8/10	-
2	MEN	e1	72	2	-	3/7/8/10	-
2	MEN	ZK	72	2	-	5/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	GQ	72	2	-	4/7/8/10	-
2	MEN	mG	72	2	-	3/7/8/10	-
2	MEN	U9	72	2	-	2/7/8/10	-
2	MEN	iO	72	2	-	4/7/8/10	-
2	MEN	iM	72	2	-	4/7/8/10	-
2	MEN	ZJ	72	2	-	4/7/8/10	-
2	MEN	RF	72	2,82	-	2/7/8/10	-
2	MEN	HI	72	2	-	4/7/8/10	-
2	MEN	wC	72	2	-	2/7/8/10	-
2	MEN	LA	72	2	-	5/7/8/10	-
69	MEN	H3	71	69	-	4/7/8/10	-
2	MEN	1C	72	2	-	4/7/8/10	-
2	MEN	cJ	72	2	-	4/7/8/10	-
2	MEN	FK	72	2,82	-	2/7/8/10	-
2	MEN	JM	72	2	-	4/7/8/10	-
2	MEN	BK	72	2,82	-	2/7/8/10	-
2	MEN	s8	72	2	-	2/7/8/10	-
2	MEN	NP	72	2	-	4/7/8/10	-
2	MEN	FJ	72	2	-	4/7/8/10	-
2	MEN	PF	72	2,82	-	3/7/8/10	-
2	MEN	V4	72	2	-	2/7/8/10	-
2	MEN	XK	72	2,82	-	2/7/8/10	-
2	MEN	T7	72	2,75	-	6/7/8/10	-
2	MEN	dF	72	2,82	-	3/7/8/10	-
2	MEN	BB	72	2	-	5/7/8/10	-
69	MEN	L3	71	69	-	4/7/8/10	-
2	MEN	RO	72	2	-	4/7/8/10	-
2	MEN	S5	72	2	-	4/7/8/10	-
10	MEN	J4	72	10	-	2/7/8/10	-
2	MEN	O9	72	2	-	4/7/8/10	-
10	MEN	FH	72	10	-	2/7/8/10	-
2	MEN	Y5	72	2	-	4/7/8/10	-
2	MEN	D9	72	2	-	2/7/8/10	-
10	MEN	NG	72	10	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	T1	72	2	-	5/7/8/10	-
69	MEN	f3	71	69	-	4/7/8/10	-
2	MEN	eJ	72	2	-	4/7/8/10	-
2	MEN	bB	72	2	-	4/7/8/10	-
2	MEN	ID	72	2	-	4/7/8/10	-
2	MEN	TM	72	2	-	3/7/8/10	-
2	MEN	rF	72	2,82	-	3/7/8/10	-
2	MEN	UQ	72	2	-	3/7/8/10	-
10	MEN	J1	72	10	-	1/7/8/10	-
2	MEN	aH	72	2	-	3/7/8/10	-
10	MEN	HH	72	10	-	4/7/8/10	-
10	MEN	L1	72	10	-	2/7/8/10	-
2	MEN	gJ	72	2	-	2/7/8/10	-
2	MEN	FF	72	2,82	-	2/7/8/10	-
10	MEN	JG	72	10	-	2/7/8/10	-
2	MEN	TJ	72	2	-	5/7/8/10	-
2	MEN	iG	72	2	-	3/7/8/10	-
2	MEN	NB	72	2	-	3/7/8/10	-
2	MEN	KD	72	2	-	4/7/8/10	-
10	MEN	H4	72	10	-	2/7/8/10	-
2	MEN	DM	72	2	-	5/7/8/10	-
2	MEN	hF	72	2,82	-	2/7/8/10	-
2	MEN	qC	72	2	-	3/7/8/10	-
69	MEN	I3	71	69	-	5/7/8/10	-
2	MEN	c1	72	2	-	4/7/8/10	-
2	MEN	HJ	72	2	-	4/7/8/10	-
2	MEN	WI	72	2	-	5/7/8/10	-
2	MEN	aB	72	2	-	4/7/8/10	-
2	MEN	LF	72	2,82	-	3/7/8/10	-
2	MEN	DI	72	2	-	4/7/8/10	-
2	MEN	CQ	72	2	-	4/7/8/10	-
69	MEN	n3	71	69	-	4/7/8/10	-
2	MEN	FI	72	2	-	5/7/8/10	-
2	MEN	gH	72	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kO	72	2	-	5/7/8/10	-
2	MEN	TG	72	2	-	3/7/8/10	-
69	MEN	O3	71	69	-	2/7/8/10	-
2	MEN	CD	72	2	-	4/7/8/10	-
2	MEN	GB	72	2	-	6/7/8/10	-
2	MEN	J5	72	2	-	5/7/8/10	-
2	MEN	kJ	72	2	-	4/7/8/10	-
2	MEN	mH	72	2	-	4/7/8/10	-
2	MEN	L7	72	2	-	5/7/8/10	-
2	MEN	PJ	72	2	-	4/7/8/10	-
69	MEN	B3	71	69	-	5/7/8/10	-
2	MEN	B5	72	2	-	4/7/8/10	-
2	MEN	B7	72	2	-	4/7/8/10	-
2	MEN	RM	72	2	-	4/7/8/10	-
2	MEN	YD	72	2	-	4/7/8/10	-
2	MEN	WQ	72	2	-	4/7/8/10	-
2	MEN	cO	72	2	-	2/7/8/10	-
2	MEN	lK	72	2,82	-	4/7/8/10	-
2	MEN	FP	72	2	-	5/7/8/10	-
2	MEN	PM	72	2	-	5/7/8/10	-
10	MEN	NH	72	10	-	2/7/8/10	-
2	MEN	LK	72	2,82	-	3/7/8/10	-
2	MEN	VO	72	2	-	2/7/8/10	-
2	MEN	LP	72	2	-	4/7/8/10	-
69	MEN	U3	71	69	-	6/7/8/10	-
10	MEN	FG	72	10	-	3/7/8/10	-
2	MEN	H7	72	2	-	4/7/8/10	-
69	MEN	q3	71	69	-	5/7/8/10	-
2	MEN	mM	72	2	-	4/7/8/10	-
2	MEN	VB	72	2	-	4/7/8/10	-
2	MEN	CB	72	2	-	2/7/8/10	-
2	MEN	HF	72	2,82	-	2/7/8/10	-
2	MEN	Y1	72	2	-	4/7/8/10	-
2	MEN	QI	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	NO	72	10	-	3/7/8/10	-
2	MEN	nK	72	2,82	-	3/7/8/10	-
2	MEN	YG	72	2	-	5/7/8/10	-
2	MEN	Y4	72	2	-	4/7/8/10	-
2	MEN	vF	72	2,82	-	1/7/8/10	-
2	MEN	pK	72	2,82	-	3/7/8/10	-
2	MEN	HA	72	2	-	4/7/8/10	-
2	MEN	T4	72	2	-	3/7/8/10	-
2	MEN	kM	72	2	-	4/7/8/10	-
69	MEN	o3	71	69	-	5/7/8/10	-
2	MEN	yC	72	2	-	3/7/8/10	-
2	MEN	pF	72	2,82	-	3/7/8/10	-
2	MEN	H5	72	2	-	4/7/8/10	-
2	MEN	PA	72	2	-	4/7/8/10	-
2	MEN	SD	72	2	-	4/7/8/10	-
2	MEN	eH	72	2	-	3/7/8/10	-
2	MEN	bK	72	2	-	4/7/8/10	-
2	MEN	N7	72	2	-	4/7/8/10	-
2	MEN	P7	72	2	-	4/7/8/10	-
69	MEN	u3	71	69	-	6/7/8/10	-
2	MEN	VP	72	2	-	4/7/8/10	-
2	MEN	O5	72	2	-	4/7/8/10	-
2	MEN	PG	72	2	-	3/7/8/10	-
2	MEN	LJ	72	2	-	5/7/8/10	-
10	MEN	JE	72	10	-	2/7/8/10	-
2	MEN	mE	72	2	-	3/7/8/10	-
2	MEN	i4	72	2	-	4/7/8/10	-
2	MEN	eB	72	2	-	3/7/8/10	-
2	MEN	TO	72	2	-	3/7/8/10	-
2	MEN	VA	72	2	-	4/7/8/10	-
2	MEN	e4	72	2	-	5/7/8/10	-
2	MEN	U5	72	2	-	4/7/8/10	-
2	MEN	NA	72	2	-	4/7/8/10	-
2	MEN	SB	72	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	c4	72	2	-	2/7/8/10	-
2	MEN	F9	72	2	-	2/7/8/10	-
2	MEN	gB	72	2	-	5/7/8/10	-
10	MEN	F1	72	10	-	2/7/8/10	-
2	MEN	PK	72	2,82	-	3/7/8/10	-
2	MEN	V7	72	2	-	4/7/8/10	-
2	MEN	jK	72	2,82	-	4/7/8/10	-
10	MEN	D4	72	10	-	2/7/8/10	-
2	MEN	y8	72	2	-	3/7/8/10	-
69	MEN	k3	71	69	-	4/7/8/10	-
2	MEN	NM	72	2	-	4/7/8/10	-
2	MEN	BI	72	2	-	5/7/8/10	-
2	MEN	P4	72	2	-	4/7/8/10	-
2	MEN	J7	72	2	-	1/7/8/10	-
2	MEN	RE	72	2	-	3/7/8/10	-
2	MEN	HK	72	2,82	-	2/7/8/10	-
2	MEN	R1	72	2	-	2/7/8/10	-
2	MEN	XP	72	2	-	4/7/8/10	-
2	MEN	aG	72	2	-	4/7/8/10	-
2	MEN	YB	72	2	-	4/7/8/10	-
2	MEN	JA	72	2	-	1/7/8/10	-
2	MEN	HB	72	2	-	2/7/8/10	-
2	MEN	m4	72	2	-	4/7/8/10	-
2	MEN	iE	72	2	-	3/7/8/10	-
2	MEN	vK	72	2,82	-	1/7/8/10	-
2	MEN	18	72	2	-	4/7/8/10	-
2	MEN	F5	72	2	-	4/7/8/10	-
2	MEN	gO	72	2	-	4/7/8/10	-
2	MEN	PH	72	2	-	4/7/8/10	-
2	MEN	DB	72	2	-	4/7/8/10	-
2	MEN	RH	72	2	-	2/7/8/10	-
2	MEN	FA	72	2	-	4/7/8/10	-
2	MEN	RK	72	2,82	-	2/7/8/10	-
2	MEN	eO	72	2	-	5/7/8/10	-
2	MEN	DP	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kH	72	2	-	4/7/8/10	-
2	MEN	SI	72	2	-	4/7/8/10	-
2	MEN	YE	72	2	-	5/7/8/10	-
10	MEN	H1	72	10	-	4/7/8/10	-
2	MEN	mO	72	2	-	4/7/8/10	-
2	MEN	eM	72	2	-	4/7/8/10	-
69	MEN	w3	71	69	-	6/7/8/10	-
2	MEN	NF	72	2,82	-	2/7/8/10	-
2	MEN	D7	72	2	-	3/7/8/10	-
2	MEN	YI	72	2	-	3/7/8/10	-
2	MEN	EQ	72	2	-	3/7/8/10	-
2	MEN	GD	72	2	-	4/7/8/10	-
2	MEN	OI	72	2	-	5/7/8/10	-
2	MEN	NK	72	2,82	-	2/7/8/10	-
2	MEN	VE	72	2	-	4/7/8/10	-
2	MEN	ZB	72	2	-	6/7/8/10	-
2	MEN	UD	72	2	-	3/7/8/10	-
2	MEN	TA	72	2,75	-	6/7/8/10	-
2	MEN	LM	72	2	-	4/7/8/10	-
2	MEN	cG	72	2	-	3/7/8/10	-
2	MEN	tK	72	2,82	-	4/7/8/10	-
2	MEN	BA	72	2	-	4/7/8/10	-
69	MEN	Q3	71	69	-	6/7/8/10	-
2	MEN	PP	72	2	-	4/7/8/10	-
2	MEN	XM	72	2	-	4/7/8/10	-
2	MEN	ZM	72	2	-	5/7/8/10	-
10	MEN	FE	72	10	-	3/7/8/10	-
10	MEN	DH	72	10	-	4/7/8/10	-
2	MEN	L5	72	2	-	4/7/8/10	-
2	MEN	TK	72	2,82	-	2/7/8/10	-
69	MEN	s3	71	69	-	6/7/8/10	-
2	MEN	DK	72	2,82	-	2/7/8/10	-
10	MEN	FO	72	10	-	3/7/8/10	-
2	MEN	ED	72	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	mJ	72	2	-	4/7/8/10	-
2	MEN	OD	72	2	-	2/7/8/10	-
2	MEN	TF	72	2,82	-	2/7/8/10	-
2	MEN	VK	72	2,82	-	4/7/8/10	-
2	MEN	BP	72	2	-	4/7/8/10	-
10	MEN	HE	72	10	-	4/7/8/10	-
2	MEN	RJ	72	2	-	4/7/8/10	-
2	MEN	PB	72	2	-	4/7/8/10	-
2	MEN	aO	72	2	-	3/7/8/10	-
2	MEN	W5	72	2	-	4/7/8/10	-
2	MEN	HP	72	2	-	4/7/8/10	-
2	MEN	Q9	72	2	-	2/7/8/10	-
2	MEN	iH	72	2	-	4/7/8/10	-
10	MEN	L4	72	10	-	4/7/8/10	-
2	MEN	JJ	72	2	-	3/7/8/10	-
2	MEN	a1	72	2	-	3/7/8/10	-
2	MEN	a4	72	2	-	3/7/8/10	-
10	MEN	LE	72	10	-	4/7/8/10	-
10	MEN	NE	72	10	-	4/7/8/10	-
2	MEN	sC	72	2	-	2/7/8/10	-
2	MEN	PO	72	2	-	4/7/8/10	-
2	MEN	ZF	72	2	-	5/7/8/10	-
2	MEN	QQ	72	2	-	4/7/8/10	-
2	MEN	i1	72	2	-	4/7/8/10	-
2	MEN	S9	72	2	-	2/7/8/10	-
2	MEN	JK	72	2,82	-	2/7/8/10	-
2	MEN	LI	72	2	-	4/7/8/10	-
10	MEN	DE	72	11,10	-	4/7/8/10	-
10	MEN	F4	72	10	-	3/7/8/10	-
2	MEN	XF	72	2,82	-	2/7/8/10	-
2	MEN	XJ	72	2	-	5/7/8/10	-
2	MEN	cH	72	2	-	4/7/8/10	-
2	MEN	JF	72	2,82	-	2/7/8/10	-
2	MEN	gG	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kE	72	2	-	4/7/8/10	-
10	MEN	HG	72	10	-	4/7/8/10	-
2	MEN	MQ	72	2	-	2/7/8/10	-

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	S3	71	MEN	CE2-ND2	67.26	2.65	1.45
69	Q3	71	MEN	CE2-ND2	67.24	2.65	1.45
69	s3	71	MEN	CE2-ND2	67.24	2.65	1.45
69	U3	71	MEN	CE2-ND2	67.22	2.65	1.45
69	w3	71	MEN	CE2-ND2	67.21	2.65	1.45
69	u3	71	MEN	CE2-ND2	67.19	2.65	1.45
69	D3	71	MEN	O-C	33.20	2.52	1.19
69	q3	71	MEN	O-C	33.20	2.52	1.19
69	f3	71	MEN	O-C	33.19	2.52	1.19
69	I3	71	MEN	O-C	33.19	2.52	1.19
69	h3	71	MEN	O-C	33.19	2.52	1.19
69	M3	71	MEN	O-C	33.18	2.52	1.19
69	L3	71	MEN	O-C	33.18	2.52	1.19
69	n3	71	MEN	O-C	33.18	2.52	1.19
69	d3	71	MEN	O-C	33.18	2.52	1.19
69	B3	71	MEN	O-C	33.17	2.52	1.19
69	o3	71	MEN	O-C	33.17	2.52	1.19
69	F3	71	MEN	O-C	33.17	2.52	1.19
69	k3	71	MEN	O-C	33.17	2.52	1.19
69	j3	71	MEN	O-C	33.16	2.52	1.19
69	H3	71	MEN	O-C	33.16	2.52	1.19
69	w3	71	MEN	CG-ND2	15.54	2.07	1.34
69	s3	71	MEN	CG-ND2	15.53	2.07	1.34
69	u3	71	MEN	CG-ND2	15.53	2.07	1.34
69	Q3	71	MEN	CG-ND2	15.53	2.07	1.34
69	S3	71	MEN	CG-ND2	15.53	2.07	1.34
69	U3	71	MEN	CG-ND2	15.52	2.07	1.34
69	F3	71	MEN	CB-CG	15.26	1.86	1.51
69	S3	71	MEN	CB-CA	15.25	1.86	1.53
69	D3	71	MEN	CB-CG	15.25	1.86	1.51
69	u3	71	MEN	CB-CA	15.24	1.86	1.53
69	o3	71	MEN	CB-CG	15.24	1.86	1.51
69	L3	71	MEN	CB-CG	15.24	1.86	1.51
69	k3	71	MEN	CB-CG	15.24	1.86	1.51
69	H3	71	MEN	CB-CG	15.24	1.86	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	q3	71	MEN	CB-CG	15.24	1.86	1.51
69	j3	71	MEN	CB-CG	15.24	1.86	1.51
69	n3	71	MEN	CB-CG	15.24	1.86	1.51
69	B3	71	MEN	CB-CG	15.23	1.86	1.51
69	s3	71	MEN	CB-CA	15.23	1.86	1.53
69	I3	71	MEN	CB-CG	15.23	1.86	1.51
69	f3	71	MEN	CB-CG	15.23	1.86	1.51
69	Q3	71	MEN	CB-CA	15.23	1.86	1.53
69	w3	71	MEN	CB-CA	15.23	1.86	1.53
69	h3	71	MEN	CB-CG	15.22	1.86	1.51
69	U3	71	MEN	CB-CA	15.22	1.86	1.53
69	d3	71	MEN	CB-CG	15.22	1.86	1.51
69	M3	71	MEN	CB-CG	15.21	1.86	1.51
69	s3	71	MEN	CB-CG	-11.51	1.25	1.51
69	Q3	71	MEN	CB-CG	-11.49	1.25	1.51
69	u3	71	MEN	CB-CG	-11.49	1.25	1.51
69	w3	71	MEN	CB-CG	-11.49	1.25	1.51
69	S3	71	MEN	CB-CG	-11.47	1.25	1.51
69	U3	71	MEN	CB-CG	-11.45	1.25	1.51
69	s3	71	MEN	O-C	9.84	1.59	1.19
69	U3	71	MEN	O-C	9.84	1.59	1.19
69	u3	71	MEN	O-C	9.84	1.59	1.19
69	Q3	71	MEN	O-C	9.83	1.59	1.19
69	w3	71	MEN	O-C	9.81	1.59	1.19
69	S3	71	MEN	O-C	9.80	1.59	1.19
69	S3	71	MEN	OD1-CG	6.75	1.37	1.23
69	s3	71	MEN	OD1-CG	6.73	1.36	1.23
69	Q3	71	MEN	OD1-CG	6.72	1.36	1.23
69	U3	71	MEN	OD1-CG	6.70	1.36	1.23
69	w3	71	MEN	OD1-CG	6.70	1.36	1.23
69	u3	71	MEN	OD1-CG	6.70	1.36	1.23
2	FF	72	MEN	OD1-CG	4.51	1.32	1.23
2	XK	72	MEN	OD1-CG	4.47	1.32	1.23
2	XF	72	MEN	OD1-CG	4.46	1.32	1.23
2	FK	72	MEN	OD1-CG	4.38	1.32	1.23
2	LK	72	MEN	OD1-CG	4.11	1.31	1.23
2	LF	72	MEN	OD1-CG	4.10	1.31	1.23
2	RK	72	MEN	OD1-CG	4.03	1.31	1.23
2	RF	72	MEN	OD1-CG	3.98	1.31	1.23
2	BK	72	MEN	OD1-CG	3.59	1.30	1.23
2	BF	72	MEN	OD1-CG	3.54	1.30	1.23
2	HF	72	MEN	OD1-CG	3.52	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	HK	72	MEN	OD1-CG	3.48	1.30	1.23
2	DK	72	MEN	OD1-CG	3.45	1.30	1.23
2	DF	72	MEN	OD1-CG	3.44	1.30	1.23
2	PK	72	MEN	OD1-CG	3.38	1.30	1.23
2	PF	72	MEN	OD1-CG	3.30	1.30	1.23
2	NK	72	MEN	OD1-CG	3.23	1.29	1.23
2	NF	72	MEN	OD1-CG	3.21	1.29	1.23
2	JK	72	MEN	OD1-CG	3.19	1.29	1.23
2	JF	72	MEN	OD1-CG	3.13	1.29	1.23
2	TK	72	MEN	OD1-CG	2.97	1.29	1.23
2	TF	72	MEN	OD1-CG	2.94	1.29	1.23
2	nF	72	MEN	OD1-CG	2.93	1.29	1.23
2	nK	72	MEN	OD1-CG	2.84	1.29	1.23
2	VK	72	MEN	OD1-CG	2.81	1.29	1.23
2	vK	72	MEN	OD1-CG	2.78	1.28	1.23
2	VF	72	MEN	OD1-CG	2.77	1.28	1.23
2	dK	72	MEN	OD1-CG	2.77	1.28	1.23
2	dF	72	MEN	OD1-CG	2.75	1.28	1.23
2	vF	72	MEN	OD1-CG	2.75	1.28	1.23
2	jF	72	MEN	OD1-CG	2.70	1.28	1.23
2	jK	72	MEN	OD1-CG	2.62	1.28	1.23
2	fF	72	MEN	OD1-CG	2.55	1.28	1.23
2	fK	72	MEN	OD1-CG	2.52	1.28	1.23
2	tF	72	MEN	OD1-CG	2.37	1.28	1.23
2	hF	72	MEN	OD1-CG	2.35	1.28	1.23
2	tK	72	MEN	OD1-CG	2.34	1.28	1.23
2	rF	72	MEN	OD1-CG	2.33	1.28	1.23
2	hK	72	MEN	OD1-CG	2.28	1.27	1.23
69	q3	71	MEN	CE2-ND2	2.24	1.49	1.45
69	k3	71	MEN	CE2-ND2	2.22	1.49	1.45
69	n3	71	MEN	CE2-ND2	2.22	1.49	1.45
69	I3	71	MEN	CE2-ND2	2.22	1.49	1.45
69	F3	71	MEN	CE2-ND2	2.22	1.49	1.45
69	h3	71	MEN	CE2-ND2	2.22	1.49	1.45
69	B3	71	MEN	CE2-ND2	2.21	1.49	1.45
69	j3	71	MEN	CE2-ND2	2.21	1.49	1.45
69	f3	71	MEN	CE2-ND2	2.21	1.49	1.45
69	L3	71	MEN	CE2-ND2	2.20	1.49	1.45
69	o3	71	MEN	CE2-ND2	2.20	1.49	1.45
2	rK	72	MEN	OD1-CG	2.19	1.27	1.23
69	H3	71	MEN	CE2-ND2	2.19	1.49	1.45
69	D3	71	MEN	CE2-ND2	2.18	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	d3	71	MEN	CE2-ND2	2.18	1.49	1.45
69	M3	71	MEN	CE2-ND2	2.15	1.49	1.45

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	U3	71	MEN	OD1-CG-CB	-38.81	64.66	121.50
69	S3	71	MEN	OD1-CG-CB	-38.79	64.69	121.50
69	s3	71	MEN	OD1-CG-CB	-38.79	64.69	121.50
69	Q3	71	MEN	OD1-CG-CB	-38.78	64.69	121.50
69	w3	71	MEN	OD1-CG-CB	-38.78	64.69	121.50
69	u3	71	MEN	OD1-CG-CB	-38.77	64.71	121.50
69	q3	71	MEN	CB-CA-C	-24.39	65.74	111.47
69	L3	71	MEN	CB-CA-C	-24.39	65.75	111.47
69	F3	71	MEN	CB-CA-C	-24.39	65.75	111.47
69	h3	71	MEN	CB-CA-C	-24.38	65.77	111.47
69	D3	71	MEN	CB-CA-C	-24.38	65.77	111.47
69	d3	71	MEN	CB-CA-C	-24.38	65.77	111.47
69	j3	71	MEN	CB-CA-C	-24.38	65.77	111.47
69	f3	71	MEN	CB-CA-C	-24.38	65.77	111.47
69	n3	71	MEN	CB-CA-C	-24.37	65.78	111.47
69	M3	71	MEN	CB-CA-C	-24.37	65.78	111.47
69	H3	71	MEN	CB-CA-C	-24.37	65.78	111.47
69	I3	71	MEN	CB-CA-C	-24.37	65.79	111.47
69	o3	71	MEN	CB-CA-C	-24.36	65.79	111.47
69	k3	71	MEN	CB-CA-C	-24.36	65.80	111.47
69	B3	71	MEN	CB-CA-C	-24.36	65.81	111.47
69	M3	71	MEN	OD1-CG-CB	23.53	155.96	121.50
69	B3	71	MEN	OD1-CG-CB	23.51	155.93	121.50
69	L3	71	MEN	OD1-CG-CB	23.51	155.93	121.50
69	h3	71	MEN	OD1-CG-CB	23.51	155.93	121.50
69	q3	71	MEN	OD1-CG-CB	23.51	155.92	121.50
69	H3	71	MEN	OD1-CG-CB	23.49	155.90	121.50
69	j3	71	MEN	OD1-CG-CB	23.49	155.90	121.50
69	k3	71	MEN	OD1-CG-CB	23.49	155.89	121.50
69	I3	71	MEN	OD1-CG-CB	23.49	155.89	121.50
69	n3	71	MEN	OD1-CG-CB	23.48	155.89	121.50
69	f3	71	MEN	OD1-CG-CB	23.48	155.89	121.50
69	o3	71	MEN	OD1-CG-CB	23.48	155.88	121.50
69	D3	71	MEN	OD1-CG-CB	23.48	155.88	121.50
69	F3	71	MEN	OD1-CG-CB	23.47	155.87	121.50
69	d3	71	MEN	OD1-CG-CB	23.47	155.87	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	H3	71	MEN	CA-CB-CG	-16.30	66.31	112.70
69	M3	71	MEN	CA-CB-CG	-16.30	66.31	112.70
69	D3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	q3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	h3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	F3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	d3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	k3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	f3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	j3	71	MEN	CA-CB-CG	-16.30	66.32	112.70
69	n3	71	MEN	CA-CB-CG	-16.30	66.33	112.70
69	I3	71	MEN	CA-CB-CG	-16.30	66.33	112.70
69	L3	71	MEN	CA-CB-CG	-16.29	66.33	112.70
69	B3	71	MEN	CA-CB-CG	-16.29	66.34	112.70
69	o3	71	MEN	CA-CB-CG	-16.29	66.35	112.70
69	Q3	71	MEN	OD1-CG-ND2	-14.64	46.10	122.36
69	j3	71	MEN	CB-CG-ND2	-14.64	95.79	115.48
69	u3	71	MEN	OD1-CG-ND2	-14.64	46.10	122.36
69	S3	71	MEN	OD1-CG-ND2	-14.64	46.10	122.36
69	k3	71	MEN	CB-CG-ND2	-14.64	95.79	115.48
69	w3	71	MEN	OD1-CG-ND2	-14.64	46.12	122.36
69	F3	71	MEN	CB-CG-ND2	-14.64	95.80	115.48
69	s3	71	MEN	OD1-CG-ND2	-14.64	46.13	122.36
69	d3	71	MEN	CB-CG-ND2	-14.64	95.80	115.48
69	n3	71	MEN	CB-CG-ND2	-14.63	95.80	115.48
69	o3	71	MEN	CB-CG-ND2	-14.63	95.80	115.48
69	L3	71	MEN	CB-CG-ND2	-14.63	95.81	115.48
69	U3	71	MEN	OD1-CG-ND2	-14.63	46.17	122.36
69	B3	71	MEN	CB-CG-ND2	-14.62	95.82	115.48
69	D3	71	MEN	CB-CG-ND2	-14.62	95.83	115.48
69	H3	71	MEN	CB-CG-ND2	-14.61	95.83	115.48
69	f3	71	MEN	CB-CG-ND2	-14.61	95.83	115.48
69	q3	71	MEN	CB-CG-ND2	-14.61	95.84	115.48
69	I3	71	MEN	CB-CG-ND2	-14.61	95.84	115.48
69	h3	71	MEN	CB-CG-ND2	-14.59	95.86	115.48
69	M3	71	MEN	CB-CG-ND2	-14.56	95.90	115.48
69	D3	71	MEN	OD1-CG-ND2	-11.66	61.66	122.36
69	h3	71	MEN	OD1-CG-ND2	-11.65	61.67	122.36
69	I3	71	MEN	OD1-CG-ND2	-11.65	61.67	122.36
69	f3	71	MEN	OD1-CG-ND2	-11.65	61.68	122.36
69	d3	71	MEN	OD1-CG-ND2	-11.65	61.68	122.36
69	H3	71	MEN	OD1-CG-ND2	-11.65	61.68	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	F3	71	MEN	OD1-CG-ND2	-11.65	61.68	122.36
69	M3	71	MEN	OD1-CG-ND2	-11.65	61.69	122.36
69	n3	71	MEN	OD1-CG-ND2	-11.65	61.69	122.36
69	q3	71	MEN	OD1-CG-ND2	-11.65	61.71	122.36
69	o3	71	MEN	OD1-CG-ND2	-11.65	61.71	122.36
69	k3	71	MEN	OD1-CG-ND2	-11.65	61.71	122.36
69	L3	71	MEN	OD1-CG-ND2	-11.64	61.72	122.36
69	B3	71	MEN	OD1-CG-ND2	-11.64	61.72	122.36
69	j3	71	MEN	OD1-CG-ND2	-11.64	61.73	122.36
2	LF	72	MEN	CB-CG-ND2	-8.42	104.16	115.48
2	LK	72	MEN	CB-CG-ND2	-8.41	104.17	115.48
2	FK	72	MEN	CB-CG-ND2	-7.93	104.83	115.48
2	FF	72	MEN	CB-CG-ND2	-7.84	104.94	115.48
2	XF	72	MEN	CB-CG-ND2	-6.87	106.25	115.48
2	XK	72	MEN	CB-CG-ND2	-6.85	106.27	115.48
2	RF	72	MEN	CB-CG-ND2	-6.73	106.43	115.48
2	RK	72	MEN	CB-CG-ND2	-6.73	106.43	115.48
2	T7	72	MEN	CB-CG-ND2	6.63	124.40	115.48
2	TA	72	MEN	CB-CG-ND2	6.62	124.39	115.48
2	BK	72	MEN	CB-CG-ND2	-6.54	106.69	115.48
2	BF	72	MEN	CB-CG-ND2	-6.51	106.72	115.48
69	s3	71	MEN	CB-CA-C	5.77	122.29	111.47
69	U3	71	MEN	CB-CA-C	5.76	122.27	111.47
69	S3	71	MEN	CB-CA-C	5.75	122.26	111.47
69	u3	71	MEN	CB-CA-C	5.75	122.25	111.47
69	w3	71	MEN	CB-CA-C	5.74	122.24	111.47
69	Q3	71	MEN	CB-CA-C	5.73	122.21	111.47
10	L1	72	MEN	CB-CG-ND2	5.67	123.11	115.48
10	LH	72	MEN	CB-CG-ND2	5.61	123.03	115.48
2	NK	72	MEN	CB-CG-ND2	-5.41	108.20	115.48
2	PK	72	MEN	CB-CG-ND2	-5.34	108.30	115.48
2	PF	72	MEN	CB-CG-ND2	-5.34	108.31	115.48
2	NF	72	MEN	CB-CG-ND2	-5.28	108.39	115.48
69	Q3	71	MEN	CB-CG-ND2	-4.91	108.88	115.48
69	S3	71	MEN	CB-CG-ND2	-4.90	108.90	115.48
69	w3	71	MEN	CB-CG-ND2	-4.89	108.91	115.48
69	s3	71	MEN	CB-CG-ND2	-4.89	108.91	115.48
69	u3	71	MEN	CB-CG-ND2	-4.89	108.91	115.48
69	U3	71	MEN	CB-CG-ND2	-4.87	108.93	115.48
2	HK	72	MEN	CB-CG-ND2	-4.81	109.01	115.48
2	HF	72	MEN	CB-CG-ND2	-4.79	109.04	115.48
2	TK	72	MEN	CB-CA-C	-4.39	103.23	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	JF	72	MEN	CB-CG-ND2	-4.39	109.58	115.48
2	TF	72	MEN	CB-CA-C	-4.38	103.27	111.47
2	DK	72	MEN	CB-CG-ND2	-4.29	109.72	115.48
2	JK	72	MEN	CB-CG-ND2	-4.24	109.78	115.48
2	B5	72	MEN	CB-CA-C	-4.23	103.54	111.47
2	fK	72	MEN	CB-CG-ND2	-4.21	109.82	115.48
2	fF	72	MEN	CB-CG-ND2	-4.19	109.85	115.48
2	DF	72	MEN	CB-CG-ND2	-4.18	109.86	115.48
2	L5	72	MEN	CB-CA-C	-4.11	103.76	111.47
2	dF	72	MEN	CB-CG-ND2	-4.07	110.01	115.48
2	cH	72	MEN	CB-CA-C	-4.04	103.89	111.47
2	dK	72	MEN	CB-CG-ND2	-4.04	110.05	115.48
2	c1	72	MEN	CB-CA-C	-4.03	103.92	111.47
2	Y5	72	MEN	CB-CA-C	-4.01	103.94	111.47
2	HJ	72	MEN	CB-CA-C	-3.93	104.09	111.47
2	H7	72	MEN	CB-CA-C	-3.84	104.26	111.47
2	HA	72	MEN	CB-CA-C	-3.83	104.30	111.47
2	DF	72	MEN	CB-CA-C	-3.81	104.32	111.47
2	DK	72	MEN	CB-CA-C	-3.77	104.40	111.47
69	u3	71	MEN	CA-CB-CG	3.74	123.34	112.70
69	w3	71	MEN	CA-CB-CG	3.74	123.34	112.70
69	U3	71	MEN	CA-CB-CG	3.74	123.33	112.70
69	s3	71	MEN	CA-CB-CG	3.73	123.32	112.70
69	Q3	71	MEN	CA-CB-CG	3.73	123.32	112.70
69	S3	71	MEN	CA-CB-CG	3.72	123.29	112.70
2	RP	72	MEN	CB-CA-C	-3.71	104.52	111.47
2	U5	72	MEN	CB-CA-C	-3.67	104.59	111.47
2	jK	72	MEN	CB-CG-ND2	-3.66	110.56	115.48
2	B9	72	MEN	CB-CA-C	-3.64	104.64	111.47
2	H5	72	MEN	CB-CA-C	-3.63	104.67	111.47
10	JO	72	MEN	CB-CG-ND2	3.61	120.34	115.48
10	J4	72	MEN	CB-CG-ND2	3.60	120.33	115.48
2	O5	72	MEN	CB-CA-C	-3.59	104.73	111.47
2	IQ	72	MEN	CB-CG-ND2	3.57	120.28	115.48
2	Q5	72	MEN	CB-CA-C	-3.56	104.79	111.47
2	jF	72	MEN	CB-CG-ND2	-3.55	110.71	115.48
2	XP	72	MEN	CB-CA-C	-3.52	104.86	111.47
2	YD	72	MEN	CB-CA-C	-3.51	104.89	111.47
2	FJ	72	MEN	CB-CA-C	-3.48	104.94	111.47
2	HM	72	MEN	CB-CA-C	-3.48	104.94	111.47
2	TH	72	MEN	CB-CA-C	-3.47	104.96	111.47
2	ID	72	MEN	CB-CG-ND2	3.47	120.15	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T1	72	MEN	CB-CA-C	-3.46	104.97	111.47
2	W5	72	MEN	CB-CA-C	-3.46	104.98	111.47
2	YQ	72	MEN	CB-CA-C	-3.46	104.98	111.47
2	L9	72	MEN	CB-CA-C	-3.46	104.99	111.47
2	lF	72	MEN	CB-CA-C	-3.45	105.00	111.47
2	lK	72	MEN	CB-CA-C	-3.44	105.02	111.47
2	F5	72	MEN	CB-CA-C	-3.42	105.06	111.47
2	O9	72	MEN	CB-CA-C	-3.42	105.06	111.47
2	MD	72	MEN	CB-CG-ND2	3.42	120.08	115.48
2	MQ	72	MEN	CB-CG-ND2	3.41	120.07	115.48
2	S5	72	MEN	CB-CA-C	-3.40	105.09	111.47
10	H4	72	MEN	CB-CG-ND2	3.37	120.01	115.48
2	q8	72	MEN	CB-CA-C	-3.36	105.16	111.47
10	J1	72	MEN	CB-CA-C	-3.36	105.18	111.47
2	qC	72	MEN	CB-CA-C	-3.33	105.22	111.47
10	JH	72	MEN	CB-CA-C	-3.33	105.23	111.47
2	ZM	72	MEN	CB-CA-C	-3.32	105.24	111.47
2	FM	72	MEN	CB-CA-C	-3.31	105.26	111.47
10	HO	72	MEN	CB-CG-ND2	3.31	119.94	115.48
2	VJ	72	MEN	CB-CA-C	-3.30	105.27	111.47
2	QD	72	MEN	CB-CA-C	-3.30	105.28	111.47
2	FP	72	MEN	CB-CA-C	-3.30	105.29	111.47
2	D5	72	MEN	CB-CA-C	-3.28	105.33	111.47
2	VM	72	MEN	CB-CA-C	-3.27	105.34	111.47
2	gM	72	MEN	CB-CA-C	-3.27	105.35	111.47
2	RJ	72	MEN	CB-CA-C	-3.26	105.35	111.47
10	FG	72	MEN	CB-CG-ND2	3.25	119.85	115.48
2	LP	72	MEN	CB-CA-C	-3.24	105.39	111.47
2	QQ	72	MEN	CB-CA-C	-3.24	105.39	111.47
2	JM	72	MEN	CB-CA-C	-3.21	105.44	111.47
2	BP	72	MEN	CB-CA-C	-3.20	105.47	111.47
2	GQ	72	MEN	CB-CA-C	-3.20	105.48	111.47
10	L4	72	MEN	CB-CG-ND2	3.19	119.77	115.48
2	F9	72	MEN	CB-CA-C	-3.19	105.50	111.47
10	FE	72	MEN	CB-CG-ND2	3.18	119.76	115.48
2	mM	72	MEN	CB-CA-C	-3.17	105.53	111.47
2	VF	72	MEN	CB-CA-C	-3.16	105.54	111.47
2	GD	72	MEN	CB-CA-C	-3.16	105.54	111.47
2	UQ	72	MEN	CB-CA-C	-3.16	105.54	111.47
2	UD	72	MEN	CB-CA-C	-3.16	105.55	111.47
2	JI	72	MEN	CB-CA-C	-3.15	105.55	111.47
2	gH	72	MEN	CB-CA-C	-3.15	105.56	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	LO	72	MEN	CB-CG-ND2	3.14	119.70	115.48
2	VK	72	MEN	CB-CA-C	-3.14	105.59	111.47
2	FF	72	MEN	CB-CA-C	-3.13	105.60	111.47
10	FO	72	MEN	CB-CG-ND2	3.13	119.69	115.48
2	g1	72	MEN	CB-CA-C	-3.12	105.61	111.47
10	JG	72	MEN	CB-CG-ND2	3.12	119.68	115.48
2	FI	72	MEN	CB-CA-C	-3.12	105.62	111.47
2	eM	72	MEN	CB-CA-C	-3.11	105.63	111.47
2	FK	72	MEN	CB-CA-C	-3.11	105.63	111.47
10	JE	72	MEN	CB-CG-ND2	3.11	119.66	115.48
2	kO	72	MEN	CB-CA-C	-3.09	105.67	111.47
2	HP	72	MEN	CB-CA-C	-3.09	105.67	111.47
2	J5	72	MEN	CB-CA-C	-3.09	105.67	111.47
10	L4	72	MEN	CB-CA-C	-3.08	105.69	111.47
2	VH	72	MEN	CB-CA-C	-3.08	105.69	111.47
2	DP	72	MEN	CB-CA-C	-3.08	105.70	111.47
10	LO	72	MEN	CB-CA-C	-3.08	105.70	111.47
10	F4	72	MEN	CB-CG-ND2	3.07	119.62	115.48
2	V1	72	MEN	CB-CA-C	-3.06	105.73	111.47
2	aG	72	MEN	CB-CA-C	-3.06	105.73	111.47
2	pK	72	MEN	CB-CA-C	-3.06	105.73	111.47
2	aE	72	MEN	CB-CA-C	-3.06	105.74	111.47
2	k4	72	MEN	CB-CA-C	-3.05	105.75	111.47
2	NF	72	MEN	CB-CA-C	-3.05	105.76	111.47
2	VP	72	MEN	CB-CA-C	-3.04	105.76	111.47
2	LI	72	MEN	CA-CB-CG	-3.04	104.04	112.70
2	kG	72	MEN	CB-CA-C	-3.03	105.78	111.47
2	N7	72	MEN	CB-CA-C	-3.03	105.79	111.47
2	NA	72	MEN	CB-CA-C	-3.02	105.80	111.47
2	ED	72	MEN	CB-CA-C	-3.02	105.81	111.47
2	PP	72	MEN	CB-CA-C	-3.02	105.81	111.47
2	kE	72	MEN	CB-CA-C	-3.01	105.82	111.47
2	EQ	72	MEN	CB-CA-C	-3.01	105.82	111.47
2	NP	72	MEN	CB-CA-C	-3.01	105.83	111.47
2	pF	72	MEN	CB-CA-C	-3.01	105.83	111.47
2	BI	72	MEN	CB-CA-C	-3.00	105.84	111.47
2	NK	72	MEN	CB-CA-C	-2.99	105.86	111.47
2	e4	72	MEN	CB-CA-C	-2.98	105.88	111.47
2	L9	72	MEN	CA-CB-CG	-2.98	104.22	112.70
2	JP	72	MEN	CB-CA-C	-2.97	105.90	111.47
10	DE	72	MEN	CB-CA-C	-2.97	105.90	111.47
2	SI	72	MEN	CB-CA-C	-2.97	105.91	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	eO	72	MEN	CB-CA-C	-2.96	105.92	111.47
2	TP	72	MEN	CB-CA-C	-2.96	105.92	111.47
2	kM	72	MEN	CB-CA-C	-2.96	105.92	111.47
2	PG	72	MEN	CB-CA-C	-2.96	105.93	111.47
10	DG	72	MEN	CB-CA-C	-2.96	105.93	111.47
2	gE	72	MEN	CB-CA-C	-2.96	105.93	111.47
2	gG	72	MEN	CB-CA-C	-2.96	105.93	111.47
2	PE	72	MEN	CB-CA-C	-2.95	105.94	111.47
2	B9	72	MEN	CA-CB-CG	-2.94	104.34	112.70
2	tK	72	MEN	CB-CA-C	-2.93	105.97	111.47
2	PA	72	MEN	CB-CA-C	-2.90	106.02	111.47
2	y8	72	MEN	CB-CA-C	-2.90	106.02	111.47
2	iH	72	MEN	CB-CA-C	-2.90	106.03	111.47
2	iM	72	MEN	CB-CA-C	-2.90	106.04	111.47
2	i1	72	MEN	CB-CA-C	-2.89	106.05	111.47
2	UI	72	MEN	CB-CA-C	-2.89	106.05	111.47
2	P1	72	MEN	CB-CA-C	-2.89	106.05	111.47
2	P7	72	MEN	CB-CA-C	-2.88	106.06	111.47
2	tF	72	MEN	CB-CA-C	-2.88	106.06	111.47
2	XJ	72	MEN	CB-CA-C	-2.86	106.10	111.47
2	WQ	72	MEN	CB-CA-C	-2.86	106.11	111.47
10	HH	72	MEN	CB-CA-C	-2.86	106.11	111.47
2	yC	72	MEN	CB-CA-C	-2.86	106.11	111.47
2	LM	72	MEN	CB-CA-C	-2.85	106.12	111.47
2	PH	72	MEN	CB-CA-C	-2.85	106.13	111.47
2	PM	72	MEN	CB-CA-C	-2.85	106.13	111.47
2	aH	72	MEN	CB-CG-ND2	2.84	119.30	115.48
10	H1	72	MEN	CB-CA-C	-2.84	106.15	111.47
2	i4	72	MEN	CB-CA-C	-2.82	106.17	111.47
2	WD	72	MEN	CB-CA-C	-2.82	106.18	111.47
2	a1	72	MEN	CB-CG-ND2	2.81	119.26	115.48
2	WI	72	MEN	CB-CA-C	-2.80	106.22	111.47
2	gJ	72	MEN	CB-CA-C	-2.80	106.22	111.47
2	GQ	72	MEN	CA-CB-CG	-2.80	104.74	112.70
2	iO	72	MEN	CB-CA-C	-2.79	106.23	111.47
2	GD	72	MEN	CA-CB-CG	-2.79	104.77	112.70
2	OI	72	MEN	CB-CA-C	-2.78	106.26	111.47
2	TO	72	MEN	CB-CA-C	-2.77	106.27	111.47
2	F7	72	MEN	CB-CA-C	-2.77	106.27	111.47
2	H9	72	MEN	CB-CG-ND2	2.77	119.20	115.48
2	FA	72	MEN	CB-CA-C	-2.76	106.29	111.47
2	T4	72	MEN	CB-CA-C	-2.76	106.29	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	FH	72	MEN	CB-CA-C	-2.74	106.32	111.47
10	F1	72	MEN	CB-CA-C	-2.73	106.35	111.47
2	nK	72	MEN	CB-CG-ND2	-2.72	111.82	115.48
2	PJ	72	MEN	CB-CA-C	-2.72	106.37	111.47
10	LE	72	MEN	CB-CG-ND2	2.70	119.12	115.48
2	YO	72	MEN	CB-CA-C	-2.69	106.42	111.47
2	KD	72	MEN	CB-CA-C	-2.69	106.42	111.47
10	HG	72	MEN	CB-CG-ND2	2.69	119.10	115.48
69	h3	71	MEN	CE2-ND2-CG	2.69	142.44	121.93
69	M3	71	MEN	CE2-ND2-CG	2.69	142.43	121.93
69	H3	71	MEN	CE2-ND2-CG	2.69	142.42	121.93
69	I3	71	MEN	CE2-ND2-CG	2.68	142.41	121.93
69	q3	71	MEN	CE2-ND2-CG	2.68	142.41	121.93
69	D3	71	MEN	CE2-ND2-CG	2.68	142.40	121.93
2	XM	72	MEN	CB-CA-C	-2.68	106.44	111.47
69	f3	71	MEN	CE2-ND2-CG	2.68	142.40	121.93
69	k3	71	MEN	CE2-ND2-CG	2.68	142.39	121.93
69	n3	71	MEN	CE2-ND2-CG	2.68	142.39	121.93
69	o3	71	MEN	CE2-ND2-CG	2.68	142.38	121.93
69	F3	71	MEN	CE2-ND2-CG	2.68	142.38	121.93
69	L3	71	MEN	CE2-ND2-CG	2.68	142.37	121.93
69	d3	71	MEN	CE2-ND2-CG	2.68	142.35	121.93
69	B3	71	MEN	CE2-ND2-CG	2.68	142.35	121.93
69	j3	71	MEN	CE2-ND2-CG	2.67	142.34	121.93
2	KQ	72	MEN	CB-CA-C	-2.66	106.48	111.47
2	Y4	72	MEN	CB-CA-C	-2.66	106.48	111.47
2	HI	72	MEN	CB-CA-C	-2.65	106.50	111.47
2	gO	72	MEN	CB-CA-C	-2.65	106.51	111.47
2	sC	72	MEN	CB-CG-ND2	2.64	119.04	115.48
2	s8	72	MEN	CB-CG-ND2	2.64	119.03	115.48
2	cM	72	MEN	CB-CA-C	-2.63	106.54	111.47
10	LE	72	MEN	CB-CA-C	-2.62	106.56	111.47
2	JA	72	MEN	CB-CA-C	-2.62	106.56	111.47
2	VE	72	MEN	CB-CA-C	-2.61	106.57	111.47
2	mJ	72	MEN	CB-CA-C	-2.61	106.57	111.47
2	J9	72	MEN	CB-CG-ND2	2.61	118.99	115.48
10	DH	72	MEN	CB-CA-C	-2.61	106.58	111.47
10	LG	72	MEN	CB-CG-ND2	2.60	118.98	115.48
2	g4	72	MEN	CB-CA-C	-2.60	106.60	111.47
2	XJ	72	MEN	CA-CB-CG	-2.60	105.31	112.70
2	YG	72	MEN	CB-CG-ND2	2.59	118.97	115.48
2	NJ	72	MEN	CB-CA-C	-2.59	106.61	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	LG	72	MEN	CB-CA-C	-2.59	106.61	111.47
2	nF	72	MEN	CB-CG-ND2	-2.59	112.00	115.48
2	XA	72	MEN	CB-CA-C	-2.59	106.61	111.47
2	mE	72	MEN	CB-CA-C	-2.59	106.61	111.47
2	VG	72	MEN	CB-CA-C	-2.59	106.61	111.47
2	X7	72	MEN	CB-CA-C	-2.59	106.62	111.47
2	DI	72	MEN	CB-CA-C	-2.59	106.62	111.47
2	mG	72	MEN	CB-CA-C	-2.58	106.62	111.47
2	m4	72	MEN	CB-CG-ND2	2.58	118.95	115.48
2	J7	72	MEN	CB-CA-C	-2.58	106.64	111.47
10	HE	72	MEN	CB-CG-ND2	2.57	118.94	115.48
10	D1	72	MEN	CB-CA-C	-2.56	106.66	111.47
10	D1	72	MEN	CA-CB-CG	-2.56	105.40	112.70
2	TG	72	MEN	CB-CA-C	-2.56	106.67	111.47
2	1C	72	MEN	CB-CA-C	-2.55	106.68	111.47
2	CD	72	MEN	CB-CA-C	-2.55	106.68	111.47
10	NE	72	MEN	CB-CA-C	-2.55	106.69	111.47
10	DH	72	MEN	CA-CB-CG	-2.55	105.44	112.70
2	eG	72	MEN	CB-CA-C	-2.55	106.69	111.47
2	kJ	72	MEN	CB-CA-C	-2.55	106.69	111.47
2	T7	72	MEN	OD1-CG-CB	-2.55	117.77	121.50
2	18	72	MEN	CB-CA-C	-2.54	106.70	111.47
2	YE	72	MEN	CB-CG-ND2	2.54	118.90	115.48
2	eE	72	MEN	CB-CA-C	-2.54	106.71	111.47
2	CQ	72	MEN	CB-CA-C	-2.54	106.71	111.47
10	NG	72	MEN	CB-CA-C	-2.53	106.72	111.47
2	TE	72	MEN	CB-CA-C	-2.53	106.72	111.47
2	RE	72	MEN	CB-CA-C	-2.53	106.73	111.47
2	W9	72	MEN	CB-CA-C	-2.53	106.73	111.47
2	FA	72	MEN	CB-CG-ND2	2.51	118.86	115.48
2	mO	72	MEN	CB-CG-ND2	2.51	118.86	115.48
2	RG	72	MEN	CB-CA-C	-2.51	106.77	111.47
2	X7	72	MEN	CB-CG-ND2	2.50	118.85	115.48
2	JJ	72	MEN	CB-CA-C	-2.50	106.79	111.47
2	BB	72	MEN	CA-CB-CG	-2.50	105.60	112.70
2	YB	72	MEN	CA-CB-CG	-2.49	105.60	112.70
2	RM	72	MEN	CB-CA-C	-2.49	106.80	111.47
2	uC	72	MEN	CB-CA-C	-2.48	106.81	111.47
2	HB	72	MEN	CA-CB-CG	-2.48	105.63	112.70
2	NM	72	MEN	CB-CG-ND2	2.48	118.82	115.48
2	S9	72	MEN	CB-CA-C	-2.48	106.82	111.47
2	F7	72	MEN	CB-CG-ND2	2.47	118.81	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	NE	72	MEN	CB-CG-ND2	2.47	118.80	115.48
2	TO	72	MEN	CB-CG-ND2	2.46	118.80	115.48
10	NG	72	MEN	CB-CG-ND2	2.46	118.80	115.48
10	J4	72	MEN	CB-CA-C	-2.46	106.86	111.47
2	u8	72	MEN	CB-CA-C	-2.46	106.86	111.47
2	T4	72	MEN	CB-CG-ND2	2.46	118.79	115.48
2	TM	72	MEN	CB-CA-C	-2.46	106.86	111.47
2	cJ	72	MEN	CB-CA-C	-2.45	106.88	111.47
2	V7	72	MEN	CB-CA-C	-2.44	106.89	111.47
2	TA	72	MEN	OD1-CG-CB	-2.44	117.92	121.50
2	LK	72	MEN	OD1-CG-CB	2.44	125.07	121.50
10	JO	72	MEN	CB-CA-C	-2.44	106.90	111.47
2	XA	72	MEN	CB-CG-ND2	2.43	118.76	115.48
2	TF	72	MEN	CB-CG-ND2	-2.43	112.21	115.48
2	SD	72	MEN	CB-CA-C	-2.43	106.92	111.47
2	TK	72	MEN	CB-CG-ND2	-2.42	112.22	115.48
2	LI	72	MEN	CB-CA-C	-2.42	106.93	111.47
2	YI	72	MEN	CB-CA-C	-2.42	106.93	111.47
2	SQ	72	MEN	CB-CA-C	-2.42	106.94	111.47
2	aO	72	MEN	CB-CG-ND2	2.41	118.72	115.48
2	eJ	72	MEN	CB-CA-C	-2.40	106.96	111.47
2	VA	72	MEN	CB-CA-C	-2.40	106.97	111.47
2	a4	72	MEN	CB-CG-ND2	2.40	118.71	115.48
2	JF	72	MEN	CB-CA-C	-2.40	106.97	111.47
2	LF	72	MEN	OD1-CG-CB	2.38	124.99	121.50
2	JK	72	MEN	CB-CA-C	-2.38	107.00	111.47
2	Q9	72	MEN	CB-CG-ND2	2.38	118.69	115.48
2	LJ	72	MEN	CB-CA-C	-2.38	107.01	111.47
2	NJ	72	MEN	CB-CG-ND2	2.37	118.68	115.48
2	fK	72	MEN	CB-CA-C	-2.37	107.02	111.47
2	fF	72	MEN	CB-CA-C	-2.36	107.04	111.47
10	DO	72	MEN	CB-CG-ND2	2.36	118.66	115.48
2	PH	72	MEN	CB-CG-ND2	2.36	118.65	115.48
2	TJ	72	MEN	CB-CA-C	-2.35	107.06	111.47
2	XK	72	MEN	CA-CB-CG	2.35	119.40	112.70
2	O9	72	MEN	CA-CB-CG	-2.35	106.01	112.70
2	GB	72	MEN	CA-CB-CG	-2.35	106.01	112.70
10	DG	72	MEN	CA-CB-CG	-2.33	106.08	112.70
2	FK	72	MEN	OD1-CG-CB	2.32	124.90	121.50
2	D9	72	MEN	CB-CA-C	-2.32	107.11	111.47
2	18	72	MEN	CB-CG-ND2	2.32	118.61	115.48
2	IB	72	MEN	CA-CB-CG	-2.32	106.10	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	XF	72	MEN	CA-CB-CG	2.32	119.30	112.70
10	DE	72	MEN	CA-CB-CG	-2.32	106.10	112.70
2	F9	72	MEN	CA-CB-CG	-2.31	106.12	112.70
10	D4	72	MEN	CB-CG-ND2	2.30	118.58	115.48
2	1C	72	MEN	CB-CG-ND2	2.30	118.58	115.48
2	T1	72	MEN	CB-CG-ND2	2.30	118.57	115.48
2	RB	72	MEN	CA-CB-CG	-2.29	106.18	112.70
10	NO	72	MEN	CB-CA-C	-2.29	107.17	111.47
2	RP	72	MEN	CA-CB-CG	-2.29	106.19	112.70
2	OB	72	MEN	CA-CB-CG	-2.29	106.19	112.70
2	ZK	72	MEN	CA-CB-CG	-2.28	106.20	112.70
2	mH	72	MEN	CB-CA-C	-2.28	107.19	111.47
2	FF	72	MEN	OD1-CG-CB	2.28	124.84	121.50
2	LF	72	MEN	CB-CA-C	-2.28	107.20	111.47
2	P1	72	MEN	CB-CG-ND2	2.28	118.55	115.48
2	VO	72	MEN	CB-CG-ND2	2.28	118.55	115.48
2	CD	72	MEN	CB-CG-ND2	2.27	118.54	115.48
2	HK	72	MEN	CB-CA-C	-2.27	107.21	111.47
2	RO	72	MEN	CB-CG-ND2	2.27	118.54	115.48
2	m4	72	MEN	CB-CA-C	-2.27	107.21	111.47
2	LB	72	MEN	CA-CB-CG	-2.27	106.24	112.70
2	RK	72	MEN	OD1-CG-CB	2.27	124.82	121.50
2	JJ	72	MEN	CB-CG-ND2	2.27	118.53	115.48
10	N4	72	MEN	CB-CA-C	-2.26	107.22	111.47
2	kH	72	MEN	CB-CA-C	-2.26	107.23	111.47
2	aO	72	MEN	CB-CA-C	-2.26	107.23	111.47
2	CQ	72	MEN	CB-CG-ND2	2.26	118.52	115.48
2	Q9	72	MEN	CB-CA-C	-2.26	107.24	111.47
2	DM	72	MEN	CB-CA-C	-2.26	107.24	111.47
2	RF	72	MEN	OD1-CG-CB	2.25	124.80	121.50
2	mO	72	MEN	CB-CA-C	-2.25	107.26	111.47
2	R4	72	MEN	CB-CG-ND2	2.24	118.50	115.48
2	gM	72	MEN	CB-CG-ND2	2.24	118.50	115.48
2	k1	72	MEN	CB-CA-C	-2.24	107.27	111.47
10	N4	72	MEN	CB-CG-ND2	2.24	118.49	115.48
2	aG	72	MEN	CB-CG-ND2	2.24	118.49	115.48
2	TH	72	MEN	CB-CG-ND2	2.23	118.49	115.48
2	m1	72	MEN	CB-CA-C	-2.23	107.29	111.47
2	H9	72	MEN	CB-CA-C	-2.23	107.29	111.47
2	Y9	72	MEN	CB-CA-C	-2.22	107.30	111.47
2	YH	72	MEN	CB-CA-C	-2.22	107.31	111.47
69	s3	71	MEN	CE2-ND2-CG	-2.22	105.00	121.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	U3	71	MEN	CE2-ND2-CG	-2.22	105.00	121.93
2	ZF	72	MEN	CA-CB-CG	-2.22	106.39	112.70
69	w3	71	MEN	CE2-ND2-CG	-2.22	105.02	121.93
69	u3	71	MEN	CE2-ND2-CG	-2.22	105.02	121.93
69	Q3	71	MEN	CE2-ND2-CG	-2.21	105.03	121.93
69	S3	71	MEN	CE2-ND2-CG	-2.21	105.03	121.93
2	LK	72	MEN	CB-CA-C	-2.20	107.33	111.47
2	cO	72	MEN	CB-CA-C	-2.20	107.34	111.47
10	NO	72	MEN	CB-CG-ND2	2.20	118.45	115.48
2	H5	72	MEN	CB-CG-ND2	2.20	118.45	115.48
2	aE	72	MEN	CB-CG-ND2	2.20	118.44	115.48
2	HF	72	MEN	CB-CA-C	-2.20	107.35	111.47
2	U9	72	MEN	CB-CG-ND2	2.20	118.44	115.48
2	Y1	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	c4	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	iJ	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	eH	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	V4	72	MEN	CB-CG-ND2	2.18	118.42	115.48
2	RO	72	MEN	CB-CA-C	-2.18	107.38	111.47
2	ZJ	72	MEN	CB-CA-C	-2.18	107.39	111.47
2	a4	72	MEN	CB-CA-C	-2.17	107.40	111.47
2	R4	72	MEN	CB-CA-C	-2.17	107.40	111.47
2	QI	72	MEN	CA-CB-CG	-2.17	106.53	112.70
2	V1	72	MEN	CB-CG-ND2	2.17	118.40	115.48
2	eO	72	MEN	CA-CB-CG	-2.16	106.54	112.70
2	U9	72	MEN	CB-CA-C	-2.16	107.41	111.47
2	bK	72	MEN	CB-CA-C	-2.16	107.42	111.47
2	bF	72	MEN	CB-CA-C	-2.16	107.42	111.47
2	MQ	72	MEN	CB-CA-C	-2.16	107.43	111.47
10	L1	72	MEN	CB-CA-C	-2.15	107.44	111.47
2	e1	72	MEN	CB-CA-C	-2.15	107.44	111.47
2	JI	72	MEN	CA-CB-CG	-2.15	106.59	112.70
2	e4	72	MEN	CA-CB-CG	-2.15	106.59	112.70
2	J5	72	MEN	CB-CG-ND2	2.15	118.37	115.48
2	VH	72	MEN	CB-CG-ND2	2.14	118.37	115.48
2	VO	72	MEN	CB-CA-C	-2.14	107.45	111.47
2	CB	72	MEN	CA-CB-CG	-2.14	106.61	112.70
2	DA	72	MEN	CB-CG-ND2	2.14	118.36	115.48
2	V4	72	MEN	CB-CA-C	-2.12	107.49	111.47
2	D7	72	MEN	CB-CG-ND2	2.12	118.34	115.48
10	LH	72	MEN	CB-CA-C	-2.12	107.50	111.47
2	XM	72	MEN	CA-CB-CG	-2.11	106.70	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	eB	72	MEN	CA-CB-CG	-2.11	106.70	112.70
2	MD	72	MEN	CB-CA-C	-2.11	107.52	111.47
2	BA	72	MEN	CB-CA-C	-2.10	107.54	111.47
2	B7	72	MEN	CB-CA-C	-2.10	107.54	111.47
2	RH	72	MEN	CB-CG-ND2	2.09	118.30	115.48
2	QQ	72	MEN	CB-CG-ND2	2.09	118.30	115.48
2	OQ	72	MEN	CB-CG-ND2	2.08	118.29	115.48
2	PK	72	MEN	OD1-CG-CB	2.08	124.55	121.50
2	OD	72	MEN	CB-CG-ND2	2.08	118.28	115.48
2	rK	72	MEN	CB-CA-C	-2.08	107.57	111.47
2	sC	72	MEN	CB-CA-C	-2.08	107.58	111.47
2	kJ	72	MEN	CB-CG-ND2	2.07	118.27	115.48
2	VE	72	MEN	CB-CG-ND2	2.07	118.27	115.48
2	s8	72	MEN	CB-CA-C	-2.07	107.59	111.47
2	VG	72	MEN	CB-CG-ND2	2.06	118.26	115.48
2	R1	72	MEN	CB-CG-ND2	2.06	118.26	115.48
2	rF	72	MEN	CB-CA-C	-2.06	107.61	111.47
2	PF	72	MEN	OD1-CG-CB	2.05	124.50	121.50
2	lF	72	MEN	CB-CG-ND2	2.05	118.24	115.48
2	OQ	72	MEN	CB-CA-C	-2.05	107.63	111.47
2	iG	72	MEN	CB-CA-C	-2.05	107.63	111.47
2	vF	72	MEN	CB-CA-C	-2.04	107.64	111.47
10	DO	72	MEN	CB-CA-C	-2.04	107.64	111.47
2	g1	72	MEN	CB-CG-ND2	2.04	118.22	115.48
2	NK	72	MEN	OD1-CG-CB	2.04	124.48	121.50
2	YI	72	MEN	CA-CB-CG	-2.04	106.91	112.70
2	cG	72	MEN	CB-CA-C	-2.03	107.65	111.47
2	LJ	72	MEN	CA-CB-CG	-2.03	106.92	112.70
2	jF	72	MEN	CB-CA-C	-2.03	107.66	111.47
10	D4	72	MEN	CB-CA-C	-2.03	107.67	111.47
2	gH	72	MEN	CB-CG-ND2	2.03	118.21	115.48
2	eJ	72	MEN	CA-CB-CG	-2.03	106.93	112.70
2	NM	72	MEN	CB-CA-C	-2.02	107.67	111.47
2	JM	72	MEN	CB-CG-ND2	2.02	118.21	115.48
10	H4	72	MEN	CB-CA-C	-2.02	107.68	111.47
2	OD	72	MEN	CB-CA-C	-2.02	107.68	111.47
2	lK	72	MEN	CB-CG-ND2	2.02	118.20	115.48
2	PM	72	MEN	CB-CG-ND2	2.01	118.19	115.48
2	cE	72	MEN	CB-CA-C	-2.01	107.70	111.47
2	VB	72	MEN	CA-CB-CG	-2.01	106.98	112.70
2	QD	72	MEN	CB-CG-ND2	2.01	118.19	115.48
10	HG	72	MEN	CB-CA-C	-2.01	107.71	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	XB	72	MEN	CA-CB-CG	-2.01	106.99	112.70
2	iE	72	MEN	CB-CA-C	-2.00	107.71	111.47

There are no chirality outliers.

All (1235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BA	72	MEN	N-CA-CB-CG
2	DA	72	MEN	O-C-CA-CB
2	FA	72	MEN	C-CA-CB-CG
2	LA	72	MEN	O-C-CA-CB
2	LA	72	MEN	C-CA-CB-CG
2	NA	72	MEN	C-CA-CB-CG
2	PA	72	MEN	C-CA-CB-CG
2	RA	72	MEN	C-CA-CB-CG
2	TA	72	MEN	C-CA-CB-CG
2	TA	72	MEN	CB-CG-ND2-CE2
2	TA	72	MEN	OD1-CG-ND2-CE2
2	VA	72	MEN	C-CA-CB-CG
2	BB	72	MEN	N-CA-CB-CG
2	BB	72	MEN	C-CA-CB-CG
2	BB	72	MEN	CB-CG-ND2-CE2
2	CB	72	MEN	C-CA-CB-CG
2	DB	72	MEN	CB-CG-ND2-CE2
2	FB	72	MEN	C-CA-CB-CG
2	GB	72	MEN	C-CA-CB-CG
2	GB	72	MEN	CB-CG-ND2-CE2
2	HB	72	MEN	C-CA-CB-CG
2	IB	72	MEN	O-C-CA-CB
2	IB	72	MEN	N-CA-CB-CG
2	IB	72	MEN	C-CA-CB-CG
2	LB	72	MEN	CB-CG-ND2-CE2
2	LB	72	MEN	OD1-CG-ND2-CE2
2	MB	72	MEN	C-CA-CB-CG
2	NB	72	MEN	O-C-CA-CB
2	NB	72	MEN	CB-CG-ND2-CE2
2	NB	72	MEN	OD1-CG-ND2-CE2
2	OB	72	MEN	N-CA-CB-CG
2	OB	72	MEN	C-CA-CB-CG
2	OB	72	MEN	CB-CG-ND2-CE2
2	PB	72	MEN	C-CA-CB-CG
2	QB	72	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	QB	72	MEN	C-CA-CB-CG
2	QB	72	MEN	CB-CG-ND2-CE2
2	RB	72	MEN	O-C-CA-CB
2	RB	72	MEN	CB-CG-ND2-CE2
2	RB	72	MEN	OD1-CG-ND2-CE2
2	SB	72	MEN	C-CA-CB-CG
2	VB	72	MEN	C-CA-CB-CG
2	VB	72	MEN	CB-CG-ND2-CE2
2	XB	72	MEN	O-C-CA-CB
2	XB	72	MEN	C-CA-CB-CG
2	XB	72	MEN	CB-CG-ND2-CE2
2	YB	72	MEN	CB-CG-ND2-CE2
2	ZB	72	MEN	C-CA-CB-CG
2	ZB	72	MEN	CB-CG-ND2-CE2
2	CD	72	MEN	C-CA-CB-CG
2	GD	72	MEN	C-CA-CB-CG
2	KD	72	MEN	C-CA-CB-CG
2	MD	72	MEN	C-CA-CB-CG
2	QD	72	MEN	N-CA-CB-CG
2	QD	72	MEN	C-CA-CB-CG
2	WD	72	MEN	C-CA-CB-CG
2	YD	72	MEN	N-CA-CB-CG
10	DE	72	MEN	C-CA-CB-CG
10	HE	72	MEN	C-CA-CB-CG
10	LE	72	MEN	C-CA-CB-CG
2	RE	72	MEN	C-CA-CB-CG
2	YE	72	MEN	O-C-CA-CB
2	YE	72	MEN	C-CA-CB-CG
2	LF	72	MEN	O-C-CA-CB
2	PF	72	MEN	O-C-CA-CB
2	ZF	72	MEN	O-C-CA-CB
2	ZF	72	MEN	C-CA-CB-CG
10	DG	72	MEN	C-CA-CB-CG
10	HG	72	MEN	C-CA-CB-CG
10	LG	72	MEN	C-CA-CB-CG
2	RG	72	MEN	C-CA-CB-CG
2	YG	72	MEN	O-C-CA-CB
2	YG	72	MEN	C-CA-CB-CG
10	DH	72	MEN	C-CA-CB-CG
10	HH	72	MEN	N-CA-CB-CG
10	HH	72	MEN	C-CA-CB-CG
2	PH	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	RH	72	MEN	C-CA-CB-CG
2	TH	72	MEN	O-C-CA-CB
2	TH	72	MEN	N-CA-CB-CG
2	TH	72	MEN	C-CA-CB-CG
2	BI	72	MEN	O-C-CA-CB
2	BI	72	MEN	C-CA-CB-CG
2	DI	72	MEN	C-CA-CB-CG
2	FI	72	MEN	O-C-CA-CB
2	FI	72	MEN	C-CA-CB-CG
2	HI	72	MEN	C-CA-CB-CG
2	JI	72	MEN	O-C-CA-CB
2	JI	72	MEN	C-CA-CB-CG
2	LI	72	MEN	C-CA-CB-CG
2	OI	72	MEN	O-C-CA-CB
2	OI	72	MEN	C-CA-CB-CG
2	QI	72	MEN	C-CA-CB-CG
2	SI	72	MEN	C-CA-CB-CG
2	UI	72	MEN	N-CA-CB-CG
2	UI	72	MEN	C-CA-CB-CG
2	WI	72	MEN	O-C-CA-CB
2	WI	72	MEN	C-CA-CB-CG
2	YI	72	MEN	C-CA-CB-CG
2	DJ	72	MEN	C-CA-CB-CG
2	FJ	72	MEN	N-CA-CB-CG
2	FJ	72	MEN	C-CA-CB-CG
2	HJ	72	MEN	C-CA-CB-CG
2	LJ	72	MEN	O-C-CA-CB
2	LJ	72	MEN	C-CA-CB-CG
2	NJ	72	MEN	O-C-CA-CB
2	NJ	72	MEN	C-CA-CB-CG
2	TJ	72	MEN	O-C-CA-CB
2	TJ	72	MEN	C-CA-CB-CG
2	VJ	72	MEN	C-CA-CB-CG
2	XJ	72	MEN	O-C-CA-CB
2	XJ	72	MEN	C-CA-CB-CG
2	ZJ	72	MEN	C-CA-CB-CG
2	LK	72	MEN	O-C-CA-CB
2	PK	72	MEN	O-C-CA-CB
2	ZK	72	MEN	O-C-CA-CB
2	ZK	72	MEN	C-CA-CB-CG
2	DM	72	MEN	O-C-CA-CB
2	DM	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	FM	72	MEN	C-CA-CB-CG
2	HM	72	MEN	O-C-CA-CB
2	JM	72	MEN	C-CA-CB-CG
2	LM	72	MEN	C-CA-CB-CG
2	NM	72	MEN	O-C-CA-CB
2	NM	72	MEN	C-CA-CB-CG
2	PM	72	MEN	O-C-CA-CB
2	RM	72	MEN	C-CA-CB-CG
2	TM	72	MEN	O-C-CA-CB
2	TM	72	MEN	C-CA-CB-CG
2	VM	72	MEN	C-CA-CB-CG
2	XM	72	MEN	O-C-CA-CB
2	XM	72	MEN	C-CA-CB-CG
2	ZM	72	MEN	O-C-CA-CB
2	ZM	72	MEN	C-CA-CB-CG
10	NO	72	MEN	O-C-CA-CB
2	PO	72	MEN	C-CA-CB-CG
2	RO	72	MEN	C-CA-CB-CG
2	YO	72	MEN	C-CA-CB-CG
2	BP	72	MEN	C-CA-CB-CG
2	DP	72	MEN	C-CA-CB-CG
2	FP	72	MEN	O-C-CA-CB
2	FP	72	MEN	C-CA-CB-CG
2	HP	72	MEN	C-CA-CB-CG
2	JP	72	MEN	C-CA-CB-CG
2	LP	72	MEN	C-CA-CB-CG
2	NP	72	MEN	C-CA-CB-CG
2	PP	72	MEN	C-CA-CB-CG
2	TP	72	MEN	C-CA-CB-CG
2	VP	72	MEN	C-CA-CB-CG
2	XP	72	MEN	C-CA-CB-CG
2	CQ	72	MEN	C-CA-CB-CG
2	GQ	72	MEN	C-CA-CB-CG
2	KQ	72	MEN	C-CA-CB-CG
2	MQ	72	MEN	C-CA-CB-CG
2	QQ	72	MEN	N-CA-CB-CG
2	QQ	72	MEN	C-CA-CB-CG
2	WQ	72	MEN	C-CA-CB-CG
2	YQ	72	MEN	N-CA-CB-CG
2	P1	72	MEN	C-CA-CB-CG
2	R1	72	MEN	C-CA-CB-CG
2	T1	72	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	T1	72	MEN	N-CA-CB-CG
2	T1	72	MEN	C-CA-CB-CG
10	D1	72	MEN	C-CA-CB-CG
10	H1	72	MEN	N-CA-CB-CG
10	H1	72	MEN	C-CA-CB-CG
2	g1	72	MEN	O-C-CA-CB
2	g1	72	MEN	CA-CB-CG-OD1
2	g1	72	MEN	CA-CB-CG-ND2
2	i1	72	MEN	C-CA-CB-CG
2	c1	72	MEN	C-CA-CB-CG
2	e1	72	MEN	O-C-CA-CB
69	B3	71	MEN	O-C-CA-CB
69	B3	71	MEN	CB-CG-ND2-CE2
69	D3	71	MEN	O-C-CA-CB
69	D3	71	MEN	CB-CG-ND2-CE2
69	F3	71	MEN	CB-CG-ND2-CE2
69	H3	71	MEN	CB-CG-ND2-CE2
69	I3	71	MEN	O-C-CA-CB
69	I3	71	MEN	CB-CG-ND2-CE2
69	L3	71	MEN	CB-CG-ND2-CE2
69	M3	71	MEN	CB-CG-ND2-CE2
69	Q3	71	MEN	O-C-CA-CB
69	Q3	71	MEN	CB-CG-ND2-CE2
69	S3	71	MEN	O-C-CA-CB
69	S3	71	MEN	CB-CG-ND2-CE2
69	U3	71	MEN	O-C-CA-CB
69	U3	71	MEN	CB-CG-ND2-CE2
69	d3	71	MEN	O-C-CA-CB
69	d3	71	MEN	CB-CG-ND2-CE2
69	f3	71	MEN	CB-CG-ND2-CE2
69	h3	71	MEN	O-C-CA-CB
69	h3	71	MEN	CB-CG-ND2-CE2
69	j3	71	MEN	CB-CG-ND2-CE2
69	k3	71	MEN	CB-CG-ND2-CE2
69	n3	71	MEN	CB-CG-ND2-CE2
69	o3	71	MEN	O-C-CA-CB
69	o3	71	MEN	CB-CG-ND2-CE2
69	q3	71	MEN	O-C-CA-CB
69	q3	71	MEN	CB-CG-ND2-CE2
69	s3	71	MEN	O-C-CA-CB
69	s3	71	MEN	CB-CG-ND2-CE2
69	u3	71	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
69	u3	71	MEN	CB-CG-ND2-CE2
69	w3	71	MEN	O-C-CA-CB
69	w3	71	MEN	CB-CG-ND2-CE2
10	N4	72	MEN	O-C-CA-CB
2	P4	72	MEN	C-CA-CB-CG
2	R4	72	MEN	C-CA-CB-CG
2	Y4	72	MEN	C-CA-CB-CG
2	i4	72	MEN	C-CA-CB-CG
2	k4	72	MEN	O-C-CA-CB
2	k4	72	MEN	C-CA-CB-CG
2	m4	72	MEN	C-CA-CB-CG
2	e4	72	MEN	O-C-CA-CB
2	g4	72	MEN	C-CA-CB-CG
2	B5	72	MEN	N-CA-CB-CG
2	B5	72	MEN	C-CA-CB-CG
2	F5	72	MEN	C-CA-CB-CG
2	H5	72	MEN	C-CA-CB-CG
2	J5	72	MEN	O-C-CA-CB
2	L5	72	MEN	C-CA-CB-CG
2	O5	72	MEN	C-CA-CB-CG
2	Q5	72	MEN	C-CA-CB-CG
2	S5	72	MEN	N-CA-CB-CG
2	S5	72	MEN	C-CA-CB-CG
2	W5	72	MEN	C-CA-CB-CG
2	Y5	72	MEN	C-CA-CB-CG
2	B7	72	MEN	N-CA-CB-CG
2	D7	72	MEN	O-C-CA-CB
2	F7	72	MEN	C-CA-CB-CG
2	L7	72	MEN	O-C-CA-CB
2	L7	72	MEN	C-CA-CB-CG
2	N7	72	MEN	C-CA-CB-CG
2	P7	72	MEN	C-CA-CB-CG
2	R7	72	MEN	C-CA-CB-CG
2	T7	72	MEN	C-CA-CB-CG
2	T7	72	MEN	CB-CG-ND2-CE2
2	T7	72	MEN	OD1-CG-ND2-CE2
2	V7	72	MEN	C-CA-CB-CG
2	q8	72	MEN	N-CA-CB-CG
2	O9	72	MEN	C-CA-CB-CG
2	aB	72	MEN	C-CA-CB-CG
2	bB	72	MEN	CB-CG-ND2-CE2
2	dB	72	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	dB	72	MEN	C-CA-CB-CG
2	dB	72	MEN	CB-CG-ND2-CE2
2	eB	72	MEN	C-CA-CB-CG
2	gB	72	MEN	O-C-CA-CB
2	gB	72	MEN	C-CA-CB-CG
2	qC	72	MEN	N-CA-CB-CG
2	aE	72	MEN	C-CA-CB-CG
2	cE	72	MEN	O-C-CA-CB
2	kE	72	MEN	C-CA-CB-CG
2	bF	72	MEN	N-CA-CB-CG
2	bF	72	MEN	C-CA-CB-CG
2	dF	72	MEN	O-C-CA-CB
2	jF	72	MEN	C-CA-CB-CG
2	nF	72	MEN	C-CA-CB-CG
2	pF	72	MEN	O-C-CA-CB
2	rF	72	MEN	O-C-CA-CB
2	tF	72	MEN	C-CA-CB-CG
2	aG	72	MEN	C-CA-CB-CG
2	cG	72	MEN	O-C-CA-CB
2	kG	72	MEN	C-CA-CB-CG
2	gH	72	MEN	O-C-CA-CB
2	gH	72	MEN	CA-CB-CG-OD1
2	gH	72	MEN	CA-CB-CG-ND2
2	iH	72	MEN	C-CA-CB-CG
2	cH	72	MEN	C-CA-CB-CG
2	eH	72	MEN	O-C-CA-CB
2	eJ	72	MEN	C-CA-CB-CG
2	iJ	72	MEN	C-CA-CB-CG
2	kJ	72	MEN	C-CA-CB-CG
2	mJ	72	MEN	C-CA-CB-CG
2	bK	72	MEN	N-CA-CB-CG
2	bK	72	MEN	C-CA-CB-CG
2	dK	72	MEN	O-C-CA-CB
2	jK	72	MEN	C-CA-CB-CG
2	nK	72	MEN	C-CA-CB-CG
2	pK	72	MEN	O-C-CA-CB
2	rK	72	MEN	O-C-CA-CB
2	tK	72	MEN	C-CA-CB-CG
2	eM	72	MEN	C-CA-CB-CG
2	gM	72	MEN	O-C-CA-CB
2	gM	72	MEN	C-CA-CB-CG
2	iM	72	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	iM	72	MEN	C-CA-CB-CG
2	kM	72	MEN	C-CA-CB-CG
2	mM	72	MEN	C-CA-CB-CG
2	iO	72	MEN	C-CA-CB-CG
2	kO	72	MEN	O-C-CA-CB
2	kO	72	MEN	C-CA-CB-CG
2	mO	72	MEN	C-CA-CB-CG
2	eO	72	MEN	O-C-CA-CB
2	gO	72	MEN	C-CA-CB-CG
2	FA	72	MEN	CA-CB-CG-OD1
2	OD	72	MEN	CA-CB-CG-OD1
2	SD	72	MEN	CA-CB-CG-OD1
2	YD	72	MEN	CA-CB-CG-OD1
2	VE	72	MEN	CA-CB-CG-OD1
2	VG	72	MEN	CA-CB-CG-OD1
2	VH	72	MEN	CA-CB-CG-OD1
2	JM	72	MEN	CA-CB-CG-OD1
2	OQ	72	MEN	CA-CB-CG-OD1
2	SQ	72	MEN	CA-CB-CG-OD1
2	YQ	72	MEN	CA-CB-CG-OD1
2	V1	72	MEN	CA-CB-CG-OD1
2	k1	72	MEN	CA-CB-CG-OD1
2	m4	72	MEN	CA-CB-CG-OD1
2	F5	72	MEN	CA-CB-CG-OD1
2	H5	72	MEN	CA-CB-CG-OD1
2	J5	72	MEN	CA-CB-CG-OD1
2	S5	72	MEN	CA-CB-CG-OD1
2	W5	72	MEN	CA-CB-CG-OD1
2	F7	72	MEN	CA-CB-CG-OD1
2	aE	72	MEN	CA-CB-CG-OD1
2	aG	72	MEN	CA-CB-CG-OD1
2	kH	72	MEN	CA-CB-CG-OD1
2	mO	72	MEN	CA-CB-CG-OD1
2	FA	72	MEN	CA-CB-CG-ND2
2	OD	72	MEN	CA-CB-CG-ND2
2	SD	72	MEN	CA-CB-CG-ND2
2	YD	72	MEN	CA-CB-CG-ND2
2	VE	72	MEN	CA-CB-CG-ND2
2	VG	72	MEN	CA-CB-CG-ND2
10	LH	72	MEN	CA-CB-CG-ND2
2	VH	72	MEN	CA-CB-CG-ND2
2	PJ	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	JM	72	MEN	CA-CB-CG-ND2
2	PM	72	MEN	CA-CB-CG-ND2
2	TO	72	MEN	CA-CB-CG-ND2
2	OQ	72	MEN	CA-CB-CG-ND2
2	SQ	72	MEN	CA-CB-CG-ND2
2	YQ	72	MEN	CA-CB-CG-ND2
10	L1	72	MEN	CA-CB-CG-ND2
2	V1	72	MEN	CA-CB-CG-ND2
2	k1	72	MEN	CA-CB-CG-ND2
2	T4	72	MEN	CA-CB-CG-ND2
2	k4	72	MEN	CA-CB-CG-ND2
2	m4	72	MEN	CA-CB-CG-ND2
2	F5	72	MEN	CA-CB-CG-ND2
2	H5	72	MEN	CA-CB-CG-ND2
2	J5	72	MEN	CA-CB-CG-ND2
2	S5	72	MEN	CA-CB-CG-ND2
2	W5	72	MEN	CA-CB-CG-ND2
2	F7	72	MEN	CA-CB-CG-ND2
2	aE	72	MEN	CA-CB-CG-ND2
2	tF	72	MEN	CA-CB-CG-ND2
2	aG	72	MEN	CA-CB-CG-ND2
2	kH	72	MEN	CA-CB-CG-ND2
2	mJ	72	MEN	CA-CB-CG-ND2
2	tK	72	MEN	CA-CB-CG-ND2
2	cM	72	MEN	CA-CB-CG-ND2
2	gM	72	MEN	CA-CB-CG-ND2
2	kM	72	MEN	CA-CB-CG-ND2
2	kO	72	MEN	CA-CB-CG-ND2
2	mO	72	MEN	CA-CB-CG-ND2
2	BB	72	MEN	OD1-CG-ND2-CE2
2	DB	72	MEN	OD1-CG-ND2-CE2
2	OB	72	MEN	OD1-CG-ND2-CE2
2	VB	72	MEN	OD1-CG-ND2-CE2
2	XB	72	MEN	OD1-CG-ND2-CE2
2	YB	72	MEN	OD1-CG-ND2-CE2
69	B3	71	MEN	OD1-CG-ND2-CE2
69	D3	71	MEN	OD1-CG-ND2-CE2
69	F3	71	MEN	OD1-CG-ND2-CE2
69	H3	71	MEN	OD1-CG-ND2-CE2
69	I3	71	MEN	OD1-CG-ND2-CE2
69	L3	71	MEN	OD1-CG-ND2-CE2
69	M3	71	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
69	d3	71	MEN	OD1-CG-ND2-CE2
69	f3	71	MEN	OD1-CG-ND2-CE2
69	h3	71	MEN	OD1-CG-ND2-CE2
69	j3	71	MEN	OD1-CG-ND2-CE2
69	k3	71	MEN	OD1-CG-ND2-CE2
69	n3	71	MEN	OD1-CG-ND2-CE2
69	o3	71	MEN	OD1-CG-ND2-CE2
69	q3	71	MEN	OD1-CG-ND2-CE2
2	dB	72	MEN	OD1-CG-ND2-CE2
2	FA	72	MEN	N-CA-CB-CG
2	PA	72	MEN	N-CA-CB-CG
2	RA	72	MEN	N-CA-CB-CG
2	TA	72	MEN	N-CA-CB-CG
2	VA	72	MEN	N-CA-CB-CG
2	CB	72	MEN	N-CA-CB-CG
2	DB	72	MEN	N-CA-CB-CG
2	FB	72	MEN	N-CA-CB-CG
2	GB	72	MEN	N-CA-CB-CG
2	HB	72	MEN	N-CA-CB-CG
2	LB	72	MEN	N-CA-CB-CG
2	MB	72	MEN	N-CA-CB-CG
2	PB	72	MEN	N-CA-CB-CG
2	QB	72	MEN	N-CA-CB-CG
2	SB	72	MEN	N-CA-CB-CG
2	VB	72	MEN	N-CA-CB-CG
2	XB	72	MEN	N-CA-CB-CG
2	YB	72	MEN	N-CA-CB-CG
2	ZB	72	MEN	N-CA-CB-CG
2	CD	72	MEN	N-CA-CB-CG
2	GD	72	MEN	N-CA-CB-CG
2	KD	72	MEN	N-CA-CB-CG
2	MD	72	MEN	N-CA-CB-CG
2	SD	72	MEN	N-CA-CB-CG
2	WD	72	MEN	N-CA-CB-CG
10	DE	72	MEN	N-CA-CB-CG
2	RE	72	MEN	N-CA-CB-CG
2	ZF	72	MEN	N-CA-CB-CG
10	DG	72	MEN	N-CA-CB-CG
10	HG	72	MEN	N-CA-CB-CG
2	RG	72	MEN	N-CA-CB-CG
10	DH	72	MEN	N-CA-CB-CG
2	PH	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	RH	72	MEN	N-CA-CB-CG
2	VH	72	MEN	N-CA-CB-CG
2	BI	72	MEN	N-CA-CB-CG
2	DI	72	MEN	N-CA-CB-CG
2	FI	72	MEN	N-CA-CB-CG
2	HI	72	MEN	N-CA-CB-CG
2	JI	72	MEN	N-CA-CB-CG
2	LI	72	MEN	N-CA-CB-CG
2	OI	72	MEN	N-CA-CB-CG
2	QI	72	MEN	N-CA-CB-CG
2	SI	72	MEN	N-CA-CB-CG
2	WI	72	MEN	N-CA-CB-CG
2	YI	72	MEN	N-CA-CB-CG
2	DJ	72	MEN	N-CA-CB-CG
2	HJ	72	MEN	N-CA-CB-CG
2	LJ	72	MEN	N-CA-CB-CG
2	NJ	72	MEN	N-CA-CB-CG
2	RJ	72	MEN	N-CA-CB-CG
2	TJ	72	MEN	N-CA-CB-CG
2	VJ	72	MEN	N-CA-CB-CG
2	XJ	72	MEN	N-CA-CB-CG
2	ZJ	72	MEN	N-CA-CB-CG
2	ZK	72	MEN	N-CA-CB-CG
2	DM	72	MEN	N-CA-CB-CG
2	FM	72	MEN	N-CA-CB-CG
2	HM	72	MEN	N-CA-CB-CG
2	JM	72	MEN	N-CA-CB-CG
2	LM	72	MEN	N-CA-CB-CG
2	NM	72	MEN	N-CA-CB-CG
2	TM	72	MEN	N-CA-CB-CG
2	VM	72	MEN	N-CA-CB-CG
2	XM	72	MEN	N-CA-CB-CG
2	ZM	72	MEN	N-CA-CB-CG
2	YO	72	MEN	N-CA-CB-CG
2	BP	72	MEN	N-CA-CB-CG
2	DP	72	MEN	N-CA-CB-CG
2	HP	72	MEN	N-CA-CB-CG
2	JP	72	MEN	N-CA-CB-CG
2	LP	72	MEN	N-CA-CB-CG
2	NP	72	MEN	N-CA-CB-CG
2	PP	72	MEN	N-CA-CB-CG
2	TP	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	VP	72	MEN	N-CA-CB-CG
2	XP	72	MEN	N-CA-CB-CG
2	CQ	72	MEN	N-CA-CB-CG
2	GQ	72	MEN	N-CA-CB-CG
2	KQ	72	MEN	N-CA-CB-CG
2	MQ	72	MEN	N-CA-CB-CG
2	SQ	72	MEN	N-CA-CB-CG
2	WQ	72	MEN	N-CA-CB-CG
2	P1	72	MEN	N-CA-CB-CG
2	R1	72	MEN	N-CA-CB-CG
10	D1	72	MEN	N-CA-CB-CG
2	V1	72	MEN	N-CA-CB-CG
2	i1	72	MEN	N-CA-CB-CG
2	c1	72	MEN	N-CA-CB-CG
69	Q3	71	MEN	N-CA-CB-CG
69	S3	71	MEN	N-CA-CB-CG
69	U3	71	MEN	N-CA-CB-CG
69	s3	71	MEN	N-CA-CB-CG
69	u3	71	MEN	N-CA-CB-CG
69	w3	71	MEN	N-CA-CB-CG
2	Y4	72	MEN	N-CA-CB-CG
2	i4	72	MEN	N-CA-CB-CG
2	k4	72	MEN	N-CA-CB-CG
2	g4	72	MEN	N-CA-CB-CG
2	F5	72	MEN	N-CA-CB-CG
2	H5	72	MEN	N-CA-CB-CG
2	J5	72	MEN	N-CA-CB-CG
2	L5	72	MEN	N-CA-CB-CG
2	O5	72	MEN	N-CA-CB-CG
2	Q5	72	MEN	N-CA-CB-CG
2	U5	72	MEN	N-CA-CB-CG
2	W5	72	MEN	N-CA-CB-CG
2	Y5	72	MEN	N-CA-CB-CG
2	F7	72	MEN	N-CA-CB-CG
2	P7	72	MEN	N-CA-CB-CG
2	R7	72	MEN	N-CA-CB-CG
2	T7	72	MEN	N-CA-CB-CG
2	V7	72	MEN	N-CA-CB-CG
2	18	72	MEN	N-CA-CB-CG
2	O9	72	MEN	N-CA-CB-CG
2	aB	72	MEN	N-CA-CB-CG
2	dB	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	eB	72	MEN	N-CA-CB-CG
2	gB	72	MEN	N-CA-CB-CG
2	1C	72	MEN	N-CA-CB-CG
2	aE	72	MEN	N-CA-CB-CG
2	kE	72	MEN	N-CA-CB-CG
2	lF	72	MEN	N-CA-CB-CG
2	tF	72	MEN	N-CA-CB-CG
2	aG	72	MEN	N-CA-CB-CG
2	kG	72	MEN	N-CA-CB-CG
2	iH	72	MEN	N-CA-CB-CG
2	cH	72	MEN	N-CA-CB-CG
2	cJ	72	MEN	N-CA-CB-CG
2	eJ	72	MEN	N-CA-CB-CG
2	iJ	72	MEN	N-CA-CB-CG
2	kJ	72	MEN	N-CA-CB-CG
2	mJ	72	MEN	N-CA-CB-CG
2	lK	72	MEN	N-CA-CB-CG
2	tK	72	MEN	N-CA-CB-CG
2	cM	72	MEN	N-CA-CB-CG
2	eM	72	MEN	N-CA-CB-CG
2	gM	72	MEN	N-CA-CB-CG
2	iM	72	MEN	N-CA-CB-CG
2	kM	72	MEN	N-CA-CB-CG
2	mM	72	MEN	N-CA-CB-CG
2	iO	72	MEN	N-CA-CB-CG
2	kO	72	MEN	N-CA-CB-CG
2	gO	72	MEN	N-CA-CB-CG
10	LH	72	MEN	CA-CB-CG-OD1
2	PJ	72	MEN	CA-CB-CG-OD1
2	PM	72	MEN	CA-CB-CG-OD1
2	TO	72	MEN	CA-CB-CG-OD1
10	L1	72	MEN	CA-CB-CG-OD1
2	k4	72	MEN	CA-CB-CG-OD1
2	tF	72	MEN	CA-CB-CG-OD1
2	tK	72	MEN	CA-CB-CG-OD1
2	kM	72	MEN	CA-CB-CG-OD1
2	kO	72	MEN	CA-CB-CG-OD1
2	PA	72	MEN	CA-CB-CG-ND2
2	PH	72	MEN	CA-CB-CG-ND2
2	P1	72	MEN	CA-CB-CG-ND2
2	D5	72	MEN	CA-CB-CG-ND2
2	O5	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	P7	72	MEN	CA-CB-CG-ND2
2	rF	72	MEN	CA-CB-CG-ND2
2	rK	72	MEN	CA-CB-CG-ND2
2	mM	72	MEN	CA-CB-CG-ND2
2	GB	72	MEN	OD1-CG-ND2-CE2
2	QB	72	MEN	OD1-CG-ND2-CE2
2	ZB	72	MEN	OD1-CG-ND2-CE2
69	Q3	71	MEN	OD1-CG-ND2-CE2
69	S3	71	MEN	OD1-CG-ND2-CE2
69	U3	71	MEN	OD1-CG-ND2-CE2
69	s3	71	MEN	OD1-CG-ND2-CE2
69	u3	71	MEN	OD1-CG-ND2-CE2
69	w3	71	MEN	OD1-CG-ND2-CE2
2	bB	72	MEN	OD1-CG-ND2-CE2
2	PA	72	MEN	CA-CB-CG-OD1
2	RA	72	MEN	CA-CB-CG-OD1
2	PB	72	MEN	CA-CB-CG-OD1
2	GD	72	MEN	CA-CB-CG-OD1
10	LE	72	MEN	CA-CB-CG-OD1
2	PE	72	MEN	CA-CB-CG-OD1
2	TE	72	MEN	CA-CB-CG-OD1
2	BF	72	MEN	CA-CB-CG-OD1
2	JF	72	MEN	CA-CB-CG-OD1
2	LF	72	MEN	CA-CB-CG-OD1
2	NF	72	MEN	CA-CB-CG-OD1
2	RF	72	MEN	CA-CB-CG-OD1
2	XF	72	MEN	CA-CB-CG-OD1
10	LG	72	MEN	CA-CB-CG-OD1
2	PG	72	MEN	CA-CB-CG-OD1
2	TG	72	MEN	CA-CB-CG-OD1
10	DH	72	MEN	CA-CB-CG-OD1
10	FH	72	MEN	CA-CB-CG-OD1
10	NH	72	MEN	CA-CB-CG-OD1
2	PH	72	MEN	CA-CB-CG-OD1
2	BI	72	MEN	CA-CB-CG-OD1
2	FI	72	MEN	CA-CB-CG-OD1
2	HI	72	MEN	CA-CB-CG-OD1
2	OI	72	MEN	CA-CB-CG-OD1
2	QI	72	MEN	CA-CB-CG-OD1
2	SI	72	MEN	CA-CB-CG-OD1
2	FJ	72	MEN	CA-CB-CG-OD1
2	BK	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	JK	72	MEN	CA-CB-CG-OD1
2	NK	72	MEN	CA-CB-CG-OD1
2	RK	72	MEN	CA-CB-CG-OD1
2	XK	72	MEN	CA-CB-CG-OD1
2	FM	72	MEN	CA-CB-CG-OD1
2	LM	72	MEN	CA-CB-CG-OD1
2	VM	72	MEN	CA-CB-CG-OD1
10	DO	72	MEN	CA-CB-CG-OD1
10	HO	72	MEN	CA-CB-CG-OD1
2	RO	72	MEN	CA-CB-CG-OD1
2	BP	72	MEN	CA-CB-CG-OD1
2	RP	72	MEN	CA-CB-CG-OD1
2	GQ	72	MEN	CA-CB-CG-OD1
10	N1	72	MEN	CA-CB-CG-OD1
2	P1	72	MEN	CA-CB-CG-OD1
10	D1	72	MEN	CA-CB-CG-OD1
10	F1	72	MEN	CA-CB-CG-OD1
10	H4	72	MEN	CA-CB-CG-OD1
10	D4	72	MEN	CA-CB-CG-OD1
2	R4	72	MEN	CA-CB-CG-OD1
2	T4	72	MEN	CA-CB-CG-OD1
2	D5	72	MEN	CA-CB-CG-OD1
2	L5	72	MEN	CA-CB-CG-OD1
2	O5	72	MEN	CA-CB-CG-OD1
2	P7	72	MEN	CA-CB-CG-OD1
2	R7	72	MEN	CA-CB-CG-OD1
2	F9	72	MEN	CA-CB-CG-OD1
2	H9	72	MEN	CA-CB-CG-OD1
2	J9	72	MEN	CA-CB-CG-OD1
2	S9	72	MEN	CA-CB-CG-OD1
2	Y9	72	MEN	CA-CB-CG-OD1
2	gB	72	MEN	CA-CB-CG-OD1
2	bF	72	MEN	CA-CB-CG-OD1
2	dF	72	MEN	CA-CB-CG-OD1
2	rF	72	MEN	CA-CB-CG-OD1
2	eJ	72	MEN	CA-CB-CG-OD1
2	kJ	72	MEN	CA-CB-CG-OD1
2	mJ	72	MEN	CA-CB-CG-OD1
2	bK	72	MEN	CA-CB-CG-OD1
2	dK	72	MEN	CA-CB-CG-OD1
2	rK	72	MEN	CA-CB-CG-OD1
2	cM	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	gM	72	MEN	CA-CB-CG-OD1
2	mM	72	MEN	CA-CB-CG-OD1
2	BA	72	MEN	CA-CB-CG-ND2
2	HA	72	MEN	CA-CB-CG-ND2
2	RA	72	MEN	CA-CB-CG-ND2
2	VA	72	MEN	CA-CB-CG-ND2
2	XA	72	MEN	CA-CB-CG-ND2
2	PB	72	MEN	CA-CB-CG-ND2
2	ZB	72	MEN	CA-CB-CG-ND2
2	ED	72	MEN	CA-CB-CG-ND2
2	GD	72	MEN	CA-CB-CG-ND2
2	KD	72	MEN	CA-CB-CG-ND2
2	UD	72	MEN	CA-CB-CG-ND2
2	WD	72	MEN	CA-CB-CG-ND2
10	DE	72	MEN	CA-CB-CG-ND2
10	NE	72	MEN	CA-CB-CG-ND2
2	FF	72	MEN	CA-CB-CG-ND2
2	JF	72	MEN	CA-CB-CG-ND2
2	NF	72	MEN	CA-CB-CG-ND2
2	ZF	72	MEN	CA-CB-CG-ND2
10	DG	72	MEN	CA-CB-CG-ND2
10	NG	72	MEN	CA-CB-CG-ND2
10	DH	72	MEN	CA-CB-CG-ND2
10	FH	72	MEN	CA-CB-CG-ND2
10	NH	72	MEN	CA-CB-CG-ND2
2	TH	72	MEN	CA-CB-CG-ND2
2	FI	72	MEN	CA-CB-CG-ND2
2	JI	72	MEN	CA-CB-CG-ND2
2	QI	72	MEN	CA-CB-CG-ND2
2	UI	72	MEN	CA-CB-CG-ND2
2	WI	72	MEN	CA-CB-CG-ND2
2	HJ	72	MEN	CA-CB-CG-ND2
2	NJ	72	MEN	CA-CB-CG-ND2
2	RJ	72	MEN	CA-CB-CG-ND2
2	FK	72	MEN	CA-CB-CG-ND2
2	JK	72	MEN	CA-CB-CG-ND2
2	NK	72	MEN	CA-CB-CG-ND2
2	ZK	72	MEN	CA-CB-CG-ND2
2	DM	72	MEN	CA-CB-CG-ND2
2	FM	72	MEN	CA-CB-CG-ND2
2	LM	72	MEN	CA-CB-CG-ND2
2	RM	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	VM	72	MEN	CA-CB-CG-ND2
2	ZM	72	MEN	CA-CB-CG-ND2
10	DO	72	MEN	CA-CB-CG-ND2
2	RO	72	MEN	CA-CB-CG-ND2
2	BP	72	MEN	CA-CB-CG-ND2
2	DP	72	MEN	CA-CB-CG-ND2
2	FP	72	MEN	CA-CB-CG-ND2
2	HP	72	MEN	CA-CB-CG-ND2
2	JP	72	MEN	CA-CB-CG-ND2
2	LP	72	MEN	CA-CB-CG-ND2
2	PP	72	MEN	CA-CB-CG-ND2
2	TP	72	MEN	CA-CB-CG-ND2
2	VP	72	MEN	CA-CB-CG-ND2
2	XP	72	MEN	CA-CB-CG-ND2
2	EQ	72	MEN	CA-CB-CG-ND2
2	GQ	72	MEN	CA-CB-CG-ND2
2	KQ	72	MEN	CA-CB-CG-ND2
2	UQ	72	MEN	CA-CB-CG-ND2
2	WQ	72	MEN	CA-CB-CG-ND2
10	N1	72	MEN	CA-CB-CG-ND2
2	T1	72	MEN	CA-CB-CG-ND2
10	D1	72	MEN	CA-CB-CG-ND2
10	F1	72	MEN	CA-CB-CG-ND2
2	Y1	72	MEN	CA-CB-CG-ND2
2	m1	72	MEN	CA-CB-CG-ND2
2	c1	72	MEN	CA-CB-CG-ND2
69	O3	71	MEN	CA-CB-CG-ND2
10	D4	72	MEN	CA-CB-CG-ND2
2	R4	72	MEN	CA-CB-CG-ND2
2	i4	72	MEN	CA-CB-CG-ND2
2	c4	72	MEN	CA-CB-CG-ND2
2	L5	72	MEN	CA-CB-CG-ND2
2	Q5	72	MEN	CA-CB-CG-ND2
2	U5	72	MEN	CA-CB-CG-ND2
2	Y5	72	MEN	CA-CB-CG-ND2
2	B7	72	MEN	CA-CB-CG-ND2
2	H7	72	MEN	CA-CB-CG-ND2
2	R7	72	MEN	CA-CB-CG-ND2
2	V7	72	MEN	CA-CB-CG-ND2
2	X7	72	MEN	CA-CB-CG-ND2
2	B9	72	MEN	CA-CB-CG-ND2
2	D9	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	F9	72	MEN	CA-CB-CG-ND2
2	H9	72	MEN	CA-CB-CG-ND2
2	Q9	72	MEN	CA-CB-CG-ND2
2	S9	72	MEN	CA-CB-CG-ND2
2	U9	72	MEN	CA-CB-CG-ND2
2	W9	72	MEN	CA-CB-CG-ND2
2	gE	72	MEN	CA-CB-CG-ND2
2	mE	72	MEN	CA-CB-CG-ND2
2	bF	72	MEN	CA-CB-CG-ND2
2	dF	72	MEN	CA-CB-CG-ND2
2	fF	72	MEN	CA-CB-CG-ND2
2	lF	72	MEN	CA-CB-CG-ND2
2	gG	72	MEN	CA-CB-CG-ND2
2	mG	72	MEN	CA-CB-CG-ND2
2	mH	72	MEN	CA-CB-CG-ND2
2	cH	72	MEN	CA-CB-CG-ND2
2	cJ	72	MEN	CA-CB-CG-ND2
2	eJ	72	MEN	CA-CB-CG-ND2
2	kJ	72	MEN	CA-CB-CG-ND2
2	dK	72	MEN	CA-CB-CG-ND2
2	fK	72	MEN	CA-CB-CG-ND2
2	lK	72	MEN	CA-CB-CG-ND2
2	eM	72	MEN	CA-CB-CG-ND2
2	iO	72	MEN	CA-CB-CG-ND2
2	cO	72	MEN	CA-CB-CG-ND2
2	HA	72	MEN	N-CA-CB-CG
2	RB	72	MEN	N-CA-CB-CG
10	HE	72	MEN	N-CA-CB-CG
2	RM	72	MEN	N-CA-CB-CG
10	NO	72	MEN	N-CA-CB-CG
2	m1	72	MEN	N-CA-CB-CG
69	B3	71	MEN	N-CA-CB-CG
69	D3	71	MEN	N-CA-CB-CG
69	F3	71	MEN	N-CA-CB-CG
69	H3	71	MEN	N-CA-CB-CG
69	I3	71	MEN	N-CA-CB-CG
69	L3	71	MEN	N-CA-CB-CG
69	M3	71	MEN	N-CA-CB-CG
69	d3	71	MEN	N-CA-CB-CG
69	f3	71	MEN	N-CA-CB-CG
69	h3	71	MEN	N-CA-CB-CG
69	j3	71	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
69	k3	71	MEN	N-CA-CB-CG
69	n3	71	MEN	N-CA-CB-CG
69	o3	71	MEN	N-CA-CB-CG
69	q3	71	MEN	N-CA-CB-CG
10	N4	72	MEN	N-CA-CB-CG
2	H7	72	MEN	N-CA-CB-CG
2	bB	72	MEN	N-CA-CB-CG
2	jF	72	MEN	N-CA-CB-CG
2	mH	72	MEN	N-CA-CB-CG
2	jK	72	MEN	N-CA-CB-CG
2	BA	72	MEN	CA-CB-CG-OD1
2	HA	72	MEN	CA-CB-CG-OD1
2	VA	72	MEN	CA-CB-CG-OD1
2	ED	72	MEN	CA-CB-CG-OD1
2	KD	72	MEN	CA-CB-CG-OD1
2	UD	72	MEN	CA-CB-CG-OD1
10	DE	72	MEN	CA-CB-CG-OD1
10	JE	72	MEN	CA-CB-CG-OD1
10	NE	72	MEN	CA-CB-CG-OD1
2	YE	72	MEN	CA-CB-CG-OD1
2	FF	72	MEN	CA-CB-CG-OD1
2	HF	72	MEN	CA-CB-CG-OD1
2	PF	72	MEN	CA-CB-CG-OD1
2	ZF	72	MEN	CA-CB-CG-OD1
10	DG	72	MEN	CA-CB-CG-OD1
10	JG	72	MEN	CA-CB-CG-OD1
10	NG	72	MEN	CA-CB-CG-OD1
2	YG	72	MEN	CA-CB-CG-OD1
2	TH	72	MEN	CA-CB-CG-OD1
2	YH	72	MEN	CA-CB-CG-OD1
2	DI	72	MEN	CA-CB-CG-OD1
2	JI	72	MEN	CA-CB-CG-OD1
2	UI	72	MEN	CA-CB-CG-OD1
2	WI	72	MEN	CA-CB-CG-OD1
2	HJ	72	MEN	CA-CB-CG-OD1
2	NJ	72	MEN	CA-CB-CG-OD1
2	RJ	72	MEN	CA-CB-CG-OD1
2	VJ	72	MEN	CA-CB-CG-OD1
2	XJ	72	MEN	CA-CB-CG-OD1
2	ZJ	72	MEN	CA-CB-CG-OD1
2	FK	72	MEN	CA-CB-CG-OD1
2	HK	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	LK	72	MEN	CA-CB-CG-OD1
2	PK	72	MEN	CA-CB-CG-OD1
2	ZK	72	MEN	CA-CB-CG-OD1
2	DM	72	MEN	CA-CB-CG-OD1
2	RM	72	MEN	CA-CB-CG-OD1
2	ZM	72	MEN	CA-CB-CG-OD1
2	VO	72	MEN	CA-CB-CG-OD1
2	DP	72	MEN	CA-CB-CG-OD1
2	HP	72	MEN	CA-CB-CG-OD1
2	JP	72	MEN	CA-CB-CG-OD1
2	LP	72	MEN	CA-CB-CG-OD1
2	PP	72	MEN	CA-CB-CG-OD1
2	TP	72	MEN	CA-CB-CG-OD1
2	XP	72	MEN	CA-CB-CG-OD1
2	EQ	72	MEN	CA-CB-CG-OD1
2	KQ	72	MEN	CA-CB-CG-OD1
2	UQ	72	MEN	CA-CB-CG-OD1
2	T1	72	MEN	CA-CB-CG-OD1
2	Y1	72	MEN	CA-CB-CG-OD1
2	m1	72	MEN	CA-CB-CG-OD1
2	a1	72	MEN	CA-CB-CG-OD1
2	c1	72	MEN	CA-CB-CG-OD1
69	O3	71	MEN	CA-CB-CG-OD1
2	V4	72	MEN	CA-CB-CG-OD1
2	i4	72	MEN	CA-CB-CG-OD1
2	a4	72	MEN	CA-CB-CG-OD1
2	c4	72	MEN	CA-CB-CG-OD1
2	g4	72	MEN	CA-CB-CG-OD1
2	Q5	72	MEN	CA-CB-CG-OD1
2	U5	72	MEN	CA-CB-CG-OD1
2	B7	72	MEN	CA-CB-CG-OD1
2	H7	72	MEN	CA-CB-CG-OD1
2	V7	72	MEN	CA-CB-CG-OD1
2	y8	72	MEN	CA-CB-CG-OD1
2	s8	72	MEN	CA-CB-CG-OD1
2	B9	72	MEN	CA-CB-CG-OD1
2	D9	72	MEN	CA-CB-CG-OD1
2	L9	72	MEN	CA-CB-CG-OD1
2	Q9	72	MEN	CA-CB-CG-OD1
2	U9	72	MEN	CA-CB-CG-OD1
2	W9	72	MEN	CA-CB-CG-OD1
2	yC	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	sC	72	MEN	CA-CB-CG-OD1
2	cE	72	MEN	CA-CB-CG-OD1
2	gE	72	MEN	CA-CB-CG-OD1
2	kE	72	MEN	CA-CB-CG-OD1
2	mE	72	MEN	CA-CB-CG-OD1
2	fF	72	MEN	CA-CB-CG-OD1
2	jF	72	MEN	CA-CB-CG-OD1
2	pF	72	MEN	CA-CB-CG-OD1
2	cG	72	MEN	CA-CB-CG-OD1
2	gG	72	MEN	CA-CB-CG-OD1
2	kG	72	MEN	CA-CB-CG-OD1
2	mG	72	MEN	CA-CB-CG-OD1
2	mH	72	MEN	CA-CB-CG-OD1
2	aH	72	MEN	CA-CB-CG-OD1
2	cH	72	MEN	CA-CB-CG-OD1
2	cJ	72	MEN	CA-CB-CG-OD1
2	fK	72	MEN	CA-CB-CG-OD1
2	jK	72	MEN	CA-CB-CG-OD1
2	pK	72	MEN	CA-CB-CG-OD1
2	iO	72	MEN	CA-CB-CG-OD1
2	aO	72	MEN	CA-CB-CG-OD1
2	cO	72	MEN	CA-CB-CG-OD1
2	gO	72	MEN	CA-CB-CG-OD1
2	LA	72	MEN	CA-CB-CG-ND2
10	LE	72	MEN	CA-CB-CG-ND2
2	PE	72	MEN	CA-CB-CG-ND2
2	TE	72	MEN	CA-CB-CG-ND2
2	YE	72	MEN	CA-CB-CG-ND2
2	BF	72	MEN	CA-CB-CG-ND2
2	LF	72	MEN	CA-CB-CG-ND2
2	RF	72	MEN	CA-CB-CG-ND2
2	VF	72	MEN	CA-CB-CG-ND2
10	LG	72	MEN	CA-CB-CG-ND2
2	PG	72	MEN	CA-CB-CG-ND2
2	TG	72	MEN	CA-CB-CG-ND2
2	YG	72	MEN	CA-CB-CG-ND2
10	HH	72	MEN	CA-CB-CG-ND2
2	YH	72	MEN	CA-CB-CG-ND2
2	HI	72	MEN	CA-CB-CG-ND2
2	SI	72	MEN	CA-CB-CG-ND2
2	VJ	72	MEN	CA-CB-CG-ND2
2	XJ	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	BK	72	MEN	CA-CB-CG-ND2
2	LK	72	MEN	CA-CB-CG-ND2
2	RK	72	MEN	CA-CB-CG-ND2
2	VK	72	MEN	CA-CB-CG-ND2
10	HO	72	MEN	CA-CB-CG-ND2
10	JO	72	MEN	CA-CB-CG-ND2
2	NP	72	MEN	CA-CB-CG-ND2
2	RP	72	MEN	CA-CB-CG-ND2
10	H1	72	MEN	CA-CB-CG-ND2
2	a1	72	MEN	CA-CB-CG-ND2
10	H4	72	MEN	CA-CB-CG-ND2
10	J4	72	MEN	CA-CB-CG-ND2
2	18	72	MEN	CA-CB-CG-ND2
2	J9	72	MEN	CA-CB-CG-ND2
2	L9	72	MEN	CA-CB-CG-ND2
2	Y9	72	MEN	CA-CB-CG-ND2
2	1C	72	MEN	CA-CB-CG-ND2
2	kE	72	MEN	CA-CB-CG-ND2
2	hF	72	MEN	CA-CB-CG-ND2
2	pF	72	MEN	CA-CB-CG-ND2
2	kG	72	MEN	CA-CB-CG-ND2
2	aH	72	MEN	CA-CB-CG-ND2
2	bK	72	MEN	CA-CB-CG-ND2
2	hK	72	MEN	CA-CB-CG-ND2
2	pK	72	MEN	CA-CB-CG-ND2
2	BA	72	MEN	C-CA-CB-CG
2	HA	72	MEN	C-CA-CB-CG
2	XA	72	MEN	C-CA-CB-CG
2	DB	72	MEN	C-CA-CB-CG
2	LB	72	MEN	C-CA-CB-CG
2	RB	72	MEN	C-CA-CB-CG
2	YB	72	MEN	C-CA-CB-CG
2	ID	72	MEN	C-CA-CB-CG
2	SD	72	MEN	C-CA-CB-CG
2	YD	72	MEN	C-CA-CB-CG
10	NE	72	MEN	C-CA-CB-CG
2	VE	72	MEN	C-CA-CB-CG
2	VF	72	MEN	C-CA-CB-CG
10	NG	72	MEN	C-CA-CB-CG
2	VG	72	MEN	C-CA-CB-CG
2	VH	72	MEN	C-CA-CB-CG
2	YH	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	PJ	72	MEN	C-CA-CB-CG
2	RJ	72	MEN	C-CA-CB-CG
2	VK	72	MEN	C-CA-CB-CG
2	HM	72	MEN	C-CA-CB-CG
2	PM	72	MEN	C-CA-CB-CG
10	LO	72	MEN	C-CA-CB-CG
2	RP	72	MEN	C-CA-CB-CG
2	IQ	72	MEN	C-CA-CB-CG
2	SQ	72	MEN	C-CA-CB-CG
2	YQ	72	MEN	C-CA-CB-CG
2	V1	72	MEN	C-CA-CB-CG
2	Y1	72	MEN	C-CA-CB-CG
2	k1	72	MEN	C-CA-CB-CG
2	a1	72	MEN	C-CA-CB-CG
69	Q3	71	MEN	C-CA-CB-CG
69	S3	71	MEN	C-CA-CB-CG
69	U3	71	MEN	C-CA-CB-CG
69	s3	71	MEN	C-CA-CB-CG
69	u3	71	MEN	C-CA-CB-CG
69	w3	71	MEN	C-CA-CB-CG
10	L4	72	MEN	C-CA-CB-CG
2	e4	72	MEN	C-CA-CB-CG
2	D5	72	MEN	C-CA-CB-CG
2	J5	72	MEN	C-CA-CB-CG
2	U5	72	MEN	C-CA-CB-CG
2	B7	72	MEN	C-CA-CB-CG
2	H7	72	MEN	C-CA-CB-CG
2	X7	72	MEN	C-CA-CB-CG
2	y8	72	MEN	C-CA-CB-CG
2	18	72	MEN	C-CA-CB-CG
2	q8	72	MEN	C-CA-CB-CG
2	u8	72	MEN	C-CA-CB-CG
2	w8	72	MEN	C-CA-CB-CG
2	yC	72	MEN	C-CA-CB-CG
2	1C	72	MEN	C-CA-CB-CG
2	qC	72	MEN	C-CA-CB-CG
2	uC	72	MEN	C-CA-CB-CG
2	wC	72	MEN	C-CA-CB-CG
2	gE	72	MEN	C-CA-CB-CG
2	iE	72	MEN	C-CA-CB-CG
2	lF	72	MEN	C-CA-CB-CG
2	gG	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	iG	72	MEN	C-CA-CB-CG
2	kH	72	MEN	C-CA-CB-CG
2	aH	72	MEN	C-CA-CB-CG
2	cJ	72	MEN	C-CA-CB-CG
2	lK	72	MEN	C-CA-CB-CG
2	cM	72	MEN	C-CA-CB-CG
2	eO	72	MEN	C-CA-CB-CG
2	DA	72	MEN	CA-CB-CG-OD1
2	ZB	72	MEN	CA-CB-CG-OD1
2	QD	72	MEN	CA-CB-CG-OD1
2	WD	72	MEN	CA-CB-CG-OD1
2	VF	72	MEN	CA-CB-CG-OD1
10	HG	72	MEN	CA-CB-CG-OD1
2	LJ	72	MEN	CA-CB-CG-OD1
2	VK	72	MEN	CA-CB-CG-OD1
2	FP	72	MEN	CA-CB-CG-OD1
2	VP	72	MEN	CA-CB-CG-OD1
2	QQ	72	MEN	CA-CB-CG-OD1
2	WQ	72	MEN	CA-CB-CG-OD1
2	e4	72	MEN	CA-CB-CG-OD1
2	B5	72	MEN	CA-CB-CG-OD1
2	Y5	72	MEN	CA-CB-CG-OD1
2	D7	72	MEN	CA-CB-CG-OD1
2	X7	72	MEN	CA-CB-CG-OD1
2	18	72	MEN	CA-CB-CG-OD1
2	O9	72	MEN	CA-CB-CG-OD1
2	1C	72	MEN	CA-CB-CG-OD1
2	lF	72	MEN	CA-CB-CG-OD1
2	lK	72	MEN	CA-CB-CG-OD1
2	eM	72	MEN	CA-CB-CG-OD1
2	eO	72	MEN	CA-CB-CG-OD1
2	DA	72	MEN	CA-CB-CG-ND2
2	NA	72	MEN	CA-CB-CG-ND2
2	GB	72	MEN	CA-CB-CG-ND2
2	CD	72	MEN	CA-CB-CG-ND2
2	ID	72	MEN	CA-CB-CG-ND2
2	QD	72	MEN	CA-CB-CG-ND2
10	HE	72	MEN	CA-CB-CG-ND2
10	JE	72	MEN	CA-CB-CG-ND2
2	DF	72	MEN	CA-CB-CG-ND2
2	HF	72	MEN	CA-CB-CG-ND2
2	PF	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	TF	72	MEN	CA-CB-CG-ND2
2	XF	72	MEN	CA-CB-CG-ND2
10	HG	72	MEN	CA-CB-CG-ND2
10	JG	72	MEN	CA-CB-CG-ND2
2	BI	72	MEN	CA-CB-CG-ND2
2	DI	72	MEN	CA-CB-CG-ND2
2	OI	72	MEN	CA-CB-CG-ND2
2	FJ	72	MEN	CA-CB-CG-ND2
2	LJ	72	MEN	CA-CB-CG-ND2
2	ZJ	72	MEN	CA-CB-CG-ND2
2	DK	72	MEN	CA-CB-CG-ND2
2	HK	72	MEN	CA-CB-CG-ND2
2	PK	72	MEN	CA-CB-CG-ND2
2	TK	72	MEN	CA-CB-CG-ND2
2	XK	72	MEN	CA-CB-CG-ND2
10	LO	72	MEN	CA-CB-CG-ND2
2	PO	72	MEN	CA-CB-CG-ND2
2	VO	72	MEN	CA-CB-CG-ND2
2	YO	72	MEN	CA-CB-CG-ND2
2	IQ	72	MEN	CA-CB-CG-ND2
2	QQ	72	MEN	CA-CB-CG-ND2
2	i1	72	MEN	CA-CB-CG-ND2
69	Q3	71	MEN	CA-CB-CG-ND2
69	S3	71	MEN	CA-CB-CG-ND2
69	U3	71	MEN	CA-CB-CG-ND2
69	s3	71	MEN	CA-CB-CG-ND2
69	u3	71	MEN	CA-CB-CG-ND2
69	w3	71	MEN	CA-CB-CG-ND2
10	L4	72	MEN	CA-CB-CG-ND2
2	P4	72	MEN	CA-CB-CG-ND2
2	V4	72	MEN	CA-CB-CG-ND2
2	Y4	72	MEN	CA-CB-CG-ND2
2	a4	72	MEN	CA-CB-CG-ND2
2	e4	72	MEN	CA-CB-CG-ND2
2	g4	72	MEN	CA-CB-CG-ND2
2	B5	72	MEN	CA-CB-CG-ND2
2	D7	72	MEN	CA-CB-CG-ND2
2	L7	72	MEN	CA-CB-CG-ND2
2	N7	72	MEN	CA-CB-CG-ND2
2	y8	72	MEN	CA-CB-CG-ND2
2	s8	72	MEN	CA-CB-CG-ND2
2	O9	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	aB	72	MEN	CA-CB-CG-ND2
2	gB	72	MEN	CA-CB-CG-ND2
2	yC	72	MEN	CA-CB-CG-ND2
2	sC	72	MEN	CA-CB-CG-ND2
2	cE	72	MEN	CA-CB-CG-ND2
2	jF	72	MEN	CA-CB-CG-ND2
2	cG	72	MEN	CA-CB-CG-ND2
2	iH	72	MEN	CA-CB-CG-ND2
2	jK	72	MEN	CA-CB-CG-ND2
2	aO	72	MEN	CA-CB-CG-ND2
2	eO	72	MEN	CA-CB-CG-ND2
2	gO	72	MEN	CA-CB-CG-ND2
2	LA	72	MEN	N-CA-CB-CG
2	NA	72	MEN	N-CA-CB-CG
10	LE	72	MEN	N-CA-CB-CG
10	NE	72	MEN	N-CA-CB-CG
2	VE	72	MEN	N-CA-CB-CG
2	YE	72	MEN	N-CA-CB-CG
10	LG	72	MEN	N-CA-CB-CG
10	NG	72	MEN	N-CA-CB-CG
2	VG	72	MEN	N-CA-CB-CG
2	YG	72	MEN	N-CA-CB-CG
2	PJ	72	MEN	N-CA-CB-CG
10	LO	72	MEN	N-CA-CB-CG
2	PO	72	MEN	N-CA-CB-CG
2	RO	72	MEN	N-CA-CB-CG
2	FP	72	MEN	N-CA-CB-CG
10	L4	72	MEN	N-CA-CB-CG
2	P4	72	MEN	N-CA-CB-CG
2	R4	72	MEN	N-CA-CB-CG
2	m4	72	MEN	N-CA-CB-CG
2	e4	72	MEN	N-CA-CB-CG
2	D5	72	MEN	N-CA-CB-CG
2	L7	72	MEN	N-CA-CB-CG
2	N7	72	MEN	N-CA-CB-CG
2	gE	72	MEN	N-CA-CB-CG
2	gG	72	MEN	N-CA-CB-CG
2	gJ	72	MEN	N-CA-CB-CG
2	mO	72	MEN	N-CA-CB-CG
2	eO	72	MEN	N-CA-CB-CG
2	NA	72	MEN	CA-CB-CG-OD1
2	XA	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	GB	72	MEN	CA-CB-CG-OD1
2	ID	72	MEN	CA-CB-CG-OD1
10	HE	72	MEN	CA-CB-CG-OD1
2	DF	72	MEN	CA-CB-CG-OD1
2	TF	72	MEN	CA-CB-CG-OD1
2	DK	72	MEN	CA-CB-CG-OD1
2	TK	72	MEN	CA-CB-CG-OD1
10	JO	72	MEN	CA-CB-CG-OD1
10	LO	72	MEN	CA-CB-CG-OD1
2	YO	72	MEN	CA-CB-CG-OD1
2	NP	72	MEN	CA-CB-CG-OD1
2	IQ	72	MEN	CA-CB-CG-OD1
2	i1	72	MEN	CA-CB-CG-OD1
10	J4	72	MEN	CA-CB-CG-OD1
10	L4	72	MEN	CA-CB-CG-OD1
2	Y4	72	MEN	CA-CB-CG-OD1
2	N7	72	MEN	CA-CB-CG-OD1
2	aB	72	MEN	CA-CB-CG-OD1
2	hF	72	MEN	CA-CB-CG-OD1
2	iH	72	MEN	CA-CB-CG-OD1
2	hK	72	MEN	CA-CB-CG-OD1
2	CQ	72	MEN	CA-CB-CG-ND2
2	u8	72	MEN	CA-CB-CG-ND2
2	uC	72	MEN	CA-CB-CG-ND2
2	LA	72	MEN	CA-CB-CG-OD1
2	CD	72	MEN	CA-CB-CG-OD1
10	HH	72	MEN	CA-CB-CG-OD1
2	PO	72	MEN	CA-CB-CG-OD1
2	CQ	72	MEN	CA-CB-CG-OD1
10	H1	72	MEN	CA-CB-CG-OD1
2	P4	72	MEN	CA-CB-CG-OD1
2	L7	72	MEN	CA-CB-CG-OD1
2	u8	72	MEN	CA-CB-CG-OD1
2	uC	72	MEN	CA-CB-CG-OD1
2	XA	72	MEN	N-CA-CB-CG
2	ED	72	MEN	N-CA-CB-CG
2	ID	72	MEN	N-CA-CB-CG
2	UD	72	MEN	N-CA-CB-CG
10	FE	72	MEN	N-CA-CB-CG
2	TE	72	MEN	N-CA-CB-CG
2	VF	72	MEN	N-CA-CB-CG
10	FG	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	TG	72	MEN	N-CA-CB-CG
2	YH	72	MEN	N-CA-CB-CG
2	VK	72	MEN	N-CA-CB-CG
2	PM	72	MEN	N-CA-CB-CG
10	FO	72	MEN	N-CA-CB-CG
2	TO	72	MEN	N-CA-CB-CG
2	RP	72	MEN	N-CA-CB-CG
2	EQ	72	MEN	N-CA-CB-CG
2	IQ	72	MEN	N-CA-CB-CG
2	UQ	72	MEN	N-CA-CB-CG
2	Y1	72	MEN	N-CA-CB-CG
2	k1	72	MEN	N-CA-CB-CG
10	F4	72	MEN	N-CA-CB-CG
2	T4	72	MEN	N-CA-CB-CG
2	a4	72	MEN	N-CA-CB-CG
2	X7	72	MEN	N-CA-CB-CG
2	B9	72	MEN	N-CA-CB-CG
2	iE	72	MEN	N-CA-CB-CG
2	nF	72	MEN	N-CA-CB-CG
2	iG	72	MEN	N-CA-CB-CG
2	kH	72	MEN	N-CA-CB-CG
2	nK	72	MEN	N-CA-CB-CG
2	aO	72	MEN	N-CA-CB-CG
2	iJ	72	MEN	CA-CB-CG-OD1
2	JA	72	MEN	CA-CB-CG-OD1
2	RB	72	MEN	CA-CB-CG-OD1
2	LI	72	MEN	CA-CB-CG-OD1
2	e1	72	MEN	CA-CB-CG-OD1
2	J7	72	MEN	CA-CB-CG-OD1
2	nF	72	MEN	CA-CB-CG-OD1
2	eH	72	MEN	CA-CB-CG-OD1
2	nK	72	MEN	CA-CB-CG-OD1
2	iM	72	MEN	CA-CB-CG-OD1
2	TJ	72	MEN	CA-CB-CG-ND2
10	FO	72	MEN	CA-CB-CG-ND2
10	F4	72	MEN	CA-CB-CG-ND2
2	eE	72	MEN	CA-CB-CG-ND2
2	eG	72	MEN	CA-CB-CG-ND2
2	PE	72	MEN	N-CA-CB-CG
2	PG	72	MEN	N-CA-CB-CG
2	JJ	72	MEN	N-CA-CB-CG
2	JJ	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
10	NO	72	MEN	C-CA-CB-CG
2	m1	72	MEN	C-CA-CB-CG
69	B3	71	MEN	C-CA-CB-CG
69	D3	71	MEN	C-CA-CB-CG
69	F3	71	MEN	C-CA-CB-CG
69	H3	71	MEN	C-CA-CB-CG
69	I3	71	MEN	C-CA-CB-CG
69	L3	71	MEN	C-CA-CB-CG
69	M3	71	MEN	C-CA-CB-CG
69	d3	71	MEN	C-CA-CB-CG
69	f3	71	MEN	C-CA-CB-CG
69	h3	71	MEN	C-CA-CB-CG
69	j3	71	MEN	C-CA-CB-CG
69	k3	71	MEN	C-CA-CB-CG
69	n3	71	MEN	C-CA-CB-CG
69	o3	71	MEN	C-CA-CB-CG
69	q3	71	MEN	C-CA-CB-CG
10	N4	72	MEN	C-CA-CB-CG
2	B9	72	MEN	C-CA-CB-CG
2	bB	72	MEN	C-CA-CB-CG
2	mE	72	MEN	C-CA-CB-CG
2	mG	72	MEN	C-CA-CB-CG
2	mH	72	MEN	C-CA-CB-CG
2	gJ	72	MEN	C-CA-CB-CG
2	eB	72	MEN	OD1-CG-ND2-CE2
2	TA	72	MEN	CA-CB-CG-OD1
2	BB	72	MEN	CA-CB-CG-OD1
2	FB	72	MEN	CA-CB-CG-OD1
2	IB	72	MEN	CA-CB-CG-OD1
2	QB	72	MEN	CA-CB-CG-OD1
10	FE	72	MEN	CA-CB-CG-OD1
2	RE	72	MEN	CA-CB-CG-OD1
10	FG	72	MEN	CA-CB-CG-OD1
2	RG	72	MEN	CA-CB-CG-OD1
10	JH	72	MEN	CA-CB-CG-OD1
2	YI	72	MEN	CA-CB-CG-OD1
2	DJ	72	MEN	CA-CB-CG-OD1
2	JJ	72	MEN	CA-CB-CG-OD1
2	TJ	72	MEN	CA-CB-CG-OD1
2	HM	72	MEN	CA-CB-CG-OD1
2	NM	72	MEN	CA-CB-CG-OD1
2	XM	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
10	FO	72	MEN	CA-CB-CG-OD1
10	J1	72	MEN	CA-CB-CG-OD1
10	F4	72	MEN	CA-CB-CG-OD1
2	T7	72	MEN	CA-CB-CG-OD1
2	q8	72	MEN	CA-CB-CG-OD1
2	qC	72	MEN	CA-CB-CG-OD1
2	eE	72	MEN	CA-CB-CG-OD1
2	iE	72	MEN	CA-CB-CG-OD1
2	vF	72	MEN	CA-CB-CG-OD1
2	eG	72	MEN	CA-CB-CG-OD1
2	iG	72	MEN	CA-CB-CG-OD1
2	vK	72	MEN	CA-CB-CG-OD1
2	TA	72	MEN	CA-CB-CG-ND2
2	RB	72	MEN	CA-CB-CG-ND2
2	SB	72	MEN	CA-CB-CG-ND2
10	FE	72	MEN	CA-CB-CG-ND2
10	FG	72	MEN	CA-CB-CG-ND2
2	LI	72	MEN	CA-CB-CG-ND2
2	e1	72	MEN	CA-CB-CG-ND2
2	T7	72	MEN	CA-CB-CG-ND2
2	w8	72	MEN	CA-CB-CG-ND2
2	wC	72	MEN	CA-CB-CG-ND2
2	eH	72	MEN	CA-CB-CG-ND2
2	iJ	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2437 ligands modelled in this entry, 8 are monoatomic - leaving 2429 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PEB	rC	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.13	19 (35%)
82	PEB	F5	203	2	46,46,46	2.53	12 (26%)	54,67,67	2.10	19 (35%)
82	PEB	cK	203	1,2	46,46,46	2.60	14 (30%)	54,67,67	2.73	23 (42%)
87	CLA	42	608	60	54,58,73	1.42	10 (18%)	65,95,113	1.77	17 (26%)
87	CLA	I2	102	-	69,73,73	1.22	9 (13%)	83,113,113	1.37	6 (7%)
82	PEB	TH	202	2	46,46,46	2.63	11 (23%)	54,67,67	1.93	16 (29%)
87	CLA	8N	305	-	49,53,73	1.48	8 (16%)	59,89,113	1.52	7 (11%)
82	PEB	RK	202	2	46,46,46	2.66	14 (30%)	54,67,67	2.30	20 (37%)
87	CLA	BN	817	-	63,67,73	1.33	9 (14%)	75,105,113	1.41	11 (14%)
82	PEB	dO	201	1	46,46,46	2.55	11 (23%)	54,67,67	2.21	20 (37%)
87	CLA	BN	834	-	69,73,73	1.28	11 (15%)	83,113,113	1.36	11 (13%)
87	CLA	R2	201	87	49,53,73	1.51	7 (14%)	59,89,113	1.55	7 (11%)
82	PEB	WM	201	1	46,46,46	2.61	12 (26%)	54,67,67	2.18	18 (33%)
82	PEB	dG	202	1,2	46,46,46	2.57	10 (21%)	54,67,67	2.35	21 (38%)
82	PEB	j1	203	1,2	46,46,46	2.71	16 (34%)	54,67,67	2.43	19 (35%)
82	PEB	QD	202	2	46,46,46	2.74	15 (32%)	54,67,67	1.92	16 (29%)
87	CLA	AL	405	15	54,58,73	1.41	10 (18%)	65,95,113	1.61	11 (16%)
82	PEB	YH	202	2	46,46,46	2.72	12 (26%)	54,67,67	2.09	19 (35%)
87	CLA	6N	604	87,62	46,50,73	1.52	8 (17%)	55,85,113	1.45	5 (9%)
82	PEB	fG	202	1	46,46,46	2.66	15 (32%)	54,67,67	1.96	17 (31%)
82	PEB	g4	203	2	46,46,46	2.71	13 (28%)	54,67,67	2.02	15 (27%)
82	PEB	C7	202	1	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	WH	202	1	46,46,46	2.65	13 (28%)	54,67,67	2.33	22 (40%)
82	PEB	iK	201	1,2	46,46,46	2.60	12 (26%)	54,67,67	2.35	18 (33%)
87	CLA	BN	829	-	47,51,73	1.46	9 (19%)	56,86,113	1.57	4 (7%)
82	PEB	CJ	202	1	46,46,46	2.44	13 (28%)	54,67,67	2.09	16 (29%)
82	PEB	SP	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.18	22 (40%)
87	CLA	8N	301	64,103	50,54,73	1.57	12 (24%)	60,90,113	1.73	16 (26%)
84	CYC	H4	1001	10	46,46,46	2.37	17 (36%)	61,67,67	3.00	29 (47%)
82	PEB	z8	201	1	46,46,46	2.71	13 (28%)	54,67,67	2.23	26 (48%)
82	PEB	lM	201	1,2	46,46,46	2.54	13 (28%)	54,67,67	2.32	21 (38%)
87	CLA	2N	312	58	49,53,73	1.50	9 (18%)	59,89,113	1.66	9 (15%)
82	PEB	QF	203	1,2	46,46,46	2.71	14 (30%)	54,67,67	3.06	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	dL	401	18	69,73,73	1.25	10 (14%)	83,113,113	1.50	7 (8%)
97	GOL	i6	102	-	5,5,5	0.24	0	5,5,5	0.20	0
84	CYC	V3	1001	-	46,46,46	2.52	15 (32%)	61,67,67	3.07	32 (52%)
82	PEB	lJ	201	1,2	46,46,46	2.51	12 (26%)	54,67,67	2.45	22 (40%)
85	BCR	d6	405	-	41,41,41	0.80	0	56,56,56	2.02	17 (30%)
82	PEB	IM	201	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.42	20 (37%)
87	CLA	B2	804	41	69,73,73	1.29	10 (14%)	83,113,113	1.40	11 (13%)
82	PEB	FM	202	2	46,46,46	2.61	14 (30%)	54,67,67	2.20	19 (35%)
83	PUB	AJ	304	13	45,46,46	2.72	9 (20%)	46,67,67	3.11	23 (50%)
87	CLA	H6	103	22	69,73,73	1.25	10 (14%)	83,113,113	1.26	8 (9%)
87	CLA	1N	601	57	49,53,73	1.47	9 (18%)	59,89,113	1.58	6 (10%)
82	PEB	UM	203	1	46,46,46	2.57	13 (28%)	54,67,67	2.25	18 (33%)
82	PEB	J7	201	3,2	46,46,46	2.67	12 (26%)	54,67,67	2.14	16 (29%)
99	SF4	BN	804	-	0,12,12	-	-	-		
82	PEB	Q9	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.30	23 (42%)
82	PEB	NO	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.13	19 (35%)
82	PEB	GK	203	1	46,46,46	2.63	13 (28%)	54,67,67	2.45	25 (46%)
82	PEB	HG	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	2.00	16 (29%)
82	PEB	IA	202	1	46,46,46	2.69	13 (28%)	54,67,67	1.90	17 (31%)
87	CLA	BN	806	41	69,73,73	1.22	8 (11%)	83,113,113	1.41	9 (10%)
82	PEB	XQ	201	1,2	46,46,46	2.59	12 (26%)	54,67,67	2.36	19 (35%)
87	CLA	B2	835	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
82	PEB	WA	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	YE	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.29	21 (38%)
82	PEB	ID	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.18	21 (38%)
82	PEB	LD	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.28	19 (35%)
82	PEB	VK	202	2	46,46,46	2.67	14 (30%)	54,67,67	2.46	22 (40%)
82	PEB	OK	203	1	46,46,46	2.62	11 (23%)	54,67,67	2.08	20 (37%)
87	CLA	D6	403	-	69,73,73	1.24	10 (14%)	83,113,113	1.31	6 (7%)
100	3XQ	JN	104	-	24,24,24	0.20	0	25,25,25	0.23	0
82	PEB	wC	202	2	46,46,46	2.71	12 (26%)	54,67,67	2.41	17 (31%)
92	LMG	B6	619	16	39,39,55	1.03	2 (5%)	47,47,63	1.27	5 (10%)
84	CYC	T3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
95	DGD	D6	410	18,22	63,63,67	0.85	2 (3%)	77,77,81	1.10	4 (5%)
87	CLA	12	605	57	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	VF	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.46	23 (42%)
87	CLA	d6	406	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	8 (9%)
84	CYC	73	1002	73	46,46,46	2.46	18 (39%)	61,67,67	3.01	29 (47%)
87	CLA	12	606	-	49,53,73	1.47	8 (16%)	59,89,113	1.35	5 (8%)
82	PEB	sF	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.09	16 (29%)
82	PEB	PH	201	11,2	46,46,46	2.60	13 (28%)	54,67,67	2.20	19 (35%)
82	PEB	MB	201	2	46,46,46	2.53	11 (23%)	54,67,67	2.12	18 (33%)
82	PEB	RQ	202	1	46,46,46	2.69	13 (28%)	54,67,67	1.93	16 (29%)
87	CLA	62	307	87	49,53,73	1.50	9 (18%)	59,89,113	1.48	7 (11%)
95	DGD	J6	101	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	5 (6%)
82	PEB	aF	203	1	46,46,46	2.72	11 (23%)	54,67,67	2.27	21 (38%)
82	PEB	RO	201	11,2	46,46,46	2.64	13 (28%)	54,67,67	2.40	16 (29%)
82	PEB	QB	202	2,5	46,46,46	2.61	13 (28%)	54,67,67	2.05	16 (29%)
95	DGD	BL	607	-	41,41,67	1.05	2 (4%)	55,55,81	1.12	4 (7%)
82	PEB	C7	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.52	20 (37%)
82	PEB	B7	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.83	22 (40%)
82	PEB	jF	201	2	46,46,46	2.63	12 (26%)	54,67,67	2.65	22 (40%)
85	BCR	KN	101	40,49	41,41,41	0.78	1 (2%)	56,56,56	2.75	19 (33%)
87	CLA	B6	616	16	69,73,73	1.36	11 (15%)	83,113,113	1.64	6 (7%)
82	PEB	ZB	202	2	46,46,46	2.60	12 (26%)	54,67,67	2.04	14 (25%)
82	PEB	G7	201	1	46,46,46	2.50	9 (19%)	54,67,67	2.31	16 (29%)
82	PEB	RA	202	2	46,46,46	2.50	11 (23%)	54,67,67	2.93	21 (38%)
82	PEB	J7	203	2	46,46,46	2.69	12 (26%)	54,67,67	2.15	19 (35%)
84	CYC	D1	1003	10,9	46,46,46	2.26	15 (32%)	61,67,67	2.88	26 (42%)
82	PEB	NK	201	2	46,46,46	2.59	11 (23%)	54,67,67	2.90	17 (31%)
82	PEB	TF	201	2	46,46,46	2.51	10 (21%)	54,67,67	2.80	17 (31%)
82	PEB	SF	201	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.54	22 (40%)
87	CLA	B2	801	41	62,66,73	1.42	9 (14%)	74,104,113	1.65	15 (20%)
82	PEB	VD	203	1,2	46,46,46	2.70	15 (32%)	54,67,67	2.36	20 (37%)
87	CLA	B2	815	41	59,63,73	1.34	8 (13%)	71,101,113	1.49	7 (9%)
84	CYC	k3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	D5	203	2	46,46,46	2.55	11 (23%)	54,67,67	2.00	18 (33%)
87	CLA	A2	813	-	69,73,73	1.21	9 (13%)	83,113,113	1.34	5 (6%)
87	CLA	CL	510	-	69,73,73	1.27	10 (14%)	83,113,113	1.60	13 (15%)
84	CYC	A3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	26 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	PP	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	19 (35%)
87	CLA	FN	205	45	69,73,73	1.36	9 (13%)	83,113,113	1.66	12 (14%)
92	LMG	JL	103	18,24	33,33,55	1.15	2 (6%)	41,41,63	1.22	3 (7%)
85	BCR	A6	401	-	41,41,41	0.74	0	56,56,56	2.25	19 (33%)
82	PEB	fB	301	76,2	46,46,46	2.65	13 (28%)	54,67,67	1.93	16 (29%)
82	PEB	C9	201	1	46,46,46	2.62	15 (32%)	54,67,67	1.97	17 (31%)
82	PEB	MD	202	2	46,46,46	2.60	11 (23%)	54,67,67	2.00	15 (27%)
82	PEB	QG	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.13	19 (35%)
82	PEB	TD	203	1	46,46,46	2.67	11 (23%)	54,67,67	2.12	14 (25%)
82	PEB	MM	203	1	46,46,46	2.44	14 (30%)	54,67,67	2.18	18 (33%)
82	PEB	h4	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.28	22 (40%)
82	PEB	KM	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.08	15 (27%)
87	CLA	CL	514	-	59,63,73	1.36	11 (18%)	71,101,113	1.45	5 (7%)
82	PEB	UP	203	1,2	46,46,46	3.08	13 (28%)	54,67,67	3.08	20 (37%)
84	CYC	S3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	cL	509	-	69,73,73	1.24	10 (14%)	83,113,113	1.51	12 (14%)
87	CLA	RN	202	54	49,53,73	1.50	8 (16%)	59,89,113	1.52	8 (13%)
84	CYC	n3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	s8	203	2	46,46,46	2.73	12 (26%)	54,67,67	1.89	17 (31%)
82	PEB	cF	201	1	46,46,46	2.63	12 (26%)	54,67,67	2.28	20 (37%)
87	CLA	B2	813	-	49,53,73	1.46	9 (18%)	59,89,113	1.54	5 (8%)
87	CLA	3N	305	59,87	69,73,73	1.35	10 (14%)	83,113,113	1.87	15 (18%)
93	BCT	AL	412	15,90,18	2,3,3	1.16	0	2,3,3	3.89	1 (50%)
103	ZEX	8N	310	64,87	42,43,43	1.78	9 (21%)	55,60,60	3.89	31 (56%)
82	PEB	W9	202	2	46,46,46	2.73	13 (28%)	54,67,67	2.29	20 (37%)
82	PEB	Y9	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.22	18 (33%)
82	PEB	nK	202	2	46,46,46	2.82	15 (32%)	54,67,67	1.97	16 (29%)
84	CYC	D3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	w8	204	2	46,46,46	2.74	13 (28%)	54,67,67	2.00	16 (29%)
82	PEB	aJ	201	13,1	46,46,46	2.56	13 (28%)	54,67,67	2.09	14 (25%)
82	PEB	Q5	201	74,2	46,46,46	2.56	13 (28%)	54,67,67	2.01	19 (35%)
82	PEB	N7	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.24	20 (37%)
82	PEB	VK	201	2	46,46,46	2.60	11 (23%)	54,67,67	2.43	18 (33%)
82	PEB	hF	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.43	21 (38%)
82	PEB	FO	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.23	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	62	301	62	49,53,73	1.49	10 (20%)	59,89,113	1.39	4 (6%)
82	PEB	IK	201	1	46,46,46	2.53	12 (26%)	54,67,67	3.17	23 (42%)
82	PEB	a4	203	2	46,46,46	2.68	14 (30%)	54,67,67	1.98	17 (31%)
87	CLA	bL	621	-	69,73,73	1.22	8 (11%)	83,113,113	1.42	7 (8%)
87	CLA	c6	607	17	69,73,73	1.23	8 (11%)	83,113,113	1.33	6 (7%)
84	CYC	r3	1001	-	46,46,46	0.79	0	61,67,67	0.76	1 (1%)
82	PEB	IQ	201	2,77	46,46,46	2.69	14 (30%)	54,67,67	2.77	23 (42%)
82	PEB	cH	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.34	21 (38%)
85	BCR	Z6	101	39	41,41,41	0.78	1 (2%)	56,56,56	3.40	25 (44%)
87	CLA	AN	811	-	69,73,73	1.29	11 (15%)	83,113,113	1.56	10 (12%)
84	CYC	I3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
93	BCT	A6	409	15,90,18	2,3,3	1.23	0	2,3,3	3.83	2 (100%)
82	PEB	j1	202	1	46,46,46	2.72	14 (30%)	54,67,67	2.20	20 (37%)
85	BCR	F2	204	-	41,41,41	0.72	0	56,56,56	1.94	13 (23%)
83	PUB	Z5	303	1,74	45,46,46	2.79	11 (24%)	46,67,67	3.47	18 (39%)
82	PEB	U7	201	1	46,46,46	2.58	11 (23%)	54,67,67	2.61	18 (33%)
82	PEB	HP	201	56,2	46,46,46	2.65	14 (30%)	54,67,67	2.04	17 (31%)
87	CLA	c6	605	17	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
88	LHG	m6	102	-	38,38,48	1.04	2 (5%)	41,44,54	1.09	4 (9%)
88	LHG	CL	521	-	36,36,48	1.08	2 (5%)	39,42,54	1.12	3 (7%)
87	CLA	B2	831	-	64,68,73	1.31	10 (15%)	77,107,113	1.44	9 (11%)
82	PEB	LP	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.01	16 (29%)
92	LMG	J6	102	-	43,43,55	1.01	3 (6%)	51,51,63	2.16	12 (23%)
82	PEB	LF	201	2	46,46,46	2.59	12 (26%)	54,67,67	3.16	21 (38%)
85	BCR	cL	504	17	41,41,41	0.85	1 (2%)	56,56,56	2.32	17 (30%)
88	LHG	d6	402	-	45,45,48	0.96	2 (4%)	48,51,54	1.11	3 (6%)
87	CLA	BN	811	-	69,73,73	1.27	11 (15%)	83,113,113	1.49	7 (8%)
82	PEB	V1	203	2	46,46,46	2.69	13 (28%)	54,67,67	2.14	17 (31%)
95	DGD	h6	101	22	63,63,67	0.91	2 (3%)	77,77,81	1.00	3 (3%)
92	LMG	C6	501	-	55,55,55	0.86	2 (3%)	63,63,63	0.99	2 (3%)
82	PEB	UG	201	1,2	46,46,46	2.59	11 (23%)	54,67,67	2.39	19 (35%)
82	PEB	K5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	20 (37%)
87	CLA	42	603	-	49,53,73	1.47	11 (22%)	59,89,113	1.57	9 (15%)
87	CLA	12	611	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	7 (11%)
82	PEB	fM	202	1	46,46,46	2.60	12 (26%)	54,67,67	2.16	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	b6	612	-	69,73,73	1.26	9 (13%)	83,113,113	1.40	10 (12%)
82	PEB	U5	201	74,2	46,46,46	2.77	14 (30%)	54,67,67	2.11	18 (33%)
82	PEB	U7	202	1	46,46,46	2.64	13 (28%)	54,67,67	1.93	16 (29%)
82	PEB	KE	201	10,9	46,46,46	2.60	13 (28%)	54,67,67	2.08	17 (31%)
82	PEB	DA	202	2	46,46,46	2.51	12 (26%)	54,67,67	2.46	21 (38%)
82	PEB	QA	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.02	14 (25%)
82	PEB	BQ	201	1	46,46,46	2.52	12 (26%)	54,67,67	2.31	20 (37%)
82	PEB	IK	203	1,2	46,46,46	2.51	12 (26%)	54,67,67	2.86	24 (44%)
82	PEB	i1	202	2	46,46,46	2.75	12 (26%)	54,67,67	1.88	15 (27%)
82	PEB	V5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
87	CLA	O2	202	53	54,58,73	1.49	7 (12%)	65,95,113	1.92	13 (20%)
82	PEB	dM	202	1	46,46,46	2.61	13 (28%)	54,67,67	1.98	14 (25%)
87	CLA	6N	611	62	49,53,73	1.44	6 (12%)	59,89,113	1.43	4 (6%)
82	PEB	XM	201	2	46,46,46	2.71	13 (28%)	54,67,67	2.07	19 (35%)
82	PEB	XJ	202	2	46,46,46	2.56	13 (28%)	54,67,67	2.19	22 (40%)
82	PEB	RA	203	2	46,46,46	2.62	13 (28%)	54,67,67	2.40	26 (48%)
82	PEB	CF	203	1	46,46,46	2.62	13 (28%)	54,67,67	2.05	20 (37%)
82	PEB	O1	202	1	46,46,46	2.65	12 (26%)	54,67,67	2.11	18 (33%)
82	PEB	yF	301	14	46,46,46	2.64	13 (28%)	54,67,67	2.13	18 (33%)
87	CLA	HL	101	22	69,73,73	1.24	9 (13%)	83,113,113	1.43	10 (12%)
82	PEB	OE	203	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.23	21 (38%)
88	LHG	BL	610	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
82	PEB	A9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	wF	301	13	46,46,46	2.57	12 (26%)	54,67,67	2.18	20 (37%)
85	BCR	FN	202	-	41,41,41	0.72	0	56,56,56	2.11	18 (32%)
82	PEB	PK	202	2	46,46,46	2.87	15 (32%)	54,67,67	2.31	20 (37%)
87	CLA	62	308	62	49,53,73	1.50	9 (18%)	59,89,113	1.54	7 (11%)
82	PEB	WK	203	1	46,46,46	2.70	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	MQ	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.16	18 (33%)
87	CLA	B2	833	-	51,55,73	1.44	12 (23%)	61,91,113	1.48	12 (19%)
82	PEB	ZO	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.81	23 (42%)
82	PEB	M5	305	74	46,46,46	2.57	13 (28%)	54,67,67	2.36	24 (44%)
82	PEB	E9	202	1	46,46,46	2.73	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	Q1	203	1	46,46,46	2.61	13 (28%)	54,67,67	2.12	18 (33%)
87	CLA	cL	512	-	69,73,73	1.26	10 (14%)	83,113,113	1.55	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PEB	LD	203	1	46,46,46	2.66	10 (21%)	54,67,67	2.06	18 (33%)
87	CLA	cL	506	-	69,73,73	1.28	11 (15%)	83,113,113	1.35	9 (10%)
82	PEB	uF	203	1	46,46,46	2.78	13 (28%)	54,67,67	1.87	17 (31%)
87	CLA	4N	605	60	49,53,73	1.48	9 (18%)	59,89,113	1.99	11 (18%)
82	PEB	qK	203	1	46,46,46	2.76	13 (28%)	54,67,67	2.16	19 (35%)
82	PEB	TK	201	2	46,46,46	2.51	9 (19%)	54,67,67	2.80	17 (31%)
82	PEB	Y1	202	2	46,46,46	2.73	13 (28%)	54,67,67	2.10	19 (35%)
82	PEB	e1	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.09	20 (37%)
95	DGD	CL	520	-	43,43,67	1.08	2 (4%)	57,57,81	1.27	6 (10%)
87	CLA	BN	832	-	69,73,73	1.24	10 (14%)	83,113,113	1.40	8 (9%)
82	PEB	OD	201	3,2,82	46,46,46	2.66	12 (26%)	54,67,67	2.07	16 (29%)
82	PEB	II	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	mG	203	2	46,46,46	2.65	14 (30%)	54,67,67	2.04	14 (25%)
87	CLA	22	611	-	46,50,73	1.49	9 (19%)	55,85,113	1.64	7 (12%)
87	CLA	6N	603	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
82	PEB	yK	301	14	46,46,46	2.64	13 (28%)	54,67,67	2.12	18 (33%)
87	CLA	4N	606	-	49,53,73	1.49	9 (18%)	59,89,113	1.48	6 (10%)
87	CLA	52	610	-	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
82	PEB	GG	1002	10,9	46,46,46	2.55	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	J7	202	2	46,46,46	2.54	12 (26%)	54,67,67	2.52	20 (37%)
82	PEB	eF	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.32	23 (42%)
82	PEB	lG	201	1,2	46,46,46	2.62	13 (28%)	54,67,67	2.17	17 (31%)
82	PEB	R7	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.19	19 (35%)
84	CYC	F4	1001	10	46,46,46	2.32	15 (32%)	61,67,67	2.90	26 (42%)
82	PEB	Q4	201	1	46,46,46	2.61	13 (28%)	54,67,67	2.77	27 (50%)
82	PEB	HD	201	1,2	46,46,46	2.50	12 (26%)	54,67,67	2.42	20 (37%)
82	PEB	SF	203	1	46,46,46	2.62	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	FD	202	1	46,46,46	2.70	12 (26%)	54,67,67	1.98	17 (31%)
82	PEB	II	203	1,2	46,46,46	2.29	13 (28%)	54,67,67	3.23	24 (44%)
82	PEB	TJ	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.05	17 (31%)
82	PEB	dE	203	1	46,46,46	2.67	14 (30%)	54,67,67	2.06	20 (37%)
82	PEB	JB	201	1	46,46,46	2.70	13 (28%)	54,67,67	2.77	21 (38%)
85	BCR	C6	507	-	41,41,41	0.82	1 (2%)	56,56,56	2.03	16 (28%)
94	PL9	a6	601	15	55,55,55	0.62	2 (3%)	68,69,69	1.92	22 (32%)
82	PEB	xF	304	13	46,46,46	2.68	11 (23%)	54,67,67	2.07	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	sC	203	2	46,46,46	2.73	12 (26%)	54,67,67	1.90	17 (31%)
84	CYC	M3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	CK	203	1	46,46,46	2.63	13 (28%)	54,67,67	2.04	20 (37%)
82	PEB	GK	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.95	28 (51%)
84	CYC	o3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	bH	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.03	18 (33%)
82	PEB	uC	201	2	46,46,46	2.68	15 (32%)	54,67,67	2.32	23 (42%)
82	PEB	S1	202	1	46,46,46	2.69	12 (26%)	54,67,67	2.24	18 (33%)
82	PEB	YK	202	1	46,46,46	2.67	12 (26%)	54,67,67	1.87	16 (29%)
82	PEB	QH	201	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.44	22 (40%)
82	PEB	MJ	202	1	46,46,46	2.47	11 (23%)	54,67,67	2.40	20 (37%)
82	PEB	MA	202	1	46,46,46	2.60	12 (26%)	54,67,67	1.91	13 (24%)
82	PEB	YD	201	2,82	46,46,46	2.71	13 (28%)	54,67,67	1.99	15 (27%)
87	CLA	BN	836	87,41,57	69,73,73	1.23	8 (11%)	83,113,113	1.66	9 (10%)
82	PEB	pF	201	2	46,46,46	2.60	11 (23%)	54,67,67	2.41	22 (40%)
82	PEB	jG	201	1	46,46,46	2.64	13 (28%)	54,67,67	2.08	19 (35%)
87	CLA	B2	827	-	69,73,73	1.32	10 (14%)	83,113,113	1.44	11 (13%)
82	PEB	BI	202	1,2	46,46,46	2.31	12 (26%)	54,67,67	2.80	23 (42%)
87	CLA	AL	403	15	69,73,73	1.29	12 (17%)	83,113,113	1.46	11 (13%)
82	PEB	b4	201	1	46,46,46	2.68	11 (23%)	54,67,67	2.32	22 (40%)
87	CLA	A2	818	-	49,53,73	1.47	9 (18%)	59,89,113	1.48	5 (8%)
82	PEB	OA	201	1	46,46,46	2.55	11 (23%)	54,67,67	2.94	25 (46%)
82	PEB	GM	203	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.39	19 (35%)
82	PEB	w8	202	2	46,46,46	2.70	12 (26%)	54,67,67	2.40	17 (31%)
82	PEB	MB	202	2	46,46,46	2.83	13 (28%)	54,67,67	2.19	22 (40%)
87	CLA	A2	808	-	69,73,73	1.26	11 (15%)	83,113,113	1.38	8 (9%)
82	PEB	YJ	201	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.41	22 (40%)
82	PEB	WG	203	1,2	46,46,46	2.50	11 (23%)	54,67,67	2.32	22 (40%)
82	PEB	qF	203	1	46,46,46	2.74	14 (30%)	54,67,67	2.15	20 (37%)
95	DGD	AL	416	-	41,41,67	1.11	3 (7%)	55,55,81	1.50	8 (14%)
87	CLA	7N	605	-	49,53,73	1.49	9 (18%)	59,89,113	1.52	7 (11%)
82	PEB	UO	202	1	46,46,46	2.53	11 (23%)	54,67,67	1.99	14 (25%)
88	LHG	BL	615	-	40,40,48	0.99	2 (5%)	43,46,54	1.04	3 (6%)
87	CLA	DL	404	-	69,73,73	1.26	10 (14%)	83,113,113	1.30	7 (8%)
91	PHO	A6	407	-	58,69,69	2.61	13 (22%)	56,99,99	2.75	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	X5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	DD	201	1,2	46,46,46	2.49	13 (28%)	54,67,67	2.43	21 (38%)
87	CLA	12	608	57	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
82	PEB	YA	304	3,82	46,46,46	2.63	14 (30%)	54,67,67	2.32	18 (33%)
87	CLA	ON	203	53	49,53,73	1.63	11 (22%)	59,89,113	1.47	7 (11%)
82	PEB	AE	304	3	46,46,46	2.60	12 (26%)	54,67,67	2.10	20 (37%)
82	PEB	FK	201	2	46,46,46	2.59	12 (26%)	54,67,67	3.54	18 (33%)
82	PEB	XK	203	2	46,46,46	2.75	15 (32%)	54,67,67	2.27	22 (40%)
82	PEB	lG	203	1	46,46,46	2.64	14 (30%)	54,67,67	1.95	17 (31%)
85	BCR	kL	100	-	41,41,41	0.83	0	56,56,56	2.73	23 (41%)
82	PEB	AG	304	3	46,46,46	2.59	12 (26%)	54,67,67	2.10	19 (35%)
84	CYC	l3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.91	26 (42%)
82	PEB	KQ	202	2	46,46,46	2.61	12 (26%)	54,67,67	1.98	18 (33%)
82	PEB	HD	203	1	46,46,46	2.75	12 (26%)	54,67,67	2.07	16 (29%)
82	PEB	YI	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.07	18 (33%)
87	CLA	72	603	-	49,53,73	1.47	8 (16%)	59,89,113	1.53	8 (13%)
82	PEB	kF	201	1	46,46,46	2.72	13 (28%)	54,67,67	2.07	16 (29%)
82	PEB	YK	201	1	46,46,46	2.67	11 (23%)	54,67,67	2.13	19 (35%)
95	DGD	a6	604	15,17	54,54,67	0.91	2 (3%)	68,68,81	1.10	6 (8%)
82	PEB	SE	202	1,2	46,46,46	2.56	11 (23%)	54,67,67	2.49	20 (37%)
87	CLA	B2	822	-	69,73,73	1.27	11 (15%)	83,113,113	1.35	13 (15%)
82	PEB	JI	202	2	46,46,46	2.65	13 (28%)	54,67,67	1.94	17 (31%)
87	CLA	A2	824	40	55,59,73	1.38	8 (14%)	66,96,113	1.57	6 (9%)
87	CLA	8N	308	-	49,53,73	1.49	11 (22%)	59,89,113	2.07	12 (20%)
82	PEB	SD	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.10	15 (27%)
82	PEB	Y4	203	2	46,46,46	2.59	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	BK	202	2	46,46,46	2.73	13 (28%)	54,67,67	2.26	17 (31%)
82	PEB	DD	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.79	24 (44%)
82	PEB	d1	201	1,2	46,46,46	2.60	10 (21%)	54,67,67	2.29	18 (33%)
84	CYC	p3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	24 (39%)
87	CLA	AN	819	40	66,70,73	1.30	10 (15%)	79,109,113	1.51	9 (11%)
82	PEB	EA	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.00	16 (29%)
82	PEB	GP	201	1,2	46,46,46	3.11	13 (28%)	54,67,67	3.10	20 (37%)
82	PEB	PA	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	QH	202	1	46,46,46	2.58	11 (23%)	54,67,67	2.35	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	A4	301	3	46,46,46	2.62	12 (26%)	54,67,67	1.99	17 (31%)
82	PEB	eE	203	2	46,46,46	2.80	14 (30%)	54,67,67	2.41	22 (40%)
82	PEB	I9	202	1	46,46,46	2.74	14 (30%)	54,67,67	2.41	21 (38%)
82	PEB	A1	302	3	46,46,46	2.68	13 (28%)	54,67,67	1.98	16 (29%)
82	PEB	KD	201	2	46,46,46	2.62	13 (28%)	54,67,67	1.95	15 (27%)
82	PEB	QE	201	1,2	46,46,46	2.58	13 (28%)	54,67,67	2.68	24 (44%)
82	PEB	kK	202	1	46,46,46	2.72	12 (26%)	54,67,67	1.79	15 (27%)
82	PEB	BQ	203	1,2	46,46,46	2.34	11 (23%)	54,67,67	2.48	18 (33%)
84	CYC	H3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
88	LHG	I6	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.13	5 (9%)
87	CLA	AN	807	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	7 (8%)
102	BGC	32	301	-	11,11,12	0.36	0	15,15,17	1.38	1 (6%)
82	PEB	Y7	304	3,82	46,46,46	2.63	14 (30%)	54,67,67	2.32	18 (33%)
82	PEB	Q5	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.50	21 (38%)
82	PEB	aB	201	2	46,46,46	2.54	12 (26%)	54,67,67	2.25	19 (35%)
82	PEB	lK	203	1,2	46,46,46	2.71	16 (34%)	54,67,67	2.49	23 (42%)
87	CLA	AN	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	7 (8%)
82	PEB	PJ	201	2	46,46,46	2.68	13 (28%)	54,67,67	2.16	21 (38%)
87	CLA	B6	615	16	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
87	CLA	LN	203	85,50,41	69,73,73	1.24	8 (11%)	83,113,113	1.47	6 (7%)
82	PEB	bP	502	2	46,46,46	2.52	11 (23%)	54,67,67	2.16	19 (35%)
84	CYC	LE	1001	10	46,46,46	2.38	18 (39%)	61,67,67	3.02	29 (47%)
95	DGD	c6	620	-	49,49,67	0.95	2 (4%)	63,63,81	1.07	4 (6%)
82	PEB	UJ	201	1,2	46,46,46	2.54	11 (23%)	54,67,67	2.47	24 (44%)
87	CLA	B6	603	-	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
84	CYC	f3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	bL	620	16,85	60,64,73	1.31	10 (16%)	72,102,113	1.43	6 (8%)
82	PEB	VM	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.15	17 (31%)
87	CLA	FN	203	45	49,53,73	1.53	12 (24%)	59,89,113	1.43	9 (15%)
82	PEB	QJ	202	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.30	21 (38%)
82	PEB	F9	201	74,2	46,46,46	2.73	13 (28%)	54,67,67	2.30	18 (33%)
82	PEB	GM	202	1	46,46,46	2.58	14 (30%)	54,67,67	2.06	16 (29%)
87	CLA	c6	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	8 (9%)
87	CLA	AN	826	-	69,73,73	1.27	11 (15%)	83,113,113	1.41	11 (13%)
82	PEB	Q7	201	1	46,46,46	2.56	12 (26%)	54,67,67	2.71	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	oK	202	1	46,46,46	2.70	12 (26%)	54,67,67	1.98	18 (33%)
87	CLA	22	608	58	49,53,73	1.52	8 (16%)	59,89,113	1.50	11 (18%)
82	PEB	XI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	20 (37%)
82	PEB	EM	202	1	46,46,46	2.64	11 (23%)	54,67,67	2.10	18 (33%)
82	PEB	UO	201	1	46,46,46	2.52	12 (26%)	54,67,67	2.94	26 (48%)
82	PEB	S4	201	1	46,46,46	2.67	14 (30%)	54,67,67	2.64	25 (46%)
96	HEM	fL	102	-	50,50,50	1.63	9 (18%)	66,82,82	1.68	15 (22%)
95	DGD	CL	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	2 (2%)
82	PEB	VA	202	2	46,46,46	2.51	11 (23%)	54,67,67	2.62	23 (42%)
82	PEB	hG	202	1	46,46,46	2.65	14 (30%)	54,67,67	1.99	17 (31%)
82	PEB	rF	202	2	46,46,46	2.80	16 (34%)	54,67,67	2.23	19 (35%)
87	CLA	BN	831	-	64,68,73	1.31	10 (15%)	77,107,113	1.42	9 (11%)
82	PEB	aH	202	2	46,46,46	2.77	13 (28%)	54,67,67	2.00	17 (31%)
82	PEB	O7	201	1	46,46,46	2.55	11 (23%)	54,67,67	2.94	25 (46%)
82	PEB	SG	202	-	46,46,46	0.64	0	54,67,67	0.80	1 (1%)
82	PEB	qK	202	1	46,46,46	2.60	13 (28%)	54,67,67	3.09	23 (42%)
85	BCR	H6	101	-	41,41,41	0.81	2 (4%)	56,56,56	2.14	18 (32%)
84	CYC	K3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
87	CLA	nL	101	-	69,73,73	1.24	10 (14%)	83,113,113	1.45	10 (12%)
84	CYC	I4	1001	9	46,46,46	2.31	17 (36%)	61,67,67	2.84	26 (42%)
84	CYC	GO	1001	9	46,46,46	2.40	15 (32%)	61,67,67	2.79	24 (39%)
82	PEB	wC	204	2	46,46,46	2.74	14 (30%)	54,67,67	1.99	15 (27%)
85	BCR	b6	601	-	41,41,41	0.89	2 (4%)	56,56,56	2.10	17 (30%)
87	CLA	B2	830	-	69,73,73	1.23	9 (13%)	83,113,113	1.30	4 (4%)
82	PEB	fF	201	13,2	46,46,46	2.53	10 (21%)	54,67,67	2.92	18 (33%)
82	PEB	fE	202	1	46,46,46	2.67	16 (34%)	54,67,67	1.96	17 (31%)
82	PEB	NJ	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.48	21 (38%)
82	PEB	m4	203	2	46,46,46	2.70	13 (28%)	54,67,67	2.03	20 (37%)
82	PEB	i4	203	2	46,46,46	2.74	13 (28%)	54,67,67	1.86	16 (29%)
87	CLA	BL	606	-	69,73,73	1.24	8 (11%)	83,113,113	1.39	5 (6%)
95	DGD	a6	603	-	41,41,67	1.07	2 (4%)	55,55,81	1.33	5 (9%)
87	CLA	82	306	64,103	50,54,73	1.57	12 (24%)	60,90,113	1.73	16 (26%)
87	CLA	1N	609	-	46,50,73	1.50	9 (19%)	55,85,113	1.66	8 (14%)
82	PEB	mO	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.37	20 (37%)
87	CLA	A2	812	-	59,63,73	1.34	9 (15%)	71,101,113	1.46	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	CYC	y3	1001	71	46,46,46	2.54	17 (36%)	61,67,67	3.17	31 (50%)
82	PEB	WE	201	1	46,46,46	2.60	14 (30%)	54,67,67	2.36	22 (40%)
82	PEB	cM	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.25	17 (31%)
82	PEB	Y7	303	3,82	46,46,46	2.60	13 (28%)	54,67,67	2.58	22 (40%)
82	PEB	KK	201	1,2	46,46,46	2.48	11 (23%)	54,67,67	2.59	19 (35%)
87	CLA	AN	812	-	59,63,73	1.34	9 (15%)	71,101,113	1.45	6 (8%)
82	PEB	aM	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.05	14 (25%)
95	DGD	AL	415	-	41,41,67	1.07	2 (4%)	55,55,81	1.20	5 (9%)
82	PEB	DM	202	2	46,46,46	2.63	14 (30%)	54,67,67	2.07	20 (37%)
82	PEB	GQ	202	2	46,46,46	2.68	11 (23%)	54,67,67	2.13	21 (38%)
82	PEB	SB	202	2	46,46,46	2.52	13 (28%)	54,67,67	2.12	19 (35%)
87	CLA	C6	519	-	59,63,73	1.34	10 (16%)	71,101,113	1.37	7 (9%)
82	PEB	p8	201	1	46,46,46	2.66	12 (26%)	54,67,67	2.00	18 (33%)
82	PEB	IM	203	1	46,46,46	2.53	12 (26%)	54,67,67	2.11	18 (33%)
82	PEB	JM	202	2	46,46,46	2.65	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	LQ	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.23	15 (27%)
85	BCR	bL	603	-	41,41,41	0.74	0	56,56,56	1.77	13 (23%)
82	PEB	U9	202	2	46,46,46	2.60	11 (23%)	54,67,67	2.28	20 (37%)
87	CLA	A2	807	-	69,73,73	1.26	10 (14%)	83,113,113	1.39	6 (7%)
82	PEB	RO	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.48	22 (40%)
82	PEB	B9	203	2	46,46,46	2.66	12 (26%)	54,67,67	2.06	14 (25%)
84	CYC	u3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	6N	602	62	69,73,73	1.27	9 (13%)	83,113,113	1.28	9 (10%)
87	CLA	72	602	62,63	69,73,73	1.39	10 (14%)	83,113,113	1.79	18 (21%)
82	PEB	FJ	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.21	21 (38%)
94	PL9	A6	410	-	55,55,55	0.61	1 (1%)	68,69,69	2.28	21 (30%)
82	PEB	eB	201	2	46,46,46	2.56	13 (28%)	54,67,67	2.05	16 (29%)
82	PEB	PF	201	2	46,46,46	2.60	11 (23%)	54,67,67	3.03	19 (35%)
82	PEB	OG	203	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.24	21 (38%)
82	PEB	QG	201	1,2	46,46,46	2.58	13 (28%)	54,67,67	2.67	24 (44%)
87	CLA	c6	610	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	7 (8%)
87	CLA	AN	833	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
82	PEB	TD	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.10	17 (31%)
82	PEB	S9	202	2	46,46,46	2.56	13 (28%)	54,67,67	2.28	22 (40%)
91	PHO	a6	613	-	58,69,69	2.65	13 (22%)	56,99,99	2.69	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
95	DGD	cL	502	-	63,63,67	0.84	2 (3%)	77,77,81	1.27	8 (10%)
87	CLA	AN	816	-	49,53,73	1.51	9 (18%)	59,89,113	1.50	6 (10%)
84	CYC	t3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
84	CYC	N4	1001	10	46,46,46	2.48	19 (41%)	61,67,67	2.83	27 (44%)
82	PEB	uK	201	1	46,46,46	2.74	13 (28%)	54,67,67	2.05	16 (29%)
82	PEB	PD	201	1,2	46,46,46	2.66	14 (30%)	54,67,67	2.04	18 (33%)
99	SF4	C2	101	42	0,12,12	-	-	-		
92	LMG	BL	611	-	40,40,55	1.01	2 (5%)	48,48,63	1.34	6 (12%)
85	BCR	C6	508	-	41,41,41	0.80	1 (2%)	56,56,56	2.61	22 (39%)
87	CLA	6N	605	62	49,53,73	1.47	8 (16%)	59,89,113	1.54	7 (11%)
82	PEB	HQ	203	1	46,46,46	2.73	13 (28%)	54,67,67	2.08	16 (29%)
82	PEB	xK	304	13	46,46,46	2.72	11 (23%)	54,67,67	2.10	19 (35%)
85	BCR	KL	100	-	41,41,41	0.83	0	56,56,56	2.73	23 (41%)
82	PEB	CP	202	1	46,46,46	2.60	14 (30%)	54,67,67	2.20	20 (37%)
87	CLA	6N	606	87	49,53,73	1.50	9 (18%)	59,89,113	1.48	7 (11%)
82	PEB	VJ	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.19	20 (37%)
82	PEB	R9	202	1	46,46,46	2.73	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	AA	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.04	16 (29%)
82	PEB	ZE	202	1	46,46,46	2.62	14 (30%)	54,67,67	2.25	19 (35%)
82	PEB	hF	202	2	46,46,46	2.68	12 (26%)	54,67,67	1.97	19 (35%)
82	PEB	F5	201	74,2	46,46,46	2.70	12 (26%)	54,67,67	2.33	24 (44%)
87	CLA	5N	605	61	49,53,73	1.49	9 (18%)	59,89,113	1.51	6 (10%)
82	PEB	JH	1002	10	46,46,46	2.54	13 (28%)	54,67,67	2.20	17 (31%)
82	PEB	J5	203	2	46,46,46	2.54	13 (28%)	54,67,67	2.06	19 (35%)
87	CLA	1N	610	57	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
82	PEB	M5	301	74	46,46,46	2.56	12 (26%)	54,67,67	2.22	20 (37%)
82	PEB	KA	202	1	46,46,46	2.67	13 (28%)	54,67,67	1.89	14 (25%)
82	PEB	V1	201	2	46,46,46	2.62	14 (30%)	54,67,67	2.30	20 (37%)
82	PEB	aO	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.29	18 (33%)
87	CLA	cL	507	-	69,73,73	1.26	9 (13%)	83,113,113	1.39	6 (7%)
82	PEB	S7	201	1	46,46,46	2.57	11 (23%)	54,67,67	2.78	21 (38%)
87	CLA	BN	824	-	69,73,73	1.28	11 (15%)	83,113,113	1.47	13 (15%)
82	PEB	hH	202	1	46,46,46	0.64	0	54,67,67	0.79	1 (1%)
82	PEB	T1	201	11,2	46,46,46	2.60	15 (32%)	54,67,67	2.32	24 (44%)
82	PEB	OJ	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.04	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	FB	201	2,5	46,46,46	2.49	12 (26%)	54,67,67	2.22	15 (27%)
87	CLA	42	607	60	49,53,73	1.52	10 (20%)	59,89,113	1.65	9 (15%)
82	PEB	tF	201	2	46,46,46	2.68	11 (23%)	54,67,67	2.73	17 (31%)
82	PEB	X9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	GJ	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.19	20 (37%)
87	CLA	BN	814	-	49,53,73	1.45	9 (18%)	59,89,113	1.54	4 (6%)
82	PEB	TB	201	1	46,46,46	2.70	13 (28%)	54,67,67	2.77	21 (38%)
82	PEB	hB	301	76,2	46,46,46	2.64	12 (26%)	54,67,67	1.93	16 (29%)
82	PEB	pK	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.31	20 (37%)
88	LHG	l6	101	26,16	48,48,48	0.90	2 (4%)	51,54,54	1.13	4 (7%)
82	PEB	dF	202	2	46,46,46	2.92	15 (32%)	54,67,67	2.19	19 (35%)
82	PEB	CF	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	A4	305	3	46,46,46	2.62	12 (26%)	54,67,67	2.02	16 (29%)
87	CLA	KN	105	40,49	53,57,73	1.37	10 (18%)	62,93,113	1.34	10 (16%)
92	LMG	j6	102	18,24	33,33,55	1.12	2 (6%)	41,41,63	1.17	4 (9%)
82	PEB	lF	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.42	17 (31%)
82	PEB	YG	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.29	21 (38%)
87	CLA	AN	820	-	69,73,73	1.28	10 (14%)	83,113,113	1.50	14 (16%)
87	CLA	b6	611	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	6 (7%)
83	PUB	yF	302	14	45,46,46	2.62	8 (17%)	46,67,67	2.96	20 (43%)
95	DGD	C6	521	-	63,63,67	0.84	2 (3%)	77,77,81	1.16	7 (9%)
82	PEB	vK	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.03	19 (35%)
82	PEB	jH	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.21	19 (35%)
87	CLA	4N	603	-	49,53,73	1.47	11 (22%)	59,89,113	1.56	9 (15%)
82	PEB	GF	203	1	46,46,46	2.63	13 (28%)	54,67,67	2.46	26 (48%)
82	PEB	gF	203	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.49	19 (35%)
87	CLA	42	601	60	49,53,73	1.46	9 (18%)	59,89,113	1.55	7 (11%)
84	CYC	FG	1001	10	46,46,46	2.33	15 (32%)	61,67,67	2.90	24 (39%)
82	PEB	FH	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.17	16 (29%)
87	CLA	22	612	58	49,53,73	1.50	9 (18%)	59,89,113	1.64	9 (15%)
95	DGD	cL	520	-	49,49,67	0.98	2 (4%)	63,63,81	1.12	4 (6%)
82	PEB	hH	201	1	46,46,46	2.67	13 (28%)	54,67,67	2.16	18 (33%)
87	CLA	B2	819	41	49,53,73	1.48	11 (22%)	59,89,113	1.56	7 (11%)
84	CYC	GG	1001	10,9	46,46,46	2.38	15 (32%)	61,67,67	2.87	27 (44%)
82	PEB	BA	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.83	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	oF	202	1	46,46,46	2.69	12 (26%)	54,67,67	1.98	17 (31%)
91	PHO	AL	410	-	58,69,69	2.58	13 (22%)	56,99,99	2.58	15 (26%)
82	PEB	KF	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.30	17 (31%)
82	PEB	NP	201	2	46,46,46	2.62	13 (28%)	54,67,67	1.97	18 (33%)
94	PL9	aL	601	15	55,55,55	0.75	3 (5%)	68,69,69	1.97	19 (27%)
87	CLA	b6	618	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
82	PEB	TE	201	2	46,46,46	2.59	12 (26%)	54,67,67	2.25	19 (35%)
83	PUB	AO	303	3	45,46,46	2.65	9 (20%)	46,67,67	2.86	16 (34%)
83	PUB	NQ	201	1,3	45,46,46	2.85	11 (24%)	46,67,67	3.08	18 (39%)
82	PEB	SH	202	1	46,46,46	2.67	11 (23%)	54,67,67	2.23	18 (33%)
82	PEB	s8	202	2	46,46,46	2.79	13 (28%)	54,67,67	2.34	18 (33%)
87	CLA	DL	406	-	69,73,73	1.22	10 (14%)	83,113,113	1.38	6 (7%)
82	PEB	ZG	201	1,2	46,46,46	2.54	11 (23%)	54,67,67	2.52	23 (42%)
82	PEB	SM	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.05	14 (25%)
82	PEB	dF	201	2	46,46,46	2.62	11 (23%)	54,67,67	2.38	18 (33%)
82	PEB	c4	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.22	17 (31%)
82	PEB	YD	202	2	46,46,46	2.68	13 (28%)	54,67,67	1.94	14 (25%)
82	PEB	LA	203	2	46,46,46	2.66	12 (26%)	54,67,67	1.89	19 (35%)
87	CLA	BL	622	16	69,73,73	1.24	9 (13%)	83,113,113	1.45	7 (8%)
85	BCR	FN	204	-	41,41,41	0.72	0	56,56,56	1.95	13 (23%)
82	PEB	Q1	201	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.43	22 (40%)
82	PEB	KA	201	1	46,46,46	2.73	15 (32%)	54,67,67	2.42	21 (38%)
82	PEB	R4	202	2	46,46,46	2.57	13 (28%)	54,67,67	2.49	22 (40%)
87	CLA	B2	805	41	69,73,73	1.22	8 (11%)	83,113,113	1.41	9 (10%)
82	PEB	EJ	202	1	46,46,46	2.58	11 (23%)	54,67,67	2.07	14 (25%)
87	CLA	5N	604	61	46,50,73	1.48	10 (21%)	55,85,113	1.60	6 (10%)
82	PEB	UF	202	1	46,46,46	2.60	11 (23%)	54,67,67	2.08	16 (29%)
82	PEB	CI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
87	CLA	cL	510	-	69,73,73	1.27	9 (13%)	83,113,113	1.46	7 (8%)
84	CYC	HE	1001	10	46,46,46	2.27	16 (34%)	61,67,67	3.02	27 (44%)
82	PEB	18	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.16	15 (27%)
85	BCR	A2	846	-	41,41,41	0.76	0	56,56,56	2.75	19 (33%)
82	PEB	DH	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.06	17 (31%)
82	PEB	vC	201	1	46,46,46	2.69	14 (30%)	54,67,67	2.03	16 (29%)
85	BCR	K2	105	-	41,41,41	0.83	0	56,56,56	2.48	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	dE	202	1,2	46,46,46	2.57	12 (26%)	54,67,67	2.35	21 (38%)
82	PEB	GI	201	1,2	46,46,46	2.34	13 (28%)	54,67,67	3.06	24 (44%)
82	PEB	A1	301	3	46,46,46	2.69	11 (23%)	54,67,67	2.02	15 (27%)
82	PEB	PM	201	2	46,46,46	2.70	15 (32%)	54,67,67	2.37	20 (37%)
82	PEB	VQ	201	1	46,46,46	2.52	11 (23%)	54,67,67	2.10	18 (33%)
87	CLA	6N	613	62	49,53,73	1.49	10 (20%)	59,89,113	1.39	4 (6%)
82	PEB	hK	201	2	46,46,46	2.61	13 (28%)	54,67,67	2.44	22 (40%)
82	PEB	NM	202	2	46,46,46	2.62	14 (30%)	54,67,67	2.19	17 (31%)
82	PEB	jM	202	1	46,46,46	2.63	11 (23%)	54,67,67	2.75	18 (33%)
82	PEB	VD	201	1	46,46,46	2.51	11 (23%)	54,67,67	2.10	18 (33%)
82	PEB	KK	203	1	46,46,46	2.63	11 (23%)	54,67,67	2.12	21 (38%)
82	PEB	WB	402	6,2	46,46,46	2.66	12 (26%)	54,67,67	2.33	25 (46%)
82	PEB	L5	201	74,2	46,46,46	2.55	13 (28%)	54,67,67	2.03	18 (33%)
87	CLA	BN	808	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
82	PEB	JQ	201	1	46,46,46	2.68	12 (26%)	54,67,67	2.11	18 (33%)
87	CLA	6N	601	62	49,53,73	1.47	8 (16%)	59,89,113	1.42	4 (6%)
82	PEB	CJ	201	1	46,46,46	2.50	11 (23%)	54,67,67	2.23	20 (37%)
82	PEB	P1	201	11,2	46,46,46	2.59	13 (28%)	54,67,67	2.21	19 (35%)
82	PEB	D9	202	2	46,46,46	2.66	14 (30%)	54,67,67	2.21	19 (35%)
82	PEB	AO	301	3	46,46,46	2.61	11 (23%)	54,67,67	1.98	17 (31%)
82	PEB	l1	201	1,2	46,46,46	2.65	12 (26%)	54,67,67	2.34	19 (35%)
82	PEB	H7	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.08	17 (31%)
82	PEB	f1	201	1	46,46,46	2.66	14 (30%)	54,67,67	1.93	17 (31%)
82	PEB	eH	203	1,2	46,46,46	2.61	14 (30%)	54,67,67	2.53	18 (33%)
82	PEB	U1	201	1,2	46,46,46	2.64	13 (28%)	54,67,67	2.39	19 (35%)
83	PUB	QJ	201	14,1	45,46,46	2.67	10 (22%)	46,67,67	3.10	21 (45%)
88	LHG	C6	505	-	36,36,48	1.04	2 (5%)	39,42,54	1.23	4 (10%)
82	PEB	LQ	203	1	46,46,46	2.66	10 (21%)	54,67,67	2.06	18 (33%)
82	PEB	NB	201	2	46,46,46	2.53	12 (26%)	54,67,67	2.14	19 (35%)
82	PEB	v8	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.66	22 (40%)
82	PEB	WG	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.37	23 (42%)
87	CLA	B2	832	-	69,73,73	1.24	10 (14%)	83,113,113	1.41	9 (10%)
87	CLA	BL	621	-	69,73,73	1.27	11 (15%)	83,113,113	1.56	10 (12%)
82	PEB	DK	203	2	46,46,46	2.70	14 (30%)	54,67,67	2.07	20 (37%)
82	PEB	BP	202	2	46,46,46	2.65	11 (23%)	54,67,67	2.09	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	wK	303	13	46,46,46	2.73	14 (30%)	54,67,67	2.12	20 (37%)
82	PEB	JP	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.01	17 (31%)
87	CLA	2N	310	58	45,49,73	1.48	9 (20%)	54,84,113	1.58	7 (12%)
82	PEB	mH	202	2	46,46,46	2.84	11 (23%)	54,67,67	1.87	15 (27%)
82	PEB	wK	302	13	46,46,46	2.61	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	hJ	203	1	46,46,46	2.58	12 (26%)	54,67,67	2.19	19 (35%)
82	PEB	IQ	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.18	21 (38%)
84	CYC	P3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	cL	511	17	69,73,73	1.23	11 (15%)	83,113,113	1.40	7 (8%)
87	CLA	3N	306	-	49,53,73	1.45	8 (16%)	59,89,113	1.52	8 (13%)
85	BCR	BN	840	41	41,41,41	0.73	0	56,56,56	1.79	16 (28%)
87	CLA	BN	801	-	69,73,73	1.23	12 (17%)	83,113,113	1.33	7 (8%)
82	PEB	WI	202	1,2	46,46,46	2.46	13 (28%)	54,67,67	2.87	21 (38%)
84	CYC	j3	1001	73,69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
94	PL9	DL	401	18,26	55,55,55	0.73	3 (5%)	68,69,69	1.88	15 (22%)
82	PEB	u8	203	2	46,46,46	2.70	13 (28%)	54,67,67	1.98	20 (37%)
87	CLA	HL	102	22	69,73,73	1.24	9 (13%)	83,113,113	1.31	8 (9%)
88	LHG	A2	844	-	39,39,48	1.04	2 (5%)	42,45,54	1.08	2 (4%)
82	PEB	MP	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.05	17 (31%)
82	PEB	oF	203	1	46,46,46	2.68	13 (28%)	54,67,67	2.19	18 (33%)
87	CLA	d6	401	18	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
82	PEB	JD	201	1	46,46,46	2.65	14 (30%)	54,67,67	2.11	18 (33%)
87	CLA	A2	810	40	69,73,73	1.18	10 (14%)	83,113,113	1.42	7 (8%)
82	PEB	eB	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.13	19 (35%)
87	CLA	72	607	63	54,58,73	1.45	9 (16%)	65,95,113	1.48	9 (13%)
83	PUB	yF	303	14	45,46,46	2.61	9 (20%)	46,67,67	3.04	19 (41%)
82	PEB	F9	203	2	46,46,46	2.61	11 (23%)	54,67,67	2.14	18 (33%)
82	PEB	sK	202	1	46,46,46	2.72	12 (26%)	54,67,67	1.98	19 (35%)
82	PEB	kO	201	2	46,46,46	2.63	14 (30%)	54,67,67	1.93	14 (25%)
82	PEB	KI	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	L5	203	2	46,46,46	2.52	13 (28%)	54,67,67	2.17	18 (33%)
84	CYC	G3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	25 (40%)
82	PEB	RB	202	2	46,46,46	2.61	11 (23%)	54,67,67	2.11	20 (37%)
82	PEB	TI	201	1,2	46,46,46	2.37	13 (28%)	54,67,67	2.87	22 (40%)
82	PEB	FA	202	2	46,46,46	2.50	12 (26%)	54,67,67	2.69	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	DI	201	12,2	46,46,46	2.70	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	W5	203	2	46,46,46	2.57	11 (23%)	54,67,67	2.00	17 (31%)
87	CLA	ON	201	-	45,49,73	1.51	8 (17%)	54,84,113	1.54	6 (11%)
82	PEB	I7	202	1	46,46,46	2.69	13 (28%)	54,67,67	1.91	17 (31%)
82	PEB	kJ	201	2	46,46,46	2.70	14 (30%)	54,67,67	2.08	18 (33%)
82	PEB	SI	202	2	46,46,46	2.58	11 (23%)	54,67,67	1.95	15 (27%)
82	PEB	VE	201	2	46,46,46	2.60	14 (30%)	54,67,67	2.10	18 (33%)
82	PEB	ZG	202	1	46,46,46	2.62	13 (28%)	54,67,67	2.25	21 (38%)
82	PEB	M9	305	74	46,46,46	2.53	13 (28%)	54,67,67	2.34	21 (38%)
87	CLA	K2	103	-	49,53,73	1.48	12 (24%)	59,89,113	1.49	7 (11%)
87	CLA	A2	806	-	59,63,73	1.33	10 (16%)	71,101,113	1.49	8 (11%)
82	PEB	IF	202	1	46,46,46	0.64	0	54,67,67	0.78	1 (1%)
82	PEB	mH	201	2	46,46,46	2.73	15 (32%)	54,67,67	2.02	17 (31%)
82	PEB	W1	203	1,2	46,46,46	2.66	14 (30%)	54,67,67	2.25	21 (38%)
87	CLA	a6	607	15	69,73,73	1.25	10 (14%)	83,113,113	1.35	8 (9%)
82	PEB	h1	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.16	18 (33%)
87	CLA	AN	841	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	9 (10%)
85	BCR	cL	518	-	41,41,41	0.69	0	56,56,56	2.99	26 (46%)
87	CLA	c6	615	-	59,63,73	1.34	8 (13%)	71,101,113	1.40	8 (11%)
92	LMG	x6	601	37	50,50,55	0.91	2 (4%)	58,58,63	1.14	4 (6%)
82	PEB	W9	203	2	46,46,46	2.64	12 (26%)	54,67,67	2.00	16 (29%)
87	CLA	BN	825	41	69,73,73	1.30	9 (13%)	83,113,113	1.48	12 (14%)
87	CLA	AN	852	59,40	49,53,73	1.79	11 (22%)	59,89,113	2.61	19 (32%)
87	CLA	62	306	62	49,53,73	1.47	8 (16%)	59,89,113	1.54	7 (11%)
88	LHG	M6	101	-	38,38,48	1.02	2 (5%)	41,44,54	1.27	4 (9%)
82	PEB	pC	202	1	46,46,46	2.81	13 (28%)	54,67,67	2.69	23 (42%)
87	CLA	BL	603	-	69,73,73	1.26	10 (14%)	83,113,113	1.54	10 (12%)
82	PEB	BD	203	1,2	46,46,46	2.34	11 (23%)	54,67,67	2.47	18 (33%)
82	PEB	B5	201	74,2,82	46,46,46	2.63	14 (30%)	54,67,67	2.08	18 (33%)
82	PEB	B7	201	2,82	46,46,46	2.63	13 (28%)	54,67,67	2.21	20 (37%)
88	LHG	A2	843	40	48,48,48	0.93	2 (4%)	51,54,54	0.91	2 (3%)
82	PEB	MP	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.23	22 (40%)
83	PUB	BM	302	14	45,46,46	2.64	9 (20%)	46,67,67	3.02	18 (39%)
82	PEB	IP	202	1	46,46,46	2.64	11 (23%)	54,67,67	2.29	19 (35%)
101	FES	NN	101	-	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	RK	201	2	46,46,46	2.50	9 (19%)	54,67,67	3.43	21 (38%)
82	PEB	gO	203	2	46,46,46	2.72	13 (28%)	54,67,67	2.02	16 (29%)
85	BCR	B6	601	-	41,41,41	0.80	1 (2%)	56,56,56	2.08	21 (37%)
82	PEB	YQ	201	2,82	46,46,46	2.72	14 (30%)	54,67,67	1.99	15 (27%)
82	PEB	L7	202	2	46,46,46	2.49	12 (26%)	54,67,67	2.68	22 (40%)
84	CYC	DH	1003	10,9	46,46,46	2.26	15 (32%)	61,67,67	2.89	25 (40%)
85	BCR	L2	201	-	41,41,41	0.75	0	56,56,56	1.87	12 (21%)
87	CLA	c6	612	17	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
82	PEB	F9	202	2	46,46,46	2.61	11 (23%)	54,67,67	2.32	22 (40%)
82	PEB	lK	201	2	46,46,46	2.64	14 (30%)	54,67,67	2.41	17 (31%)
82	PEB	AJ	301	13	46,46,46	2.49	12 (26%)	54,67,67	2.14	19 (35%)
82	PEB	lJ	203	1	46,46,46	2.50	13 (28%)	54,67,67	2.16	20 (37%)
82	PEB	fG	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.11	21 (38%)
82	PEB	R5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
87	CLA	BN	812	-	59,63,73	1.33	10 (16%)	71,101,113	1.47	8 (11%)
82	PEB	IJ	202	1	46,46,46	2.53	13 (28%)	54,67,67	2.33	17 (31%)
87	CLA	AN	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
82	PEB	UH	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.19	19 (35%)
87	CLA	B6	606	-	69,73,73	1.25	9 (13%)	83,113,113	1.43	8 (9%)
82	PEB	AI	202	1	46,46,46	2.53	14 (30%)	54,67,67	2.10	20 (37%)
82	PEB	JK	201	2	46,46,46	2.54	11 (23%)	54,67,67	2.87	19 (35%)
87	CLA	7N	607	63	54,58,73	1.45	9 (16%)	65,95,113	1.48	9 (13%)
82	PEB	d1	202	1	46,46,46	2.67	13 (28%)	54,67,67	2.07	16 (29%)
82	PEB	EI	202	1	46,46,46	2.54	13 (28%)	54,67,67	2.11	20 (37%)
88	LHG	DL	407	18	48,48,48	0.91	2 (4%)	51,54,54	1.04	4 (7%)
82	PEB	C5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
82	PEB	aM	204	1,2	46,46,46	2.61	12 (26%)	54,67,67	2.26	18 (33%)
83	PUB	Y7	302	3	45,46,46	2.68	11 (24%)	46,67,67	2.93	20 (43%)
82	PEB	XF	203	2	46,46,46	2.75	15 (32%)	54,67,67	2.28	22 (40%)
82	PEB	nK	201	2	46,46,46	2.71	12 (26%)	54,67,67	3.00	20 (37%)
82	PEB	ZH	202	1	46,46,46	2.63	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	DQ	201	1,2	46,46,46	2.48	13 (28%)	54,67,67	2.42	20 (37%)
82	PEB	dM	203	1	46,46,46	2.62	12 (26%)	54,67,67	2.30	16 (29%)
82	PEB	wC	203	2	46,46,46	2.68	12 (26%)	54,67,67	1.94	15 (27%)
82	PEB	xC	202	1	46,46,46	2.75	13 (28%)	54,67,67	2.68	25 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	3N	313	-	49,53,73	1.49	9 (18%)	59,89,113	1.53	8 (13%)
82	PEB	HP	202	2	46,46,46	2.61	12 (26%)	54,67,67	2.08	17 (31%)
82	PEB	E7	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.01	16 (29%)
84	CYC	JH	1003	10,9	46,46,46	2.30	16 (34%)	61,67,67	2.71	27 (44%)
96	HEM	f6	101	19,20	50,50,50	1.69	9 (18%)	66,82,82	1.58	16 (24%)
82	PEB	MP	203	1,2	46,46,46	3.03	13 (28%)	54,67,67	3.15	20 (37%)
85	BCR	LN	205	50	41,41,41	0.77	0	56,56,56	3.24	24 (42%)
82	PEB	P5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	GE	1002	10,9	46,46,46	2.54	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	TM	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.17	18 (33%)
82	PEB	hE	203	1	46,46,46	2.64	11 (23%)	54,67,67	1.98	16 (29%)
84	CYC	H1	1001	10	46,46,46	2.34	17 (36%)	61,67,67	2.88	29 (47%)
82	PEB	P7	201	2	46,46,46	2.61	13 (28%)	54,67,67	2.16	16 (29%)
82	PEB	U9	204	1,2	46,46,46	2.74	13 (28%)	54,67,67	2.16	17 (31%)
85	BCR	k6	102	-	41,41,41	0.73	0	56,56,56	2.76	23 (41%)
82	PEB	DE	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	2.09	18 (33%)
82	PEB	gJ	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.10	22 (40%)
82	PEB	PQ	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.09	14 (25%)
85	BCR	b6	603	-	41,41,41	0.85	1 (2%)	56,56,56	2.15	18 (32%)
82	PEB	dQ	401	2,77	46,46,46	2.62	12 (26%)	54,67,67	2.24	18 (33%)
82	PEB	YM	201	1,2	46,46,46	2.48	12 (26%)	54,67,67	2.54	22 (40%)
82	PEB	UH	201	1,2	46,46,46	2.63	13 (28%)	54,67,67	2.39	19 (35%)
87	CLA	42	609	60	45,49,73	1.48	8 (17%)	54,84,113	1.68	8 (14%)
92	LMG	BL	612	16	39,39,55	1.06	2 (5%)	47,47,63	1.21	5 (10%)
87	CLA	AN	836	-	49,53,73	1.47	9 (18%)	59,89,113	1.58	6 (10%)
82	PEB	MK	202	1	46,46,46	2.72	12 (26%)	54,67,67	1.93	18 (33%)
91	PHO	aL	610	-	58,69,69	2.62	13 (22%)	56,99,99	2.51	13 (23%)
87	CLA	b6	605	16	69,73,73	1.43	10 (14%)	83,113,113	1.78	11 (13%)
82	PEB	D5	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.17	18 (33%)
82	PEB	R7	203	2	46,46,46	2.63	13 (28%)	54,67,67	2.41	26 (48%)
97	GOL	wL	101	-	5,5,5	0.24	0	5,5,5	0.35	0
100	3XQ	J2	104	-	24,24,24	0.20	0	25,25,25	0.23	0
82	PEB	QQ	202	2	46,46,46	2.73	15 (32%)	54,67,67	1.93	16 (29%)
87	CLA	62	309	62	54,58,73	2.13	12 (22%)	65,95,113	7.24	27 (41%)
82	PEB	OI	202	1,2	46,46,46	2.32	12 (26%)	54,67,67	3.16	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	c1	201	2	46,46,46	2.64	13 (28%)	54,67,67	2.15	20 (37%)
82	PEB	lM	203	1	46,46,46	2.56	14 (30%)	54,67,67	2.14	19 (35%)
87	CLA	A2	811	-	69,73,73	1.28	11 (15%)	83,113,113	1.56	10 (12%)
87	CLA	L2	202	50	61,65,73	1.29	8 (13%)	73,103,113	1.31	6 (8%)
87	CLA	bL	608	-	69,73,73	1.27	10 (14%)	83,113,113	1.38	7 (8%)
82	PEB	QB	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.36	18 (33%)
87	CLA	BN	835	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	6 (7%)
82	PEB	J9	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.26	22 (40%)
82	PEB	RI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
87	CLA	A2	803	40,50,53	56,60,73	1.40	11 (19%)	67,97,113	1.37	7 (10%)
92	LMG	ML	101	-	41,41,55	1.05	3 (7%)	49,49,63	1.65	9 (18%)
84	CYC	FE	1002	10	46,46,46	2.33	16 (34%)	61,67,67	2.90	24 (39%)
83	PUB	AG	302	3	45,46,46	2.70	10 (22%)	46,67,67	3.07	23 (50%)
82	PEB	VE	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.12	17 (31%)
82	PEB	OJ	203	1,2	46,46,46	2.49	12 (26%)	54,67,67	2.60	24 (44%)
82	PEB	M7	202	1	46,46,46	2.60	12 (26%)	54,67,67	1.92	13 (24%)
82	PEB	LH	1003	10	46,46,46	2.46	12 (26%)	54,67,67	2.33	17 (31%)
82	PEB	y8	201	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	OB	201	2,5	46,46,46	2.56	12 (26%)	54,67,67	2.24	17 (31%)
82	PEB	FP	201	56,2	46,46,46	2.65	14 (30%)	54,67,67	2.03	18 (33%)
82	PEB	FI	201	2	46,46,46	2.59	14 (30%)	54,67,67	2.06	19 (35%)
82	PEB	KB	303	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	OG	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.34	21 (38%)
82	PEB	cF	203	1,2	46,46,46	2.62	13 (28%)	54,67,67	2.73	23 (42%)
87	CLA	62	302	62	49,53,73	1.48	9 (18%)	59,89,113	1.41	4 (6%)
82	PEB	AK	202	1	46,46,46	2.72	13 (28%)	54,67,67	1.82	15 (27%)
82	PEB	PG	201	11,2	46,46,46	2.64	13 (28%)	54,67,67	2.35	22 (40%)
82	PEB	XK	201	2	46,46,46	2.57	10 (21%)	54,67,67	3.43	20 (37%)
87	CLA	AN	815	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	12 (14%)
92	LMG	b6	620	16	39,39,55	1.05	2 (5%)	47,47,63	1.33	5 (10%)
82	PEB	fJ	202	1	46,46,46	2.63	14 (30%)	54,67,67	2.23	19 (35%)
87	CLA	b6	616	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
83	PUB	xF	306	13	45,46,46	2.74	10 (22%)	46,67,67	2.93	19 (41%)
87	CLA	CL	515	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	6 (7%)
92	LMG	m6	101	85	41,41,55	1.01	2 (4%)	49,49,63	1.15	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	AP	203	1,2	46,46,46	3.05	13 (28%)	54,67,67	3.11	19 (35%)
82	PEB	V9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	SJ	203	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.40	21 (38%)
82	PEB	EF	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.08	20 (37%)
82	PEB	eE	201	2	46,46,46	2.65	13 (28%)	54,67,67	1.91	15 (27%)
82	PEB	Z9	304	74	46,46,46	2.54	14 (30%)	54,67,67	2.34	21 (38%)
88	LHG	mL	102	-	38,38,48	1.05	2 (5%)	41,44,54	1.08	2 (4%)
87	CLA	52	601	61	49,53,73	1.47	8 (16%)	59,89,113	1.59	7 (11%)
87	CLA	A2	840	-	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
85	BCR	bL	602	-	41,41,41	0.79	0	56,56,56	2.29	19 (33%)
87	CLA	4N	610	-	46,50,73	1.50	7 (15%)	55,85,113	1.65	7 (12%)
83	PUB	AH	304	3	45,46,46	2.95	11 (24%)	46,67,67	3.30	22 (47%)
82	PEB	QB	203	2	46,46,46	2.57	11 (23%)	54,67,67	2.04	16 (29%)
82	PEB	cE	202	2	46,46,46	2.67	11 (23%)	54,67,67	1.94	15 (27%)
82	PEB	B5	203	2	46,46,46	2.52	12 (26%)	54,67,67	2.02	19 (35%)
82	PEB	B7	203	2	46,46,46	2.66	11 (23%)	54,67,67	2.06	20 (37%)
84	CYC	c3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	12	603	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	6 (10%)
82	PEB	fE	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.12	19 (35%)
82	PEB	eG	203	2	46,46,46	2.79	14 (30%)	54,67,67	2.40	22 (40%)
87	CLA	BN	828	41	49,53,73	1.49	11 (22%)	59,89,113	1.49	7 (11%)
82	PEB	qC	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.04	16 (29%)
87	CLA	12	601	57	49,53,73	1.47	9 (18%)	59,89,113	1.58	6 (10%)
82	PEB	aM	201	13,1	46,46,46	2.61	13 (28%)	54,67,67	2.08	16 (29%)
82	PEB	iO	203	2	46,46,46	2.75	12 (26%)	54,67,67	1.85	15 (27%)
82	PEB	VG	202	2	46,46,46	2.66	13 (28%)	54,67,67	2.13	17 (31%)
82	PEB	VI	203	1,2	46,46,46	2.15	10 (21%)	54,67,67	3.09	23 (42%)
87	CLA	b6	610	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	7 (8%)
87	CLA	AN	849	40	69,73,73	1.25	10 (14%)	83,113,113	1.50	9 (10%)
82	PEB	J4	1002	10	46,46,46	2.65	14 (30%)	54,67,67	2.09	19 (35%)
96	HEM	G2	201	46	50,50,50	1.79	10 (20%)	66,82,82	1.39	7 (10%)
87	CLA	A2	835	-	69,73,73	1.20	10 (14%)	83,113,113	1.38	8 (9%)
82	PEB	lE	203	1	46,46,46	2.64	14 (30%)	54,67,67	1.96	17 (31%)
82	PEB	fJ	201	1	46,46,46	2.61	10 (21%)	54,67,67	1.99	16 (29%)
87	CLA	6N	607	62	49,53,73	1.50	9 (18%)	59,89,113	1.55	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	QO	202	1	46,46,46	0.65	0	54,67,67	0.79	1 (1%)
87	CLA	4N	607	60	49,53,73	1.52	9 (18%)	59,89,113	1.66	9 (15%)
82	PEB	DB	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.02	19 (35%)
102	BGC	3N	302	-	11,11,12	0.36	0	15,15,17	1.38	1 (6%)
82	PEB	S5	202	2	46,46,46	2.53	13 (28%)	54,67,67	2.21	16 (29%)
82	PEB	1C	203	2	46,46,46	2.73	10 (21%)	54,67,67	1.84	14 (25%)
85	BCR	F2	203	-	41,41,41	0.73	0	56,56,56	2.11	18 (32%)
87	CLA	72	605	-	49,53,73	1.48	9 (18%)	59,89,113	1.53	7 (11%)
87	CLA	5N	607	61	54,58,73	1.39	8 (14%)	65,95,113	1.57	9 (13%)
87	CLA	3N	309	59	54,58,73	1.36	7 (12%)	65,95,113	1.86	13 (20%)
82	PEB	RD	202	1	46,46,46	2.70	12 (26%)	54,67,67	1.94	16 (29%)
82	PEB	dK	202	2	46,46,46	2.91	15 (32%)	54,67,67	2.19	19 (35%)
84	CYC	EO	1001	9	46,46,46	2.34	18 (39%)	61,67,67	2.88	24 (39%)
82	PEB	dH	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.07	16 (29%)
92	LMG	qL	301	-	43,43,55	0.99	2 (4%)	51,51,63	1.18	6 (11%)
82	PEB	KJ	202	1	46,46,46	2.37	13 (28%)	54,67,67	2.62	20 (37%)
82	PEB	c1	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.35	21 (38%)
87	CLA	72	601	63	49,53,73	1.47	7 (14%)	59,89,113	1.57	6 (10%)
82	PEB	YK	203	1,2	46,46,46	2.68	15 (32%)	54,67,67	2.55	22 (40%)
82	PEB	J9	203	2	46,46,46	2.68	13 (28%)	54,67,67	2.09	16 (29%)
87	CLA	BN	816	41	59,63,73	1.34	7 (11%)	71,101,113	1.48	7 (9%)
82	PEB	aJ	203	1	46,46,46	2.58	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	R1	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.17	22 (40%)
82	PEB	sF	202	1	46,46,46	2.73	12 (26%)	54,67,67	1.99	19 (35%)
85	BCR	bL	601	87	41,41,41	0.76	0	56,56,56	1.58	11 (19%)
82	PEB	uF	202	1	46,46,46	2.73	12 (26%)	54,67,67	2.03	17 (31%)
82	PEB	QF	201	1	46,46,46	2.50	11 (23%)	54,67,67	2.37	21 (38%)
87	CLA	4N	601	60	49,53,73	1.47	9 (18%)	59,89,113	1.56	7 (11%)
82	PEB	Z1	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	g4	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.02	17 (31%)
82	PEB	f4	202	1	46,46,46	2.62	13 (28%)	54,67,67	1.96	17 (31%)
82	PEB	PK	201	2	46,46,46	2.59	10 (21%)	54,67,67	3.01	19 (35%)
85	BCR	hL	102	-	41,41,41	0.72	0	56,56,56	1.81	14 (25%)
101	FES	N2	101	-	0,4,4	-	-	-		
82	PEB	TI	203	1	46,46,46	2.53	12 (26%)	54,67,67	2.10	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	gG	202	2	46,46,46	2.68	12 (26%)	54,67,67	2.12	19 (35%)
84	CYC	DG	1001	10	46,46,46	2.29	16 (34%)	61,67,67	2.94	28 (45%)
87	CLA	5N	601	61	49,53,73	1.47	7 (14%)	59,89,113	1.61	7 (11%)
82	PEB	WF	202	1	46,46,46	2.71	12 (26%)	54,67,67	2.33	24 (44%)
82	PEB	Y7	301	3	46,46,46	2.87	13 (28%)	54,67,67	2.60	24 (44%)
82	PEB	kE	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.30	20 (37%)
87	CLA	2N	302	58	49,53,73	1.45	6 (12%)	59,89,113	1.64	6 (10%)
82	PEB	zK	501	78,2	46,46,46	2.50	11 (23%)	54,67,67	2.41	19 (35%)
87	CLA	BL	605	-	69,73,73	1.23	11 (15%)	83,113,113	1.44	6 (7%)
82	PEB	fJ	203	1,2	46,46,46	2.53	13 (28%)	54,67,67	2.28	19 (35%)
82	PEB	LK	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.54	20 (37%)
84	CYC	i3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	25 (40%)
82	PEB	lE	202	-	46,46,46	0.63	0	54,67,67	0.78	1 (1%)
82	PEB	TA	201	2	46,46,46	2.66	12 (26%)	54,67,67	2.19	16 (29%)
82	PEB	cE	201	2	46,46,46	2.62	13 (28%)	54,67,67	2.10	18 (33%)
82	PEB	KP	201	1,2	46,46,46	3.00	13 (28%)	54,67,67	3.06	19 (35%)
82	PEB	UM	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.40	20 (37%)
87	CLA	F2	201	45	49,53,73	1.52	12 (24%)	59,89,113	1.43	9 (15%)
98	PQN	A2	842	-	34,34,34	1.53	2 (5%)	42,45,45	1.00	2 (4%)
87	CLA	3N	308	59	49,53,73	2.34	6 (12%)	59,89,113	3.49	15 (25%)
82	PEB	u8	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.30	17 (31%)
87	CLA	22	605	58,41	58,62,73	1.45	10 (17%)	73,100,113	1.63	12 (16%)
87	CLA	32	309	59	54,58,73	1.36	7 (12%)	65,95,113	1.86	13 (20%)
82	PEB	WB	401	6,2	46,46,46	2.48	12 (26%)	54,67,67	2.12	19 (35%)
94	PL9	dL	406	18,26	55,55,55	0.70	3 (5%)	68,69,69	1.79	16 (23%)
82	PEB	DA	203	2	46,46,46	2.69	13 (28%)	54,67,67	2.15	20 (37%)
82	PEB	C5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
87	CLA	JN	101	48	46,50,73	1.52	10 (21%)	55,85,113	1.56	7 (12%)
85	BCR	AN	848	-	41,41,41	0.83	1 (2%)	56,56,56	2.57	20 (35%)
87	CLA	32	303	59,87	49,53,73	1.53	6 (12%)	59,89,113	1.81	11 (18%)
87	CLA	C6	520	-	69,73,73	1.23	9 (13%)	83,113,113	1.35	5 (6%)
83	PUB	AD	302	1,3	45,46,46	2.72	9 (20%)	46,67,67	3.03	18 (39%)
87	CLA	K2	101	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
82	PEB	AB	501	2,4	46,46,46	2.52	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	JA	203	2	46,46,46	2.68	12 (26%)	54,67,67	2.14	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	gM	202	2	46,46,46	2.70	11 (23%)	54,67,67	2.06	19 (35%)
87	CLA	B6	613	-	69,73,73	1.24	10 (14%)	83,113,113	1.31	5 (6%)
82	PEB	eM	201	13,2	46,46,46	2.68	14 (30%)	54,67,67	2.26	19 (35%)
87	CLA	B6	605	16	69,73,73	1.23	10 (14%)	83,113,113	1.31	6 (7%)
82	PEB	YB	201	2	46,46,46	2.60	14 (30%)	54,67,67	2.14	17 (31%)
84	CYC	DE	1001	10	46,46,46	2.29	16 (34%)	61,67,67	2.91	28 (45%)
82	PEB	QM	202	1,2	46,46,46	2.54	11 (23%)	54,67,67	2.42	20 (37%)
82	PEB	m1	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.03	18 (33%)
85	BCR	CL	502	17	41,41,41	0.88	0	56,56,56	2.37	18 (32%)
82	PEB	dD	401	2,77	46,46,46	2.61	12 (26%)	54,67,67	2.24	18 (33%)
82	PEB	YP	501	2	46,46,46	2.56	11 (23%)	54,67,67	2.08	16 (29%)
82	PEB	LK	201	2	46,46,46	2.58	12 (26%)	54,67,67	3.15	20 (37%)
82	PEB	H9	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.40	18 (33%)
82	PEB	cK	201	1	46,46,46	2.63	12 (26%)	54,67,67	2.27	19 (35%)
87	CLA	O2	203	53	49,53,73	1.64	11 (22%)	59,89,113	1.48	7 (11%)
85	BCR	FL	101	20	41,41,41	0.74	0	56,56,56	2.39	25 (44%)
87	CLA	7N	608	63	45,49,73	1.52	7 (15%)	54,84,113	1.60	8 (14%)
82	PEB	dH	201	1,2	46,46,46	2.60	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	bP	501	56,2	46,46,46	2.54	13 (28%)	54,67,67	2.05	17 (31%)
88	LHG	AL	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	4 (7%)
82	PEB	F7	202	2	46,46,46	2.49	12 (26%)	54,67,67	2.70	23 (42%)
87	CLA	K2	104	-	46,50,73	1.47	10 (21%)	55,85,113	1.73	8 (14%)
82	PEB	VM	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.04	18 (33%)
82	PEB	GA	202	1	46,46,46	2.65	13 (28%)	54,67,67	1.96	20 (37%)
92	LMG	m6	103	-	41,41,55	1.00	2 (4%)	49,49,63	1.12	5 (10%)
82	PEB	S5	203	2	46,46,46	2.49	13 (28%)	54,67,67	1.99	18 (33%)
82	PEB	SG	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.14	20 (37%)
82	PEB	PI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	fO	201	1	46,46,46	2.64	11 (23%)	54,67,67	2.24	21 (38%)
82	PEB	BI	201	2	46,46,46	2.66	14 (30%)	54,67,67	2.26	22 (40%)
82	PEB	hM	203	1	46,46,46	2.57	12 (26%)	54,67,67	2.51	18 (33%)
83	PUB	wF	304	13	45,46,46	2.59	10 (22%)	46,67,67	2.96	20 (43%)
82	PEB	UD	202	2	46,46,46	2.73	11 (23%)	54,67,67	1.97	18 (33%)
82	PEB	K5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
85	BCR	cL	503	-	41,41,41	0.72	0	56,56,56	1.82	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	QK	203	1,2	46,46,46	2.69	14 (30%)	54,67,67	3.08	22 (40%)
87	CLA	AN	827	-	59,63,73	1.36	10 (16%)	71,101,113	1.44	13 (18%)
87	CLA	bL	622	-	69,73,73	1.25	11 (15%)	83,113,113	1.38	6 (7%)
82	PEB	lF	203	1,2	46,46,46	2.72	16 (34%)	54,67,67	2.50	23 (42%)
82	PEB	aF	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.15	18 (33%)
82	PEB	R4	201	11,2	46,46,46	2.63	13 (28%)	54,67,67	2.40	17 (31%)
82	PEB	JJ	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.15	19 (35%)
82	PEB	MM	201	1,2	46,46,46	2.48	12 (26%)	54,67,67	2.49	23 (42%)
82	PEB	y8	203	2	46,46,46	2.77	13 (28%)	54,67,67	1.96	17 (31%)
87	CLA	22	604	-	46,50,73	1.49	10 (21%)	55,85,113	1.63	10 (18%)
88	LHG	dL	408	-	45,45,48	0.96	2 (4%)	48,51,54	1.04	3 (6%)
82	PEB	X5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	20 (37%)
85	BCR	HL	103	-	41,41,41	0.73	0	56,56,56	1.70	12 (21%)
82	PEB	JQ	203	1,2	46,46,46	2.48	14 (30%)	54,67,67	2.18	17 (31%)
92	LMG	bL	624	16	39,39,55	1.06	2 (5%)	47,47,63	1.20	3 (6%)
82	PEB	KQ	201	2	46,46,46	2.62	12 (26%)	54,67,67	1.95	15 (27%)
83	PUB	AH	303	3	45,46,46	2.85	10 (22%)	46,67,67	3.03	19 (41%)
87	CLA	B2	809	-	69,73,73	1.25	9 (13%)	83,113,113	1.51	6 (7%)
82	PEB	XM	202	2	46,46,46	2.65	15 (32%)	54,67,67	2.14	19 (35%)
92	LMG	jL	101	18,24	33,33,55	1.16	2 (6%)	41,41,63	1.26	4 (9%)
82	PEB	F7	201	3,2	46,46,46	2.62	9 (19%)	54,67,67	2.07	19 (35%)
82	PEB	SE	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.14	19 (35%)
82	PEB	BD	201	1	46,46,46	2.51	13 (28%)	54,67,67	2.30	19 (35%)
82	PEB	OM	201	1	46,46,46	2.63	12 (26%)	54,67,67	2.20	17 (31%)
82	PEB	AD	304	3,82	46,46,46	2.70	13 (28%)	54,67,67	2.20	18 (33%)
82	PEB	gO	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.02	17 (31%)
82	PEB	a4	201	2	46,46,46	2.59	13 (28%)	54,67,67	2.30	18 (33%)
82	PEB	UJ	203	1	46,46,46	2.54	12 (26%)	54,67,67	2.16	19 (35%)
82	PEB	W5	201	2	46,46,46	2.53	12 (26%)	54,67,67	2.28	20 (37%)
82	PEB	H1	1002	10	46,46,46	2.76	14 (30%)	54,67,67	2.24	19 (35%)
82	PEB	Z4	202	1	46,46,46	2.56	12 (26%)	54,67,67	2.01	14 (25%)
82	PEB	gM	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.07	20 (37%)
87	CLA	AN	822	40	49,53,73	1.47	10 (20%)	59,89,113	1.63	8 (13%)
85	BCR	L2	205	50	41,41,41	0.76	0	56,56,56	3.24	23 (41%)
82	PEB	yC	201	2	46,46,46	0.64	0	54,67,67	0.78	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	fK	202	2	46,46,46	2.95	14 (30%)	54,67,67	2.32	22 (40%)
85	BCR	AL	401	-	41,41,41	0.69	0	56,56,56	1.74	11 (19%)
82	PEB	BI	203	2	46,46,46	2.57	11 (23%)	54,67,67	2.18	18 (33%)
82	PEB	LE	1002	10,9	46,46,46	2.71	14 (30%)	54,67,67	2.03	18 (33%)
82	PEB	EK	202	1	46,46,46	2.62	13 (28%)	54,67,67	2.08	20 (37%)
82	PEB	mF	201	1	46,46,46	2.68	11 (23%)	54,67,67	2.01	18 (33%)
82	PEB	WA	201	1	46,46,46	2.44	12 (26%)	54,67,67	2.37	21 (38%)
87	CLA	42	605	60	49,53,73	1.49	9 (18%)	59,89,113	1.99	11 (18%)
84	CYC	K4	1001	9	46,46,46	2.36	16 (34%)	61,67,67	2.84	25 (40%)
82	PEB	HK	202	2	46,46,46	2.66	12 (26%)	54,67,67	2.24	20 (37%)
83	PUB	KA	203	1,3	45,46,46	2.69	9 (20%)	46,67,67	3.07	19 (41%)
82	PEB	jM	201	1	46,46,46	2.69	12 (26%)	54,67,67	2.26	17 (31%)
82	PEB	Z5	304	74,82	46,46,46	2.57	13 (28%)	54,67,67	2.92	22 (40%)
82	PEB	OK	201	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.48	22 (40%)
82	PEB	XD	201	1,2	46,46,46	2.59	11 (23%)	54,67,67	2.36	19 (35%)
82	PEB	KB	302	2,5	46,46,46	2.54	13 (28%)	54,67,67	2.18	16 (29%)
82	PEB	ZM	202	2	46,46,46	2.64	15 (32%)	54,67,67	2.15	17 (31%)
82	PEB	QM	203	1	46,46,46	2.65	12 (26%)	54,67,67	2.03	13 (24%)
82	PEB	SA	202	1	46,46,46	2.50	11 (23%)	54,67,67	2.02	14 (25%)
82	PEB	AE	301	3	46,46,46	2.58	13 (28%)	54,67,67	2.10	19 (35%)
87	CLA	12	610	57	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
87	CLA	52	609	61	46,50,73	1.51	8 (17%)	55,85,113	1.68	6 (10%)
82	PEB	IJ	201	1,2	46,46,46	2.52	11 (23%)	54,67,67	2.40	21 (38%)
84	CYC	73	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	DF	202	1,2	46,46,46	2.49	11 (23%)	54,67,67	2.71	23 (42%)
82	PEB	DK	202	1,2	46,46,46	2.48	11 (23%)	54,67,67	2.69	23 (42%)
82	PEB	RQ	201	1	46,46,46	2.66	13 (28%)	54,67,67	1.95	17 (31%)
82	PEB	UE	201	1,2	46,46,46	2.60	11 (23%)	54,67,67	2.39	19 (35%)
87	CLA	8N	306	64	49,53,73	1.57	12 (24%)	59,89,113	1.75	11 (18%)
84	CYC	B3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.10	28 (45%)
82	PEB	RA	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.19	19 (35%)
82	PEB	QI	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.01	19 (35%)
82	PEB	RD	203	1,2	46,46,46	2.68	14 (30%)	54,67,67	2.18	20 (37%)
87	CLA	F2	205	45	69,73,73	1.36	9 (13%)	83,113,113	1.67	12 (14%)
95	DGD	O6	301	-	41,41,67	1.05	2 (4%)	55,55,81	1.13	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	T1	202	2	46,46,46	2.63	11 (23%)	54,67,67	1.91	15 (27%)
82	PEB	fK	201	13,2	46,46,46	2.56	11 (23%)	54,67,67	2.93	18 (33%)
87	CLA	1N	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.49	6 (10%)
82	PEB	TG	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.25	20 (37%)
85	BCR	B2	841	41	41,41,41	0.77	0	56,56,56	2.31	21 (37%)
87	CLA	DL	403	18	69,73,73	1.25	12 (17%)	83,113,113	1.53	11 (13%)
82	PEB	eK	203	1	46,46,46	2.69	12 (26%)	54,67,67	2.13	17 (31%)
87	CLA	A6	402	15	69,73,73	1.25	9 (13%)	83,113,113	1.40	11 (13%)
87	CLA	D6	402	18	69,73,73	1.23	10 (14%)	83,113,113	1.36	6 (7%)
87	CLA	8N	304	64	49,53,73	1.49	10 (20%)	59,89,113	1.64	11 (18%)
82	PEB	ED	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.10	18 (33%)
82	PEB	PQ	201	1,2	46,46,46	2.67	14 (30%)	54,67,67	2.03	18 (33%)
82	PEB	kK	203	1,2	46,46,46	2.57	13 (28%)	54,67,67	2.41	19 (35%)
82	PEB	SO	201	1	46,46,46	2.68	13 (28%)	54,67,67	2.65	25 (46%)
83	PUB	A1	304	3	45,46,46	2.97	11 (24%)	46,67,67	3.30	22 (47%)
82	PEB	pF	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.29	20 (37%)
92	LMG	aL	611	-	42,42,55	1.05	2 (4%)	50,50,63	1.32	8 (16%)
82	PEB	LM	202	2	46,46,46	2.65	12 (26%)	54,67,67	2.16	21 (38%)
82	PEB	gK	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.04	18 (33%)
82	PEB	HJ	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.28	20 (37%)
82	PEB	PA	203	2	46,46,46	2.59	13 (28%)	54,67,67	2.11	18 (33%)
82	PEB	SA	201	1	46,46,46	2.58	11 (23%)	54,67,67	2.78	22 (40%)
87	CLA	AN	830	-	69,73,73	1.24	12 (17%)	83,113,113	1.35	8 (9%)
84	CYC	E3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	24 (39%)
82	PEB	HA	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.43	22 (40%)
82	PEB	fH	203	1,2	46,46,46	2.68	13 (28%)	54,67,67	2.00	17 (31%)
82	PEB	NQ	204	1,2	46,46,46	2.73	13 (28%)	54,67,67	2.20	20 (37%)
82	PEB	DK	201	2	46,46,46	2.53	10 (21%)	54,67,67	2.91	20 (37%)
82	PEB	RO	203	2	46,46,46	2.59	11 (23%)	54,67,67	1.88	15 (27%)
82	PEB	z8	202	1	46,46,46	2.72	14 (30%)	54,67,67	2.34	22 (40%)
84	CYC	ME	1001	10,9	46,46,46	2.34	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	A2	814	40	58,62,73	1.36	10 (17%)	69,99,113	1.43	6 (8%)
82	PEB	B9	202	2	46,46,46	2.63	14 (30%)	54,67,67	2.70	24 (44%)
87	CLA	D6	405	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)
82	PEB	iK	202	1	46,46,46	2.64	12 (26%)	54,67,67	2.29	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PEB	dH	203	1	46,46,46	2.69	13 (28%)	54,67,67	2.39	20 (37%)
82	PEB	W1	202	1	46,46,46	2.63	12 (26%)	54,67,67	2.32	21 (38%)
82	PEB	d4	202	1	46,46,46	2.64	14 (30%)	54,67,67	1.93	15 (27%)
82	PEB	YM	202	1	46,46,46	2.61	11 (23%)	54,67,67	2.14	15 (27%)
87	CLA	42	604	60	46,50,73	2.16	10 (21%)	55,85,113	4.30	22 (40%)
82	PEB	cB	401	6,2	46,46,46	2.66	11 (23%)	54,67,67	2.17	16 (29%)
82	PEB	iO	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.30	19 (35%)
82	PEB	mG	201	2	46,46,46	2.69	16 (34%)	54,67,67	1.95	15 (27%)
82	PEB	T5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	gH	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.00	19 (35%)
82	PEB	ZJ	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.10	17 (31%)
82	PEB	Y4	202	2	46,46,46	2.56	13 (28%)	54,67,67	2.35	22 (40%)
82	PEB	VH	202	2	46,46,46	2.70	13 (28%)	54,67,67	2.12	17 (31%)
82	PEB	AK	201	1	46,46,46	2.61	12 (26%)	54,67,67	2.28	19 (35%)
87	CLA	BL	623	16	69,73,73	1.26	11 (15%)	83,113,113	1.46	8 (9%)
87	CLA	C6	513	-	69,73,73	1.23	10 (14%)	83,113,113	1.33	5 (6%)
82	PEB	VA	203	2	46,46,46	2.70	13 (28%)	54,67,67	1.98	20 (37%)
82	PEB	hG	203	1	46,46,46	2.64	12 (26%)	54,67,67	1.97	16 (29%)
87	CLA	42	602	60	69,73,73	1.28	11 (15%)	83,113,113	1.36	7 (8%)
82	PEB	CA	202	1	46,46,46	0.64	0	54,67,67	0.79	1 (1%)
87	CLA	22	609	58	54,58,73	1.49	10 (18%)	65,95,113	1.89	14 (21%)
82	PEB	e4	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.29	22 (40%)
82	PEB	hM	202	1	46,46,46	2.64	13 (28%)	54,67,67	2.07	16 (29%)
87	CLA	A2	817	-	46,50,73	1.48	9 (19%)	55,85,113	1.58	6 (10%)
82	PEB	WQ	202	2	46,46,46	2.73	15 (32%)	54,67,67	1.92	17 (31%)
84	CYC	IO	1001	9	46,46,46	2.32	17 (36%)	61,67,67	2.83	26 (42%)
87	CLA	32	307	59	49,53,73	2.34	7 (14%)	59,89,113	3.49	14 (23%)
87	CLA	5N	611	61	49,53,73	1.49	8 (16%)	59,89,113	1.60	9 (15%)
82	PEB	cK	202	1	46,46,46	2.66	11 (23%)	54,67,67	2.04	18 (33%)
82	PEB	gH	202	2	46,46,46	2.72	13 (28%)	54,67,67	2.19	16 (29%)
82	PEB	L7	201	2,82	46,46,46	2.69	13 (28%)	54,67,67	2.15	18 (33%)
87	CLA	BL	608	-	69,73,73	1.27	9 (13%)	83,113,113	1.42	8 (9%)
82	PEB	YE	201	2	46,46,46	2.54	13 (28%)	54,67,67	2.59	22 (40%)
82	PEB	dE	201	1,3	46,46,46	2.65	13 (28%)	54,67,67	2.18	19 (35%)
92	LMG	XL	601	37	50,50,55	0.99	2 (4%)	58,58,63	1.25	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	fE	203	1,2	46,46,46	2.66	13 (28%)	54,67,67	2.14	16 (29%)
82	PEB	b1	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.03	18 (33%)
82	PEB	MA	201	1	46,46,46	2.54	11 (23%)	54,67,67	2.36	19 (35%)
95	DGD	C6	503	-	43,43,67	1.01	3 (6%)	57,57,81	1.62	11 (19%)
84	CYC	D4	1001	10	46,46,46	2.27	15 (32%)	61,67,67	2.86	26 (42%)
87	CLA	AN	817	-	46,50,73	1.49	9 (19%)	55,85,113	1.57	6 (10%)
82	PEB	Z5	301	74	46,46,46	2.55	13 (28%)	54,67,67	2.22	20 (37%)
82	PEB	SD	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.07	20 (37%)
82	PEB	r8	202	1	46,46,46	2.79	13 (28%)	54,67,67	2.38	20 (37%)
84	CYC	HO	1001	10	46,46,46	2.38	16 (34%)	61,67,67	3.01	29 (47%)
82	PEB	y8	202	2	46,46,46	2.69	11 (23%)	54,67,67	2.30	19 (35%)
87	CLA	82	303	64	49,53,73	1.50	10 (20%)	59,89,113	1.65	11 (18%)
87	CLA	7N	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	8 (13%)
82	PEB	X7	201	2,75	46,46,46	2.75	13 (28%)	54,67,67	2.29	20 (37%)
87	CLA	B6	604	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
82	PEB	OF	201	1,2	46,46,46	2.56	13 (28%)	54,67,67	2.48	22 (40%)
82	PEB	Q1	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.35	19 (35%)
82	PEB	YF	202	1	46,46,46	2.68	12 (26%)	54,67,67	1.89	17 (31%)
82	PEB	DA	201	3,2	46,46,46	2.64	14 (30%)	54,67,67	2.24	17 (31%)
82	PEB	QP	203	1,2	46,46,46	3.07	14 (30%)	54,67,67	3.04	21 (38%)
87	CLA	LN	206	50	60,64,73	1.29	9 (15%)	72,102,113	1.45	9 (12%)
82	PEB	J5	202	2	46,46,46	2.53	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	RE	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.07	18 (33%)
82	PEB	F1	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.18	16 (29%)
82	PEB	XF	202	2	46,46,46	2.49	12 (26%)	54,67,67	2.51	20 (37%)
82	PEB	XJ	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.14	19 (35%)
82	PEB	BB	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	17 (31%)
87	CLA	A2	820	-	69,73,73	1.28	10 (14%)	83,113,113	1.50	14 (16%)
95	DGD	C6	523	-	49,49,67	0.95	2 (4%)	63,63,81	1.07	4 (6%)
92	LMG	d6	409	18	54,54,55	0.89	2 (3%)	62,62,63	1.00	3 (4%)
82	PEB	Z1	203	1	46,46,46	2.76	13 (28%)	54,67,67	2.22	19 (35%)
87	CLA	C6	514	87	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
82	PEB	O1	201	1	46,46,46	2.62	14 (30%)	54,67,67	2.15	21 (38%)
82	PEB	YO	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.35	21 (38%)
82	PEB	q8	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.41	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	cO	203	2	46,46,46	2.69	13 (28%)	54,67,67	1.92	14 (25%)
85	BCR	J2	102	-	41,41,41	0.73	0	56,56,56	2.01	16 (28%)
82	PEB	HQ	202	1	46,46,46	2.63	14 (30%)	54,67,67	2.31	20 (37%)
87	CLA	6N	610	-	46,50,73	1.51	9 (19%)	55,85,113	1.70	8 (14%)
82	PEB	fG	203	1,2	46,46,46	2.65	13 (28%)	54,67,67	2.14	16 (29%)
84	CYC	HG	1001	10	46,46,46	2.26	15 (32%)	61,67,67	3.02	27 (44%)
87	CLA	A2	852	59,40	49,53,73	1.79	11 (22%)	59,89,113	2.61	19 (32%)
82	PEB	PJ	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.07	22 (40%)
82	PEB	B5	202	2	46,46,46	2.70	13 (28%)	54,67,67	2.25	20 (37%)
82	PEB	gB	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.09	15 (27%)
82	PEB	iJ	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.21	20 (37%)
82	PEB	WJ	203	1,2	46,46,46	2.45	11 (23%)	54,67,67	2.68	23 (42%)
82	PEB	eG	202	2	46,46,46	2.62	11 (23%)	54,67,67	2.25	20 (37%)
87	CLA	3N	303	59,60	49,53,73	1.57	8 (16%)	59,89,113	2.08	13 (22%)
82	PEB	AH	305	3	46,46,46	2.68	12 (26%)	54,67,67	2.10	16 (29%)
82	PEB	H4	1002	10	46,46,46	2.54	13 (28%)	54,67,67	2.05	16 (29%)
92	LMG	D6	409	18	54,54,55	0.88	2 (3%)	62,62,63	1.01	3 (4%)
82	PEB	mK	202	1	46,46,46	2.68	12 (26%)	54,67,67	2.18	17 (31%)
87	CLA	3N	304	59,87	49,53,73	1.53	6 (12%)	59,89,113	1.81	11 (18%)
82	PEB	H7	203	2	46,46,46	2.70	13 (28%)	54,67,67	2.24	19 (35%)
82	PEB	TP	202	2	46,46,46	2.66	12 (26%)	54,67,67	2.06	20 (37%)
82	PEB	O5	203	2	46,46,46	2.52	12 (26%)	54,67,67	2.11	19 (35%)
82	PEB	hE	202	1	46,46,46	2.65	14 (30%)	54,67,67	1.98	17 (31%)
85	BCR	JN	103	40,48	41,41,41	0.70	0	56,56,56	2.08	16 (28%)
87	CLA	A2	830	-	69,73,73	1.24	12 (17%)	83,113,113	1.36	8 (9%)
82	PEB	CB	202	2	46,46,46	2.73	14 (30%)	54,67,67	2.20	20 (37%)
82	PEB	CM	202	1	46,46,46	2.52	14 (30%)	54,67,67	2.18	20 (37%)
82	PEB	UA	202	1	46,46,46	2.63	13 (28%)	54,67,67	1.94	16 (29%)
82	PEB	gJ	201	2	46,46,46	2.72	14 (30%)	54,67,67	2.25	21 (38%)
87	CLA	BN	820	41	49,53,73	1.47	11 (22%)	59,89,113	1.55	8 (13%)
82	PEB	Y4	201	2	46,46,46	2.61	13 (28%)	54,67,67	2.16	20 (37%)
87	CLA	b6	607	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
82	PEB	MD	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.17	18 (33%)
82	PEB	AF	202	1	46,46,46	2.70	14 (30%)	54,67,67	1.81	15 (27%)
82	PEB	e4	201	2	46,46,46	2.58	14 (30%)	54,67,67	2.18	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	VH	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.28	20 (37%)
82	PEB	KB	301	2,5	46,46,46	2.55	12 (26%)	54,67,67	2.21	23 (42%)
82	PEB	CK	202	1	46,46,46	2.50	9 (19%)	54,67,67	2.41	19 (35%)
82	PEB	iF	202	1	46,46,46	2.65	12 (26%)	54,67,67	2.29	22 (40%)
82	PEB	eA	301	1,75	46,46,46	2.55	12 (26%)	54,67,67	2.03	15 (27%)
87	CLA	RN	201	87	49,53,73	1.50	7 (14%)	59,89,113	1.54	7 (11%)
82	PEB	cB	403	6,2	46,46,46	2.63	12 (26%)	54,67,67	2.26	24 (44%)
82	PEB	dB	201	2	46,46,46	2.54	13 (28%)	54,67,67	2.02	16 (29%)
82	PEB	CQ	201	3,2	46,46,46	2.63	14 (30%)	54,67,67	2.33	21 (38%)
84	CYC	E1	1001	10,9	46,46,46	2.35	17 (36%)	61,67,67	3.17	28 (45%)
82	PEB	iJ	201	13,2	46,46,46	2.69	13 (28%)	54,67,67	2.10	19 (35%)
87	CLA	22	610	58	45,49,73	1.49	9 (20%)	54,84,113	1.58	7 (12%)
82	PEB	P7	203	2	46,46,46	2.60	13 (28%)	54,67,67	2.10	18 (33%)
82	PEB	GQ	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.14	19 (35%)
82	PEB	ZF	201	2	46,46,46	2.67	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	CP	203	1	46,46,46	2.62	13 (28%)	54,67,67	1.98	19 (35%)
82	PEB	O4	202	1	46,46,46	2.56	14 (30%)	54,67,67	1.94	15 (27%)
82	PEB	k4	202	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	xF	302	13	46,46,46	2.71	16 (34%)	54,67,67	2.30	16 (29%)
87	CLA	BN	810	-	69,73,73	1.24	9 (13%)	83,113,113	1.51	6 (7%)
83	PUB	AO	302	3	45,46,46	2.70	9 (20%)	46,67,67	2.90	17 (36%)
87	CLA	4N	604	60	46,50,73	2.15	9 (19%)	55,85,113	4.29	22 (40%)
87	CLA	AN	803	40,50,53	56,60,73	1.40	11 (19%)	67,97,113	1.38	7 (10%)
95	DGD	c6	601	-	63,63,67	1.08	4 (6%)	77,77,81	1.82	16 (20%)
82	PEB	TJ	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.26	20 (37%)
85	BCR	AN	845	40	41,41,41	0.71	0	56,56,56	1.97	12 (21%)
82	PEB	TI	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	SM	203	1,2	46,46,46	2.57	12 (26%)	54,67,67	2.26	19 (35%)
82	PEB	LQ	201	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.28	19 (35%)
87	CLA	32	304	59,87	69,73,73	1.35	10 (14%)	83,113,113	1.87	15 (18%)
87	CLA	A2	821	-	69,73,73	1.24	10 (14%)	83,113,113	1.45	10 (12%)
82	PEB	bO	202	1	46,46,46	2.65	12 (26%)	54,67,67	1.97	15 (27%)
82	PEB	HI	202	1,2	46,46,46	2.32	13 (28%)	54,67,67	3.04	24 (44%)
82	PEB	hO	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.28	21 (38%)
82	PEB	UA	201	1	46,46,46	2.58	11 (23%)	54,67,67	2.61	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	BN	813	-	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
87	CLA	72	604	63	46,50,73	1.50	10 (21%)	55,85,113	1.60	8 (14%)
87	CLA	3N	310	59,87	45,49,73	1.51	8 (17%)	54,84,113	1.85	9 (16%)
82	PEB	PA	202	2	46,46,46	2.41	12 (26%)	54,67,67	2.67	24 (44%)
82	PEB	PO	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.45	23 (42%)
82	PEB	fH	202	1	46,46,46	2.86	11 (23%)	54,67,67	2.29	19 (35%)
87	CLA	L2	203	85,50,41	69,73,73	1.24	8 (11%)	83,113,113	1.47	6 (7%)
82	PEB	KI	201	1,2	46,46,46	2.45	14 (30%)	54,67,67	2.84	21 (38%)
87	CLA	8N	303	64	69,73,73	1.33	12 (17%)	83,113,113	1.78	14 (16%)
82	PEB	UP	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.25	19 (35%)
84	CYC	NO	1001	10	46,46,46	2.48	19 (41%)	61,67,67	2.84	27 (44%)
82	PEB	FA	201	3,2	46,46,46	2.61	10 (21%)	54,67,67	2.07	19 (35%)
82	PEB	g1	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.20	16 (29%)
85	BCR	K2	102	40,49	41,41,41	0.80	1 (2%)	56,56,56	2.74	19 (33%)
83	PUB	AE	302	3	45,46,46	2.70	10 (22%)	46,67,67	3.07	22 (47%)
82	PEB	OP	201	1,2	46,46,46	3.01	13 (28%)	54,67,67	2.87	20 (37%)
82	PEB	vF	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.01	19 (35%)
82	PEB	kG	201	3,2	46,46,46	2.65	13 (28%)	54,67,67	2.30	19 (35%)
82	PEB	V7	201	2,75	46,46,46	2.58	12 (26%)	54,67,67	2.09	15 (27%)
88	LHG	a6	610	15	42,42,48	0.97	2 (4%)	45,48,54	1.10	2 (4%)
84	CYC	FO	1001	10	46,46,46	2.31	15 (32%)	61,67,67	2.89	26 (42%)
87	CLA	KN	102	-	49,53,73	1.49	12 (24%)	59,89,113	1.49	6 (10%)
82	PEB	W4	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.64	24 (44%)
84	CYC	g3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	CL	513	17	64,68,73	1.35	9 (14%)	77,107,113	1.61	16 (20%)
87	CLA	82	305	64	49,53,73	1.57	13 (26%)	59,89,113	1.75	11 (18%)
82	PEB	DB	203	2	46,46,46	2.51	12 (26%)	54,67,67	2.16	18 (33%)
82	PEB	mO	201	2	46,46,46	2.63	12 (26%)	54,67,67	2.14	17 (31%)
82	PEB	H5	202	2	46,46,46	2.56	11 (23%)	54,67,67	2.24	18 (33%)
82	PEB	d1	203	1	46,46,46	2.69	11 (23%)	54,67,67	2.41	20 (37%)
82	PEB	lE	201	1,2	46,46,46	2.61	14 (30%)	54,67,67	2.15	17 (31%)
84	CYC	DH	1001	10	46,46,46	2.37	17 (36%)	61,67,67	2.78	24 (39%)
82	PEB	l4	202	-	46,46,46	2.62	13 (28%)	54,67,67	2.03	18 (33%)
82	PEB	XQ	203	1	46,46,46	2.70	12 (26%)	54,67,67	1.95	14 (25%)
82	PEB	EF	201	1	46,46,46	2.49	11 (23%)	54,67,67	2.37	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	CYC	JO	1001	10	46,46,46	2.31	18 (39%)	61,67,67	2.95	27 (44%)
82	PEB	GB	201	2	46,46,46	2.60	13 (28%)	54,67,67	2.13	17 (31%)
82	PEB	qF	201	1,2	46,46,46	2.63	13 (28%)	54,67,67	2.51	23 (42%)
92	LMG	dL	407	18	54,54,55	0.92	2 (3%)	62,62,63	1.34	6 (9%)
82	PEB	G5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	20 (37%)
82	PEB	UF	201	1	46,46,46	2.52	11 (23%)	54,67,67	3.22	25 (46%)
82	PEB	t8	201	1	46,46,46	2.72	14 (30%)	54,67,67	1.84	17 (31%)
82	PEB	N7	203	2	46,46,46	2.57	12 (26%)	54,67,67	2.53	22 (40%)
82	PEB	d4	201	1	46,46,46	2.54	11 (23%)	54,67,67	2.22	21 (38%)
82	PEB	OI	203	2	46,46,46	2.61	11 (23%)	54,67,67	1.98	17 (31%)
87	CLA	AN	835	-	69,73,73	1.20	10 (14%)	83,113,113	1.38	8 (9%)
87	CLA	82	302	64	69,73,73	1.33	12 (17%)	83,113,113	1.77	14 (16%)
87	CLA	AN	805	40	69,73,73	1.29	10 (14%)	83,113,113	1.32	8 (9%)
85	BCR	BN	841	41	41,41,41	0.77	0	56,56,56	2.31	21 (37%)
82	PEB	WP	201	1,2	46,46,46	3.07	13 (28%)	54,67,67	3.14	20 (37%)
82	PEB	LO	1002	10	46,46,46	2.56	13 (28%)	54,67,67	2.53	20 (37%)
82	PEB	Y5	201	74,2	46,46,46	2.54	12 (26%)	54,67,67	2.20	19 (35%)
98	PQN	B2	837	41	34,34,34	1.88	4 (11%)	42,45,45	2.53	14 (33%)
87	CLA	c6	606	17	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
82	PEB	I5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	DQ	203	1	46,46,46	2.69	12 (26%)	54,67,67	2.24	17 (31%)
82	PEB	mM	202	2	46,46,46	2.69	15 (32%)	54,67,67	2.16	21 (38%)
92	LMG	k6	101	25	55,55,55	0.89	2 (3%)	63,63,63	0.89	2 (3%)
99	SF4	CN	101	42	0,12,12	-	-	-		
82	PEB	MF	203	1,2	46,46,46	2.59	14 (30%)	54,67,67	2.56	19 (35%)
82	PEB	PP	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.11	17 (31%)
82	PEB	aE	202	2	46,46,46	2.60	14 (30%)	54,67,67	2.09	17 (31%)
82	PEB	DP	201	2	46,46,46	2.59	13 (28%)	54,67,67	2.04	16 (29%)
82	PEB	P4	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.47	23 (42%)
88	LHG	ML	102	-	38,38,48	1.03	2 (5%)	41,44,54	1.09	3 (7%)
87	CLA	BN	805	41	69,73,73	1.29	10 (14%)	83,113,113	1.40	11 (13%)
82	PEB	RM	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.19	18 (33%)
82	PEB	mE	201	2	46,46,46	2.70	16 (34%)	54,67,67	1.95	15 (27%)
82	PEB	OO	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.53	25 (46%)
82	PEB	AQ	301	3	46,46,46	2.61	12 (26%)	54,67,67	2.05	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	BP	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.02	19 (35%)
95	DGD	JL	101	-	63,63,67	0.83	2 (3%)	77,77,81	0.94	2 (2%)
87	CLA	8N	307	-	46,50,73	1.48	8 (17%)	55,85,113	1.47	6 (10%)
82	PEB	a1	202	2	46,46,46	2.75	13 (28%)	54,67,67	2.01	16 (29%)
82	PEB	kO	203	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	EJ	203	1	46,46,46	2.48	13 (28%)	54,67,67	2.14	18 (33%)
87	CLA	C6	517	-	69,73,73	1.26	10 (14%)	83,113,113	1.34	7 (8%)
82	PEB	D7	202	2	46,46,46	2.52	12 (26%)	54,67,67	2.46	21 (38%)
82	PEB	hJ	202	1	46,46,46	2.60	13 (28%)	54,67,67	1.99	17 (31%)
82	PEB	LI	202	2	46,46,46	2.53	12 (26%)	54,67,67	2.02	16 (29%)
87	CLA	I2	103	47,50	69,73,73	1.25	9 (13%)	83,113,113	1.38	9 (10%)
82	PEB	DD	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.28	17 (31%)
82	PEB	OK	202	1	46,46,46	2.53	11 (23%)	54,67,67	2.26	21 (38%)
87	CLA	AN	809	-	69,73,73	1.24	9 (13%)	83,113,113	1.51	15 (18%)
82	PEB	JO	1002	10	46,46,46	2.65	14 (30%)	54,67,67	2.10	19 (35%)
82	PEB	PE	201	11,2	46,46,46	2.65	13 (28%)	54,67,67	2.35	22 (40%)
82	PEB	RP	201	56,2	46,46,46	2.61	14 (30%)	54,67,67	2.03	17 (31%)
82	PEB	JJ	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.28	18 (33%)
82	PEB	PO	203	2	46,46,46	2.56	11 (23%)	54,67,67	1.86	16 (29%)
87	CLA	A2	849	40	69,73,73	1.26	10 (14%)	83,113,113	1.50	9 (10%)
87	CLA	A2	819	40	66,70,73	1.30	10 (15%)	79,109,113	1.52	9 (11%)
87	CLA	A2	815	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	11 (13%)
82	PEB	QK	201	1	46,46,46	2.49	11 (23%)	54,67,67	2.35	21 (38%)
82	PEB	aH	201	2	46,46,46	2.62	10 (21%)	54,67,67	2.12	19 (35%)
84	CYC	w3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
92	LMG	bL	623	-	41,41,55	0.98	2 (4%)	49,49,63	1.30	5 (10%)
82	PEB	gF	202	1	46,46,46	2.66	13 (28%)	54,67,67	2.03	18 (33%)
82	PEB	P4	201	2	46,46,46	2.64	12 (26%)	54,67,67	2.19	18 (33%)
87	CLA	bL	617	-	69,73,73	1.28	10 (14%)	83,113,113	1.54	8 (9%)
84	CYC	F1	1001	10	46,46,46	2.34	16 (34%)	61,67,67	2.84	25 (40%)
87	CLA	CL	503	-	69,73,73	1.24	11 (15%)	83,113,113	1.52	10 (12%)
98	PQN	AN	842	-	34,34,34	1.53	2 (5%)	42,45,45	1.01	2 (4%)
82	PEB	HO	1002	10	46,46,46	2.56	13 (28%)	54,67,67	2.05	16 (29%)
89	OEX	AL	408	15	0,14,14	-	-	-		
82	PEB	V4	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.20	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	AJ	302	13	46,46,46	2.58	11 (23%)	54,67,67	2.03	15 (27%)
87	CLA	AN	838	-	69,73,73	1.25	11 (15%)	83,113,113	1.38	9 (10%)
87	CLA	B2	818	-	69,73,73	1.26	10 (14%)	83,113,113	1.40	7 (8%)
82	PEB	gB	203	2	46,46,46	2.71	14 (30%)	54,67,67	2.28	22 (40%)
82	PEB	aK	203	1	46,46,46	2.70	10 (21%)	54,67,67	2.27	21 (38%)
82	PEB	QQ	201	3,2	46,46,46	2.72	12 (26%)	54,67,67	2.21	22 (40%)
82	PEB	IB	203	2	46,46,46	2.54	12 (26%)	54,67,67	2.15	18 (33%)
82	PEB	FD	203	1,2	46,46,46	2.82	15 (32%)	54,67,67	2.99	22 (40%)
82	PEB	N9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
85	BCR	B2	843	-	41,41,41	0.77	0	56,56,56	2.01	18 (32%)
82	PEB	LI	201	12,2	46,46,46	2.59	13 (28%)	54,67,67	2.04	19 (35%)
82	PEB	R1	202	2	46,46,46	2.72	13 (28%)	54,67,67	1.87	14 (25%)
82	PEB	TQ	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.10	18 (33%)
87	CLA	BL	604	-	63,67,73	1.31	11 (17%)	75,105,113	1.28	6 (8%)
82	PEB	G9	202	1	46,46,46	2.73	14 (30%)	54,67,67	2.41	20 (37%)
87	CLA	A2	826	-	69,73,73	1.28	11 (15%)	83,113,113	1.40	11 (13%)
82	PEB	K7	202	1	46,46,46	2.67	13 (28%)	54,67,67	1.89	15 (27%)
82	PEB	SB	201	2	46,46,46	2.53	12 (26%)	54,67,67	2.13	17 (31%)
87	CLA	J2	101	48	46,50,73	1.52	10 (21%)	55,85,113	1.55	8 (14%)
82	PEB	k1	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.06	21 (38%)
82	PEB	PG	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.33	24 (44%)
82	PEB	WI	203	2	46,46,46	2.64	13 (28%)	54,67,67	1.92	17 (31%)
85	BCR	AN	846	-	41,41,41	0.76	0	56,56,56	2.75	19 (33%)
82	PEB	YG	201	2	46,46,46	2.52	12 (26%)	54,67,67	2.58	22 (40%)
87	CLA	b6	604	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	5 (6%)
82	PEB	N9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.41	20 (37%)
87	CLA	B6	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
82	PEB	tK	202	2	46,46,46	2.81	13 (28%)	54,67,67	2.26	19 (35%)
87	CLA	cL	515	17	64,68,73	1.35	9 (14%)	77,107,113	1.61	14 (18%)
92	LMG	bL	611	37,16	50,50,55	0.98	2 (4%)	58,58,63	1.17	5 (8%)
87	CLA	A2	825	-	59,63,73	1.38	11 (18%)	71,101,113	1.47	9 (12%)
87	CLA	B2	824	41	69,73,73	1.30	9 (13%)	83,113,113	1.47	12 (14%)
82	PEB	HE	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	1.99	16 (29%)
82	PEB	A7	202	1	46,46,46	2.66	14 (30%)	54,67,67	2.03	16 (29%)
82	PEB	S7	202	1	46,46,46	2.50	12 (26%)	54,67,67	2.02	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	NA	202	2	46,46,46	2.40	10 (21%)	54,67,67	3.00	23 (42%)
85	BCR	B2	842	-	41,41,41	0.76	0	56,56,56	2.28	17 (30%)
82	PEB	oF	201	1	46,46,46	2.74	13 (28%)	54,67,67	2.11	19 (35%)
82	PEB	kK	201	1	46,46,46	2.71	12 (26%)	54,67,67	2.06	15 (27%)
82	PEB	BM	301	14	46,46,46	2.63	13 (28%)	54,67,67	2.34	19 (35%)
87	CLA	32	313	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	8 (13%)
87	CLA	6N	612	62	49,53,73	1.66	8 (16%)	59,89,113	2.06	15 (25%)
85	BCR	BN	842	-	41,41,41	0.77	0	56,56,56	2.28	17 (30%)
82	PEB	G9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	mO	203	2	46,46,46	2.70	14 (30%)	54,67,67	2.03	21 (38%)
82	PEB	RJ	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.20	18 (33%)
87	CLA	A2	832	40	54,58,73	1.41	11 (20%)	65,95,113	1.60	9 (13%)
82	PEB	ND	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.02	16 (29%)
82	PEB	L4	1002	10	46,46,46	2.56	13 (28%)	54,67,67	2.52	20 (37%)
82	PEB	II	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.11	20 (37%)
82	PEB	h1	203	1	46,46,46	0.64	0	54,67,67	0.79	1 (1%)
82	PEB	xK	302	13	46,46,46	2.71	15 (32%)	54,67,67	2.31	16 (29%)
87	CLA	B2	836	87,41,57	69,73,73	1.23	8 (11%)	83,113,113	1.66	9 (10%)
88	LHG	c6	619	17	31,31,48	1.11	2 (6%)	34,37,54	1.31	3 (8%)
84	CYC	J3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
96	HEM	vL	201	35	50,50,50	1.67	10 (20%)	66,82,82	1.76	16 (24%)
85	BCR	fL	101	20	41,41,41	0.74	0	56,56,56	2.42	25 (44%)
82	PEB	c4	201	2	46,46,46	2.63	11 (23%)	54,67,67	1.99	14 (25%)
84	CYC	J4	1001	10	46,46,46	2.31	18 (39%)	61,67,67	2.96	28 (45%)
84	CYC	JH	1001	10	46,46,46	2.31	18 (39%)	61,67,67	2.89	30 (49%)
82	PEB	T9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
82	PEB	eK	201	1,2	46,46,46	2.71	14 (30%)	54,67,67	2.18	19 (35%)
82	PEB	GM	201	1	46,46,46	2.64	12 (26%)	54,67,67	2.08	15 (27%)
82	PEB	jJ	203	1,2	46,46,46	2.54	13 (28%)	54,67,67	2.37	21 (38%)
85	BCR	b6	602	-	41,41,41	0.76	0	56,56,56	2.48	24 (42%)
82	PEB	wF	302	13	46,46,46	2.62	12 (26%)	54,67,67	2.06	18 (33%)
87	CLA	BN	821	54,41	47,51,73	1.43	8 (17%)	56,86,113	1.25	6 (10%)
82	PEB	XA	201	2,75	46,46,46	2.75	13 (28%)	54,67,67	2.29	20 (37%)
82	PEB	QP	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.13	20 (37%)
82	PEB	CP	201	1,2	46,46,46	2.98	14 (30%)	54,67,67	2.95	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	L2	206	50	60,64,73	1.29	9 (15%)	72,102,113	1.46	9 (12%)
87	CLA	b6	608	16	69,73,73	1.22	11 (15%)	83,113,113	1.51	10 (12%)
82	PEB	R7	202	2	46,46,46	2.48	12 (26%)	54,67,67	2.93	21 (38%)
82	PEB	JF	202	2	46,46,46	2.78	13 (28%)	54,67,67	2.42	23 (42%)
87	CLA	82	304	-	49,53,73	1.48	8 (16%)	59,89,113	1.52	7 (11%)
82	PEB	ZE	201	1,2	46,46,46	2.53	11 (23%)	54,67,67	2.51	23 (42%)
82	PEB	tC	201	1	46,46,46	2.73	14 (30%)	54,67,67	1.85	17 (31%)
84	CYC	E4	1001	9	46,46,46	2.34	18 (39%)	61,67,67	2.89	24 (39%)
93	BCT	d6	410	15,90,18	2,3,3	1.26	0	2,3,3	4.07	1 (50%)
82	PEB	hG	201	1,2	46,46,46	2.69	14 (30%)	54,67,67	2.26	15 (27%)
82	PEB	H5	201	74,2	46,46,46	2.85	16 (34%)	54,67,67	2.37	17 (31%)
87	CLA	C6	511	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
82	PEB	18	201	2	46,46,46	2.77	12 (26%)	54,67,67	2.00	17 (31%)
87	CLA	B6	608	16	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
82	PEB	YH	201	2	46,46,46	2.74	14 (30%)	54,67,67	2.25	23 (42%)
82	PEB	LF	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.54	20 (37%)
82	PEB	dJ	201	1,2	46,46,46	2.59	13 (28%)	54,67,67	2.29	19 (35%)
89	OEX	A6	405	15	0,14,14	-	-	-		
87	CLA	62	312	62	49,53,73	1.44	6 (12%)	59,89,113	1.44	4 (6%)
82	PEB	uC	202	2	46,46,46	2.59	14 (30%)	54,67,67	2.30	17 (31%)
82	PEB	IP	203	1,2	46,46,46	3.05	13 (28%)	54,67,67	3.09	19 (35%)
82	PEB	KM	202	1	46,46,46	2.48	13 (28%)	54,67,67	2.13	19 (35%)
82	PEB	jG	202	1	46,46,46	2.68	12 (26%)	54,67,67	1.89	14 (25%)
82	PEB	NF	202	2	46,46,46	2.83	14 (30%)	54,67,67	2.40	19 (35%)
87	CLA	cL	513	17	69,73,73	1.28	8 (11%)	83,113,113	1.32	6 (7%)
82	PEB	JD	202	1	46,46,46	2.59	12 (26%)	54,67,67	1.97	14 (25%)
82	PEB	S9	203	2	46,46,46	2.64	12 (26%)	54,67,67	2.08	19 (35%)
84	CYC	M1	201	10,9	46,46,46	2.30	16 (34%)	61,67,67	2.73	27 (44%)
82	PEB	eO	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.30	22 (40%)
84	CYC	C3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
87	CLA	A2	816	-	49,53,73	1.51	9 (18%)	59,89,113	1.50	5 (8%)
85	BCR	BL	618	-	41,41,41	0.73	0	56,56,56	1.83	13 (23%)
83	PUB	Z5	302	1,74	45,46,46	2.80	13 (28%)	46,67,67	3.59	25 (54%)
82	PEB	j4	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.02	16 (29%)
82	PEB	ZH	203	1	46,46,46	2.76	13 (28%)	54,67,67	2.22	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	VA	201	2,75	46,46,46	2.56	12 (26%)	54,67,67	2.08	15 (27%)
82	PEB	JA	202	2	46,46,46	2.54	12 (26%)	54,67,67	2.52	20 (37%)
82	PEB	NA	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.23	21 (38%)
82	PEB	cM	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.06	19 (35%)
84	CYC	LO	1001	10	46,46,46	2.35	18 (39%)	61,67,67	2.93	28 (45%)
87	CLA	32	302	59,60	49,53,73	1.57	8 (16%)	59,89,113	2.09	12 (20%)
87	CLA	ON	202	53	54,58,73	1.49	7 (12%)	65,95,113	1.93	13 (20%)
82	PEB	rK	202	2	46,46,46	2.80	16 (34%)	54,67,67	2.23	19 (35%)
92	LMG	bL	610	-	41,41,55	0.31	0	49,49,63	0.48	0
82	PEB	Z1	201	1,2	46,46,46	2.64	11 (23%)	54,67,67	2.96	28 (51%)
82	PEB	NI	203	1,2	46,46,46	2.39	13 (28%)	54,67,67	2.66	21 (38%)
82	PEB	dG	204	1	46,46,46	2.68	14 (30%)	54,67,67	1.99	16 (29%)
99	SF4	CN	102	42	0,12,12	-	-	-		
82	PEB	M7	201	1	46,46,46	2.56	11 (23%)	54,67,67	2.36	19 (35%)
87	CLA	b6	617	-	69,73,73	1.25	9 (13%)	83,113,113	1.33	7 (8%)
82	PEB	ZE	203	1,2	46,46,46	2.59	13 (28%)	54,67,67	2.19	18 (33%)
82	PEB	jE	202	1	46,46,46	2.67	12 (26%)	54,67,67	1.89	14 (25%)
87	CLA	1N	611	-	49,53,73	1.50	9 (18%)	59,89,113	1.49	8 (13%)
82	PEB	wC	201	2	46,46,46	2.68	12 (26%)	54,67,67	1.98	17 (31%)
87	CLA	c6	608	85,92	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
82	PEB	DJ	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	18 (33%)
82	PEB	hJ	201	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.33	20 (37%)
82	PEB	pC	201	1	46,46,46	2.66	12 (26%)	54,67,67	2.00	18 (33%)
87	CLA	cL	516	-	59,63,73	1.35	9 (15%)	71,101,113	1.43	5 (7%)
82	PEB	KF	201	1,2	46,46,46	2.48	11 (23%)	54,67,67	2.59	20 (37%)
82	PEB	YA	301	3	46,46,46	2.87	13 (28%)	54,67,67	2.60	24 (44%)
85	BCR	B6	621	92	41,41,41	0.88	2 (4%)	56,56,56	2.38	19 (33%)
82	PEB	VI	202	1	46,46,46	2.54	13 (28%)	54,67,67	2.11	20 (37%)
82	PEB	TK	202	2	46,46,46	2.77	15 (32%)	54,67,67	2.40	23 (42%)
82	PEB	AG	301	3	46,46,46	2.57	13 (28%)	54,67,67	2.08	18 (33%)
82	PEB	YP	502	2	46,46,46	2.49	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	SJ	202	1	46,46,46	2.58	13 (28%)	54,67,67	2.07	17 (31%)
95	DGD	AL	414	15	63,63,67	0.83	2 (3%)	77,77,81	1.33	9 (11%)
82	PEB	S9	201	74,2	46,46,46	2.71	14 (30%)	54,67,67	2.45	18 (33%)
82	PEB	OD	202	2	46,46,46	2.73	16 (34%)	54,67,67	1.94	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	aO	203	2	46,46,46	2.69	14 (30%)	54,67,67	1.98	17 (31%)
82	PEB	bF	202	2	46,46,46	2.93	14 (30%)	54,67,67	2.54	22 (40%)
82	PEB	I7	201	1	46,46,46	2.60	14 (30%)	54,67,67	2.14	15 (27%)
87	CLA	2N	309	58	54,58,73	1.50	10 (18%)	65,95,113	1.88	14 (21%)
82	PEB	xC	201	1	46,46,46	2.69	12 (26%)	54,67,67	1.87	15 (27%)
87	CLA	aL	605	15	69,73,73	1.26	10 (14%)	83,113,113	1.49	10 (12%)
82	PEB	HF	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.23	19 (35%)
82	PEB	AQ	303	3,82	46,46,46	2.71	14 (30%)	54,67,67	2.11	20 (37%)
94	PL9	d6	408	18,26	55,55,55	0.62	2 (3%)	68,69,69	1.98	21 (30%)
89	OEX	aL	608	15	0,14,14	-	-	-		
87	CLA	CL	505	-	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
87	CLA	H6	102	22	69,73,73	1.23	10 (14%)	83,113,113	1.32	8 (9%)
82	PEB	IB	202	2	46,46,46	2.45	13 (28%)	54,67,67	2.14	20 (37%)
87	CLA	BN	819	-	69,73,73	1.27	9 (13%)	83,113,113	1.39	7 (8%)
82	PEB	PB	201	2	46,46,46	2.66	12 (26%)	54,67,67	2.26	19 (35%)
82	PEB	Q4	202	1	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	R9	201	1	46,46,46	2.62	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	N5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	iM	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.06	19 (35%)
82	PEB	uK	202	1	46,46,46	2.77	13 (28%)	54,67,67	1.86	17 (31%)
95	DGD	C6	502	-	63,63,67	1.08	4 (6%)	77,77,81	1.82	16 (20%)
84	CYC	D1	1001	10	46,46,46	2.35	15 (32%)	61,67,67	2.79	24 (39%)
82	PEB	uC	203	2	46,46,46	2.71	13 (28%)	54,67,67	1.98	19 (35%)
88	LHG	C6	522	17	31,31,48	1.12	2 (6%)	34,37,54	1.57	4 (11%)
87	CLA	CL	506	-	69,73,73	1.24	11 (15%)	83,113,113	1.63	12 (14%)
95	DGD	cL	519	-	63,63,67	0.84	2 (3%)	77,77,81	0.95	3 (3%)
82	PEB	R4	203	2	46,46,46	2.59	11 (23%)	54,67,67	1.87	14 (25%)
82	PEB	Q9	201	2	46,46,46	2.72	12 (26%)	54,67,67	2.04	15 (27%)
87	CLA	5N	610	-	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
82	PEB	BA	203	2	46,46,46	2.65	12 (26%)	54,67,67	2.06	18 (33%)
87	CLA	42	606	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
87	CLA	A6	404	15	54,58,73	1.38	9 (16%)	65,95,113	1.53	8 (12%)
85	BCR	AN	804	-	41,41,41	0.76	0	56,56,56	2.07	17 (30%)
82	PEB	SH	203	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.41	22 (40%)
82	PEB	NM	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.45	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	a6	608	-	64,68,73	1.29	10 (15%)	77,107,113	1.43	11 (14%)
82	PEB	DQ	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.80	26 (48%)
82	PEB	bF	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.07	18 (33%)
82	PEB	lG	202	1	46,46,46	2.59	14 (30%)	54,67,67	1.97	15 (27%)
82	PEB	RD	201	1	46,46,46	2.67	13 (28%)	54,67,67	1.95	16 (29%)
84	CYC	m3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	bL	618	-	69,73,73	1.25	11 (15%)	83,113,113	1.53	10 (12%)
82	PEB	ID	201	2,77	46,46,46	2.68	14 (30%)	54,67,67	2.79	23 (42%)
82	PEB	KJ	201	1	46,46,46	2.57	11 (23%)	54,67,67	2.22	18 (33%)
82	PEB	r8	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.14	19 (35%)
87	CLA	BN	833	-	51,55,73	1.44	12 (23%)	61,91,113	1.48	11 (18%)
82	PEB	jJ	202	1	46,46,46	2.68	11 (23%)	54,67,67	2.03	17 (31%)
82	PEB	M9	302	74	46,46,46	2.57	11 (23%)	54,67,67	2.31	22 (40%)
82	PEB	O9	203	2	46,46,46	2.68	14 (30%)	54,67,67	2.08	19 (35%)
88	LHG	bL	612	16	48,48,48	0.94	2 (4%)	51,54,54	1.07	3 (5%)
96	HEM	GN	201	46	50,50,50	1.79	10 (20%)	66,82,82	1.39	7 (10%)
82	PEB	iG	201	2	46,46,46	2.67	13 (28%)	54,67,67	1.96	16 (29%)
82	PEB	VF	201	2	46,46,46	2.58	11 (23%)	54,67,67	2.40	18 (33%)
87	CLA	BL	619	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	8 (9%)
82	PEB	WF	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.59	27 (50%)
82	PEB	FQ	202	1	46,46,46	2.70	13 (28%)	54,67,67	1.97	18 (33%)
82	PEB	E7	201	1	46,46,46	2.73	14 (30%)	54,67,67	2.22	17 (31%)
82	PEB	vK	201	2	46,46,46	2.69	12 (26%)	54,67,67	2.74	21 (38%)
82	PEB	QJ	204	1	46,46,46	2.57	13 (28%)	54,67,67	2.12	15 (27%)
82	PEB	jK	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.17	17 (31%)
84	CYC	KG	202	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.78	24 (39%)
82	PEB	mF	202	1	46,46,46	2.68	12 (26%)	54,67,67	2.17	17 (31%)
84	CYC	LH	1001	10,9	46,46,46	2.37	14 (30%)	61,67,67	2.99	28 (45%)
87	CLA	A2	834	-	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)
82	PEB	cJ	202	2	46,46,46	2.65	12 (26%)	54,67,67	2.25	19 (35%)
87	CLA	7N	601	63	49,53,73	1.48	7 (14%)	59,89,113	1.57	6 (10%)
82	PEB	ZB	201	2	46,46,46	2.62	13 (28%)	54,67,67	1.97	18 (33%)
82	PEB	jO	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.01	16 (29%)
82	PEB	OG	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.08	17 (31%)
87	CLA	RN	204	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	sK	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.11	16 (29%)
82	PEB	MI	401	-	46,46,46	0.63	0	54,67,67	0.78	1 (1%)
82	PEB	GD	202	2	46,46,46	2.69	12 (26%)	54,67,67	2.14	21 (38%)
87	CLA	cL	508	-	69,73,73	1.25	11 (15%)	83,113,113	1.53	10 (12%)
82	PEB	cO	201	2	46,46,46	2.62	11 (23%)	54,67,67	1.98	14 (25%)
83	PUB	xK	305	13	45,46,46	2.76	9 (20%)	46,67,67	2.88	19 (41%)
84	CYC	N3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	25 (40%)
82	PEB	SO	202	1,76	46,46,46	2.53	14 (30%)	54,67,67	2.00	16 (29%)
82	PEB	QE	202	1	46,46,46	2.64	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	YA	303	3,82	46,46,46	2.62	13 (28%)	54,67,67	2.59	22 (40%)
82	PEB	aB	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.01	20 (37%)
82	PEB	KJ	203	1,2	46,46,46	2.45	12 (26%)	54,67,67	2.69	21 (38%)
82	PEB	SP	201	1,2	46,46,46	3.03	13 (28%)	54,67,67	2.94	20 (37%)
87	CLA	1N	604	-	46,50,73	1.49	10 (21%)	55,85,113	1.54	6 (10%)
82	PEB	AP	202	1	46,46,46	2.60	14 (30%)	54,67,67	2.00	17 (31%)
83	PUB	wK	304	13	45,46,46	2.58	11 (24%)	46,67,67	2.96	20 (43%)
84	CYC	L4	1001	10	46,46,46	2.35	18 (39%)	61,67,67	2.93	28 (45%)
82	PEB	T7	201	2	46,46,46	2.65	12 (26%)	54,67,67	2.19	17 (31%)
82	PEB	SM	201	1	46,46,46	2.64	12 (26%)	54,67,67	1.97	14 (25%)
82	PEB	sF	203	1,2	46,46,46	2.75	15 (32%)	54,67,67	2.55	20 (37%)
82	PEB	zC	202	1	46,46,46	2.72	12 (26%)	54,67,67	2.33	22 (40%)
82	PEB	mJ	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.05	18 (33%)
83	PUB	A4	303	3	45,46,46	2.66	9 (20%)	46,67,67	2.86	15 (32%)
84	CYC	BG	1001	10,8	46,46,46	2.44	18 (39%)	61,67,67	2.82	28 (45%)
82	PEB	DF	201	2	46,46,46	2.54	10 (21%)	54,67,67	2.92	21 (38%)
82	PEB	OP	203	1	46,46,46	2.53	12 (26%)	54,67,67	2.39	19 (35%)
82	PEB	T4	203	2	46,46,46	2.60	11 (23%)	54,67,67	1.91	16 (29%)
84	CYC	q3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	W9	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.28	18 (33%)
82	PEB	WF	203	1	46,46,46	2.69	13 (28%)	54,67,67	1.97	16 (29%)
84	CYC	G4	1001	9	46,46,46	2.40	16 (34%)	61,67,67	2.79	25 (40%)
87	CLA	BN	827	-	69,73,73	1.32	10 (14%)	83,113,113	1.45	11 (13%)
82	PEB	WK	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.32	24 (44%)
82	PEB	YO	203	2	46,46,46	2.60	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	qC	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.41	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	BCR	BL	617	-	41,41,41	0.78	0	56,56,56	2.24	18 (32%)
87	CLA	A2	822	40	49,53,73	1.47	10 (20%)	59,89,113	1.63	8 (13%)
82	PEB	m4	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.37	20 (37%)
82	PEB	CI	202	1	46,46,46	2.53	13 (28%)	54,67,67	2.11	20 (37%)
94	PL9	D6	408	18,26	55,55,55	0.64	2 (3%)	68,69,69	2.02	23 (33%)
82	PEB	cB	402	6,2	46,46,46	2.54	11 (23%)	54,67,67	2.21	19 (35%)
82	PEB	j1	201	1	46,46,46	2.61	12 (26%)	54,67,67	2.22	19 (35%)
82	PEB	GI	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	jH	203	1,2	46,46,46	2.69	16 (34%)	54,67,67	2.42	19 (35%)
87	CLA	AN	828	40	69,73,73	1.36	9 (13%)	83,113,113	1.58	13 (15%)
82	PEB	Y9	203	2	46,46,46	2.60	12 (26%)	54,67,67	2.04	15 (27%)
82	PEB	AO	304	3	46,46,46	2.60	11 (23%)	54,67,67	2.07	17 (31%)
82	PEB	ZG	203	1	46,46,46	2.58	13 (28%)	54,67,67	2.18	18 (33%)
87	CLA	42	611	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	4 (6%)
88	LHG	L6	101	26	48,48,48	0.90	2 (4%)	51,54,54	1.13	4 (7%)
88	LHG	d6	407	18	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
82	PEB	gK	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.51	21 (38%)
82	PEB	gF	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.53	21 (38%)
82	PEB	UJ	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.36	21 (38%)
99	SF4	B2	803	-	0,12,12	-	-	-		
82	PEB	NH	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.03	14 (25%)
82	PEB	mJ	201	13,2	46,46,46	2.73	13 (28%)	54,67,67	2.43	21 (38%)
82	PEB	bO	201	1	46,46,46	2.66	11 (23%)	54,67,67	2.31	21 (38%)
82	PEB	CD	202	2	46,46,46	2.66	12 (26%)	54,67,67	1.99	17 (31%)
82	PEB	WE	202	1,77	46,46,46	2.54	13 (28%)	54,67,67	2.10	17 (31%)
87	CLA	1N	608	57	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
87	CLA	A2	841	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	9 (10%)
82	PEB	fM	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.03	14 (25%)
87	CLA	B2	823	-	69,73,73	1.27	11 (15%)	83,113,113	1.46	13 (15%)
82	PEB	T4	202	2	46,46,46	2.61	14 (30%)	54,67,67	2.27	20 (37%)
97	GOL	WL	101	-	5,5,5	0.22	0	5,5,5	0.34	0
82	PEB	QA	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.72	20 (37%)
82	PEB	F4	1002	10	46,46,46	2.57	12 (26%)	54,67,67	2.24	21 (38%)
87	CLA	CL	518	-	50,54,73	1.44	10 (20%)	60,90,113	1.45	6 (10%)
87	CLA	IN	103	47,50	69,73,73	1.25	9 (13%)	83,113,113	1.39	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	B6	611	-	69,73,73	1.25	9 (13%)	83,113,113	1.37	7 (8%)
87	CLA	AN	839	-	69,73,73	1.24	8 (11%)	83,113,113	1.41	9 (10%)
87	CLA	O2	201	-	45,49,73	1.50	8 (17%)	54,84,113	1.52	6 (11%)
82	PEB	m4	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.15	17 (31%)
82	PEB	mE	203	2	46,46,46	2.65	14 (30%)	54,67,67	2.04	15 (27%)
87	CLA	c6	614	17	64,68,73	1.30	8 (12%)	77,107,113	1.41	10 (12%)
87	CLA	bL	614	-	69,73,73	1.25	8 (11%)	83,113,113	1.46	9 (10%)
87	CLA	CL	509	17	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
85	BCR	aL	604	-	41,41,41	0.70	0	56,56,56	1.72	11 (19%)
87	CLA	BL	620	16	69,73,73	1.28	12 (17%)	83,113,113	1.41	6 (7%)
82	PEB	jM	203	1,2	46,46,46	2.57	13 (28%)	54,67,67	2.32	17 (31%)
82	PEB	AH	301	3	46,46,46	2.70	11 (23%)	54,67,67	2.03	15 (27%)
82	PEB	e7	301	1,75	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
87	CLA	82	308	-	49,53,73	1.49	11 (22%)	59,89,113	2.07	12 (20%)
87	CLA	12	609	-	46,50,73	1.50	9 (19%)	55,85,113	1.67	9 (16%)
82	PEB	X7	203	2	46,46,46	2.61	14 (30%)	54,67,67	2.34	23 (42%)
87	CLA	A2	801	40,45	69,73,73	1.27	9 (13%)	83,113,113	1.43	10 (12%)
82	PEB	L9	203	2	46,46,46	2.64	12 (26%)	54,67,67	2.08	18 (33%)
87	CLA	62	303	62	69,73,73	1.28	8 (11%)	83,113,113	1.29	10 (12%)
82	PEB	MF	202	1	46,46,46	2.71	13 (28%)	54,67,67	1.92	18 (33%)
82	PEB	IJ	203	1	46,46,46	2.53	14 (30%)	54,67,67	2.36	18 (33%)
87	CLA	c6	604	17	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
82	PEB	dO	202	1	46,46,46	2.63	14 (30%)	54,67,67	1.92	15 (27%)
82	PEB	fM	203	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.38	20 (37%)
82	PEB	RB	201	6,2	46,46,46	2.75	12 (26%)	54,67,67	2.24	18 (33%)
87	CLA	2N	307	58	49,53,73	1.47	8 (16%)	59,89,113	1.51	9 (15%)
87	CLA	R2	202	54	49,53,73	1.50	8 (16%)	59,89,113	1.54	8 (13%)
84	CYC	v3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	25 (40%)
97	GOL	I6	102	-	5,5,5	0.24	0	5,5,5	0.21	0
82	PEB	PF	202	2	46,46,46	2.88	15 (32%)	54,67,67	2.31	20 (37%)
82	PEB	WH	201	1	46,46,46	2.57	11 (23%)	54,67,67	2.25	18 (33%)
82	PEB	AI	203	1,2	46,46,46	2.40	14 (30%)	54,67,67	2.83	22 (40%)
95	DGD	aL	603	15	54,54,67	0.91	2 (3%)	68,68,81	1.04	2 (2%)
82	PEB	aJ	204	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.57	22 (40%)
82	PEB	IF	201	1	46,46,46	2.53	12 (26%)	54,67,67	3.18	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	1C	201	2	46,46,46	2.78	13 (28%)	54,67,67	2.01	17 (31%)
82	PEB	U9	203	2	46,46,46	2.69	11 (23%)	54,67,67	1.98	15 (27%)
87	CLA	1N	602	57	69,73,73	1.21	6 (8%)	83,113,113	1.44	9 (10%)
82	PEB	M9	304	74	46,46,46	2.69	13 (28%)	54,67,67	2.24	18 (33%)
82	PEB	E5	202	1	46,46,46	2.58	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	LA	202	2	46,46,46	2.48	12 (26%)	54,67,67	2.69	23 (42%)
92	LMG	B6	622	37,16	50,50,55	0.92	2 (4%)	58,58,63	1.04	4 (6%)
85	BCR	KN	104	-	41,41,41	0.83	0	56,56,56	2.48	19 (33%)
82	PEB	lM	202	1	46,46,46	2.58	11 (23%)	54,67,67	2.16	17 (31%)
82	PEB	SQ	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.09	15 (27%)
82	PEB	HK	201	2	46,46,46	2.48	13 (28%)	54,67,67	2.89	27 (50%)
82	PEB	q8	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.04	16 (29%)
83	PUB	AQ	302	1,3	45,46,46	2.73	9 (20%)	46,67,67	3.03	18 (39%)
87	CLA	BN	815	41	46,50,73	1.47	10 (21%)	55,85,113	1.62	8 (14%)
82	PEB	PD	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.10	15 (27%)
85	BCR	JN	102	-	41,41,41	0.74	0	56,56,56	2.00	16 (28%)
82	PEB	AD	301	3	46,46,46	2.63	12 (26%)	54,67,67	2.06	21 (38%)
82	PEB	eF	201	1,2	46,46,46	2.71	14 (30%)	54,67,67	2.19	21 (38%)
85	BCR	K6	102	-	41,41,41	0.73	0	56,56,56	2.77	23 (41%)
82	PEB	P1	202	2	46,46,46	2.69	12 (26%)	54,67,67	2.02	18 (33%)
84	CYC	FE	1001	10,9	46,46,46	2.36	18 (39%)	61,67,67	2.78	25 (40%)
82	PEB	D1	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.05	17 (31%)
87	CLA	12	604	-	46,50,73	1.49	10 (21%)	55,85,113	1.55	6 (10%)
82	PEB	ED	201	2,77	46,46,46	2.62	14 (30%)	54,67,67	2.36	20 (37%)
82	PEB	IA	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.14	15 (27%)
88	LHG	aL	607	15	42,42,48	0.98	2 (4%)	45,48,54	1.09	2 (4%)
82	PEB	PI	202	1	46,46,46	2.54	14 (30%)	54,67,67	2.11	20 (37%)
82	PEB	CQ	202	2	46,46,46	2.66	12 (26%)	54,67,67	1.96	16 (29%)
82	PEB	IF	203	1,2	46,46,46	2.50	12 (26%)	54,67,67	2.85	24 (44%)
87	CLA	A2	836	-	49,53,73	1.48	9 (18%)	59,89,113	1.57	6 (10%)
82	PEB	aO	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.47	22 (40%)
95	DGD	B2	844	41	67,67,67	0.87	2 (2%)	81,81,81	1.00	4 (4%)
82	PEB	eF	203	1	46,46,46	2.69	12 (26%)	54,67,67	2.14	17 (31%)
82	PEB	OE	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.09	18 (33%)
82	PEB	WJ	202	1	46,46,46	2.47	13 (28%)	54,67,67	2.54	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	62	310	-	45,49,73	1.51	8 (17%)	54,84,113	1.54	6 (11%)
82	PEB	AF	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	T7	203	2	46,46,46	2.63	12 (26%)	54,67,67	2.26	21 (38%)
82	PEB	LA	201	2,82	46,46,46	2.67	13 (28%)	54,67,67	2.13	18 (33%)
96	HEM	V6	201	35	50,50,50	1.61	10 (20%)	66,82,82	1.72	18 (27%)
87	CLA	A2	839	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	9 (10%)
82	PEB	DO	1002	10	46,46,46	2.59	12 (26%)	54,67,67	2.16	18 (33%)
82	PEB	ND	204	1,2	46,46,46	2.72	11 (23%)	54,67,67	2.19	19 (35%)
82	PEB	G7	202	1	46,46,46	2.65	12 (26%)	54,67,67	1.97	20 (37%)
95	DGD	BN	844	41	67,67,67	0.87	2 (2%)	81,81,81	0.99	4 (4%)
87	CLA	22	601	58	49,53,73	1.45	6 (12%)	59,89,113	1.63	6 (10%)
88	LHG	CL	522	17	31,31,48	1.11	2 (6%)	34,37,54	1.54	5 (14%)
82	PEB	f1	202	1	46,46,46	2.85	11 (23%)	54,67,67	2.29	19 (35%)
82	PEB	TO	202	2	46,46,46	2.60	13 (28%)	54,67,67	2.26	20 (37%)
82	PEB	ZH	201	1,2	46,46,46	2.63	11 (23%)	54,67,67	2.95	28 (51%)
82	PEB	i1	201	2	46,46,46	2.67	14 (30%)	54,67,67	2.10	16 (29%)
82	PEB	RP	202	2	46,46,46	2.55	11 (23%)	54,67,67	2.09	19 (35%)
84	CYC	O3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.10	28 (45%)
87	CLA	72	606	63	49,53,73	1.53	10 (20%)	59,89,113	1.53	7 (11%)
82	PEB	L7	203	2	46,46,46	2.66	12 (26%)	54,67,67	1.89	18 (33%)
82	PEB	oK	201	1	46,46,46	2.72	12 (26%)	54,67,67	2.11	19 (35%)
82	PEB	LJ	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.11	17 (31%)
84	CYC	KO	1001	9	46,46,46	2.36	16 (34%)	61,67,67	2.84	25 (40%)
87	CLA	c6	616	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
87	CLA	C6	518	-	64,68,73	1.30	10 (15%)	77,107,113	1.35	4 (5%)
87	CLA	bL	606	-	69,73,73	1.27	13 (18%)	83,113,113	1.32	7 (8%)
82	PEB	k4	201	2	46,46,46	2.62	14 (30%)	54,67,67	1.93	14 (25%)
82	PEB	NI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	19 (35%)
87	CLA	7N	610	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
82	PEB	OH	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.13	18 (33%)
87	CLA	2N	301	58,41	58,62,73	1.45	10 (17%)	73,100,113	1.63	12 (16%)
87	CLA	B2	829	-	47,51,73	1.45	9 (19%)	56,86,113	1.56	4 (7%)
82	PEB	jH	202	1	46,46,46	2.72	13 (28%)	54,67,67	2.20	19 (35%)
82	PEB	OM	202	1	46,46,46	2.58	15 (32%)	54,67,67	2.37	23 (42%)
82	PEB	rC	202	1	46,46,46	2.78	14 (30%)	54,67,67	2.37	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
83	PUB	AG	303	3	45,46,46	2.71	9 (20%)	46,67,67	2.85	16 (34%)
82	PEB	DG	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	2.09	18 (33%)
87	CLA	6N	609	-	45,49,73	1.51	7 (15%)	54,84,113	1.53	6 (11%)
82	PEB	YI	201	12,2	46,46,46	2.51	13 (28%)	54,67,67	2.08	19 (35%)
82	PEB	V7	202	2	46,46,46	2.51	12 (26%)	54,67,67	2.61	23 (42%)
82	PEB	WD	202	2	46,46,46	2.72	15 (32%)	54,67,67	1.92	16 (29%)
87	CLA	R2	203	54,41	50,54,73	1.45	8 (16%)	60,90,113	1.43	5 (8%)
82	PEB	CM	203	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.60	23 (42%)
82	PEB	bK	202	2	46,46,46	2.93	12 (26%)	54,67,67	2.52	21 (38%)
87	CLA	AN	814	40	58,62,73	1.37	10 (17%)	69,99,113	1.44	6 (8%)
82	PEB	BB	203	2	46,46,46	2.60	12 (26%)	54,67,67	2.20	19 (35%)
82	PEB	HB	203	2	46,46,46	2.58	12 (26%)	54,67,67	2.19	17 (31%)
85	BCR	BN	839	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
82	PEB	O1	203	1,2	46,46,46	2.56	11 (23%)	54,67,67	2.37	21 (38%)
82	PEB	BK	201	2	46,46,46	2.56	12 (26%)	54,67,67	3.32	19 (35%)
87	CLA	7N	604	63	46,50,73	1.51	10 (21%)	55,85,113	1.59	8 (14%)
82	PEB	gK	203	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.47	19 (35%)
82	PEB	GB	202	2	46,46,46	2.53	11 (23%)	54,67,67	2.06	17 (31%)
82	PEB	M9	301	74,2	46,46,46	2.54	12 (26%)	54,67,67	1.86	16 (29%)
82	PEB	EA	201	1	46,46,46	2.74	14 (30%)	54,67,67	2.23	17 (31%)
82	PEB	18	203	2	46,46,46	2.71	11 (23%)	54,67,67	1.84	14 (25%)
82	PEB	Y1	201	2	46,46,46	2.75	14 (30%)	54,67,67	2.25	23 (42%)
87	CLA	cL	505	-	69,73,73	1.24	9 (13%)	83,113,113	1.49	11 (13%)
93	BCT	aL	612	15,90,18	2,3,3	1.22	0	2,3,3	3.86	1 (50%)
95	DGD	CL	523	-	49,49,67	0.97	2 (4%)	63,63,81	1.12	4 (6%)
88	LHG	dL	405	18	48,48,48	0.90	2 (4%)	51,54,54	1.02	3 (5%)
82	PEB	iK	203	1	46,46,46	2.70	13 (28%)	54,67,67	1.92	16 (29%)
82	PEB	h4	202	1	46,46,46	2.63	12 (26%)	54,67,67	1.95	16 (29%)
87	CLA	B2	806	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	6 (7%)
82	PEB	J1	1002	10	46,46,46	2.53	13 (28%)	54,67,67	2.19	17 (31%)
82	PEB	OH	201	1	46,46,46	2.61	14 (30%)	54,67,67	2.15	21 (38%)
95	DGD	a6	602	-	41,41,67	1.04	2 (4%)	55,55,81	1.16	4 (7%)
82	PEB	J9	201	2	46,46,46	2.76	15 (32%)	54,67,67	2.25	18 (33%)
87	CLA	c6	613	17	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
84	CYC	U3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	TQ	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.13	14 (25%)
82	PEB	lJ	202	1	46,46,46	2.55	13 (28%)	54,67,67	2.44	21 (38%)
82	PEB	eG	201	2	46,46,46	2.66	14 (30%)	54,67,67	1.92	16 (29%)
82	PEB	e4	203	2	46,46,46	2.56	11 (23%)	54,67,67	1.92	13 (24%)
92	LMG	bL	609	-	41,41,55	0.31	0	49,49,63	0.56	0
87	CLA	cL	517	-	69,73,73	1.26	10 (14%)	83,113,113	1.34	6 (7%)
87	CLA	BN	823	-	69,73,73	1.27	11 (15%)	83,113,113	1.34	13 (15%)
87	CLA	LN	204	50	54,58,73	1.46	10 (18%)	65,95,113	1.75	11 (16%)
82	PEB	gH	203	1,74,2	46,46,46	2.62	13 (28%)	54,67,67	2.29	19 (35%)
82	PEB	EM	201	1,2	46,46,46	2.60	13 (28%)	54,67,67	2.33	20 (37%)
82	PEB	CB	201	2,4	46,46,46	2.62	12 (26%)	54,67,67	2.23	20 (37%)
82	PEB	EP	202	1	46,46,46	2.60	12 (26%)	54,67,67	2.04	16 (29%)
82	PEB	VQ	202	1	46,46,46	2.79	12 (26%)	54,67,67	1.94	15 (27%)
84	CYC	R3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	24 (39%)
87	CLA	bL	615	-	69,73,73	1.23	10 (14%)	83,113,113	1.32	8 (9%)
87	CLA	AN	851	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
87	CLA	A2	831	-	69,73,73	1.32	11 (15%)	83,113,113	1.50	11 (13%)
95	DGD	b6	621	-	41,41,67	1.10	2 (4%)	55,55,81	1.35	7 (12%)
92	LMG	CL	519	-	55,55,55	0.87	2 (3%)	63,63,63	1.06	4 (6%)
87	CLA	CL	508	87	69,73,73	1.28	10 (14%)	83,113,113	1.48	9 (10%)
82	PEB	VD	202	1	46,46,46	2.78	12 (26%)	54,67,67	1.94	15 (27%)
85	BCR	F6	101	20	41,41,41	0.81	1 (2%)	56,56,56	2.31	17 (30%)
85	BCR	B6	602	-	41,41,41	0.79	0	56,56,56	2.15	17 (30%)
82	PEB	u8	201	2	46,46,46	2.68	15 (32%)	54,67,67	2.31	22 (40%)
82	PEB	XQ	202	1	46,46,46	2.70	14 (30%)	54,67,67	1.90	16 (29%)
83	PUB	QM	201	14,1	45,46,46	2.77	10 (22%)	46,67,67	2.95	20 (43%)
82	PEB	N4	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.14	20 (37%)
82	PEB	P9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
82	PEB	YF	203	1,2	46,46,46	2.69	13 (28%)	54,67,67	2.56	22 (40%)
82	PEB	LB	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.20	17 (31%)
87	CLA	AN	813	-	69,73,73	1.20	9 (13%)	83,113,113	1.34	5 (6%)
84	CYC	Q3	1001	73,69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	RH	202	2	46,46,46	2.72	13 (28%)	54,67,67	1.88	15 (27%)
82	PEB	xK	303	13	46,46,46	2.64	12 (26%)	54,67,67	1.88	12 (22%)
82	PEB	FF	202	2	46,46,46	2.66	14 (30%)	54,67,67	2.37	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	NB	202	2	46,46,46	2.53	12 (26%)	54,67,67	2.06	16 (29%)
82	PEB	JM	201	2	46,46,46	2.68	13 (28%)	54,67,67	2.06	19 (35%)
82	PEB	L1	1002	10	46,46,46	2.47	12 (26%)	54,67,67	2.33	17 (31%)
82	PEB	U5	202	2	46,46,46	2.58	11 (23%)	54,67,67	2.25	18 (33%)
82	PEB	GP	203	1	46,46,46	2.62	14 (30%)	54,67,67	1.95	16 (29%)
82	PEB	OH	203	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.38	20 (37%)
82	PEB	RG	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.23	20 (37%)
82	PEB	K9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.42	21 (38%)
82	PEB	SG	203	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.50	20 (37%)
96	HEM	v6	201	35	50,50,50	1.60	10 (20%)	66,82,82	1.72	17 (25%)
82	PEB	V5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.06	18 (33%)
96	HEM	FL	102	-	50,50,50	1.66	8 (16%)	66,82,82	1.68	15 (22%)
84	CYC	NE	201	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.78	25 (40%)
82	PEB	JA	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.14	16 (29%)
82	PEB	W7	202	1	46,46,46	2.68	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	FA	203	2	46,46,46	2.74	13 (28%)	54,67,67	1.93	21 (38%)
83	PUB	AJ	303	13	45,46,46	2.61	9 (20%)	46,67,67	3.19	21 (45%)
82	PEB	VG	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.11	18 (33%)
87	CLA	A2	805	40	69,73,73	1.28	10 (14%)	83,113,113	1.33	8 (9%)
82	PEB	EP	201	1	46,46,46	2.57	14 (30%)	54,67,67	2.07	17 (31%)
82	PEB	HI	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.12	19 (35%)
82	PEB	bE	201	1	46,46,46	2.65	13 (28%)	54,67,67	2.20	17 (31%)
87	CLA	AN	821	-	69,73,73	1.23	11 (15%)	83,113,113	1.44	10 (12%)
87	CLA	2N	303	58	69,73,73	1.45	6 (8%)	83,113,113	2.61	18 (21%)
87	CLA	b6	613	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
82	PEB	A9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.41	20 (37%)
87	CLA	A2	833	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
82	PEB	WM	203	1,2	46,46,46	2.47	11 (23%)	54,67,67	2.48	20 (37%)
82	PEB	GA	201	1	46,46,46	2.50	11 (23%)	54,67,67	2.32	16 (29%)
87	CLA	C6	512	-	69,73,73	1.23	9 (13%)	83,113,113	1.35	6 (7%)
82	PEB	ZK	202	2	46,46,46	2.82	15 (32%)	54,67,67	2.14	20 (37%)
95	DGD	L6	102	26	59,59,67	0.87	2 (3%)	73,73,81	1.17	7 (9%)
82	PEB	A1	305	3	46,46,46	2.69	14 (30%)	54,67,67	2.09	17 (31%)
87	CLA	52	605	61	49,53,73	1.48	9 (18%)	59,89,113	1.50	6 (10%)
82	PEB	ZO	202	1	46,46,46	2.56	12 (26%)	54,67,67	2.00	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	kO	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.35	20 (37%)
82	PEB	XB	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.23	20 (37%)
85	BCR	A2	848	-	41,41,41	0.83	1 (2%)	56,56,56	2.57	20 (35%)
87	CLA	B2	814	41	46,50,73	1.47	10 (21%)	55,85,113	1.63	8 (14%)
82	PEB	b1	202	1	46,46,46	2.76	11 (23%)	54,67,67	2.29	22 (40%)
82	PEB	S5	201	74,2	46,46,46	2.70	14 (30%)	54,67,67	2.22	20 (37%)
82	PEB	TF	202	2	46,46,46	2.76	15 (32%)	54,67,67	2.39	24 (44%)
87	CLA	FN	201	45	45,49,73	1.54	8 (17%)	54,84,113	1.71	8 (14%)
87	CLA	2N	311	-	46,50,73	1.49	9 (19%)	55,85,113	1.65	7 (12%)
82	PEB	hM	201	1,2	46,46,46	2.52	13 (28%)	54,67,67	2.29	19 (35%)
82	PEB	D4	1002	10	46,46,46	2.60	12 (26%)	54,67,67	2.16	18 (33%)
82	PEB	FJ	201	79,2	46,46,46	2.74	12 (26%)	54,67,67	2.50	20 (37%)
82	PEB	kH	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.06	21 (38%)
82	PEB	AO	305	3	46,46,46	2.62	12 (26%)	54,67,67	2.02	17 (31%)
88	LHG	i6	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.77	2 (3%)
82	PEB	Y5	203	2	46,46,46	2.50	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	uF	201	1,2	46,46,46	2.68	14 (30%)	54,67,67	2.16	15 (27%)
83	PUB	xF	305	13	45,46,46	2.76	9 (20%)	46,67,67	2.88	20 (43%)
87	CLA	AN	810	40	69,73,73	1.19	10 (14%)	83,113,113	1.43	7 (8%)
82	PEB	f4	201	1	46,46,46	2.66	12 (26%)	54,67,67	2.24	21 (38%)
82	PEB	RI	202	1	46,46,46	2.53	13 (28%)	54,67,67	2.11	20 (37%)
82	PEB	IM	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.20	16 (29%)
82	PEB	cF	202	1,10	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
87	CLA	BN	822	-	59,63,73	1.36	10 (16%)	71,101,113	1.42	7 (9%)
82	PEB	eK	202	1	46,46,46	2.60	12 (26%)	54,67,67	2.32	22 (40%)
85	BCR	BN	838	-	41,41,41	0.74	0	56,56,56	2.49	21 (37%)
87	CLA	A2	851	-	69,73,73	1.23	10 (14%)	83,113,113	1.40	8 (9%)
82	PEB	N7	202	2	46,46,46	2.41	10 (21%)	54,67,67	2.99	23 (42%)
87	CLA	b6	615	-	69,73,73	1.23	10 (14%)	83,113,113	1.30	6 (7%)
82	PEB	IK	202	1	46,46,46	0.65	0	54,67,67	0.79	1 (1%)
87	CLA	BN	802	41	62,66,73	1.41	9 (14%)	74,104,113	1.65	14 (18%)
82	PEB	HI	203	2	46,46,46	2.59	12 (26%)	54,67,67	2.06	17 (31%)
82	PEB	VO	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.50	23 (42%)
82	PEB	AQ	304	3,82	46,46,46	2.70	13 (28%)	54,67,67	2.20	18 (33%)
82	PEB	VP	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.12	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PEB	AD	303	3,82	46,46,46	2.71	14 (30%)	54,67,67	2.11	20 (37%)
87	CLA	72	610	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	6 (10%)
84	CYC	DO	1001	10	46,46,46	2.27	15 (32%)	61,67,67	2.87	26 (42%)
82	PEB	tK	201	2	46,46,46	2.68	11 (23%)	54,67,67	2.73	19 (35%)
82	PEB	lK	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.11	19 (35%)
82	PEB	FP	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.13	19 (35%)
82	PEB	AA	201	1	46,46,46	2.68	14 (30%)	54,67,67	2.14	22 (40%)
82	PEB	eJ	201	13,2	46,46,46	2.64	13 (28%)	54,67,67	2.16	19 (35%)
87	CLA	4N	608	60	54,58,73	1.42	10 (18%)	65,95,113	1.77	17 (26%)
82	PEB	bB	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.21	19 (35%)
82	PEB	S1	201	1	46,46,46	2.62	13 (28%)	54,67,67	2.27	16 (29%)
82	PEB	aK	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.15	19 (35%)
82	PEB	KP	202	1	46,46,46	2.50	12 (26%)	54,67,67	2.24	19 (35%)
82	PEB	KB	304	2,5	46,46,46	2.49	12 (26%)	54,67,67	2.07	20 (37%)
84	CYC	FH	1001	10	46,46,46	2.34	16 (34%)	61,67,67	2.85	25 (40%)
82	PEB	cG	202	2	46,46,46	2.68	12 (26%)	54,67,67	1.94	15 (27%)
87	CLA	B2	828	41	49,53,73	1.49	11 (22%)	59,89,113	1.49	7 (11%)
87	CLA	dL	404	-	69,73,73	1.23	8 (11%)	83,113,113	1.41	9 (10%)
82	PEB	LP	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.04	17 (31%)
84	CYC	C4	1001	9	46,46,46	2.36	16 (34%)	61,67,67	2.88	28 (45%)
87	CLA	AN	823	40	69,73,73	1.23	11 (15%)	83,113,113	1.45	10 (12%)
87	CLA	B2	820	54,41	47,51,73	1.42	9 (19%)	56,86,113	1.26	6 (10%)
82	PEB	U5	203	2	46,46,46	2.59	13 (28%)	54,67,67	1.96	17 (31%)
87	CLA	BN	807	-	69,73,73	1.26	11 (15%)	83,113,113	1.28	6 (7%)
82	PEB	JK	202	2	46,46,46	2.78	14 (30%)	54,67,67	2.41	23 (42%)
82	PEB	Y5	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.27	18 (33%)
91	PHO	d6	404	-	58,69,69	2.66	13 (22%)	56,99,99	2.72	19 (33%)
82	PEB	ZM	201	2	46,46,46	2.72	14 (30%)	54,67,67	2.23	19 (35%)
82	PEB	H5	203	2	46,46,46	2.60	11 (23%)	54,67,67	1.88	16 (29%)
83	PUB	Z9	305	1,74	45,46,46	2.92	11 (24%)	46,67,67	4.11	25 (54%)
85	BCR	I2	101	-	41,41,41	0.77	0	56,56,56	2.36	15 (26%)
84	CYC	N1	1001	10,8	46,46,46	2.41	18 (39%)	61,67,67	2.74	28 (45%)
87	CLA	b6	614	-	63,67,73	1.30	10 (15%)	75,105,113	1.38	6 (8%)
87	CLA	7N	606	63	49,53,73	1.53	9 (18%)	59,89,113	1.54	7 (11%)
82	PEB	OM	203	1,2	46,46,46	2.63	12 (26%)	54,67,67	2.27	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	C6	509	-	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
95	DGD	lL	101	26	59,59,67	0.91	2 (3%)	73,73,81	1.58	11 (15%)
82	PEB	YB	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.04	18 (33%)
82	PEB	YO	201	2	46,46,46	2.60	13 (28%)	54,67,67	2.16	20 (37%)
82	PEB	V7	203	2	46,46,46	2.69	13 (28%)	54,67,67	1.97	19 (35%)
87	CLA	32	310	59,87	45,49,73	1.51	9 (20%)	54,84,113	1.84	9 (16%)
82	PEB	QP	201	1	46,46,46	2.61	14 (30%)	54,67,67	2.10	17 (31%)
82	PEB	FM	201	79,2	46,46,46	2.73	13 (28%)	54,67,67	2.31	21 (38%)
82	PEB	pK	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.42	21 (38%)
82	PEB	H9	201	74,2	46,46,46	2.67	13 (28%)	54,67,67	1.97	16 (29%)
95	DGD	b6	622	-	43,43,67	1.06	3 (6%)	57,57,81	1.22	5 (8%)
88	LHG	cL	501	17	31,31,48	1.11	2 (6%)	34,37,54	1.50	5 (14%)
85	BCR	CL	516	-	41,41,41	0.72	0	56,56,56	2.91	21 (37%)
87	CLA	B2	816	-	63,67,73	1.34	10 (15%)	75,105,113	1.42	9 (12%)
82	PEB	P7	202	2	46,46,46	2.43	12 (26%)	54,67,67	2.67	24 (44%)
85	BCR	IN	101	-	41,41,41	0.76	0	56,56,56	2.36	15 (26%)
82	PEB	Z9	301	74	46,46,46	2.58	11 (23%)	54,67,67	2.31	22 (40%)
84	CYC	F3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	AN	831	-	69,73,73	1.31	11 (15%)	83,113,113	1.50	11 (13%)
82	PEB	L9	201	2	46,46,46	2.68	14 (30%)	54,67,67	2.00	15 (27%)
82	PEB	MQ	202	2	46,46,46	2.59	11 (23%)	54,67,67	2.00	15 (27%)
82	PEB	iH	202	2	46,46,46	2.76	12 (26%)	54,67,67	1.88	13 (24%)
82	PEB	HA	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.08	17 (31%)
103	ZEX	8N	309	64	42,43,43	0.82	1 (2%)	55,60,60	2.15	16 (29%)
87	CLA	C6	510	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	8 (9%)
84	CYC	CO	1001	9	46,46,46	2.37	16 (34%)	61,67,67	2.87	27 (44%)
82	PEB	kM	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.11	19 (35%)
82	PEB	lH	202	1	46,46,46	2.77	13 (28%)	54,67,67	2.30	19 (35%)
87	CLA	1N	607	57	54,58,73	1.39	8 (14%)	65,95,113	1.53	10 (15%)
82	PEB	yC	203	2	46,46,46	2.77	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	GP	202	1	46,46,46	2.55	12 (26%)	54,67,67	2.29	18 (33%)
82	PEB	C9	202	1	46,46,46	2.74	13 (28%)	54,67,67	2.42	20 (37%)
82	PEB	kG	202	2	46,46,46	2.63	14 (30%)	54,67,67	2.11	15 (27%)
82	PEB	DF	203	2	46,46,46	2.68	14 (30%)	54,67,67	2.08	20 (37%)
82	PEB	CK	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.15	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	A5	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	j4	201	1	46,46,46	2.64	13 (28%)	54,67,67	2.29	22 (40%)
82	PEB	gE	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	17 (31%)
82	PEB	P9	202	1	46,46,46	2.74	13 (28%)	54,67,67	2.41	21 (38%)
85	BCR	A2	847	-	41,41,41	0.80	0	56,56,56	1.99	18 (32%)
83	PUB	K7	203	1,3	45,46,46	2.69	9 (20%)	46,67,67	3.07	19 (41%)
82	PEB	AP	201	1	46,46,46	2.51	11 (23%)	54,67,67	2.23	17 (31%)
82	PEB	iO	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.05	18 (33%)
87	CLA	AN	850	40	69,73,73	1.28	9 (13%)	83,113,113	1.36	8 (9%)
87	CLA	BL	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.33	7 (8%)
82	PEB	XD	203	1	46,46,46	2.68	12 (26%)	54,67,67	1.96	15 (27%)
87	CLA	3N	312	59	49,53,73	1.48	9 (18%)	59,89,113	1.50	7 (11%)
82	PEB	qF	202	1	46,46,46	2.59	13 (28%)	54,67,67	3.09	23 (42%)
87	CLA	dL	402	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	9 (10%)
85	BCR	B2	802	87,50,41	41,41,41	0.77	0	56,56,56	3.37	24 (42%)
82	PEB	QF	202	1	46,46,46	2.61	12 (26%)	54,67,67	1.92	17 (31%)
82	PEB	G5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	M5	304	74,82	46,46,46	2.58	13 (28%)	54,67,67	2.92	22 (40%)
84	CYC	M4	1001	9	46,46,46	2.30	15 (32%)	61,67,67	2.85	22 (36%)
82	PEB	jE	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.08	19 (35%)
87	CLA	4N	602	60	69,73,73	1.28	11 (15%)	83,113,113	1.35	7 (8%)
82	PEB	kE	202	2	46,46,46	2.63	11 (23%)	54,67,67	2.12	17 (31%)
82	PEB	XI	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.12	20 (37%)
82	PEB	WQ	201	3,2	46,46,46	2.63	13 (28%)	54,67,67	2.30	19 (35%)
82	PEB	Z4	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.83	25 (46%)
82	PEB	UI	201	2	46,46,46	2.65	14 (30%)	54,67,67	2.10	21 (38%)
82	PEB	XK	202	2	46,46,46	2.50	12 (26%)	54,67,67	2.51	20 (37%)
82	PEB	UM	202	1	46,46,46	2.60	13 (28%)	54,67,67	2.20	15 (27%)
82	PEB	JB	202	1	46,46,46	2.70	13 (28%)	54,67,67	2.50	20 (37%)
82	PEB	c4	203	2	46,46,46	2.70	13 (28%)	54,67,67	1.92	14 (25%)
87	CLA	F2	202	45	45,49,73	1.54	8 (17%)	54,84,113	1.71	8 (14%)
84	CYC	L1	1001	10	46,46,46	2.53	20 (43%)	61,67,67	3.05	34 (55%)
82	PEB	QB	204	2	46,46,46	2.66	13 (28%)	54,67,67	2.10	17 (31%)
82	PEB	EK	201	1	46,46,46	2.48	11 (23%)	54,67,67	2.37	17 (31%)
82	PEB	GK	202	1	46,46,46	2.49	12 (26%)	54,67,67	3.22	25 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	qK	201	1,2	46,46,46	2.62	13 (28%)	54,67,67	2.49	23 (42%)
82	PEB	UG	203	1	46,46,46	2.64	13 (28%)	54,67,67	2.02	18 (33%)
87	CLA	B2	825	-	69,73,73	1.22	12 (17%)	83,113,113	1.33	7 (8%)
82	PEB	HB	202	2	46,46,46	2.57	12 (26%)	54,67,67	2.12	18 (33%)
82	PEB	XP	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.07	17 (31%)
87	CLA	2N	308	58	49,53,73	1.52	8 (16%)	59,89,113	1.51	11 (18%)
83	PUB	xK	306	13	45,46,46	2.75	10 (22%)	46,67,67	2.93	19 (41%)
87	CLA	5N	609	61	46,50,73	1.50	9 (19%)	55,85,113	1.70	6 (10%)
82	PEB	XF	201	2	46,46,46	2.55	10 (21%)	54,67,67	3.42	20 (37%)
83	PUB	M5	303	1,74	45,46,46	2.80	11 (24%)	46,67,67	3.46	18 (39%)
82	PEB	HF	201	2	46,46,46	2.48	13 (28%)	54,67,67	2.89	28 (51%)
84	CYC	EE	1001	10,9	46,46,46	2.42	19 (41%)	61,67,67	2.80	26 (42%)
83	PUB	YA	302	3	45,46,46	2.67	11 (24%)	46,67,67	2.93	21 (45%)
87	CLA	IN	102	-	69,73,73	1.23	9 (13%)	83,113,113	1.36	6 (7%)
82	PEB	iH	201	2	46,46,46	2.67	14 (30%)	54,67,67	2.10	16 (29%)
82	PEB	EQ	201	2,77	46,46,46	2.61	14 (30%)	54,67,67	2.35	21 (38%)
82	PEB	WP	202	1	46,46,46	2.55	12 (26%)	54,67,67	2.22	18 (33%)
83	PUB	Z9	302	74	45,46,46	2.85	11 (24%)	46,67,67	3.45	20 (43%)
82	PEB	KK	202	1	46,46,46	2.67	12 (26%)	54,67,67	2.30	17 (31%)
87	CLA	AN	834	-	69,73,73	1.24	10 (14%)	83,113,113	1.44	9 (10%)
82	PEB	MK	203	1,2	46,46,46	2.59	14 (30%)	54,67,67	2.55	19 (35%)
82	PEB	xF	303	13	46,46,46	2.64	11 (23%)	54,67,67	1.89	13 (24%)
82	PEB	w8	201	2	46,46,46	2.68	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	1C	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.16	15 (27%)
82	PEB	PE	202	2	46,46,46	2.63	12 (26%)	54,67,67	2.33	24 (44%)
82	PEB	hO	202	1	46,46,46	2.63	12 (26%)	54,67,67	1.95	16 (29%)
83	PUB	M9	303	74	45,46,46	2.85	11 (24%)	46,67,67	3.45	21 (45%)
82	PEB	mK	201	1	46,46,46	2.68	11 (23%)	54,67,67	2.03	19 (35%)
84	CYC	W3	1001	71	46,46,46	2.54	17 (36%)	61,67,67	3.18	31 (50%)
82	PEB	hE	201	1,2	46,46,46	2.69	15 (32%)	54,67,67	2.26	15 (27%)
82	PEB	kF	202	1	46,46,46	2.72	13 (28%)	54,67,67	1.80	15 (27%)
82	PEB	dB	202	2	46,46,46	2.63	12 (26%)	54,67,67	2.13	16 (29%)
82	PEB	NA	203	2	46,46,46	2.56	12 (26%)	54,67,67	2.53	22 (40%)
82	PEB	CM	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.11	15 (27%)
95	DGD	DL	408	18	63,63,67	0.86	2 (3%)	77,77,81	1.07	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	DB	202	2	46,46,46	2.52	13 (28%)	54,67,67	2.10	18 (33%)
82	PEB	HB	201	2	46,46,46	2.70	13 (28%)	54,67,67	2.47	19 (35%)
82	PEB	VP	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.02	19 (35%)
82	PEB	eJ	202	2	46,46,46	2.57	12 (26%)	54,67,67	2.22	23 (42%)
82	PEB	MF	201	1	46,46,46	2.61	11 (23%)	54,67,67	1.95	14 (25%)
87	CLA	bL	604	-	50,54,73	1.44	9 (18%)	60,90,113	1.55	5 (8%)
82	PEB	RQ	203	1,2	46,46,46	2.67	14 (30%)	54,67,67	2.18	20 (37%)
82	PEB	NE	202	10,9	46,46,46	2.61	15 (32%)	54,67,67	2.11	17 (31%)
82	PEB	gE	202	2	46,46,46	2.67	11 (23%)	54,67,67	2.12	19 (35%)
91	PHO	dL	403	-	58,69,69	2.58	13 (22%)	56,99,99	2.75	19 (33%)
82	PEB	q8	203	2	46,46,46	2.67	12 (26%)	54,67,67	2.01	17 (31%)
83	PUB	AE	303	3	45,46,46	2.69	9 (20%)	46,67,67	2.85	16 (34%)
87	CLA	62	304	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	4 (6%)
84	CYC	IE	1001	10,9	46,46,46	2.40	16 (34%)	61,67,67	2.89	25 (40%)
82	PEB	LD	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.23	15 (27%)
85	BCR	a6	605	-	41,41,41	0.81	1 (2%)	56,56,56	1.92	18 (32%)
82	PEB	B9	201	2	46,46,46	2.67	12 (26%)	54,67,67	2.15	16 (29%)
87	CLA	5N	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.42	4 (6%)
82	PEB	TD	201	1,2	46,46,46	2.57	15 (32%)	54,67,67	2.23	16 (29%)
87	CLA	CL	504	-	69,73,73	1.29	10 (14%)	83,113,113	1.34	9 (10%)
82	PEB	F7	203	2	46,46,46	2.75	13 (28%)	54,67,67	1.94	20 (37%)
82	PEB	QG	202	1	46,46,46	2.64	13 (28%)	54,67,67	2.04	18 (33%)
82	PEB	MM	202	1	46,46,46	2.51	13 (28%)	54,67,67	2.24	16 (29%)
82	PEB	SI	201	2	46,46,46	2.54	13 (28%)	54,67,67	2.08	18 (33%)
82	PEB	K7	201	1	46,46,46	2.73	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	NG	201	10,9	46,46,46	2.60	15 (32%)	54,67,67	2.11	17 (31%)
82	PEB	MJ	203	1	46,46,46	2.34	13 (28%)	54,67,67	2.31	18 (33%)
87	CLA	1N	605	57	49,53,73	1.48	7 (14%)	59,89,113	1.50	6 (10%)
82	PEB	T5	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.27	20 (37%)
82	PEB	Q9	203	2	46,46,46	2.71	12 (26%)	54,67,67	1.98	19 (35%)
82	PEB	O4	201	1	46,46,46	2.59	12 (26%)	54,67,67	2.54	24 (44%)
82	PEB	Z9	303	74	46,46,46	2.69	13 (28%)	54,67,67	2.25	18 (33%)
82	PEB	i4	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.31	19 (35%)
84	CYC	EG	1001	10,9	46,46,46	2.41	19 (41%)	61,67,67	2.80	26 (42%)
82	PEB	BJ	301	14	46,46,46	2.59	13 (28%)	54,67,67	2.35	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	CYC	MG	1001	10,9	46,46,46	2.35	18 (39%)	61,67,67	2.91	25 (40%)
87	CLA	M2	101	51,41	49,53,73	1.48	11 (22%)	59,89,113	1.62	11 (18%)
87	CLA	82	301	64	49,53,73	1.52	11 (22%)	59,89,113	1.68	9 (15%)
82	PEB	EQ	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.11	18 (33%)
82	PEB	TQ	201	1,2	46,46,46	2.56	15 (32%)	54,67,67	2.24	16 (29%)
82	PEB	D7	201	3,2	46,46,46	2.65	14 (30%)	54,67,67	2.24	17 (31%)
88	LHG	AL	407	15	42,42,48	0.97	2 (4%)	45,48,54	1.08	2 (4%)
82	PEB	PD	202	1	46,46,46	2.77	12 (26%)	54,67,67	2.16	18 (33%)
87	CLA	7N	602	62,63	69,73,73	1.38	10 (14%)	83,113,113	1.79	18 (21%)
82	PEB	w8	203	2	46,46,46	2.68	12 (26%)	54,67,67	1.94	16 (29%)
82	PEB	PH	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.01	18 (33%)
82	PEB	a4	202	2	46,46,46	2.60	13 (28%)	54,67,67	2.48	23 (42%)
84	CYC	L3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	jK	201	2	46,46,46	2.63	11 (23%)	54,67,67	2.66	22 (40%)
82	PEB	Q7	202	1	46,46,46	2.53	12 (26%)	54,67,67	2.02	14 (25%)
85	BCR	h6	102	-	41,41,41	0.80	0	56,56,56	2.08	14 (25%)
82	PEB	QH	203	1	46,46,46	2.61	11 (23%)	54,67,67	2.12	18 (33%)
82	PEB	SP	203	1	46,46,46	2.83	13 (28%)	54,67,67	2.03	17 (31%)
92	LMG	b6	623	-	41,41,55	0.27	0	49,49,63	0.35	0
82	PEB	BF	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.26	18 (33%)
92	LMG	j6	101	-	43,43,55	1.00	3 (6%)	51,51,63	2.16	12 (23%)
82	PEB	yC	202	2	46,46,46	2.70	11 (23%)	54,67,67	2.30	19 (35%)
82	PEB	iE	202	2	46,46,46	2.68	12 (26%)	54,67,67	1.98	18 (33%)
82	PEB	iF	203	1	46,46,46	2.69	12 (26%)	54,67,67	1.93	16 (29%)
82	PEB	WM	202	1	46,46,46	2.52	12 (26%)	54,67,67	2.42	19 (35%)
87	CLA	6N	608	62	54,58,73	2.14	12 (22%)	65,95,113	7.23	27 (41%)
87	CLA	72	608	63	45,49,73	1.52	7 (15%)	54,84,113	1.59	8 (14%)
82	PEB	YJ	203	1	46,46,46	2.36	13 (28%)	54,67,67	2.17	20 (37%)
82	PEB	b4	202	1	46,46,46	2.66	12 (26%)	54,67,67	1.97	15 (27%)
82	PEB	H9	203	2	46,46,46	2.70	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	GF	202	1	46,46,46	2.49	12 (26%)	54,67,67	3.21	25 (46%)
82	PEB	YF	201	1	46,46,46	2.64	11 (23%)	54,67,67	2.12	19 (35%)
82	PEB	V1	202	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.41	21 (38%)
82	PEB	TH	201	11,2	46,46,46	2.59	15 (32%)	54,67,67	2.31	23 (42%)
82	PEB	NJ	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.28	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	J5	201	2	46,46,46	2.63	12 (26%)	54,67,67	2.16	19 (35%)
85	BCR	AN	847	-	41,41,41	0.79	0	56,56,56	1.99	18 (32%)
92	LMG	mL	101	-	41,41,55	1.06	3 (7%)	49,49,63	1.63	8 (16%)
82	PEB	RE	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.23	19 (35%)
82	PEB	QD	201	3,2	46,46,46	2.73	11 (23%)	54,67,67	2.21	23 (42%)
82	PEB	eM	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.09	17 (31%)
82	PEB	aM	203	1	46,46,46	2.59	12 (26%)	54,67,67	2.40	17 (31%)
96	HEM	VL	201	35	50,50,50	1.67	11 (22%)	66,82,82	1.76	16 (24%)
87	CLA	A2	827	-	59,63,73	1.36	10 (16%)	71,101,113	1.43	13 (18%)
82	PEB	HQ	201	1,2	46,46,46	2.51	12 (26%)	54,67,67	2.41	20 (37%)
82	PEB	IB	201	2	46,46,46	2.52	12 (26%)	54,67,67	2.08	16 (29%)
82	PEB	m1	202	2	46,46,46	2.84	12 (26%)	54,67,67	1.86	14 (25%)
87	CLA	4N	611	-	49,53,73	1.47	10 (20%)	59,89,113	1.49	4 (6%)
82	PEB	UE	203	1	46,46,46	2.64	14 (30%)	54,67,67	2.02	18 (33%)
84	CYC	h3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	aG	201	2	46,46,46	2.62	13 (28%)	54,67,67	2.19	20 (37%)
82	PEB	FD	201	1	46,46,46	2.53	14 (30%)	54,67,67	2.60	22 (40%)
87	CLA	A2	809	-	69,73,73	1.25	9 (13%)	83,113,113	1.52	15 (18%)
82	PEB	TB	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.50	20 (37%)
82	PEB	kF	203	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.40	18 (33%)
82	PEB	UB	301	2,5	46,46,46	2.65	13 (28%)	54,67,67	2.17	18 (33%)
82	PEB	BF	201	2	46,46,46	2.56	12 (26%)	54,67,67	3.30	19 (35%)
82	PEB	CF	202	1	46,46,46	2.52	9 (19%)	54,67,67	2.41	19 (35%)
82	PEB	LG	1002	10,9	46,46,46	2.72	13 (28%)	54,67,67	2.04	19 (35%)
82	PEB	iE	201	2	46,46,46	2.68	13 (28%)	54,67,67	1.96	16 (29%)
82	PEB	WI	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.23	20 (37%)
87	CLA	42	610	-	46,50,73	1.49	7 (15%)	55,85,113	1.64	7 (12%)
92	LMG	AL	411	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)
87	CLA	BL	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	8 (9%)
82	PEB	aE	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.19	20 (37%)
82	PEB	YJ	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.25	20 (37%)
87	CLA	52	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.42	4 (6%)
87	CLA	B6	612	-	63,67,73	1.29	10 (15%)	75,105,113	1.38	6 (8%)
87	CLA	dL	409	-	54,58,73	1.40	9 (16%)	65,95,113	1.55	9 (13%)
82	PEB	BD	202	1	46,46,46	2.61	11 (23%)	54,67,67	1.98	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	CYC	K1	1001	10,9	46,46,46	2.30	14 (30%)	61,67,67	2.94	28 (45%)
82	PEB	KD	202	2	46,46,46	2.62	13 (28%)	54,67,67	1.97	18 (33%)
84	CYC	BE	1001	10,8	46,46,46	2.43	18 (39%)	61,67,67	2.84	28 (45%)
87	CLA	c6	611	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	10 (12%)
82	PEB	JI	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.06	21 (38%)
82	PEB	RJ	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.30	18 (33%)
83	PUB	BJ	302	14	45,46,46	2.53	8 (17%)	46,67,67	3.02	14 (30%)
92	LMG	A6	408	-	51,51,55	0.93	2 (3%)	59,59,63	1.21	6 (10%)
85	BCR	CL	501	-	41,41,41	0.74	0	56,56,56	1.77	16 (28%)
82	PEB	VJ	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.20	24 (44%)
82	PEB	N1	1002	10	46,46,46	2.60	14 (30%)	54,67,67	2.04	13 (24%)
82	PEB	a1	201	2	46,46,46	2.62	11 (23%)	54,67,67	2.11	19 (35%)
82	PEB	XP	201	2	46,46,46	2.57	13 (28%)	54,67,67	2.06	16 (29%)
98	PQN	BN	837	41	34,34,34	1.88	4 (11%)	42,45,45	2.53	14 (33%)
87	CLA	22	606	58	49,53,73	1.45	7 (14%)	59,89,113	1.57	5 (8%)
82	PEB	mG	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.32	18 (33%)
84	CYC	J1	1001	10	46,46,46	2.32	18 (39%)	61,67,67	2.90	30 (49%)
82	PEB	EJ	201	1,2	46,46,46	2.44	12 (26%)	54,67,67	2.54	22 (40%)
87	CLA	R2	204	-	49,53,73	1.46	10 (20%)	59,89,113	1.50	7 (11%)
92	LMG	b6	624	-	36,36,55	1.16	2 (5%)	44,44,63	1.25	4 (9%)
82	PEB	eH	202	2	46,46,46	2.70	13 (28%)	54,67,67	1.93	16 (29%)
82	PEB	jF	202	2	46,46,46	2.72	13 (28%)	54,67,67	2.15	16 (29%)
87	CLA	12	602	57	69,73,73	1.21	6 (8%)	83,113,113	1.44	9 (10%)
84	CYC	e3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
82	PEB	O9	202	2	46,46,46	2.62	13 (28%)	54,67,67	3.12	26 (48%)
96	HEM	E6	101	19	50,50,50	1.69	8 (16%)	66,82,82	1.53	13 (19%)
82	PEB	SF	202	1	46,46,46	2.59	14 (30%)	54,67,67	2.33	18 (33%)
82	PEB	PO	201	2	46,46,46	2.64	12 (26%)	54,67,67	2.18	18 (33%)
82	PEB	nF	202	2	46,46,46	2.81	15 (32%)	54,67,67	1.96	16 (29%)
82	PEB	YM	203	1	46,46,46	2.50	14 (30%)	54,67,67	2.08	16 (29%)
92	LMG	JL	102	-	43,43,55	0.96	2 (4%)	51,51,63	1.28	5 (9%)
82	PEB	EP	203	1,2	46,46,46	3.10	13 (28%)	54,67,67	3.00	19 (35%)
82	PEB	VB	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.20	19 (35%)
84	CYC	IG	1001	10,9	46,46,46	2.41	16 (34%)	61,67,67	2.90	25 (40%)
82	PEB	dM	201	1,2	46,46,46	2.56	13 (28%)	54,67,67	2.46	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	C6	515	17	69,73,73	1.24	10 (14%)	83,113,113	1.27	6 (7%)
82	PEB	hK	202	2	46,46,46	2.67	13 (28%)	54,67,67	1.99	20 (37%)
82	PEB	vF	201	2	46,46,46	2.68	12 (26%)	54,67,67	2.75	21 (38%)
87	CLA	C6	516	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	9 (10%)
82	PEB	I9	201	1	46,46,46	2.62	15 (32%)	54,67,67	1.97	17 (31%)
82	PEB	zF	501	78,2	46,46,46	2.50	9 (19%)	54,67,67	2.42	19 (35%)
82	PEB	eO	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.18	17 (31%)
82	PEB	XD	202	1	46,46,46	2.70	13 (28%)	54,67,67	1.92	16 (29%)
82	PEB	X7	202	2	46,46,46	2.43	10 (21%)	54,67,67	2.77	24 (44%)
87	CLA	a6	609	-	54,58,73	1.40	10 (18%)	65,95,113	1.49	8 (12%)
87	CLA	CL	512	-	69,73,73	1.27	10 (14%)	83,113,113	1.32	6 (7%)
82	PEB	EI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	aK	201	1,2	46,46,46	2.71	14 (30%)	54,67,67	2.29	20 (37%)
82	PEB	QM	204	1	46,46,46	2.55	13 (28%)	54,67,67	1.92	12 (22%)
87	CLA	3N	307	-	46,50,73	1.50	9 (19%)	55,85,113	1.61	8 (14%)
87	CLA	22	603	-	49,53,73	1.47	8 (16%)	59,89,113	1.44	4 (6%)
82	PEB	v8	201	1	46,46,46	2.68	14 (30%)	54,67,67	2.04	16 (29%)
82	PEB	lO	202	1	46,46,46	2.63	13 (28%)	54,67,67	2.05	17 (31%)
82	PEB	GJ	202	1	46,46,46	2.55	12 (26%)	54,67,67	2.01	16 (29%)
83	PUB	xF	301	13	45,46,46	2.66	10 (22%)	46,67,67	3.16	23 (50%)
87	CLA	K2	106	40,49	53,57,73	1.37	10 (18%)	62,93,113	1.34	11 (17%)
99	SF4	C2	102	42	0,12,12	-	-	-		
87	CLA	B2	811	-	59,63,73	1.33	10 (16%)	71,101,113	1.47	8 (11%)
82	PEB	eH	201	2	46,46,46	2.70	14 (30%)	54,67,67	2.09	20 (37%)
82	PEB	WG	202	1,77	46,46,46	2.53	13 (28%)	54,67,67	2.09	17 (31%)
82	PEB	aJ	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.15	19 (35%)
87	CLA	AN	825	-	59,63,73	1.38	11 (18%)	71,101,113	1.47	9 (12%)
82	PEB	sC	202	2	46,46,46	2.78	13 (28%)	54,67,67	2.34	18 (33%)
82	PEB	O9	201	2	46,46,46	2.65	14 (30%)	54,67,67	2.23	19 (35%)
82	PEB	K9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
82	PEB	t8	202	1	46,46,46	2.75	13 (28%)	54,67,67	2.46	20 (37%)
82	PEB	JP	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.10	17 (31%)
82	PEB	nF	201	2	46,46,46	2.70	12 (26%)	54,67,67	2.98	20 (37%)
82	PEB	UB	303	2,5	46,46,46	2.53	12 (26%)	54,67,67	2.05	17 (31%)
82	PEB	O5	202	2	46,46,46	2.60	13 (28%)	54,67,67	2.33	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	HD	202	1	46,46,46	2.64	14 (30%)	54,67,67	2.31	20 (37%)
87	CLA	22	602	58	69,73,73	1.44	6 (8%)	83,113,113	2.60	18 (21%)
82	PEB	I5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
82	PEB	mM	201	13,2	46,46,46	2.70	14 (30%)	54,67,67	2.12	17 (31%)
87	CLA	B6	607	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	6 (7%)
87	CLA	BN	818	41	64,68,73	1.26	9 (14%)	77,107,113	1.45	9 (11%)
82	PEB	oK	203	1	46,46,46	2.69	13 (28%)	54,67,67	2.19	17 (31%)
82	PEB	AM	302	13	46,46,46	2.59	11 (23%)	54,67,67	1.99	17 (31%)
82	PEB	QE	203	1	46,46,46	2.63	12 (26%)	54,67,67	2.12	19 (35%)
82	PEB	SK	203	1	46,46,46	2.61	11 (23%)	54,67,67	2.15	16 (29%)
82	PEB	ZK	201	2	46,46,46	2.68	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	U4	202	1	46,46,46	2.53	12 (26%)	54,67,67	1.98	14 (25%)
82	PEB	AH	302	3	46,46,46	2.67	12 (26%)	54,67,67	1.98	16 (29%)
82	PEB	OQ	202	2	46,46,46	2.73	15 (32%)	54,67,67	1.94	16 (29%)
87	CLA	K6	101	25	69,73,73	1.25	9 (13%)	83,113,113	1.37	10 (12%)
82	PEB	bH	202	1	46,46,46	2.76	12 (26%)	54,67,67	2.29	22 (40%)
83	PUB	ND	201	1,3	45,46,46	2.85	11 (24%)	46,67,67	3.07	18 (39%)
82	PEB	HJ	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.13	17 (31%)
82	PEB	WJ	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.27	21 (38%)
87	CLA	A2	838	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	9 (10%)
82	PEB	QO	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.77	27 (50%)
82	PEB	NI	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.12	20 (37%)
84	CYC	BG	1002	10,8	46,46,46	2.43	18 (39%)	61,67,67	2.98	29 (47%)
94	PL9	AL	413	-	55,55,55	0.72	2 (3%)	68,69,69	2.61	17 (25%)
82	PEB	HH	1002	10	46,46,46	2.76	13 (28%)	54,67,67	2.23	19 (35%)
82	PEB	UI	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.11	19 (35%)
82	PEB	RM	202	2	46,46,46	2.66	12 (26%)	54,67,67	2.19	21 (38%)
82	PEB	T4	201	2	46,46,46	2.60	13 (28%)	54,67,67	2.22	19 (35%)
82	PEB	L9	202	2	46,46,46	2.68	12 (26%)	54,67,67	2.23	21 (38%)
84	CYC	GE	1001	10,9	46,46,46	2.39	16 (34%)	61,67,67	2.86	26 (42%)
82	PEB	BQ	202	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	OA	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.04	19 (35%)
82	PEB	kJ	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.14	21 (38%)
83	PUB	M5	302	1,74	45,46,46	2.80	13 (28%)	46,67,67	3.59	25 (54%)
82	PEB	sC	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.25	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	3N	301	59	49,53,73	1.44	9 (18%)	59,89,113	1.48	8 (13%)
82	PEB	OI	201	2	46,46,46	2.68	15 (32%)	54,67,67	2.17	18 (33%)
92	LMG	D6	407	18,24	33,33,55	1.13	2 (6%)	41,41,63	1.51	8 (19%)
92	LMG	DL	402	18	54,54,55	0.92	2 (3%)	62,62,63	1.33	7 (11%)
82	PEB	EB	501	2,4	46,46,46	2.55	11 (23%)	54,67,67	2.07	18 (33%)
82	PEB	h1	201	1,74,2	46,46,46	2.62	13 (28%)	54,67,67	2.29	19 (35%)
87	CLA	LN	202	50	61,65,73	1.30	8 (13%)	73,103,113	1.31	6 (8%)
82	PEB	E9	201	1	46,46,46	2.61	12 (26%)	54,67,67	1.97	17 (31%)
87	CLA	B2	808	-	69,73,73	1.28	11 (15%)	83,113,113	1.35	6 (7%)
82	PEB	dJ	202	1	46,46,46	2.60	13 (28%)	54,67,67	2.07	15 (27%)
82	PEB	HM	202	2	46,46,46	2.70	14 (30%)	54,67,67	2.25	24 (44%)
82	PEB	fH	201	1	46,46,46	2.66	14 (30%)	54,67,67	1.92	16 (29%)
87	CLA	B2	812	-	69,73,73	1.25	10 (14%)	83,113,113	1.40	10 (12%)
87	CLA	5N	606	61	49,53,73	1.43	6 (12%)	59,89,113	1.78	7 (11%)
82	PEB	O5	201	74,2,82	46,46,46	2.56	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	JF	201	2	46,46,46	2.54	12 (26%)	54,67,67	2.89	19 (35%)
82	PEB	DM	201	14,2	46,46,46	2.70	13 (28%)	54,67,67	2.13	18 (33%)
91	PHO	D6	404	-	58,69,69	2.63	13 (22%)	56,99,99	2.74	19 (33%)
83	PUB	A4	302	3	45,46,46	2.70	9 (20%)	46,67,67	2.89	18 (39%)
82	PEB	cH	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.14	20 (37%)
85	BCR	B2	838	-	41,41,41	0.73	0	56,56,56	2.49	21 (37%)
103	ZEX	82	309	64	42,43,43	0.82	2 (4%)	55,60,60	2.15	16 (29%)
82	PEB	FK	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.37	20 (37%)
82	PEB	NQ	202	1	46,46,46	2.69	14 (30%)	54,67,67	1.89	16 (29%)
82	PEB	U4	201	1	46,46,46	2.51	12 (26%)	54,67,67	2.94	26 (48%)
87	CLA	32	308	59	49,53,73	1.43	9 (18%)	59,89,113	1.47	7 (11%)
87	CLA	52	604	61	46,50,73	1.49	10 (21%)	55,85,113	1.60	6 (10%)
92	LMG	b6	619	-	41,41,55	1.02	2 (4%)	49,49,63	1.21	4 (8%)
82	PEB	vC	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.66	22 (40%)
82	PEB	cO	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.22	17 (31%)
82	PEB	PM	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.03	20 (37%)
84	CYC	CG	1001	10,9	46,46,46	2.37	18 (39%)	61,67,67	2.77	25 (40%)
82	PEB	WE	203	1,2	46,46,46	2.49	11 (23%)	54,67,67	2.32	22 (40%)
82	PEB	b1	203	1,2	46,46,46	2.62	14 (30%)	54,67,67	2.53	18 (33%)
82	PEB	GJ	203	1,2	46,46,46	2.49	12 (26%)	54,67,67	2.49	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
92	LMG	B6	618	-	40,40,55	1.04	2 (5%)	48,48,63	1.36	6 (12%)
82	PEB	W1	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.26	18 (33%)
82	PEB	Q5	203	2	46,46,46	2.53	13 (28%)	54,67,67	2.07	17 (31%)
82	PEB	BB	202	2	46,46,46	2.53	11 (23%)	54,67,67	2.12	18 (33%)
82	PEB	PQ	202	1	46,46,46	2.77	12 (26%)	54,67,67	2.16	19 (35%)
82	PEB	l1	202	1	46,46,46	2.68	12 (26%)	54,67,67	2.02	17 (31%)
82	PEB	H7	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.43	22 (40%)
82	PEB	OQ	201	3,2,82	46,46,46	2.66	12 (26%)	54,67,67	2.07	16 (29%)
84	CYC	LH	1002	10	46,46,46	2.53	20 (43%)	61,67,67	3.04	34 (55%)
85	BCR	BL	616	-	41,41,41	0.80	0	56,56,56	1.59	11 (19%)
87	CLA	62	305	87,62	46,50,73	1.51	8 (17%)	55,85,113	1.45	6 (10%)
87	CLA	aL	606	-	64,68,73	1.44	10 (15%)	77,107,113	2.04	16 (20%)
87	CLA	B2	826	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
85	BCR	J2	103	40,48	41,41,41	0.71	0	56,56,56	2.09	16 (28%)
82	PEB	O7	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.05	19 (35%)
82	PEB	wF	303	13	46,46,46	2.71	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	D9	201	2	46,46,46	2.64	13 (28%)	54,67,67	2.16	18 (33%)
82	PEB	NK	202	2	46,46,46	2.84	13 (28%)	54,67,67	2.41	19 (35%)
87	CLA	bL	607	-	69,73,73	1.29	11 (15%)	83,113,113	1.65	12 (14%)
85	BCR	c6	602	-	41,41,41	0.81	0	56,56,56	2.21	22 (39%)
87	CLA	BN	826	-	69,73,73	1.25	11 (15%)	83,113,113	1.34	8 (9%)
82	PEB	TA	203	2	46,46,46	2.62	12 (26%)	54,67,67	2.27	21 (38%)
82	PEB	KM	203	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.55	23 (42%)
87	CLA	32	306	-	46,50,73	1.50	9 (19%)	55,85,113	1.59	8 (14%)
87	CLA	d6	403	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
87	CLA	AN	802	40,45	69,73,73	1.27	9 (13%)	83,113,113	1.44	10 (12%)
82	PEB	SQ	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.07	20 (37%)
82	PEB	TM	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.15	21 (38%)
82	PEB	jO	201	1	46,46,46	2.65	13 (28%)	54,67,67	2.30	22 (40%)
82	PEB	x8	202	1	46,46,46	2.76	13 (28%)	54,67,67	2.67	25 (46%)
82	PEB	DJ	201	14,2	46,46,46	2.68	13 (28%)	54,67,67	2.23	22 (40%)
85	BCR	BN	843	-	41,41,41	0.77	0	56,56,56	2.01	18 (32%)
87	CLA	52	608	61	45,49,73	1.54	9 (20%)	54,84,113	1.71	9 (16%)
87	CLA	5N	602	61	69,73,73	1.24	9 (13%)	83,113,113	1.37	9 (10%)
82	PEB	HM	201	2	46,46,46	2.70	13 (28%)	54,67,67	2.36	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	UQ	202	2	46,46,46	2.73	12 (26%)	54,67,67	1.96	17 (31%)
82	PEB	A7	201	1	46,46,46	2.67	14 (30%)	54,67,67	2.14	21 (38%)
95	DGD	C6	504	-	43,43,67	1.01	3 (6%)	57,57,81	1.53	10 (17%)
103	ZEX	82	310	64,87	42,43,43	1.77	9 (21%)	55,60,60	3.88	30 (54%)
87	CLA	B6	609	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	8 (9%)
84	CYC	MO	1001	9	46,46,46	2.29	15 (32%)	61,67,67	2.87	22 (36%)
87	CLA	2N	304	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	4 (6%)
85	BCR	BN	803	87,50,41	41,41,41	0.76	0	56,56,56	3.37	24 (42%)
82	PEB	e1	202	2	46,46,46	2.70	13 (28%)	54,67,67	1.94	15 (27%)
82	PEB	SJ	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.18	17 (31%)
82	PEB	Z5	305	74	46,46,46	2.57	13 (28%)	54,67,67	2.36	25 (46%)
82	PEB	T7	202	2	46,46,46	2.35	10 (21%)	54,67,67	3.03	27 (50%)
87	CLA	bL	619	-	63,67,73	1.30	10 (15%)	75,105,113	1.35	8 (10%)
82	PEB	UD	201	3,2	46,46,46	2.71	15 (32%)	54,67,67	2.03	19 (35%)
82	PEB	A4	304	3	46,46,46	2.62	13 (28%)	54,67,67	2.06	17 (31%)
82	PEB	DP	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.07	19 (35%)
82	PEB	bG	201	1	46,46,46	2.67	13 (28%)	54,67,67	2.20	16 (29%)
82	PEB	lH	201	1	46,46,46	2.68	14 (30%)	54,67,67	2.02	17 (31%)
87	CLA	A2	823	40	69,73,73	1.23	11 (15%)	83,113,113	1.43	10 (12%)
84	CYC	EH	1001	10,9	46,46,46	2.36	17 (36%)	61,67,67	3.17	28 (45%)
87	CLA	AN	801	-	48,52,73	1.46	10 (20%)	56,87,113	1.70	9 (16%)
82	PEB	QJ	203	1	46,46,46	2.59	12 (26%)	54,67,67	2.03	15 (27%)
87	CLA	b6	606	16	69,73,73	1.24	9 (13%)	83,113,113	1.38	8 (9%)
95	DGD	c6	618	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
82	PEB	MK	201	1	46,46,46	2.60	11 (23%)	54,67,67	1.95	16 (29%)
82	PEB	bE	202	1	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	iG	202	2	46,46,46	2.67	13 (28%)	54,67,67	1.99	16 (29%)
82	PEB	LJ	201	2	46,46,46	2.67	12 (26%)	54,67,67	2.36	18 (33%)
82	PEB	aF	201	1,2	46,46,46	2.71	13 (28%)	54,67,67	2.28	21 (38%)
95	DGD	BL	613	-	41,41,67	1.11	3 (7%)	55,55,81	1.47	7 (12%)
84	CYC	d3	1001	73,69	46,46,46	2.52	17 (36%)	61,67,67	3.12	28 (45%)
87	CLA	RN	203	54,41	50,54,73	1.46	8 (16%)	60,90,113	1.43	5 (8%)
87	CLA	52	606	61	49,53,73	1.43	7 (14%)	59,89,113	1.79	7 (11%)
82	PEB	ZF	202	2	46,46,46	2.81	15 (32%)	54,67,67	2.12	21 (38%)
82	PEB	WO	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.64	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PEB	SH	201	1	46,46,46	2.62	13 (28%)	54,67,67	2.28	16 (29%)
82	PEB	MJ	201	1,2	46,46,46	2.50	11 (23%)	54,67,67	2.55	23 (42%)
84	CYC	C1	1001	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.84	27 (44%)
82	PEB	N5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	W7	201	1	46,46,46	2.44	12 (26%)	54,67,67	2.39	21 (38%)
82	PEB	D9	203	2	46,46,46	2.70	12 (26%)	54,67,67	1.95	15 (27%)
82	PEB	gG	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.09	17 (31%)
82	PEB	SB	203	2	46,46,46	2.53	11 (23%)	54,67,67	2.13	15 (27%)
83	PUB	A1	303	3	45,46,46	2.83	10 (22%)	46,67,67	3.03	19 (41%)
82	PEB	GI	203	1	46,46,46	2.54	13 (28%)	54,67,67	2.11	20 (37%)
87	CLA	AN	829	-	69,73,73	1.24	9 (13%)	83,113,113	1.52	8 (9%)
82	PEB	UQ	201	3,2	46,46,46	2.70	15 (32%)	54,67,67	2.03	19 (35%)
82	PEB	tC	202	1	46,46,46	2.75	13 (28%)	54,67,67	2.46	20 (37%)
82	PEB	bK	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.08	18 (33%)
82	PEB	AM	301	13	46,46,46	2.58	13 (28%)	54,67,67	2.07	19 (35%)
82	PEB	YQ	202	2	46,46,46	2.67	13 (28%)	54,67,67	1.93	14 (25%)
82	PEB	p8	202	1	46,46,46	2.80	13 (28%)	54,67,67	2.69	22 (40%)
82	PEB	FI	202	2	46,46,46	2.57	11 (23%)	54,67,67	2.08	18 (33%)
82	PEB	NF	201	2	46,46,46	2.59	11 (23%)	54,67,67	2.91	19 (35%)
87	CLA	A2	837	-	55,59,73	1.41	11 (20%)	66,96,113	1.69	15 (22%)
82	PEB	UG	202	1	46,46,46	2.63	13 (28%)	54,67,67	2.06	18 (33%)
87	CLA	L2	204	50	54,58,73	1.46	10 (18%)	65,95,113	1.74	13 (20%)
82	PEB	BA	201	2,82	46,46,46	2.63	13 (28%)	54,67,67	2.21	20 (37%)
82	PEB	Y9	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.11	17 (31%)
82	PEB	JQ	202	1	46,46,46	2.60	11 (23%)	54,67,67	1.99	14 (25%)
82	PEB	OP	202	1	46,46,46	2.53	11 (23%)	54,67,67	2.14	18 (33%)
82	PEB	R5	202	1	46,46,46	2.58	13 (28%)	54,67,67	2.06	18 (33%)
87	CLA	B2	807	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	6 (7%)
82	PEB	l1	203	1	46,46,46	2.76	14 (30%)	54,67,67	2.29	19 (35%)
82	PEB	NB	203	2	46,46,46	2.56	13 (28%)	54,67,67	2.21	19 (35%)
87	CLA	BN	830	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	4 (4%)
82	PEB	f1	203	1,2	46,46,46	2.70	13 (28%)	54,67,67	2.02	17 (31%)
84	CYC	LG	1001	10	46,46,46	2.40	17 (36%)	61,67,67	3.02	28 (45%)
87	CLA	MN	101	51,41	49,53,73	1.48	11 (22%)	59,89,113	1.63	10 (16%)
82	PEB	TO	203	2	46,46,46	2.59	11 (23%)	54,67,67	1.91	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	V4	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.49	22 (40%)
82	PEB	x8	201	1	46,46,46	2.68	12 (26%)	54,67,67	1.87	16 (29%)
82	PEB	NP	202	2	46,46,46	2.63	12 (26%)	54,67,67	2.12	17 (31%)
83	PUB	yK	303	14	45,46,46	2.62	9 (20%)	46,67,67	3.03	19 (41%)
83	PUB	xK	301	13	45,46,46	2.66	10 (22%)	46,67,67	3.18	23 (50%)
85	BCR	c6	617	-	41,41,41	0.76	0	56,56,56	3.02	21 (37%)
82	PEB	dE	204	1	46,46,46	2.67	14 (30%)	54,67,67	1.99	16 (29%)
82	PEB	rK	201	13,2	46,46,46	2.63	12 (26%)	54,67,67	2.17	14 (25%)
82	PEB	sK	203	1,2	46,46,46	2.76	15 (32%)	54,67,67	2.55	20 (37%)
87	CLA	AN	806	-	59,63,73	1.33	9 (15%)	71,101,113	1.49	8 (11%)
87	CLA	A2	850	40	69,73,73	1.27	8 (11%)	83,113,113	1.37	9 (10%)
82	PEB	RF	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.30	21 (38%)
82	PEB	KI	203	1	46,46,46	2.53	13 (28%)	54,67,67	2.11	20 (37%)
87	CLA	62	311	-	46,50,73	1.51	8 (17%)	55,85,113	1.70	8 (14%)
87	CLA	8N	302	64	49,53,73	1.52	11 (22%)	59,89,113	1.67	9 (15%)
82	PEB	FQ	201	1	46,46,46	2.54	12 (26%)	54,67,67	2.61	22 (40%)
87	CLA	A2	802	-	48,52,73	1.46	9 (18%)	56,87,113	1.70	9 (16%)
82	PEB	VO	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.19	19 (35%)
87	CLA	B6	610	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	7 (8%)
87	CLA	82	307	-	46,50,73	1.48	10 (21%)	55,85,113	1.46	6 (10%)
95	DGD	B6	620	16	59,59,67	0.90	2 (3%)	73,73,81	0.98	3 (4%)
82	PEB	JD	203	1,2	46,46,46	2.48	12 (26%)	54,67,67	2.17	16 (29%)
82	PEB	U1	203	1	46,46,46	2.71	11 (23%)	54,67,67	2.19	20 (37%)
82	PEB	XA	203	2	46,46,46	2.60	14 (30%)	54,67,67	2.34	23 (42%)
87	CLA	52	602	61	69,73,73	1.24	9 (13%)	83,113,113	1.37	8 (9%)
87	CLA	AL	404	87	64,68,73	1.26	9 (14%)	77,107,113	1.44	8 (10%)
82	PEB	VB	202	1,2	46,46,46	2.64	12 (26%)	54,67,67	2.04	15 (27%)
82	PEB	S4	202	1,76	46,46,46	2.53	14 (30%)	54,67,67	1.98	16 (29%)
84	CYC	HH	1001	10	46,46,46	2.35	18 (39%)	61,67,67	2.88	29 (47%)
85	BCR	A2	804	-	41,41,41	0.75	0	56,56,56	2.07	17 (30%)
82	PEB	P5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	D7	203	2	46,46,46	2.68	13 (28%)	54,67,67	2.14	20 (37%)
87	CLA	B2	821	-	59,63,73	1.35	10 (16%)	71,101,113	1.41	6 (8%)
87	CLA	KN	103	-	46,50,73	1.47	10 (21%)	55,85,113	1.74	8 (14%)
82	PEB	ND	202	1	46,46,46	2.67	13 (28%)	54,67,67	1.87	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	GB	203	2	46,46,46	2.59	12 (26%)	54,67,67	2.12	18 (33%)
87	CLA	B2	817	41	64,68,73	1.26	9 (14%)	77,107,113	1.45	9 (11%)
87	CLA	2N	306	58	49,53,73	1.46	8 (16%)	59,89,113	1.56	5 (8%)
82	PEB	OE	201	1	46,46,46	2.58	13 (28%)	54,67,67	2.32	21 (38%)
82	PEB	VI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	GD	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.14	19 (35%)
89	OEX	a6	611	15,17	0,14,14	-	-	-		
84	CYC	BE	1002	10,8	46,46,46	2.43	17 (36%)	61,67,67	2.97	29 (47%)
82	PEB	RH	201	2	46,46,46	2.62	14 (30%)	54,67,67	2.17	22 (40%)
87	CLA	A6	403	87	64,68,73	1.27	10 (15%)	77,107,113	1.41	7 (9%)
82	PEB	mE	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.32	18 (33%)
82	PEB	FF	201	2	46,46,46	2.59	12 (26%)	54,67,67	3.56	17 (31%)
82	PEB	KG	201	10,9	46,46,46	2.58	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	dG	201	1,3	46,46,46	2.65	12 (26%)	54,67,67	2.18	20 (37%)
84	CYC	CH	1001	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.83	27 (44%)
85	BCR	B2	840	41	41,41,41	0.72	0	56,56,56	1.79	16 (28%)
87	CLA	AN	808	-	69,73,73	1.25	11 (15%)	83,113,113	1.37	8 (9%)
82	PEB	rF	201	13,2	46,46,46	2.62	12 (26%)	54,67,67	2.17	14 (25%)
82	PEB	OF	202	1	46,46,46	2.52	11 (23%)	54,67,67	2.26	21 (38%)
82	PEB	UH	202	1	46,46,46	2.69	15 (32%)	54,67,67	2.02	17 (31%)
87	CLA	A2	829	-	69,73,73	1.24	9 (13%)	83,113,113	1.53	8 (9%)
82	PEB	OJ	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.68	21 (38%)
87	CLA	CL	507	-	69,73,73	1.24	11 (15%)	83,113,113	1.60	11 (13%)
82	PEB	FQ	203	1,2	46,46,46	2.82	15 (32%)	54,67,67	2.98	22 (40%)
82	PEB	U9	201	74,2	46,46,46	2.73	13 (28%)	54,67,67	2.03	15 (27%)
91	PHO	DL	405	-	58,69,69	2.61	13 (22%)	56,99,99	2.81	16 (28%)
82	PEB	WK	201	1,2	46,46,46	2.52	12 (26%)	54,67,67	2.59	27 (50%)
87	CLA	12	607	57	54,58,73	1.39	9 (16%)	65,95,113	1.53	10 (15%)
87	CLA	cL	514	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
82	PEB	tF	202	2	46,46,46	2.80	14 (30%)	54,67,67	2.26	19 (35%)
87	CLA	BL	602	-	69,73,73	1.29	10 (14%)	83,113,113	1.46	7 (8%)
84	CYC	63	901	73	46,46,46	2.36	17 (36%)	61,67,67	2.98	30 (49%)
82	PEB	iM	201	13,2	46,46,46	2.75	15 (32%)	54,67,67	2.22	19 (35%)
82	PEB	X9	202	1	46,46,46	2.74	14 (30%)	54,67,67	2.42	21 (38%)
82	PEB	g4	202	2	46,46,46	2.56	11 (23%)	54,67,67	2.32	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	UE	202	1	46,46,46	2.62	13 (28%)	54,67,67	2.06	17 (31%)
82	PEB	ZJ	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.37	20 (37%)
82	PEB	RF	201	2	46,46,46	2.50	10 (21%)	54,67,67	3.44	21 (38%)
82	PEB	kH	203	1,2	46,46,46	2.64	12 (26%)	54,67,67	2.34	20 (37%)
82	PEB	VQ	203	1,2	46,46,46	2.70	15 (32%)	54,67,67	2.37	19 (35%)
84	CYC	NH	1001	10,8	46,46,46	2.41	18 (39%)	61,67,67	2.75	29 (47%)
82	PEB	UB	302	2,5	46,46,46	2.70	13 (28%)	54,67,67	2.31	21 (38%)
82	PEB	lF	202	2	46,46,46	2.72	13 (28%)	54,67,67	2.12	18 (33%)
87	CLA	AN	824	40	55,59,73	1.38	8 (14%)	66,96,113	1.57	6 (9%)
82	PEB	OO	202	1	46,46,46	2.54	14 (30%)	54,67,67	1.94	14 (25%)
82	PEB	CA	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.54	20 (37%)
82	PEB	NQ	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.02	16 (29%)
82	PEB	XB	201	2	46,46,46	2.55	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	V9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.42	21 (38%)
82	PEB	TA	202	2	46,46,46	2.35	10 (21%)	54,67,67	3.04	27 (50%)
82	PEB	s8	201	2	46,46,46	2.72	15 (32%)	54,67,67	2.25	19 (35%)
87	CLA	62	313	62	49,53,73	1.67	8 (16%)	59,89,113	2.06	15 (25%)
82	PEB	UK	202	1	46,46,46	2.61	11 (23%)	54,67,67	2.10	17 (31%)
87	CLA	32	312	59	49,53,73	1.48	10 (20%)	59,89,113	1.51	7 (11%)
87	CLA	B2	810	-	69,73,73	1.27	12 (17%)	83,113,113	1.49	8 (9%)
82	PEB	A5	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	dG	203	1	46,46,46	2.66	14 (30%)	54,67,67	2.07	20 (37%)
82	PEB	jJ	201	1	46,46,46	2.64	11 (23%)	54,67,67	2.14	16 (29%)
87	CLA	2N	305	-	46,50,73	1.49	10 (21%)	55,85,113	1.63	10 (18%)
87	CLA	BN	809	-	69,73,73	1.28	11 (15%)	83,113,113	1.34	6 (7%)
82	PEB	tK	203	1,2	46,46,46	2.70	14 (30%)	54,67,67	2.16	16 (29%)
82	PEB	GF	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.96	27 (50%)
87	CLA	3N	311	-	46,50,73	1.51	10 (21%)	55,85,113	1.60	8 (14%)
82	PEB	WH	203	1,2	46,46,46	2.67	14 (30%)	54,67,67	2.22	21 (38%)
82	PEB	CJ	203	1,2	46,46,46	2.49	11 (23%)	54,67,67	2.53	23 (42%)
82	PEB	k1	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.10	20 (37%)
82	PEB	qC	203	2	46,46,46	2.67	12 (26%)	54,67,67	2.02	17 (31%)
82	PEB	eE	202	2	46,46,46	2.62	10 (21%)	54,67,67	2.25	19 (35%)
82	PEB	QK	202	1	46,46,46	2.60	11 (23%)	54,67,67	1.92	18 (33%)
87	CLA	b6	609	-	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	22	607	58	49,53,73	1.47	8 (16%)	59,89,113	1.49	9 (15%)
85	BCR	c6	603	87,17	41,41,41	0.79	0	56,56,56	2.59	25 (44%)
82	PEB	lO	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.30	21 (38%)
95	DGD	BL	614	-	59,59,67	0.94	3 (5%)	73,73,81	1.57	12 (16%)
82	PEB	IP	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	cJ	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.18	18 (33%)
82	PEB	iF	201	1,2	46,46,46	2.61	12 (26%)	54,67,67	2.35	18 (33%)
87	CLA	A2	828	40	69,73,73	1.36	9 (13%)	83,113,113	1.58	13 (15%)
82	PEB	KF	203	1	46,46,46	2.62	12 (26%)	54,67,67	2.11	22 (40%)
88	LHG	iL	101	-	48,48,48	0.96	2 (4%)	51,54,54	0.96	3 (5%)
82	PEB	cG	201	2	46,46,46	2.62	13 (28%)	54,67,67	2.11	18 (33%)
83	PUB	yK	302	14	45,46,46	2.59	8 (17%)	46,67,67	2.96	20 (43%)
87	CLA	bL	613	16	69,73,73	1.26	11 (15%)	83,113,113	1.49	8 (9%)
82	PEB	WD	201	3,2	46,46,46	2.62	14 (30%)	54,67,67	2.30	19 (35%)
87	CLA	32	305	-	49,53,73	1.45	8 (16%)	59,89,113	1.52	8 (13%)
82	PEB	F5	202	2	46,46,46	2.42	12 (26%)	54,67,67	2.47	23 (42%)
85	BCR	LN	201	-	41,41,41	0.75	0	56,56,56	1.87	11 (19%)
87	CLA	B2	834	-	69,73,73	1.28	11 (15%)	83,113,113	1.37	11 (13%)
87	CLA	bL	605	-	69,73,73	1.23	9 (13%)	83,113,113	1.28	7 (8%)
82	PEB	TP	201	56,2	46,46,46	2.68	14 (30%)	54,67,67	2.02	18 (33%)
87	CLA	AN	837	-	55,59,73	1.40	11 (20%)	66,96,113	1.68	15 (22%)
82	PEB	SK	202	1	46,46,46	2.59	14 (30%)	54,67,67	2.33	18 (33%)
88	LHG	AN	844	-	39,39,48	1.03	2 (5%)	42,45,54	1.08	2 (4%)
82	PEB	fO	202	1	46,46,46	2.65	14 (30%)	54,67,67	1.96	17 (31%)
84	CYC	KH	1001	10,9	46,46,46	2.29	13 (28%)	61,67,67	2.93	28 (45%)
82	PEB	LM	201	2	46,46,46	2.68	13 (28%)	54,67,67	2.09	18 (33%)
82	PEB	OF	203	1	46,46,46	2.60	10 (21%)	54,67,67	2.06	20 (37%)
85	BCR	A2	845	40	41,41,41	0.72	0	56,56,56	1.97	12 (21%)
82	PEB	UP	202	1	46,46,46	2.71	14 (30%)	54,67,67	2.33	19 (35%)
82	PEB	L5	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.11	19 (35%)
87	CLA	32	311	-	46,50,73	1.50	10 (21%)	55,85,113	1.58	8 (14%)
82	PEB	E5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	AI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
84	CYC	x3	1001	-	46,46,46	2.53	16 (34%)	61,67,67	3.07	32 (52%)
82	PEB	zC	201	1	46,46,46	2.70	13 (28%)	54,67,67	2.23	26 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	RI	203	1,2	46,46,46	2.29	11 (23%)	54,67,67	2.97	22 (40%)
83	PUB	AM	303	13	45,46,46	2.70	10 (22%)	46,67,67	3.06	19 (41%)
82	PEB	YP	503	56,2	46,46,46	2.57	13 (28%)	54,67,67	2.07	16 (29%)
82	PEB	T9	202	1	46,46,46	2.74	13 (28%)	54,67,67	2.41	21 (38%)
82	PEB	RG	202	2	46,46,46	2.60	12 (26%)	54,67,67	2.08	18 (33%)
95	DGD	hL	101	22	63,63,67	0.86	2 (3%)	77,77,81	1.04	5 (6%)
82	PEB	U1	202	1	46,46,46	2.70	14 (30%)	54,67,67	2.02	18 (33%)
87	CLA	52	611	61	49,53,73	1.49	8 (16%)	59,89,113	1.59	9 (15%)
82	PEB	XA	202	2	46,46,46	2.42	10 (21%)	54,67,67	2.76	23 (42%)
82	PEB	eO	203	2	46,46,46	2.55	11 (23%)	54,67,67	1.91	13 (24%)
83	PUB	AM	304	13	45,46,46	2.67	10 (22%)	46,67,67	2.97	18 (39%)
87	CLA	7N	609	-	46,50,73	1.51	9 (19%)	55,85,113	1.59	7 (12%)
82	PEB	UK	201	1	46,46,46	2.53	11 (23%)	54,67,67	3.21	25 (46%)
88	LHG	D6	406	18	48,48,48	0.89	2 (4%)	51,54,54	1.09	3 (5%)
92	LMG	a6	614	87	42,42,55	1.04	2 (4%)	50,50,63	1.22	4 (8%)
82	PEB	i4	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.06	18 (33%)
82	PEB	fF	202	2	46,46,46	2.93	14 (30%)	54,67,67	2.31	22 (40%)
84	CYC	I1	1001	10,9	46,46,46	2.38	14 (30%)	61,67,67	3.00	28 (45%)
82	PEB	j4	203	-	46,46,46	2.60	13 (28%)	54,67,67	2.32	20 (37%)
82	PEB	EM	203	1	46,46,46	2.52	12 (26%)	54,67,67	2.09	15 (27%)
87	CLA	52	607	61	54,58,73	1.38	8 (14%)	65,95,113	1.57	10 (15%)
87	CLA	AN	832	40	54,58,73	1.41	11 (20%)	65,95,113	1.60	9 (13%)
82	PEB	SK	201	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.55	22 (40%)
82	PEB	gO	202	2	46,46,46	2.57	10 (21%)	54,67,67	2.33	21 (38%)
85	BCR	B2	839	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
82	PEB	W5	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.20	20 (37%)
87	CLA	1N	606	-	49,53,73	1.48	9 (18%)	59,89,113	1.36	5 (8%)
82	PEB	kM	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.16	19 (35%)
82	PEB	ZB	203	2	46,46,46	2.76	12 (26%)	54,67,67	2.16	17 (31%)
87	CLA	CL	511	-	69,73,73	1.25	10 (14%)	83,113,113	1.47	12 (14%)
82	PEB	HA	203	2	46,46,46	2.72	14 (30%)	54,67,67	2.25	19 (35%)
88	LHG	AN	843	40	48,48,48	0.93	2 (4%)	51,54,54	0.91	2 (3%)
82	PEB	CD	201	3,2	46,46,46	2.63	14 (30%)	54,67,67	2.34	21 (38%)
87	CLA	5N	608	61	45,49,73	1.53	9 (20%)	54,84,113	1.72	9 (16%)
82	PEB	g1	201	2	46,46,46	2.74	13 (28%)	54,67,67	2.00	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	bL	616	-	69,73,73	1.26	11 (15%)	83,113,113	1.34	9 (10%)
87	CLA	4N	609	60	45,49,73	1.49	8 (17%)	54,84,113	1.69	8 (14%)
82	PEB	TO	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.22	19 (35%)
82	PEB	DI	202	2	46,46,46	2.59	11 (23%)	54,67,67	2.00	15 (27%)
82	PEB	wK	301	13	46,46,46	2.54	12 (26%)	54,67,67	2.17	22 (40%)
82	PEB	D5	201	74,2	46,46,46	2.55	13 (28%)	54,67,67	2.17	20 (37%)
82	PEB	dK	201	2	46,46,46	2.62	11 (23%)	54,67,67	2.38	19 (35%)
82	PEB	kH	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.11	20 (37%)
82	PEB	l4	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.29	21 (38%)
82	PEB	aG	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.09	17 (31%)
82	PEB	ZI	401	12,2	46,46,46	2.79	16 (34%)	54,67,67	3.04	22 (40%)
87	CLA	72	609	-	46,50,73	1.51	8 (17%)	55,85,113	1.57	7 (12%)
88	LHG	B6	617	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	2 (3%)
88	LHG	D6	401	-	42,42,48	0.97	2 (4%)	45,48,54	1.10	2 (4%)
92	LMG	yL	101	-	55,55,55	0.34	0	63,63,63	0.53	0
82	PEB	gB	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.08	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	rC	201	1	-	9/26/74/74	0/4/4/4
82	PEB	F5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	cK	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	42	608	60	-	11/21/97/115	-
87	CLA	I2	102	-	-	12/39/115/115	-
82	PEB	TH	202	2	-	15/26/74/74	0/4/4/4
87	CLA	8N	305	-	-	7/15/91/115	-
82	PEB	RK	202	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	817	-	-	8/32/108/115	-
82	PEB	dO	201	1	-	9/26/74/74	0/4/4/4
87	CLA	BN	834	-	-	15/39/115/115	-
87	CLA	R2	201	87	-	7/15/91/115	-
82	PEB	WM	201	1	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	dG	202	1,2	-	6/26/74/74	0/4/4/4
82	PEB	j1	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	QD	202	2	-	11/26/74/74	0/4/4/4
87	CLA	AL	405	15	-	8/21/97/115	-
82	PEB	YH	202	2	-	8/26/74/74	0/4/4/4
87	CLA	6N	604	87,62	-	9/12/88/115	-
82	PEB	fG	202	1	-	8/26/74/74	0/4/4/4
82	PEB	g4	203	2	-	11/26/74/74	0/4/4/4
82	PEB	C7	202	1	-	13/26/74/74	0/4/4/4
82	PEB	WH	202	1	-	9/26/74/74	0/4/4/4
82	PEB	iK	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	BN	829	-	-	7/13/89/115	-
82	PEB	CJ	202	1	-	10/26/74/74	0/4/4/4
82	PEB	SP	202	1	-	4/26/74/74	0/4/4/4
87	CLA	8N	301	64,103	-	10/17/93/115	-
84	CYC	H4	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	z8	201	1	-	10/26/74/74	0/4/4/4
82	PEB	lM	201	1,2	-	8/26/74/74	0/4/4/4
87	CLA	2N	312	58	-	7/15/91/115	-
82	PEB	QF	203	1,2	-	7/26/74/74	0/4/4/4
87	CLA	dL	401	18	-	14/39/115/115	-
97	GOL	i6	102	-	-	0/4/4/4	-
84	CYC	V3	1001	-	-	10/26/74/74	0/4/4/4
82	PEB	lJ	201	1,2	-	8/26/74/74	0/4/4/4
85	BCR	d6	405	-	-	12/29/63/63	0/2/2/2
82	PEB	IM	201	1,2	-	6/26/74/74	0/4/4/4
87	CLA	B2	804	41	-	8/39/115/115	-
82	PEB	FM	202	2	-	9/26/74/74	0/4/4/4
83	PUB	AJ	304	13	-	8/26/74/74	0/4/4/4
87	CLA	H6	103	22	-	19/39/115/115	-
87	CLA	1N	601	57	-	12/15/91/115	-
82	PEB	UM	203	1	-	9/26/74/74	0/4/4/4
82	PEB	J7	201	3,2	-	4/26/74/74	0/4/4/4
99	SF4	BN	804	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	Q9	202	2	-	7/26/74/74	0/4/4/4
82	PEB	NO	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	GK	203	1	-	9/26/74/74	0/4/4/4
82	PEB	HG	1002	10,9	-	8/26/74/74	0/4/4/4
82	PEB	IA	202	1	-	11/26/74/74	0/4/4/4
87	CLA	BN	806	41	-	18/39/115/115	-
82	PEB	XQ	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	B2	835	-	-	22/39/115/115	-
82	PEB	WA	202	1	-	12/26/74/74	0/4/4/4
82	PEB	YE	202	2	-	11/26/74/74	0/4/4/4
82	PEB	ID	202	2	-	7/26/74/74	0/4/4/4
82	PEB	LD	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	VK	202	2	-	12/26/74/74	0/4/4/4
82	PEB	OK	203	1	-	9/26/74/74	0/4/4/4
87	CLA	D6	403	-	-	19/39/115/115	-
100	3XQ	JN	104	-	-	17/24/24/24	-
82	PEB	wC	202	2	-	5/26/74/74	0/4/4/4
92	LMG	B6	619	16	-	7/34/54/70	0/1/1/1
84	CYC	T3	1001	68	-	8/26/74/74	0/4/4/4
95	DGD	D6	410	18,22	-	12/51/91/95	0/2/2/2
87	CLA	12	605	57	-	9/15/91/115	-
82	PEB	VF	202	2	-	12/26/74/74	0/4/4/4
87	CLA	d6	406	-	-	21/39/115/115	-
84	CYC	73	1002	73	-	6/26/74/74	0/4/4/4
87	CLA	12	606	-	-	8/15/91/115	-
82	PEB	sF	201	1	-	12/26/74/74	0/4/4/4
82	PEB	PH	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	MB	201	2	-	3/26/74/74	0/4/4/4
82	PEB	RQ	202	1	-	10/26/74/74	0/4/4/4
87	CLA	62	307	87	-	8/15/91/115	-
95	DGD	J6	101	-	-	13/51/91/95	0/2/2/2
82	PEB	aF	203	1	-	12/26/74/74	0/4/4/4
82	PEB	RO	201	11,2	-	3/26/74/74	0/4/4/4
82	PEB	QB	202	2,5	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	DGD	BL	607	-	-	5/29/69/95	0/2/2/2
82	PEB	C7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	B7	202	2	-	8/26/74/74	0/4/4/4
82	PEB	jF	201	2	-	7/26/74/74	0/4/4/4
85	BCR	KN	101	40,49	-	13/29/63/63	0/2/2/2
87	CLA	B6	616	16	-	16/39/115/115	-
82	PEB	ZB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	G7	201	1	-	6/26/74/74	0/4/4/4
82	PEB	RA	202	2	-	10/26/74/74	0/4/4/4
82	PEB	J7	203	2	-	16/26/74/74	0/4/4/4
84	CYC	D1	1003	10,9	-	10/26/74/74	0/4/4/4
82	PEB	NK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	TF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	SF	201	1,2	-	4/26/74/74	0/4/4/4
87	CLA	B2	801	41	-	13/31/107/115	-
82	PEB	VD	203	1,2	-	14/26/74/74	0/4/4/4
87	CLA	B2	815	41	-	8/27/103/115	-
84	CYC	k3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	D5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	A2	813	-	-	13/39/115/115	-
87	CLA	CL	510	-	-	11/39/115/115	-
84	CYC	A3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	PP	201	2	-	7/26/74/74	0/4/4/4
87	CLA	FN	205	45	-	19/39/115/115	-
92	LMG	JL	103	18,24	-	6/28/48/70	0/1/1/1
85	BCR	A6	401	-	-	4/29/63/63	0/2/2/2
82	PEB	fB	301	76,2	-	10/26/74/74	0/4/4/4
82	PEB	C9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	MD	202	2	-	9/26/74/74	0/4/4/4
82	PEB	QG	203	1	-	10/26/74/74	0/4/4/4
82	PEB	TD	203	1	-	13/26/74/74	0/4/4/4
82	PEB	MM	203	1	-	10/26/74/74	0/4/4/4
82	PEB	h4	201	1	-	10/26/74/74	0/4/4/4
82	PEB	KM	201	1	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	CL	514	-	-	11/27/103/115	-
82	PEB	UP	203	1,2	-	11/26/74/74	0/4/4/4
84	CYC	S3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	cL	509	-	-	21/39/115/115	-
87	CLA	RN	202	54	-	9/15/91/115	-
84	CYC	n3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	s8	203	2	-	7/26/74/74	0/4/4/4
82	PEB	cF	201	1	-	10/26/74/74	0/4/4/4
87	CLA	B2	813	-	-	4/15/91/115	-
87	CLA	3N	305	59,87	-	15/39/115/115	-
103	ZEX	8N	310	64,87	-	11/29/67/67	0/2/2/2
82	PEB	W9	202	2	-	12/26/74/74	0/4/4/4
82	PEB	Y9	202	2	-	7/26/74/74	0/4/4/4
82	PEB	nK	202	2	-	11/26/74/74	0/4/4/4
84	CYC	D3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	w8	204	2	-	8/26/74/74	0/4/4/4
82	PEB	aJ	201	13,1	-	12/26/74/74	0/4/4/4
82	PEB	Q5	201	74,2	-	8/26/74/74	0/4/4/4
82	PEB	N7	201	2	-	3/26/74/74	0/4/4/4
82	PEB	VK	201	2	-	10/26/74/74	0/4/4/4
82	PEB	hF	201	2	-	8/26/74/74	0/4/4/4
82	PEB	FO	1002	10	-	9/26/74/74	0/4/4/4
87	CLA	62	301	62	-	6/15/91/115	-
82	PEB	IK	201	1	-	9/26/74/74	0/4/4/4
82	PEB	a4	203	2	-	11/26/74/74	0/4/4/4
87	CLA	bL	621	-	-	8/39/115/115	-
87	CLA	c6	607	17	-	17/39/115/115	-
84	CYC	r3	1001	-	-	12/26/74/74	0/4/4/4
82	PEB	IQ	201	2,77	-	7/26/74/74	0/4/4/4
82	PEB	cH	202	2	-	11/26/74/74	0/4/4/4
85	BCR	Z6	101	39	-	3/29/63/63	0/2/2/2
87	CLA	AN	811	-	-	21/39/115/115	-
84	CYC	I3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	j1	202	1	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	BCR	F2	204	-	-	6/29/63/63	0/2/2/2
83	PUB	Z5	303	1,74	-	8/26/74/74	0/4/4/4
82	PEB	U7	201	1	-	4/26/74/74	0/4/4/4
82	PEB	HP	201	56,2	-	7/26/74/74	0/4/4/4
87	CLA	c6	605	17	-	17/39/115/115	-
88	LHG	m6	102	-	-	19/43/43/53	-
88	LHG	CL	521	-	-	14/41/41/53	-
87	CLA	B2	831	-	-	17/33/109/115	-
82	PEB	LP	201	2	-	7/26/74/74	0/4/4/4
92	LMG	J6	102	-	-	17/38/58/70	0/1/1/1
82	PEB	LF	201	2	-	9/26/74/74	0/4/4/4
85	BCR	cL	504	17	-	5/29/63/63	0/2/2/2
88	LHG	d6	402	-	-	17/50/50/53	-
87	CLA	BN	811	-	-	20/39/115/115	-
82	PEB	V1	203	2	-	7/26/74/74	0/4/4/4
95	DGD	h6	101	22	-	12/51/91/95	0/2/2/2
92	LMG	C6	501	-	-	17/50/70/70	0/1/1/1
82	PEB	UG	201	1,2	-	5/26/74/74	0/4/4/4
82	PEB	K5	201	1	-	11/26/74/74	0/4/4/4
87	CLA	42	603	-	-	5/15/91/115	-
87	CLA	12	611	-	-	8/15/91/115	-
82	PEB	fM	202	1	-	13/26/74/74	0/4/4/4
87	CLA	b6	612	-	-	17/39/115/115	-
82	PEB	U5	201	74,2	-	11/26/74/74	0/4/4/4
82	PEB	U7	202	1	-	10/26/74/74	0/4/4/4
82	PEB	KE	201	10,9	-	6/26/74/74	0/4/4/4
82	PEB	DA	202	2	-	12/26/74/74	0/4/4/4
82	PEB	QA	202	1	-	9/26/74/74	0/4/4/4
82	PEB	BQ	201	1	-	9/26/74/74	0/4/4/4
82	PEB	IK	203	1,2	-	5/26/74/74	0/4/4/4
82	PEB	i1	202	2	-	9/26/74/74	0/4/4/4
82	PEB	V5	201	1	-	11/26/74/74	0/4/4/4
87	CLA	O2	202	53	-	10/21/97/115	-
82	PEB	dM	202	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	6N	611	62	-	10/15/91/115	-
82	PEB	XM	201	2	-	9/26/74/74	0/4/4/4
82	PEB	XJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	RA	203	2	-	10/26/74/74	0/4/4/4
82	PEB	CF	203	1	-	10/26/74/74	0/4/4/4
82	PEB	O1	202	1	-	7/26/74/74	0/4/4/4
82	PEB	yF	301	14	-	8/26/74/74	0/4/4/4
87	CLA	HL	101	22	-	10/39/115/115	-
82	PEB	OE	203	1,2	-	6/26/74/74	0/4/4/4
88	LHG	BL	610	-	-	13/53/53/53	-
82	PEB	A9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	wF	301	13	-	11/26/74/74	0/4/4/4
85	BCR	FN	202	-	-	6/29/63/63	0/2/2/2
82	PEB	PK	202	2	-	14/26/74/74	0/4/4/4
87	CLA	62	308	62	-	5/15/91/115	-
82	PEB	WK	203	1	-	13/26/74/74	0/4/4/4
82	PEB	MQ	201	2	-	7/26/74/74	0/4/4/4
87	CLA	B2	833	-	-	8/18/94/115	-
82	PEB	ZO	201	1	-	7/26/74/74	0/4/4/4
82	PEB	M5	305	74	-	13/26/74/74	0/4/4/4
82	PEB	E9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	Q1	203	1	-	9/26/74/74	0/4/4/4
87	CLA	cL	512	-	-	8/39/115/115	-
82	PEB	LD	203	1	-	12/26/74/74	0/4/4/4
87	CLA	cL	506	-	-	16/39/115/115	-
82	PEB	uF	203	1	-	10/26/74/74	0/4/4/4
87	CLA	4N	605	60	-	9/15/91/115	-
82	PEB	qK	203	1	-	10/26/74/74	0/4/4/4
82	PEB	TK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	Y1	202	2	-	8/26/74/74	0/4/4/4
82	PEB	e1	201	2	-	8/26/74/74	0/4/4/4
95	DGD	CL	520	-	-	5/31/71/95	0/2/2/2
87	CLA	BN	832	-	-	12/39/115/115	-
82	PEB	OD	201	3,2,82	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	II	201	1	-	9/26/74/74	0/4/4/4
82	PEB	mG	203	2	-	8/26/74/74	0/4/4/4
87	CLA	22	611	-	-	7/12/88/115	-
87	CLA	6N	603	-	-	9/15/91/115	-
82	PEB	yK	301	14	-	8/26/74/74	0/4/4/4
87	CLA	4N	606	-	-	8/15/91/115	-
87	CLA	52	610	-	-	5/15/91/115	-
82	PEB	GG	1002	10,9	-	9/26/74/74	0/4/4/4
82	PEB	J7	202	2	-	8/26/74/74	0/4/4/4
82	PEB	eF	202	1	-	8/26/74/74	0/4/4/4
82	PEB	lG	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	R7	201	2	-	5/26/74/74	0/4/4/4
84	CYC	F4	1001	10	-	11/26/74/74	0/4/4/4
82	PEB	Q4	201	1	-	8/26/74/74	0/4/4/4
82	PEB	HD	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	SF	203	1	-	9/26/74/74	0/4/4/4
82	PEB	FD	202	1	-	10/26/74/74	0/4/4/4
82	PEB	II	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	TJ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	dE	203	1	-	8/26/74/74	0/4/4/4
82	PEB	JB	201	1	-	8/26/74/74	0/4/4/4
85	BCR	C6	507	-	-	1/29/63/63	0/2/2/2
94	PL9	a6	601	15	-	11/53/73/73	0/1/1/1
82	PEB	xF	304	13	-	8/26/74/74	0/4/4/4
82	PEB	sC	203	2	-	7/26/74/74	0/4/4/4
84	CYC	M3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	CK	203	1	-	10/26/74/74	0/4/4/4
82	PEB	GK	201	1,2	-	8/26/74/74	0/4/4/4
84	CYC	o3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	bH	201	1	-	10/26/74/74	0/4/4/4
82	PEB	uC	201	2	-	10/26/74/74	0/4/4/4
82	PEB	S1	202	1	-	9/26/74/74	0/4/4/4
82	PEB	YK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	QH	201	1,2	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	MJ	202	1	-	5/26/74/74	0/4/4/4
82	PEB	MA	202	1	-	13/26/74/74	0/4/4/4
82	PEB	YD	201	2,82	-	7/26/74/74	0/4/4/4
87	CLA	BN	836	87,41,57	-	18/39/115/115	-
82	PEB	pF	201	2	-	8/26/74/74	0/4/4/4
82	PEB	jG	201	1	-	9/26/74/74	0/4/4/4
87	CLA	B2	827	-	-	15/39/115/115	-
82	PEB	BI	202	1,2	-	10/26/74/74	0/4/4/4
87	CLA	AL	403	15	-	12/39/115/115	-
82	PEB	b4	201	1	-	9/26/74/74	0/4/4/4
87	CLA	A2	818	-	-	8/15/91/115	-
82	PEB	OA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	GM	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	w8	202	2	-	5/26/74/74	0/4/4/4
82	PEB	MB	202	2	-	9/26/74/74	0/4/4/4
87	CLA	A2	808	-	-	17/39/115/115	-
82	PEB	YJ	201	1,2	-	6/26/74/74	0/4/4/4
82	PEB	WG	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	qF	203	1	-	10/26/74/74	0/4/4/4
95	DGD	AL	416	-	-	8/29/69/95	0/2/2/2
87	CLA	7N	605	-	-	8/15/91/115	-
82	PEB	UO	202	1	-	10/26/74/74	0/4/4/4
88	LHG	BL	615	-	-	17/45/45/53	-
87	CLA	DL	404	-	-	15/39/115/115	-
91	PHO	A6	407	-	3/3/17/22	11/37/103/103	0/5/6/6
82	PEB	X5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	DD	201	1,2	-	11/26/74/74	0/4/4/4
87	CLA	12	608	57	-	7/10/86/115	-
82	PEB	YA	304	3,82	-	13/26/74/74	0/4/4/4
87	CLA	ON	203	53	-	10/15/91/115	-
82	PEB	AE	304	3	-	5/26/74/74	0/4/4/4
82	PEB	FK	201	2	-	5/26/74/74	0/4/4/4
82	PEB	XK	203	2	-	11/26/74/74	0/4/4/4
82	PEB	lG	203	1	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	BCR	kL	100	-	-	13/29/63/63	0/2/2/2
82	PEB	AG	304	3	-	5/26/74/74	0/4/4/4
84	CYC	l3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	KQ	202	2	-	12/26/74/74	0/4/4/4
82	PEB	HD	203	1	-	12/26/74/74	0/4/4/4
82	PEB	YI	202	2	-	5/26/74/74	0/4/4/4
87	CLA	72	603	-	-	7/15/91/115	-
82	PEB	kF	201	1	-	12/26/74/74	0/4/4/4
82	PEB	YK	201	1	-	7/26/74/74	0/4/4/4
95	DGD	a6	604	15,17	-	4/42/82/95	0/2/2/2
82	PEB	SE	202	1,2	-	7/26/74/74	0/4/4/4
87	CLA	B2	822	-	-	16/39/115/115	-
82	PEB	JI	202	2	-	9/26/74/74	0/4/4/4
87	CLA	A2	824	40	-	10/23/99/115	-
87	CLA	8N	308	-	-	12/15/91/115	-
82	PEB	SD	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	Y4	203	2	-	11/26/74/74	0/4/4/4
82	PEB	BK	202	2	-	13/26/74/74	0/4/4/4
82	PEB	DD	202	1	-	9/26/74/74	0/4/4/4
82	PEB	d1	201	1,2	-	5/26/74/74	0/4/4/4
84	CYC	p3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	AN	819	40	-	12/36/112/115	-
82	PEB	EA	202	1	-	11/26/74/74	0/4/4/4
82	PEB	GP	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	PA	201	2	-	4/26/74/74	0/4/4/4
82	PEB	QH	202	1	-	12/26/74/74	0/4/4/4
82	PEB	A4	301	3	-	7/26/74/74	0/4/4/4
82	PEB	eE	203	2	-	13/26/74/74	0/4/4/4
82	PEB	I9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	A1	302	3	-	11/26/74/74	0/4/4/4
82	PEB	KD	201	2	-	9/26/74/74	0/4/4/4
82	PEB	QE	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	kK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	BQ	203	1,2	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	CYC	H3	1001	73,69	-	4/26/74/74	0/4/4/4
88	LHG	I6	101	-	-	21/53/53/53	-
87	CLA	AN	807	-	-	12/39/115/115	-
102	BGC	32	301	-	-	0/2/19/22	0/1/1/1
82	PEB	Y7	304	3,82	-	13/26/74/74	0/4/4/4
82	PEB	Q5	202	2	-	10/26/74/74	0/4/4/4
82	PEB	aB	201	2	-	2/26/74/74	0/4/4/4
82	PEB	lK	203	1,2	-	10/26/74/74	0/4/4/4
87	CLA	AN	840	-	-	14/39/115/115	-
82	PEB	PJ	201	2	-	6/26/74/74	0/4/4/4
87	CLA	B6	615	16	-	20/39/115/115	-
87	CLA	LN	203	85,50,41	-	22/39/115/115	-
82	PEB	bP	502	2	-	9/26/74/74	0/4/4/4
84	CYC	LE	1001	10	-	11/26/74/74	0/4/4/4
95	DGD	c6	620	-	-	13/37/77/95	0/2/2/2
82	PEB	UJ	201	1,2	-	8/26/74/74	0/4/4/4
87	CLA	B6	603	-	-	13/39/115/115	-
84	CYC	f3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	bL	620	16,85	-	11/29/105/115	-
82	PEB	VM	201	2	-	6/26/74/74	0/4/4/4
87	CLA	FN	203	45	-	10/15/91/115	-
82	PEB	QJ	202	1,2	-	8/26/74/74	0/4/4/4
82	PEB	F9	201	74,2	-	12/26/74/74	0/4/4/4
82	PEB	GM	202	1	-	12/26/74/74	0/4/4/4
87	CLA	c6	609	-	-	19/39/115/115	-
87	CLA	AN	826	-	-	11/39/115/115	-
82	PEB	Q7	201	1	-	5/26/74/74	0/4/4/4
82	PEB	oK	202	1	-	10/26/74/74	0/4/4/4
87	CLA	22	608	58	-	7/15/91/115	-
82	PEB	XI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	EM	202	1	-	8/26/74/74	0/4/4/4
82	PEB	UO	201	1	-	7/26/74/74	0/4/4/4
82	PEB	S4	201	1	-	10/26/74/74	0/4/4/4
96	HEM	fL	102	-	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	DGD	CL	517	-	-	5/51/91/95	0/2/2/2
82	PEB	VA	202	2	-	10/26/74/74	0/4/4/4
82	PEB	hG	202	1	-	11/26/74/74	0/4/4/4
82	PEB	rF	202	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	831	-	-	17/33/109/115	-
82	PEB	aH	202	2	-	10/26/74/74	0/4/4/4
82	PEB	O7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	SG	202	-	-	10/26/74/74	0/4/4/4
82	PEB	qK	202	1	-	17/26/74/74	0/4/4/4
85	BCR	H6	101	-	-	3/29/63/63	0/2/2/2
84	CYC	K3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	nL	101	-	-	18/39/115/115	-
84	CYC	I4	1001	9	-	11/26/74/74	0/4/4/4
84	CYC	GO	1001	9	-	8/26/74/74	0/4/4/4
82	PEB	wC	204	2	-	8/26/74/74	0/4/4/4
85	BCR	b6	601	-	-	2/29/63/63	0/2/2/2
87	CLA	B2	830	-	-	15/39/115/115	-
82	PEB	fF	201	13,2	-	10/26/74/74	0/4/4/4
82	PEB	fE	202	1	-	8/26/74/74	0/4/4/4
82	PEB	NJ	201	2	-	8/26/74/74	0/4/4/4
82	PEB	m4	203	2	-	7/26/74/74	0/4/4/4
82	PEB	i4	203	2	-	10/26/74/74	0/4/4/4
87	CLA	BL	606	-	-	2/39/115/115	-
95	DGD	a6	603	-	-	10/29/69/95	0/2/2/2
87	CLA	82	306	64,103	-	10/17/93/115	-
87	CLA	1N	609	-	-	6/12/88/115	-
82	PEB	mO	202	2	-	8/26/74/74	0/4/4/4
87	CLA	A2	812	-	-	11/27/103/115	-
84	CYC	y3	1001	71	-	10/26/74/74	0/4/4/4
82	PEB	WE	201	1	-	7/26/74/74	0/4/4/4
82	PEB	cM	201	2	-	10/26/74/74	0/4/4/4
82	PEB	Y7	303	3,82	-	13/26/74/74	0/4/4/4
82	PEB	KK	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	AN	812	-	-	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	aM	202	1	-	7/26/74/74	0/4/4/4
95	DGD	AL	415	-	-	1/29/69/95	0/2/2/2
82	PEB	DM	202	2	-	9/26/74/74	0/4/4/4
82	PEB	GQ	202	2	-	13/26/74/74	0/4/4/4
82	PEB	SB	202	2	-	7/26/74/74	0/4/4/4
87	CLA	C6	519	-	-	11/27/103/115	-
82	PEB	p8	201	1	-	12/26/74/74	0/4/4/4
82	PEB	IM	203	1	-	9/26/74/74	0/4/4/4
82	PEB	JM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	LQ	202	1	-	9/26/74/74	0/4/4/4
85	BCR	bL	603	-	-	4/29/63/63	0/2/2/2
82	PEB	U9	202	2	-	11/26/74/74	0/4/4/4
87	CLA	A2	807	-	-	12/39/115/115	-
82	PEB	RO	202	2	-	10/26/74/74	0/4/4/4
82	PEB	B9	203	2	-	7/26/74/74	0/4/4/4
84	CYC	u3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	6N	602	62	-	18/39/115/115	-
87	CLA	72	602	62,63	-	14/39/115/115	-
82	PEB	FJ	202	2	-	7/26/74/74	0/4/4/4
94	PL9	A6	410	-	-	17/53/73/73	0/1/1/1
82	PEB	eB	201	2	-	6/26/74/74	0/4/4/4
82	PEB	PF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	OG	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	QG	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	c6	610	-	-	11/39/115/115	-
87	CLA	AN	833	-	-	13/39/115/115	-
82	PEB	TD	202	1	-	9/26/74/74	0/4/4/4
82	PEB	S9	202	2	-	9/26/74/74	0/4/4/4
91	PHO	a6	613	-	3/3/17/22	11/37/103/103	0/5/6/6
95	DGD	cL	502	-	-	12/51/91/95	0/2/2/2
87	CLA	AN	816	-	-	8/15/91/115	-
84	CYC	t3	1001	68	-	8/26/74/74	0/4/4/4
84	CYC	N4	1001	10	-	13/26/74/74	0/4/4/4
82	PEB	uK	201	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	PD	201	1,2	-	8/26/74/74	0/4/4/4
99	SF4	C2	101	42	-	-	0/6/5/5
92	LMG	BL	611	-	-	12/35/55/70	0/1/1/1
85	BCR	C6	508	-	-	10/29/63/63	0/2/2/2
87	CLA	6N	605	62	-	8/15/91/115	-
82	PEB	HQ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	xK	304	13	-	8/26/74/74	0/4/4/4
85	BCR	KL	100	-	-	13/29/63/63	0/2/2/2
82	PEB	CP	202	1	-	6/26/74/74	0/4/4/4
87	CLA	6N	606	87	-	8/15/91/115	-
82	PEB	VJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	R9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	AA	202	1	-	13/26/74/74	0/4/4/4
82	PEB	ZE	202	1	-	9/26/74/74	0/4/4/4
82	PEB	hF	202	2	-	9/26/74/74	0/4/4/4
82	PEB	F5	201	74,2	-	11/26/74/74	0/4/4/4
87	CLA	5N	605	61	-	6/15/91/115	-
82	PEB	JH	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	J5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	1N	610	57	-	8/15/91/115	-
82	PEB	M5	301	74	-	8/26/74/74	0/4/4/4
82	PEB	KA	202	1	-	11/26/74/74	0/4/4/4
82	PEB	V1	201	2	-	2/26/74/74	0/4/4/4
82	PEB	aO	201	2	-	2/26/74/74	0/4/4/4
87	CLA	cL	507	-	-	12/39/115/115	-
82	PEB	S7	201	1	-	4/26/74/74	0/4/4/4
87	CLA	BN	824	-	-	8/39/115/115	-
82	PEB	hH	202	1	-	11/26/74/74	0/4/4/4
82	PEB	T1	201	11,2	-	9/26/74/74	0/4/4/4
82	PEB	OJ	201	1	-	5/26/74/74	0/4/4/4
82	PEB	FB	201	2,5	-	12/26/74/74	0/4/4/4
87	CLA	42	607	60	-	8/15/91/115	-
82	PEB	tF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	X9	201	1	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	GJ	201	1	-	6/26/74/74	0/4/4/4
87	CLA	BN	814	-	-	4/15/91/115	-
82	PEB	TB	201	1	-	8/26/74/74	0/4/4/4
82	PEB	hB	301	76,2	-	10/26/74/74	0/4/4/4
82	PEB	pK	202	2	-	11/26/74/74	0/4/4/4
88	LHG	l6	101	26,16	-	18/53/53/53	-
82	PEB	dF	202	2	-	14/26/74/74	0/4/4/4
82	PEB	CF	201	1	-	6/26/74/74	0/4/4/4
82	PEB	A4	305	3	-	11/26/74/74	0/4/4/4
87	CLA	KN	105	40,49	-	11/20/96/115	-
92	LMG	j6	102	18,24	-	10/28/48/70	0/1/1/1
82	PEB	lF	201	2	-	11/26/74/74	0/4/4/4
82	PEB	YG	202	2	-	12/26/74/74	0/4/4/4
87	CLA	AN	820	-	-	12/39/115/115	-
87	CLA	b6	611	-	-	19/39/115/115	-
83	PUB	yF	302	14	-	3/26/74/74	0/4/4/4
95	DGD	C6	521	-	-	14/51/91/95	0/2/2/2
82	PEB	vK	202	2	-	9/26/74/74	0/4/4/4
82	PEB	jH	201	1	-	9/26/74/74	0/4/4/4
87	CLA	4N	603	-	-	5/15/91/115	-
82	PEB	GF	203	1	-	9/26/74/74	0/4/4/4
82	PEB	gF	203	1,2	-	9/26/74/74	0/4/4/4
87	CLA	42	601	60	-	8/15/91/115	-
84	CYC	FG	1001	10	-	7/26/74/74	0/4/4/4
82	PEB	FH	1002	10	-	11/26/74/74	0/4/4/4
87	CLA	22	612	58	-	7/15/91/115	-
95	DGD	cL	520	-	-	11/37/77/95	0/2/2/2
82	PEB	hH	201	1	-	11/26/74/74	0/4/4/4
87	CLA	B2	819	41	-	8/15/91/115	-
84	CYC	GG	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	BA	202	2	-	8/26/74/74	0/4/4/4
82	PEB	oF	202	1	-	10/26/74/74	0/4/4/4
91	PHO	AL	410	-	3/3/17/22	14/37/103/103	0/5/6/6
82	PEB	KF	202	1	-	4/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	NP	201	2	-	8/26/74/74	0/4/4/4
94	PL9	aL	601	15	-	10/53/73/73	0/1/1/1
87	CLA	b6	618	-	-	19/39/115/115	-
82	PEB	TE	201	2	-	3/26/74/74	0/4/4/4
83	PUB	AO	303	3	-	6/26/74/74	0/4/4/4
83	PUB	NQ	201	1,3	-	1/26/74/74	0/4/4/4
82	PEB	SH	202	1	-	9/26/74/74	0/4/4/4
82	PEB	s8	202	2	-	8/26/74/74	0/4/4/4
87	CLA	DL	406	-	-	18/39/115/115	-
82	PEB	ZG	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	SM	202	1	-	11/26/74/74	0/4/4/4
82	PEB	dF	201	2	-	9/26/74/74	0/4/4/4
82	PEB	c4	202	2	-	11/26/74/74	0/4/4/4
82	PEB	YD	202	2	-	8/26/74/74	0/4/4/4
82	PEB	LA	203	2	-	10/26/74/74	0/4/4/4
87	CLA	BL	622	16	-	9/39/115/115	-
85	BCR	FN	204	-	-	6/29/63/63	0/2/2/2
82	PEB	Q1	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	KA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	R4	202	2	-	10/26/74/74	0/4/4/4
87	CLA	B2	805	41	-	18/39/115/115	-
82	PEB	EJ	202	1	-	5/26/74/74	0/4/4/4
87	CLA	5N	604	61	-	6/12/88/115	-
82	PEB	UF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	CI	201	1	-	9/26/74/74	0/4/4/4
87	CLA	cL	510	-	-	23/39/115/115	-
84	CYC	HE	1001	10	-	9/26/74/74	0/4/4/4
82	PEB	18	202	2	-	6/26/74/74	0/4/4/4
85	BCR	A2	846	-	-	10/29/63/63	0/2/2/2
82	PEB	DH	1002	10	-	11/26/74/74	0/4/4/4
82	PEB	vC	201	1	-	10/26/74/74	0/4/4/4
85	BCR	K2	105	-	-	8/29/63/63	0/2/2/2
82	PEB	dE	202	1,2	-	6/26/74/74	0/4/4/4
82	PEB	GI	201	1,2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	A1	301	3	-	7/26/74/74	0/4/4/4
82	PEB	PM	201	2	-	10/26/74/74	0/4/4/4
82	PEB	VQ	201	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	613	62	-	6/15/91/115	-
82	PEB	hK	201	2	-	8/26/74/74	0/4/4/4
82	PEB	NM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	jM	202	1	-	12/26/74/74	0/4/4/4
82	PEB	VD	201	1	-	12/26/74/74	0/4/4/4
82	PEB	KK	203	1	-	8/26/74/74	0/4/4/4
82	PEB	WB	402	6,2	-	6/26/74/74	0/4/4/4
82	PEB	L5	201	74,2	-	10/26/74/74	0/4/4/4
87	CLA	BN	808	-	-	11/39/115/115	-
82	PEB	JQ	201	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	601	62	-	7/15/91/115	-
82	PEB	CJ	201	1	-	4/26/74/74	0/4/4/4
82	PEB	P1	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	D9	202	2	-	9/26/74/74	0/4/4/4
82	PEB	AO	301	3	-	7/26/74/74	0/4/4/4
82	PEB	l1	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	H7	201	2	-	5/26/74/74	0/4/4/4
82	PEB	f1	201	1	-	9/26/74/74	0/4/4/4
82	PEB	eH	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	U1	201	1,2	-	9/26/74/74	0/4/4/4
83	PUB	QJ	201	14,1	-	5/26/74/74	0/4/4/4
88	LHG	C6	505	-	-	14/41/41/53	-
82	PEB	LQ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	NB	201	2	-	6/26/74/74	0/4/4/4
82	PEB	v8	202	1	-	15/26/74/74	0/4/4/4
82	PEB	WG	201	1	-	7/26/74/74	0/4/4/4
87	CLA	B2	832	-	-	12/39/115/115	-
87	CLA	BL	621	-	-	15/39/115/115	-
82	PEB	DK	203	2	-	12/26/74/74	0/4/4/4
82	PEB	BP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	wK	303	13	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	JP	201	2	-	6/26/74/74	0/4/4/4
87	CLA	2N	310	58	-	5/10/86/115	-
82	PEB	mH	202	2	-	10/26/74/74	0/4/4/4
82	PEB	wK	302	13	-	10/26/74/74	0/4/4/4
82	PEB	hJ	203	1	-	14/26/74/74	0/4/4/4
82	PEB	IQ	202	2	-	7/26/74/74	0/4/4/4
84	CYC	P3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	cL	511	17	-	13/39/115/115	-
87	CLA	3N	306	-	-	8/15/91/115	-
85	BCR	BN	840	41	-	7/29/63/63	0/2/2/2
87	CLA	BN	801	-	-	17/39/115/115	-
82	PEB	WI	202	1,2	-	9/26/74/74	0/4/4/4
84	CYC	j3	1001	73,69	-	4/26/74/74	0/4/4/4
94	PL9	DL	401	18,26	-	12/53/73/73	0/1/1/1
82	PEB	u8	203	2	-	2/26/74/74	0/4/4/4
87	CLA	HL	102	22	-	15/39/115/115	-
88	LHG	A2	844	-	-	17/44/44/53	-
82	PEB	MP	202	1	-	9/26/74/74	0/4/4/4
82	PEB	oF	203	1	-	15/26/74/74	0/4/4/4
87	CLA	d6	401	18	-	17/39/115/115	-
82	PEB	JD	201	1	-	12/26/74/74	0/4/4/4
87	CLA	A2	810	40	-	23/39/115/115	-
82	PEB	eB	202	2	-	5/26/74/74	0/4/4/4
87	CLA	72	607	63	-	9/21/97/115	-
83	PUB	yF	303	14	-	4/26/74/74	0/4/4/4
82	PEB	F9	203	2	-	9/26/74/74	0/4/4/4
82	PEB	sK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	kO	201	2	-	8/26/74/74	0/4/4/4
82	PEB	KI	202	1	-	9/26/74/74	0/4/4/4
82	PEB	L5	203	2	-	12/26/74/74	0/4/4/4
84	CYC	G3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	RB	202	2	-	11/26/74/74	0/4/4/4
82	PEB	TI	201	1,2	-	10/26/74/74	0/4/4/4
82	PEB	FA	202	2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	DI	201	12,2	-	6/26/74/74	0/4/4/4
82	PEB	W5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	ON	201	-	-	7/10/86/115	-
82	PEB	I7	202	1	-	11/26/74/74	0/4/4/4
82	PEB	kJ	201	2	-	9/26/74/74	0/4/4/4
82	PEB	SI	202	2	-	9/26/74/74	0/4/4/4
82	PEB	VE	201	2	-	8/26/74/74	0/4/4/4
82	PEB	ZG	202	1	-	9/26/74/74	0/4/4/4
82	PEB	M9	305	74	-	10/26/74/74	0/4/4/4
87	CLA	K2	103	-	-	5/15/91/115	-
87	CLA	A2	806	-	-	9/27/103/115	-
82	PEB	IF	202	1	-	15/26/74/74	0/4/4/4
82	PEB	mH	201	2	-	8/26/74/74	0/4/4/4
82	PEB	W1	203	1,2	-	8/26/74/74	0/4/4/4
87	CLA	a6	607	15	-	13/39/115/115	-
82	PEB	h1	202	1	-	11/26/74/74	0/4/4/4
87	CLA	AN	841	-	-	14/39/115/115	-
85	BCR	cL	518	-	-	4/29/63/63	0/2/2/2
87	CLA	c6	615	-	-	10/27/103/115	-
92	LMG	x6	601	37	-	8/45/65/70	0/1/1/1
82	PEB	W9	203	2	-	6/26/74/74	0/4/4/4
87	CLA	BN	825	41	-	20/39/115/115	-
87	CLA	AN	852	59,40	-	8/15/91/115	-
87	CLA	62	306	62	-	8/15/91/115	-
88	LHG	M6	101	-	-	13/43/43/53	-
82	PEB	pC	202	1	-	16/26/74/74	0/4/4/4
87	CLA	BL	603	-	-	13/39/115/115	-
82	PEB	BD	203	1,2	-	12/26/74/74	0/4/4/4
82	PEB	B5	201	74,2,82	-	11/26/74/74	0/4/4/4
82	PEB	B7	201	2,82	-	8/26/74/74	0/4/4/4
88	LHG	A2	843	40	-	16/53/53/53	-
82	PEB	MP	201	1	-	5/26/74/74	0/4/4/4
83	PUB	BM	302	14	-	9/26/74/74	0/4/4/4
82	PEB	IP	202	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
101	FES	NN	101	-	-	-	0/1/1/1
82	PEB	RK	201	2	-	8/26/74/74	0/4/4/4
82	PEB	gO	203	2	-	11/26/74/74	0/4/4/4
85	BCR	B6	601	-	-	0/29/63/63	0/2/2/2
82	PEB	YQ	201	2,82	-	7/26/74/74	0/4/4/4
82	PEB	L7	202	2	-	9/26/74/74	0/4/4/4
84	CYC	DH	1003	10,9	-	10/26/74/74	0/4/4/4
85	BCR	L2	201	-	-	13/29/63/63	0/2/2/2
87	CLA	c6	612	17	-	19/39/115/115	-
82	PEB	F9	202	2	-	8/26/74/74	0/4/4/4
82	PEB	lK	201	2	-	11/26/74/74	0/4/4/4
82	PEB	AJ	301	13	-	12/26/74/74	0/4/4/4
82	PEB	lJ	203	1	-	11/26/74/74	0/4/4/4
82	PEB	fG	201	1	-	10/26/74/74	0/4/4/4
82	PEB	R5	201	1	-	11/26/74/74	0/4/4/4
87	CLA	BN	812	-	-	7/27/103/115	-
82	PEB	IJ	202	1	-	7/26/74/74	0/4/4/4
87	CLA	AN	818	-	-	8/15/91/115	-
82	PEB	UH	203	1	-	9/26/74/74	0/4/4/4
87	CLA	B6	606	-	-	13/39/115/115	-
82	PEB	AI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	JK	201	2	-	8/26/74/74	0/4/4/4
87	CLA	7N	607	63	-	9/21/97/115	-
82	PEB	d1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	EI	202	1	-	10/26/74/74	0/4/4/4
88	LHG	DL	407	18	-	16/53/53/53	-
82	PEB	C5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	aM	204	1,2	-	9/26/74/74	0/4/4/4
83	PUB	Y7	302	3	-	3/26/74/74	0/4/4/4
82	PEB	XF	203	2	-	11/26/74/74	0/4/4/4
82	PEB	nK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	ZH	202	1	-	9/26/74/74	0/4/4/4
82	PEB	DQ	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	dM	203	1	-	13/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	wC	203	2	-	6/26/74/74	0/4/4/4
82	PEB	xC	202	1	-	15/26/74/74	0/4/4/4
87	CLA	3N	313	-	-	8/15/91/115	-
82	PEB	HP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	E7	202	1	-	11/26/74/74	0/4/4/4
84	CYC	JH	1003	10,9	-	11/26/74/74	0/4/4/4
96	HEM	f6	101	19,20	-	2/14/54/54	-
82	PEB	MP	203	1,2	-	13/26/74/74	0/4/4/4
85	BCR	LN	205	50	-	11/29/63/63	0/2/2/2
82	PEB	P5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	GE	1002	10,9	-	9/26/74/74	0/4/4/4
82	PEB	TM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	hE	203	1	-	7/26/74/74	0/4/4/4
84	CYC	H1	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	P7	201	2	-	4/26/74/74	0/4/4/4
82	PEB	U9	204	1,2	-	8/26/74/74	0/4/4/4
85	BCR	k6	102	-	-	12/29/63/63	0/2/2/2
82	PEB	DE	1002	10,9	-	8/26/74/74	0/4/4/4
82	PEB	gJ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	PQ	203	1	-	12/26/74/74	0/4/4/4
85	BCR	b6	603	-	-	2/29/63/63	0/2/2/2
82	PEB	dQ	401	2,77	-	12/26/74/74	0/4/4/4
82	PEB	YM	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	UH	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	42	609	60	-	5/10/86/115	-
92	LMG	BL	612	16	-	5/34/54/70	0/1/1/1
87	CLA	AN	836	-	-	7/15/91/115	-
91	PHO	aL	610	-	3/3/17/22	14/37/103/103	0/5/6/6
82	PEB	MK	202	1	-	10/26/74/74	0/4/4/4
87	CLA	b6	605	16	-	15/39/115/115	-
82	PEB	D5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	R7	203	2	-	10/26/74/74	0/4/4/4
97	GOL	wL	101	-	-	2/4/4/4	-
100	3XQ	J2	104	-	-	14/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	QQ	202	2	-	11/26/74/74	0/4/4/4
87	CLA	62	309	62	-	10/21/97/115	-
82	PEB	OI	202	1,2	-	10/26/74/74	0/4/4/4
82	PEB	c1	201	2	-	7/26/74/74	0/4/4/4
82	PEB	lM	203	1	-	12/26/74/74	0/4/4/4
87	CLA	A2	811	-	-	21/39/115/115	-
87	CLA	L2	202	50	-	16/30/106/115	-
87	CLA	bL	608	-	-	10/39/115/115	-
82	PEB	QB	201	2	-	15/26/74/74	0/4/4/4
87	CLA	BN	835	-	-	22/39/115/115	-
82	PEB	J9	202	2	-	8/26/74/74	0/4/4/4
82	PEB	RI	201	1	-	9/26/74/74	0/4/4/4
87	CLA	A2	803	40,50,53	-	13/24/100/115	-
92	LMG	ML	101	-	-	11/36/56/70	0/1/1/1
84	CYC	FE	1002	10	-	7/26/74/74	0/4/4/4
83	PUB	AG	302	3	-	9/26/74/74	0/4/4/4
82	PEB	VE	202	2	-	10/26/74/74	0/4/4/4
82	PEB	OJ	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	M7	202	1	-	13/26/74/74	0/4/4/4
82	PEB	LH	1003	10	-	8/26/74/74	0/4/4/4
82	PEB	y8	201	2	-	16/26/74/74	0/4/4/4
82	PEB	OB	201	2,5	-	11/26/74/74	0/4/4/4
82	PEB	FP	201	56,2	-	7/26/74/74	0/4/4/4
82	PEB	FI	201	2	-	12/26/74/74	0/4/4/4
82	PEB	KB	303	2	-	12/26/74/74	0/4/4/4
82	PEB	OG	201	1	-	9/26/74/74	0/4/4/4
82	PEB	cF	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	62	302	62	-	7/15/91/115	-
82	PEB	AK	202	1	-	11/26/74/74	0/4/4/4
82	PEB	PG	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	XK	201	2	-	9/26/74/74	0/4/4/4
87	CLA	AN	815	-	-	20/39/115/115	-
92	LMG	b6	620	16	-	12/34/54/70	0/1/1/1
82	PEB	fJ	202	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	b6	616	-	-	12/39/115/115	-
83	PUB	xF	306	13	-	6/26/74/74	0/4/4/4
87	CLA	CL	515	-	-	8/39/115/115	-
92	LMG	m6	101	85	-	16/36/56/70	0/1/1/1
82	PEB	AP	203	1,2	-	12/26/74/74	0/4/4/4
82	PEB	V9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	SJ	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	EF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	eE	201	2	-	9/26/74/74	0/4/4/4
82	PEB	Z9	304	74	-	10/26/74/74	0/4/4/4
88	LHG	mL	102	-	-	17/43/43/53	-
87	CLA	52	601	61	-	11/15/91/115	-
87	CLA	A2	840	-	-	14/39/115/115	-
85	BCR	bL	602	-	-	1/29/63/63	0/2/2/2
87	CLA	4N	610	-	-	7/12/88/115	-
83	PUB	AH	304	3	-	15/26/74/74	0/4/4/4
82	PEB	QB	203	2	-	9/26/74/74	0/4/4/4
82	PEB	cE	202	2	-	10/26/74/74	0/4/4/4
82	PEB	B5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	B7	203	2	-	12/26/74/74	0/4/4/4
84	CYC	c3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	12	603	-	-	4/15/91/115	-
82	PEB	fE	201	1	-	10/26/74/74	0/4/4/4
82	PEB	eG	203	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	828	41	-	7/15/91/115	-
82	PEB	qC	201	2	-	5/26/74/74	0/4/4/4
87	CLA	12	601	57	-	12/15/91/115	-
82	PEB	aM	201	13,1	-	10/26/74/74	0/4/4/4
82	PEB	iO	203	2	-	10/26/74/74	0/4/4/4
82	PEB	VG	202	2	-	10/26/74/74	0/4/4/4
82	PEB	VI	203	1,2	-	10/26/74/74	0/4/4/4
87	CLA	b6	610	-	-	17/39/115/115	-
87	CLA	AN	849	40	-	11/39/115/115	-
82	PEB	J4	1002	10	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	HEM	G2	201	46	-	6/14/54/54	-
87	CLA	A2	835	-	-	16/39/115/115	-
82	PEB	lE	203	1	-	7/26/74/74	0/4/4/4
82	PEB	fJ	201	1	-	5/26/74/74	0/4/4/4
87	CLA	6N	607	62	-	5/15/91/115	-
82	PEB	QO	202	1	-	8/26/74/74	0/4/4/4
87	CLA	4N	607	60	-	8/15/91/115	-
82	PEB	DB	201	2	-	8/26/74/74	0/4/4/4
102	BGC	3N	302	-	-	0/2/19/22	0/1/1/1
82	PEB	S5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	1C	203	2	-	6/26/74/74	0/4/4/4
85	BCR	F2	203	-	-	6/29/63/63	0/2/2/2
87	CLA	72	605	-	-	8/15/91/115	-
87	CLA	5N	607	61	-	8/21/97/115	-
87	CLA	3N	309	59	-	14/21/97/115	-
82	PEB	RD	202	1	-	10/26/74/74	0/4/4/4
82	PEB	dK	202	2	-	14/26/74/74	0/4/4/4
84	CYC	EO	1001	9	-	10/26/74/74	0/4/4/4
82	PEB	dH	202	1	-	10/26/74/74	0/4/4/4
92	LMG	qL	301	-	-	10/38/58/70	0/1/1/1
82	PEB	KJ	202	1	-	16/26/74/74	0/4/4/4
82	PEB	c1	202	2	-	11/26/74/74	0/4/4/4
87	CLA	72	601	63	-	12/15/91/115	-
82	PEB	YK	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	J9	203	2	-	9/26/74/74	0/4/4/4
87	CLA	BN	816	41	-	8/27/103/115	-
82	PEB	aJ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	R1	201	2	-	7/26/74/74	0/4/4/4
82	PEB	sF	202	1	-	10/26/74/74	0/4/4/4
85	BCR	bL	601	87	-	8/29/63/63	0/2/2/2
82	PEB	uF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	QF	201	1	-	7/26/74/74	0/4/4/4
87	CLA	4N	601	60	-	8/15/91/115	-
82	PEB	Z1	202	1	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	g4	201	2	-	4/26/74/74	0/4/4/4
82	PEB	f4	202	1	-	11/26/74/74	0/4/4/4
82	PEB	PK	201	2	-	7/26/74/74	0/4/4/4
85	BCR	hL	102	-	-	3/29/63/63	0/2/2/2
101	FES	N2	101	-	-	-	0/1/1/1
82	PEB	TI	203	1	-	10/26/74/74	0/4/4/4
82	PEB	gG	202	2	-	11/26/74/74	0/4/4/4
84	CYC	DG	1001	10	-	13/26/74/74	0/4/4/4
87	CLA	5N	601	61	-	11/15/91/115	-
82	PEB	WF	202	1	-	8/26/74/74	0/4/4/4
82	PEB	Y7	301	3	-	18/26/74/74	0/4/4/4
82	PEB	kE	201	3,2	-	9/26/74/74	0/4/4/4
87	CLA	2N	302	58	-	7/15/91/115	-
82	PEB	zK	501	78,2	-	7/26/74/74	0/4/4/4
87	CLA	BL	605	-	-	16/39/115/115	-
82	PEB	fJ	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	LK	202	2	-	14/26/74/74	0/4/4/4
84	CYC	i3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	lE	202	-	-	13/26/74/74	0/4/4/4
82	PEB	TA	201	2	-	5/26/74/74	0/4/4/4
82	PEB	cE	201	2	-	6/26/74/74	0/4/4/4
82	PEB	KP	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	UM	201	1,2	-	6/26/74/74	0/4/4/4
87	CLA	F2	201	45	-	10/15/91/115	-
98	PQN	A2	842	-	-	6/23/43/43	0/2/2/2
87	CLA	3N	308	59	-	5/15/91/115	-
82	PEB	u8	202	2	-	7/26/74/74	0/4/4/4
87	CLA	22	605	58,41	-	11/25/101/115	-
87	CLA	32	309	59	-	14/21/97/115	-
82	PEB	WB	401	6,2	-	10/26/74/74	0/4/4/4
94	PL9	dL	406	18,26	-	13/53/73/73	0/1/1/1
82	PEB	DA	203	2	-	11/26/74/74	0/4/4/4
82	PEB	C5	202	1	-	11/26/74/74	0/4/4/4
87	CLA	JN	101	48	-	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	BCR	AN	848	-	-	16/29/63/63	0/2/2/2
87	CLA	32	303	59,87	-	8/15/91/115	-
87	CLA	C6	520	-	-	15/39/115/115	-
83	PUB	AD	302	1,3	-	8/26/74/74	0/4/4/4
87	CLA	K2	101	-	-	12/39/115/115	-
82	PEB	AB	501	2,4	-	10/26/74/74	0/4/4/4
82	PEB	JA	203	2	-	16/26/74/74	0/4/4/4
82	PEB	gM	202	2	-	10/26/74/74	0/4/4/4
87	CLA	B6	613	-	-	17/39/115/115	-
82	PEB	eM	201	13,2	-	6/26/74/74	0/4/4/4
87	CLA	B6	605	16	-	16/39/115/115	-
82	PEB	YB	201	2	-	5/26/74/74	0/4/4/4
84	CYC	DE	1001	10	-	13/26/74/74	0/4/4/4
82	PEB	QM	202	1,2	-	7/26/74/74	0/4/4/4
82	PEB	m1	201	2	-	8/26/74/74	0/4/4/4
85	BCR	CL	502	17	-	5/29/63/63	0/2/2/2
82	PEB	dD	401	2,77	-	12/26/74/74	0/4/4/4
82	PEB	YP	501	2	-	4/26/74/74	0/4/4/4
82	PEB	LK	201	2	-	9/26/74/74	0/4/4/4
82	PEB	H9	202	2	-	8/26/74/74	0/4/4/4
82	PEB	cK	201	1	-	10/26/74/74	0/4/4/4
87	CLA	O2	203	53	-	10/15/91/115	-
85	BCR	FL	101	20	-	8/29/63/63	0/2/2/2
87	CLA	7N	608	63	-	6/10/86/115	-
82	PEB	dH	201	1,2	-	5/26/74/74	0/4/4/4
82	PEB	bP	501	56,2	-	10/26/74/74	0/4/4/4
88	LHG	AL	406	-	-	22/53/53/53	-
82	PEB	F7	202	2	-	10/26/74/74	0/4/4/4
87	CLA	K2	104	-	-	4/12/88/115	-
82	PEB	VM	202	2	-	9/26/74/74	0/4/4/4
82	PEB	GA	202	1	-	12/26/74/74	0/4/4/4
92	LMG	m6	103	-	-	10/36/56/70	0/1/1/1
82	PEB	S5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	SG	201	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	PI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	fO	201	1	-	11/26/74/74	0/4/4/4
82	PEB	BI	201	2	-	9/26/74/74	0/4/4/4
82	PEB	hM	203	1	-	11/26/74/74	0/4/4/4
83	PUB	wF	304	13	-	7/26/74/74	0/4/4/4
82	PEB	UD	202	2	-	7/26/74/74	0/4/4/4
82	PEB	K5	202	1	-	11/26/74/74	0/4/4/4
85	BCR	cL	503	-	-	2/29/63/63	0/2/2/2
82	PEB	QK	203	1,2	-	8/26/74/74	0/4/4/4
87	CLA	AN	827	-	-	9/27/103/115	-
87	CLA	bL	622	-	-	15/39/115/115	-
82	PEB	lF	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	aF	202	1	-	9/26/74/74	0/4/4/4
82	PEB	R4	201	11,2	-	3/26/74/74	0/4/4/4
82	PEB	JJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	MM	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	y8	203	2	-	9/26/74/74	0/4/4/4
87	CLA	22	604	-	-	3/12/88/115	-
88	LHG	dL	408	-	-	12/50/50/53	-
82	PEB	X5	201	1	-	11/26/74/74	0/4/4/4
85	BCR	HL	103	-	-	4/29/63/63	0/2/2/2
82	PEB	JQ	203	1,2	-	14/26/74/74	0/4/4/4
92	LMG	bL	624	16	-	7/34/54/70	0/1/1/1
82	PEB	KQ	201	2	-	9/26/74/74	0/4/4/4
83	PUB	AH	303	3	-	5/26/74/74	0/4/4/4
87	CLA	B2	809	-	-	11/39/115/115	-
82	PEB	XM	202	2	-	9/26/74/74	0/4/4/4
92	LMG	jL	101	18,24	-	8/28/48/70	0/1/1/1
82	PEB	F7	201	3,2	-	5/26/74/74	0/4/4/4
82	PEB	SE	201	1	-	10/26/74/74	0/4/4/4
82	PEB	BD	201	1	-	9/26/74/74	0/4/4/4
82	PEB	OM	201	1	-	7/26/74/74	0/4/4/4
82	PEB	AD	304	3,82	-	11/26/74/74	0/4/4/4
82	PEB	gO	201	2	-	4/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	a4	201	2	-	2/26/74/74	0/4/4/4
82	PEB	UJ	203	1	-	9/26/74/74	0/4/4/4
82	PEB	W5	201	2	-	7/26/74/74	0/4/4/4
82	PEB	H1	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	Z4	202	1	-	9/26/74/74	0/4/4/4
82	PEB	gM	201	2	-	8/26/74/74	0/4/4/4
87	CLA	AN	822	40	-	8/15/91/115	-
85	BCR	L2	205	50	-	11/29/63/63	0/2/2/2
82	PEB	yC	201	2	-	12/26/74/74	0/4/4/4
82	PEB	fK	202	2	-	13/26/74/74	0/4/4/4
85	BCR	AL	401	-	-	5/29/63/63	0/2/2/2
82	PEB	BI	203	2	-	7/26/74/74	0/4/4/4
82	PEB	LE	1002	10,9	-	11/26/74/74	0/4/4/4
82	PEB	EK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	mF	201	1	-	6/26/74/74	0/4/4/4
82	PEB	WA	201	1	-	7/26/74/74	0/4/4/4
87	CLA	42	605	60	-	9/15/91/115	-
84	CYC	K4	1001	9	-	9/26/74/74	0/4/4/4
82	PEB	HK	202	2	-	12/26/74/74	0/4/4/4
83	PUB	KA	203	1,3	-	6/26/74/74	0/4/4/4
82	PEB	jM	201	1	-	10/26/74/74	0/4/4/4
82	PEB	Z5	304	74,82	-	8/26/74/74	0/4/4/4
82	PEB	OK	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	XD	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	KB	302	2,5	-	7/26/74/74	0/4/4/4
82	PEB	ZM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	QM	203	1	-	10/26/74/74	0/4/4/4
82	PEB	SA	202	1	-	8/26/74/74	0/4/4/4
82	PEB	AE	301	3	-	10/26/74/74	0/4/4/4
87	CLA	12	610	57	-	8/15/91/115	-
87	CLA	52	609	61	-	6/12/88/115	-
82	PEB	IJ	201	1,2	-	6/26/74/74	0/4/4/4
84	CYC	73	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	DF	202	1,2	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	DK	202	1,2	-	12/26/74/74	0/4/4/4
82	PEB	RQ	201	1	-	11/26/74/74	0/4/4/4
82	PEB	UE	201	1,2	-	5/26/74/74	0/4/4/4
87	CLA	8N	306	64	-	9/15/91/115	-
84	CYC	B3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	RA	201	2	-	5/26/74/74	0/4/4/4
82	PEB	QI	201	2	-	6/26/74/74	0/4/4/4
82	PEB	RD	203	1,2	-	10/26/74/74	0/4/4/4
87	CLA	F2	205	45	-	19/39/115/115	-
95	DGD	O6	301	-	-	7/29/69/95	0/2/2/2
82	PEB	T1	202	2	-	15/26/74/74	0/4/4/4
82	PEB	fK	201	13,2	-	10/26/74/74	0/4/4/4
87	CLA	1N	603	-	-	4/15/91/115	-
82	PEB	TG	201	2	-	3/26/74/74	0/4/4/4
85	BCR	B2	841	41	-	4/29/63/63	0/2/2/2
87	CLA	DL	403	18	-	10/39/115/115	-
82	PEB	eK	203	1	-	8/26/74/74	0/4/4/4
87	CLA	A6	402	15	-	22/39/115/115	-
87	CLA	D6	402	18	-	17/39/115/115	-
87	CLA	8N	304	64	-	8/15/91/115	-
82	PEB	ED	202	2	-	7/26/74/74	0/4/4/4
82	PEB	PQ	201	1,2	-	8/26/74/74	0/4/4/4
82	PEB	kK	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	SO	201	1	-	10/26/74/74	0/4/4/4
83	PUB	A1	304	3	-	15/26/74/74	0/4/4/4
82	PEB	pF	202	2	-	11/26/74/74	0/4/4/4
92	LMG	aL	611	-	-	9/37/57/70	0/1/1/1
82	PEB	LM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	gK	202	1	-	11/26/74/74	0/4/4/4
82	PEB	HJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	PA	203	2	-	8/26/74/74	0/4/4/4
82	PEB	SA	201	1	-	4/26/74/74	0/4/4/4
87	CLA	AN	830	-	-	14/39/115/115	-
84	CYC	E3	1001	68	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	HA	202	2	-	8/26/74/74	0/4/4/4
82	PEB	fH	203	1,2	-	12/26/74/74	0/4/4/4
82	PEB	NQ	204	1,2	-	13/26/74/74	0/4/4/4
82	PEB	DK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	RO	203	2	-	7/26/74/74	0/4/4/4
82	PEB	z8	202	1	-	11/26/74/74	0/4/4/4
84	CYC	ME	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	A2	814	40	-	10/26/102/115	-
82	PEB	B9	202	2	-	8/26/74/74	0/4/4/4
87	CLA	D6	405	-	-	13/39/115/115	-
82	PEB	iK	202	1	-	11/26/74/74	0/4/4/4
82	PEB	dH	203	1	-	10/26/74/74	0/4/4/4
82	PEB	W1	202	1	-	9/26/74/74	0/4/4/4
82	PEB	d4	202	1	-	8/26/74/74	0/4/4/4
82	PEB	YM	202	1	-	8/26/74/74	0/4/4/4
87	CLA	42	604	60	-	7/12/88/115	-
82	PEB	cB	401	6,2	-	6/26/74/74	0/4/4/4
82	PEB	iO	202	2	-	8/26/74/74	0/4/4/4
82	PEB	mG	201	2	-	6/26/74/74	0/4/4/4
82	PEB	T5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	gH	201	2	-	9/26/74/74	0/4/4/4
82	PEB	ZJ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	Y4	202	2	-	6/26/74/74	0/4/4/4
82	PEB	VH	202	2	-	7/26/74/74	0/4/4/4
82	PEB	AK	201	1	-	9/26/74/74	0/4/4/4
87	CLA	BL	623	16	-	11/39/115/115	-
87	CLA	C6	513	-	-	21/39/115/115	-
82	PEB	VA	203	2	-	7/26/74/74	0/4/4/4
82	PEB	hG	203	1	-	7/26/74/74	0/4/4/4
87	CLA	42	602	60	-	16/39/115/115	-
82	PEB	CA	202	1	-	13/26/74/74	0/4/4/4
87	CLA	22	609	58	-	11/21/97/115	-
82	PEB	e4	202	2	-	10/26/74/74	0/4/4/4
82	PEB	hM	202	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	A2	817	-	-	7/12/88/115	-
82	PEB	WQ	202	2	-	8/26/74/74	0/4/4/4
84	CYC	IO	1001	9	-	11/26/74/74	0/4/4/4
87	CLA	32	307	59	-	5/15/91/115	-
87	CLA	5N	611	61	-	10/15/91/115	-
82	PEB	cK	202	1	-	13/26/74/74	0/4/4/4
82	PEB	gH	202	2	-	5/26/74/74	0/4/4/4
82	PEB	L7	201	2,82	-	7/26/74/74	0/4/4/4
87	CLA	BL	608	-	-	17/39/115/115	-
82	PEB	YE	201	2	-	11/26/74/74	0/4/4/4
82	PEB	dE	201	1,3	-	11/26/74/74	0/4/4/4
92	LMG	XL	601	37	-	15/45/65/70	0/1/1/1
82	PEB	fE	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	b1	201	1	-	10/26/74/74	0/4/4/4
82	PEB	MA	201	1	-	8/26/74/74	0/4/4/4
95	DGD	C6	503	-	-	13/31/71/95	0/2/2/2
84	CYC	D4	1001	10	-	10/26/74/74	0/4/4/4
87	CLA	AN	817	-	-	7/12/88/115	-
82	PEB	Z5	301	74	-	8/26/74/74	0/4/4/4
82	PEB	SD	202	2	-	10/26/74/74	0/4/4/4
82	PEB	r8	202	1	-	16/26/74/74	0/4/4/4
84	CYC	HO	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	y8	202	2	-	9/26/74/74	0/4/4/4
87	CLA	82	303	64	-	8/15/91/115	-
87	CLA	7N	603	-	-	7/15/91/115	-
82	PEB	X7	201	2,75	-	5/26/74/74	0/4/4/4
87	CLA	B6	604	-	-	14/39/115/115	-
82	PEB	OF	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	Q1	202	1	-	12/26/74/74	0/4/4/4
82	PEB	YF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	DA	201	3,2	-	11/26/74/74	0/4/4/4
82	PEB	QP	203	1,2	-	12/26/74/74	0/4/4/4
87	CLA	LN	206	50	-	5/29/105/115	-
82	PEB	J5	202	2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	RE	202	2	-	12/26/74/74	0/4/4/4
82	PEB	F1	1002	10	-	11/26/74/74	0/4/4/4
82	PEB	XF	202	2	-	6/26/74/74	0/4/4/4
82	PEB	XJ	201	2	-	5/26/74/74	0/4/4/4
82	PEB	BB	201	2	-	3/26/74/74	0/4/4/4
87	CLA	A2	820	-	-	12/39/115/115	-
95	DGD	C6	523	-	-	13/37/77/95	0/2/2/2
92	LMG	d6	409	18	-	17/49/69/70	0/1/1/1
82	PEB	Z1	203	1	-	7/26/74/74	0/4/4/4
87	CLA	C6	514	87	-	24/39/115/115	-
82	PEB	O1	201	1	-	11/26/74/74	0/4/4/4
82	PEB	YO	202	2	-	6/26/74/74	0/4/4/4
82	PEB	q8	202	2	-	9/26/74/74	0/4/4/4
82	PEB	cO	203	2	-	11/26/74/74	0/4/4/4
85	BCR	J2	102	-	-	7/29/63/63	0/2/2/2
82	PEB	HQ	202	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	610	-	-	5/12/88/115	-
82	PEB	fG	203	1,2	-	9/26/74/74	0/4/4/4
84	CYC	HG	1001	10	-	9/26/74/74	0/4/4/4
87	CLA	A2	852	59,40	-	8/15/91/115	-
82	PEB	PJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	B5	202	2	-	9/26/74/74	0/4/4/4
82	PEB	gB	202	2	-	8/26/74/74	0/4/4/4
82	PEB	iJ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	WJ	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	eG	202	2	-	7/26/74/74	0/4/4/4
87	CLA	3N	303	59,60	-	9/15/91/115	-
82	PEB	AH	305	3	-	12/26/74/74	0/4/4/4
82	PEB	H4	1002	10	-	8/26/74/74	0/4/4/4
92	LMG	D6	409	18	-	16/49/69/70	0/1/1/1
82	PEB	mK	202	1	-	11/26/74/74	0/4/4/4
87	CLA	3N	304	59,87	-	8/15/91/115	-
82	PEB	H7	203	2	-	12/26/74/74	0/4/4/4
82	PEB	TP	202	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	O5	203	2	-	14/26/74/74	0/4/4/4
82	PEB	hE	202	1	-	11/26/74/74	0/4/4/4
85	BCR	JN	103	40,48	-	13/29/63/63	0/2/2/2
87	CLA	A2	830	-	-	14/39/115/115	-
82	PEB	CB	202	2	-	9/26/74/74	0/4/4/4
82	PEB	CM	202	1	-	11/26/74/74	0/4/4/4
82	PEB	UA	202	1	-	10/26/74/74	0/4/4/4
82	PEB	gJ	201	2	-	9/26/74/74	0/4/4/4
87	CLA	BN	820	41	-	8/15/91/115	-
82	PEB	Y4	201	2	-	4/26/74/74	0/4/4/4
87	CLA	b6	607	-	-	15/39/115/115	-
82	PEB	MD	201	2	-	7/26/74/74	0/4/4/4
82	PEB	AF	202	1	-	11/26/74/74	0/4/4/4
82	PEB	e4	201	2	-	5/26/74/74	0/4/4/4
82	PEB	VH	201	2	-	2/26/74/74	0/4/4/4
82	PEB	KB	301	2,5	-	9/26/74/74	0/4/4/4
82	PEB	CK	202	1	-	7/26/74/74	0/4/4/4
82	PEB	iF	202	1	-	11/26/74/74	0/4/4/4
82	PEB	eA	301	1,75	-	9/26/74/74	0/4/4/4
87	CLA	RN	201	87	-	7/15/91/115	-
82	PEB	cB	403	6,2	-	6/26/74/74	0/4/4/4
82	PEB	dB	201	2	-	9/26/74/74	0/4/4/4
82	PEB	CQ	201	3,2	-	4/26/74/74	0/4/4/4
84	CYC	E1	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	iJ	201	13,2	-	5/26/74/74	0/4/4/4
87	CLA	22	610	58	-	5/10/86/115	-
82	PEB	P7	203	2	-	8/26/74/74	0/4/4/4
82	PEB	GQ	201	2	-	4/26/74/74	0/4/4/4
82	PEB	ZF	201	2	-	9/26/74/74	0/4/4/4
82	PEB	CP	203	1	-	9/26/74/74	0/4/4/4
82	PEB	O4	202	1	-	6/26/74/74	0/4/4/4
82	PEB	k4	202	2	-	12/26/74/74	0/4/4/4
82	PEB	xF	302	13	-	13/26/74/74	0/4/4/4
87	CLA	BN	810	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PUB	AO	302	3	-	2/26/74/74	0/4/4/4
87	CLA	4N	604	60	-	7/12/88/115	-
87	CLA	AN	803	40,50,53	-	13/24/100/115	-
95	DGD	c6	601	-	-	26/51/91/95	0/2/2/2
82	PEB	TJ	201	2	-	7/26/74/74	0/4/4/4
85	BCR	AN	845	40	-	11/29/63/63	0/2/2/2
82	PEB	TI	202	1	-	9/26/74/74	0/4/4/4
82	PEB	SM	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	LQ	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	32	304	59,87	-	15/39/115/115	-
87	CLA	A2	821	-	-	18/39/115/115	-
82	PEB	bO	202	1	-	8/26/74/74	0/4/4/4
82	PEB	HI	202	1,2	-	10/26/74/74	0/4/4/4
82	PEB	hO	201	1	-	10/26/74/74	0/4/4/4
82	PEB	UA	201	1	-	4/26/74/74	0/4/4/4
87	CLA	BN	813	-	-	28/39/115/115	-
87	CLA	72	604	63	-	7/12/88/115	-
87	CLA	3N	310	59,87	-	5/10/86/115	-
82	PEB	PA	202	2	-	7/26/74/74	0/4/4/4
82	PEB	PO	202	2	-	6/26/74/74	0/4/4/4
82	PEB	fH	202	1	-	10/26/74/74	0/4/4/4
87	CLA	L2	203	85,50,41	-	22/39/115/115	-
82	PEB	KI	201	1,2	-	10/26/74/74	0/4/4/4
87	CLA	8N	303	64	-	19/39/115/115	-
82	PEB	UP	201	1	-	4/26/74/74	0/4/4/4
84	CYC	NO	1001	10	-	13/26/74/74	0/4/4/4
82	PEB	FA	201	3,2	-	5/26/74/74	0/4/4/4
82	PEB	g1	202	2	-	5/26/74/74	0/4/4/4
85	BCR	K2	102	40,49	-	13/29/63/63	0/2/2/2
83	PUB	AE	302	3	-	9/26/74/74	0/4/4/4
82	PEB	OP	201	1,2	-	10/26/74/74	0/4/4/4
82	PEB	vF	202	2	-	9/26/74/74	0/4/4/4
82	PEB	kG	201	3,2	-	9/26/74/74	0/4/4/4
82	PEB	V7	201	2,75	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	LHG	a6	610	15	-	14/47/47/53	-
84	CYC	FO	1001	10	-	11/26/74/74	0/4/4/4
87	CLA	KN	102	-	-	5/15/91/115	-
82	PEB	W4	201	1	-	6/26/74/74	0/4/4/4
84	CYC	g3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	CL	513	17	-	16/33/109/115	-
87	CLA	82	305	64	-	9/15/91/115	-
82	PEB	DB	203	2	-	15/26/74/74	0/4/4/4
82	PEB	mO	201	2	-	9/26/74/74	0/4/4/4
82	PEB	H5	202	2	-	8/26/74/74	0/4/4/4
82	PEB	d1	203	1	-	10/26/74/74	0/4/4/4
82	PEB	lE	201	1,2	-	9/26/74/74	0/4/4/4
84	CYC	DH	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	l4	202	-	-	10/26/74/74	0/4/4/4
82	PEB	XQ	203	1	-	10/26/74/74	0/4/4/4
82	PEB	EF	201	1	-	9/26/74/74	0/4/4/4
84	CYC	JO	1001	10	-	11/26/74/74	0/4/4/4
82	PEB	GB	201	2	-	6/26/74/74	0/4/4/4
82	PEB	qF	201	1,2	-	9/26/74/74	0/4/4/4
92	LMG	dL	407	18	-	23/49/69/70	0/1/1/1
82	PEB	G5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	UF	201	1	-	8/26/74/74	0/4/4/4
82	PEB	t8	201	1	-	9/26/74/74	0/4/4/4
82	PEB	N7	203	2	-	8/26/74/74	0/4/4/4
82	PEB	d4	201	1	-	9/26/74/74	0/4/4/4
82	PEB	OI	203	2	-	8/26/74/74	0/4/4/4
87	CLA	AN	835	-	-	16/39/115/115	-
87	CLA	82	302	64	-	19/39/115/115	-
87	CLA	AN	805	40	-	23/39/115/115	-
85	BCR	BN	841	41	-	4/29/63/63	0/2/2/2
82	PEB	WP	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	LO	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	Y5	201	74,2	-	10/26/74/74	0/4/4/4
98	PQN	B2	837	41	-	5/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	c6	606	17	-	16/39/115/115	-
82	PEB	I5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	DQ	203	1	-	10/26/74/74	0/4/4/4
82	PEB	mM	202	2	-	9/26/74/74	0/4/4/4
92	LMG	k6	101	25	-	15/50/70/70	0/1/1/1
99	SF4	CN	101	42	-	-	0/6/5/5
82	PEB	MF	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	PP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	aE	202	2	-	14/26/74/74	0/4/4/4
82	PEB	DP	201	2	-	6/26/74/74	0/4/4/4
82	PEB	P4	202	2	-	6/26/74/74	0/4/4/4
88	LHG	ML	102	-	-	15/43/43/53	-
87	CLA	BN	805	41	-	8/39/115/115	-
82	PEB	RM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	mE	201	2	-	6/26/74/74	0/4/4/4
82	PEB	OO	201	1	-	8/26/74/74	0/4/4/4
82	PEB	AQ	301	3	-	11/26/74/74	0/4/4/4
82	PEB	BP	201	2	-	9/26/74/74	0/4/4/4
95	DGD	JL	101	-	-	8/51/91/95	0/2/2/2
87	CLA	8N	307	-	-	5/12/88/115	-
82	PEB	a1	202	2	-	10/26/74/74	0/4/4/4
82	PEB	kO	203	2	-	12/26/74/74	0/4/4/4
82	PEB	EJ	203	1	-	11/26/74/74	0/4/4/4
87	CLA	C6	517	-	-	13/39/115/115	-
82	PEB	D7	202	2	-	12/26/74/74	0/4/4/4
82	PEB	hJ	202	1	-	6/26/74/74	0/4/4/4
82	PEB	LI	202	2	-	6/26/74/74	0/4/4/4
87	CLA	I2	103	47,50	-	20/39/115/115	-
82	PEB	DD	203	1	-	10/26/74/74	0/4/4/4
82	PEB	OK	202	1	-	9/26/74/74	0/4/4/4
87	CLA	AN	809	-	-	15/39/115/115	-
82	PEB	JO	1002	10	-	11/26/74/74	0/4/4/4
82	PEB	PE	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	RP	201	56,2	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	JJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	PO	203	2	-	6/26/74/74	0/4/4/4
87	CLA	A2	849	40	-	11/39/115/115	-
87	CLA	A2	819	40	-	12/36/112/115	-
87	CLA	A2	815	-	-	20/39/115/115	-
82	PEB	QK	201	1	-	7/26/74/74	0/4/4/4
82	PEB	aH	201	2	-	6/26/74/74	0/4/4/4
84	CYC	w3	1001	73,69	-	4/26/74/74	0/4/4/4
92	LMG	bL	623	-	-	11/36/56/70	0/1/1/1
82	PEB	gF	202	1	-	11/26/74/74	0/4/4/4
82	PEB	P4	201	2	-	5/26/74/74	0/4/4/4
87	CLA	bL	617	-	-	13/39/115/115	-
84	CYC	F1	1001	10	-	8/26/74/74	0/4/4/4
87	CLA	CL	503	-	-	22/39/115/115	-
98	PQN	AN	842	-	-	6/23/43/43	0/2/2/2
82	PEB	HO	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	V4	201	2	-	4/26/74/74	0/4/4/4
82	PEB	AJ	302	13	-	8/26/74/74	0/4/4/4
87	CLA	AN	838	-	-	15/39/115/115	-
87	CLA	B2	818	-	-	16/39/115/115	-
82	PEB	gB	203	2	-	14/26/74/74	0/4/4/4
82	PEB	aK	203	1	-	12/26/74/74	0/4/4/4
82	PEB	QQ	201	3,2	-	3/26/74/74	0/4/4/4
82	PEB	IB	203	2	-	8/26/74/74	0/4/4/4
82	PEB	FD	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	N9	201	1	-	7/26/74/74	0/4/4/4
85	BCR	B2	843	-	-	6/29/63/63	0/2/2/2
82	PEB	LI	201	12,2	-	10/26/74/74	0/4/4/4
82	PEB	R1	202	2	-	12/26/74/74	0/4/4/4
82	PEB	TQ	202	1	-	9/26/74/74	0/4/4/4
87	CLA	BL	604	-	-	7/32/108/115	-
82	PEB	G9	202	1	-	15/26/74/74	0/4/4/4
87	CLA	A2	826	-	-	11/39/115/115	-
82	PEB	K7	202	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	SB	201	2	-	4/26/74/74	0/4/4/4
87	CLA	J2	101	48	-	5/12/88/115	-
82	PEB	k1	201	2	-	8/26/74/74	0/4/4/4
82	PEB	PG	202	2	-	13/26/74/74	0/4/4/4
82	PEB	WI	203	2	-	6/26/74/74	0/4/4/4
85	BCR	AN	846	-	-	10/29/63/63	0/2/2/2
82	PEB	YG	201	2	-	11/26/74/74	0/4/4/4
87	CLA	b6	604	-	-	16/39/115/115	-
82	PEB	N9	202	1	-	15/26/74/74	0/4/4/4
87	CLA	B6	614	-	-	8/39/115/115	-
82	PEB	tK	202	2	-	11/26/74/74	0/4/4/4
87	CLA	cL	515	17	-	17/33/109/115	-
92	LMG	bL	611	37,16	-	14/45/65/70	0/1/1/1
87	CLA	A2	825	-	-	7/27/103/115	-
87	CLA	B2	824	41	-	20/39/115/115	-
82	PEB	HE	1002	10,9	-	8/26/74/74	0/4/4/4
82	PEB	A7	202	1	-	13/26/74/74	0/4/4/4
82	PEB	S7	202	1	-	8/26/74/74	0/4/4/4
82	PEB	NA	202	2	-	9/26/74/74	0/4/4/4
85	BCR	B2	842	-	-	13/29/63/63	0/2/2/2
82	PEB	oF	201	1	-	13/26/74/74	0/4/4/4
82	PEB	kK	201	1	-	12/26/74/74	0/4/4/4
82	PEB	BM	301	14	-	13/26/74/74	0/4/4/4
87	CLA	32	313	-	-	8/15/91/115	-
87	CLA	6N	612	62	-	9/15/91/115	-
85	BCR	BN	842	-	-	13/29/63/63	0/2/2/2
82	PEB	G9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	mO	203	2	-	7/26/74/74	0/4/4/4
82	PEB	RJ	202	2	-	9/26/74/74	0/4/4/4
87	CLA	A2	832	40	-	10/21/97/115	-
82	PEB	ND	203	1	-	12/26/74/74	0/4/4/4
82	PEB	L4	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	II	202	1	-	10/26/74/74	0/4/4/4
82	PEB	h1	203	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	xK	302	13	-	13/26/74/74	0/4/4/4
87	CLA	B2	836	87,41,57	-	18/39/115/115	-
88	LHG	c6	619	17	-	11/36/36/53	-
84	CYC	J3	1001	68	-	8/26/74/74	0/4/4/4
96	HEM	vL	201	35	-	2/14/54/54	-
85	BCR	fL	101	20	-	8/29/63/63	0/2/2/2
82	PEB	c4	201	2	-	7/26/74/74	0/4/4/4
84	CYC	J4	1001	10	-	11/26/74/74	0/4/4/4
84	CYC	JH	1001	10	-	7/26/74/74	0/4/4/4
82	PEB	T9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	eK	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	GM	201	1	-	8/26/74/74	0/4/4/4
82	PEB	jJ	203	1,2	-	7/26/74/74	0/4/4/4
85	BCR	b6	602	-	-	1/29/63/63	0/2/2/2
82	PEB	wF	302	13	-	10/26/74/74	0/4/4/4
87	CLA	BN	821	54,41	-	2/13/89/115	-
82	PEB	XA	201	2,75	-	6/26/74/74	0/4/4/4
82	PEB	QP	202	1	-	11/26/74/74	0/4/4/4
82	PEB	CP	201	1,2	-	13/26/74/74	0/4/4/4
87	CLA	L2	206	50	-	5/29/105/115	-
87	CLA	b6	608	16	-	17/39/115/115	-
82	PEB	R7	202	2	-	10/26/74/74	0/4/4/4
82	PEB	JF	202	2	-	15/26/74/74	0/4/4/4
87	CLA	82	304	-	-	7/15/91/115	-
82	PEB	ZE	201	1,2	-	8/26/74/74	0/4/4/4
82	PEB	tC	201	1	-	9/26/74/74	0/4/4/4
84	CYC	E4	1001	9	-	10/26/74/74	0/4/4/4
82	PEB	hG	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	H5	201	74,2	-	11/26/74/74	0/4/4/4
87	CLA	C6	511	-	-	15/39/115/115	-
82	PEB	18	201	2	-	11/26/74/74	0/4/4/4
87	CLA	B6	608	16	-	16/39/115/115	-
82	PEB	YH	201	2	-	6/26/74/74	0/4/4/4
82	PEB	LF	202	2	-	14/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	dJ	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	62	312	62	-	10/15/91/115	-
82	PEB	uC	202	2	-	7/26/74/74	0/4/4/4
82	PEB	IP	203	1,2	-	13/26/74/74	0/4/4/4
82	PEB	KM	202	1	-	14/26/74/74	0/4/4/4
82	PEB	jG	202	1	-	7/26/74/74	0/4/4/4
82	PEB	NF	202	2	-	12/26/74/74	0/4/4/4
87	CLA	cL	513	17	-	9/39/115/115	-
82	PEB	JD	202	1	-	12/26/74/74	0/4/4/4
82	PEB	S9	203	2	-	11/26/74/74	0/4/4/4
84	CYC	M1	201	10,9	-	11/26/74/74	0/4/4/4
82	PEB	eO	202	2	-	10/26/74/74	0/4/4/4
84	CYC	C3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	A2	816	-	-	8/15/91/115	-
85	BCR	BL	618	-	-	4/29/63/63	0/2/2/2
83	PUB	Z5	302	1,74	-	7/26/74/74	0/4/4/4
82	PEB	j4	202	1	-	7/26/74/74	0/4/4/4
82	PEB	ZH	203	1	-	7/26/74/74	0/4/4/4
82	PEB	VA	201	2,75	-	11/26/74/74	0/4/4/4
82	PEB	JA	202	2	-	8/26/74/74	0/4/4/4
82	PEB	NA	201	2	-	3/26/74/74	0/4/4/4
82	PEB	cM	202	2	-	10/26/74/74	0/4/4/4
84	CYC	LO	1001	10	-	6/26/74/74	0/4/4/4
87	CLA	32	302	59,60	-	9/15/91/115	-
87	CLA	ON	202	53	-	10/21/97/115	-
82	PEB	rK	202	2	-	13/26/74/74	0/4/4/4
92	LMG	bL	610	-	-	17/36/56/70	0/1/1/1
82	PEB	Z1	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	NI	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	dG	204	1	-	12/26/74/74	0/4/4/4
99	SF4	CN	102	42	-	-	0/6/5/5
82	PEB	M7	201	1	-	8/26/74/74	0/4/4/4
87	CLA	b6	617	-	-	17/39/115/115	-
82	PEB	ZE	203	1,2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	jE	202	1	-	7/26/74/74	0/4/4/4
87	CLA	1N	611	-	-	8/15/91/115	-
82	PEB	wC	201	2	-	12/26/74/74	0/4/4/4
87	CLA	c6	608	85,92	-	23/39/115/115	-
82	PEB	DJ	202	2	-	11/26/74/74	0/4/4/4
82	PEB	hJ	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	pC	201	1	-	13/26/74/74	0/4/4/4
87	CLA	cL	516	-	-	10/27/103/115	-
82	PEB	KF	201	1,2	-	6/26/74/74	0/4/4/4
82	PEB	YA	301	3	-	18/26/74/74	0/4/4/4
85	BCR	B6	621	92	-	0/29/63/63	0/2/2/2
82	PEB	VI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	TK	202	2	-	17/26/74/74	0/4/4/4
82	PEB	AG	301	3	-	10/26/74/74	0/4/4/4
82	PEB	YP	502	2	-	12/26/74/74	0/4/4/4
82	PEB	SJ	202	1	-	12/26/74/74	0/4/4/4
95	DGD	AL	414	15	-	17/51/91/95	0/2/2/2
82	PEB	S9	201	74,2	-	12/26/74/74	0/4/4/4
82	PEB	OD	202	2	-	14/26/74/74	0/4/4/4
82	PEB	aO	203	2	-	11/26/74/74	0/4/4/4
82	PEB	bF	202	2	-	11/26/74/74	0/4/4/4
82	PEB	I7	201	1	-	13/26/74/74	0/4/4/4
87	CLA	2N	309	58	-	11/21/97/115	-
82	PEB	xC	201	1	-	11/26/74/74	0/4/4/4
87	CLA	aL	605	15	-	12/39/115/115	-
82	PEB	HF	202	2	-	12/26/74/74	0/4/4/4
82	PEB	AQ	303	3,82	-	11/26/74/74	0/4/4/4
94	PL9	d6	408	18,26	-	15/53/73/73	0/1/1/1
87	CLA	CL	505	-	-	16/39/115/115	-
87	CLA	H6	102	22	-	8/39/115/115	-
82	PEB	IB	202	2	-	8/26/74/74	0/4/4/4
87	CLA	BN	819	-	-	16/39/115/115	-
82	PEB	PB	201	2	-	5/26/74/74	0/4/4/4
82	PEB	Q4	202	1	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	R9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	N5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	iM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	uK	202	1	-	9/26/74/74	0/4/4/4
95	DGD	C6	502	-	-	26/51/91/95	0/2/2/2
84	CYC	D1	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	uC	203	2	-	2/26/74/74	0/4/4/4
88	LHG	C6	522	17	-	13/36/36/53	-
87	CLA	CL	506	-	-	17/39/115/115	-
95	DGD	cL	519	-	-	7/51/91/95	0/2/2/2
82	PEB	R4	203	2	-	7/26/74/74	0/4/4/4
82	PEB	Q9	201	2	-	10/26/74/74	0/4/4/4
87	CLA	5N	610	-	-	5/15/91/115	-
82	PEB	BA	203	2	-	12/26/74/74	0/4/4/4
87	CLA	42	606	-	-	8/15/91/115	-
87	CLA	A6	404	15	-	4/21/97/115	-
85	BCR	AN	804	-	-	2/29/63/63	0/2/2/2
82	PEB	SH	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	NM	201	2	-	9/26/74/74	0/4/4/4
87	CLA	a6	608	-	-	13/33/109/115	-
82	PEB	DQ	202	1	-	9/26/74/74	0/4/4/4
82	PEB	bF	201	2	-	4/26/74/74	0/4/4/4
82	PEB	lG	202	1	-	14/26/74/74	0/4/4/4
82	PEB	RD	201	1	-	11/26/74/74	0/4/4/4
84	CYC	m3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	bL	618	-	-	11/39/115/115	-
82	PEB	ID	201	2,77	-	7/26/74/74	0/4/4/4
82	PEB	KJ	201	1	-	6/26/74/74	0/4/4/4
82	PEB	r8	201	1	-	9/26/74/74	0/4/4/4
87	CLA	BN	833	-	-	8/18/94/115	-
82	PEB	jJ	202	1	-	11/26/74/74	0/4/4/4
82	PEB	M9	302	74	-	16/26/74/74	0/4/4/4
82	PEB	O9	203	2	-	7/26/74/74	0/4/4/4
88	LHG	bL	612	16	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	HEM	GN	201	46	-	6/14/54/54	-
82	PEB	iG	201	2	-	10/26/74/74	0/4/4/4
82	PEB	VF	201	2	-	10/26/74/74	0/4/4/4
87	CLA	BL	619	-	-	6/39/115/115	-
82	PEB	WF	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	FQ	202	1	-	10/26/74/74	0/4/4/4
82	PEB	E7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	vK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	QJ	204	1	-	10/26/74/74	0/4/4/4
82	PEB	jK	202	2	-	12/26/74/74	0/4/4/4
84	CYC	KG	202	10,9	-	11/26/74/74	0/4/4/4
82	PEB	mF	202	1	-	11/26/74/74	0/4/4/4
84	CYC	LH	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	A2	834	-	-	20/39/115/115	-
82	PEB	cJ	202	2	-	10/26/74/74	0/4/4/4
87	CLA	7N	601	63	-	12/15/91/115	-
82	PEB	ZB	201	2	-	10/26/74/74	0/4/4/4
82	PEB	jO	202	1	-	7/26/74/74	0/4/4/4
82	PEB	OG	202	1	-	10/26/74/74	0/4/4/4
87	CLA	RN	204	-	-	11/15/91/115	-
82	PEB	sK	201	1	-	12/26/74/74	0/4/4/4
82	PEB	MI	401	-	-	10/26/74/74	0/4/4/4
82	PEB	GD	202	2	-	13/26/74/74	0/4/4/4
87	CLA	cL	508	-	-	18/39/115/115	-
82	PEB	cO	201	2	-	7/26/74/74	0/4/4/4
83	PUB	xK	305	13	-	8/26/74/74	0/4/4/4
84	CYC	N3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	SO	202	1,76	-	10/26/74/74	0/4/4/4
82	PEB	QE	202	1	-	9/26/74/74	0/4/4/4
82	PEB	YA	303	3,82	-	13/26/74/74	0/4/4/4
82	PEB	aB	202	2	-	6/26/74/74	0/4/4/4
82	PEB	KJ	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	SP	201	1,2	-	11/26/74/74	0/4/4/4
87	CLA	1N	604	-	-	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	AP	202	1	-	9/26/74/74	0/4/4/4
83	PUB	wK	304	13	-	7/26/74/74	0/4/4/4
84	CYC	L4	1001	10	-	6/26/74/74	0/4/4/4
82	PEB	T7	201	2	-	5/26/74/74	0/4/4/4
82	PEB	SM	201	1	-	10/26/74/74	0/4/4/4
82	PEB	sF	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	zC	202	1	-	11/26/74/74	0/4/4/4
82	PEB	mJ	202	2	-	7/26/74/74	0/4/4/4
83	PUB	A4	303	3	-	6/26/74/74	0/4/4/4
84	CYC	BG	1001	10,8	-	13/26/74/74	0/4/4/4
82	PEB	DF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	OP	203	1	-	12/26/74/74	0/4/4/4
82	PEB	T4	203	2	-	10/26/74/74	0/4/4/4
84	CYC	q3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	W9	201	2	-	12/26/74/74	0/4/4/4
82	PEB	WF	203	1	-	13/26/74/74	0/4/4/4
84	CYC	G4	1001	9	-	8/26/74/74	0/4/4/4
87	CLA	BN	827	-	-	15/39/115/115	-
82	PEB	WK	202	1	-	8/26/74/74	0/4/4/4
82	PEB	YO	203	2	-	11/26/74/74	0/4/4/4
82	PEB	qC	202	2	-	9/26/74/74	0/4/4/4
85	BCR	BL	617	-	-	3/29/63/63	0/2/2/2
87	CLA	A2	822	40	-	8/15/91/115	-
82	PEB	m4	202	2	-	8/26/74/74	0/4/4/4
82	PEB	CI	202	1	-	10/26/74/74	0/4/4/4
94	PL9	D6	408	18,26	-	12/53/73/73	0/1/1/1
82	PEB	cB	402	6,2	-	12/26/74/74	0/4/4/4
82	PEB	j1	201	1	-	9/26/74/74	0/4/4/4
82	PEB	GI	202	1	-	9/26/74/74	0/4/4/4
82	PEB	jH	203	1,2	-	9/26/74/74	0/4/4/4
87	CLA	AN	828	40	-	13/39/115/115	-
82	PEB	Y9	203	2	-	7/26/74/74	0/4/4/4
82	PEB	AO	304	3	-	9/26/74/74	0/4/4/4
82	PEB	ZG	203	1	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	42	611	-	-	6/15/91/115	-
88	LHG	L6	101	26	-	18/53/53/53	-
88	LHG	d6	407	18	-	15/53/53/53	-
82	PEB	gK	201	1	-	6/26/74/74	0/4/4/4
82	PEB	gF	201	1	-	6/26/74/74	0/4/4/4
82	PEB	UJ	202	1	-	5/26/74/74	0/4/4/4
99	SF4	B2	803	-	-	-	0/6/5/5
82	PEB	NH	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	mJ	201	13,2	-	8/26/74/74	0/4/4/4
82	PEB	bO	201	1	-	9/26/74/74	0/4/4/4
82	PEB	CD	202	2	-	7/26/74/74	0/4/4/4
82	PEB	WE	202	1,77	-	7/26/74/74	0/4/4/4
87	CLA	1N	608	57	-	7/10/86/115	-
87	CLA	A2	841	-	-	14/39/115/115	-
82	PEB	fM	201	1	-	6/26/74/74	0/4/4/4
87	CLA	B2	823	-	-	8/39/115/115	-
82	PEB	T4	202	2	-	5/26/74/74	0/4/4/4
97	GOL	WL	101	-	-	2/4/4/4	-
82	PEB	QA	201	1	-	5/26/74/74	0/4/4/4
82	PEB	F4	1002	10	-	9/26/74/74	0/4/4/4
87	CLA	CL	518	-	-	12/17/93/115	-
87	CLA	IN	103	47,50	-	20/39/115/115	-
87	CLA	B6	611	-	-	19/39/115/115	-
87	CLA	AN	839	-	-	9/39/115/115	-
87	CLA	O2	201	-	-	7/10/86/115	-
82	PEB	m4	201	2	-	9/26/74/74	0/4/4/4
82	PEB	mE	203	2	-	8/26/74/74	0/4/4/4
87	CLA	c6	614	17	-	12/33/109/115	-
87	CLA	bL	614	-	-	11/39/115/115	-
87	CLA	CL	509	17	-	14/39/115/115	-
85	BCR	aL	604	-	-	6/29/63/63	0/2/2/2
87	CLA	BL	620	16	-	11/39/115/115	-
82	PEB	jM	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	AH	301	3	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	e7	301	1,75	-	9/26/74/74	0/4/4/4
87	CLA	82	308	-	-	12/15/91/115	-
87	CLA	12	609	-	-	6/12/88/115	-
82	PEB	X7	203	2	-	12/26/74/74	0/4/4/4
87	CLA	A2	801	40,45	-	16/39/115/115	-
82	PEB	L9	203	2	-	7/26/74/74	0/4/4/4
87	CLA	62	303	62	-	18/39/115/115	-
82	PEB	MF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	IJ	203	1	-	10/26/74/74	0/4/4/4
87	CLA	c6	604	17	-	27/39/115/115	-
82	PEB	dO	202	1	-	8/26/74/74	0/4/4/4
82	PEB	fM	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	RB	201	6,2	-	6/26/74/74	0/4/4/4
87	CLA	2N	307	58	-	8/15/91/115	-
87	CLA	R2	202	54	-	9/15/91/115	-
84	CYC	v3	1001	68	-	8/26/74/74	0/4/4/4
97	GOL	I6	102	-	-	0/4/4/4	-
82	PEB	PF	202	2	-	14/26/74/74	0/4/4/4
82	PEB	WH	201	1	-	8/26/74/74	0/4/4/4
82	PEB	AI	203	1,2	-	10/26/74/74	0/4/4/4
95	DGD	aL	603	15	-	7/42/82/95	0/2/2/2
82	PEB	aJ	204	1,2	-	6/26/74/74	0/4/4/4
82	PEB	IF	201	1	-	9/26/74/74	0/4/4/4
82	PEB	1C	201	2	-	11/26/74/74	0/4/4/4
82	PEB	U9	203	2	-	7/26/74/74	0/4/4/4
87	CLA	1N	602	57	-	15/39/115/115	-
82	PEB	M9	304	74	-	11/26/74/74	0/4/4/4
82	PEB	E5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	LA	202	2	-	9/26/74/74	0/4/4/4
92	LMG	B6	622	37,16	-	12/45/65/70	0/1/1/1
85	BCR	KN	104	-	-	8/29/63/63	0/2/2/2
82	PEB	lM	202	1	-	6/26/74/74	0/4/4/4
82	PEB	SQ	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	HK	201	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	q8	201	2	-	5/26/74/74	0/4/4/4
83	PUB	AQ	302	1,3	-	8/26/74/74	0/4/4/4
87	CLA	BN	815	41	-	5/12/88/115	-
82	PEB	PD	203	1	-	12/26/74/74	0/4/4/4
85	BCR	JN	102	-	-	7/29/63/63	0/2/2/2
82	PEB	AD	301	3	-	11/26/74/74	0/4/4/4
82	PEB	eF	201	1,2	-	12/26/74/74	0/4/4/4
85	BCR	K6	102	-	-	12/29/63/63	0/2/2/2
82	PEB	P1	202	2	-	8/26/74/74	0/4/4/4
84	CYC	FE	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	D1	1002	10	-	11/26/74/74	0/4/4/4
87	CLA	12	604	-	-	3/12/88/115	-
82	PEB	ED	201	2,77	-	12/26/74/74	0/4/4/4
82	PEB	IA	201	1	-	13/26/74/74	0/4/4/4
88	LHG	aL	607	15	-	18/47/47/53	-
82	PEB	PI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	CQ	202	2	-	7/26/74/74	0/4/4/4
82	PEB	IF	203	1,2	-	5/26/74/74	0/4/4/4
87	CLA	A2	836	-	-	7/15/91/115	-
82	PEB	aO	202	2	-	7/26/74/74	0/4/4/4
95	DGD	B2	844	41	-	19/55/95/95	0/2/2/2
82	PEB	eF	203	1	-	8/26/74/74	0/4/4/4
82	PEB	OE	202	1	-	10/26/74/74	0/4/4/4
82	PEB	WJ	202	1	-	14/26/74/74	0/4/4/4
87	CLA	62	310	-	-	5/10/86/115	-
82	PEB	AF	201	1	-	9/26/74/74	0/4/4/4
82	PEB	T7	203	2	-	7/26/74/74	0/4/4/4
82	PEB	LA	201	2,82	-	6/26/74/74	0/4/4/4
96	HEM	V6	201	35	-	2/14/54/54	-
87	CLA	A2	839	-	-	9/39/115/115	-
82	PEB	DO	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	ND	204	1,2	-	13/26/74/74	0/4/4/4
82	PEB	G7	202	1	-	12/26/74/74	0/4/4/4
95	DGD	BN	844	41	-	19/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	22	601	58	-	7/15/91/115	-
88	LHG	CL	522	17	-	10/36/36/53	-
82	PEB	f1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	TO	202	2	-	5/26/74/74	0/4/4/4
82	PEB	ZH	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	i1	201	2	-	7/26/74/74	0/4/4/4
82	PEB	RP	202	2	-	6/26/74/74	0/4/4/4
84	CYC	O3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	72	606	63	-	7/15/91/115	-
82	PEB	L7	203	2	-	10/26/74/74	0/4/4/4
82	PEB	oK	201	1	-	13/26/74/74	0/4/4/4
82	PEB	LJ	202	2	-	10/26/74/74	0/4/4/4
84	CYC	KO	1001	9	-	9/26/74/74	0/4/4/4
87	CLA	c6	616	-	-	12/39/115/115	-
87	CLA	C6	518	-	-	14/33/109/115	-
87	CLA	bL	606	-	-	11/39/115/115	-
82	PEB	k4	201	2	-	8/26/74/74	0/4/4/4
82	PEB	NI	201	1	-	9/26/74/74	0/4/4/4
87	CLA	7N	610	-	-	5/15/91/115	-
82	PEB	OH	202	1	-	7/26/74/74	0/4/4/4
87	CLA	2N	301	58,41	-	11/25/101/115	-
87	CLA	B2	829	-	-	7/13/89/115	-
82	PEB	jH	202	1	-	8/26/74/74	0/4/4/4
82	PEB	OM	202	1	-	9/26/74/74	0/4/4/4
82	PEB	rC	202	1	-	16/26/74/74	0/4/4/4
83	PUB	AG	303	3	-	9/26/74/74	0/4/4/4
82	PEB	DG	1002	10,9	-	8/26/74/74	0/4/4/4
87	CLA	6N	609	-	-	5/10/86/115	-
82	PEB	YI	201	12,2	-	10/26/74/74	0/4/4/4
82	PEB	V7	202	2	-	10/26/74/74	0/4/4/4
82	PEB	WD	202	2	-	8/26/74/74	0/4/4/4
87	CLA	R2	203	54,41	-	8/17/93/115	-
82	PEB	CM	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	bK	202	2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	AN	814	40	-	10/26/102/115	-
82	PEB	BB	203	2	-	8/26/74/74	0/4/4/4
82	PEB	HB	203	2	-	12/26/74/74	0/4/4/4
85	BCR	BN	839	-	-	6/29/63/63	0/2/2/2
82	PEB	O1	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	BK	201	2	-	9/26/74/74	0/4/4/4
87	CLA	7N	604	63	-	7/12/88/115	-
82	PEB	gK	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	GB	202	2	-	9/26/74/74	0/4/4/4
82	PEB	M9	301	74,2	-	6/26/74/74	0/4/4/4
82	PEB	EA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	18	203	2	-	6/26/74/74	0/4/4/4
82	PEB	Y1	201	2	-	6/26/74/74	0/4/4/4
87	CLA	cL	505	-	-	23/39/115/115	-
95	DGD	CL	523	-	-	11/37/77/95	0/2/2/2
88	LHG	dL	405	18	-	15/53/53/53	-
82	PEB	iK	203	1	-	13/26/74/74	0/4/4/4
82	PEB	h4	202	1	-	8/26/74/74	0/4/4/4
87	CLA	B2	806	-	-	20/39/115/115	-
82	PEB	J1	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	OH	201	1	-	11/26/74/74	0/4/4/4
95	DGD	a6	602	-	-	10/29/69/95	0/2/2/2
82	PEB	J9	201	2	-	12/26/74/74	0/4/4/4
87	CLA	c6	613	17	-	14/39/115/115	-
84	CYC	U3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	TQ	203	1	-	13/26/74/74	0/4/4/4
82	PEB	lJ	202	1	-	7/26/74/74	0/4/4/4
82	PEB	eG	201	2	-	9/26/74/74	0/4/4/4
82	PEB	e4	203	2	-	6/26/74/74	0/4/4/4
92	LMG	bL	609	-	3/3/8/8	21/36/56/70	0/1/1/1
87	CLA	cL	517	-	-	10/39/115/115	-
87	CLA	BN	823	-	-	16/39/115/115	-
87	CLA	LN	204	50	-	13/21/97/115	-
82	PEB	gH	203	1,74,2	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	EM	201	1,2	-	6/26/74/74	0/4/4/4
82	PEB	CB	201	2,4	-	3/26/74/74	0/4/4/4
82	PEB	EP	202	1	-	11/26/74/74	0/4/4/4
82	PEB	VQ	202	1	-	12/26/74/74	0/4/4/4
84	CYC	R3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	bL	615	-	-	15/39/115/115	-
87	CLA	AN	851	-	-	22/39/115/115	-
87	CLA	A2	831	-	-	13/39/115/115	-
95	DGD	b6	621	-	-	9/29/69/95	0/2/2/2
92	LMG	CL	519	-	-	22/50/70/70	0/1/1/1
87	CLA	CL	508	87	-	23/39/115/115	-
82	PEB	VD	202	1	-	12/26/74/74	0/4/4/4
85	BCR	F6	101	20	-	9/29/63/63	0/2/2/2
85	BCR	B6	602	-	-	2/29/63/63	0/2/2/2
82	PEB	u8	201	2	-	10/26/74/74	0/4/4/4
82	PEB	XQ	202	1	-	12/26/74/74	0/4/4/4
83	PUB	QM	201	14,1	-	7/26/74/74	0/4/4/4
82	PEB	N4	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	P9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	YF	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	LB	201	2	-	10/26/74/74	0/4/4/4
87	CLA	AN	813	-	-	13/39/115/115	-
84	CYC	Q3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	RH	202	2	-	12/26/74/74	0/4/4/4
82	PEB	xK	303	13	-	12/26/74/74	0/4/4/4
82	PEB	FF	202	2	-	11/26/74/74	0/4/4/4
82	PEB	NB	202	2	-	8/26/74/74	0/4/4/4
82	PEB	JM	201	2	-	6/26/74/74	0/4/4/4
82	PEB	L1	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	U5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	GP	203	1	-	10/26/74/74	0/4/4/4
82	PEB	OH	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	RG	201	2	-	8/26/74/74	0/4/4/4
82	PEB	K9	202	1	-	15/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	SG	203	1,2	-	7/26/74/74	0/4/4/4
96	HEM	v6	201	35	-	2/14/54/54	-
82	PEB	V5	202	1	-	11/26/74/74	0/4/4/4
96	HEM	FL	102	-	-	6/14/54/54	-
84	CYC	NE	201	10,9	-	10/26/74/74	0/4/4/4
82	PEB	JA	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	W7	202	1	-	12/26/74/74	0/4/4/4
82	PEB	FA	203	2	-	11/26/74/74	0/4/4/4
83	PUB	AJ	303	13	-	13/26/74/74	0/4/4/4
82	PEB	VG	201	2	-	8/26/74/74	0/4/4/4
87	CLA	A2	805	40	-	23/39/115/115	-
82	PEB	EP	201	1	-	7/26/74/74	0/4/4/4
82	PEB	HI	201	2	-	8/26/74/74	0/4/4/4
82	PEB	bE	201	1	-	6/26/74/74	0/4/4/4
87	CLA	AN	821	-	-	18/39/115/115	-
87	CLA	2N	303	58	-	16/39/115/115	-
87	CLA	b6	613	-	-	17/39/115/115	-
82	PEB	A9	202	1	-	15/26/74/74	0/4/4/4
87	CLA	A2	833	-	-	13/39/115/115	-
82	PEB	WM	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	GA	201	1	-	6/26/74/74	0/4/4/4
87	CLA	C6	512	-	-	13/39/115/115	-
82	PEB	ZK	202	2	-	10/26/74/74	0/4/4/4
95	DGD	L6	102	26	-	24/47/87/95	0/2/2/2
82	PEB	A1	305	3	-	12/26/74/74	0/4/4/4
87	CLA	52	605	61	-	6/15/91/115	-
82	PEB	ZO	202	1	-	9/26/74/74	0/4/4/4
82	PEB	kO	202	2	-	13/26/74/74	0/4/4/4
82	PEB	XB	202	2	-	10/26/74/74	0/4/4/4
85	BCR	A2	848	-	-	16/29/63/63	0/2/2/2
87	CLA	B2	814	41	-	5/12/88/115	-
82	PEB	b1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	S5	201	74,2	-	11/26/74/74	0/4/4/4
82	PEB	TF	202	2	-	17/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	FN	201	45	-	5/10/86/115	-
87	CLA	2N	311	-	-	7/12/88/115	-
82	PEB	hM	201	1,2	-	8/26/74/74	0/4/4/4
82	PEB	D4	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	FJ	201	79,2	-	7/26/74/74	0/4/4/4
82	PEB	kH	201	2	-	8/26/74/74	0/4/4/4
82	PEB	AO	305	3	-	11/26/74/74	0/4/4/4
88	LHG	i6	101	-	-	17/53/53/53	-
82	PEB	Y5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	uF	201	1,2	-	11/26/74/74	0/4/4/4
83	PUB	xF	305	13	-	8/26/74/74	0/4/4/4
87	CLA	AN	810	40	-	23/39/115/115	-
82	PEB	f4	201	1	-	11/26/74/74	0/4/4/4
82	PEB	RI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	IM	202	1	-	7/26/74/74	0/4/4/4
82	PEB	cF	202	1,10	-	9/26/74/74	0/4/4/4
87	CLA	BN	822	-	-	13/27/103/115	-
82	PEB	eK	202	1	-	8/26/74/74	0/4/4/4
85	BCR	BN	838	-	-	5/29/63/63	0/2/2/2
87	CLA	A2	851	-	-	22/39/115/115	-
82	PEB	N7	202	2	-	9/26/74/74	0/4/4/4
87	CLA	b6	615	-	-	17/39/115/115	-
82	PEB	IK	202	1	-	15/26/74/74	0/4/4/4
87	CLA	BN	802	41	-	13/31/107/115	-
82	PEB	HI	203	2	-	6/26/74/74	0/4/4/4
82	PEB	VO	202	2	-	12/26/74/74	0/4/4/4
82	PEB	AQ	304	3,82	-	11/26/74/74	0/4/4/4
82	PEB	VP	202	2	-	7/26/74/74	0/4/4/4
82	PEB	AD	303	3,82	-	11/26/74/74	0/4/4/4
87	CLA	72	610	-	-	5/15/91/115	-
84	CYC	DO	1001	10	-	10/26/74/74	0/4/4/4
82	PEB	tK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	lK	202	2	-	13/26/74/74	0/4/4/4
82	PEB	FP	202	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	AA	201	1	-	11/26/74/74	0/4/4/4
82	PEB	eJ	201	13,2	-	6/26/74/74	0/4/4/4
87	CLA	4N	608	60	-	11/21/97/115	-
82	PEB	bB	201	2	-	11/26/74/74	0/4/4/4
82	PEB	S1	201	1	-	7/26/74/74	0/4/4/4
82	PEB	aK	202	1	-	9/26/74/74	0/4/4/4
82	PEB	KP	202	1	-	4/26/74/74	0/4/4/4
82	PEB	KB	304	2,5	-	9/26/74/74	0/4/4/4
84	CYC	FH	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	cG	202	2	-	10/26/74/74	0/4/4/4
87	CLA	B2	828	41	-	7/15/91/115	-
87	CLA	dL	404	-	-	17/39/115/115	-
82	PEB	LP	202	2	-	6/26/74/74	0/4/4/4
84	CYC	C4	1001	9	-	11/26/74/74	0/4/4/4
87	CLA	AN	823	40	-	20/39/115/115	-
87	CLA	B2	820	54,41	-	2/13/89/115	-
82	PEB	U5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	BN	807	-	-	20/39/115/115	-
82	PEB	JK	202	2	-	15/26/74/74	0/4/4/4
91	PHO	d6	404	-	3/3/17/22	3/37/103/103	0/5/6/6
82	PEB	Y5	202	2	-	12/26/74/74	0/4/4/4
82	PEB	ZM	201	2	-	8/26/74/74	0/4/4/4
82	PEB	H5	203	2	-	12/26/74/74	0/4/4/4
83	PUB	Z9	305	1,74	-	14/26/74/74	0/4/4/4
85	BCR	I2	101	-	-	12/29/63/63	0/2/2/2
84	CYC	N1	1001	10,8	-	10/26/74/74	0/4/4/4
87	CLA	b6	614	-	-	10/32/108/115	-
87	CLA	7N	606	63	-	7/15/91/115	-
82	PEB	OM	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	C6	509	-	-	19/39/115/115	-
95	DGD	lL	101	26	-	20/47/87/95	0/2/2/2
82	PEB	YB	202	2	-	8/26/74/74	0/4/4/4
82	PEB	YO	201	2	-	3/26/74/74	0/4/4/4
82	PEB	V7	203	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	32	310	59,87	-	5/10/86/115	-
82	PEB	QP	201	1	-	7/26/74/74	0/4/4/4
82	PEB	FM	201	79,2	-	6/26/74/74	0/4/4/4
82	PEB	pK	201	2	-	8/26/74/74	0/4/4/4
82	PEB	H9	201	74,2	-	10/26/74/74	0/4/4/4
95	DGD	b6	622	-	-	10/31/71/95	0/2/2/2
88	LHG	cL	501	17	-	7/36/36/53	-
85	BCR	CL	516	-	-	5/29/63/63	0/2/2/2
87	CLA	B2	816	-	-	8/32/108/115	-
82	PEB	P7	202	2	-	7/26/74/74	0/4/4/4
85	BCR	IN	101	-	-	12/29/63/63	0/2/2/2
82	PEB	Z9	301	74	-	16/26/74/74	0/4/4/4
84	CYC	F3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	AN	831	-	-	14/39/115/115	-
82	PEB	L9	201	2	-	10/26/74/74	0/4/4/4
82	PEB	MQ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	iH	202	2	-	9/26/74/74	0/4/4/4
82	PEB	HA	201	2	-	5/26/74/74	0/4/4/4
103	ZEX	8N	309	64	-	11/29/67/67	0/2/2/2
87	CLA	C6	510	-	-	17/39/115/115	-
84	CYC	CO	1001	9	-	11/26/74/74	0/4/4/4
82	PEB	kM	202	2	-	9/26/74/74	0/4/4/4
82	PEB	lH	202	1	-	13/26/74/74	0/4/4/4
87	CLA	1N	607	57	-	11/21/97/115	-
82	PEB	yC	203	2	-	9/26/74/74	0/4/4/4
82	PEB	GP	202	1	-	4/26/74/74	0/4/4/4
82	PEB	C9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	kG	202	2	-	11/26/74/74	0/4/4/4
82	PEB	DF	203	2	-	12/26/74/74	0/4/4/4
82	PEB	CK	201	1	-	6/26/74/74	0/4/4/4
82	PEB	A5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	j4	201	1	-	10/26/74/74	0/4/4/4
82	PEB	gE	201	2	-	6/26/74/74	0/4/4/4
82	PEB	P9	202	1	-	15/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	BCR	A2	847	-	-	8/29/63/63	0/2/2/2
83	PUB	K7	203	1,3	-	6/26/74/74	0/4/4/4
82	PEB	AP	201	1	-	4/26/74/74	0/4/4/4
82	PEB	iO	201	2	-	7/26/74/74	0/4/4/4
87	CLA	AN	850	40	-	6/39/115/115	-
87	CLA	BL	601	-	-	15/39/115/115	-
82	PEB	XD	203	1	-	10/26/74/74	0/4/4/4
87	CLA	3N	312	59	-	9/15/91/115	-
82	PEB	qF	202	1	-	17/26/74/74	0/4/4/4
87	CLA	dL	402	-	-	8/39/115/115	-
85	BCR	B2	802	87,50,41	-	11/29/63/63	0/2/2/2
82	PEB	QF	202	1	-	7/26/74/74	0/4/4/4
82	PEB	G5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	M5	304	74,82	-	8/26/74/74	0/4/4/4
84	CYC	M4	1001	9	-	10/26/74/74	0/4/4/4
82	PEB	jE	201	1	-	9/26/74/74	0/4/4/4
87	CLA	4N	602	60	-	16/39/115/115	-
82	PEB	kE	202	2	-	11/26/74/74	0/4/4/4
82	PEB	XI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	WQ	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	Z4	201	1	-	7/26/74/74	0/4/4/4
82	PEB	UI	201	2	-	7/26/74/74	0/4/4/4
82	PEB	XK	202	2	-	6/26/74/74	0/4/4/4
82	PEB	UM	202	1	-	4/26/74/74	0/4/4/4
82	PEB	JB	202	1	-	11/26/74/74	0/4/4/4
82	PEB	c4	203	2	-	11/26/74/74	0/4/4/4
87	CLA	F2	202	45	-	5/10/86/115	-
84	CYC	L1	1001	10	-	12/26/74/74	0/4/4/4
82	PEB	QB	204	2	-	11/26/74/74	0/4/4/4
82	PEB	EK	201	1	-	9/26/74/74	0/4/4/4
82	PEB	GK	202	1	-	7/26/74/74	0/4/4/4
82	PEB	qK	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	UG	203	1	-	12/26/74/74	0/4/4/4
87	CLA	B2	825	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	HB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	XP	202	2	-	8/26/74/74	0/4/4/4
87	CLA	2N	308	58	-	7/15/91/115	-
83	PUB	xK	306	13	-	6/26/74/74	0/4/4/4
87	CLA	5N	609	61	-	6/12/88/115	-
82	PEB	XF	201	2	-	10/26/74/74	0/4/4/4
83	PUB	M5	303	1,74	-	8/26/74/74	0/4/4/4
82	PEB	HF	201	2	-	7/26/74/74	0/4/4/4
84	CYC	EE	1001	10,9	-	8/26/74/74	0/4/4/4
83	PUB	YA	302	3	-	3/26/74/74	0/4/4/4
87	CLA	IN	102	-	-	11/39/115/115	-
82	PEB	iH	201	2	-	7/26/74/74	0/4/4/4
82	PEB	EQ	201	2,77	-	12/26/74/74	0/4/4/4
82	PEB	WP	202	1	-	4/26/74/74	0/4/4/4
83	PUB	Z9	302	74	-	7/26/74/74	0/4/4/4
82	PEB	KK	202	1	-	4/26/74/74	0/4/4/4
87	CLA	AN	834	-	-	20/39/115/115	-
82	PEB	MK	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	xF	303	13	-	12/26/74/74	0/4/4/4
82	PEB	w8	201	2	-	12/26/74/74	0/4/4/4
82	PEB	1C	202	2	-	6/26/74/74	0/4/4/4
82	PEB	PE	202	2	-	13/26/74/74	0/4/4/4
82	PEB	hO	202	1	-	8/26/74/74	0/4/4/4
83	PUB	M9	303	74	-	7/26/74/74	0/4/4/4
82	PEB	mK	201	1	-	6/26/74/74	0/4/4/4
84	CYC	W3	1001	71	-	10/26/74/74	0/4/4/4
82	PEB	hE	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	kF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	dB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	NA	203	2	-	8/26/74/74	0/4/4/4
82	PEB	CM	201	1	-	8/26/74/74	0/4/4/4
95	DGD	DL	408	18	-	9/51/91/95	0/2/2/2
82	PEB	DB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	HB	201	2	-	15/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	VP	201	2	-	7/26/74/74	0/4/4/4
82	PEB	eJ	202	2	-	11/26/74/74	0/4/4/4
82	PEB	MF	201	1	-	6/26/74/74	0/4/4/4
87	CLA	bL	604	-	-	8/17/93/115	-
82	PEB	RQ	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	NE	202	10,9	-	9/26/74/74	0/4/4/4
91	PHO	dL	403	-	3/3/17/22	8/37/103/103	0/5/6/6
82	PEB	gE	202	2	-	11/26/74/74	0/4/4/4
82	PEB	q8	203	2	-	6/26/74/74	0/4/4/4
83	PUB	AE	303	3	-	9/26/74/74	0/4/4/4
87	CLA	62	304	-	-	9/15/91/115	-
84	CYC	IE	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	LD	202	1	-	9/26/74/74	0/4/4/4
85	BCR	a6	605	-	-	6/29/63/63	0/2/2/2
82	PEB	B9	201	2	-	10/26/74/74	0/4/4/4
87	CLA	5N	603	-	-	8/15/91/115	-
82	PEB	TD	201	1,2	-	13/26/74/74	0/4/4/4
87	CLA	CL	504	-	-	18/39/115/115	-
82	PEB	F7	203	2	-	11/26/74/74	0/4/4/4
82	PEB	QG	202	1	-	9/26/74/74	0/4/4/4
82	PEB	MM	202	1	-	6/26/74/74	0/4/4/4
82	PEB	SI	201	2	-	12/26/74/74	0/4/4/4
82	PEB	K7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	NG	201	10,9	-	9/26/74/74	0/4/4/4
82	PEB	MJ	203	1	-	9/26/74/74	0/4/4/4
87	CLA	1N	605	57	-	9/15/91/115	-
82	PEB	T5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	Q9	203	2	-	7/26/74/74	0/4/4/4
82	PEB	O4	201	1	-	8/26/74/74	0/4/4/4
82	PEB	Z9	303	74	-	11/26/74/74	0/4/4/4
82	PEB	i4	202	2	-	8/26/74/74	0/4/4/4
84	CYC	EG	1001	10,9	-	8/26/74/74	0/4/4/4
82	PEB	BJ	301	14	-	9/26/74/74	0/4/4/4
84	CYC	MG	1001	10,9	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	M2	101	51,41	-	10/15/91/115	-
87	CLA	82	301	64	-	10/15/91/115	-
82	PEB	EQ	202	2	-	7/26/74/74	0/4/4/4
82	PEB	TQ	201	1,2	-	13/26/74/74	0/4/4/4
82	PEB	D7	201	3,2	-	11/26/74/74	0/4/4/4
88	LHG	AL	407	15	-	16/47/47/53	-
82	PEB	PD	202	1	-	9/26/74/74	0/4/4/4
87	CLA	7N	602	62,63	-	14/39/115/115	-
82	PEB	w8	203	2	-	6/26/74/74	0/4/4/4
82	PEB	PH	202	2	-	8/26/74/74	0/4/4/4
82	PEB	a4	202	2	-	7/26/74/74	0/4/4/4
84	CYC	L3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	jK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	Q7	202	1	-	9/26/74/74	0/4/4/4
85	BCR	h6	102	-	-	3/29/63/63	0/2/2/2
82	PEB	QH	203	1	-	9/26/74/74	0/4/4/4
82	PEB	SP	203	1	-	11/26/74/74	0/4/4/4
92	LMG	b6	623	-	-	21/36/56/70	0/1/1/1
82	PEB	BF	202	2	-	13/26/74/74	0/4/4/4
92	LMG	j6	101	-	-	17/38/58/70	0/1/1/1
82	PEB	yC	202	2	-	9/26/74/74	0/4/4/4
82	PEB	iE	202	2	-	10/26/74/74	0/4/4/4
82	PEB	iF	203	1	-	13/26/74/74	0/4/4/4
82	PEB	WM	202	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	608	62	-	10/21/97/115	-
87	CLA	72	608	63	-	6/10/86/115	-
82	PEB	YJ	203	1	-	9/26/74/74	0/4/4/4
82	PEB	b4	202	1	-	8/26/74/74	0/4/4/4
82	PEB	H9	203	2	-	9/26/74/74	0/4/4/4
82	PEB	GF	202	1	-	7/26/74/74	0/4/4/4
82	PEB	YF	201	1	-	7/26/74/74	0/4/4/4
82	PEB	V1	202	1,2	-	8/26/74/74	0/4/4/4
82	PEB	TH	201	11,2	-	9/26/74/74	0/4/4/4
82	PEB	NJ	202	2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	J5	201	2	-	9/26/74/74	0/4/4/4
85	BCR	AN	847	-	-	8/29/63/63	0/2/2/2
92	LMG	mL	101	-	-	8/36/56/70	0/1/1/1
82	PEB	RE	201	2	-	8/26/74/74	0/4/4/4
82	PEB	QD	201	3,2	-	3/26/74/74	0/4/4/4
82	PEB	eM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	aM	203	1	-	15/26/74/74	0/4/4/4
96	HEM	VL	201	35	-	2/14/54/54	-
87	CLA	A2	827	-	-	9/27/103/115	-
82	PEB	HQ	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	IB	201	2	-	7/26/74/74	0/4/4/4
82	PEB	m1	202	2	-	10/26/74/74	0/4/4/4
87	CLA	4N	611	-	-	6/15/91/115	-
82	PEB	UE	203	1	-	12/26/74/74	0/4/4/4
84	CYC	h3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	aG	201	2	-	5/26/74/74	0/4/4/4
82	PEB	FD	201	1	-	11/26/74/74	0/4/4/4
87	CLA	A2	809	-	-	15/39/115/115	-
82	PEB	TB	202	1	-	11/26/74/74	0/4/4/4
82	PEB	kF	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	UB	301	2,5	-	9/26/74/74	0/4/4/4
82	PEB	BF	201	2	-	9/26/74/74	0/4/4/4
82	PEB	CF	202	1	-	7/26/74/74	0/4/4/4
82	PEB	LG	1002	10,9	-	11/26/74/74	0/4/4/4
82	PEB	iE	201	2	-	10/26/74/74	0/4/4/4
82	PEB	WI	201	2	-	8/26/74/74	0/4/4/4
87	CLA	42	610	-	-	7/12/88/115	-
92	LMG	AL	411	-	-	12/46/66/70	0/1/1/1
87	CLA	BL	609	-	-	18/39/115/115	-
82	PEB	aE	201	2	-	5/26/74/74	0/4/4/4
82	PEB	YJ	202	1	-	6/26/74/74	0/4/4/4
87	CLA	52	603	-	-	8/15/91/115	-
87	CLA	B6	612	-	-	14/32/108/115	-
87	CLA	dL	409	-	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	BD	202	1	-	10/26/74/74	0/4/4/4
84	CYC	K1	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	KD	202	2	-	12/26/74/74	0/4/4/4
84	CYC	BE	1001	10,8	-	13/26/74/74	0/4/4/4
87	CLA	c6	611	-	-	10/39/115/115	-
82	PEB	JI	201	2	-	8/26/74/74	0/4/4/4
82	PEB	RJ	201	2	-	6/26/74/74	0/4/4/4
83	PUB	BJ	302	14	-	7/26/74/74	0/4/4/4
92	LMG	A6	408	-	-	8/46/66/70	0/1/1/1
85	BCR	CL	501	-	-	1/29/63/63	0/2/2/2
82	PEB	VJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	N1	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	a1	201	2	-	6/26/74/74	0/4/4/4
82	PEB	XP	201	2	-	6/26/74/74	0/4/4/4
98	PQN	BN	837	41	-	5/23/43/43	0/2/2/2
87	CLA	22	606	58	-	9/15/91/115	-
82	PEB	mG	202	2	-	8/26/74/74	0/4/4/4
84	CYC	J1	1001	10	-	6/26/74/74	0/4/4/4
82	PEB	EJ	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	R2	204	-	-	11/15/91/115	-
92	LMG	b6	624	-	-	11/31/51/70	0/1/1/1
82	PEB	eH	202	2	-	11/26/74/74	0/4/4/4
82	PEB	jF	202	2	-	12/26/74/74	0/4/4/4
87	CLA	12	602	57	-	15/39/115/115	-
84	CYC	e3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	O9	202	2	-	8/26/74/74	0/4/4/4
96	HEM	E6	101	19	-	2/14/54/54	-
82	PEB	SF	202	1	-	8/26/74/74	0/4/4/4
82	PEB	PO	201	2	-	5/26/74/74	0/4/4/4
82	PEB	nF	202	2	-	11/26/74/74	0/4/4/4
82	PEB	YM	203	1	-	13/26/74/74	0/4/4/4
92	LMG	JL	102	-	-	16/38/58/70	0/1/1/1
82	PEB	EP	203	1,2	-	13/26/74/74	0/4/4/4
82	PEB	VB	201	2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	CYC	IG	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	dM	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	C6	515	17	-	13/39/115/115	-
82	PEB	hK	202	2	-	9/26/74/74	0/4/4/4
82	PEB	vF	201	2	-	7/26/74/74	0/4/4/4
87	CLA	C6	516	-	-	10/39/115/115	-
82	PEB	I9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	zF	501	78,2	-	7/26/74/74	0/4/4/4
82	PEB	eO	201	2	-	5/26/74/74	0/4/4/4
82	PEB	XD	202	1	-	12/26/74/74	0/4/4/4
82	PEB	X7	202	2	-	9/26/74/74	0/4/4/4
87	CLA	a6	609	-	-	6/21/97/115	-
87	CLA	CL	512	-	-	6/39/115/115	-
82	PEB	EI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	aK	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	QM	204	1	-	10/26/74/74	0/4/4/4
87	CLA	3N	307	-	-	4/12/88/115	-
87	CLA	22	603	-	-	9/15/91/115	-
82	PEB	v8	201	1	-	10/26/74/74	0/4/4/4
82	PEB	lO	202	1	-	10/26/74/74	0/4/4/4
82	PEB	GJ	202	1	-	6/26/74/74	0/4/4/4
83	PUB	xF	301	13	-	6/26/74/74	0/4/4/4
87	CLA	K2	106	40,49	-	10/20/96/115	-
99	SF4	C2	102	42	-	-	0/6/5/5
87	CLA	B2	811	-	-	7/27/103/115	-
82	PEB	eH	201	2	-	8/26/74/74	0/4/4/4
82	PEB	WG	202	1,77	-	7/26/74/74	0/4/4/4
82	PEB	aJ	202	1	-	7/26/74/74	0/4/4/4
87	CLA	AN	825	-	-	7/27/103/115	-
82	PEB	sC	202	2	-	8/26/74/74	0/4/4/4
82	PEB	O9	201	2	-	12/26/74/74	0/4/4/4
82	PEB	K9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	t8	202	1	-	18/26/74/74	0/4/4/4
82	PEB	JP	202	2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	nF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	UB	303	2,5	-	8/26/74/74	0/4/4/4
82	PEB	O5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	HD	202	1	-	12/26/74/74	0/4/4/4
87	CLA	22	602	58	-	16/39/115/115	-
82	PEB	I5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	mM	201	13,2	-	7/26/74/74	0/4/4/4
87	CLA	B6	607	-	-	16/39/115/115	-
87	CLA	BN	818	41	-	12/33/109/115	-
82	PEB	oK	203	1	-	15/26/74/74	0/4/4/4
82	PEB	AM	302	13	-	8/26/74/74	0/4/4/4
82	PEB	QE	203	1	-	10/26/74/74	0/4/4/4
82	PEB	SK	203	1	-	9/26/74/74	0/4/4/4
82	PEB	ZK	201	2	-	9/26/74/74	0/4/4/4
82	PEB	U4	202	1	-	10/26/74/74	0/4/4/4
82	PEB	AH	302	3	-	11/26/74/74	0/4/4/4
82	PEB	OQ	202	2	-	14/26/74/74	0/4/4/4
87	CLA	K6	101	25	-	14/39/115/115	-
82	PEB	bH	202	1	-	10/26/74/74	0/4/4/4
83	PUB	ND	201	1,3	-	1/26/74/74	0/4/4/4
82	PEB	HJ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	WJ	201	1	-	4/26/74/74	0/4/4/4
87	CLA	A2	838	-	-	15/39/115/115	-
82	PEB	QO	201	1	-	8/26/74/74	0/4/4/4
82	PEB	NI	202	1	-	10/26/74/74	0/4/4/4
84	CYC	BG	1002	10,8	-	7/26/74/74	0/4/4/4
94	PL9	AL	413	-	-	13/53/73/73	0/1/1/1
82	PEB	HH	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	UI	202	2	-	6/26/74/74	0/4/4/4
82	PEB	RM	202	2	-	11/26/74/74	0/4/4/4
82	PEB	T4	201	2	-	5/26/74/74	0/4/4/4
82	PEB	L9	202	2	-	8/26/74/74	0/4/4/4
84	CYC	GE	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	BQ	202	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	OA	202	1	-	10/26/74/74	0/4/4/4
82	PEB	kJ	202	2	-	7/26/74/74	0/4/4/4
83	PUB	M5	302	1,74	-	7/26/74/74	0/4/4/4
82	PEB	sC	201	2	-	7/26/74/74	0/4/4/4
87	CLA	3N	301	59	-	5/15/91/115	-
82	PEB	OI	201	2	-	8/26/74/74	0/4/4/4
92	LMG	D6	407	18,24	-	7/28/48/70	0/1/1/1
92	LMG	DL	402	18	-	18/49/69/70	0/1/1/1
82	PEB	EB	501	2,4	-	10/26/74/74	0/4/4/4
82	PEB	h1	201	1,74,2	-	9/26/74/74	0/4/4/4
87	CLA	LN	202	50	-	16/30/106/115	-
82	PEB	E9	201	1	-	7/26/74/74	0/4/4/4
87	CLA	B2	808	-	-	14/39/115/115	-
82	PEB	dJ	202	1	-	6/26/74/74	0/4/4/4
82	PEB	HM	202	2	-	11/26/74/74	0/4/4/4
82	PEB	fH	201	1	-	9/26/74/74	0/4/4/4
87	CLA	B2	812	-	-	28/39/115/115	-
87	CLA	5N	606	61	-	6/15/91/115	-
82	PEB	O5	201	74,2,82	-	9/26/74/74	0/4/4/4
82	PEB	JF	201	2	-	8/26/74/74	0/4/4/4
91	PHO	D6	404	-	3/3/17/22	7/37/103/103	0/5/6/6
82	PEB	DM	201	14,2	-	10/26/74/74	0/4/4/4
83	PUB	A4	302	3	-	2/26/74/74	0/4/4/4
82	PEB	cH	201	2	-	7/26/74/74	0/4/4/4
85	BCR	B2	838	-	-	5/29/63/63	0/2/2/2
103	ZEX	82	309	64	-	11/29/67/67	0/2/2/2
82	PEB	FK	202	2	-	11/26/74/74	0/4/4/4
82	PEB	NQ	202	1	-	11/26/74/74	0/4/4/4
82	PEB	U4	201	1	-	8/26/74/74	0/4/4/4
87	CLA	32	308	59	-	5/15/91/115	-
87	CLA	52	604	61	-	6/12/88/115	-
92	LMG	b6	619	-	-	5/36/56/70	0/1/1/1
82	PEB	vC	202	1	-	15/26/74/74	0/4/4/4
82	PEB	cO	202	2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	PM	202	2	-	7/26/74/74	0/4/4/4
84	CYC	CG	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	WE	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	b1	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	GJ	203	1,2	-	8/26/74/74	0/4/4/4
92	LMG	B6	618	-	-	10/35/55/70	0/1/1/1
82	PEB	W1	201	1	-	8/26/74/74	0/4/4/4
82	PEB	Q5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	BB	202	2	-	7/26/74/74	0/4/4/4
82	PEB	PQ	202	1	-	9/26/74/74	0/4/4/4
82	PEB	l1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	H7	202	2	-	8/26/74/74	0/4/4/4
82	PEB	OQ	201	3,2,82	-	8/26/74/74	0/4/4/4
84	CYC	LH	1002	10	-	12/26/74/74	0/4/4/4
85	BCR	BL	616	-	-	4/29/63/63	0/2/2/2
87	CLA	62	305	87,62	-	9/12/88/115	-
87	CLA	aL	606	-	1/1/14/20	10/33/109/115	-
87	CLA	B2	826	-	-	18/39/115/115	-
85	BCR	J2	103	40,48	-	13/29/63/63	0/2/2/2
82	PEB	O7	202	1	-	10/26/74/74	0/4/4/4
82	PEB	wF	303	13	-	7/26/74/74	0/4/4/4
82	PEB	D9	201	2	-	10/26/74/74	0/4/4/4
82	PEB	NK	202	2	-	12/26/74/74	0/4/4/4
87	CLA	bL	607	-	-	16/39/115/115	-
85	BCR	c6	602	-	-	3/29/63/63	0/2/2/2
87	CLA	BN	826	-	-	18/39/115/115	-
82	PEB	TA	203	2	-	7/26/74/74	0/4/4/4
82	PEB	KM	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	32	306	-	-	4/12/88/115	-
87	CLA	d6	403	-	-	18/39/115/115	-
87	CLA	AN	802	40,45	-	16/39/115/115	-
82	PEB	SQ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	TM	202	2	-	7/26/74/74	0/4/4/4
82	PEB	jO	201	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	x8	202	1	-	15/26/74/74	0/4/4/4
82	PEB	DJ	201	14,2	-	8/26/74/74	0/4/4/4
85	BCR	BN	843	-	-	6/29/63/63	0/2/2/2
87	CLA	52	608	61	-	6/10/86/115	-
87	CLA	5N	602	61	-	12/39/115/115	-
82	PEB	HM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	UQ	202	2	-	7/26/74/74	0/4/4/4
82	PEB	A7	201	1	-	11/26/74/74	0/4/4/4
95	DGD	C6	504	-	-	12/31/71/95	0/2/2/2
103	ZEX	82	310	64,87	-	10/29/67/67	0/2/2/2
87	CLA	B6	609	-	-	14/39/115/115	-
84	CYC	MO	1001	9	-	10/26/74/74	0/4/4/4
87	CLA	2N	304	-	-	9/15/91/115	-
85	BCR	BN	803	87,50,41	-	11/29/63/63	0/2/2/2
82	PEB	e1	202	2	-	11/26/74/74	0/4/4/4
82	PEB	SJ	201	1	-	8/26/74/74	0/4/4/4
82	PEB	Z5	305	74	-	13/26/74/74	0/4/4/4
82	PEB	T7	202	2	-	9/26/74/74	0/4/4/4
87	CLA	bL	619	-	-	8/32/108/115	-
82	PEB	UD	201	3,2	-	9/26/74/74	0/4/4/4
82	PEB	A4	304	3	-	9/26/74/74	0/4/4/4
82	PEB	DP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	bG	201	1	-	6/26/74/74	0/4/4/4
82	PEB	lH	201	1	-	10/26/74/74	0/4/4/4
87	CLA	A2	823	40	-	20/39/115/115	-
84	CYC	EH	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	AN	801	-	-	9/13/90/115	-
82	PEB	QJ	203	1	-	7/26/74/74	0/4/4/4
87	CLA	b6	606	16	-	10/39/115/115	-
95	DGD	c6	618	-	-	10/51/91/95	0/2/2/2
82	PEB	MK	201	1	-	6/26/74/74	0/4/4/4
82	PEB	bE	202	1	-	12/26/74/74	0/4/4/4
82	PEB	iG	202	2	-	10/26/74/74	0/4/4/4
82	PEB	LJ	201	2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	aF	201	1,2	-	9/26/74/74	0/4/4/4
95	DGD	BL	613	-	-	7/29/69/95	0/2/2/2
84	CYC	d3	1001	73,69	-	4/26/74/74	0/4/4/4
87	CLA	RN	203	54,41	-	8/17/93/115	-
87	CLA	52	606	61	-	6/15/91/115	-
82	PEB	ZF	202	2	-	10/26/74/74	0/4/4/4
82	PEB	WO	201	1	-	6/26/74/74	0/4/4/4
82	PEB	SH	201	1	-	7/26/74/74	0/4/4/4
82	PEB	MJ	201	1,2	-	7/26/74/74	0/4/4/4
84	CYC	C1	1001	10,9	-	8/26/74/74	0/4/4/4
82	PEB	N5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	W7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	D9	203	2	-	7/26/74/74	0/4/4/4
82	PEB	gG	201	2	-	6/26/74/74	0/4/4/4
82	PEB	SB	203	2	-	8/26/74/74	0/4/4/4
83	PUB	A1	303	3	-	5/26/74/74	0/4/4/4
82	PEB	GI	203	1	-	10/26/74/74	0/4/4/4
87	CLA	AN	829	-	-	17/39/115/115	-
82	PEB	UQ	201	3,2	-	9/26/74/74	0/4/4/4
82	PEB	tC	202	1	-	18/26/74/74	0/4/4/4
82	PEB	bK	201	2	-	4/26/74/74	0/4/4/4
82	PEB	AM	301	13	-	12/26/74/74	0/4/4/4
82	PEB	YQ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	p8	202	1	-	16/26/74/74	0/4/4/4
82	PEB	FI	202	2	-	9/26/74/74	0/4/4/4
82	PEB	NF	201	2	-	7/26/74/74	0/4/4/4
87	CLA	A2	837	-	-	8/23/99/115	-
82	PEB	UG	202	1	-	9/26/74/74	0/4/4/4
87	CLA	L2	204	50	-	13/21/97/115	-
82	PEB	BA	201	2,82	-	8/26/74/74	0/4/4/4
82	PEB	Y9	201	2	-	10/26/74/74	0/4/4/4
82	PEB	JQ	202	1	-	12/26/74/74	0/4/4/4
82	PEB	OP	202	1	-	4/26/74/74	0/4/4/4
82	PEB	R5	202	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	B2	807	-	-	11/39/115/115	-
82	PEB	l1	203	1	-	13/26/74/74	0/4/4/4
82	PEB	NB	203	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	830	-	-	15/39/115/115	-
82	PEB	f1	203	1,2	-	12/26/74/74	0/4/4/4
84	CYC	LG	1001	10	-	11/26/74/74	0/4/4/4
87	CLA	MN	101	51,41	-	10/15/91/115	-
82	PEB	TO	203	2	-	10/26/74/74	0/4/4/4
82	PEB	V4	202	2	-	12/26/74/74	0/4/4/4
82	PEB	x8	201	1	-	11/26/74/74	0/4/4/4
82	PEB	NP	202	2	-	6/26/74/74	0/4/4/4
83	PUB	yK	303	14	-	5/26/74/74	0/4/4/4
83	PUB	xK	301	13	-	6/26/74/74	0/4/4/4
85	BCR	c6	617	-	-	9/29/63/63	0/2/2/2
82	PEB	dE	204	1	-	12/26/74/74	0/4/4/4
82	PEB	rK	201	13,2	-	11/26/74/74	0/4/4/4
82	PEB	sK	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	AN	806	-	-	9/27/103/115	-
87	CLA	A2	850	40	-	6/39/115/115	-
82	PEB	RF	202	2	-	13/26/74/74	0/4/4/4
82	PEB	KI	203	1	-	10/26/74/74	0/4/4/4
87	CLA	62	311	-	-	5/12/88/115	-
87	CLA	8N	302	64	-	10/15/91/115	-
82	PEB	FQ	201	1	-	11/26/74/74	0/4/4/4
87	CLA	A2	802	-	-	9/13/90/115	-
82	PEB	VO	201	2	-	4/26/74/74	0/4/4/4
87	CLA	B6	610	-	-	11/39/115/115	-
87	CLA	82	307	-	-	5/12/88/115	-
95	DGD	B6	620	16	-	12/47/87/95	0/2/2/2
82	PEB	JD	203	1,2	-	14/26/74/74	0/4/4/4
82	PEB	U1	203	1	-	9/26/74/74	0/4/4/4
82	PEB	XA	203	2	-	12/26/74/74	0/4/4/4
87	CLA	52	602	61	-	12/39/115/115	-
87	CLA	AL	404	87	-	6/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	VB	202	1,2	-	10/26/74/74	0/4/4/4
82	PEB	S4	202	1,76	-	10/26/74/74	0/4/4/4
84	CYC	HH	1001	10	-	8/26/74/74	0/4/4/4
85	BCR	A2	804	-	-	2/29/63/63	0/2/2/2
82	PEB	P5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	D7	203	2	-	11/26/74/74	0/4/4/4
87	CLA	B2	821	-	-	13/27/103/115	-
87	CLA	KN	103	-	-	4/12/88/115	-
82	PEB	ND	202	1	-	11/26/74/74	0/4/4/4
82	PEB	GB	203	2	-	12/26/74/74	0/4/4/4
87	CLA	B2	817	41	-	12/33/109/115	-
87	CLA	2N	306	58	-	9/15/91/115	-
82	PEB	OE	201	1	-	9/26/74/74	0/4/4/4
82	PEB	VI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	GD	201	2	-	4/26/74/74	0/4/4/4
84	CYC	BE	1002	10,8	-	7/26/74/74	0/4/4/4
82	PEB	RH	201	2	-	7/26/74/74	0/4/4/4
87	CLA	A6	403	87	-	9/33/109/115	-
82	PEB	mE	202	2	-	8/26/74/74	0/4/4/4
82	PEB	FF	201	2	-	5/26/74/74	0/4/4/4
82	PEB	KG	201	10,9	-	6/26/74/74	0/4/4/4
82	PEB	dG	201	1,3	-	10/26/74/74	0/4/4/4
84	CYC	CH	1001	10,9	-	8/26/74/74	0/4/4/4
85	BCR	B2	840	41	-	7/29/63/63	0/2/2/2
87	CLA	AN	808	-	-	17/39/115/115	-
82	PEB	rF	201	13,2	-	11/26/74/74	0/4/4/4
82	PEB	OF	202	1	-	9/26/74/74	0/4/4/4
82	PEB	UH	202	1	-	7/26/74/74	0/4/4/4
87	CLA	A2	829	-	-	17/39/115/115	-
82	PEB	OJ	202	1	-	16/26/74/74	0/4/4/4
87	CLA	CL	507	-	-	19/39/115/115	-
82	PEB	FQ	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	U9	201	74,2	-	10/26/74/74	0/4/4/4
91	PHO	DL	405	-	3/3/17/22	8/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	WK	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	12	607	57	-	11/21/97/115	-
87	CLA	cL	514	-	-	6/39/115/115	-
82	PEB	tF	202	2	-	11/26/74/74	0/4/4/4
87	CLA	BL	602	-	-	16/39/115/115	-
84	CYC	63	901	73	-	7/26/74/74	0/4/4/4
82	PEB	iM	201	13,2	-	8/26/74/74	0/4/4/4
82	PEB	X9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	g4	202	2	-	8/26/74/74	0/4/4/4
82	PEB	UE	202	1	-	9/26/74/74	0/4/4/4
82	PEB	ZJ	201	2	-	5/26/74/74	0/4/4/4
82	PEB	RF	201	2	-	8/26/74/74	0/4/4/4
82	PEB	kH	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	VQ	203	1,2	-	14/26/74/74	0/4/4/4
84	CYC	NH	1001	10,8	-	10/26/74/74	0/4/4/4
82	PEB	UB	302	2,5	-	9/26/74/74	0/4/4/4
82	PEB	lF	202	2	-	13/26/74/74	0/4/4/4
87	CLA	AN	824	40	-	10/23/99/115	-
82	PEB	OO	202	1	-	6/26/74/74	0/4/4/4
82	PEB	CA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	NQ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	XB	201	2	-	9/26/74/74	0/4/4/4
82	PEB	V9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	TA	202	2	-	9/26/74/74	0/4/4/4
82	PEB	s8	201	2	-	7/26/74/74	0/4/4/4
87	CLA	62	313	62	-	9/15/91/115	-
82	PEB	UK	202	1	-	10/26/74/74	0/4/4/4
87	CLA	32	312	59	-	9/15/91/115	-
87	CLA	B2	810	-	-	20/39/115/115	-
82	PEB	A5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	dG	203	1	-	8/26/74/74	0/4/4/4
82	PEB	jJ	201	1	-	6/26/74/74	0/4/4/4
87	CLA	2N	305	-	-	3/12/88/115	-
87	CLA	BN	809	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	tK	203	1,2	-	11/26/74/74	0/4/4/4
82	PEB	GF	201	1,2	-	8/26/74/74	0/4/4/4
87	CLA	3N	311	-	-	9/12/88/115	-
82	PEB	WH	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	CJ	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	k1	202	2	-	8/26/74/74	0/4/4/4
82	PEB	qC	203	2	-	6/26/74/74	0/4/4/4
82	PEB	eE	202	2	-	7/26/74/74	0/4/4/4
82	PEB	QK	202	1	-	7/26/74/74	0/4/4/4
87	CLA	b6	609	-	-	19/39/115/115	-
87	CLA	22	607	58	-	8/15/91/115	-
85	BCR	c6	603	87,17	-	10/29/63/63	0/2/2/2
82	PEB	lO	201	1	-	8/26/74/74	0/4/4/4
95	DGD	BL	614	-	-	15/47/87/95	0/2/2/2
82	PEB	IP	201	1	-	5/26/74/74	0/4/4/4
82	PEB	cJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	iF	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	A2	828	40	-	13/39/115/115	-
82	PEB	KF	203	1	-	8/26/74/74	0/4/4/4
88	LHG	iL	101	-	-	16/53/53/53	-
82	PEB	cG	201	2	-	6/26/74/74	0/4/4/4
83	PUB	yK	302	14	-	3/26/74/74	0/4/4/4
87	CLA	bL	613	16	-	13/39/115/115	-
82	PEB	WD	201	3,2	-	4/26/74/74	0/4/4/4
87	CLA	32	305	-	-	8/15/91/115	-
82	PEB	F5	202	2	-	10/26/74/74	0/4/4/4
85	BCR	LN	201	-	-	12/29/63/63	0/2/2/2
87	CLA	B2	834	-	-	15/39/115/115	-
87	CLA	bL	605	-	-	8/39/115/115	-
82	PEB	TP	201	56,2	-	7/26/74/74	0/4/4/4
87	CLA	AN	837	-	-	8/23/99/115	-
82	PEB	SK	202	1	-	8/26/74/74	0/4/4/4
88	LHG	AN	844	-	-	17/44/44/53	-
82	PEB	fO	202	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	CYC	KH	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	LM	201	2	-	4/26/74/74	0/4/4/4
82	PEB	OF	203	1	-	9/26/74/74	0/4/4/4
85	BCR	A2	845	40	-	11/29/63/63	0/2/2/2
82	PEB	UP	202	1	-	10/26/74/74	0/4/4/4
82	PEB	L5	202	2	-	10/26/74/74	0/4/4/4
87	CLA	32	311	-	-	9/12/88/115	-
82	PEB	E5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	AI	201	1	-	9/26/74/74	0/4/4/4
84	CYC	x3	1001	-	-	10/26/74/74	0/4/4/4
82	PEB	zC	201	1	-	10/26/74/74	0/4/4/4
82	PEB	RI	203	1,2	-	10/26/74/74	0/4/4/4
83	PUB	AM	303	13	-	11/26/74/74	0/4/4/4
82	PEB	YP	503	56,2	-	7/26/74/74	0/4/4/4
82	PEB	T9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	RG	202	2	-	12/26/74/74	0/4/4/4
95	DGD	hL	101	22	-	18/51/91/95	0/2/2/2
82	PEB	U1	202	1	-	7/26/74/74	0/4/4/4
87	CLA	52	611	61	-	10/15/91/115	-
82	PEB	XA	202	2	-	9/26/74/74	0/4/4/4
82	PEB	eO	203	2	-	6/26/74/74	0/4/4/4
83	PUB	AM	304	13	-	8/26/74/74	0/4/4/4
87	CLA	7N	609	-	-	7/12/88/115	-
82	PEB	UK	201	1	-	8/26/74/74	0/4/4/4
88	LHG	D6	406	18	-	11/53/53/53	-
92	LMG	a6	614	87	-	3/37/57/70	0/1/1/1
82	PEB	i4	201	2	-	7/26/74/74	0/4/4/4
82	PEB	fF	202	2	-	13/26/74/74	0/4/4/4
84	CYC	I1	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	j4	203	-	-	13/26/74/74	0/4/4/4
82	PEB	EM	203	1	-	12/26/74/74	0/4/4/4
87	CLA	52	607	61	-	8/21/97/115	-
87	CLA	AN	832	40	-	10/21/97/115	-
82	PEB	SK	201	1,2	-	4/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	gO	202	2	-	8/26/74/74	0/4/4/4
85	BCR	B2	839	-	-	6/29/63/63	0/2/2/2
82	PEB	W5	202	2	-	11/26/74/74	0/4/4/4
87	CLA	1N	606	-	-	8/15/91/115	-
82	PEB	kM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	ZB	203	2	-	11/26/74/74	0/4/4/4
87	CLA	CL	511	-	-	11/39/115/115	-
82	PEB	HA	203	2	-	12/26/74/74	0/4/4/4
88	LHG	AN	843	40	-	16/53/53/53	-
82	PEB	CD	201	3,2	-	4/26/74/74	0/4/4/4
87	CLA	5N	608	61	-	6/10/86/115	-
82	PEB	g1	201	2	-	9/26/74/74	0/4/4/4
87	CLA	bL	616	-	-	16/39/115/115	-
87	CLA	4N	609	60	-	5/10/86/115	-
82	PEB	TO	201	2	-	5/26/74/74	0/4/4/4
82	PEB	DI	202	2	-	6/26/74/74	0/4/4/4
82	PEB	wK	301	13	-	11/26/74/74	0/4/4/4
82	PEB	D5	201	74,2	-	6/26/74/74	0/4/4/4
82	PEB	dK	201	2	-	9/26/74/74	0/4/4/4
82	PEB	kH	202	2	-	8/26/74/74	0/4/4/4
82	PEB	l4	201	1	-	8/26/74/74	0/4/4/4
82	PEB	aG	202	2	-	14/26/74/74	0/4/4/4
82	PEB	ZI	401	12,2	-	7/26/74/74	0/4/4/4
87	CLA	72	609	-	-	7/12/88/115	-
88	LHG	B6	617	-	-	15/53/53/53	-
88	LHG	D6	401	-	-	16/47/47/53	-
92	LMG	yL	101	-	-	29/50/70/70	0/1/1/1
82	PEB	gB	201	2	-	11/26/74/74	0/4/4/4

All (26459) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	A1	304	PUB	C3A-C2A	13.51	1.49	1.34
83	AH	304	PUB	C3A-C2A	13.34	1.49	1.34
83	M9	303	PUB	C3A-C2A	12.80	1.49	1.34
83	Z9	302	PUB	C3A-C2A	12.78	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WP	201	PEB	C4C-C3C	12.62	1.56	1.37
82	GP	201	PEB	C4C-C3C	12.53	1.55	1.37
83	Z9	305	PUB	C3A-C2A	12.48	1.48	1.34
82	MP	203	PEB	C4C-C3C	12.40	1.55	1.37
82	IP	203	PEB	C4C-C3C	12.34	1.55	1.37
82	UP	203	PEB	C4C-C3C	12.32	1.55	1.37
82	EP	203	PEB	C4C-C3C	12.27	1.55	1.37
82	AP	203	PEB	C4C-C3C	12.25	1.55	1.37
82	KP	201	PEB	C4C-C3C	12.23	1.55	1.37
82	QP	203	PEB	C4C-C3C	12.20	1.55	1.37
82	SP	201	PEB	C4C-C3C	12.03	1.55	1.37
83	xK	305	PUB	C3A-C2A	12.01	1.48	1.34
83	M5	303	PUB	C3A-C2A	11.98	1.48	1.34
83	xF	305	PUB	C3A-C2A	11.96	1.48	1.34
83	Z5	303	PUB	C3A-C2A	11.87	1.47	1.34
83	AJ	304	PUB	C3A-C2A	11.84	1.47	1.34
82	CP	201	PEB	C4C-C3C	11.82	1.54	1.37
82	OP	201	PEB	C4C-C3C	11.81	1.54	1.37
83	QM	201	PUB	C3A-C2A	11.72	1.47	1.34
83	AQ	302	PUB	C3A-C2A	11.67	1.47	1.34
83	ND	201	PUB	C3A-C2A	11.67	1.47	1.34
83	xK	306	PUB	C3A-C2A	11.66	1.47	1.34
83	NQ	201	PUB	C3A-C2A	11.65	1.47	1.34
83	AH	303	PUB	C3A-C2A	11.63	1.47	1.34
83	AO	302	PUB	C3A-C2A	11.58	1.47	1.34
83	AD	302	PUB	C3A-C2A	11.57	1.47	1.34
83	xF	306	PUB	C3A-C2A	11.56	1.47	1.34
83	xK	301	PUB	C3A-C2A	11.55	1.47	1.34
83	AG	302	PUB	C3A-C2A	11.55	1.47	1.34
83	xF	301	PUB	C3A-C2A	11.53	1.47	1.34
83	A4	302	PUB	C3A-C2A	11.53	1.47	1.34
83	A1	303	PUB	C3A-C2A	11.48	1.47	1.34
83	AG	303	PUB	C3A-C2A	11.48	1.47	1.34
83	AE	302	PUB	C3A-C2A	11.45	1.47	1.34
83	KA	203	PUB	C3A-C2A	11.45	1.47	1.34
82	fH	202	PEB	C2D-C3D	11.43	1.49	1.34
83	AE	303	PUB	C3A-C2A	11.40	1.47	1.34
83	K7	203	PUB	C3A-C2A	11.37	1.47	1.34
82	f1	202	PEB	C2D-C3D	11.36	1.49	1.34
82	bK	202	PEB	C4C-C3C	11.30	1.54	1.37
83	A4	303	PUB	C3A-C2A	11.30	1.47	1.34
83	AM	304	PUB	C3A-C2A	11.29	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	Y7	302	PUB	C3A-C2A	11.22	1.47	1.34
82	fK	202	PEB	C4C-C3C	11.18	1.53	1.37
83	yF	303	PUB	C3A-C2A	11.18	1.47	1.34
82	fF	202	PEB	C4C-C3C	11.18	1.53	1.37
82	bF	202	PEB	C4C-C3C	11.17	1.53	1.37
83	AM	303	PUB	C3A-C2A	11.14	1.47	1.34
83	AO	303	PUB	C3A-C2A	11.13	1.47	1.34
83	yK	303	PUB	C3A-C2A	11.10	1.47	1.34
83	BM	302	PUB	C3A-C2A	11.10	1.47	1.34
83	YA	302	PUB	C3A-C2A	11.08	1.46	1.34
83	yF	302	PUB	C3A-C2A	11.07	1.46	1.34
82	Y7	301	PEB	C4C-C3C	10.99	1.53	1.37
83	QJ	201	PUB	C3A-C2A	10.97	1.46	1.34
82	YA	301	PEB	C4C-C3C	10.97	1.53	1.37
82	PF	202	PEB	C4C-C3C	10.96	1.53	1.37
83	yK	302	PUB	C3A-C2A	10.95	1.46	1.34
82	PK	202	PEB	C4C-C3C	10.94	1.53	1.37
82	NF	202	PEB	C4C-C3C	10.87	1.53	1.37
83	BJ	302	PUB	C3A-C2A	10.83	1.46	1.34
83	AJ	303	PUB	C3A-C2A	10.78	1.46	1.34
82	NK	202	PEB	C4C-C3C	10.73	1.53	1.37
82	H5	201	PEB	C2D-C3D	10.72	1.48	1.34
82	U5	201	PEB	C2D-C3D	10.69	1.48	1.34
83	M5	302	PUB	C3A-C2A	10.55	1.46	1.34
83	Z5	302	PUB	C3A-C2A	10.52	1.46	1.34
82	U1	203	PEB	C2D-C3D	10.52	1.48	1.34
82	UH	203	PEB	C2D-C3D	10.46	1.48	1.34
83	wF	304	PUB	C3A-C2A	10.46	1.46	1.34
82	JB	202	PEB	C4C-C3C	10.43	1.52	1.37
83	wK	304	PUB	C3A-C2A	10.42	1.46	1.34
82	TK	202	PEB	C4C-C3C	10.41	1.52	1.37
82	TB	202	PEB	C4C-C3C	10.39	1.52	1.37
82	dF	202	PEB	C4C-C3C	10.37	1.52	1.37
82	j1	202	PEB	C2D-C3D	10.37	1.47	1.34
82	TF	202	PEB	C4C-C3C	10.35	1.52	1.37
82	jH	202	PEB	C2D-C3D	10.32	1.47	1.34
82	HH	1002	PEB	C2D-C3D	10.32	1.47	1.34
82	z8	201	PEB	C2D-C3D	10.31	1.47	1.34
82	JF	202	PEB	C4C-C3C	10.30	1.52	1.37
82	HB	201	PEB	C4C-C3C	10.25	1.52	1.37
82	RB	201	PEB	C2D-C3D	10.24	1.47	1.34
82	WQ	201	PEB	C2D-C3D	10.24	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	zC	201	PEB	C2D-C3D	10.23	1.47	1.34
82	jJ	202	PEB	C2D-C3D	10.23	1.47	1.34
82	JK	202	PEB	C4C-C3C	10.23	1.52	1.37
82	bH	202	PEB	C2D-C3D	10.22	1.47	1.34
82	dK	202	PEB	C4C-C3C	10.22	1.52	1.37
87	3N	308	CLA	C4B-NB	10.21	1.50	1.37
82	b1	202	PEB	C2D-C3D	10.21	1.47	1.34
82	H1	1002	PEB	C2D-C3D	10.20	1.47	1.34
82	cB	401	PEB	C2D-C3D	10.20	1.47	1.34
87	32	307	CLA	C4B-NB	10.19	1.50	1.37
82	ZH	203	PEB	C2D-C3D	10.19	1.47	1.34
82	rF	202	PEB	C4C-C3C	10.18	1.52	1.37
82	w8	204	PEB	C2D-C3D	10.18	1.47	1.34
82	1C	203	PEB	C2D-C3D	10.16	1.47	1.34
82	wC	204	PEB	C2D-C3D	10.15	1.47	1.34
82	m1	201	PEB	C2D-C3D	10.15	1.47	1.34
82	Z1	203	PEB	C2D-C3D	10.14	1.47	1.34
82	y8	202	PEB	C2D-C3D	10.14	1.47	1.34
82	g1	201	PEB	C2D-C3D	10.12	1.47	1.34
82	mH	201	PEB	C2D-C3D	10.12	1.47	1.34
82	yC	202	PEB	C2D-C3D	10.12	1.47	1.34
82	CQ	201	PEB	C2D-C3D	10.11	1.47	1.34
82	uF	203	PEB	C2D-C3D	10.11	1.47	1.34
82	xK	304	PEB	C2D-C3D	10.11	1.47	1.34
82	UQ	202	PEB	C2D-C3D	10.11	1.47	1.34
82	OH	202	PEB	C2D-C3D	10.11	1.47	1.34
82	WD	201	PEB	C2D-C3D	10.10	1.47	1.34
82	rK	202	PEB	C4C-C3C	10.10	1.52	1.37
82	tK	201	PEB	C2D-C3D	10.09	1.47	1.34
82	i1	201	PEB	C2D-C3D	10.09	1.47	1.34
82	UD	202	PEB	C2D-C3D	10.09	1.47	1.34
82	XB	202	PEB	C4C-C3C	10.07	1.52	1.37
82	18	201	PEB	C2D-C3D	10.06	1.47	1.34
82	CD	201	PEB	C2D-C3D	10.06	1.47	1.34
82	AD	303	PEB	C2D-C3D	10.06	1.47	1.34
82	iH	201	PEB	C2D-C3D	10.06	1.47	1.34
82	gH	201	PEB	C2D-C3D	10.05	1.47	1.34
82	j1	203	PEB	C2D-C3D	10.04	1.47	1.34
82	vF	201	PEB	C2D-C3D	10.04	1.47	1.34
82	O1	202	PEB	C2D-C3D	10.04	1.47	1.34
82	EA	201	PEB	C2D-C3D	10.03	1.47	1.34
82	lH	202	PEB	C2D-C3D	10.03	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	uK	201	PEB	C2D-C3D	10.03	1.47	1.34
82	VB	201	PEB	C4C-C3C	10.03	1.52	1.37
82	xF	302	PEB	C2D-C3D	10.03	1.47	1.34
82	xK	302	PEB	C2D-C3D	10.03	1.47	1.34
82	q8	201	PEB	C2D-C3D	10.02	1.47	1.34
82	sC	202	PEB	C2D-C3D	10.02	1.47	1.34
82	s8	202	PEB	C2D-C3D	10.02	1.47	1.34
82	xF	304	PEB	C2D-C3D	10.01	1.47	1.34
82	B5	202	PEB	C2D-C3D	10.01	1.47	1.34
82	1C	201	PEB	C2D-C3D	10.01	1.47	1.34
82	aF	203	PEB	C2D-C3D	10.01	1.47	1.34
82	aK	203	PEB	C2D-C3D	10.01	1.47	1.34
82	rC	202	PEB	C2D-C3D	10.00	1.47	1.34
82	r8	202	PEB	C2D-C3D	10.00	1.47	1.34
82	PD	203	PEB	C2D-C3D	10.00	1.47	1.34
82	qC	201	PEB	C2D-C3D	10.00	1.47	1.34
82	tF	201	PEB	C2D-C3D	10.00	1.47	1.34
82	b4	201	PEB	C2D-C3D	9.99	1.47	1.34
82	M5	304	PEB	C2D-C3D	9.99	1.47	1.34
82	PQ	203	PEB	C2D-C3D	9.99	1.47	1.34
82	uK	202	PEB	C2D-C3D	9.99	1.47	1.34
82	SH	202	PEB	C2D-C3D	9.99	1.47	1.34
82	WD	202	PEB	C2D-C3D	9.99	1.47	1.34
82	18	203	PEB	C2D-C3D	9.98	1.47	1.34
82	W9	202	PEB	C2D-C3D	9.98	1.47	1.34
82	vK	201	PEB	C2D-C3D	9.98	1.47	1.34
82	ZF	202	PEB	C4C-C3C	9.98	1.52	1.37
82	aH	202	PEB	C2D-C3D	9.98	1.47	1.34
82	YD	201	PEB	C2D-C3D	9.98	1.47	1.34
82	gJ	202	PEB	C2D-C3D	9.98	1.47	1.34
82	c1	201	PEB	C2D-C3D	9.97	1.47	1.34
82	GD	202	PEB	C2D-C3D	9.97	1.47	1.34
82	oF	201	PEB	C2D-C3D	9.97	1.47	1.34
82	E7	201	PEB	C2D-C3D	9.97	1.47	1.34
82	wC	203	PEB	C2D-C3D	9.97	1.47	1.34
82	mK	202	PEB	C2D-C3D	9.97	1.47	1.34
82	L9	202	PEB	C2D-C3D	9.97	1.47	1.34
82	WQ	202	PEB	C2D-C3D	9.97	1.47	1.34
82	S1	202	PEB	C2D-C3D	9.97	1.47	1.34
82	m1	202	PEB	C2D-C3D	9.96	1.47	1.34
82	qK	203	PEB	C2D-C3D	9.96	1.47	1.34
82	OD	201	PEB	C2D-C3D	9.96	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Z5	304	PEB	C2D-C3D	9.96	1.47	1.34
82	PB	201	PEB	C2D-C3D	9.96	1.47	1.34
82	mH	202	PEB	C2D-C3D	9.95	1.47	1.34
82	OD	202	PEB	C2D-C3D	9.95	1.47	1.34
82	Y9	202	PEB	C2D-C3D	9.95	1.47	1.34
82	DD	203	PEB	C4C-C3C	9.95	1.52	1.37
82	AQ	303	PEB	C2D-C3D	9.94	1.47	1.34
82	w8	203	PEB	C2D-C3D	9.94	1.47	1.34
82	nK	201	PEB	C2D-C3D	9.94	1.47	1.34
82	uF	202	PEB	C2D-C3D	9.94	1.47	1.34
82	l1	203	PEB	C2D-C3D	9.94	1.47	1.34
82	sK	202	PEB	C2D-C3D	9.94	1.47	1.34
82	sC	203	PEB	C2D-C3D	9.93	1.47	1.34
82	GQ	202	PEB	C2D-C3D	9.93	1.47	1.34
82	eK	201	PEB	C2D-C3D	9.93	1.47	1.34
82	VD	202	PEB	C2D-C3D	9.93	1.47	1.34
82	VQ	202	PEB	C2D-C3D	9.93	1.47	1.34
82	MK	202	PEB	C2D-C3D	9.93	1.47	1.34
82	Q9	202	PEB	C2D-C3D	9.93	1.47	1.34
82	f4	201	PEB	C2D-C3D	9.93	1.47	1.34
82	QG	203	PEB	C2D-C3D	9.93	1.47	1.34
82	b1	203	PEB	C2D-C3D	9.93	1.47	1.34
82	jM	201	PEB	C2D-C3D	9.92	1.47	1.34
82	yC	203	PEB	C2D-C3D	9.92	1.47	1.34
82	s8	203	PEB	C2D-C3D	9.92	1.47	1.34
82	B9	202	PEB	C2D-C3D	9.92	1.47	1.34
82	OQ	201	PEB	C2D-C3D	9.91	1.47	1.34
82	wC	201	PEB	C2D-C3D	9.91	1.47	1.34
82	rK	201	PEB	C2D-C3D	9.91	1.47	1.34
82	WA	202	PEB	C2D-C3D	9.91	1.47	1.34
82	nF	201	PEB	C2D-C3D	9.91	1.47	1.34
82	VB	202	PEB	C2D-C3D	9.91	1.47	1.34
82	YD	202	PEB	C2D-C3D	9.91	1.47	1.34
82	Z1	201	PEB	C2D-C3D	9.91	1.47	1.34
82	YA	301	PEB	C2D-C3D	9.91	1.47	1.34
82	HD	203	PEB	C2D-C3D	9.90	1.47	1.34
82	XF	203	PEB	C4C-C3C	9.90	1.52	1.37
82	qK	202	PEB	C2D-C3D	9.90	1.47	1.34
82	LA	201	PEB	C2D-C3D	9.90	1.47	1.34
82	ZK	202	PEB	C4C-C3C	9.90	1.52	1.37
82	C9	202	PEB	C2D-C3D	9.90	1.47	1.34
82	ZH	201	PEB	C2D-C3D	9.89	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	K7	201	PEB	C2D-C3D	9.89	1.47	1.34
82	ZB	203	PEB	C4C-C3C	9.89	1.52	1.37
82	N1	1002	PEB	C2D-C3D	9.89	1.47	1.34
82	dH	203	PEB	C2D-C3D	9.89	1.47	1.34
82	OQ	202	PEB	C2D-C3D	9.89	1.47	1.34
82	bO	201	PEB	C2D-C3D	9.89	1.47	1.34
82	GQ	201	PEB	C2D-C3D	9.89	1.47	1.34
82	L7	201	PEB	C2D-C3D	9.89	1.47	1.34
82	MF	202	PEB	C2D-C3D	9.89	1.47	1.34
82	w8	201	PEB	C2D-C3D	9.88	1.47	1.34
82	N9	202	PEB	C2D-C3D	9.88	1.47	1.34
82	y8	203	PEB	C2D-C3D	9.88	1.47	1.34
82	DA	203	PEB	C2D-C3D	9.88	1.47	1.34
82	I7	202	PEB	C2D-C3D	9.88	1.47	1.34
82	DQ	203	PEB	C4C-C3C	9.88	1.52	1.37
82	wC	202	PEB	C2D-C3D	9.87	1.47	1.34
82	KA	201	PEB	C2D-C3D	9.87	1.47	1.34
82	YQ	201	PEB	C2D-C3D	9.87	1.47	1.34
82	IA	202	PEB	C2D-C3D	9.87	1.47	1.34
82	cH	201	PEB	C2D-C3D	9.87	1.47	1.34
82	TP	202	PEB	C2D-C3D	9.87	1.47	1.34
82	Y7	301	PEB	C2D-C3D	9.87	1.47	1.34
82	mF	202	PEB	C2D-C3D	9.87	1.47	1.34
82	QQ	201	PEB	C2D-C3D	9.86	1.47	1.34
82	eH	203	PEB	C2D-C3D	9.86	1.47	1.34
82	tK	202	PEB	C2D-C3D	9.86	1.47	1.34
82	kK	202	PEB	C2D-C3D	9.86	1.47	1.34
82	GA	202	PEB	C2D-C3D	9.86	1.47	1.34
82	I9	202	PEB	C2D-C3D	9.85	1.47	1.34
82	gK	202	PEB	C2D-C3D	9.85	1.47	1.34
82	c1	202	PEB	C2D-C3D	9.85	1.47	1.34
82	qC	202	PEB	C2D-C3D	9.85	1.47	1.34
82	qF	202	PEB	C2D-C3D	9.85	1.47	1.34
82	gH	202	PEB	C2D-C3D	9.85	1.47	1.34
82	r8	201	PEB	C2D-C3D	9.85	1.47	1.34
82	X9	202	PEB	C2D-C3D	9.85	1.47	1.34
82	qF	203	PEB	C2D-C3D	9.85	1.47	1.34
82	oK	202	PEB	C2D-C3D	9.85	1.47	1.34
82	sK	203	PEB	C2D-C3D	9.85	1.47	1.34
82	U9	203	PEB	C2D-C3D	9.84	1.47	1.34
82	MB	202	PEB	C2D-C3D	9.84	1.47	1.34
82	oK	201	PEB	C2D-C3D	9.84	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	W1	202	PEB	C2D-C3D	9.84	1.47	1.34
82	XK	203	PEB	C4C-C3C	9.84	1.52	1.37
82	H7	201	PEB	C2D-C3D	9.84	1.47	1.34
82	QD	201	PEB	C2D-C3D	9.84	1.47	1.34
82	mE	201	PEB	C2D-C3D	9.84	1.47	1.34
82	BK	202	PEB	C4C-C3C	9.84	1.52	1.37
82	NO	1002	PEB	C2D-C3D	9.84	1.47	1.34
82	WH	202	PEB	C2D-C3D	9.83	1.47	1.34
82	pF	201	PEB	C2D-C3D	9.83	1.47	1.34
82	sF	202	PEB	C2D-C3D	9.83	1.47	1.34
82	lF	201	PEB	C2D-C3D	9.83	1.47	1.34
82	J7	203	PEB	C2D-C3D	9.83	1.47	1.34
82	q8	203	PEB	C2D-C3D	9.83	1.47	1.34
82	fJ	202	PEB	C2D-C3D	9.83	1.47	1.34
82	T9	202	PEB	C2D-C3D	9.83	1.47	1.34
82	A1	302	PEB	C2D-C3D	9.83	1.47	1.34
82	d1	203	PEB	C2D-C3D	9.83	1.47	1.34
82	E9	202	PEB	C2D-C3D	9.83	1.47	1.34
82	MF	201	PEB	C2D-C3D	9.83	1.47	1.34
82	hG	202	PEB	C2D-C3D	9.83	1.47	1.34
82	b4	202	PEB	C2D-C3D	9.83	1.47	1.34
82	D7	203	PEB	C2D-C3D	9.83	1.47	1.34
82	GD	201	PEB	C2D-C3D	9.83	1.47	1.34
82	QP	202	PEB	C2D-C3D	9.83	1.47	1.34
82	kH	202	PEB	C2D-C3D	9.82	1.47	1.34
82	jH	203	PEB	C2D-C3D	9.82	1.47	1.34
82	fO	201	PEB	C2D-C3D	9.82	1.47	1.34
82	FM	201	PEB	C4C-C3C	9.82	1.52	1.37
82	iO	201	PEB	C2D-C3D	9.82	1.47	1.34
82	P9	202	PEB	C2D-C3D	9.82	1.47	1.34
82	eH	201	PEB	C2D-C3D	9.82	1.47	1.34
82	SQ	201	PEB	C2D-C3D	9.82	1.47	1.34
82	a1	202	PEB	C2D-C3D	9.82	1.47	1.34
82	Z1	202	PEB	C2D-C3D	9.82	1.47	1.34
82	A9	202	PEB	C2D-C3D	9.81	1.47	1.34
82	VH	202	PEB	C2D-C3D	9.81	1.47	1.34
82	V9	202	PEB	C2D-C3D	9.81	1.47	1.34
82	AH	302	PEB	C2D-C3D	9.81	1.47	1.34
82	G9	202	PEB	C2D-C3D	9.81	1.47	1.34
82	mF	201	PEB	C2D-C3D	9.80	1.47	1.34
82	JA	203	PEB	C2D-C3D	9.80	1.47	1.34
82	Y1	201	PEB	C2D-C3D	9.80	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FA	203	PEB	C2D-C3D	9.80	1.47	1.34
82	k1	202	PEB	C2D-C3D	9.80	1.47	1.34
82	SD	201	PEB	C2D-C3D	9.80	1.47	1.34
82	tF	202	PEB	C2D-C3D	9.80	1.47	1.34
82	oF	202	PEB	C2D-C3D	9.80	1.47	1.34
82	HM	201	PEB	C4C-C3C	9.80	1.51	1.37
82	W7	202	PEB	C2D-C3D	9.80	1.47	1.34
82	L7	203	PEB	C2D-C3D	9.79	1.47	1.34
82	rC	201	PEB	C2D-C3D	9.79	1.47	1.34
82	jH	201	PEB	C2D-C3D	9.79	1.47	1.34
82	VA	203	PEB	C2D-C3D	9.79	1.47	1.34
82	XQ	203	PEB	C2D-C3D	9.79	1.47	1.34
82	N4	1002	PEB	C2D-C3D	9.79	1.47	1.34
82	H9	203	PEB	C2D-C3D	9.79	1.47	1.34
82	Q9	203	PEB	C2D-C3D	9.79	1.47	1.34
82	iO	203	PEB	C2D-C3D	9.79	1.47	1.34
82	NH	1002	PEB	C2D-C3D	9.79	1.47	1.34
82	G7	202	PEB	C2D-C3D	9.79	1.47	1.34
82	K9	202	PEB	C2D-C3D	9.79	1.47	1.34
82	R9	202	PEB	C2D-C3D	9.79	1.47	1.34
82	tC	201	PEB	C2D-C3D	9.79	1.47	1.34
82	YO	203	PEB	C2D-C3D	9.79	1.47	1.34
82	g4	203	PEB	C2D-C3D	9.78	1.47	1.34
82	H7	202	PEB	C2D-C3D	9.78	1.47	1.34
82	iH	202	PEB	C2D-C3D	9.78	1.47	1.34
82	jJ	201	PEB	C2D-C3D	9.78	1.47	1.34
82	q8	202	PEB	C2D-C3D	9.78	1.47	1.34
82	lK	201	PEB	C2D-C3D	9.78	1.47	1.34
82	YQ	202	PEB	C2D-C3D	9.78	1.47	1.34
82	eK	203	PEB	C2D-C3D	9.77	1.47	1.34
82	iE	201	PEB	C2D-C3D	9.77	1.47	1.34
82	U9	201	PEB	C2D-C3D	9.77	1.47	1.34
82	rF	201	PEB	C2D-C3D	9.77	1.47	1.34
82	gG	202	PEB	C2D-C3D	9.77	1.47	1.34
82	J9	202	PEB	C2D-C3D	9.77	1.47	1.34
82	w8	202	PEB	C2D-C3D	9.77	1.47	1.34
82	sF	203	PEB	C2D-C3D	9.77	1.47	1.34
82	gB	203	PEB	C4C-C3C	9.77	1.51	1.37
82	V7	203	PEB	C2D-C3D	9.77	1.47	1.34
82	aJ	203	PEB	C2D-C3D	9.77	1.47	1.34
82	S9	201	PEB	C4C-C3C	9.76	1.51	1.37
82	IP	202	PEB	C2D-C3D	9.76	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mM	202	PEB	C2D-C3D	9.76	1.47	1.34
82	nK	202	PEB	C4C-C3C	9.76	1.51	1.37
82	eF	201	PEB	C2D-C3D	9.76	1.47	1.34
82	LO	1002	PEB	C2D-C3D	9.76	1.47	1.34
82	D9	203	PEB	C2D-C3D	9.76	1.47	1.34
82	hE	202	PEB	C2D-C3D	9.76	1.47	1.34
82	iE	202	PEB	C2D-C3D	9.76	1.47	1.34
82	bF	201	PEB	C2D-C3D	9.76	1.47	1.34
82	lG	203	PEB	C2D-C3D	9.76	1.47	1.34
82	cH	202	PEB	C2D-C3D	9.76	1.47	1.34
82	BF	202	PEB	C4C-C3C	9.76	1.51	1.37
82	i1	202	PEB	C2D-C3D	9.76	1.47	1.34
82	iK	203	PEB	C2D-C3D	9.76	1.47	1.34
82	PH	202	PEB	C2D-C3D	9.75	1.47	1.34
82	t8	201	PEB	C2D-C3D	9.75	1.47	1.34
82	fM	201	PEB	C2D-C3D	9.75	1.47	1.34
82	gM	202	PEB	C2D-C3D	9.75	1.47	1.34
82	kF	202	PEB	C2D-C3D	9.75	1.47	1.34
82	YH	201	PEB	C2D-C3D	9.75	1.47	1.34
82	pF	202	PEB	C2D-C3D	9.75	1.47	1.34
82	HA	201	PEB	C2D-C3D	9.75	1.47	1.34
82	OM	202	PEB	C2D-C3D	9.75	1.47	1.34
82	AH	301	PEB	C2D-C3D	9.75	1.47	1.34
82	B9	201	PEB	C2D-C3D	9.75	1.47	1.34
82	F7	203	PEB	C2D-C3D	9.75	1.47	1.34
82	ND	204	PEB	C2D-C3D	9.75	1.47	1.34
82	eF	203	PEB	C2D-C3D	9.75	1.47	1.34
82	g1	202	PEB	C2D-C3D	9.74	1.47	1.34
82	uC	203	PEB	C2D-C3D	9.74	1.47	1.34
82	iF	202	PEB	C2D-C3D	9.74	1.47	1.34
82	YH	202	PEB	C2D-C3D	9.74	1.47	1.34
82	L4	1002	PEB	C2D-C3D	9.74	1.47	1.34
82	gF	202	PEB	C2D-C3D	9.74	1.47	1.34
82	lK	203	PEB	C2D-C3D	9.74	1.47	1.34
82	QE	203	PEB	C2D-C3D	9.74	1.47	1.34
82	u8	203	PEB	C2D-C3D	9.74	1.47	1.34
82	vC	201	PEB	C2D-C3D	9.74	1.47	1.34
82	Z9	303	PEB	C2D-C3D	9.74	1.47	1.34
82	AD	301	PEB	C2D-C3D	9.74	1.47	1.34
82	AQ	304	PEB	C2D-C3D	9.74	1.47	1.34
82	c4	203	PEB	C2D-C3D	9.73	1.47	1.34
82	NQ	204	PEB	C2D-C3D	9.73	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	f1	203	PEB	C2D-C3D	9.73	1.47	1.34
82	c4	202	PEB	C2D-C3D	9.73	1.47	1.34
82	cO	201	PEB	C2D-C3D	9.73	1.47	1.34
82	M9	304	PEB	C2D-C3D	9.73	1.47	1.34
82	HA	202	PEB	C2D-C3D	9.73	1.47	1.34
82	e1	201	PEB	C2D-C3D	9.73	1.47	1.34
82	Y4	203	PEB	C2D-C3D	9.73	1.47	1.34
82	pK	202	PEB	C2D-C3D	9.73	1.47	1.34
82	mG	203	PEB	C2D-C3D	9.72	1.47	1.34
82	D9	201	PEB	C2D-C3D	9.72	1.47	1.34
82	lE	203	PEB	C2D-C3D	9.72	1.47	1.34
82	W9	203	PEB	C2D-C3D	9.72	1.47	1.34
82	c4	201	PEB	C2D-C3D	9.72	1.47	1.34
82	g4	201	PEB	C2D-C3D	9.72	1.47	1.34
82	F9	202	PEB	C2D-C3D	9.72	1.47	1.34
82	lF	203	PEB	C2D-C3D	9.72	1.47	1.34
82	V1	203	PEB	C2D-C3D	9.72	1.47	1.34
82	i4	203	PEB	C2D-C3D	9.72	1.47	1.34
82	cG	202	PEB	C2D-C3D	9.72	1.47	1.34
82	v8	201	PEB	C2D-C3D	9.72	1.47	1.34
82	U9	202	PEB	C2D-C3D	9.72	1.47	1.34
82	ND	203	PEB	C2D-C3D	9.71	1.47	1.34
82	mG	201	PEB	C2D-C3D	9.71	1.47	1.34
82	XD	203	PEB	C2D-C3D	9.71	1.47	1.34
82	QG	201	PEB	C2D-C3D	9.71	1.47	1.34
82	MQ	201	PEB	C2D-C3D	9.71	1.47	1.34
82	aK	201	PEB	C2D-C3D	9.71	1.47	1.34
82	SO	201	PEB	C2D-C3D	9.71	1.47	1.34
82	mK	201	PEB	C2D-C3D	9.71	1.47	1.34
82	ZK	202	PEB	C2D-C3D	9.71	1.47	1.34
82	VG	202	PEB	C2D-C3D	9.70	1.47	1.34
82	PQ	201	PEB	C2D-C3D	9.70	1.47	1.34
82	B9	203	PEB	C2D-C3D	9.70	1.47	1.34
82	eE	203	PEB	C2D-C3D	9.70	1.47	1.34
82	BA	202	PEB	C2D-C3D	9.70	1.47	1.34
82	U1	202	PEB	C2D-C3D	9.70	1.47	1.34
82	gO	201	PEB	C2D-C3D	9.70	1.47	1.34
82	TM	202	PEB	C2D-C3D	9.69	1.47	1.34
82	fB	301	PEB	C2D-C3D	9.69	1.47	1.34
82	UI	202	PEB	C2D-C3D	9.69	1.47	1.34
82	J9	203	PEB	C2D-C3D	9.69	1.47	1.34
82	eH	202	PEB	C2D-C3D	9.69	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	F4	1002	PEB	C2D-C3D	9.69	1.47	1.34
82	pK	201	PEB	C2D-C3D	9.69	1.47	1.34
82	LA	203	PEB	C2D-C3D	9.69	1.47	1.34
82	dJ	201	PEB	C2D-C3D	9.69	1.47	1.34
82	j1	201	PEB	C2D-C3D	9.68	1.47	1.34
82	kH	201	PEB	C2D-C3D	9.68	1.47	1.34
82	dE	203	PEB	C2D-C3D	9.68	1.47	1.34
82	P1	202	PEB	C2D-C3D	9.68	1.47	1.34
82	Y1	202	PEB	C2D-C3D	9.68	1.47	1.34
82	gK	201	PEB	C2D-C3D	9.68	1.47	1.34
82	bK	201	PEB	C2D-C3D	9.68	1.47	1.34
82	aF	201	PEB	C2D-C3D	9.68	1.47	1.34
82	cK	202	PEB	C2D-C3D	9.68	1.47	1.34
82	AD	304	PEB	C2D-C3D	9.68	1.47	1.34
82	QB	201	PEB	C4C-C3C	9.68	1.51	1.37
82	cE	202	PEB	C2D-C3D	9.67	1.47	1.34
82	iG	202	PEB	C2D-C3D	9.67	1.47	1.34
82	cO	202	PEB	C2D-C3D	9.67	1.47	1.34
82	bO	202	PEB	C2D-C3D	9.67	1.47	1.34
82	D9	202	PEB	C2D-C3D	9.67	1.47	1.34
82	d1	201	PEB	C2D-C3D	9.67	1.47	1.34
82	A4	304	PEB	C2D-C3D	9.67	1.47	1.34
82	kO	201	PEB	C2D-C3D	9.67	1.47	1.34
82	lF	202	PEB	C2D-C3D	9.67	1.47	1.34
82	nF	202	PEB	C4C-C3C	9.67	1.51	1.37
82	WH	203	PEB	C2D-C3D	9.67	1.47	1.34
82	OP	203	PEB	C2D-C3D	9.67	1.47	1.34
82	mE	203	PEB	C2D-C3D	9.67	1.47	1.34
82	mJ	202	PEB	C2D-C3D	9.67	1.47	1.34
82	A1	301	PEB	C2D-C3D	9.66	1.47	1.34
82	qC	203	PEB	C2D-C3D	9.66	1.47	1.34
82	bH	201	PEB	C2D-C3D	9.66	1.47	1.34
82	MK	201	PEB	C2D-C3D	9.66	1.47	1.34
82	KF	203	PEB	C2D-C3D	9.66	1.47	1.34
82	u8	201	PEB	C2D-C3D	9.66	1.47	1.34
82	O9	203	PEB	C2D-C3D	9.66	1.47	1.34
82	ZF	202	PEB	C2D-C3D	9.66	1.47	1.34
82	dH	201	PEB	C2D-C3D	9.66	1.47	1.34
82	YF	202	PEB	C2D-C3D	9.66	1.47	1.34
82	gE	202	PEB	C2D-C3D	9.66	1.47	1.34
82	kM	201	PEB	C2D-C3D	9.66	1.47	1.34
82	AH	305	PEB	C2D-C3D	9.66	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MD	201	PEB	C2D-C3D	9.66	1.47	1.34
82	HP	202	PEB	C2D-C3D	9.66	1.47	1.34
82	rK	202	PEB	C2D-C3D	9.65	1.46	1.34
82	aM	201	PEB	C2D-C3D	9.65	1.46	1.34
82	LG	1002	PEB	C4C-C3C	9.65	1.51	1.37
82	aO	203	PEB	C2D-C3D	9.65	1.46	1.34
82	Q9	201	PEB	C2D-C3D	9.65	1.46	1.34
82	F9	201	PEB	C2D-C3D	9.65	1.46	1.34
82	VE	202	PEB	C2D-C3D	9.65	1.46	1.34
82	uC	201	PEB	C2D-C3D	9.65	1.46	1.34
82	QD	202	PEB	C2D-C3D	9.65	1.46	1.34
82	NQ	203	PEB	C2D-C3D	9.65	1.46	1.34
82	NP	202	PEB	C2D-C3D	9.65	1.46	1.34
82	FO	1002	PEB	C2D-C3D	9.65	1.46	1.34
82	gF	201	PEB	C2D-C3D	9.65	1.46	1.34
82	gO	203	PEB	C2D-C3D	9.65	1.46	1.34
82	xC	201	PEB	C2D-C3D	9.65	1.46	1.34
82	J9	201	PEB	C2D-C3D	9.64	1.46	1.34
82	H9	202	PEB	C2D-C3D	9.64	1.46	1.34
82	U9	204	PEB	C2D-C3D	9.64	1.46	1.34
82	QB	204	PEB	C4C-C3C	9.64	1.51	1.37
82	HQ	203	PEB	C2D-C3D	9.64	1.46	1.34
82	QK	202	PEB	C2D-C3D	9.64	1.46	1.34
82	kM	202	PEB	C2D-C3D	9.64	1.46	1.34
82	QF	202	PEB	C2D-C3D	9.64	1.46	1.34
82	cK	201	PEB	C2D-C3D	9.64	1.46	1.34
82	B7	203	PEB	C2D-C3D	9.64	1.46	1.34
82	dK	201	PEB	C2D-C3D	9.64	1.46	1.34
82	mO	201	PEB	C2D-C3D	9.64	1.46	1.34
82	ZH	202	PEB	C2D-C3D	9.64	1.46	1.34
82	eG	203	PEB	C2D-C3D	9.64	1.46	1.34
82	i4	201	PEB	C2D-C3D	9.63	1.46	1.34
82	EK	202	PEB	C2D-C3D	9.63	1.46	1.34
82	KK	203	PEB	C2D-C3D	9.63	1.46	1.34
82	RG	201	PEB	C2D-C3D	9.63	1.46	1.34
82	UJ	203	PEB	C2D-C3D	9.63	1.46	1.34
82	dG	201	PEB	C2D-C3D	9.63	1.46	1.34
82	PD	201	PEB	C2D-C3D	9.63	1.46	1.34
82	e4	203	PEB	C2D-C3D	9.63	1.46	1.34
82	cM	202	PEB	C2D-C3D	9.63	1.46	1.34
82	k1	201	PEB	C2D-C3D	9.63	1.46	1.34
82	YK	203	PEB	C2D-C3D	9.63	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A1	305	PEB	C2D-C3D	9.62	1.46	1.34
82	s8	201	PEB	C2D-C3D	9.62	1.46	1.34
82	F9	203	PEB	C2D-C3D	9.62	1.46	1.34
82	PD	202	PEB	C2D-C3D	9.62	1.46	1.34
82	AE	304	PEB	C2D-C3D	9.62	1.46	1.34
82	fH	203	PEB	C2D-C3D	9.62	1.46	1.34
82	ZK	201	PEB	C2D-C3D	9.62	1.46	1.34
82	S4	201	PEB	C2D-C3D	9.62	1.46	1.34
82	TD	203	PEB	C2D-C3D	9.62	1.46	1.34
82	EF	202	PEB	C2D-C3D	9.62	1.46	1.34
82	eE	201	PEB	C2D-C3D	9.62	1.46	1.34
82	GM	201	PEB	C2D-C3D	9.62	1.46	1.34
82	RD	202	PEB	C2D-C3D	9.62	1.46	1.34
82	hB	301	PEB	C2D-C3D	9.62	1.46	1.34
82	iM	201	PEB	C4C-C3C	9.61	1.51	1.37
82	S9	203	PEB	C2D-C3D	9.61	1.46	1.34
82	iG	201	PEB	C2D-C3D	9.61	1.46	1.34
82	jG	202	PEB	C2D-C3D	9.61	1.46	1.34
82	LQ	203	PEB	C2D-C3D	9.61	1.46	1.34
82	QQ	202	PEB	C2D-C3D	9.61	1.46	1.34
82	dF	202	PEB	C2D-C3D	9.61	1.46	1.34
82	aM	204	PEB	C2D-C3D	9.61	1.46	1.34
82	e1	202	PEB	C2D-C3D	9.61	1.46	1.34
82	UD	201	PEB	C2D-C3D	9.60	1.46	1.34
82	YF	203	PEB	C2D-C3D	9.60	1.46	1.34
82	dF	201	PEB	C2D-C3D	9.60	1.46	1.34
82	PQ	202	PEB	C2D-C3D	9.60	1.46	1.34
82	F9	201	PEB	C4C-C3C	9.60	1.51	1.37
82	AK	202	PEB	C2D-C3D	9.60	1.46	1.34
82	B7	202	PEB	C2D-C3D	9.60	1.46	1.34
82	x8	201	PEB	C2D-C3D	9.60	1.46	1.34
82	fE	203	PEB	C2D-C3D	9.60	1.46	1.34
82	SP	203	PEB	C4C-C3C	9.60	1.51	1.37
82	vC	202	PEB	C2D-C3D	9.59	1.46	1.34
82	hG	203	PEB	C2D-C3D	9.59	1.46	1.34
82	RH	201	PEB	C2D-C3D	9.59	1.46	1.34
82	hE	203	PEB	C2D-C3D	9.59	1.46	1.34
82	LE	1002	PEB	C4C-C3C	9.59	1.51	1.37
82	mO	203	PEB	C2D-C3D	9.59	1.46	1.34
82	cO	203	PEB	C2D-C3D	9.59	1.46	1.34
82	L9	201	PEB	C2D-C3D	9.59	1.46	1.34
82	LD	203	PEB	C2D-C3D	9.59	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UE	203	PEB	C2D-C3D	9.59	1.46	1.34
82	HA	203	PEB	C2D-C3D	9.59	1.46	1.34
82	v8	202	PEB	C2D-C3D	9.59	1.46	1.34
82	JM	202	PEB	C2D-C3D	9.59	1.46	1.34
82	fE	201	PEB	C2D-C3D	9.59	1.46	1.34
82	HI	203	PEB	C2D-C3D	9.59	1.46	1.34
82	UH	202	PEB	C2D-C3D	9.58	1.46	1.34
82	AG	304	PEB	C2D-C3D	9.58	1.46	1.34
82	Y9	201	PEB	C2D-C3D	9.58	1.46	1.34
82	dB	202	PEB	C4C-C3C	9.58	1.51	1.37
82	dG	204	PEB	C2D-C3D	9.58	1.46	1.34
82	UQ	201	PEB	C2D-C3D	9.58	1.46	1.34
82	dK	202	PEB	C2D-C3D	9.58	1.46	1.34
82	AO	304	PEB	C2D-C3D	9.58	1.46	1.34
82	m4	201	PEB	C2D-C3D	9.58	1.46	1.34
82	OK	203	PEB	C2D-C3D	9.58	1.46	1.34
82	wF	301	PEB	C2D-C3D	9.58	1.46	1.34
82	iK	202	PEB	C2D-C3D	9.58	1.46	1.34
82	AF	202	PEB	C2D-C3D	9.58	1.46	1.34
82	K7	202	PEB	C2D-C3D	9.57	1.46	1.34
82	xF	303	PEB	C2D-C3D	9.57	1.46	1.34
82	jG	201	PEB	C2D-C3D	9.57	1.46	1.34
82	mO	202	PEB	C2D-C3D	9.57	1.46	1.34
82	cF	201	PEB	C2D-C3D	9.57	1.46	1.34
82	QE	201	PEB	C2D-C3D	9.57	1.46	1.34
82	sC	201	PEB	C2D-C3D	9.57	1.46	1.34
82	eG	201	PEB	C2D-C3D	9.57	1.46	1.34
82	a1	201	PEB	C2D-C3D	9.57	1.46	1.34
82	dE	201	PEB	C2D-C3D	9.57	1.46	1.34
82	xK	303	PEB	C2D-C3D	9.57	1.46	1.34
82	LM	202	PEB	C2D-C3D	9.57	1.46	1.34
82	RE	201	PEB	C2D-C3D	9.57	1.46	1.34
82	TQ	203	PEB	C2D-C3D	9.57	1.46	1.34
82	O9	201	PEB	C2D-C3D	9.57	1.46	1.34
82	gJ	201	PEB	C2D-C3D	9.57	1.46	1.34
82	JA	201	PEB	C2D-C3D	9.56	1.46	1.34
82	YK	202	PEB	C2D-C3D	9.56	1.46	1.34
82	WF	202	PEB	C2D-C3D	9.56	1.46	1.34
82	R1	201	PEB	C2D-C3D	9.56	1.46	1.34
82	lK	202	PEB	C2D-C3D	9.56	1.46	1.34
82	aH	201	PEB	C2D-C3D	9.56	1.46	1.34
82	XD	201	PEB	C2D-C3D	9.56	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kJ	201	PEB	C2D-C3D	9.56	1.46	1.34
82	kM	201	PEB	C4C-C3C	9.56	1.51	1.37
82	UH	201	PEB	C2D-C3D	9.56	1.46	1.34
82	U1	201	PEB	C2D-C3D	9.56	1.46	1.34
82	WI	203	PEB	C2D-C3D	9.55	1.46	1.34
82	Q4	201	PEB	C2D-C3D	9.55	1.46	1.34
82	a4	203	PEB	C2D-C3D	9.55	1.46	1.34
82	RF	202	PEB	C4C-C3C	9.55	1.51	1.37
82	gG	201	PEB	C2D-C3D	9.55	1.46	1.34
82	p8	202	PEB	C2D-C3D	9.55	1.46	1.34
82	MD	202	PEB	C2D-C3D	9.55	1.46	1.34
82	T4	203	PEB	C2D-C3D	9.55	1.46	1.34
82	kE	202	PEB	C2D-C3D	9.55	1.46	1.34
82	RQ	201	PEB	C2D-C3D	9.55	1.46	1.34
82	e4	202	PEB	C2D-C3D	9.55	1.46	1.34
82	ZF	201	PEB	C2D-C3D	9.54	1.46	1.34
82	SD	202	PEB	C2D-C3D	9.54	1.46	1.34
82	CF	201	PEB	C2D-C3D	9.54	1.46	1.34
82	iM	201	PEB	C2D-C3D	9.54	1.46	1.34
82	YK	201	PEB	C2D-C3D	9.54	1.46	1.34
82	Q5	202	PEB	C2D-C3D	9.54	1.46	1.34
82	JI	202	PEB	C2D-C3D	9.54	1.46	1.34
82	CK	201	PEB	C2D-C3D	9.54	1.46	1.34
82	aM	202	PEB	C2D-C3D	9.54	1.46	1.34
82	k4	201	PEB	C2D-C3D	9.54	1.46	1.34
82	jM	202	PEB	C2D-C3D	9.54	1.46	1.34
82	rF	202	PEB	C2D-C3D	9.54	1.46	1.34
82	UG	203	PEB	C2D-C3D	9.54	1.46	1.34
82	BP	202	PEB	C2D-C3D	9.53	1.46	1.34
82	kJ	202	PEB	C2D-C3D	9.53	1.46	1.34
82	Q1	203	PEB	C2D-C3D	9.53	1.46	1.34
82	H7	203	PEB	C2D-C3D	9.53	1.46	1.34
82	W1	203	PEB	C2D-C3D	9.53	1.46	1.34
82	RJ	202	PEB	C2D-C3D	9.53	1.46	1.34
82	l1	202	PEB	C2D-C3D	9.53	1.46	1.34
82	J7	201	PEB	C2D-C3D	9.52	1.46	1.34
82	F7	201	PEB	C2D-C3D	9.52	1.46	1.34
82	WF	203	PEB	C2D-C3D	9.52	1.46	1.34
82	CK	203	PEB	C2D-C3D	9.52	1.46	1.34
82	FP	202	PEB	C2D-C3D	9.52	1.46	1.34
82	jE	202	PEB	C2D-C3D	9.52	1.46	1.34
82	cJ	202	PEB	C2D-C3D	9.52	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dG	203	PEB	C2D-C3D	9.52	1.46	1.34
82	iM	202	PEB	C2D-C3D	9.52	1.46	1.34
82	wK	301	PEB	C2D-C3D	9.52	1.46	1.34
82	AQ	301	PEB	C2D-C3D	9.51	1.46	1.34
82	ZH	201	PEB	C4C-C3C	9.51	1.51	1.37
82	jE	201	PEB	C2D-C3D	9.51	1.46	1.34
82	O9	202	PEB	C2D-C3D	9.51	1.46	1.34
82	S9	201	PEB	C2D-C3D	9.51	1.46	1.34
82	UK	202	PEB	C2D-C3D	9.51	1.46	1.34
82	h4	201	PEB	C2D-C3D	9.51	1.46	1.34
82	ZM	202	PEB	C2D-C3D	9.51	1.46	1.34
82	DQ	203	PEB	C2D-C3D	9.51	1.46	1.34
82	pC	202	PEB	C2D-C3D	9.51	1.46	1.34
82	JP	202	PEB	C2D-C3D	9.51	1.46	1.34
82	mM	201	PEB	C2D-C3D	9.51	1.46	1.34
82	Q5	202	PEB	C4C-C3C	9.51	1.51	1.37
82	RQ	202	PEB	C2D-C3D	9.51	1.46	1.34
82	x8	202	PEB	C2D-C3D	9.51	1.46	1.34
82	JH	1002	PEB	C2D-C3D	9.51	1.46	1.34
82	m4	202	PEB	C2D-C3D	9.51	1.46	1.34
82	fE	202	PEB	C2D-C3D	9.51	1.46	1.34
82	VM	202	PEB	C2D-C3D	9.50	1.46	1.34
82	eE	202	PEB	C2D-C3D	9.50	1.46	1.34
82	eG	202	PEB	C2D-C3D	9.50	1.46	1.34
82	fK	202	PEB	C2D-C3D	9.50	1.46	1.34
82	RM	202	PEB	C2D-C3D	9.50	1.46	1.34
82	IM	201	PEB	C2D-C3D	9.50	1.46	1.34
82	AO	301	PEB	C2D-C3D	9.50	1.46	1.34
82	SP	203	PEB	C2D-C3D	9.50	1.46	1.34
82	iF	203	PEB	C2D-C3D	9.50	1.46	1.34
82	eO	202	PEB	C2D-C3D	9.50	1.46	1.34
82	TM	201	PEB	C4C-C3C	9.50	1.51	1.37
82	UF	202	PEB	C2D-C3D	9.50	1.46	1.34
82	XM	202	PEB	C2D-C3D	9.50	1.46	1.34
82	FJ	201	PEB	C4C-C3C	9.49	1.51	1.37
82	KA	202	PEB	C2D-C3D	9.49	1.46	1.34
82	NQ	202	PEB	C2D-C3D	9.49	1.46	1.34
82	d4	202	PEB	C2D-C3D	9.49	1.46	1.34
82	VD	203	PEB	C2D-C3D	9.49	1.46	1.34
82	QM	203	PEB	C2D-C3D	9.49	1.46	1.34
82	Y5	202	PEB	C2D-C3D	9.49	1.46	1.34
82	bF	202	PEB	C2D-C3D	9.49	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hM	202	PEB	C2D-C3D	9.49	1.46	1.34
82	m4	203	PEB	C2D-C3D	9.49	1.46	1.34
82	dM	203	PEB	C2D-C3D	9.49	1.46	1.34
82	YF	201	PEB	C2D-C3D	9.49	1.46	1.34
82	cJ	201	PEB	C4C-C3C	9.49	1.51	1.37
82	P4	202	PEB	C2D-C3D	9.49	1.46	1.34
82	SQ	202	PEB	C2D-C3D	9.49	1.46	1.34
82	E7	202	PEB	C2D-C3D	9.49	1.46	1.34
82	WH	201	PEB	C2D-C3D	9.49	1.46	1.34
82	A4	301	PEB	C2D-C3D	9.49	1.46	1.34
82	QF	201	PEB	C2D-C3D	9.48	1.46	1.34
82	JJ	202	PEB	C2D-C3D	9.48	1.46	1.34
82	P4	201	PEB	C2D-C3D	9.48	1.46	1.34
82	PO	202	PEB	C2D-C3D	9.48	1.46	1.34
82	BA	201	PEB	C2D-C3D	9.48	1.46	1.34
82	fJ	201	PEB	C2D-C3D	9.48	1.46	1.34
82	fG	203	PEB	C2D-C3D	9.48	1.46	1.34
82	H5	203	PEB	C2D-C3D	9.48	1.46	1.34
82	RD	201	PEB	C2D-C3D	9.48	1.46	1.34
82	OM	203	PEB	C2D-C3D	9.48	1.46	1.34
82	b1	201	PEB	C2D-C3D	9.48	1.46	1.34
82	DD	203	PEB	C2D-C3D	9.47	1.46	1.34
82	VJ	201	PEB	C2D-C3D	9.47	1.46	1.34
82	WK	203	PEB	C2D-C3D	9.47	1.46	1.34
82	cG	201	PEB	C2D-C3D	9.47	1.46	1.34
82	A4	305	PEB	C2D-C3D	9.47	1.46	1.34
82	gE	201	PEB	C2D-C3D	9.47	1.46	1.34
82	Z9	301	PEB	C2D-C3D	9.47	1.46	1.34
82	18	202	PEB	C2D-C3D	9.47	1.46	1.34
82	lK	202	PEB	C4C-C3C	9.47	1.51	1.37
82	iJ	202	PEB	C2D-C3D	9.47	1.46	1.34
82	kO	202	PEB	C2D-C3D	9.47	1.46	1.34
82	kG	202	PEB	C2D-C3D	9.47	1.46	1.34
82	nK	202	PEB	C2D-C3D	9.47	1.46	1.34
82	dO	202	PEB	C2D-C3D	9.47	1.46	1.34
82	PM	202	PEB	C2D-C3D	9.46	1.46	1.34
82	bG	201	PEB	C2D-C3D	9.46	1.46	1.34
82	E9	201	PEB	C2D-C3D	9.46	1.46	1.34
82	TO	203	PEB	C2D-C3D	9.46	1.46	1.34
82	HJ	202	PEB	C2D-C3D	9.46	1.46	1.34
82	XQ	202	PEB	C2D-C3D	9.46	1.46	1.34
82	XQ	201	PEB	C2D-C3D	9.46	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	R9	201	PEB	C2D-C3D	9.46	1.46	1.34
82	OA	202	PEB	C2D-C3D	9.46	1.46	1.34
82	j4	203	PEB	C2D-C3D	9.46	1.46	1.34
82	vK	202	PEB	C2D-C3D	9.46	1.46	1.34
82	aM	203	PEB	C2D-C3D	9.46	1.46	1.34
82	Z1	201	PEB	C4C-C3C	9.45	1.51	1.37
82	CB	202	PEB	C2D-C3D	9.45	1.46	1.34
82	OF	203	PEB	C2D-C3D	9.45	1.46	1.34
82	QI	201	PEB	C2D-C3D	9.45	1.46	1.34
82	hF	201	PEB	C2D-C3D	9.45	1.46	1.34
82	M5	305	PEB	C2D-C3D	9.45	1.46	1.34
82	nF	202	PEB	C2D-C3D	9.45	1.46	1.34
82	lH	201	PEB	C2D-C3D	9.45	1.46	1.34
82	qF	201	PEB	C2D-C3D	9.45	1.46	1.34
82	L9	203	PEB	C2D-C3D	9.45	1.46	1.34
82	vF	202	PEB	C2D-C3D	9.45	1.46	1.34
82	ND	202	PEB	C2D-C3D	9.45	1.46	1.34
82	J1	1002	PEB	C2D-C3D	9.45	1.46	1.34
82	fG	201	PEB	C2D-C3D	9.45	1.46	1.34
82	zC	202	PEB	C2D-C3D	9.44	1.46	1.34
82	xC	202	PEB	C2D-C3D	9.44	1.46	1.34
82	EM	202	PEB	C2D-C3D	9.44	1.46	1.34
82	ZB	203	PEB	C2D-C3D	9.44	1.46	1.34
82	DM	202	PEB	C2D-C3D	9.44	1.46	1.34
82	I9	201	PEB	C2D-C3D	9.44	1.46	1.34
82	gM	201	PEB	C2D-C3D	9.44	1.46	1.34
82	AO	305	PEB	C2D-C3D	9.44	1.46	1.34
82	U7	202	PEB	C2D-C3D	9.44	1.46	1.34
82	QB	203	PEB	C2D-C3D	9.44	1.46	1.34
82	DI	202	PEB	C2D-C3D	9.44	1.46	1.34
82	dE	204	PEB	C2D-C3D	9.44	1.46	1.34
82	FA	201	PEB	C2D-C3D	9.44	1.46	1.34
82	PE	201	PEB	C2D-C3D	9.44	1.46	1.34
82	CF	202	PEB	C2D-C3D	9.44	1.46	1.34
82	H9	201	PEB	C2D-C3D	9.44	1.46	1.34
82	DP	202	PEB	C2D-C3D	9.44	1.46	1.34
82	z8	202	PEB	C2D-C3D	9.44	1.46	1.34
82	C9	201	PEB	C2D-C3D	9.44	1.46	1.34
82	eO	203	PEB	C2D-C3D	9.44	1.46	1.34
82	wK	303	PEB	C4C-C3C	9.44	1.51	1.37
82	AE	301	PEB	C2D-C3D	9.44	1.46	1.34
82	VF	202	PEB	C2D-C3D	9.44	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	eM	202	PEB	C2D-C3D	9.44	1.46	1.34
82	ZB	202	PEB	C2D-C3D	9.43	1.46	1.34
82	kK	201	PEB	C2D-C3D	9.43	1.46	1.34
82	JQ	201	PEB	C2D-C3D	9.43	1.46	1.34
82	dM	202	PEB	C2D-C3D	9.43	1.46	1.34
82	CA	201	PEB	C2D-C3D	9.43	1.46	1.34
82	fG	202	PEB	C2D-C3D	9.43	1.46	1.34
82	BA	203	PEB	C2D-C3D	9.43	1.46	1.34
82	CF	203	PEB	C2D-C3D	9.43	1.46	1.34
82	h4	202	PEB	C2D-C3D	9.43	1.46	1.34
82	aE	201	PEB	C2D-C3D	9.43	1.46	1.34
82	fM	203	PEB	C2D-C3D	9.43	1.46	1.34
82	M9	302	PEB	C2D-C3D	9.43	1.46	1.34
82	UP	201	PEB	C2D-C3D	9.43	1.46	1.34
82	G9	201	PEB	C2D-C3D	9.43	1.46	1.34
82	kF	201	PEB	C2D-C3D	9.43	1.46	1.34
82	RK	202	PEB	C4C-C3C	9.43	1.51	1.37
82	CD	202	PEB	C2D-C3D	9.43	1.46	1.34
82	RH	202	PEB	C2D-C3D	9.43	1.46	1.34
82	CK	202	PEB	C2D-C3D	9.43	1.46	1.34
82	gB	202	PEB	C2D-C3D	9.43	1.46	1.34
82	FD	203	PEB	C2D-C3D	9.43	1.46	1.34
82	QJ	204	PEB	C2D-C3D	9.43	1.46	1.34
82	FP	201	PEB	C2D-C3D	9.42	1.46	1.34
82	1C	202	PEB	C2D-C3D	9.42	1.46	1.34
82	FQ	202	PEB	C2D-C3D	9.42	1.46	1.34
82	dM	201	PEB	C2D-C3D	9.42	1.46	1.34
82	L7	202	PEB	C2D-C3D	9.42	1.46	1.34
82	PP	202	PEB	C2D-C3D	9.42	1.46	1.34
82	lO	201	PEB	C2D-C3D	9.42	1.46	1.34
82	FD	202	PEB	C2D-C3D	9.42	1.46	1.34
82	SJ	202	PEB	C2D-C3D	9.42	1.46	1.34
82	HM	202	PEB	C2D-C3D	9.42	1.46	1.34
82	VQ	203	PEB	C2D-C3D	9.42	1.46	1.34
82	hO	202	PEB	C2D-C3D	9.42	1.46	1.34
82	RO	203	PEB	C2D-C3D	9.42	1.46	1.34
82	R4	203	PEB	C2D-C3D	9.42	1.46	1.34
82	EA	202	PEB	C2D-C3D	9.42	1.46	1.34
82	j4	201	PEB	C2D-C3D	9.42	1.46	1.34
82	D5	203	PEB	C2D-C3D	9.42	1.46	1.34
82	AA	201	PEB	C2D-C3D	9.42	1.46	1.34
82	zK	501	PEB	C2D-C3D	9.42	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	d4	201	PEB	C2D-C3D	9.41	1.46	1.34
82	jO	201	PEB	C2D-C3D	9.41	1.46	1.34
82	K9	201	PEB	C2D-C3D	9.41	1.46	1.34
82	gF	203	PEB	C2D-C3D	9.41	1.46	1.34
82	gK	203	PEB	C2D-C3D	9.41	1.46	1.34
82	dO	201	PEB	C2D-C3D	9.41	1.46	1.34
82	lF	202	PEB	C4C-C3C	9.41	1.51	1.37
82	SM	203	PEB	C2D-C3D	9.41	1.46	1.34
82	BP	201	PEB	C2D-C3D	9.41	1.46	1.34
82	AF	201	PEB	C2D-C3D	9.41	1.46	1.34
82	t8	202	PEB	C2D-C3D	9.41	1.46	1.34
82	IF	201	PEB	C4C-C3C	9.41	1.51	1.37
82	XP	202	PEB	C2D-C3D	9.41	1.46	1.34
82	A7	201	PEB	C2D-C3D	9.41	1.46	1.34
82	XD	202	PEB	C2D-C3D	9.40	1.46	1.34
82	S9	202	PEB	C2D-C3D	9.40	1.46	1.34
82	hO	201	PEB	C2D-C3D	9.40	1.46	1.34
82	LP	202	PEB	C2D-C3D	9.40	1.46	1.34
82	DK	203	PEB	C4C-C3C	9.40	1.51	1.37
82	HP	201	PEB	C2D-C3D	9.40	1.46	1.34
82	MQ	202	PEB	C2D-C3D	9.40	1.46	1.34
82	gB	203	PEB	C2D-C3D	9.40	1.46	1.34
82	oF	203	PEB	C2D-C3D	9.40	1.46	1.34
82	BB	203	PEB	C2D-C3D	9.40	1.46	1.34
82	HF	202	PEB	C2D-C3D	9.40	1.46	1.34
82	VK	202	PEB	C2D-C3D	9.40	1.46	1.34
82	QM	202	PEB	C2D-C3D	9.40	1.46	1.34
82	B7	201	PEB	C2D-C3D	9.40	1.46	1.34
82	bE	201	PEB	C2D-C3D	9.40	1.46	1.34
82	A9	201	PEB	C2D-C3D	9.40	1.46	1.34
82	PO	201	PEB	C2D-C3D	9.39	1.46	1.34
82	UP	202	PEB	C2D-C3D	9.39	1.46	1.34
82	R4	201	PEB	C2D-C3D	9.39	1.46	1.34
82	C7	201	PEB	C2D-C3D	9.39	1.46	1.34
82	ZM	201	PEB	C2D-C3D	9.39	1.46	1.34
82	zF	501	PEB	C2D-C3D	9.39	1.46	1.34
82	BM	301	PEB	C2D-C3D	9.39	1.46	1.34
82	BJ	301	PEB	C2D-C3D	9.39	1.46	1.34
82	YM	202	PEB	C2D-C3D	9.39	1.46	1.34
82	VP	202	PEB	C2D-C3D	9.39	1.46	1.34
82	h1	201	PEB	C2D-C3D	9.39	1.46	1.34
82	GP	203	PEB	C2D-C3D	9.39	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UG	201	PEB	C2D-C3D	9.39	1.46	1.34
82	Z5	305	PEB	C2D-C3D	9.39	1.46	1.34
82	T9	201	PEB	C2D-C3D	9.39	1.46	1.34
82	hJ	202	PEB	C2D-C3D	9.39	1.46	1.34
82	TP	201	PEB	C2D-C3D	9.38	1.46	1.34
82	QK	201	PEB	C2D-C3D	9.38	1.46	1.34
82	cE	201	PEB	C2D-C3D	9.38	1.46	1.34
82	AG	301	PEB	C2D-C3D	9.38	1.46	1.34
82	MP	201	PEB	C2D-C3D	9.38	1.46	1.34
82	N9	201	PEB	C2D-C3D	9.38	1.46	1.34
82	mG	202	PEB	C2D-C3D	9.38	1.46	1.34
82	qK	201	PEB	C2D-C3D	9.38	1.46	1.34
82	mJ	201	PEB	C2D-C3D	9.38	1.46	1.34
82	P9	201	PEB	C2D-C3D	9.38	1.46	1.34
82	tC	202	PEB	C2D-C3D	9.38	1.46	1.34
82	PK	201	PEB	C2D-C3D	9.38	1.46	1.34
82	fO	202	PEB	C2D-C3D	9.38	1.46	1.34
82	wK	302	PEB	C2D-C3D	9.38	1.46	1.34
82	JJ	201	PEB	C4C-C3C	9.38	1.51	1.37
82	UB	302	PEB	C2D-C3D	9.38	1.46	1.34
82	eF	202	PEB	C2D-C3D	9.38	1.46	1.34
82	HQ	203	PEB	C4C-C3C	9.37	1.51	1.37
82	CQ	202	PEB	C2D-C3D	9.37	1.46	1.34
82	PM	201	PEB	C4C-C3C	9.37	1.51	1.37
82	eK	202	PEB	C2D-C3D	9.37	1.46	1.34
82	X9	201	PEB	C2D-C3D	9.37	1.46	1.34
82	QH	203	PEB	C2D-C3D	9.37	1.46	1.34
82	gK	201	PEB	C4C-C3C	9.37	1.51	1.37
83	Z9	305	PUB	C1B-C2B	9.37	1.51	1.37
82	WB	402	PEB	C2D-C3D	9.37	1.46	1.34
82	AK	201	PEB	C2D-C3D	9.37	1.46	1.34
82	PG	201	PEB	C2D-C3D	9.37	1.46	1.34
82	V9	201	PEB	C2D-C3D	9.37	1.46	1.34
82	X7	203	PEB	C2D-C3D	9.37	1.46	1.34
82	EP	202	PEB	C2D-C3D	9.37	1.46	1.34
82	QO	201	PEB	C2D-C3D	9.36	1.46	1.34
82	ED	202	PEB	C2D-C3D	9.36	1.46	1.34
82	RJ	201	PEB	C4C-C3C	9.36	1.51	1.37
82	PM	201	PEB	C2D-C3D	9.36	1.46	1.34
82	D5	202	PEB	C2D-C3D	9.36	1.46	1.34
82	NM	201	PEB	C4C-C3C	9.36	1.51	1.37
82	jF	202	PEB	C2D-C3D	9.36	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SE	202	PEB	C2D-C3D	9.36	1.46	1.34
82	lM	203	PEB	C2D-C3D	9.36	1.46	1.34
82	Y9	203	PEB	C2D-C3D	9.36	1.46	1.34
82	WK	202	PEB	C2D-C3D	9.36	1.46	1.34
82	EQ	202	PEB	C2D-C3D	9.36	1.46	1.34
82	YO	202	PEB	C2D-C3D	9.36	1.46	1.34
82	aB	202	PEB	C2D-C3D	9.36	1.46	1.34
82	AB	501	PEB	C2D-C3D	9.36	1.46	1.34
82	V7	201	PEB	C2D-C3D	9.36	1.46	1.34
82	SF	203	PEB	C2D-C3D	9.35	1.46	1.34
82	YB	202	PEB	C2D-C3D	9.35	1.46	1.34
82	oK	203	PEB	C2D-C3D	9.35	1.46	1.34
82	O7	202	PEB	C2D-C3D	9.35	1.46	1.34
82	pC	201	PEB	C2D-C3D	9.35	1.46	1.34
82	XA	202	PEB	C2D-C3D	9.35	1.46	1.34
82	TJ	201	PEB	C4C-C3C	9.35	1.51	1.37
82	L5	202	PEB	C2D-C3D	9.35	1.46	1.34
82	HD	203	PEB	C4C-C3C	9.35	1.51	1.37
82	wF	303	PEB	C4C-C3C	9.34	1.51	1.37
82	RO	201	PEB	C2D-C3D	9.34	1.46	1.34
82	W9	201	PEB	C2D-C3D	9.34	1.46	1.34
82	UA	202	PEB	C2D-C3D	9.34	1.46	1.34
82	GM	202	PEB	C2D-C3D	9.34	1.46	1.34
82	iO	202	PEB	C2D-C3D	9.34	1.46	1.34
82	DF	203	PEB	C4C-C3C	9.34	1.51	1.37
82	VB	201	PEB	C2D-C3D	9.34	1.46	1.34
82	RM	201	PEB	C2D-C3D	9.34	1.46	1.34
82	gH	203	PEB	C2D-C3D	9.34	1.46	1.34
82	IK	201	PEB	C4C-C3C	9.34	1.51	1.37
82	KK	202	PEB	C2D-C3D	9.34	1.46	1.34
82	R1	202	PEB	C2D-C3D	9.34	1.46	1.34
82	QG	202	PEB	C2D-C3D	9.34	1.46	1.34
82	CP	202	PEB	C2D-C3D	9.34	1.46	1.34
82	p8	201	PEB	C2D-C3D	9.34	1.46	1.34
82	KQ	201	PEB	C2D-C3D	9.34	1.46	1.34
82	HM	201	PEB	C2D-C3D	9.34	1.46	1.34
82	EM	201	PEB	C2D-C3D	9.33	1.46	1.34
82	lE	201	PEB	C2D-C3D	9.33	1.46	1.34
82	lG	201	PEB	C2D-C3D	9.33	1.46	1.34
82	RE	202	PEB	C2D-C3D	9.33	1.46	1.34
82	wF	302	PEB	C2D-C3D	9.33	1.46	1.34
82	jF	202	PEB	C4C-C3C	9.33	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UE	202	PEB	C2D-C3D	9.33	1.46	1.34
82	UG	202	PEB	C2D-C3D	9.33	1.46	1.34
82	Y4	202	PEB	C2D-C3D	9.33	1.46	1.34
82	RP	202	PEB	C2D-C3D	9.33	1.46	1.34
82	LJ	201	PEB	C4C-C3C	9.33	1.51	1.37
82	JK	202	PEB	C2D-C3D	9.33	1.46	1.34
82	NQ	202	PEB	C4C-C3C	9.33	1.51	1.37
82	gM	201	PEB	C4C-C3C	9.33	1.51	1.37
82	EM	203	PEB	C2D-C3D	9.32	1.46	1.34
82	hM	203	PEB	C2D-C3D	9.32	1.46	1.34
82	CP	203	PEB	C2D-C3D	9.32	1.46	1.34
82	XM	201	PEB	C2D-C3D	9.32	1.46	1.34
82	SG	203	PEB	C2D-C3D	9.32	1.46	1.34
82	FQ	203	PEB	C2D-C3D	9.32	1.46	1.34
82	NI	202	PEB	C2D-C3D	9.32	1.46	1.34
82	UK	201	PEB	C4C-C3C	9.32	1.51	1.37
82	gK	202	PEB	C4C-C3C	9.32	1.51	1.37
82	l4	201	PEB	C2D-C3D	9.32	1.46	1.34
82	fM	202	PEB	C2D-C3D	9.32	1.46	1.34
82	GK	203	PEB	C2D-C3D	9.32	1.46	1.34
82	AM	302	PEB	C2D-C3D	9.31	1.46	1.34
82	gO	202	PEB	C2D-C3D	9.31	1.46	1.34
82	GB	201	PEB	C2D-C3D	9.31	1.46	1.34
82	HB	202	PEB	C2D-C3D	9.31	1.46	1.34
82	GI	203	PEB	C2D-C3D	9.31	1.46	1.34
82	O5	202	PEB	C2D-C3D	9.31	1.46	1.34
82	X7	202	PEB	C2D-C3D	9.31	1.46	1.34
82	gJ	201	PEB	C4C-C3C	9.31	1.51	1.37
82	tK	202	PEB	C4C-C3C	9.31	1.51	1.37
82	YE	202	PEB	C2D-C3D	9.31	1.46	1.34
82	BQ	202	PEB	C2D-C3D	9.31	1.46	1.34
82	bK	202	PEB	C2D-C3D	9.31	1.46	1.34
82	yK	301	PEB	C2D-C3D	9.31	1.46	1.34
82	aH	202	PEB	C4C-C3C	9.31	1.51	1.37
82	RG	202	PEB	C2D-C3D	9.31	1.46	1.34
82	hJ	201	PEB	C2D-C3D	9.31	1.46	1.34
82	gF	201	PEB	C4C-C3C	9.31	1.51	1.37
82	OG	203	PEB	C2D-C3D	9.31	1.46	1.34
82	ZG	201	PEB	C2D-C3D	9.31	1.46	1.34
82	TH	202	PEB	C2D-C3D	9.31	1.46	1.34
82	SK	203	PEB	C2D-C3D	9.31	1.46	1.34
82	MB	202	PEB	C4C-C3C	9.30	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VM	201	PEB	C2D-C3D	9.30	1.46	1.34
82	jK	202	PEB	C2D-C3D	9.30	1.46	1.34
82	i4	202	PEB	C2D-C3D	9.30	1.46	1.34
82	aF	203	PEB	C4C-C3C	9.30	1.51	1.37
82	UE	201	PEB	C2D-C3D	9.30	1.46	1.34
82	M7	201	PEB	C2D-C3D	9.30	1.46	1.34
82	PG	202	PEB	C2D-C3D	9.30	1.46	1.34
82	NM	202	PEB	C2D-C3D	9.30	1.46	1.34
82	VI	202	PEB	C2D-C3D	9.30	1.46	1.34
82	AM	301	PEB	C2D-C3D	9.30	1.46	1.34
82	GP	202	PEB	C2D-C3D	9.30	1.46	1.34
82	YA	304	PEB	C2D-C3D	9.30	1.46	1.34
82	BD	202	PEB	C2D-C3D	9.30	1.46	1.34
82	PP	201	PEB	C2D-C3D	9.30	1.46	1.34
82	S1	201	PEB	C2D-C3D	9.30	1.46	1.34
82	W5	201	PEB	C2D-C3D	9.30	1.46	1.34
82	Y7	304	PEB	C2D-C3D	9.30	1.46	1.34
82	ZM	201	PEB	C4C-C3C	9.30	1.51	1.37
82	T1	202	PEB	C2D-C3D	9.29	1.46	1.34
82	VA	201	PEB	C2D-C3D	9.29	1.46	1.34
82	QP	201	PEB	C2D-C3D	9.29	1.46	1.34
82	II	202	PEB	C2D-C3D	9.29	1.46	1.34
82	PF	201	PEB	C2D-C3D	9.29	1.46	1.34
82	KF	202	PEB	C2D-C3D	9.29	1.46	1.34
82	W5	203	PEB	C2D-C3D	9.29	1.46	1.34
82	w8	204	PEB	C4C-C3C	9.29	1.51	1.37
82	OI	203	PEB	C2D-C3D	9.29	1.46	1.34
82	UH	202	PEB	C4C-C3C	9.29	1.51	1.37
82	kE	201	PEB	C2D-C3D	9.29	1.46	1.34
82	LF	202	PEB	C4C-C3C	9.29	1.51	1.37
82	AA	202	PEB	C2D-C3D	9.29	1.46	1.34
82	mE	202	PEB	C2D-C3D	9.29	1.46	1.34
82	HQ	202	PEB	C2D-C3D	9.29	1.46	1.34
82	hK	201	PEB	C2D-C3D	9.28	1.46	1.34
82	HB	203	PEB	C4C-C3C	9.28	1.51	1.37
82	LK	202	PEB	C4C-C3C	9.28	1.51	1.37
82	eO	201	PEB	C2D-C3D	9.28	1.46	1.34
82	RO	202	PEB	C2D-C3D	9.28	1.46	1.34
82	EI	202	PEB	C2D-C3D	9.28	1.46	1.34
82	NP	201	PEB	C2D-C3D	9.28	1.46	1.34
82	lM	201	PEB	C2D-C3D	9.28	1.46	1.34
82	hF	202	PEB	C4C-C3C	9.28	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	QJ	203	PEB	C2D-C3D	9.28	1.46	1.34
82	FM	202	PEB	C2D-C3D	9.28	1.46	1.34
82	UF	201	PEB	C4C-C3C	9.28	1.51	1.37
82	ZB	201	PEB	C2D-C3D	9.28	1.46	1.34
82	W1	201	PEB	C2D-C3D	9.28	1.46	1.34
82	fF	202	PEB	C2D-C3D	9.27	1.46	1.34
82	CI	202	PEB	C2D-C3D	9.27	1.46	1.34
82	AI	202	PEB	C2D-C3D	9.27	1.46	1.34
82	jK	201	PEB	C2D-C3D	9.27	1.46	1.34
82	KD	201	PEB	C2D-C3D	9.27	1.46	1.34
82	ZE	202	PEB	C2D-C3D	9.27	1.46	1.34
82	cM	201	PEB	C2D-C3D	9.27	1.46	1.34
82	XK	201	PEB	C2D-C3D	9.27	1.46	1.34
82	P7	203	PEB	C2D-C3D	9.27	1.46	1.34
82	aG	201	PEB	C2D-C3D	9.27	1.46	1.34
82	VJ	202	PEB	C2D-C3D	9.27	1.46	1.34
82	FI	202	PEB	C2D-C3D	9.26	1.46	1.34
82	gB	201	PEB	C2D-C3D	9.26	1.46	1.34
82	PJ	201	PEB	C2D-C3D	9.26	1.46	1.34
82	KD	202	PEB	C2D-C3D	9.26	1.46	1.34
82	XI	202	PEB	C2D-C3D	9.26	1.46	1.34
82	O1	201	PEB	C2D-C3D	9.26	1.46	1.34
82	FA	202	PEB	C2D-C3D	9.26	1.46	1.34
82	XA	203	PEB	C2D-C3D	9.26	1.46	1.34
82	JQ	202	PEB	C2D-C3D	9.26	1.46	1.34
82	QE	202	PEB	C2D-C3D	9.26	1.46	1.34
82	VJ	201	PEB	C4C-C3C	9.25	1.51	1.37
82	eM	201	PEB	C4C-C3C	9.25	1.51	1.37
82	S5	202	PEB	C2D-C3D	9.25	1.46	1.34
82	OE	203	PEB	C2D-C3D	9.25	1.46	1.34
82	YH	202	PEB	C4C-C3C	9.25	1.51	1.37
82	wC	204	PEB	C4C-C3C	9.25	1.51	1.37
82	WF	201	PEB	C2D-C3D	9.25	1.46	1.34
82	LA	202	PEB	C2D-C3D	9.25	1.46	1.34
82	TI	203	PEB	C2D-C3D	9.25	1.46	1.34
82	M7	202	PEB	C2D-C3D	9.25	1.46	1.34
82	Z9	304	PEB	C2D-C3D	9.25	1.46	1.34
82	D4	1002	PEB	C2D-C3D	9.25	1.46	1.34
82	Z4	202	PEB	C2D-C3D	9.25	1.46	1.34
82	WK	201	PEB	C2D-C3D	9.25	1.46	1.34
82	DM	201	PEB	C2D-C3D	9.25	1.46	1.34
82	GF	203	PEB	C2D-C3D	9.25	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	LB	201	PEB	C4C-C3C	9.25	1.51	1.37
82	a1	202	PEB	C4C-C3C	9.24	1.51	1.37
82	kF	201	PEB	C4C-C3C	9.24	1.51	1.37
82	PI	202	PEB	C2D-C3D	9.24	1.46	1.34
82	PJ	202	PEB	C2D-C3D	9.24	1.46	1.34
82	VA	202	PEB	C2D-C3D	9.24	1.46	1.34
82	QF	203	PEB	C2D-C3D	9.24	1.46	1.34
82	QJ	202	PEB	C2D-C3D	9.24	1.46	1.34
82	mJ	201	PEB	C4C-C3C	9.24	1.51	1.37
82	dJ	202	PEB	C2D-C3D	9.24	1.46	1.34
82	SP	202	PEB	C2D-C3D	9.24	1.46	1.34
82	dG	202	PEB	C2D-C3D	9.24	1.46	1.34
82	J9	203	PEB	C4C-C3C	9.24	1.51	1.37
82	U1	202	PEB	C4C-C3C	9.24	1.51	1.37
82	IA	201	PEB	C2D-C3D	9.24	1.46	1.34
82	VE	201	PEB	C2D-C3D	9.24	1.46	1.34
82	HJ	201	PEB	C4C-C3C	9.23	1.51	1.37
82	bB	201	PEB	C2D-C3D	9.23	1.46	1.34
82	YK	201	PEB	C4C-C3C	9.23	1.51	1.37
82	XP	201	PEB	C2D-C3D	9.23	1.46	1.34
82	fK	201	PEB	C2D-C3D	9.23	1.46	1.34
82	DK	203	PEB	C2D-C3D	9.23	1.46	1.34
82	RI	202	PEB	C2D-C3D	9.23	1.46	1.34
82	T4	201	PEB	C2D-C3D	9.23	1.46	1.34
82	AH	301	PEB	C4C-C3C	9.23	1.51	1.37
82	A1	301	PEB	C4C-C3C	9.23	1.51	1.37
82	KI	203	PEB	C2D-C3D	9.23	1.46	1.34
82	YH	201	PEB	C4C-C3C	9.23	1.51	1.37
82	lJ	201	PEB	C2D-C3D	9.23	1.46	1.34
82	TM	201	PEB	C2D-C3D	9.23	1.46	1.34
82	MA	202	PEB	C2D-C3D	9.23	1.46	1.34
82	DO	1002	PEB	C2D-C3D	9.23	1.46	1.34
82	F7	202	PEB	C2D-C3D	9.23	1.46	1.34
82	PE	202	PEB	C2D-C3D	9.23	1.46	1.34
82	XJ	202	PEB	C2D-C3D	9.23	1.46	1.34
82	OA	201	PEB	C2D-C3D	9.22	1.46	1.34
82	V7	202	PEB	C2D-C3D	9.22	1.46	1.34
82	VQ	203	PEB	C4C-C3C	9.22	1.51	1.37
82	SM	202	PEB	C2D-C3D	9.22	1.46	1.34
82	SH	201	PEB	C2D-C3D	9.22	1.46	1.34
82	IM	203	PEB	C2D-C3D	9.22	1.46	1.34
82	KQ	202	PEB	C2D-C3D	9.22	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VD	203	PEB	C4C-C3C	9.22	1.51	1.37
82	HK	202	PEB	C2D-C3D	9.22	1.46	1.34
82	ZO	202	PEB	C2D-C3D	9.22	1.46	1.34
82	iJ	201	PEB	C2D-C3D	9.22	1.46	1.34
82	HO	1002	PEB	C2D-C3D	9.22	1.46	1.34
82	l1	201	PEB	C4C-C3C	9.21	1.51	1.37
82	ZE	201	PEB	C2D-C3D	9.21	1.46	1.34
82	RK	201	PEB	C2D-C3D	9.21	1.46	1.34
82	aK	202	PEB	C2D-C3D	9.21	1.46	1.34
82	JD	201	PEB	C2D-C3D	9.21	1.46	1.34
82	kK	201	PEB	C4C-C3C	9.21	1.51	1.37
82	l1	201	PEB	C2D-C3D	9.21	1.46	1.34
82	ZG	202	PEB	C2D-C3D	9.21	1.46	1.34
82	hK	202	PEB	C4C-C3C	9.21	1.51	1.37
82	DK	201	PEB	C2D-C3D	9.21	1.46	1.34
82	bB	201	PEB	C4C-C3C	9.21	1.51	1.37
82	EP	201	PEB	C2D-C3D	9.21	1.46	1.34
82	A7	202	PEB	C2D-C3D	9.21	1.46	1.34
82	J7	202	PEB	C2D-C3D	9.20	1.46	1.34
82	QD	202	PEB	C4C-C3C	9.20	1.51	1.37
82	YG	202	PEB	C2D-C3D	9.20	1.46	1.34
82	UB	301	PEB	C4C-C3C	9.20	1.51	1.37
82	FF	202	PEB	C4C-C3C	9.20	1.51	1.37
82	f4	202	PEB	C2D-C3D	9.20	1.46	1.34
82	VG	201	PEB	C2D-C3D	9.20	1.46	1.34
82	U5	202	PEB	C2D-C3D	9.20	1.46	1.34
82	OM	201	PEB	C2D-C3D	9.20	1.46	1.34
82	hF	202	PEB	C2D-C3D	9.20	1.46	1.34
82	JF	202	PEB	C2D-C3D	9.19	1.46	1.34
82	ZJ	201	PEB	C4C-C3C	9.19	1.51	1.37
82	kJ	201	PEB	C4C-C3C	9.19	1.51	1.37
82	WG	203	PEB	C2D-C3D	9.19	1.46	1.34
82	jK	202	PEB	C4C-C3C	9.19	1.51	1.37
82	R7	203	PEB	C2D-C3D	9.19	1.46	1.34
82	Y5	201	PEB	C2D-C3D	9.19	1.46	1.34
82	lJ	203	PEB	C2D-C3D	9.19	1.46	1.34
82	aJ	201	PEB	C2D-C3D	9.19	1.46	1.34
82	WF	202	PEB	C4C-C3C	9.19	1.51	1.37
82	a4	202	PEB	C2D-C3D	9.19	1.46	1.34
82	MA	201	PEB	C2D-C3D	9.19	1.46	1.34
91	d6	404	PHO	C1D-C2D	9.19	1.49	1.39
82	NE	202	PEB	C2D-C3D	9.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	i1	202	PEB	C4C-C3C	9.18	1.51	1.37
82	iH	202	PEB	C4C-C3C	9.18	1.51	1.37
82	KE	201	PEB	C2D-C3D	9.18	1.46	1.34
82	HD	202	PEB	C2D-C3D	9.18	1.46	1.34
82	H5	202	PEB	C2D-C3D	9.18	1.46	1.34
82	Y1	201	PEB	C4C-C3C	9.18	1.51	1.37
82	TO	201	PEB	C2D-C3D	9.18	1.46	1.34
82	M9	305	PEB	C2D-C3D	9.18	1.46	1.34
82	iF	201	PEB	C2D-C3D	9.18	1.46	1.34
82	II	201	PEB	C2D-C3D	9.17	1.46	1.34
82	OO	201	PEB	C2D-C3D	9.17	1.46	1.34
82	JI	201	PEB	C2D-C3D	9.17	1.46	1.34
82	NK	202	PEB	C2D-C3D	9.17	1.46	1.34
82	MP	202	PEB	C2D-C3D	9.17	1.46	1.34
82	LF	201	PEB	C2D-C3D	9.17	1.46	1.34
82	SI	202	PEB	C2D-C3D	9.17	1.46	1.34
82	OH	203	PEB	C2D-C3D	9.17	1.46	1.34
82	iK	201	PEB	C2D-C3D	9.17	1.46	1.34
82	YP	503	PEB	C2D-C3D	9.17	1.46	1.34
82	L5	201	PEB	C2D-C3D	9.17	1.46	1.34
82	LB	201	PEB	C2D-C3D	9.17	1.46	1.34
82	EB	501	PEB	C2D-C3D	9.17	1.46	1.34
82	GM	203	PEB	C2D-C3D	9.17	1.46	1.34
82	tF	202	PEB	C4C-C3C	9.17	1.51	1.37
82	QB	204	PEB	C2D-C3D	9.17	1.46	1.34
82	WE	203	PEB	C2D-C3D	9.17	1.46	1.34
82	XF	201	PEB	C2D-C3D	9.16	1.46	1.34
82	I7	201	PEB	C2D-C3D	9.16	1.46	1.34
82	YI	202	PEB	C2D-C3D	9.16	1.46	1.34
82	dH	202	PEB	C2D-C3D	9.16	1.46	1.34
82	kH	203	PEB	C4C-C3C	9.16	1.51	1.37
82	OH	201	PEB	C2D-C3D	9.16	1.46	1.34
82	RF	201	PEB	C2D-C3D	9.16	1.46	1.34
82	kG	201	PEB	C2D-C3D	9.16	1.46	1.34
82	NJ	201	PEB	C4C-C3C	9.16	1.51	1.37
82	T1	202	PEB	C4C-C3C	9.16	1.51	1.37
82	sF	201	PEB	C2D-C3D	9.16	1.46	1.34
82	GF	202	PEB	C4C-C3C	9.16	1.51	1.37
82	DJ	202	PEB	C2D-C3D	9.16	1.46	1.34
82	GJ	202	PEB	C2D-C3D	9.16	1.46	1.34
82	W5	202	PEB	C2D-C3D	9.16	1.46	1.34
82	V1	201	PEB	C2D-C3D	9.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kH	203	PEB	C2D-C3D	9.15	1.46	1.34
82	RB	202	PEB	C2D-C3D	9.15	1.46	1.34
82	Y4	201	PEB	C2D-C3D	9.15	1.46	1.34
82	cM	201	PEB	C4C-C3C	9.15	1.51	1.37
82	QQ	202	PEB	C4C-C3C	9.15	1.51	1.37
82	DF	203	PEB	C2D-C3D	9.15	1.46	1.34
82	FJ	201	PEB	C2D-C3D	9.15	1.46	1.34
82	FD	203	PEB	C4C-C3C	9.15	1.51	1.37
82	W9	201	PEB	C4C-C3C	9.15	1.51	1.37
82	BK	202	PEB	C2D-C3D	9.15	1.46	1.34
82	jF	201	PEB	C2D-C3D	9.15	1.46	1.34
82	Y1	202	PEB	C4C-C3C	9.15	1.51	1.37
82	TJ	202	PEB	C2D-C3D	9.15	1.46	1.34
82	WK	202	PEB	C4C-C3C	9.15	1.51	1.37
82	NA	202	PEB	C2D-C3D	9.15	1.46	1.34
82	GI	202	PEB	C2D-C3D	9.15	1.46	1.34
82	eJ	201	PEB	C2D-C3D	9.15	1.46	1.34
82	g4	202	PEB	C2D-C3D	9.15	1.46	1.34
82	D5	201	PEB	C2D-C3D	9.15	1.46	1.34
82	WK	203	PEB	C4C-C3C	9.15	1.51	1.37
82	dE	202	PEB	C2D-C3D	9.15	1.46	1.34
82	J7	201	PEB	C4C-C3C	9.14	1.51	1.37
82	pK	202	PEB	C4C-C3C	9.14	1.51	1.37
82	YA	303	PEB	C2D-C3D	9.14	1.46	1.34
82	R4	202	PEB	C2D-C3D	9.14	1.46	1.34
82	D7	202	PEB	C2D-C3D	9.14	1.46	1.34
82	ND	202	PEB	C4C-C3C	9.14	1.51	1.37
82	RJ	201	PEB	C2D-C3D	9.14	1.46	1.34
82	hG	201	PEB	C2D-C3D	9.14	1.46	1.34
82	UM	201	PEB	C2D-C3D	9.14	1.46	1.34
82	PO	203	PEB	C2D-C3D	9.14	1.46	1.34
82	VQ	201	PEB	C2D-C3D	9.14	1.46	1.34
82	O1	203	PEB	C2D-C3D	9.14	1.46	1.34
82	dB	202	PEB	C2D-C3D	9.14	1.46	1.34
82	jO	202	PEB	C2D-C3D	9.14	1.46	1.34
82	XB	201	PEB	C2D-C3D	9.14	1.46	1.34
82	YE	201	PEB	C2D-C3D	9.14	1.46	1.34
82	ZG	203	PEB	C2D-C3D	9.14	1.46	1.34
82	WI	201	PEB	C2D-C3D	9.14	1.46	1.34
82	P7	201	PEB	C2D-C3D	9.14	1.46	1.34
82	cJ	201	PEB	C2D-C3D	9.14	1.46	1.34
82	TI	202	PEB	C2D-C3D	9.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CM	202	PEB	C2D-C3D	9.14	1.46	1.34
82	eB	202	PEB	C2D-C3D	9.14	1.46	1.34
82	ED	201	PEB	C2D-C3D	9.14	1.46	1.34
82	jM	203	PEB	C2D-C3D	9.14	1.46	1.34
82	H4	1002	PEB	C2D-C3D	9.13	1.46	1.34
91	a6	613	PHO	C1D-C2D	9.13	1.49	1.39
82	BB	201	PEB	C2D-C3D	9.13	1.46	1.34
82	IM	202	PEB	C2D-C3D	9.13	1.46	1.34
82	RP	201	PEB	C2D-C3D	9.13	1.46	1.34
82	e4	201	PEB	C2D-C3D	9.13	1.46	1.34
82	RA	203	PEB	C2D-C3D	9.13	1.46	1.34
82	YO	201	PEB	C2D-C3D	9.13	1.46	1.34
82	DP	201	PEB	C2D-C3D	9.13	1.46	1.34
82	R7	202	PEB	C2D-C3D	9.13	1.46	1.34
82	eJ	202	PEB	C2D-C3D	9.13	1.46	1.34
82	UJ	202	PEB	C2D-C3D	9.13	1.46	1.34
82	F5	201	PEB	C2D-C3D	9.13	1.46	1.34
82	lG	202	PEB	C2D-C3D	9.13	1.46	1.34
82	TO	202	PEB	C2D-C3D	9.13	1.46	1.34
82	T4	202	PEB	C2D-C3D	9.13	1.46	1.34
82	aG	202	PEB	C2D-C3D	9.13	1.46	1.34
82	LK	201	PEB	C2D-C3D	9.13	1.46	1.34
82	VQ	202	PEB	C4C-C3C	9.13	1.51	1.37
82	IQ	202	PEB	C2D-C3D	9.13	1.46	1.34
82	PJ	201	PEB	C4C-C3C	9.13	1.51	1.37
82	PI	201	PEB	C2D-C3D	9.12	1.46	1.34
82	O7	201	PEB	C2D-C3D	9.12	1.46	1.34
82	uK	202	PEB	C4C-C3C	9.12	1.51	1.37
82	VH	201	PEB	C2D-C3D	9.12	1.46	1.34
82	V4	202	PEB	C2D-C3D	9.12	1.46	1.34
82	JA	201	PEB	C4C-C3C	9.12	1.51	1.37
82	XI	201	PEB	C2D-C3D	9.12	1.46	1.34
82	LQ	201	PEB	C2D-C3D	9.12	1.46	1.34
82	FQ	203	PEB	C4C-C3C	9.12	1.51	1.37
82	aK	203	PEB	C4C-C3C	9.12	1.51	1.37
82	V4	201	PEB	C2D-C3D	9.12	1.46	1.34
82	VI	201	PEB	C2D-C3D	9.12	1.46	1.34
82	mE	202	PEB	C4C-C3C	9.12	1.51	1.37
91	D6	404	PHO	C1D-C2D	9.12	1.49	1.39
82	UI	201	PEB	C2D-C3D	9.12	1.46	1.34
82	pF	202	PEB	C4C-C3C	9.12	1.51	1.37
82	FK	202	PEB	C4C-C3C	9.11	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gF	202	PEB	C4C-C3C	9.11	1.51	1.37
82	ID	202	PEB	C2D-C3D	9.11	1.46	1.34
82	ZE	203	PEB	C2D-C3D	9.11	1.46	1.34
82	aE	202	PEB	C2D-C3D	9.11	1.46	1.34
82	UM	203	PEB	C2D-C3D	9.11	1.46	1.34
82	P7	202	PEB	C2D-C3D	9.11	1.46	1.34
82	PA	203	PEB	C2D-C3D	9.11	1.46	1.34
82	TA	203	PEB	C2D-C3D	9.11	1.46	1.34
82	NI	201	PEB	C2D-C3D	9.11	1.46	1.34
82	jJ	203	PEB	C2D-C3D	9.11	1.46	1.34
82	WM	202	PEB	C2D-C3D	9.11	1.46	1.34
82	T7	203	PEB	C2D-C3D	9.11	1.46	1.34
82	NM	201	PEB	C2D-C3D	9.11	1.46	1.34
82	yF	301	PEB	C2D-C3D	9.11	1.46	1.34
82	OJ	202	PEB	C2D-C3D	9.11	1.46	1.34
82	UJ	201	PEB	C2D-C3D	9.11	1.46	1.34
82	eJ	201	PEB	C4C-C3C	9.11	1.51	1.37
82	LP	201	PEB	C2D-C3D	9.11	1.46	1.34
82	RA	202	PEB	C2D-C3D	9.10	1.46	1.34
82	CI	201	PEB	C2D-C3D	9.10	1.46	1.34
82	VO	201	PEB	C2D-C3D	9.10	1.46	1.34
82	fF	201	PEB	C2D-C3D	9.10	1.46	1.34
82	AI	201	PEB	C2D-C3D	9.10	1.46	1.34
82	hE	201	PEB	C2D-C3D	9.10	1.46	1.34
82	m1	201	PEB	C4C-C3C	9.10	1.50	1.37
82	JK	201	PEB	C2D-C3D	9.10	1.46	1.34
82	LD	201	PEB	C2D-C3D	9.10	1.46	1.34
82	hH	201	PEB	C2D-C3D	9.10	1.46	1.34
82	EI	201	PEB	C2D-C3D	9.10	1.46	1.34
82	UQ	202	PEB	C4C-C3C	9.10	1.50	1.37
82	TH	202	PEB	C4C-C3C	9.10	1.50	1.37
82	RI	201	PEB	C2D-C3D	9.10	1.46	1.34
82	LJ	202	PEB	C2D-C3D	9.10	1.46	1.34
82	HQ	201	PEB	C2D-C3D	9.10	1.46	1.34
82	KG	201	PEB	C2D-C3D	9.09	1.46	1.34
82	mG	202	PEB	C4C-C3C	9.09	1.50	1.37
82	DA	202	PEB	C2D-C3D	9.09	1.46	1.34
82	TQ	202	PEB	C2D-C3D	9.09	1.46	1.34
82	U5	203	PEB	C2D-C3D	9.09	1.46	1.34
82	EQ	202	PEB	C4C-C3C	9.09	1.50	1.37
82	JD	202	PEB	C2D-C3D	9.09	1.46	1.34
82	jH	201	PEB	C4C-C3C	9.09	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BF	202	PEB	C2D-C3D	9.09	1.46	1.34
82	VD	202	PEB	C4C-C3C	9.09	1.50	1.37
82	VM	201	PEB	C4C-C3C	9.09	1.50	1.37
82	uF	203	PEB	C4C-C3C	9.09	1.50	1.37
82	ZJ	202	PEB	C2D-C3D	9.09	1.46	1.34
82	UK	201	PEB	C2D-C3D	9.09	1.46	1.34
82	VP	201	PEB	C2D-C3D	9.09	1.46	1.34
82	cB	402	PEB	C2D-C3D	9.09	1.46	1.34
82	SM	201	PEB	C2D-C3D	9.09	1.46	1.34
82	d1	202	PEB	C2D-C3D	9.08	1.46	1.34
82	aJ	204	PEB	C2D-C3D	9.08	1.46	1.34
82	BI	203	PEB	C2D-C3D	9.08	1.46	1.34
82	MK	203	PEB	C2D-C3D	9.08	1.46	1.34
82	JA	202	PEB	C2D-C3D	9.08	1.46	1.34
82	SD	202	PEB	C4C-C3C	9.08	1.50	1.37
83	Z5	302	PUB	C1B-C2B	9.08	1.50	1.37
82	TD	202	PEB	C2D-C3D	9.08	1.46	1.34
82	WE	201	PEB	C2D-C3D	9.08	1.46	1.34
82	mH	201	PEB	C4C-C3C	9.08	1.50	1.37
82	UD	202	PEB	C4C-C3C	9.08	1.50	1.37
82	U1	203	PEB	C4C-C3C	9.08	1.50	1.37
82	HD	201	PEB	C2D-C3D	9.08	1.46	1.34
82	XJ	201	PEB	C2D-C3D	9.08	1.46	1.34
82	EP	203	PEB	C2D-C3D	9.08	1.46	1.34
82	eF	203	PEB	C4C-C3C	9.08	1.50	1.37
82	EF	201	PEB	C2D-C3D	9.07	1.46	1.34
82	dQ	401	PEB	C2D-C3D	9.07	1.46	1.34
82	UM	202	PEB	C2D-C3D	9.07	1.46	1.34
82	aJ	202	PEB	C2D-C3D	9.07	1.46	1.34
82	FD	202	PEB	C4C-C3C	9.07	1.50	1.37
82	b4	201	PEB	C4C-C3C	9.07	1.50	1.37
82	bO	201	PEB	C4C-C3C	9.07	1.50	1.37
82	HG	1002	PEB	C2D-C3D	9.07	1.46	1.34
82	UE	201	PEB	C4C-C3C	9.07	1.50	1.37
82	18	203	PEB	C4C-C3C	9.07	1.50	1.37
82	NG	201	PEB	C2D-C3D	9.07	1.46	1.34
82	NA	201	PEB	C2D-C3D	9.07	1.46	1.34
82	1C	203	PEB	C4C-C3C	9.07	1.50	1.37
82	YF	201	PEB	C4C-C3C	9.07	1.50	1.37
82	lM	202	PEB	C2D-C3D	9.07	1.46	1.34
82	IP	201	PEB	C2D-C3D	9.07	1.46	1.34
82	DF	201	PEB	C2D-C3D	9.07	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GJ	201	PEB	C2D-C3D	9.06	1.46	1.34
82	hK	202	PEB	C2D-C3D	9.06	1.46	1.34
82	SQ	202	PEB	C4C-C3C	9.06	1.50	1.37
82	iK	202	PEB	C4C-C3C	9.06	1.50	1.37
82	KI	202	PEB	C2D-C3D	9.06	1.46	1.34
82	NJ	202	PEB	C2D-C3D	9.06	1.46	1.34
82	VF	201	PEB	C2D-C3D	9.06	1.46	1.34
82	DH	1002	PEB	C2D-C3D	9.06	1.46	1.34
82	SK	201	PEB	C2D-C3D	9.06	1.46	1.34
82	HE	1002	PEB	C2D-C3D	9.06	1.46	1.34
82	SE	201	PEB	C2D-C3D	9.06	1.46	1.34
82	N7	202	PEB	C2D-C3D	9.06	1.46	1.34
82	sK	201	PEB	C2D-C3D	9.06	1.46	1.34
82	aO	202	PEB	C2D-C3D	9.06	1.46	1.34
83	M5	302	PUB	C1B-C2B	9.06	1.50	1.37
82	AP	202	PEB	C2D-C3D	9.05	1.46	1.34
82	XB	202	PEB	C2D-C3D	9.05	1.46	1.34
82	GB	203	PEB	C2D-C3D	9.05	1.46	1.34
82	N7	201	PEB	C2D-C3D	9.05	1.46	1.34
82	ED	202	PEB	C4C-C3C	9.05	1.50	1.37
82	VD	201	PEB	C2D-C3D	9.05	1.46	1.34
82	gE	202	PEB	C4C-C3C	9.05	1.50	1.37
82	ZJ	201	PEB	C2D-C3D	9.05	1.46	1.34
82	GB	202	PEB	C2D-C3D	9.05	1.46	1.34
82	kK	203	PEB	C2D-C3D	9.05	1.46	1.34
82	eK	203	PEB	C4C-C3C	9.05	1.50	1.37
82	WF	203	PEB	C4C-C3C	9.05	1.50	1.37
82	JJ	201	PEB	C2D-C3D	9.05	1.46	1.34
82	O4	201	PEB	C2D-C3D	9.05	1.46	1.34
82	fH	202	PEB	C4C-C3C	9.05	1.50	1.37
82	SJ	203	PEB	C2D-C3D	9.04	1.46	1.34
82	lO	202	PEB	C2D-C3D	9.04	1.46	1.34
82	SF	201	PEB	C2D-C3D	9.04	1.46	1.34
82	h1	202	PEB	C2D-C3D	9.04	1.46	1.34
82	bP	502	PEB	C2D-C3D	9.04	1.46	1.34
82	YG	201	PEB	C2D-C3D	9.04	1.46	1.34
91	A6	407	PHO	C1D-C2D	9.04	1.49	1.39
82	JM	201	PEB	C2D-C3D	9.04	1.46	1.34
82	UP	203	PEB	C2D-C3D	9.04	1.46	1.34
82	IJ	201	PEB	C2D-C3D	9.04	1.46	1.34
82	GK	202	PEB	C4C-C3C	9.04	1.50	1.37
82	BI	201	PEB	C2D-C3D	9.04	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S1	202	PEB	C4C-C3C	9.03	1.50	1.37
82	GA	201	PEB	C2D-C3D	9.03	1.46	1.34
82	gG	202	PEB	C4C-C3C	9.03	1.50	1.37
82	iF	202	PEB	C4C-C3C	9.03	1.50	1.37
82	aF	202	PEB	C2D-C3D	9.03	1.46	1.34
82	eK	202	PEB	C4C-C3C	9.03	1.50	1.37
82	l4	202	PEB	C2D-C3D	9.03	1.46	1.34
82	V1	203	PEB	C4C-C3C	9.03	1.50	1.37
82	cK	201	PEB	C4C-C3C	9.03	1.50	1.37
82	QM	204	PEB	C2D-C3D	9.03	1.46	1.34
82	f1	202	PEB	C4C-C3C	9.02	1.50	1.37
82	QH	202	PEB	C2D-C3D	9.02	1.46	1.34
82	SG	201	PEB	C2D-C3D	9.02	1.46	1.34
82	D1	1002	PEB	C2D-C3D	9.02	1.46	1.34
82	UO	202	PEB	C2D-C3D	9.02	1.46	1.34
82	wK	303	PEB	C2D-C3D	9.02	1.46	1.34
82	OG	201	PEB	C2D-C3D	9.02	1.46	1.34
82	DQ	202	PEB	C2D-C3D	9.02	1.46	1.34
82	CB	201	PEB	C2D-C3D	9.02	1.46	1.34
82	LD	203	PEB	C4C-C3C	9.02	1.50	1.37
82	x8	202	PEB	C4C-C3C	9.02	1.50	1.37
82	FJ	202	PEB	C2D-C3D	9.02	1.46	1.34
82	J4	1002	PEB	C2D-C3D	9.02	1.46	1.34
82	Y7	303	PEB	C2D-C3D	9.02	1.46	1.34
82	VH	202	PEB	C4C-C3C	9.02	1.50	1.37
82	PF	202	PEB	C2D-C3D	9.02	1.46	1.34
82	SF	203	PEB	C4C-C3C	9.02	1.50	1.37
82	YB	201	PEB	C2D-C3D	9.01	1.46	1.34
82	JF	201	PEB	C2D-C3D	9.01	1.46	1.34
82	EQ	201	PEB	C2D-C3D	9.01	1.46	1.34
82	KA	201	PEB	C4C-C3C	9.01	1.50	1.37
82	MF	203	PEB	C2D-C3D	9.01	1.46	1.34
82	DB	201	PEB	C2D-C3D	9.01	1.46	1.34
82	eM	201	PEB	C2D-C3D	9.01	1.46	1.34
82	cB	403	PEB	C2D-C3D	9.01	1.46	1.34
82	QA	201	PEB	C2D-C3D	9.01	1.46	1.34
82	mM	201	PEB	C4C-C3C	9.01	1.50	1.37
82	TA	202	PEB	C2D-C3D	9.01	1.46	1.34
82	NF	202	PEB	C2D-C3D	9.01	1.46	1.34
82	PH	201	PEB	C2D-C3D	9.01	1.46	1.34
82	FQ	202	PEB	C4C-C3C	9.01	1.50	1.37
82	EJ	202	PEB	C2D-C3D	9.01	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	O5	203	PEB	C2D-C3D	9.01	1.46	1.34
82	PA	201	PEB	C2D-C3D	9.01	1.46	1.34
82	QK	203	PEB	C2D-C3D	9.00	1.46	1.34
82	UF	201	PEB	C2D-C3D	9.00	1.46	1.34
82	NJ	201	PEB	C2D-C3D	9.00	1.46	1.34
82	K7	201	PEB	C4C-C3C	9.00	1.50	1.37
82	IB	203	PEB	C2D-C3D	9.00	1.46	1.34
82	LQ	203	PEB	C4C-C3C	9.00	1.50	1.37
82	WG	201	PEB	C2D-C3D	9.00	1.46	1.34
82	CB	201	PEB	C4C-C3C	9.00	1.50	1.37
82	qK	203	PEB	C4C-C3C	9.00	1.50	1.37
82	JM	201	PEB	C4C-C3C	9.00	1.50	1.37
82	hM	201	PEB	C2D-C3D	9.00	1.46	1.34
82	e1	202	PEB	C4C-C3C	9.00	1.50	1.37
82	KF	201	PEB	C2D-C3D	9.00	1.46	1.34
82	Q1	202	PEB	C2D-C3D	8.99	1.46	1.34
82	OG	202	PEB	C2D-C3D	8.99	1.46	1.34
82	M9	301	PEB	C2D-C3D	8.99	1.46	1.34
82	SB	203	PEB	C2D-C3D	8.99	1.46	1.34
82	J9	201	PEB	C4C-C3C	8.99	1.50	1.37
82	YM	201	PEB	C2D-C3D	8.99	1.46	1.34
82	VK	201	PEB	C2D-C3D	8.99	1.46	1.34
82	J5	203	PEB	C2D-C3D	8.99	1.46	1.34
82	eF	202	PEB	C4C-C3C	8.99	1.50	1.37
82	xC	202	PEB	C4C-C3C	8.99	1.50	1.37
82	QA	202	PEB	C2D-C3D	8.98	1.46	1.34
82	HF	202	PEB	C4C-C3C	8.98	1.50	1.37
82	FM	201	PEB	C2D-C3D	8.98	1.46	1.34
82	RD	202	PEB	C4C-C3C	8.98	1.50	1.37
82	RQ	202	PEB	C4C-C3C	8.98	1.50	1.37
82	G7	201	PEB	C2D-C3D	8.98	1.46	1.34
82	U4	202	PEB	C2D-C3D	8.98	1.46	1.34
82	TJ	201	PEB	C2D-C3D	8.98	1.46	1.34
82	OP	202	PEB	C2D-C3D	8.98	1.46	1.34
82	KK	201	PEB	C2D-C3D	8.98	1.46	1.34
82	N7	203	PEB	C2D-C3D	8.98	1.46	1.34
82	UB	301	PEB	C2D-C3D	8.97	1.46	1.34
82	wF	303	PEB	C2D-C3D	8.97	1.46	1.34
82	VO	202	PEB	C2D-C3D	8.97	1.46	1.34
82	NA	203	PEB	C2D-C3D	8.97	1.46	1.34
82	S7	201	PEB	C2D-C3D	8.97	1.46	1.34
82	tK	203	PEB	C4C-C3C	8.97	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	T7	202	PEB	C2D-C3D	8.97	1.46	1.34
82	Q7	201	PEB	C2D-C3D	8.97	1.46	1.34
82	aO	201	PEB	C2D-C3D	8.96	1.46	1.34
82	SA	201	PEB	C2D-C3D	8.96	1.46	1.34
82	ZO	201	PEB	C2D-C3D	8.96	1.46	1.34
82	DM	201	PEB	C4C-C3C	8.96	1.50	1.37
82	H9	203	PEB	C4C-C3C	8.96	1.50	1.37
82	eH	202	PEB	C4C-C3C	8.96	1.50	1.37
82	TA	201	PEB	C2D-C3D	8.96	1.46	1.34
82	KM	201	PEB	C2D-C3D	8.96	1.46	1.34
82	cF	203	PEB	C2D-C3D	8.96	1.46	1.34
82	RQ	203	PEB	C2D-C3D	8.96	1.46	1.34
82	X7	201	PEB	C2D-C3D	8.96	1.46	1.34
82	PA	202	PEB	C2D-C3D	8.96	1.46	1.34
82	TD	202	PEB	C4C-C3C	8.95	1.50	1.37
82	PD	203	PEB	C4C-C3C	8.95	1.50	1.37
82	OE	202	PEB	C2D-C3D	8.95	1.46	1.34
82	eA	301	PEB	C2D-C3D	8.95	1.46	1.34
82	mK	201	PEB	C4C-C3C	8.95	1.50	1.37
82	F1	1002	PEB	C2D-C3D	8.95	1.46	1.34
82	HK	202	PEB	C4C-C3C	8.95	1.50	1.37
82	F5	201	PEB	C4C-C3C	8.95	1.50	1.37
82	nF	201	PEB	C4C-C3C	8.95	1.50	1.37
82	FH	1002	PEB	C2D-C3D	8.95	1.46	1.34
82	J5	202	PEB	C2D-C3D	8.95	1.46	1.34
82	NQ	204	PEB	C4C-C3C	8.95	1.50	1.37
82	BA	203	PEB	C4C-C3C	8.94	1.50	1.37
82	P1	201	PEB	C2D-C3D	8.94	1.46	1.34
82	iJ	201	PEB	C4C-C3C	8.94	1.50	1.37
82	OI	201	PEB	C2D-C3D	8.94	1.46	1.34
82	j4	202	PEB	C2D-C3D	8.94	1.46	1.34
82	NK	201	PEB	C2D-C3D	8.94	1.46	1.34
82	nK	201	PEB	C4C-C3C	8.94	1.50	1.37
82	MK	202	PEB	C4C-C3C	8.94	1.50	1.37
82	IK	201	PEB	C2D-C3D	8.94	1.46	1.34
82	kF	203	PEB	C2D-C3D	8.94	1.46	1.34
82	VF	202	PEB	C4C-C3C	8.94	1.50	1.37
82	HI	201	PEB	C2D-C3D	8.94	1.46	1.34
82	RD	203	PEB	C2D-C3D	8.94	1.46	1.34
82	EJ	203	PEB	C2D-C3D	8.93	1.46	1.34
82	WM	201	PEB	C2D-C3D	8.93	1.46	1.34
82	B5	203	PEB	C2D-C3D	8.93	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	RH	202	PEB	C4C-C3C	8.93	1.50	1.37
82	XM	201	PEB	C4C-C3C	8.93	1.50	1.37
82	yC	202	PEB	C4C-C3C	8.93	1.50	1.37
82	DJ	201	PEB	C2D-C3D	8.93	1.46	1.34
82	cB	403	PEB	C4C-C3C	8.93	1.50	1.37
82	OE	201	PEB	C2D-C3D	8.93	1.46	1.34
82	WI	202	PEB	C2D-C3D	8.93	1.46	1.34
82	CJ	203	PEB	C2D-C3D	8.93	1.46	1.34
82	kH	202	PEB	C4C-C3C	8.93	1.50	1.37
82	HK	201	PEB	C2D-C3D	8.93	1.46	1.34
82	J7	203	PEB	C4C-C3C	8.93	1.50	1.37
82	f4	201	PEB	C4C-C3C	8.93	1.50	1.37
82	k1	202	PEB	C4C-C3C	8.92	1.50	1.37
82	f1	201	PEB	C2D-C3D	8.92	1.46	1.34
82	s8	202	PEB	C4C-C3C	8.92	1.50	1.37
82	DA	201	PEB	C2D-C3D	8.92	1.46	1.34
82	TF	201	PEB	C2D-C3D	8.92	1.46	1.34
82	LM	201	PEB	C2D-C3D	8.92	1.46	1.34
82	D7	201	PEB	C2D-C3D	8.92	1.46	1.34
82	SH	202	PEB	C4C-C3C	8.92	1.50	1.37
82	DD	202	PEB	C2D-C3D	8.92	1.46	1.34
82	fH	201	PEB	C2D-C3D	8.92	1.46	1.34
82	Q7	202	PEB	C2D-C3D	8.92	1.46	1.34
82	KF	203	PEB	C4C-C3C	8.92	1.50	1.37
82	Q9	203	PEB	C4C-C3C	8.92	1.50	1.37
82	mF	201	PEB	C4C-C3C	8.92	1.50	1.37
82	Z4	201	PEB	C2D-C3D	8.92	1.46	1.34
82	fO	201	PEB	C4C-C3C	8.92	1.50	1.37
82	RB	201	PEB	C4C-C3C	8.92	1.50	1.37
82	dD	401	PEB	C2D-C3D	8.92	1.46	1.34
82	XA	201	PEB	C2D-C3D	8.92	1.46	1.34
82	N5	201	PEB	C2D-C3D	8.91	1.46	1.34
82	j1	201	PEB	C4C-C3C	8.91	1.50	1.37
82	H1	1002	PEB	C4C-C3C	8.91	1.50	1.37
82	WG	202	PEB	C2D-C3D	8.91	1.46	1.34
82	TK	201	PEB	C2D-C3D	8.91	1.46	1.34
82	WE	202	PEB	C2D-C3D	8.91	1.46	1.34
82	YM	203	PEB	C2D-C3D	8.91	1.46	1.34
82	JP	201	PEB	C2D-C3D	8.91	1.46	1.34
82	R5	202	PEB	C2D-C3D	8.91	1.46	1.34
82	iF	203	PEB	C4C-C3C	8.91	1.50	1.37
82	R7	201	PEB	C2D-C3D	8.91	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	R1	202	PEB	C4C-C3C	8.91	1.50	1.37
82	SB	201	PEB	C2D-C3D	8.91	1.46	1.34
82	UH	203	PEB	C4C-C3C	8.91	1.50	1.37
82	EK	201	PEB	C4C-C3C	8.91	1.50	1.37
82	sC	202	PEB	C4C-C3C	8.91	1.50	1.37
82	SH	203	PEB	C2D-C3D	8.91	1.46	1.34
82	SK	203	PEB	C4C-C3C	8.91	1.50	1.37
82	T5	202	PEB	C2D-C3D	8.90	1.46	1.34
82	LM	201	PEB	C4C-C3C	8.90	1.50	1.37
82	NQ	203	PEB	C4C-C3C	8.90	1.50	1.37
82	cF	201	PEB	C4C-C3C	8.90	1.50	1.37
82	M5	301	PEB	C2D-C3D	8.90	1.46	1.34
82	KK	203	PEB	C4C-C3C	8.90	1.50	1.37
82	g1	201	PEB	C4C-C3C	8.90	1.50	1.37
82	PQ	203	PEB	C4C-C3C	8.90	1.50	1.37
82	TQ	202	PEB	C4C-C3C	8.90	1.50	1.37
82	XQ	203	PEB	C4C-C3C	8.90	1.50	1.37
82	hG	203	PEB	C4C-C3C	8.90	1.50	1.37
82	sK	201	PEB	C4C-C3C	8.90	1.50	1.37
82	HB	203	PEB	C2D-C3D	8.90	1.46	1.34
82	YJ	201	PEB	C2D-C3D	8.90	1.46	1.34
82	RA	202	PEB	C4C-C3C	8.90	1.50	1.37
82	CM	203	PEB	C2D-C3D	8.90	1.46	1.34
82	QP	203	PEB	C2D-C3D	8.90	1.46	1.34
82	N5	202	PEB	C2D-C3D	8.90	1.46	1.34
82	NF	201	PEB	C2D-C3D	8.90	1.46	1.34
82	OJ	201	PEB	C2D-C3D	8.89	1.46	1.34
82	GK	202	PEB	C2D-C3D	8.89	1.46	1.34
82	UG	201	PEB	C4C-C3C	8.89	1.50	1.37
82	V4	202	PEB	C4C-C3C	8.89	1.50	1.37
82	cM	202	PEB	C4C-C3C	8.89	1.50	1.37
82	JO	1002	PEB	C2D-C3D	8.89	1.46	1.34
82	Q5	203	PEB	C2D-C3D	8.89	1.46	1.34
82	hE	203	PEB	C4C-C3C	8.89	1.50	1.37
82	EK	201	PEB	C2D-C3D	8.89	1.46	1.34
82	bP	501	PEB	C2D-C3D	8.89	1.46	1.34
82	IQ	201	PEB	C2D-C3D	8.89	1.46	1.34
82	E5	202	PEB	C2D-C3D	8.89	1.46	1.34
82	F5	203	PEB	C2D-C3D	8.89	1.46	1.34
82	Z5	301	PEB	C2D-C3D	8.89	1.46	1.34
82	WP	202	PEB	C2D-C3D	8.88	1.46	1.34
82	WB	402	PEB	C4C-C3C	8.88	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SJ	201	PEB	C2D-C3D	8.88	1.46	1.34
82	AP	201	PEB	C2D-C3D	8.88	1.46	1.34
82	MF	202	PEB	C4C-C3C	8.88	1.50	1.37
82	IB	201	PEB	C2D-C3D	8.88	1.46	1.34
82	AJ	302	PEB	C2D-C3D	8.88	1.46	1.34
82	OK	202	PEB	C4C-C3C	8.88	1.50	1.37
82	X5	201	PEB	C2D-C3D	8.88	1.46	1.34
82	G5	202	PEB	C2D-C3D	8.87	1.46	1.34
82	y8	202	PEB	C4C-C3C	8.87	1.50	1.37
82	O5	201	PEB	C2D-C3D	8.87	1.46	1.34
82	XK	203	PEB	C2D-C3D	8.87	1.46	1.34
82	IF	201	PEB	C2D-C3D	8.87	1.46	1.34
82	V5	201	PEB	C2D-C3D	8.87	1.46	1.34
82	RB	202	PEB	C4C-C3C	8.87	1.50	1.37
82	VK	202	PEB	C4C-C3C	8.87	1.50	1.37
82	JA	203	PEB	C4C-C3C	8.87	1.50	1.37
82	ID	201	PEB	C2D-C3D	8.87	1.45	1.34
82	U4	201	PEB	C2D-C3D	8.87	1.45	1.34
82	a4	201	PEB	C2D-C3D	8.87	1.45	1.34
82	UO	201	PEB	C2D-C3D	8.87	1.45	1.34
82	PK	202	PEB	C2D-C3D	8.86	1.45	1.34
82	DE	1002	PEB	C2D-C3D	8.86	1.45	1.34
82	pC	201	PEB	C4C-C3C	8.86	1.50	1.37
82	GE	1002	PEB	C2D-C3D	8.86	1.45	1.34
82	vF	202	PEB	C4C-C3C	8.86	1.50	1.37
82	IK	203	PEB	C2D-C3D	8.86	1.45	1.34
82	R5	201	PEB	C2D-C3D	8.86	1.45	1.34
82	I5	201	PEB	C2D-C3D	8.86	1.45	1.34
82	GD	201	PEB	C4C-C3C	8.86	1.50	1.37
82	C7	201	PEB	C4C-C3C	8.86	1.50	1.37
82	C5	202	PEB	C2D-C3D	8.86	1.45	1.34
82	V5	202	PEB	C2D-C3D	8.86	1.45	1.34
82	P5	202	PEB	C2D-C3D	8.86	1.45	1.34
82	Q5	201	PEB	C2D-C3D	8.86	1.45	1.34
82	E5	201	PEB	C2D-C3D	8.85	1.45	1.34
82	X5	202	PEB	C2D-C3D	8.85	1.45	1.34
82	IP	202	PEB	C4C-C3C	8.85	1.50	1.37
82	OJ	203	PEB	C2D-C3D	8.85	1.45	1.34
82	qF	203	PEB	C4C-C3C	8.85	1.50	1.37
82	cK	202	PEB	C4C-C3C	8.85	1.50	1.37
82	QH	201	PEB	C2D-C3D	8.85	1.45	1.34
82	p8	201	PEB	C4C-C3C	8.85	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GP	201	PEB	C2D-C3D	8.85	1.45	1.34
82	B7	203	PEB	C4C-C3C	8.85	1.50	1.37
82	RA	201	PEB	C2D-C3D	8.85	1.45	1.34
82	A5	202	PEB	C2D-C3D	8.85	1.45	1.34
82	MM	201	PEB	C2D-C3D	8.85	1.45	1.34
82	I5	202	PEB	C2D-C3D	8.85	1.45	1.34
82	PG	201	PEB	C4C-C3C	8.85	1.50	1.37
82	T7	201	PEB	C2D-C3D	8.84	1.45	1.34
82	OF	202	PEB	C4C-C3C	8.84	1.50	1.37
82	KM	203	PEB	C2D-C3D	8.84	1.45	1.34
82	DI	201	PEB	C2D-C3D	8.84	1.45	1.34
82	K5	202	PEB	C2D-C3D	8.84	1.45	1.34
82	G5	201	PEB	C2D-C3D	8.84	1.45	1.34
82	HH	1002	PEB	C4C-C3C	8.84	1.50	1.37
82	XF	203	PEB	C2D-C3D	8.84	1.45	1.34
82	K5	201	PEB	C2D-C3D	8.84	1.45	1.34
82	Z1	202	PEB	C4C-C3C	8.83	1.50	1.37
82	HB	201	PEB	C2D-C3D	8.83	1.45	1.34
82	uF	202	PEB	C4C-C3C	8.83	1.50	1.37
82	SK	202	PEB	C2D-C3D	8.83	1.45	1.34
82	XD	203	PEB	C4C-C3C	8.83	1.50	1.37
82	cK	203	PEB	C2D-C3D	8.83	1.45	1.34
82	oF	201	PEB	C4C-C3C	8.83	1.50	1.37
82	OK	202	PEB	C2D-C3D	8.83	1.45	1.34
82	Z1	203	PEB	C4C-C3C	8.83	1.50	1.37
82	C5	201	PEB	C2D-C3D	8.83	1.45	1.34
91	DL	405	PHO	C1D-C2D	8.83	1.49	1.39
82	LG	1002	PEB	C2D-C3D	8.83	1.45	1.34
82	sC	201	PEB	C4C-C3C	8.83	1.50	1.37
82	SA	202	PEB	C2D-C3D	8.83	1.45	1.34
82	DF	201	PEB	C4C-C3C	8.83	1.50	1.37
82	CM	201	PEB	C2D-C3D	8.83	1.45	1.34
82	KP	201	PEB	C2D-C3D	8.83	1.45	1.34
82	CA	201	PEB	C4C-C3C	8.82	1.50	1.37
82	P5	201	PEB	C2D-C3D	8.82	1.45	1.34
82	ND	203	PEB	C4C-C3C	8.82	1.50	1.37
82	U7	202	PEB	C4C-C3C	8.82	1.50	1.37
82	sF	202	PEB	C4C-C3C	8.82	1.50	1.37
82	J4	1002	PEB	C4C-C3C	8.82	1.50	1.37
82	LI	202	PEB	C2D-C3D	8.82	1.45	1.34
82	CF	202	PEB	C4C-C3C	8.82	1.50	1.37
82	l4	201	PEB	C4C-C3C	8.82	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hH	201	PEB	C4C-C3C	8.82	1.50	1.37
82	AJ	302	PEB	C4C-C3C	8.81	1.50	1.37
82	s8	201	PEB	C4C-C3C	8.81	1.50	1.37
82	gH	201	PEB	C4C-C3C	8.81	1.50	1.37
82	RD	203	PEB	C4C-C3C	8.81	1.50	1.37
82	sF	201	PEB	C4C-C3C	8.81	1.50	1.37
82	ND	204	PEB	C4C-C3C	8.81	1.50	1.37
82	PE	201	PEB	C4C-C3C	8.81	1.50	1.37
82	c4	203	PEB	C4C-C3C	8.81	1.50	1.37
82	ZO	201	PEB	C4C-C3C	8.81	1.50	1.37
82	tK	203	PEB	C2D-C3D	8.81	1.45	1.34
82	iK	203	PEB	C4C-C3C	8.81	1.50	1.37
82	OK	203	PEB	C4C-C3C	8.81	1.50	1.37
82	jO	201	PEB	C4C-C3C	8.80	1.50	1.37
82	ZH	203	PEB	C4C-C3C	8.80	1.50	1.37
82	EF	201	PEB	C4C-C3C	8.80	1.50	1.37
82	uF	201	PEB	C4C-C3C	8.80	1.50	1.37
82	T5	201	PEB	C2D-C3D	8.80	1.45	1.34
82	LD	202	PEB	C2D-C3D	8.80	1.45	1.34
82	TD	203	PEB	C4C-C3C	8.80	1.50	1.37
82	RQ	203	PEB	C4C-C3C	8.79	1.50	1.37
82	LE	1002	PEB	C2D-C3D	8.79	1.45	1.34
82	L5	203	PEB	C2D-C3D	8.79	1.45	1.34
82	h1	202	PEB	C4C-C3C	8.79	1.50	1.37
82	jF	201	PEB	C4C-C3C	8.79	1.50	1.37
82	GQ	201	PEB	C4C-C3C	8.79	1.50	1.37
82	WM	203	PEB	C2D-C3D	8.79	1.45	1.34
82	AK	201	PEB	C4C-C3C	8.79	1.50	1.37
82	V1	202	PEB	C2D-C3D	8.79	1.45	1.34
82	JO	1002	PEB	C4C-C3C	8.79	1.50	1.37
82	DB	202	PEB	C2D-C3D	8.79	1.45	1.34
82	Y9	203	PEB	C4C-C3C	8.79	1.50	1.37
82	BF	201	PEB	C2D-C3D	8.79	1.45	1.34
82	J5	201	PEB	C2D-C3D	8.79	1.45	1.34
82	U9	201	PEB	C4C-C3C	8.78	1.50	1.37
82	AF	201	PEB	C4C-C3C	8.78	1.50	1.37
82	B9	203	PEB	C4C-C3C	8.78	1.50	1.37
82	yF	301	PEB	C4C-C3C	8.78	1.50	1.37
82	GJ	203	PEB	C2D-C3D	8.78	1.45	1.34
82	QB	202	PEB	C2D-C3D	8.78	1.45	1.34
82	IF	203	PEB	C2D-C3D	8.78	1.45	1.34
82	l1	202	PEB	C4C-C3C	8.78	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FK	201	PEB	C2D-C3D	8.77	1.45	1.34
82	A5	201	PEB	C2D-C3D	8.77	1.45	1.34
82	LQ	202	PEB	C2D-C3D	8.77	1.45	1.34
82	y8	203	PEB	C4C-C3C	8.77	1.50	1.37
82	GF	202	PEB	C2D-C3D	8.77	1.45	1.34
82	GG	1002	PEB	C2D-C3D	8.77	1.45	1.34
82	DJ	201	PEB	C4C-C3C	8.77	1.50	1.37
82	HF	201	PEB	C2D-C3D	8.77	1.45	1.34
82	bH	202	PEB	C4C-C3C	8.77	1.50	1.37
82	KI	201	PEB	C2D-C3D	8.77	1.45	1.34
82	B5	202	PEB	C4C-C3C	8.77	1.50	1.37
82	GQ	202	PEB	C4C-C3C	8.77	1.50	1.37
82	fE	203	PEB	C4C-C3C	8.77	1.50	1.37
82	S7	202	PEB	C2D-C3D	8.76	1.45	1.34
82	O4	202	PEB	C2D-C3D	8.76	1.45	1.34
82	BQ	201	PEB	C2D-C3D	8.76	1.45	1.34
82	Q1	201	PEB	C2D-C3D	8.76	1.45	1.34
82	fJ	203	PEB	C2D-C3D	8.76	1.45	1.34
82	uK	201	PEB	C4C-C3C	8.76	1.50	1.37
82	OF	202	PEB	C2D-C3D	8.76	1.45	1.34
82	Y9	201	PEB	C4C-C3C	8.76	1.50	1.37
82	b1	202	PEB	C4C-C3C	8.76	1.50	1.37
82	GD	202	PEB	C4C-C3C	8.76	1.50	1.37
82	SO	202	PEB	C2D-C3D	8.75	1.45	1.34
82	R7	202	PEB	C4C-C3C	8.75	1.50	1.37
91	aL	610	PHO	C1D-C2D	8.75	1.49	1.39
82	ZH	202	PEB	C4C-C3C	8.75	1.50	1.37
82	MM	202	PEB	C2D-C3D	8.75	1.45	1.34
82	TE	201	PEB	C2D-C3D	8.75	1.45	1.34
82	yC	203	PEB	C4C-C3C	8.75	1.50	1.37
82	WO	201	PEB	C2D-C3D	8.75	1.45	1.34
82	TQ	203	PEB	C4C-C3C	8.74	1.50	1.37
82	eB	201	PEB	C2D-C3D	8.74	1.45	1.34
82	oK	201	PEB	C4C-C3C	8.74	1.50	1.37
82	D9	203	PEB	C4C-C3C	8.74	1.50	1.37
82	vK	202	PEB	C4C-C3C	8.74	1.50	1.37
82	RF	202	PEB	C2D-C3D	8.74	1.45	1.34
83	AH	303	PUB	C1B-C2B	8.74	1.50	1.37
82	FF	201	PEB	C2D-C3D	8.74	1.45	1.34
82	EJ	201	PEB	C2D-C3D	8.74	1.45	1.34
82	MJ	201	PEB	C2D-C3D	8.74	1.45	1.34
82	gM	202	PEB	C4C-C3C	8.73	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SF	202	PEB	C2D-C3D	8.73	1.45	1.34
82	eE	203	PEB	C4C-C3C	8.73	1.50	1.37
82	Z4	201	PEB	C4C-C3C	8.73	1.50	1.37
82	DI	202	PEB	C4C-C3C	8.73	1.50	1.37
82	OK	201	PEB	C2D-C3D	8.73	1.45	1.34
82	S9	203	PEB	C4C-C3C	8.73	1.50	1.37
82	j4	201	PEB	C4C-C3C	8.72	1.50	1.37
82	KJ	203	PEB	C2D-C3D	8.72	1.45	1.34
82	LJ	201	PEB	C2D-C3D	8.72	1.45	1.34
82	AP	203	PEB	C2D-C3D	8.72	1.45	1.34
82	QG	203	PEB	C4C-C3C	8.72	1.50	1.37
82	UB	303	PEB	C2D-C3D	8.72	1.45	1.34
82	OF	203	PEB	C4C-C3C	8.72	1.50	1.37
82	JQ	202	PEB	C4C-C3C	8.72	1.50	1.37
82	PQ	202	PEB	C4C-C3C	8.72	1.50	1.37
82	HJ	201	PEB	C2D-C3D	8.72	1.45	1.34
82	fG	203	PEB	C4C-C3C	8.72	1.50	1.37
82	cO	203	PEB	C4C-C3C	8.72	1.50	1.37
82	NB	202	PEB	C2D-C3D	8.72	1.45	1.34
82	SP	201	PEB	C2D-C3D	8.72	1.45	1.34
82	TG	201	PEB	C2D-C3D	8.71	1.45	1.34
82	BK	201	PEB	C2D-C3D	8.71	1.45	1.34
82	S5	203	PEB	C2D-C3D	8.71	1.45	1.34
82	KM	202	PEB	C2D-C3D	8.71	1.45	1.34
82	W4	201	PEB	C2D-C3D	8.71	1.45	1.34
82	hJ	203	PEB	C2D-C3D	8.71	1.45	1.34
82	uF	201	PEB	C2D-C3D	8.71	1.45	1.34
82	p8	202	PEB	C4C-C3C	8.71	1.50	1.37
82	S4	202	PEB	C2D-C3D	8.71	1.45	1.34
82	AJ	301	PEB	C2D-C3D	8.71	1.45	1.34
82	lH	201	PEB	C4C-C3C	8.71	1.50	1.37
82	pC	202	PEB	C4C-C3C	8.71	1.50	1.37
82	XJ	201	PEB	C4C-C3C	8.70	1.50	1.37
82	O5	202	PEB	C4C-C3C	8.70	1.50	1.37
82	T1	201	PEB	C2D-C3D	8.70	1.45	1.34
82	KP	202	PEB	C2D-C3D	8.70	1.45	1.34
82	UA	202	PEB	C4C-C3C	8.70	1.50	1.37
82	jK	201	PEB	C4C-C3C	8.70	1.50	1.37
82	bK	201	PEB	C4C-C3C	8.70	1.50	1.37
82	FI	201	PEB	C2D-C3D	8.70	1.45	1.34
83	A1	303	PUB	C1B-C2B	8.70	1.50	1.37
82	aB	202	PEB	C4C-C3C	8.70	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kH	201	PEB	C4C-C3C	8.69	1.50	1.37
82	fH	201	PEB	C4C-C3C	8.69	1.50	1.37
82	IJ	203	PEB	C2D-C3D	8.69	1.45	1.34
82	QE	201	PEB	C4C-C3C	8.69	1.50	1.37
82	JB	202	PEB	C2D-C3D	8.69	1.45	1.34
82	cH	201	PEB	C4C-C3C	8.69	1.50	1.37
82	DG	1002	PEB	C2D-C3D	8.69	1.45	1.34
82	OO	202	PEB	C2D-C3D	8.69	1.45	1.34
82	D7	203	PEB	C4C-C3C	8.69	1.50	1.37
82	RK	202	PEB	C2D-C3D	8.69	1.45	1.34
82	PD	202	PEB	C4C-C3C	8.68	1.50	1.37
82	c1	201	PEB	C4C-C3C	8.68	1.50	1.37
82	yK	301	PEB	C4C-C3C	8.68	1.50	1.37
82	VO	202	PEB	C4C-C3C	8.68	1.50	1.37
82	WP	201	PEB	C2D-C3D	8.68	1.45	1.34
82	OQ	202	PEB	C4C-C3C	8.68	1.50	1.37
83	QM	201	PUB	C1B-C2B	8.68	1.50	1.37
82	YK	202	PEB	C4C-C3C	8.67	1.50	1.37
82	k1	201	PEB	C4C-C3C	8.67	1.50	1.37
82	lO	201	PEB	C4C-C3C	8.67	1.50	1.37
82	QB	201	PEB	C2D-C3D	8.67	1.45	1.34
82	DK	201	PEB	C4C-C3C	8.67	1.50	1.37
82	F9	203	PEB	C4C-C3C	8.67	1.50	1.37
82	U7	201	PEB	C2D-C3D	8.67	1.45	1.34
82	dH	201	PEB	C4C-C3C	8.67	1.50	1.37
82	TB	202	PEB	C2D-C3D	8.66	1.45	1.34
82	lJ	202	PEB	C2D-C3D	8.66	1.45	1.34
82	iO	203	PEB	C4C-C3C	8.66	1.50	1.37
82	QH	203	PEB	C4C-C3C	8.66	1.50	1.37
82	WQ	202	PEB	C4C-C3C	8.66	1.50	1.37
82	eG	203	PEB	C4C-C3C	8.66	1.50	1.37
82	JD	202	PEB	C4C-C3C	8.66	1.50	1.37
82	QK	201	PEB	C4C-C3C	8.66	1.50	1.37
82	TF	202	PEB	C2D-C3D	8.66	1.45	1.34
82	OB	201	PEB	C2D-C3D	8.66	1.45	1.34
82	AK	202	PEB	C4C-C3C	8.65	1.50	1.37
82	S5	201	PEB	C4C-C3C	8.65	1.50	1.37
82	jG	202	PEB	C4C-C3C	8.65	1.50	1.37
82	YJ	202	PEB	C2D-C3D	8.65	1.45	1.34
82	QF	201	PEB	C4C-C3C	8.65	1.50	1.37
82	V7	202	PEB	C4C-C3C	8.65	1.50	1.37
82	OP	201	PEB	C2D-C3D	8.65	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SB	202	PEB	C2D-C3D	8.65	1.45	1.34
82	UA	201	PEB	C2D-C3D	8.64	1.45	1.34
82	bF	201	PEB	C4C-C3C	8.64	1.50	1.37
82	WJ	201	PEB	C2D-C3D	8.64	1.45	1.34
82	i4	203	PEB	C4C-C3C	8.64	1.50	1.37
82	CB	202	PEB	C4C-C3C	8.64	1.50	1.37
82	QE	203	PEB	C4C-C3C	8.64	1.50	1.37
82	AF	202	PEB	C4C-C3C	8.64	1.50	1.37
82	GA	202	PEB	C4C-C3C	8.64	1.50	1.37
82	PB	201	PEB	C4C-C3C	8.64	1.50	1.37
82	O9	203	PEB	C4C-C3C	8.64	1.50	1.37
82	zF	501	PEB	C4C-C3C	8.64	1.50	1.37
82	DA	203	PEB	C4C-C3C	8.64	1.50	1.37
82	f1	203	PEB	C4C-C3C	8.64	1.50	1.37
82	TK	202	PEB	C2D-C3D	8.64	1.45	1.34
82	OD	202	PEB	C4C-C3C	8.64	1.50	1.37
82	JI	202	PEB	C4C-C3C	8.63	1.50	1.37
82	QG	201	PEB	C4C-C3C	8.63	1.50	1.37
82	Y5	203	PEB	C4C-C3C	8.63	1.50	1.37
82	sK	202	PEB	C4C-C3C	8.63	1.50	1.37
82	l1	203	PEB	C4C-C3C	8.63	1.50	1.37
82	G7	202	PEB	C4C-C3C	8.63	1.50	1.37
82	gO	203	PEB	C4C-C3C	8.63	1.50	1.37
82	A1	302	PEB	C4C-C3C	8.62	1.50	1.37
82	CK	202	PEB	C4C-C3C	8.62	1.50	1.37
82	u8	202	PEB	C2D-C3D	8.62	1.45	1.34
82	Y5	203	PEB	C2D-C3D	8.62	1.45	1.34
82	fH	203	PEB	C4C-C3C	8.61	1.50	1.37
82	dO	202	PEB	C4C-C3C	8.61	1.50	1.37
83	Z9	302	PUB	C1B-C2B	8.61	1.50	1.37
82	Q1	203	PEB	C4C-C3C	8.61	1.50	1.37
82	pK	201	PEB	C4C-C3C	8.61	1.50	1.37
82	KJ	201	PEB	C2D-C3D	8.61	1.45	1.34
82	WD	202	PEB	C4C-C3C	8.61	1.50	1.37
82	e4	202	PEB	C4C-C3C	8.61	1.50	1.37
82	lH	202	PEB	C4C-C3C	8.61	1.50	1.37
82	VA	202	PEB	C4C-C3C	8.60	1.50	1.37
82	QD	201	PEB	C4C-C3C	8.60	1.50	1.37
82	iE	202	PEB	C4C-C3C	8.60	1.50	1.37
82	AQ	301	PEB	C4C-C3C	8.60	1.50	1.37
82	uC	202	PEB	C2D-C3D	8.60	1.45	1.34
82	UP	202	PEB	C4C-C3C	8.60	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	s8	203	PEB	C4C-C3C	8.60	1.50	1.37
82	BD	202	PEB	C4C-C3C	8.60	1.50	1.37
82	H9	201	PEB	C4C-C3C	8.60	1.50	1.37
82	eO	202	PEB	C4C-C3C	8.60	1.50	1.37
82	AH	302	PEB	C4C-C3C	8.60	1.50	1.37
82	B7	202	PEB	C4C-C3C	8.60	1.50	1.37
87	6N	608	CLA	C1D-ND	8.60	1.48	1.37
82	AH	305	PEB	C4C-C3C	8.60	1.50	1.37
82	LI	201	PEB	C2D-C3D	8.60	1.45	1.34
82	Z5	301	PEB	C4C-C3C	8.59	1.50	1.37
82	kF	202	PEB	C4C-C3C	8.59	1.50	1.37
82	fJ	201	PEB	C4C-C3C	8.59	1.50	1.37
82	FK	202	PEB	C2D-C3D	8.59	1.45	1.34
82	XD	202	PEB	C4C-C3C	8.59	1.50	1.37
82	XQ	202	PEB	C4C-C3C	8.59	1.50	1.37
82	M5	301	PEB	C4C-C3C	8.59	1.50	1.37
82	AD	301	PEB	C4C-C3C	8.59	1.50	1.37
82	OF	201	PEB	C2D-C3D	8.59	1.45	1.34
82	cH	202	PEB	C4C-C3C	8.59	1.50	1.37
82	i1	201	PEB	C4C-C3C	8.58	1.50	1.37
82	cB	401	PEB	C4C-C3C	8.58	1.50	1.37
82	m1	202	PEB	C4C-C3C	8.58	1.50	1.37
82	WO	201	PEB	C4C-C3C	8.58	1.50	1.37
82	F7	203	PEB	C4C-C3C	8.58	1.50	1.37
82	YQ	201	PEB	C4C-C3C	8.58	1.50	1.37
82	mH	202	PEB	C4C-C3C	8.58	1.50	1.37
82	zK	501	PEB	C4C-C3C	8.58	1.50	1.37
82	j4	202	PEB	C4C-C3C	8.58	1.50	1.37
82	jM	201	PEB	C4C-C3C	8.58	1.50	1.37
82	f1	201	PEB	C4C-C3C	8.57	1.50	1.37
82	eE	202	PEB	C4C-C3C	8.57	1.50	1.37
91	dL	403	PHO	C1D-C2D	8.57	1.49	1.39
82	gH	202	PEB	C4C-C3C	8.57	1.50	1.37
82	NB	203	PEB	C4C-C3C	8.57	1.50	1.37
82	MQ	202	PEB	C4C-C3C	8.57	1.50	1.37
82	FA	203	PEB	C4C-C3C	8.57	1.50	1.37
87	62	309	CLA	C1D-ND	8.56	1.48	1.37
82	Y4	201	PEB	C4C-C3C	8.56	1.50	1.37
82	WH	203	PEB	C4C-C3C	8.56	1.50	1.37
82	QI	201	PEB	C4C-C3C	8.56	1.50	1.37
82	g1	202	PEB	C4C-C3C	8.56	1.50	1.37
82	aH	201	PEB	C4C-C3C	8.56	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MA	202	PEB	C4C-C3C	8.56	1.50	1.37
82	c1	202	PEB	C4C-C3C	8.56	1.50	1.37
82	M7	202	PEB	C4C-C3C	8.56	1.50	1.37
82	BD	201	PEB	C2D-C3D	8.56	1.45	1.34
82	fO	202	PEB	C4C-C3C	8.56	1.50	1.37
83	M9	303	PUB	C1B-C2B	8.56	1.50	1.37
82	LA	203	PEB	C4C-C3C	8.56	1.50	1.37
82	xK	304	PEB	C4C-C3C	8.56	1.50	1.37
82	UQ	201	PEB	C4C-C3C	8.55	1.50	1.37
82	UF	202	PEB	C4C-C3C	8.55	1.50	1.37
82	d1	201	PEB	C4C-C3C	8.55	1.50	1.37
82	zC	202	PEB	C4C-C3C	8.55	1.50	1.37
82	hO	202	PEB	C4C-C3C	8.55	1.50	1.37
82	ZG	201	PEB	C4C-C3C	8.55	1.50	1.37
82	sC	203	PEB	C4C-C3C	8.55	1.50	1.37
82	A1	305	PEB	C4C-C3C	8.55	1.50	1.37
82	OO	201	PEB	C4C-C3C	8.55	1.50	1.37
82	iG	202	PEB	C4C-C3C	8.55	1.50	1.37
82	d4	202	PEB	C4C-C3C	8.55	1.50	1.37
82	aE	201	PEB	C4C-C3C	8.55	1.50	1.37
82	jE	202	PEB	C4C-C3C	8.54	1.50	1.37
82	DD	202	PEB	C4C-C3C	8.54	1.50	1.37
82	DQ	202	PEB	C4C-C3C	8.54	1.50	1.37
82	h4	202	PEB	C4C-C3C	8.54	1.50	1.37
82	eG	202	PEB	C4C-C3C	8.54	1.50	1.37
82	EM	202	PEB	C4C-C3C	8.54	1.50	1.37
82	q8	203	PEB	C4C-C3C	8.54	1.50	1.37
82	UD	201	PEB	C4C-C3C	8.54	1.50	1.37
82	lG	202	PEB	C4C-C3C	8.54	1.50	1.37
82	eF	201	PEB	C4C-C3C	8.54	1.50	1.37
82	CJ	201	PEB	C2D-C3D	8.54	1.45	1.34
82	TH	201	PEB	C2D-C3D	8.54	1.45	1.34
82	P1	202	PEB	C4C-C3C	8.54	1.50	1.37
82	RO	202	PEB	C4C-C3C	8.54	1.50	1.37
82	YF	202	PEB	C4C-C3C	8.54	1.50	1.37
83	xK	305	PUB	C1B-C2B	8.54	1.50	1.37
82	WI	203	PEB	C4C-C3C	8.54	1.50	1.37
82	dE	201	PEB	C4C-C3C	8.54	1.50	1.37
82	AQ	303	PEB	C4C-C3C	8.54	1.50	1.37
82	J9	202	PEB	C4C-C3C	8.54	1.50	1.37
82	L5	202	PEB	C4C-C3C	8.53	1.50	1.37
82	B5	201	PEB	C2D-C3D	8.53	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	qC	203	PEB	C4C-C3C	8.53	1.50	1.37
82	mF	202	PEB	C4C-C3C	8.53	1.50	1.37
82	AD	304	PEB	C4C-C3C	8.53	1.50	1.37
82	T9	202	PEB	C4C-C3C	8.53	1.50	1.37
82	vK	201	PEB	C4C-C3C	8.53	1.50	1.37
83	yK	303	PUB	C1B-C2B	8.53	1.50	1.37
82	KJ	202	PEB	C2D-C3D	8.53	1.45	1.34
82	kK	202	PEB	C4C-C3C	8.53	1.50	1.37
82	YP	502	PEB	C2D-C3D	8.53	1.45	1.34
82	g4	203	PEB	C4C-C3C	8.53	1.50	1.37
82	lF	203	PEB	C4C-C3C	8.53	1.50	1.37
82	TI	201	PEB	C2D-C3D	8.53	1.45	1.34
82	NB	201	PEB	C2D-C3D	8.53	1.45	1.34
82	IJ	202	PEB	C2D-C3D	8.53	1.45	1.34
82	e1	201	PEB	C4C-C3C	8.53	1.50	1.37
82	d4	201	PEB	C4C-C3C	8.53	1.50	1.37
82	qC	201	PEB	C4C-C3C	8.53	1.50	1.37
83	xK	301	PUB	C1B-C2B	8.53	1.50	1.37
82	1C	201	PEB	C4C-C3C	8.52	1.50	1.37
82	dG	201	PEB	C4C-C3C	8.52	1.50	1.37
82	vF	201	PEB	C4C-C3C	8.52	1.50	1.37
82	gJ	202	PEB	C4C-C3C	8.52	1.50	1.37
82	TB	201	PEB	C2D-C3D	8.52	1.45	1.34
82	P9	202	PEB	C4C-C3C	8.52	1.50	1.37
82	X9	201	PEB	C4C-C3C	8.52	1.50	1.37
82	aK	201	PEB	C4C-C3C	8.52	1.50	1.37
82	q8	201	PEB	C4C-C3C	8.52	1.50	1.37
82	Z9	303	PEB	C4C-C3C	8.52	1.50	1.37
82	JB	201	PEB	C2D-C3D	8.51	1.45	1.34
82	F9	202	PEB	C4C-C3C	8.51	1.50	1.37
82	tF	201	PEB	C4C-C3C	8.51	1.50	1.37
82	BA	202	PEB	C4C-C3C	8.51	1.50	1.37
82	BQ	202	PEB	C4C-C3C	8.51	1.50	1.37
82	OE	203	PEB	C4C-C3C	8.51	1.50	1.37
82	W1	203	PEB	C4C-C3C	8.51	1.50	1.37
82	L9	203	PEB	C4C-C3C	8.51	1.50	1.37
82	MD	202	PEB	C4C-C3C	8.51	1.50	1.37
82	YO	201	PEB	C4C-C3C	8.51	1.50	1.37
82	z8	202	PEB	C4C-C3C	8.51	1.50	1.37
82	I9	202	PEB	C4C-C3C	8.51	1.50	1.37
82	pF	201	PEB	C4C-C3C	8.51	1.50	1.37
82	WJ	202	PEB	C2D-C3D	8.51	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DF	202	PEB	C2D-C3D	8.51	1.45	1.34
82	CK	203	PEB	C4C-C3C	8.51	1.50	1.37
82	aB	201	PEB	C2D-C3D	8.51	1.45	1.34
83	xF	301	PUB	C1B-C2B	8.51	1.50	1.37
82	dO	201	PEB	C4C-C3C	8.51	1.50	1.37
82	MK	201	PEB	C4C-C3C	8.51	1.50	1.37
82	A9	201	PEB	C4C-C3C	8.51	1.50	1.37
82	iH	201	PEB	C4C-C3C	8.50	1.50	1.37
82	RO	201	PEB	C4C-C3C	8.50	1.50	1.37
82	VB	202	PEB	C4C-C3C	8.50	1.50	1.37
82	L9	201	PEB	C4C-C3C	8.50	1.50	1.37
82	C9	201	PEB	C4C-C3C	8.50	1.50	1.37
82	jO	202	PEB	C4C-C3C	8.50	1.50	1.37
82	SO	201	PEB	C4C-C3C	8.50	1.50	1.37
82	M9	304	PEB	C4C-C3C	8.50	1.50	1.37
82	G9	201	PEB	C4C-C3C	8.49	1.50	1.37
82	aF	201	PEB	C4C-C3C	8.49	1.50	1.37
83	xF	305	PUB	C1B-C2B	8.49	1.50	1.37
82	KB	302	PEB	C2D-C3D	8.49	1.45	1.34
82	D9	201	PEB	C4C-C3C	8.49	1.50	1.37
82	X9	202	PEB	C4C-C3C	8.49	1.50	1.37
82	V9	202	PEB	C4C-C3C	8.49	1.50	1.37
82	eK	201	PEB	C4C-C3C	8.49	1.50	1.37
82	R9	202	PEB	C4C-C3C	8.49	1.50	1.37
82	aG	201	PEB	C4C-C3C	8.49	1.50	1.37
82	P4	202	PEB	C4C-C3C	8.49	1.50	1.37
82	I9	201	PEB	C4C-C3C	8.49	1.50	1.37
82	K9	201	PEB	C4C-C3C	8.49	1.50	1.37
82	N9	201	PEB	C4C-C3C	8.49	1.50	1.37
82	oF	203	PEB	C4C-C3C	8.49	1.50	1.37
82	VA	203	PEB	C4C-C3C	8.48	1.50	1.37
82	LP	201	PEB	C4C-C3C	8.48	1.50	1.37
82	O4	201	PEB	C4C-C3C	8.48	1.50	1.37
82	KD	202	PEB	C4C-C3C	8.48	1.50	1.37
82	JQ	201	PEB	C4C-C3C	8.48	1.50	1.37
82	b4	202	PEB	C4C-C3C	8.48	1.50	1.37
82	eH	201	PEB	C4C-C3C	8.48	1.50	1.37
82	D5	202	PEB	C4C-C3C	8.48	1.50	1.37
82	wF	302	PEB	C4C-C3C	8.48	1.50	1.37
82	XP	201	PEB	C4C-C3C	8.48	1.50	1.37
82	W4	201	PEB	C4C-C3C	8.48	1.50	1.37
82	C9	202	PEB	C4C-C3C	8.48	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kE	201	PEB	C4C-C3C	8.48	1.50	1.37
82	HA	203	PEB	C4C-C3C	8.48	1.50	1.37
82	E9	202	PEB	C4C-C3C	8.48	1.50	1.37
82	R9	201	PEB	C4C-C3C	8.48	1.50	1.37
82	OM	203	PEB	C4C-C3C	8.47	1.50	1.37
82	DB	203	PEB	C4C-C3C	8.47	1.50	1.37
82	QQ	201	PEB	C4C-C3C	8.47	1.50	1.37
82	ZK	201	PEB	C4C-C3C	8.47	1.50	1.37
82	K9	202	PEB	C4C-C3C	8.47	1.50	1.37
82	18	201	PEB	C4C-C3C	8.47	1.50	1.37
82	SE	202	PEB	C4C-C3C	8.47	1.50	1.37
82	fG	202	PEB	C4C-C3C	8.47	1.50	1.37
82	CQ	202	PEB	C4C-C3C	8.47	1.50	1.37
83	QJ	201	PUB	C1B-C2B	8.47	1.50	1.37
82	W5	203	PEB	C4C-C3C	8.47	1.50	1.37
82	N9	202	PEB	C4C-C3C	8.46	1.50	1.37
82	WJ	203	PEB	C2D-C3D	8.46	1.45	1.34
82	XK	202	PEB	C2D-C3D	8.46	1.45	1.34
82	kG	201	PEB	C4C-C3C	8.46	1.50	1.37
82	cJ	202	PEB	C4C-C3C	8.46	1.50	1.37
82	bO	202	PEB	C4C-C3C	8.46	1.50	1.37
82	oK	203	PEB	C4C-C3C	8.46	1.50	1.37
82	AD	303	PEB	C4C-C3C	8.46	1.50	1.37
82	H7	203	PEB	C4C-C3C	8.46	1.50	1.37
82	T9	201	PEB	C4C-C3C	8.46	1.50	1.37
82	aF	202	PEB	C4C-C3C	8.46	1.50	1.37
82	KA	202	PEB	C4C-C3C	8.45	1.50	1.37
82	BB	202	PEB	C2D-C3D	8.45	1.45	1.34
82	CJ	202	PEB	C2D-C3D	8.45	1.45	1.34
82	SG	203	PEB	C4C-C3C	8.45	1.50	1.37
82	eE	201	PEB	C4C-C3C	8.45	1.50	1.37
82	P9	201	PEB	C4C-C3C	8.45	1.50	1.37
82	VM	202	PEB	C4C-C3C	8.45	1.50	1.37
82	a4	203	PEB	C4C-C3C	8.45	1.50	1.37
82	OI	203	PEB	C4C-C3C	8.45	1.50	1.37
82	hE	202	PEB	C4C-C3C	8.45	1.50	1.37
82	SM	201	PEB	C4C-C3C	8.45	1.50	1.37
82	U9	202	PEB	C4C-C3C	8.45	1.50	1.37
82	AA	202	PEB	C4C-C3C	8.45	1.50	1.37
82	CD	202	PEB	C4C-C3C	8.45	1.50	1.37
82	a1	201	PEB	C4C-C3C	8.45	1.50	1.37
82	mJ	202	PEB	C4C-C3C	8.45	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	tK	201	PEB	C4C-C3C	8.45	1.50	1.37
82	DK	202	PEB	C2D-C3D	8.45	1.45	1.34
82	PF	201	PEB	C4C-C3C	8.45	1.50	1.37
82	L7	203	PEB	C4C-C3C	8.45	1.50	1.37
82	bG	201	PEB	C4C-C3C	8.44	1.50	1.37
82	KQ	202	PEB	C4C-C3C	8.44	1.50	1.37
82	OG	203	PEB	C4C-C3C	8.44	1.50	1.37
82	G9	202	PEB	C4C-C3C	8.44	1.50	1.37
82	dE	203	PEB	C4C-C3C	8.44	1.50	1.37
82	U5	203	PEB	C4C-C3C	8.44	1.50	1.37
82	A9	202	PEB	C4C-C3C	8.44	1.50	1.37
82	ZE	201	PEB	C4C-C3C	8.44	1.50	1.37
82	EK	202	PEB	C4C-C3C	8.44	1.50	1.37
82	YP	501	PEB	C2D-C3D	8.44	1.45	1.34
82	dG	203	PEB	C4C-C3C	8.44	1.50	1.37
82	O9	201	PEB	C4C-C3C	8.44	1.50	1.37
83	yF	303	PUB	C1B-C2B	8.44	1.50	1.37
82	YD	201	PEB	C4C-C3C	8.43	1.50	1.37
82	R4	202	PEB	C4C-C3C	8.43	1.50	1.37
82	O5	203	PEB	C4C-C3C	8.43	1.50	1.37
82	xC	201	PEB	C4C-C3C	8.43	1.50	1.37
82	fE	202	PEB	C4C-C3C	8.43	1.50	1.37
83	K7	203	PUB	C1B-C2B	8.43	1.50	1.37
82	FD	201	PEB	C2D-C3D	8.43	1.45	1.34
82	DP	202	PEB	C4C-C3C	8.43	1.50	1.37
82	aK	202	PEB	C4C-C3C	8.43	1.50	1.37
82	FF	202	PEB	C2D-C3D	8.43	1.45	1.34
82	XF	202	PEB	C2D-C3D	8.43	1.45	1.34
82	JP	202	PEB	C4C-C3C	8.43	1.50	1.37
82	f4	202	PEB	C4C-C3C	8.43	1.50	1.37
82	Y4	202	PEB	C4C-C3C	8.43	1.50	1.37
82	x8	201	PEB	C4C-C3C	8.43	1.50	1.37
82	M9	302	PEB	C4C-C3C	8.43	1.50	1.37
83	AH	304	PUB	C1B-C2B	8.42	1.50	1.37
83	A1	304	PUB	C1B-C2B	8.42	1.50	1.37
82	JI	201	PEB	C4C-C3C	8.42	1.50	1.37
82	K7	202	PEB	C4C-C3C	8.42	1.50	1.37
82	R4	201	PEB	C4C-C3C	8.42	1.50	1.37
82	V9	201	PEB	C4C-C3C	8.42	1.50	1.37
82	V7	203	PEB	C4C-C3C	8.42	1.50	1.37
82	E9	201	PEB	C4C-C3C	8.42	1.50	1.37
82	U9	203	PEB	C4C-C3C	8.42	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	AJ	304	PUB	C1B-C2B	8.42	1.50	1.37
82	G7	201	PEB	C4C-C3C	8.42	1.50	1.37
82	kJ	202	PEB	C4C-C3C	8.42	1.50	1.37
82	FI	202	PEB	C4C-C3C	8.41	1.50	1.37
82	eG	201	PEB	C4C-C3C	8.41	1.50	1.37
82	lK	203	PEB	C4C-C3C	8.41	1.50	1.37
82	aO	203	PEB	C4C-C3C	8.41	1.50	1.37
82	Z9	301	PEB	C4C-C3C	8.41	1.50	1.37
82	VP	202	PEB	C4C-C3C	8.41	1.50	1.37
82	S5	201	PEB	C2D-C3D	8.41	1.45	1.34
82	d1	202	PEB	C4C-C3C	8.41	1.50	1.37
82	WB	401	PEB	C2D-C3D	8.41	1.45	1.34
82	ZO	202	PEB	C4C-C3C	8.41	1.50	1.37
82	AI	203	PEB	C2D-C3D	8.41	1.45	1.34
83	AM	303	PUB	C1B-C2B	8.41	1.50	1.37
82	PO	202	PEB	C4C-C3C	8.40	1.50	1.37
82	OH	202	PEB	C4C-C3C	8.40	1.49	1.37
82	hG	202	PEB	C4C-C3C	8.40	1.49	1.37
82	Q5	203	PEB	C4C-C3C	8.40	1.49	1.37
82	MF	201	PEB	C4C-C3C	8.40	1.49	1.37
82	cG	202	PEB	C4C-C3C	8.40	1.49	1.37
82	oK	202	PEB	C4C-C3C	8.40	1.49	1.37
82	OF	201	PEB	C4C-C3C	8.40	1.49	1.37
82	O1	202	PEB	C4C-C3C	8.40	1.49	1.37
82	TH	201	PEB	C4C-C3C	8.40	1.49	1.37
82	BP	201	PEB	C4C-C3C	8.39	1.49	1.37
82	JJ	202	PEB	C4C-C3C	8.39	1.49	1.37
82	GK	201	PEB	C4C-C3C	8.39	1.49	1.37
82	SI	201	PEB	C2D-C3D	8.39	1.45	1.34
82	XM	202	PEB	C4C-C3C	8.39	1.49	1.37
82	PH	202	PEB	C4C-C3C	8.39	1.49	1.37
82	GA	201	PEB	C4C-C3C	8.38	1.49	1.37
82	cE	202	PEB	C4C-C3C	8.38	1.49	1.37
82	B5	201	PEB	C4C-C3C	8.38	1.49	1.37
82	dH	202	PEB	C4C-C3C	8.38	1.49	1.37
82	hO	201	PEB	C4C-C3C	8.38	1.49	1.37
82	bE	201	PEB	C4C-C3C	8.38	1.49	1.37
82	J5	203	PEB	C4C-C3C	8.38	1.49	1.37
82	TA	202	PEB	C4C-C3C	8.38	1.49	1.37
82	QB	202	PEB	C4C-C3C	8.38	1.49	1.37
82	L1	1002	PEB	C2D-C3D	8.38	1.45	1.34
82	i4	202	PEB	C4C-C3C	8.38	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EA	201	PEB	C4C-C3C	8.37	1.49	1.37
82	A4	301	PEB	C4C-C3C	8.37	1.49	1.37
82	cO	202	PEB	C4C-C3C	8.37	1.49	1.37
82	JA	202	PEB	C4C-C3C	8.37	1.49	1.37
82	UK	202	PEB	C4C-C3C	8.37	1.49	1.37
82	U1	201	PEB	C4C-C3C	8.37	1.49	1.37
82	dE	202	PEB	C4C-C3C	8.37	1.49	1.37
82	xF	302	PEB	C4C-C3C	8.37	1.49	1.37
82	LF	202	PEB	C2D-C3D	8.37	1.45	1.34
82	ZG	202	PEB	C4C-C3C	8.37	1.49	1.37
82	SD	201	PEB	C4C-C3C	8.37	1.49	1.37
82	ZF	201	PEB	C4C-C3C	8.37	1.49	1.37
82	G5	202	PEB	C4C-C3C	8.37	1.49	1.37
82	FQ	201	PEB	C2D-C3D	8.37	1.45	1.34
82	EF	202	PEB	C4C-C3C	8.37	1.49	1.37
82	AQ	304	PEB	C4C-C3C	8.37	1.49	1.37
82	T7	202	PEB	C4C-C3C	8.37	1.49	1.37
82	DB	201	PEB	C4C-C3C	8.37	1.49	1.37
82	w8	201	PEB	C4C-C3C	8.37	1.49	1.37
82	TG	201	PEB	C4C-C3C	8.36	1.49	1.37
82	GJ	201	PEB	C4C-C3C	8.36	1.49	1.37
82	GF	201	PEB	C4C-C3C	8.36	1.49	1.37
82	HP	201	PEB	C4C-C3C	8.36	1.49	1.37
82	v8	202	PEB	C4C-C3C	8.36	1.49	1.37
82	cF	203	PEB	C4C-C3C	8.36	1.49	1.37
82	mK	202	PEB	C4C-C3C	8.36	1.49	1.37
82	l4	202	PEB	C4C-C3C	8.36	1.49	1.37
82	wC	203	PEB	C4C-C3C	8.36	1.49	1.37
82	wK	302	PEB	C4C-C3C	8.36	1.49	1.37
82	BP	202	PEB	C4C-C3C	8.36	1.49	1.37
82	IB	202	PEB	C2D-C3D	8.36	1.45	1.34
82	VD	201	PEB	C4C-C3C	8.36	1.49	1.37
82	cE	201	PEB	C4C-C3C	8.36	1.49	1.37
82	JH	1002	PEB	C4C-C3C	8.36	1.49	1.37
82	QM	203	PEB	C4C-C3C	8.36	1.49	1.37
82	U4	201	PEB	C4C-C3C	8.36	1.49	1.37
82	EM	201	PEB	C4C-C3C	8.36	1.49	1.37
82	BM	301	PEB	C4C-C3C	8.36	1.49	1.37
82	VQ	201	PEB	C4C-C3C	8.36	1.49	1.37
82	eO	201	PEB	C4C-C3C	8.36	1.49	1.37
82	QE	202	PEB	C4C-C3C	8.35	1.49	1.37
82	JD	201	PEB	C4C-C3C	8.35	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	xF	304	PEB	C4C-C3C	8.35	1.49	1.37
83	BM	302	PUB	C1B-C2B	8.35	1.49	1.37
82	IA	202	PEB	C4C-C3C	8.35	1.49	1.37
82	UI	202	PEB	C4C-C3C	8.35	1.49	1.37
82	dB	201	PEB	C2D-C3D	8.35	1.45	1.34
82	IK	203	PEB	C4C-C3C	8.35	1.49	1.37
82	SQ	201	PEB	C4C-C3C	8.35	1.49	1.37
82	GB	201	PEB	C4C-C3C	8.35	1.49	1.37
82	EJ	202	PEB	C4C-C3C	8.35	1.49	1.37
82	R5	202	PEB	C4C-C3C	8.35	1.49	1.37
82	VG	201	PEB	C4C-C3C	8.35	1.49	1.37
82	E5	202	PEB	C4C-C3C	8.35	1.49	1.37
82	u8	203	PEB	C4C-C3C	8.35	1.49	1.37
82	NK	201	PEB	C4C-C3C	8.35	1.49	1.37
82	uC	203	PEB	C4C-C3C	8.35	1.49	1.37
82	RA	201	PEB	C4C-C3C	8.35	1.49	1.37
82	KE	201	PEB	C4C-C3C	8.35	1.49	1.37
82	L5	203	PEB	C4C-C3C	8.35	1.49	1.37
82	T7	203	PEB	C4C-C3C	8.35	1.49	1.37
82	MB	201	PEB	C2D-C3D	8.35	1.45	1.34
82	S4	201	PEB	C4C-C3C	8.34	1.49	1.37
82	JD	203	PEB	C2D-C3D	8.34	1.45	1.34
82	KB	304	PEB	C2D-C3D	8.34	1.45	1.34
82	AA	201	PEB	C4C-C3C	8.34	1.49	1.37
82	V5	202	PEB	C4C-C3C	8.34	1.49	1.37
82	I7	202	PEB	C4C-C3C	8.34	1.49	1.37
82	T4	202	PEB	C4C-C3C	8.34	1.49	1.37
82	h4	201	PEB	C4C-C3C	8.34	1.49	1.37
82	A7	202	PEB	C4C-C3C	8.33	1.49	1.37
82	QG	202	PEB	C4C-C3C	8.33	1.49	1.37
82	HM	202	PEB	C4C-C3C	8.33	1.49	1.37
82	PO	203	PEB	C4C-C3C	8.33	1.49	1.37
82	FA	201	PEB	C4C-C3C	8.33	1.49	1.37
82	KQ	201	PEB	C4C-C3C	8.33	1.49	1.37
82	hE	201	PEB	C4C-C3C	8.33	1.49	1.37
82	WA	202	PEB	C4C-C3C	8.33	1.49	1.37
82	IF	203	PEB	C4C-C3C	8.33	1.49	1.37
82	lO	202	PEB	C4C-C3C	8.33	1.49	1.37
82	GM	201	PEB	C4C-C3C	8.33	1.49	1.37
82	kM	202	PEB	C4C-C3C	8.33	1.49	1.37
82	A5	202	PEB	C4C-C3C	8.33	1.49	1.37
82	LM	202	PEB	C4C-C3C	8.33	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OH	203	PEB	C4C-C3C	8.33	1.49	1.37
82	O1	203	PEB	C4C-C3C	8.33	1.49	1.37
82	dG	202	PEB	C4C-C3C	8.33	1.49	1.37
82	D1	1002	PEB	C4C-C3C	8.32	1.49	1.37
82	iG	201	PEB	C4C-C3C	8.32	1.49	1.37
82	WI	201	PEB	C4C-C3C	8.32	1.49	1.37
82	EQ	201	PEB	C4C-C3C	8.32	1.49	1.37
82	A7	201	PEB	C4C-C3C	8.32	1.49	1.37
82	MM	203	PEB	C2D-C3D	8.32	1.45	1.34
82	I5	202	PEB	C4C-C3C	8.32	1.49	1.37
82	ZE	202	PEB	C4C-C3C	8.32	1.49	1.37
82	gB	202	PEB	C4C-C3C	8.32	1.49	1.37
82	KB	301	PEB	C4C-C3C	8.32	1.49	1.37
82	GF	203	PEB	C4C-C3C	8.32	1.49	1.37
82	PK	201	PEB	C4C-C3C	8.32	1.49	1.37
82	J7	202	PEB	C4C-C3C	8.32	1.49	1.37
82	VJ	202	PEB	C4C-C3C	8.32	1.49	1.37
82	c4	201	PEB	C4C-C3C	8.31	1.49	1.37
82	F7	201	PEB	C4C-C3C	8.31	1.49	1.37
82	hG	201	PEB	C4C-C3C	8.31	1.49	1.37
82	PP	202	PEB	C4C-C3C	8.31	1.49	1.37
82	Q9	202	PEB	C4C-C3C	8.31	1.49	1.37
82	UO	201	PEB	C4C-C3C	8.31	1.49	1.37
82	cK	203	PEB	C4C-C3C	8.31	1.49	1.37
82	Y9	202	PEB	C4C-C3C	8.31	1.49	1.37
82	RM	202	PEB	C4C-C3C	8.31	1.49	1.37
82	X5	202	PEB	C4C-C3C	8.31	1.49	1.37
82	Y7	304	PEB	C4C-C3C	8.31	1.49	1.37
91	d6	404	PHO	C1B-C2B	8.31	1.48	1.39
82	ZB	201	PEB	C4C-C3C	8.31	1.49	1.37
82	A4	305	PEB	C4C-C3C	8.31	1.49	1.37
82	vC	202	PEB	C4C-C3C	8.31	1.49	1.37
82	NB	203	PEB	C2D-C3D	8.31	1.45	1.34
82	Q7	202	PEB	C4C-C3C	8.31	1.49	1.37
82	lF	201	PEB	C4C-C3C	8.31	1.49	1.37
82	ZB	202	PEB	C4C-C3C	8.31	1.49	1.37
82	lK	201	PEB	C4C-C3C	8.30	1.49	1.37
82	P5	202	PEB	C4C-C3C	8.30	1.49	1.37
82	YQ	202	PEB	C4C-C3C	8.30	1.49	1.37
83	AE	302	PUB	C1B-C2B	8.30	1.49	1.37
82	PJ	202	PEB	C4C-C3C	8.30	1.49	1.37
82	TP	201	PEB	C4C-C3C	8.30	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	QA	202	PEB	C4C-C3C	8.30	1.49	1.37
82	KK	202	PEB	C4C-C3C	8.30	1.49	1.37
82	dQ	401	PEB	C4C-C3C	8.30	1.49	1.37
82	T5	202	PEB	C4C-C3C	8.30	1.49	1.37
82	KD	201	PEB	C4C-C3C	8.30	1.49	1.37
82	OG	202	PEB	C4C-C3C	8.30	1.49	1.37
82	lG	201	PEB	C4C-C3C	8.30	1.49	1.37
82	aJ	202	PEB	C4C-C3C	8.30	1.49	1.37
82	MP	203	PEB	C2D-C3D	8.30	1.45	1.34
82	SF	201	PEB	C4C-C3C	8.30	1.49	1.37
82	LH	1003	PEB	C2D-C3D	8.30	1.45	1.34
82	FH	1002	PEB	C4C-C3C	8.30	1.49	1.37
82	dB	201	PEB	C4C-C3C	8.30	1.49	1.37
82	wF	301	PEB	C4C-C3C	8.30	1.49	1.37
82	mM	202	PEB	C4C-C3C	8.30	1.49	1.37
82	PH	201	PEB	C4C-C3C	8.30	1.49	1.37
82	a4	202	PEB	C4C-C3C	8.30	1.49	1.37
82	XA	201	PEB	C4C-C3C	8.29	1.49	1.37
82	fE	201	PEB	C4C-C3C	8.29	1.49	1.37
83	AO	303	PUB	C1B-C2B	8.29	1.49	1.37
82	N7	202	PEB	C4C-C3C	8.29	1.49	1.37
82	dE	204	PEB	C4C-C3C	8.29	1.49	1.37
82	hF	201	PEB	C4C-C3C	8.29	1.49	1.37
82	OE	202	PEB	C4C-C3C	8.29	1.49	1.37
82	AO	301	PEB	C4C-C3C	8.29	1.49	1.37
82	N5	202	PEB	C4C-C3C	8.29	1.49	1.37
82	w8	203	PEB	C4C-C3C	8.29	1.49	1.37
91	AL	410	PHO	C1D-C2D	8.29	1.48	1.39
82	HA	201	PEB	C4C-C3C	8.29	1.49	1.37
82	TA	203	PEB	C4C-C3C	8.29	1.49	1.37
82	UM	202	PEB	C4C-C3C	8.29	1.49	1.37
82	FI	201	PEB	C4C-C3C	8.29	1.49	1.37
82	SI	202	PEB	C4C-C3C	8.29	1.49	1.37
82	U5	202	PEB	C4C-C3C	8.29	1.49	1.37
91	a6	613	PHO	C1B-C2B	8.29	1.48	1.39
82	CM	203	PEB	C4C-C3C	8.29	1.49	1.37
82	CF	203	PEB	C4C-C3C	8.29	1.49	1.37
82	PG	202	PEB	C4C-C3C	8.29	1.49	1.37
82	g4	202	PEB	C4C-C3C	8.29	1.49	1.37
82	AO	305	PEB	C4C-C3C	8.29	1.49	1.37
82	dJ	201	PEB	C4C-C3C	8.29	1.49	1.37
82	iO	202	PEB	C4C-C3C	8.29	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	TD	201	PEB	C4C-C3C	8.28	1.49	1.37
82	Z4	202	PEB	C4C-C3C	8.28	1.49	1.37
82	YO	202	PEB	C4C-C3C	8.28	1.49	1.37
82	SB	201	PEB	C4C-C3C	8.28	1.49	1.37
82	P7	203	PEB	C4C-C3C	8.28	1.49	1.37
82	T1	201	PEB	C4C-C3C	8.28	1.49	1.37
82	YD	202	PEB	C4C-C3C	8.28	1.49	1.37
82	m4	202	PEB	C4C-C3C	8.28	1.49	1.37
82	KG	201	PEB	C4C-C3C	8.28	1.49	1.37
82	DH	1002	PEB	C4C-C3C	8.28	1.49	1.37
82	Q4	201	PEB	C4C-C3C	8.28	1.49	1.37
82	E7	201	PEB	C4C-C3C	8.28	1.49	1.37
82	W7	201	PEB	C2D-C3D	8.28	1.45	1.34
82	PP	201	PEB	C4C-C3C	8.28	1.49	1.37
82	KB	301	PEB	C2D-C3D	8.28	1.45	1.34
82	JQ	203	PEB	C2D-C3D	8.28	1.45	1.34
82	TO	202	PEB	C4C-C3C	8.28	1.49	1.37
82	b1	201	PEB	C4C-C3C	8.28	1.49	1.37
82	D4	1002	PEB	C4C-C3C	8.28	1.49	1.37
82	LP	202	PEB	C4C-C3C	8.28	1.49	1.37
82	aO	201	PEB	C4C-C3C	8.28	1.49	1.37
82	MD	201	PEB	C4C-C3C	8.27	1.49	1.37
82	PA	203	PEB	C4C-C3C	8.27	1.49	1.37
82	xF	303	PEB	C4C-C3C	8.27	1.49	1.37
82	m4	203	PEB	C4C-C3C	8.27	1.49	1.37
82	D7	202	PEB	C4C-C3C	8.27	1.49	1.37
82	YA	304	PEB	C4C-C3C	8.27	1.49	1.37
82	C5	202	PEB	C4C-C3C	8.27	1.49	1.37
83	AG	302	PUB	C1B-C2B	8.27	1.49	1.37
82	jJ	202	PEB	C4C-C3C	8.27	1.49	1.37
82	OK	201	PEB	C4C-C3C	8.27	1.49	1.37
82	DP	201	PEB	C4C-C3C	8.27	1.49	1.37
82	rC	202	PEB	C4C-C3C	8.27	1.49	1.37
82	NB	201	PEB	C4C-C3C	8.27	1.49	1.37
82	hM	202	PEB	C4C-C3C	8.27	1.49	1.37
83	KA	203	PUB	C1B-C2B	8.27	1.49	1.37
82	cO	201	PEB	C4C-C3C	8.27	1.49	1.37
82	J5	202	PEB	C4C-C3C	8.27	1.49	1.37
82	XP	202	PEB	C4C-C3C	8.26	1.49	1.37
82	R7	201	PEB	C4C-C3C	8.26	1.49	1.37
82	UE	203	PEB	C4C-C3C	8.26	1.49	1.37
83	AM	304	PUB	C1B-C2B	8.26	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GI	201	PEB	C2D-C3D	8.26	1.45	1.34
82	GK	203	PEB	C4C-C3C	8.26	1.49	1.37
82	AM	302	PEB	C4C-C3C	8.26	1.49	1.37
82	P1	201	PEB	C4C-C3C	8.26	1.49	1.37
82	kO	202	PEB	C4C-C3C	8.26	1.49	1.37
82	m4	201	PEB	C4C-C3C	8.26	1.49	1.37
82	IP	203	PEB	C2D-C3D	8.26	1.45	1.34
82	H7	201	PEB	C4C-C3C	8.26	1.49	1.37
82	WD	201	PEB	C4C-C3C	8.26	1.49	1.37
82	K5	202	PEB	C4C-C3C	8.26	1.49	1.37
82	ZI	401	PEB	C2D-C3D	8.26	1.45	1.34
82	PE	202	PEB	C4C-C3C	8.26	1.49	1.37
82	TE	201	PEB	C4C-C3C	8.26	1.49	1.37
82	hJ	202	PEB	C4C-C3C	8.26	1.49	1.37
82	TQ	201	PEB	C2D-C3D	8.26	1.45	1.34
82	N5	201	PEB	C4C-C3C	8.26	1.49	1.37
82	r8	202	PEB	C4C-C3C	8.26	1.49	1.37
82	X7	201	PEB	C4C-C3C	8.26	1.49	1.37
82	UG	203	PEB	C4C-C3C	8.25	1.49	1.37
82	fM	202	PEB	C4C-C3C	8.25	1.49	1.37
82	e4	201	PEB	C4C-C3C	8.25	1.49	1.37
82	VE	201	PEB	C4C-C3C	8.25	1.49	1.37
82	aO	202	PEB	C4C-C3C	8.25	1.49	1.37
82	MJ	202	PEB	C2D-C3D	8.25	1.45	1.34
82	WB	401	PEB	C4C-C3C	8.25	1.49	1.37
82	DO	1002	PEB	C4C-C3C	8.25	1.49	1.37
82	D7	201	PEB	C4C-C3C	8.25	1.49	1.37
82	SJ	201	PEB	C4C-C3C	8.25	1.49	1.37
82	tC	202	PEB	C4C-C3C	8.25	1.49	1.37
82	TD	201	PEB	C2D-C3D	8.25	1.45	1.34
82	WA	201	PEB	C2D-C3D	8.25	1.45	1.34
82	j1	202	PEB	C4C-C3C	8.25	1.49	1.37
82	xK	302	PEB	C4C-C3C	8.25	1.49	1.37
82	GP	201	PEB	CHC-C4C	8.25	1.59	1.49
82	NF	201	PEB	C4C-C3C	8.25	1.49	1.37
82	TP	202	PEB	C4C-C3C	8.25	1.49	1.37
82	W7	202	PEB	C4C-C3C	8.24	1.49	1.37
82	cG	201	PEB	C4C-C3C	8.24	1.49	1.37
82	CM	201	PEB	C4C-C3C	8.24	1.49	1.37
82	W9	202	PEB	C4C-C3C	8.24	1.49	1.37
82	iJ	202	PEB	C4C-C3C	8.24	1.49	1.37
82	HI	203	PEB	C4C-C3C	8.24	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MF	203	PEB	C4C-C3C	8.24	1.49	1.37
82	V4	201	PEB	C4C-C3C	8.24	1.49	1.37
82	NP	201	PEB	C4C-C3C	8.24	1.49	1.37
82	mO	203	PEB	C4C-C3C	8.24	1.49	1.37
82	TO	201	PEB	C4C-C3C	8.24	1.49	1.37
82	OJ	201	PEB	C4C-C3C	8.24	1.49	1.37
82	J1	1002	PEB	C4C-C3C	8.24	1.49	1.37
82	aM	201	PEB	C4C-C3C	8.24	1.49	1.37
82	CD	201	PEB	C4C-C3C	8.24	1.49	1.37
82	dG	204	PEB	C4C-C3C	8.24	1.49	1.37
82	jJ	201	PEB	C4C-C3C	8.24	1.49	1.37
82	c4	202	PEB	C4C-C3C	8.23	1.49	1.37
82	v8	201	PEB	C4C-C3C	8.23	1.49	1.37
82	EP	202	PEB	C4C-C3C	8.23	1.49	1.37
82	T4	201	PEB	C4C-C3C	8.23	1.49	1.37
82	wC	201	PEB	C4C-C3C	8.23	1.49	1.37
82	LK	202	PEB	C2D-C3D	8.23	1.45	1.34
82	bH	201	PEB	C4C-C3C	8.23	1.49	1.37
82	hK	201	PEB	C4C-C3C	8.23	1.49	1.37
82	D5	201	PEB	C4C-C3C	8.23	1.49	1.37
82	t8	202	PEB	C4C-C3C	8.23	1.49	1.37
82	j4	203	PEB	C4C-C3C	8.23	1.49	1.37
82	W9	203	PEB	C4C-C3C	8.23	1.49	1.37
82	fG	201	PEB	C4C-C3C	8.23	1.49	1.37
82	SA	202	PEB	C4C-C3C	8.23	1.49	1.37
82	G5	201	PEB	C4C-C3C	8.23	1.49	1.37
82	KF	202	PEB	C4C-C3C	8.23	1.49	1.37
82	R5	201	PEB	C4C-C3C	8.23	1.49	1.37
82	oF	202	PEB	C4C-C3C	8.23	1.49	1.37
82	MB	201	PEB	C4C-C3C	8.23	1.49	1.37
82	RM	201	PEB	C4C-C3C	8.23	1.49	1.37
82	CP	201	PEB	C2D-C3D	8.22	1.45	1.34
82	iE	201	PEB	C4C-C3C	8.22	1.49	1.37
83	AG	303	PUB	C1B-C2B	8.22	1.49	1.37
82	DB	203	PEB	C2D-C3D	8.22	1.45	1.34
82	IA	201	PEB	C4C-C3C	8.22	1.49	1.37
82	H5	203	PEB	C4C-C3C	8.22	1.49	1.37
82	PO	201	PEB	C4C-C3C	8.22	1.49	1.37
82	GB	203	PEB	C4C-C3C	8.22	1.49	1.37
82	DA	201	PEB	C4C-C3C	8.22	1.49	1.37
82	xK	303	PEB	C4C-C3C	8.22	1.49	1.37
82	dD	401	PEB	C4C-C3C	8.22	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HP	202	PEB	C4C-C3C	8.22	1.49	1.37
82	V5	201	PEB	C4C-C3C	8.22	1.49	1.37
82	D9	202	PEB	C4C-C3C	8.22	1.49	1.37
82	gB	201	PEB	C4C-C3C	8.21	1.49	1.37
82	C5	201	PEB	C4C-C3C	8.21	1.49	1.37
82	mE	201	PEB	C4C-C3C	8.21	1.49	1.37
82	WQ	201	PEB	C4C-C3C	8.21	1.49	1.37
82	mG	201	PEB	C4C-C3C	8.21	1.49	1.37
82	mO	201	PEB	C4C-C3C	8.21	1.49	1.37
82	P5	201	PEB	C4C-C3C	8.21	1.49	1.37
82	ED	201	PEB	C4C-C3C	8.21	1.49	1.37
82	UJ	201	PEB	C4C-C3C	8.21	1.49	1.37
82	M9	305	PEB	C4C-C3C	8.21	1.49	1.37
82	D5	203	PEB	C4C-C3C	8.21	1.49	1.37
83	ND	201	PUB	C1B-C2B	8.21	1.49	1.37
82	I7	201	PEB	C4C-C3C	8.21	1.49	1.37
82	UH	201	PEB	C4C-C3C	8.20	1.49	1.37
82	QO	201	PEB	C4C-C3C	8.20	1.49	1.37
82	a4	201	PEB	C4C-C3C	8.20	1.49	1.37
82	MQ	201	PEB	C4C-C3C	8.20	1.49	1.37
82	P4	201	PEB	C4C-C3C	8.20	1.49	1.37
82	gO	202	PEB	C4C-C3C	8.20	1.49	1.37
82	GK	201	PEB	C2D-C3D	8.20	1.45	1.34
82	XK	201	PEB	C4C-C3C	8.20	1.49	1.37
82	NP	202	PEB	C4C-C3C	8.20	1.49	1.37
82	F1	1002	PEB	C4C-C3C	8.20	1.49	1.37
82	H9	202	PEB	C4C-C3C	8.20	1.49	1.37
82	A5	201	PEB	C4C-C3C	8.20	1.49	1.37
82	aG	202	PEB	C4C-C3C	8.20	1.49	1.37
82	vC	201	PEB	C4C-C3C	8.19	1.49	1.37
82	DA	202	PEB	C4C-C3C	8.19	1.49	1.37
82	RH	201	PEB	C4C-C3C	8.19	1.49	1.37
82	SI	201	PEB	C4C-C3C	8.19	1.49	1.37
82	dM	203	PEB	C4C-C3C	8.19	1.49	1.37
82	Z9	304	PEB	C4C-C3C	8.19	1.49	1.37
82	HD	202	PEB	C4C-C3C	8.19	1.49	1.37
82	VH	201	PEB	C4C-C3C	8.19	1.49	1.37
82	T5	201	PEB	C4C-C3C	8.19	1.49	1.37
82	S7	202	PEB	C4C-C3C	8.19	1.49	1.37
82	K5	201	PEB	C4C-C3C	8.19	1.49	1.37
82	B7	201	PEB	C4C-C3C	8.18	1.49	1.37
82	DQ	201	PEB	C2D-C3D	8.18	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GF	201	PEB	C2D-C3D	8.18	1.45	1.34
82	WM	203	PEB	C4C-C3C	8.18	1.49	1.37
82	X5	201	PEB	C4C-C3C	8.18	1.49	1.37
82	H5	202	PEB	C4C-C3C	8.18	1.49	1.37
82	JM	202	PEB	C4C-C3C	8.18	1.49	1.37
82	VO	201	PEB	C4C-C3C	8.18	1.49	1.37
82	R1	201	PEB	C4C-C3C	8.18	1.49	1.37
82	w8	202	PEB	C4C-C3C	8.18	1.49	1.37
82	jG	201	PEB	C4C-C3C	8.18	1.49	1.37
82	d1	203	PEB	C4C-C3C	8.18	1.49	1.37
82	dM	202	PEB	C4C-C3C	8.18	1.49	1.37
82	DD	201	PEB	C2D-C3D	8.18	1.45	1.34
82	CQ	201	PEB	C4C-C3C	8.18	1.49	1.37
82	RD	201	PEB	C4C-C3C	8.17	1.49	1.37
82	OI	202	PEB	C2D-C3D	8.17	1.45	1.34
82	YB	201	PEB	C4C-C3C	8.17	1.49	1.37
82	aE	202	PEB	C4C-C3C	8.17	1.49	1.37
82	BA	201	PEB	C4C-C3C	8.17	1.49	1.37
82	kG	202	PEB	C4C-C3C	8.17	1.49	1.37
82	O9	202	PEB	C4C-C3C	8.17	1.49	1.37
82	WG	203	PEB	C4C-C3C	8.17	1.49	1.37
82	I5	201	PEB	C4C-C3C	8.17	1.49	1.37
82	M9	301	PEB	C4C-C3C	8.17	1.49	1.37
83	AE	303	PUB	C1B-C2B	8.17	1.49	1.37
82	OQ	201	PEB	C4C-C3C	8.17	1.49	1.37
82	U4	202	PEB	C4C-C3C	8.17	1.49	1.37
82	NA	202	PEB	C4C-C3C	8.17	1.49	1.37
82	wC	202	PEB	C4C-C3C	8.17	1.49	1.37
82	jE	201	PEB	C4C-C3C	8.16	1.49	1.37
82	WH	202	PEB	C4C-C3C	8.16	1.49	1.37
82	XF	201	PEB	C4C-C3C	8.16	1.49	1.37
82	AM	301	PEB	C4C-C3C	8.16	1.49	1.37
82	eO	203	PEB	C4C-C3C	8.16	1.49	1.37
82	jM	202	PEB	C4C-C3C	8.16	1.49	1.37
82	V1	201	PEB	C4C-C3C	8.16	1.49	1.37
82	E5	201	PEB	C4C-C3C	8.16	1.49	1.37
82	iM	202	PEB	C4C-C3C	8.16	1.49	1.37
83	A4	303	PUB	C1B-C2B	8.15	1.49	1.37
82	YI	201	PEB	C2D-C3D	8.15	1.45	1.34
82	SH	203	PEB	C4C-C3C	8.15	1.49	1.37
82	OD	201	PEB	C4C-C3C	8.15	1.49	1.37
82	PQ	201	PEB	C4C-C3C	8.15	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	L9	202	PEB	C4C-C3C	8.15	1.49	1.37
82	X7	202	PEB	C4C-C3C	8.15	1.49	1.37
82	HJ	202	PEB	C4C-C3C	8.15	1.49	1.37
82	YO	203	PEB	C4C-C3C	8.15	1.49	1.37
82	Y5	202	PEB	C4C-C3C	8.14	1.49	1.37
82	aM	202	PEB	C4C-C3C	8.14	1.49	1.37
82	SK	201	PEB	C4C-C3C	8.14	1.49	1.37
82	OM	201	PEB	C4C-C3C	8.14	1.49	1.37
82	lG	203	PEB	C4C-C3C	8.14	1.49	1.37
82	dH	203	PEB	C4C-C3C	8.13	1.49	1.37
82	XQ	201	PEB	C4C-C3C	8.13	1.49	1.37
82	gO	201	PEB	C4C-C3C	8.13	1.49	1.37
82	AP	202	PEB	C4C-C3C	8.13	1.49	1.37
82	GP	203	PEB	C4C-C3C	8.13	1.49	1.37
82	RE	201	PEB	C4C-C3C	8.13	1.49	1.37
82	e4	203	PEB	C4C-C3C	8.13	1.49	1.37
82	KK	201	PEB	C4C-C3C	8.13	1.49	1.37
82	dJ	202	PEB	C4C-C3C	8.13	1.49	1.37
82	SJ	203	PEB	C4C-C3C	8.13	1.49	1.37
82	O4	202	PEB	C4C-C3C	8.13	1.49	1.37
82	V1	202	PEB	C4C-C3C	8.12	1.49	1.37
83	yK	302	PUB	C1B-C2B	8.12	1.49	1.37
82	UA	201	PEB	C4C-C3C	8.12	1.49	1.37
82	g4	201	PEB	C4C-C3C	8.12	1.49	1.37
82	OP	203	PEB	C4C-C3C	8.12	1.49	1.37
82	mE	203	PEB	C4C-C3C	8.12	1.49	1.37
82	mG	203	PEB	C4C-C3C	8.12	1.49	1.37
82	AG	301	PEB	C4C-C3C	8.12	1.49	1.37
82	BB	203	PEB	C4C-C3C	8.12	1.49	1.37
82	WE	201	PEB	C4C-C3C	8.12	1.49	1.37
82	S4	202	PEB	C4C-C3C	8.12	1.49	1.37
82	QP	201	PEB	C4C-C3C	8.11	1.49	1.37
82	QF	203	PEB	C4C-C3C	8.11	1.49	1.37
82	O5	201	PEB	C4C-C3C	8.11	1.49	1.37
82	AE	304	PEB	C4C-C3C	8.11	1.49	1.37
82	FM	202	PEB	C4C-C3C	8.11	1.49	1.37
82	lE	203	PEB	C4C-C3C	8.11	1.49	1.37
82	eM	202	PEB	C4C-C3C	8.11	1.49	1.37
82	zC	201	PEB	C4C-C3C	8.11	1.49	1.37
82	QK	203	PEB	C4C-C3C	8.11	1.49	1.37
83	yF	302	PUB	C1B-C2B	8.11	1.49	1.37
82	RQ	201	PEB	C4C-C3C	8.11	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UO	202	PEB	C4C-C3C	8.11	1.49	1.37
82	kO	201	PEB	C4C-C3C	8.11	1.49	1.37
82	mO	202	PEB	C4C-C3C	8.11	1.49	1.37
82	B9	201	PEB	C4C-C3C	8.11	1.49	1.37
82	kE	202	PEB	C4C-C3C	8.11	1.49	1.37
82	z8	201	PEB	C4C-C3C	8.10	1.49	1.37
82	wK	301	PEB	C4C-C3C	8.10	1.49	1.37
82	IQ	202	PEB	C4C-C3C	8.10	1.49	1.37
82	Y4	203	PEB	C4C-C3C	8.10	1.49	1.37
82	NA	203	PEB	C4C-C3C	8.10	1.49	1.37
82	XA	202	PEB	C4C-C3C	8.10	1.49	1.37
82	N7	203	PEB	C4C-C3C	8.10	1.49	1.37
82	BD	203	PEB	C4C-C3C	8.10	1.49	1.37
82	DG	1002	PEB	C4C-C3C	8.10	1.49	1.37
82	gH	203	PEB	C4C-C3C	8.09	1.49	1.37
82	jH	202	PEB	C4C-C3C	8.09	1.49	1.37
82	LI	202	PEB	C4C-C3C	8.09	1.49	1.37
82	QP	202	PEB	C4C-C3C	8.09	1.49	1.37
82	BB	202	PEB	C4C-C3C	8.09	1.49	1.37
82	KF	201	PEB	C4C-C3C	8.09	1.49	1.37
82	Q9	201	PEB	C4C-C3C	8.09	1.49	1.37
82	IP	203	PEB	CHC-C4C	8.09	1.59	1.49
82	WE	203	PEB	C4C-C3C	8.09	1.49	1.37
82	AG	304	PEB	C4C-C3C	8.09	1.49	1.37
82	GB	202	PEB	C4C-C3C	8.09	1.49	1.37
82	h1	201	PEB	C4C-C3C	8.08	1.49	1.37
82	aM	204	PEB	C4C-C3C	8.08	1.49	1.37
82	F5	202	PEB	C2D-C3D	8.08	1.44	1.34
82	EP	201	PEB	C4C-C3C	8.08	1.49	1.37
82	dF	201	PEB	C4C-C3C	8.08	1.49	1.37
82	aJ	201	PEB	C4C-C3C	8.08	1.49	1.37
82	YJ	201	PEB	C4C-C3C	8.08	1.49	1.37
82	MK	203	PEB	C4C-C3C	8.08	1.49	1.37
82	U7	201	PEB	C4C-C3C	8.08	1.49	1.37
98	B2	837	PQN	C3-C2	8.08	1.50	1.35
82	LD	202	PEB	C4C-C3C	8.08	1.49	1.37
82	BI	201	PEB	C4C-C3C	8.08	1.49	1.37
82	LK	201	PEB	C4C-C3C	8.08	1.49	1.37
82	LF	201	PEB	C4C-C3C	8.08	1.49	1.37
82	TQ	201	PEB	C4C-C3C	8.07	1.49	1.37
82	QJ	202	PEB	C4C-C3C	8.07	1.49	1.37
82	CK	201	PEB	C4C-C3C	8.07	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	NQ	201	PUB	C1B-C2B	8.07	1.49	1.37
82	YB	202	PEB	C4C-C3C	8.07	1.49	1.37
82	eA	301	PEB	C4C-C3C	8.07	1.49	1.37
82	WA	201	PEB	C4C-C3C	8.07	1.49	1.37
82	PM	202	PEB	C4C-C3C	8.07	1.49	1.37
98	BN	837	PQN	C3-C2	8.07	1.49	1.35
82	DF	202	PEB	C4C-C3C	8.07	1.49	1.37
82	UI	201	PEB	C4C-C3C	8.07	1.49	1.37
82	rK	201	PEB	C4C-C3C	8.07	1.49	1.37
82	fM	201	PEB	C4C-C3C	8.07	1.49	1.37
83	AD	302	PUB	C1B-C2B	8.06	1.49	1.37
82	YJ	203	PEB	C2D-C3D	8.06	1.44	1.34
82	VK	201	PEB	C4C-C3C	8.06	1.49	1.37
82	uC	202	PEB	C4C-C3C	8.06	1.49	1.37
82	PD	201	PEB	C4C-C3C	8.06	1.49	1.37
82	NE	202	PEB	C4C-C3C	8.06	1.49	1.37
82	BQ	203	PEB	C4C-C3C	8.06	1.49	1.37
82	NG	201	PEB	C4C-C3C	8.06	1.49	1.37
82	QA	201	PEB	C4C-C3C	8.06	1.49	1.37
91	A6	407	PHO	C1B-C2B	8.06	1.48	1.39
82	k4	201	PEB	C4C-C3C	8.06	1.49	1.37
82	eJ	202	PEB	C4C-C3C	8.06	1.49	1.37
82	TI	202	PEB	C4C-C3C	8.05	1.49	1.37
82	Q7	201	PEB	C4C-C3C	8.05	1.49	1.37
91	D6	404	PHO	C1B-C2B	8.05	1.48	1.39
82	qK	201	PEB	C4C-C3C	8.05	1.49	1.37
82	FB	201	PEB	C2D-C3D	8.05	1.44	1.34
82	ID	202	PEB	C4C-C3C	8.05	1.49	1.37
82	RI	201	PEB	C4C-C3C	8.05	1.49	1.37
82	GM	203	PEB	C4C-C3C	8.05	1.49	1.37
82	KB	302	PEB	C4C-C3C	8.05	1.49	1.37
82	HI	202	PEB	C2D-C3D	8.05	1.44	1.34
82	qF	201	PEB	C4C-C3C	8.05	1.49	1.37
82	lE	201	PEB	C4C-C3C	8.05	1.49	1.37
82	gG	201	PEB	C4C-C3C	8.05	1.49	1.37
82	H7	202	PEB	C4C-C3C	8.05	1.49	1.37
82	u8	202	PEB	C4C-C3C	8.05	1.49	1.37
82	OO	202	PEB	C4C-C3C	8.05	1.49	1.37
82	QM	202	PEB	C4C-C3C	8.05	1.49	1.37
82	SP	202	PEB	C4C-C3C	8.05	1.49	1.37
82	KI	202	PEB	C4C-C3C	8.04	1.49	1.37
82	U9	204	PEB	C4C-C3C	8.04	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CP	203	PEB	C4C-C3C	8.04	1.49	1.37
82	KJ	201	PEB	C4C-C3C	8.04	1.49	1.37
82	LQ	202	PEB	C4C-C3C	8.04	1.49	1.37
82	NM	202	PEB	C4C-C3C	8.04	1.49	1.37
82	VI	201	PEB	C4C-C3C	8.04	1.49	1.37
82	TM	202	PEB	C4C-C3C	8.04	1.49	1.37
82	XD	201	PEB	C4C-C3C	8.04	1.49	1.37
83	xK	306	PUB	C1B-C2B	8.04	1.49	1.37
82	B5	203	PEB	C4C-C3C	8.04	1.49	1.37
82	DE	1002	PEB	C4C-C3C	8.04	1.49	1.37
82	tC	201	PEB	C4C-C3C	8.04	1.49	1.37
82	DQ	201	PEB	C4C-C3C	8.03	1.49	1.37
82	WG	201	PEB	C4C-C3C	8.03	1.49	1.37
82	XI	201	PEB	C4C-C3C	8.03	1.49	1.37
82	TJ	202	PEB	C4C-C3C	8.03	1.49	1.37
82	W1	202	PEB	C4C-C3C	8.03	1.49	1.37
82	IB	201	PEB	C4C-C3C	8.03	1.49	1.37
82	HQ	201	PEB	C4C-C3C	8.03	1.49	1.37
82	J5	201	PEB	C4C-C3C	8.03	1.49	1.37
82	UB	302	PEB	C4C-C3C	8.03	1.49	1.37
82	CI	201	PEB	C4C-C3C	8.03	1.49	1.37
82	t8	201	PEB	C4C-C3C	8.03	1.49	1.37
82	eB	202	PEB	C4C-C3C	8.02	1.49	1.37
82	HB	202	PEB	C4C-C3C	8.02	1.49	1.37
82	II	201	PEB	C4C-C3C	8.02	1.49	1.37
82	NI	201	PEB	C4C-C3C	8.02	1.49	1.37
82	DD	201	PEB	C4C-C3C	8.02	1.49	1.37
82	RJ	202	PEB	C4C-C3C	8.02	1.49	1.37
82	L7	201	PEB	C4C-C3C	8.02	1.49	1.37
82	RA	203	PEB	C4C-C3C	8.02	1.49	1.37
82	QJ	203	PEB	C4C-C3C	8.02	1.49	1.37
82	PA	201	PEB	C4C-C3C	8.02	1.49	1.37
82	ZM	202	PEB	C4C-C3C	8.02	1.49	1.37
82	AI	201	PEB	C4C-C3C	8.02	1.49	1.37
82	dK	201	PEB	C4C-C3C	8.02	1.49	1.37
82	uC	201	PEB	C4C-C3C	8.02	1.49	1.37
82	SA	201	PEB	C4C-C3C	8.01	1.49	1.37
82	GI	202	PEB	C4C-C3C	8.01	1.49	1.37
82	S1	201	PEB	C4C-C3C	8.01	1.49	1.37
82	qC	202	PEB	C4C-C3C	8.01	1.49	1.37
82	UB	303	PEB	C4C-C3C	8.01	1.49	1.37
82	HD	201	PEB	C4C-C3C	8.01	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	xF	306	PUB	C1B-C2B	8.01	1.49	1.37
82	M5	305	PEB	C4C-C3C	8.01	1.49	1.37
82	YI	202	PEB	C4C-C3C	8.01	1.49	1.37
82	FP	201	PEB	C4C-C3C	8.01	1.49	1.37
82	IM	202	PEB	C4C-C3C	8.01	1.49	1.37
82	NI	203	PEB	C2D-C3D	8.00	1.44	1.34
82	W7	201	PEB	C4C-C3C	8.00	1.49	1.37
82	eB	201	PEB	C4C-C3C	8.00	1.49	1.37
82	EI	201	PEB	C4C-C3C	8.00	1.49	1.37
82	PI	201	PEB	C4C-C3C	8.00	1.49	1.37
82	iF	201	PEB	C4C-C3C	8.00	1.49	1.37
82	ZE	203	PEB	C4C-C3C	8.00	1.49	1.37
82	UG	202	PEB	C4C-C3C	8.00	1.49	1.37
82	i4	201	PEB	C4C-C3C	8.00	1.49	1.37
82	cB	402	PEB	C4C-C3C	8.00	1.49	1.37
82	SM	203	PEB	C4C-C3C	8.00	1.49	1.37
82	S9	202	PEB	C4C-C3C	8.00	1.49	1.37
83	AQ	302	PUB	C1B-C2B	8.00	1.49	1.37
82	CF	201	PEB	C4C-C3C	8.00	1.49	1.37
82	S5	202	PEB	C4C-C3C	7.99	1.49	1.37
82	TO	203	PEB	C4C-C3C	7.99	1.49	1.37
82	RG	201	PEB	C4C-C3C	7.99	1.49	1.37
82	Z5	305	PEB	C4C-C3C	7.99	1.49	1.37
82	EP	203	PEB	CHC-C4C	7.99	1.59	1.49
82	M7	201	PEB	C4C-C3C	7.99	1.49	1.37
82	YA	303	PEB	C4C-C3C	7.99	1.49	1.37
82	lM	202	PEB	C4C-C3C	7.99	1.49	1.37
82	QB	203	PEB	C4C-C3C	7.99	1.49	1.37
82	SO	202	PEB	C4C-C3C	7.99	1.49	1.37
82	N1	1002	PEB	C4C-C3C	7.99	1.49	1.37
82	rF	201	PEB	C4C-C3C	7.98	1.49	1.37
82	P7	201	PEB	C4C-C3C	7.98	1.49	1.37
82	SH	201	PEB	C4C-C3C	7.98	1.49	1.37
82	R7	203	PEB	C4C-C3C	7.98	1.49	1.37
83	AJ	303	PUB	C1B-C2B	7.98	1.49	1.37
82	HQ	202	PEB	C4C-C3C	7.98	1.49	1.37
82	BD	201	PEB	C4C-C3C	7.98	1.49	1.37
82	Q1	201	PEB	C4C-C3C	7.97	1.49	1.37
82	RI	203	PEB	C2D-C3D	7.97	1.44	1.34
82	CP	202	PEB	C4C-C3C	7.97	1.49	1.37
82	NH	1002	PEB	C4C-C3C	7.97	1.49	1.37
82	HG	1002	PEB	C4C-C3C	7.97	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	T4	203	PEB	C4C-C3C	7.97	1.49	1.37
82	VE	202	PEB	C4C-C3C	7.97	1.49	1.37
82	VG	202	PEB	C4C-C3C	7.97	1.49	1.37
82	H4	1002	PEB	C4C-C3C	7.97	1.49	1.37
82	EB	501	PEB	C4C-C3C	7.97	1.49	1.37
82	q8	202	PEB	C4C-C3C	7.97	1.49	1.37
82	aJ	204	PEB	C4C-C3C	7.97	1.49	1.37
82	hM	203	PEB	C4C-C3C	7.96	1.49	1.37
82	MP	202	PEB	C4C-C3C	7.96	1.49	1.37
82	YE	201	PEB	C4C-C3C	7.96	1.49	1.37
82	HA	202	PEB	C4C-C3C	7.96	1.49	1.37
82	DB	202	PEB	C4C-C3C	7.96	1.49	1.37
87	3N	308	CLA	C3B-C4B	7.96	1.61	1.42
82	Q5	201	PEB	C4C-C3C	7.96	1.49	1.37
82	UJ	202	PEB	C4C-C3C	7.96	1.49	1.37
82	hM	201	PEB	C4C-C3C	7.96	1.49	1.37
82	Y7	303	PEB	C4C-C3C	7.96	1.49	1.37
82	P7	202	PEB	C4C-C3C	7.95	1.49	1.37
82	S7	201	PEB	C4C-C3C	7.95	1.49	1.37
82	u8	201	PEB	C4C-C3C	7.95	1.49	1.37
82	KI	203	PEB	C4C-C3C	7.95	1.49	1.37
82	AE	301	PEB	C4C-C3C	7.95	1.49	1.37
82	YP	503	PEB	C4C-C3C	7.95	1.49	1.37
82	QK	202	PEB	C4C-C3C	7.95	1.49	1.37
82	hB	301	PEB	C4C-C3C	7.95	1.49	1.37
82	bP	501	PEB	C4C-C3C	7.94	1.49	1.37
82	DM	202	PEB	C4C-C3C	7.94	1.49	1.37
82	GJ	203	PEB	C4C-C3C	7.94	1.49	1.37
82	DK	202	PEB	C4C-C3C	7.94	1.49	1.37
82	YF	203	PEB	C4C-C3C	7.94	1.49	1.37
83	wF	304	PUB	C1B-C2B	7.94	1.49	1.37
82	iO	201	PEB	C4C-C3C	7.94	1.49	1.37
87	32	307	CLA	C3B-C4B	7.94	1.61	1.42
82	NB	202	PEB	C4C-C3C	7.93	1.49	1.37
82	HO	1002	PEB	C4C-C3C	7.93	1.49	1.37
82	BQ	201	PEB	C4C-C3C	7.93	1.49	1.37
82	BJ	301	PEB	C4C-C3C	7.93	1.49	1.37
82	UM	201	PEB	C4C-C3C	7.93	1.49	1.37
82	SE	201	PEB	C4C-C3C	7.93	1.49	1.37
82	RO	203	PEB	C4C-C3C	7.93	1.49	1.37
82	iK	201	PEB	C4C-C3C	7.93	1.49	1.37
82	QF	202	PEB	C4C-C3C	7.93	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OI	201	PEB	C4C-C3C	7.93	1.49	1.37
82	VI	202	PEB	C4C-C3C	7.93	1.49	1.37
82	aB	201	PEB	C4C-C3C	7.93	1.49	1.37
82	LA	201	PEB	C4C-C3C	7.93	1.49	1.37
82	ZJ	202	PEB	C4C-C3C	7.93	1.49	1.37
82	XJ	202	PEB	C4C-C3C	7.92	1.49	1.37
82	UE	202	PEB	C4C-C3C	7.92	1.49	1.37
82	WH	201	PEB	C4C-C3C	7.92	1.49	1.37
83	M5	303	PUB	C1B-C2B	7.92	1.49	1.37
82	NI	202	PEB	C4C-C3C	7.92	1.49	1.37
82	gE	201	PEB	C4C-C3C	7.92	1.49	1.37
82	YP	501	PEB	C4C-C3C	7.92	1.49	1.37
82	PI	202	PEB	C4C-C3C	7.92	1.49	1.37
82	W5	201	PEB	C4C-C3C	7.92	1.49	1.37
82	MA	201	PEB	C4C-C3C	7.92	1.49	1.37
82	PA	202	PEB	C4C-C3C	7.92	1.49	1.37
82	RE	202	PEB	C4C-C3C	7.92	1.49	1.37
82	SG	201	PEB	C4C-C3C	7.91	1.49	1.37
82	DI	201	PEB	C4C-C3C	7.91	1.49	1.37
82	lM	201	PEB	C4C-C3C	7.91	1.49	1.37
82	UP	203	PEB	CHC-C4C	7.91	1.59	1.49
82	VP	201	PEB	C4C-C3C	7.91	1.49	1.37
82	JD	203	PEB	C4C-C3C	7.91	1.49	1.37
82	rC	201	PEB	C4C-C3C	7.91	1.49	1.37
83	YA	302	PUB	C1B-C2B	7.91	1.49	1.37
82	EI	202	PEB	C4C-C3C	7.91	1.49	1.37
82	HI	201	PEB	C4C-C3C	7.91	1.49	1.37
82	YP	502	PEB	C4C-C3C	7.91	1.49	1.37
82	RP	202	PEB	C4C-C3C	7.90	1.49	1.37
82	R4	203	PEB	C4C-C3C	7.90	1.49	1.37
82	TK	201	PEB	C4C-C3C	7.90	1.49	1.37
82	jM	203	PEB	C4C-C3C	7.90	1.49	1.37
82	WM	201	PEB	C4C-C3C	7.90	1.49	1.37
82	FQ	201	PEB	C4C-C3C	7.90	1.49	1.37
82	V7	201	PEB	C4C-C3C	7.90	1.49	1.37
82	jH	203	PEB	C4C-C3C	7.90	1.49	1.37
82	lJ	201	PEB	C4C-C3C	7.90	1.49	1.37
82	OB	201	PEB	C4C-C3C	7.90	1.49	1.37
82	XI	202	PEB	C4C-C3C	7.90	1.49	1.37
82	RI	202	PEB	C4C-C3C	7.90	1.49	1.37
82	Y5	201	PEB	C4C-C3C	7.89	1.49	1.37
82	Q1	202	PEB	C4C-C3C	7.89	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	II	202	PEB	C4C-C3C	7.89	1.49	1.37
82	TI	203	PEB	C4C-C3C	7.89	1.49	1.37
82	AJ	301	PEB	C4C-C3C	7.89	1.49	1.37
83	Z5	303	PUB	C1B-C2B	7.89	1.49	1.37
82	O7	202	PEB	C4C-C3C	7.89	1.49	1.37
82	GP	202	PEB	C4C-C3C	7.89	1.49	1.37
83	Y7	302	PUB	C1B-C2B	7.89	1.49	1.37
82	QH	202	PEB	C4C-C3C	7.89	1.49	1.37
82	FB	201	PEB	C4C-C3C	7.89	1.49	1.37
82	QH	201	PEB	C4C-C3C	7.89	1.49	1.37
82	JQ	203	PEB	C4C-C3C	7.89	1.49	1.37
82	KM	201	PEB	C4C-C3C	7.89	1.49	1.37
82	TF	201	PEB	C4C-C3C	7.88	1.49	1.37
82	IJ	201	PEB	C4C-C3C	7.88	1.49	1.37
82	YJ	202	PEB	C4C-C3C	7.88	1.49	1.37
82	LA	202	PEB	C4C-C3C	7.88	1.49	1.37
82	FD	201	PEB	C4C-C3C	7.88	1.49	1.37
82	BI	203	PEB	C4C-C3C	7.88	1.49	1.37
82	kF	203	PEB	C4C-C3C	7.88	1.49	1.37
82	NA	201	PEB	C4C-C3C	7.88	1.49	1.37
82	SK	202	PEB	C4C-C3C	7.88	1.49	1.37
82	fB	301	PEB	C4C-C3C	7.88	1.49	1.37
82	eH	203	PEB	C4C-C3C	7.88	1.49	1.37
82	OE	201	PEB	C4C-C3C	7.88	1.49	1.37
82	GE	1002	PEB	C4C-C3C	7.87	1.49	1.37
82	YG	201	PEB	C4C-C3C	7.87	1.49	1.37
82	OH	201	PEB	C4C-C3C	7.87	1.49	1.37
82	CI	202	PEB	C4C-C3C	7.87	1.49	1.37
82	MM	201	PEB	C4C-C3C	7.87	1.49	1.37
82	KB	304	PEB	C4C-C3C	7.87	1.49	1.37
82	j1	203	PEB	C4C-C3C	7.87	1.49	1.37
82	B9	202	PEB	C4C-C3C	7.87	1.49	1.37
82	SB	203	PEB	C4C-C3C	7.87	1.49	1.37
82	FO	1002	PEB	C4C-C3C	7.86	1.49	1.37
82	OA	202	PEB	C4C-C3C	7.86	1.49	1.37
82	SJ	202	PEB	C4C-C3C	7.86	1.49	1.37
82	GI	203	PEB	C4C-C3C	7.86	1.49	1.37
82	L1	1002	PEB	C4C-C3C	7.86	1.49	1.37
82	MJ	201	PEB	C4C-C3C	7.86	1.49	1.37
82	LJ	202	PEB	C4C-C3C	7.85	1.49	1.37
82	HE	1002	PEB	C4C-C3C	7.85	1.49	1.37
82	AI	202	PEB	C4C-C3C	7.85	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OG	201	PEB	C4C-C3C	7.85	1.49	1.37
82	ZG	203	PEB	C4C-C3C	7.85	1.49	1.37
82	A4	304	PEB	C4C-C3C	7.85	1.49	1.37
82	W1	201	PEB	C4C-C3C	7.84	1.49	1.37
82	b1	203	PEB	C4C-C3C	7.84	1.49	1.37
82	O7	201	PEB	C4C-C3C	7.84	1.49	1.37
82	NJ	202	PEB	C4C-C3C	7.84	1.49	1.37
82	RG	202	PEB	C4C-C3C	7.84	1.49	1.37
82	JF	201	PEB	C4C-C3C	7.84	1.49	1.37
82	L5	201	PEB	C4C-C3C	7.83	1.49	1.37
82	LH	1003	PEB	C4C-C3C	7.83	1.49	1.37
82	RP	201	PEB	C4C-C3C	7.83	1.49	1.37
82	L7	202	PEB	C4C-C3C	7.83	1.49	1.37
91	aL	610	PHO	C1B-C2B	7.82	1.48	1.39
82	IB	203	PEB	C4C-C3C	7.82	1.49	1.37
82	GG	1002	PEB	C4C-C3C	7.82	1.49	1.37
82	SF	202	PEB	C4C-C3C	7.82	1.49	1.37
82	GM	202	PEB	C4C-C3C	7.82	1.49	1.37
82	IP	201	PEB	C4C-C3C	7.82	1.49	1.37
82	EA	202	PEB	C4C-C3C	7.82	1.49	1.37
82	QM	204	PEB	C4C-C3C	7.82	1.49	1.37
82	XB	201	PEB	C4C-C3C	7.82	1.49	1.37
82	F4	1002	PEB	C4C-C3C	7.82	1.49	1.37
83	AO	302	PUB	C1B-C2B	7.82	1.49	1.37
82	YM	201	PEB	C4C-C3C	7.82	1.49	1.37
82	F5	203	PEB	C4C-C3C	7.82	1.49	1.37
82	VF	201	PEB	C4C-C3C	7.81	1.49	1.37
82	r8	201	PEB	C4C-C3C	7.81	1.49	1.37
82	FK	201	PEB	C4C-C3C	7.81	1.49	1.37
82	aM	203	PEB	C4C-C3C	7.81	1.49	1.37
82	II	203	PEB	C2D-C3D	7.81	1.44	1.34
82	OA	201	PEB	C4C-C3C	7.81	1.49	1.37
82	F5	202	PEB	C4C-C3C	7.81	1.49	1.37
82	AO	304	PEB	C4C-C3C	7.81	1.49	1.37
82	E7	202	PEB	C4C-C3C	7.81	1.49	1.37
82	IM	201	PEB	C4C-C3C	7.80	1.49	1.37
83	A4	302	PUB	C1B-C2B	7.80	1.49	1.37
82	CJ	203	PEB	C4C-C3C	7.79	1.49	1.37
82	HF	201	PEB	C4C-C3C	7.79	1.49	1.37
82	N7	201	PEB	C4C-C3C	7.79	1.49	1.37
91	DL	405	PHO	C1B-C2B	7.79	1.48	1.39
82	kK	203	PEB	C4C-C3C	7.78	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	YM	202	PEB	C4C-C3C	7.78	1.49	1.37
82	WE	202	PEB	C4C-C3C	7.78	1.49	1.37
82	JP	201	PEB	C4C-C3C	7.78	1.49	1.37
82	O1	201	PEB	C4C-C3C	7.78	1.49	1.37
82	KM	203	PEB	C4C-C3C	7.78	1.49	1.37
83	BJ	302	PUB	C1B-C2B	7.77	1.49	1.37
82	YG	202	PEB	C4C-C3C	7.77	1.49	1.37
82	FP	202	PEB	C4C-C3C	7.77	1.49	1.37
83	wK	304	PUB	C1B-C2B	7.77	1.49	1.37
82	VA	201	PEB	C4C-C3C	7.76	1.49	1.37
82	IJ	202	PEB	C4C-C3C	7.75	1.49	1.37
82	sK	203	PEB	C4C-C3C	7.75	1.49	1.37
82	BB	201	PEB	C4C-C3C	7.75	1.49	1.37
82	DJ	202	PEB	C4C-C3C	7.73	1.49	1.37
82	S5	203	PEB	C4C-C3C	7.73	1.49	1.37
82	MP	203	PEB	CHC-C4C	7.73	1.58	1.49
82	jJ	203	PEB	C4C-C3C	7.73	1.49	1.37
91	dL	403	PHO	C1B-C2B	7.72	1.48	1.39
82	hJ	203	PEB	C4C-C3C	7.72	1.49	1.37
82	WP	201	PEB	CHC-C4C	7.72	1.58	1.49
82	BK	201	PEB	C4C-C3C	7.72	1.49	1.37
82	WG	202	PEB	C4C-C3C	7.72	1.49	1.37
82	AB	501	PEB	C4C-C3C	7.72	1.49	1.37
82	SB	202	PEB	C4C-C3C	7.72	1.49	1.37
82	W5	202	PEB	C4C-C3C	7.72	1.49	1.37
82	1C	202	PEB	C4C-C3C	7.71	1.49	1.37
82	JK	201	PEB	C4C-C3C	7.71	1.49	1.37
82	fJ	202	PEB	C4C-C3C	7.71	1.49	1.37
82	LQ	201	PEB	C4C-C3C	7.71	1.49	1.37
82	fJ	203	PEB	C4C-C3C	7.70	1.49	1.37
82	RF	201	PEB	C4C-C3C	7.70	1.48	1.37
82	QP	203	PEB	CHC-C4C	7.70	1.58	1.49
82	WP	202	PEB	C4C-C3C	7.70	1.48	1.37
82	BF	201	PEB	C4C-C3C	7.70	1.48	1.37
82	TB	201	PEB	C4C-C3C	7.69	1.48	1.37
82	sF	203	PEB	C4C-C3C	7.69	1.48	1.37
82	YK	203	PEB	C4C-C3C	7.69	1.48	1.37
82	KP	202	PEB	C4C-C3C	7.68	1.48	1.37
82	fM	203	PEB	C4C-C3C	7.68	1.48	1.37
82	18	202	PEB	C4C-C3C	7.68	1.48	1.37
82	YE	202	PEB	C4C-C3C	7.66	1.48	1.37
82	hJ	201	PEB	C4C-C3C	7.66	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OP	202	PEB	C4C-C3C	7.65	1.48	1.37
82	dM	201	PEB	C4C-C3C	7.65	1.48	1.37
82	CJ	201	PEB	C4C-C3C	7.65	1.48	1.37
82	LI	201	PEB	C4C-C3C	7.65	1.48	1.37
82	HK	201	PEB	C4C-C3C	7.64	1.48	1.37
82	gF	203	PEB	C4C-C3C	7.64	1.48	1.37
82	N4	1002	PEB	C4C-C3C	7.64	1.48	1.37
82	gK	203	PEB	C4C-C3C	7.64	1.48	1.37
82	JB	201	PEB	C4C-C3C	7.63	1.48	1.37
91	AL	410	PHO	C1B-C2B	7.63	1.48	1.39
82	LD	201	PEB	C4C-C3C	7.63	1.48	1.37
82	IB	202	PEB	C4C-C3C	7.63	1.48	1.37
82	BI	202	PEB	C2D-C3D	7.60	1.44	1.34
82	FF	201	PEB	C4C-C3C	7.60	1.48	1.37
82	NO	1002	PEB	C4C-C3C	7.60	1.48	1.37
82	WF	201	PEB	C4C-C3C	7.60	1.48	1.37
82	MM	202	PEB	C4C-C3C	7.60	1.48	1.37
82	lM	203	PEB	C4C-C3C	7.60	1.48	1.37
82	FJ	202	PEB	C4C-C3C	7.59	1.48	1.37
82	fK	201	PEB	C4C-C3C	7.59	1.48	1.37
82	MJ	202	PEB	C4C-C3C	7.59	1.48	1.37
82	GJ	202	PEB	C4C-C3C	7.58	1.48	1.37
82	IM	203	PEB	C4C-C3C	7.57	1.48	1.37
82	RK	201	PEB	C4C-C3C	7.56	1.48	1.37
82	BQ	203	PEB	C2D-C3D	7.54	1.44	1.34
82	QJ	204	PEB	C4C-C3C	7.54	1.48	1.37
82	Z5	304	PEB	C4C-C3C	7.54	1.48	1.37
82	bP	502	PEB	C4C-C3C	7.54	1.48	1.37
82	lJ	202	PEB	C4C-C3C	7.54	1.48	1.37
82	WJ	201	PEB	C4C-C3C	7.54	1.48	1.37
82	M5	304	PEB	C4C-C3C	7.53	1.48	1.37
82	AP	203	PEB	CHC-C4C	7.52	1.58	1.49
82	OJ	203	PEB	C4C-C3C	7.52	1.48	1.37
82	XF	202	PEB	C4C-C3C	7.52	1.48	1.37
82	BD	203	PEB	C2D-C3D	7.52	1.44	1.34
82	UP	201	PEB	C4C-C3C	7.51	1.48	1.37
82	T7	201	PEB	C4C-C3C	7.51	1.48	1.37
82	FA	202	PEB	C4C-C3C	7.51	1.48	1.37
82	fF	201	PEB	C4C-C3C	7.51	1.48	1.37
82	TA	201	PEB	C4C-C3C	7.48	1.48	1.37
82	WK	201	PEB	C4C-C3C	7.48	1.48	1.37
82	TI	201	PEB	C4C-C3C	7.47	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GI	201	PEB	C4C-C3C	7.45	1.48	1.37
82	XK	202	PEB	C4C-C3C	7.45	1.48	1.37
87	42	604	CLA	C3D-C2D	7.45	1.59	1.39
82	F7	202	PEB	C4C-C3C	7.45	1.48	1.37
82	SM	202	PEB	C4C-C3C	7.44	1.48	1.37
98	AN	842	PQN	C3-C2	7.43	1.48	1.35
98	A2	842	PQN	C3-C2	7.43	1.48	1.35
82	EJ	201	PEB	C4C-C3C	7.43	1.48	1.37
87	42	604	CLA	C3D-C4D	7.42	1.60	1.44
82	MJ	203	PEB	C2D-C3D	7.42	1.44	1.34
87	4N	604	CLA	C3D-C2D	7.41	1.59	1.39
82	SP	201	PEB	CHC-C4C	7.41	1.58	1.49
82	KJ	203	PEB	C4C-C3C	7.40	1.48	1.37
87	4N	604	CLA	C3D-C4D	7.40	1.60	1.44
82	AP	201	PEB	C4C-C3C	7.39	1.48	1.37
82	XA	203	PEB	C4C-C3C	7.38	1.48	1.37
82	aJ	203	PEB	C4C-C3C	7.38	1.48	1.37
82	OJ	202	PEB	C4C-C3C	7.38	1.48	1.37
82	MP	201	PEB	C4C-C3C	7.38	1.48	1.37
82	OP	201	PEB	CHC-C4C	7.37	1.58	1.49
82	WJ	203	PEB	C4C-C3C	7.30	1.48	1.37
82	X7	203	PEB	C4C-C3C	7.30	1.48	1.37
82	CM	202	PEB	C4C-C3C	7.30	1.48	1.37
82	EJ	203	PEB	C4C-C3C	7.30	1.48	1.37
82	NI	203	PEB	C4C-C3C	7.28	1.48	1.37
82	IQ	201	PEB	C4C-C3C	7.26	1.48	1.37
96	GN	201	HEM	C3D-C2D	7.23	1.52	1.36
82	ZI	401	PEB	C4C-C3C	7.23	1.48	1.37
82	CP	201	PEB	CHC-C4C	7.21	1.58	1.49
82	EM	203	PEB	C4C-C3C	7.21	1.48	1.37
82	KM	202	PEB	C4C-C3C	7.21	1.48	1.37
96	G2	201	HEM	C3D-C2D	7.21	1.52	1.36
82	ID	201	PEB	C4C-C3C	7.21	1.48	1.37
82	WI	202	PEB	C4C-C3C	7.19	1.48	1.37
82	qF	202	PEB	C4C-C3C	7.18	1.48	1.37
82	CJ	202	PEB	C4C-C3C	7.17	1.48	1.37
82	OI	202	PEB	C4C-C3C	7.16	1.48	1.37
82	qK	202	PEB	C4C-C3C	7.16	1.48	1.37
82	L4	1002	PEB	C4C-C3C	7.16	1.48	1.37
82	YM	203	PEB	C4C-C3C	7.14	1.48	1.37
82	IJ	203	PEB	C4C-C3C	7.12	1.48	1.37
82	YI	201	PEB	C4C-C3C	7.12	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BI	202	PEB	C4C-C3C	7.04	1.48	1.37
82	LO	1002	PEB	C4C-C3C	7.02	1.48	1.37
82	UJ	203	PEB	C4C-C3C	7.01	1.48	1.37
82	KP	201	PEB	CHC-C4C	7.00	1.58	1.49
82	MM	203	PEB	C4C-C3C	6.98	1.47	1.37
82	H5	201	PEB	C4C-C3C	6.98	1.47	1.37
82	lJ	203	PEB	C4C-C3C	6.95	1.47	1.37
82	AI	203	PEB	C4C-C3C	6.94	1.47	1.37
82	WJ	202	PEB	C4C-C3C	6.94	1.47	1.37
82	UM	203	PEB	C4C-C3C	6.92	1.47	1.37
82	OM	202	PEB	C4C-C3C	6.88	1.47	1.37
82	RI	203	PEB	C4C-C3C	6.81	1.47	1.37
82	YJ	203	PEB	C4C-C3C	6.77	1.47	1.37
82	KJ	202	PEB	C4C-C3C	6.74	1.47	1.37
82	VI	203	PEB	C2D-C3D	6.73	1.43	1.34
82	WM	202	PEB	C4C-C3C	6.73	1.47	1.37
82	HI	202	PEB	C4C-C3C	6.72	1.47	1.37
82	U5	201	PEB	C4C-C3C	6.69	1.47	1.37
87	2N	303	CLA	C1D-ND	6.66	1.46	1.37
82	KI	201	PEB	C4C-C3C	6.65	1.47	1.37
82	II	203	PEB	C4C-C3C	6.65	1.47	1.37
87	22	602	CLA	C1D-ND	6.58	1.45	1.37
82	VI	203	PEB	C4C-C3C	6.51	1.47	1.37
82	pC	202	PEB	CHB-C4B	6.45	1.51	1.38
84	x3	1001	CYC	CHB-C1B	6.42	1.53	1.38
84	V3	1001	CYC	CHB-C1B	6.38	1.53	1.38
82	U9	204	PEB	C3B-C2B	6.38	1.50	1.36
82	sF	203	PEB	C3B-C2B	6.38	1.50	1.36
82	sK	203	PEB	C3B-C2B	6.38	1.50	1.36
82	MJ	203	PEB	C4C-C3C	6.38	1.47	1.37
82	p8	202	PEB	CHB-C4B	6.34	1.50	1.38
82	ID	201	PEB	CHB-C4B	6.31	1.50	1.38
82	IQ	201	PEB	CHB-C4B	6.30	1.50	1.38
82	ZF	201	PEB	C3B-C2B	6.27	1.50	1.36
87	A2	852	CLA	C1D-ND	6.25	1.45	1.37
87	AN	852	CLA	C1D-ND	6.25	1.45	1.37
82	FQ	203	PEB	C3B-C2B	6.24	1.50	1.36
91	aL	610	PHO	C4D-CHA	6.23	1.49	1.39
82	FD	203	PEB	C3B-C2B	6.23	1.50	1.36
83	NQ	201	PUB	CHB-C1C	6.21	1.50	1.38
82	iK	201	PEB	C3B-C2B	6.20	1.49	1.36
82	HM	202	PEB	C3B-C2B	6.19	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ZI	401	PEB	C3B-C2B	6.19	1.49	1.36
83	ND	201	PUB	CHB-C1C	6.19	1.50	1.38
82	ZK	201	PEB	C3B-C2B	6.18	1.49	1.36
82	r8	202	PEB	C3B-C2B	6.17	1.49	1.36
82	iF	201	PEB	C3B-C2B	6.17	1.49	1.36
82	LF	202	PEB	CHB-C4B	6.15	1.50	1.38
82	t8	201	PEB	CHB-C4B	6.14	1.50	1.38
82	rC	202	PEB	C3B-C2B	6.14	1.49	1.36
82	oK	203	PEB	C3B-C2B	6.14	1.49	1.36
82	LK	202	PEB	CHB-C4B	6.13	1.50	1.38
91	AL	410	PHO	C4D-CHA	6.12	1.49	1.39
82	d1	203	PEB	C3B-C2B	6.12	1.49	1.36
82	wK	303	PEB	C3B-C2B	6.12	1.49	1.36
82	tC	201	PEB	CHB-C4B	6.10	1.50	1.38
82	g4	203	PEB	C3B-C2B	6.10	1.49	1.36
82	wF	303	PEB	C3B-C2B	6.09	1.49	1.36
82	dH	203	PEB	C3B-C2B	6.09	1.49	1.36
84	v3	1001	CYC	CHA-C1A	6.08	1.50	1.38
82	l1	203	PEB	C3B-C2B	6.07	1.49	1.36
84	N3	1001	CYC	CHA-C1A	6.07	1.50	1.38
84	g3	1001	CYC	CHA-C1A	6.07	1.50	1.38
82	gO	203	PEB	C3B-C2B	6.07	1.49	1.36
84	J3	1001	CYC	CHA-C1A	6.06	1.50	1.38
84	c3	1001	CYC	CHA-C1A	6.06	1.50	1.38
84	t3	1001	CYC	CHA-C1A	6.06	1.50	1.38
84	G3	1001	CYC	CHA-C1A	6.06	1.50	1.38
87	6N	608	CLA	C1B-NB	-6.05	1.30	1.37
82	m4	203	PEB	C3B-C2B	6.05	1.49	1.36
82	mO	203	PEB	C3B-C2B	6.05	1.49	1.36
84	R3	1001	CYC	CHA-C1A	6.05	1.50	1.38
91	dL	403	PHO	C4D-CHA	6.05	1.49	1.39
82	dE	204	PEB	C3B-C2B	6.04	1.49	1.36
84	E3	1001	CYC	CHA-C1A	6.04	1.50	1.38
84	C3	1001	CYC	CHA-C1A	6.04	1.50	1.38
82	lH	202	PEB	C3B-C2B	6.04	1.49	1.36
84	T3	1001	CYC	CHA-C1A	6.04	1.50	1.38
82	oF	203	PEB	C3B-C2B	6.04	1.49	1.36
82	dG	204	PEB	C3B-C2B	6.04	1.49	1.36
84	m3	1001	CYC	CHA-C1A	6.04	1.50	1.38
84	P3	1001	CYC	CHA-C1A	6.04	1.50	1.38
84	p3	1001	CYC	CHA-C1A	6.03	1.50	1.38
84	l3	1001	CYC	CHA-C1A	6.02	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	307	CLA	C1D-ND	6.02	1.45	1.37
84	e3	1001	CYC	CHA-C1A	6.02	1.50	1.38
82	uK	202	PEB	C3B-C2B	6.02	1.49	1.36
84	i3	1001	CYC	CHA-C1A	6.01	1.50	1.38
82	x8	202	PEB	C3B-C2B	6.01	1.49	1.36
82	hG	201	PEB	CHB-C4B	6.01	1.50	1.38
84	K3	1001	CYC	CHA-C1A	6.01	1.50	1.38
82	tK	203	PEB	C3B-C2B	6.01	1.49	1.36
84	A3	1001	CYC	CHA-C1A	6.00	1.50	1.38
82	pC	202	PEB	C3B-C2B	6.00	1.49	1.36
82	z8	201	PEB	CHB-C4B	6.00	1.50	1.38
82	hE	201	PEB	CHB-C4B	5.99	1.50	1.38
82	cK	203	PEB	C3B-C2B	5.99	1.49	1.36
82	xC	202	PEB	C3B-C2B	5.99	1.49	1.36
82	18	202	PEB	C3B-C2B	5.99	1.49	1.36
84	IE	1001	CYC	C3B-C2B	5.99	1.49	1.36
84	IG	1001	CYC	C3B-C2B	5.99	1.49	1.36
87	3N	308	CLA	C1D-ND	5.98	1.45	1.37
87	62	309	CLA	C1B-NB	-5.98	1.30	1.37
82	zC	201	PEB	CHB-C4B	5.98	1.50	1.38
82	SP	203	PEB	C3B-C2B	5.98	1.49	1.36
82	uF	203	PEB	C3B-C2B	5.97	1.49	1.36
87	b6	605	CLA	C4B-NB	5.97	1.45	1.37
91	DL	405	PHO	C3B-C4B	5.97	1.48	1.41
82	fH	202	PEB	C3B-C2B	5.97	1.49	1.36
82	1C	202	PEB	C3B-C2B	5.96	1.49	1.36
82	Y7	304	PEB	C3B-C2B	5.96	1.49	1.36
82	1C	201	PEB	CHB-C4B	5.96	1.50	1.38
82	zC	202	PEB	C3B-C2B	5.96	1.49	1.36
82	t8	202	PEB	CHB-C4B	5.96	1.50	1.38
91	d6	404	PHO	C4D-CHA	5.96	1.49	1.39
82	RQ	203	PEB	C3B-C2B	5.96	1.49	1.36
82	tC	202	PEB	C3B-C2B	5.95	1.49	1.36
82	A9	202	PEB	C3B-C2B	5.95	1.49	1.36
82	I9	202	PEB	C3B-C2B	5.95	1.49	1.36
82	tC	202	PEB	CHB-C4B	5.95	1.50	1.38
82	r8	202	PEB	CHB-C4B	5.95	1.50	1.38
82	jH	202	PEB	C3B-C2B	5.94	1.49	1.36
82	p8	202	PEB	C3B-C2B	5.94	1.49	1.36
82	P9	202	PEB	C3B-C2B	5.94	1.49	1.36
82	R9	202	PEB	C3B-C2B	5.94	1.49	1.36
82	z8	202	PEB	C3B-C2B	5.94	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	t8	202	PEB	C3B-C2B	5.93	1.49	1.36
82	tF	202	PEB	CHB-C4B	5.93	1.50	1.38
82	C9	202	PEB	C3B-C2B	5.93	1.49	1.36
82	cF	203	PEB	C3B-C2B	5.93	1.49	1.36
82	YA	304	PEB	C3B-C2B	5.93	1.49	1.36
82	X9	202	PEB	C3B-C2B	5.93	1.49	1.36
82	j1	202	PEB	C3B-C2B	5.93	1.49	1.36
91	AL	410	PHO	C3B-C4B	5.92	1.48	1.41
82	XA	201	PEB	CHB-C4B	5.92	1.50	1.38
82	tK	202	PEB	CHB-C4B	5.92	1.50	1.38
82	E9	202	PEB	C3B-C2B	5.92	1.49	1.36
82	lF	203	PEB	C3B-C2B	5.92	1.49	1.36
91	dL	403	PHO	C3B-C4B	5.92	1.48	1.41
82	K9	202	PEB	C3B-C2B	5.92	1.49	1.36
82	uF	201	PEB	C3B-C2B	5.91	1.49	1.36
82	N9	202	PEB	C3B-C2B	5.91	1.49	1.36
82	X7	201	PEB	CHB-C4B	5.90	1.50	1.38
82	O1	201	PEB	C3B-C2B	5.90	1.49	1.36
91	aL	610	PHO	C3B-C4B	5.90	1.48	1.41
82	JB	201	PEB	CHA-C1B	5.90	1.54	1.40
82	UM	203	PEB	C3B-C2B	5.90	1.49	1.36
91	DL	405	PHO	C4D-CHA	5.90	1.49	1.39
82	PD	201	PEB	C3B-C2B	5.90	1.49	1.36
82	xK	302	PEB	C3B-C2B	5.90	1.49	1.36
82	T9	202	PEB	C3B-C2B	5.89	1.49	1.36
82	aF	201	PEB	C3B-C2B	5.89	1.49	1.36
82	rC	202	PEB	CHB-C4B	5.89	1.50	1.38
82	V9	202	PEB	C3B-C2B	5.89	1.49	1.36
82	m1	202	PEB	CHB-C4B	5.89	1.50	1.38
82	dF	202	PEB	CHB-C4B	5.89	1.50	1.38
82	TB	201	PEB	CHA-C1B	5.89	1.54	1.40
82	DI	201	PEB	CHB-C4B	5.89	1.50	1.38
82	lK	203	PEB	C3B-C2B	5.89	1.49	1.36
82	18	201	PEB	CHB-C4B	5.89	1.50	1.38
82	f1	202	PEB	C3B-C2B	5.88	1.49	1.36
82	RD	203	PEB	C3B-C2B	5.88	1.49	1.36
82	G9	202	PEB	C3B-C2B	5.88	1.49	1.36
82	xK	304	PEB	C3B-C2B	5.88	1.49	1.36
84	i3	1001	CYC	CHB-C1B	5.88	1.52	1.38
84	J3	1001	CYC	CHB-C1B	5.87	1.52	1.38
82	PQ	201	PEB	C3B-C2B	5.87	1.49	1.36
82	i1	202	PEB	C3B-C2B	5.87	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	C3	1001	CYC	CHB-C1B	5.87	1.52	1.38
84	v3	1001	CYC	CHB-C1B	5.87	1.52	1.38
84	m3	1001	CYC	CHB-C1B	5.87	1.52	1.38
82	mH	202	PEB	CHB-C4B	5.87	1.50	1.38
84	R3	1001	CYC	CHB-C1B	5.86	1.52	1.38
82	aK	201	PEB	C3B-C2B	5.86	1.49	1.36
84	t3	1001	CYC	CHB-C1B	5.86	1.52	1.38
83	A1	304	PUB	C2C-C3C	5.86	1.49	1.36
84	K3	1001	CYC	CHB-C1B	5.86	1.52	1.38
82	OH	201	PEB	C3B-C2B	5.86	1.49	1.36
84	A3	1001	CYC	CHB-C1B	5.86	1.52	1.38
84	G3	1001	CYC	CHB-C1B	5.86	1.52	1.38
84	P3	1001	CYC	CHB-C1B	5.86	1.52	1.38
82	AQ	304	PEB	C3B-C2B	5.85	1.49	1.36
82	KQ	202	PEB	C3B-C2B	5.85	1.49	1.36
82	B7	201	PEB	C3B-C2B	5.85	1.49	1.36
87	62	309	CLA	MG-NA	5.85	2.20	2.06
82	FF	201	PEB	CHB-C4B	5.85	1.50	1.38
84	T3	1001	CYC	CHB-C1B	5.85	1.51	1.38
82	bH	202	PEB	C3B-C2B	5.85	1.49	1.36
84	x3	1001	CYC	CHA-C1A	5.84	1.50	1.38
82	WF	203	PEB	C3B-C2B	5.84	1.49	1.36
87	62	313	CLA	C1D-ND	5.84	1.45	1.37
84	E3	1001	CYC	CHB-C1B	5.84	1.51	1.38
82	QF	203	PEB	C3B-C2B	5.84	1.49	1.36
84	p3	1001	CYC	CHB-C1B	5.84	1.51	1.38
82	VQ	203	PEB	C3B-C2B	5.84	1.49	1.36
84	g3	1001	CYC	CHB-C1B	5.84	1.51	1.38
82	gB	201	PEB	C3B-C2B	5.84	1.49	1.36
82	TP	201	PEB	CHB-C4B	5.84	1.50	1.38
82	QK	203	PEB	C3B-C2B	5.84	1.49	1.36
82	oF	201	PEB	C3B-C2B	5.84	1.49	1.36
84	e3	1001	CYC	CHB-C1B	5.84	1.51	1.38
84	c3	1001	CYC	CHB-C1B	5.84	1.51	1.38
84	l3	1001	CYC	CHB-C1B	5.84	1.51	1.38
82	KD	202	PEB	C3B-C2B	5.84	1.49	1.36
84	F4	1001	CYC	C3B-C2B	5.83	1.49	1.36
84	N3	1001	CYC	CHB-C1B	5.83	1.51	1.38
82	w8	202	PEB	CHB-C4B	5.83	1.50	1.38
82	b1	202	PEB	C3B-C2B	5.83	1.49	1.36
82	kF	202	PEB	CHB-C4B	5.83	1.50	1.38
82	XQ	202	PEB	CHB-C4B	5.83	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	KO	1001	CYC	C3B-C2B	5.82	1.49	1.36
82	nK	201	PEB	C3B-C2B	5.82	1.49	1.36
82	iO	203	PEB	C3B-C2B	5.82	1.49	1.36
82	dK	202	PEB	CHB-C4B	5.81	1.49	1.38
82	xF	302	PEB	C3B-C2B	5.81	1.49	1.36
84	NE	201	CYC	C3B-C2B	5.81	1.49	1.36
82	u8	203	PEB	CHB-C4B	5.81	1.49	1.38
87	6N	612	CLA	C1D-ND	5.81	1.44	1.37
82	BA	201	PEB	C3B-C2B	5.81	1.49	1.36
84	V3	1001	CYC	CHA-C1A	5.81	1.49	1.38
82	i4	203	PEB	C3B-C2B	5.81	1.49	1.36
82	OI	201	PEB	C3B-C2B	5.81	1.49	1.36
82	YQ	202	PEB	C3B-C2B	5.81	1.49	1.36
91	D6	404	PHO	C4D-CHA	5.80	1.48	1.39
82	YD	202	PEB	C3B-C2B	5.80	1.49	1.36
82	hH	201	PEB	C3B-C2B	5.80	1.49	1.36
84	FO	1001	CYC	C3B-C2B	5.80	1.49	1.36
82	GK	201	PEB	C3B-C2B	5.80	1.49	1.36
87	6N	608	CLA	MG-NA	5.80	2.20	2.06
84	LH	1002	CYC	CHB-C1B	5.80	1.51	1.38
82	h1	202	PEB	C3B-C2B	5.80	1.49	1.36
82	J7	203	PEB	C3B-C2B	5.79	1.49	1.36
82	F7	203	PEB	CHB-C4B	5.79	1.49	1.38
82	FQ	202	PEB	C3B-C2B	5.79	1.49	1.36
82	iH	202	PEB	C3B-C2B	5.78	1.49	1.36
82	AD	304	PEB	C3B-C2B	5.78	1.49	1.36
98	B2	837	PQN	C10-C5	5.78	1.50	1.40
82	TA	201	PEB	CHB-C4B	5.78	1.49	1.38
82	gH	201	PEB	CHB-C4B	5.78	1.49	1.38
82	O9	202	PEB	C3B-C2B	5.77	1.49	1.36
82	EA	201	PEB	C3B-C2B	5.77	1.49	1.36
82	uC	203	PEB	CHB-C4B	5.77	1.49	1.38
82	VD	203	PEB	C3B-C2B	5.77	1.49	1.36
82	eG	203	PEB	C3B-C2B	5.77	1.49	1.36
82	AF	202	PEB	C3B-C2B	5.77	1.49	1.36
82	oK	201	PEB	C3B-C2B	5.77	1.49	1.36
82	v8	201	PEB	CHB-C4B	5.77	1.49	1.38
84	E4	1001	CYC	C3B-C2B	5.77	1.49	1.36
82	FI	201	PEB	C3B-C2B	5.77	1.49	1.36
82	JA	203	PEB	C3B-C2B	5.77	1.49	1.36
82	AD	303	PEB	C3B-C2B	5.77	1.49	1.36
82	s8	202	PEB	C3B-C2B	5.77	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	vC	201	PEB	CHB-C4B	5.76	1.49	1.38
82	aG	202	PEB	C3B-C2B	5.76	1.49	1.36
84	I4	1001	CYC	C3B-C2B	5.76	1.49	1.36
84	L1	1001	CYC	CHB-C1B	5.76	1.51	1.38
82	wC	201	PEB	CHB-C4B	5.76	1.49	1.38
82	JD	201	PEB	C3B-C2B	5.76	1.49	1.36
98	BN	837	PQN	C10-C5	5.76	1.50	1.40
82	YA	303	PEB	C3B-C2B	5.76	1.49	1.36
84	EO	1001	CYC	C3B-C2B	5.76	1.49	1.36
82	A9	202	PEB	CHB-C4B	5.76	1.49	1.38
84	GO	1001	CYC	C3B-C2B	5.76	1.49	1.36
84	NO	1001	CYC	C2A-C3A	5.75	1.49	1.36
82	FD	202	PEB	C3B-C2B	5.75	1.49	1.36
82	e1	202	PEB	C3B-C2B	5.75	1.49	1.36
82	mH	202	PEB	C3B-C2B	5.75	1.49	1.36
82	HA	203	PEB	CHB-C4B	5.75	1.49	1.38
82	E7	201	PEB	C3B-C2B	5.75	1.49	1.36
82	sC	202	PEB	C3B-C2B	5.75	1.49	1.36
82	K9	202	PEB	CHB-C4B	5.75	1.49	1.38
82	WK	203	PEB	C3B-C2B	5.75	1.48	1.36
82	KI	201	PEB	C3B-C2B	5.75	1.48	1.36
82	PK	202	PEB	CHB-C4B	5.74	1.49	1.38
82	RH	202	PEB	C3B-C2B	5.74	1.48	1.36
82	JQ	201	PEB	C3B-C2B	5.74	1.48	1.36
82	nF	202	PEB	CHB-C4B	5.74	1.49	1.38
82	V7	203	PEB	CHB-C4B	5.74	1.49	1.38
82	AK	202	PEB	C3B-C2B	5.74	1.48	1.36
82	hJ	203	PEB	CHB-C4B	5.74	1.49	1.38
82	VD	202	PEB	C3B-C2B	5.74	1.48	1.36
82	VQ	202	PEB	C3B-C2B	5.74	1.48	1.36
91	D6	404	PHO	C3B-C4B	5.74	1.48	1.41
82	T9	202	PEB	CHB-C4B	5.74	1.49	1.38
82	nF	201	PEB	C3B-C2B	5.74	1.48	1.36
82	FA	203	PEB	CHB-C4B	5.74	1.49	1.38
84	C4	1001	CYC	C3B-C2B	5.73	1.48	1.36
82	G9	202	PEB	CHB-C4B	5.73	1.49	1.38
84	FE	1001	CYC	C3B-C2B	5.73	1.48	1.36
84	KG	202	CYC	C3B-C2B	5.73	1.48	1.36
82	Y7	303	PEB	C3B-C2B	5.73	1.48	1.36
82	W9	202	PEB	CHB-C4B	5.73	1.49	1.38
82	GF	201	PEB	C3B-C2B	5.73	1.48	1.36
82	w8	201	PEB	CHB-C4B	5.73	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	T7	201	PEB	CHB-C4B	5.73	1.49	1.38
82	q8	201	PEB	C3B-C2B	5.73	1.48	1.36
82	GE	1002	PEB	C3B-C2B	5.73	1.48	1.36
82	FK	201	PEB	CHB-C4B	5.73	1.49	1.38
82	wC	202	PEB	CHB-C4B	5.73	1.49	1.38
84	G4	1001	CYC	C3B-C2B	5.73	1.48	1.36
82	R9	202	PEB	CHB-C4B	5.73	1.49	1.38
84	BE	1001	CYC	C3B-C2B	5.73	1.48	1.36
82	jK	201	PEB	C3B-C2B	5.72	1.48	1.36
83	AH	304	PUB	C2C-C3C	5.72	1.48	1.36
91	a6	613	PHO	C4D-CHA	5.72	1.48	1.39
82	jF	201	PEB	C3B-C2B	5.72	1.48	1.36
82	m1	202	PEB	C3B-C2B	5.72	1.48	1.36
82	AA	202	PEB	C3B-C2B	5.72	1.48	1.36
83	Z5	303	PUB	CHB-C1C	5.72	1.49	1.38
84	IO	1001	CYC	C3B-C2B	5.72	1.48	1.36
82	g1	201	PEB	CHB-C4B	5.72	1.49	1.38
84	y3	1001	CYC	CHB-C1B	5.72	1.51	1.38
82	GG	1002	PEB	C3B-C2B	5.72	1.48	1.36
91	A6	407	PHO	C4D-CHA	5.71	1.48	1.39
82	X9	202	PEB	CHB-C4B	5.71	1.49	1.38
82	N9	202	PEB	CHB-C4B	5.71	1.49	1.38
82	X7	203	PEB	CHB-C4B	5.71	1.49	1.38
84	L3	1001	CYC	CHB-C1B	5.71	1.51	1.38
84	JH	1003	CYC	C3B-C2B	5.71	1.48	1.36
84	N4	1001	CYC	C3B-C2B	5.71	1.48	1.36
84	w3	1001	CYC	CHB-C1B	5.71	1.51	1.38
82	B9	202	PEB	C3B-C2B	5.71	1.48	1.36
84	NO	1001	CYC	C3B-C2B	5.71	1.48	1.36
82	E9	202	PEB	CHB-C4B	5.71	1.49	1.38
82	Q9	203	PEB	C3B-C2B	5.71	1.48	1.36
82	qC	201	PEB	C3B-C2B	5.71	1.48	1.36
82	kK	202	PEB	CHB-C4B	5.70	1.49	1.38
82	P9	202	PEB	CHB-C4B	5.70	1.49	1.38
84	N4	1001	CYC	C2A-C3A	5.70	1.48	1.36
84	DH	1001	CYC	C3B-C2B	5.70	1.48	1.36
84	D3	1001	CYC	CHB-C1B	5.70	1.51	1.38
82	aE	202	PEB	C3B-C2B	5.70	1.48	1.36
83	xK	306	PUB	CHB-C1C	5.70	1.49	1.38
82	I9	202	PEB	CHB-C4B	5.70	1.49	1.38
84	H3	1001	CYC	CHB-C1B	5.70	1.51	1.38
82	Q9	201	PEB	CHB-C4B	5.70	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DA	203	PEB	C3B-C2B	5.70	1.48	1.36
84	D1	1003	CYC	C3B-C2B	5.70	1.48	1.36
84	F3	1001	CYC	CHB-C1B	5.70	1.51	1.38
82	A1	301	PEB	C3B-C2B	5.70	1.48	1.36
82	eH	202	PEB	C3B-C2B	5.70	1.48	1.36
82	R1	202	PEB	C3B-C2B	5.70	1.48	1.36
82	Y7	301	PEB	C3B-C2B	5.70	1.48	1.36
84	EE	1001	CYC	C3B-C2B	5.70	1.48	1.36
83	M5	303	PUB	CHB-C1C	5.70	1.49	1.38
82	MK	203	PEB	C3B-C2B	5.70	1.48	1.36
84	o3	1001	CYC	CHB-C1B	5.70	1.51	1.38
84	h3	1001	CYC	CHB-C1B	5.69	1.51	1.38
82	xC	201	PEB	CHB-C4B	5.69	1.49	1.38
84	BG	1002	CYC	C3B-C2B	5.69	1.48	1.36
84	M1	201	CYC	C3B-C2B	5.69	1.48	1.36
82	D7	201	PEB	C3B-C2B	5.69	1.48	1.36
84	73	1001	CYC	CHB-C1B	5.69	1.51	1.38
82	C9	202	PEB	CHB-C4B	5.69	1.49	1.38
84	u3	1001	CYC	CHB-C1B	5.69	1.51	1.38
82	hJ	203	PEB	C3B-C2B	5.69	1.48	1.36
84	W3	1001	CYC	CHB-C1B	5.69	1.51	1.38
84	k3	1001	CYC	CHB-C1B	5.69	1.51	1.38
84	MG	1001	CYC	C3B-C2B	5.69	1.48	1.36
84	K4	1001	CYC	C3B-C2B	5.68	1.48	1.36
82	UP	202	PEB	C3B-C2B	5.68	1.48	1.36
84	d3	1001	CYC	CHB-C1B	5.68	1.51	1.38
84	Q3	1001	CYC	CHB-C1B	5.68	1.51	1.38
84	q3	1001	CYC	CHB-C1B	5.68	1.51	1.38
83	xF	306	PUB	CHB-C1C	5.68	1.49	1.38
82	AH	301	PEB	C3B-C2B	5.68	1.48	1.36
82	hE	201	PEB	C3B-C2B	5.68	1.48	1.36
82	jH	203	PEB	C3B-C2B	5.68	1.48	1.36
84	CO	1001	CYC	C3B-C2B	5.68	1.48	1.36
82	V9	202	PEB	CHB-C4B	5.68	1.49	1.38
82	pF	202	PEB	CHB-C4B	5.68	1.49	1.38
82	A1	302	PEB	C3B-C2B	5.68	1.48	1.36
82	A1	305	PEB	C3B-C2B	5.68	1.48	1.36
82	AQ	303	PEB	C3B-C2B	5.68	1.48	1.36
82	XD	202	PEB	CHB-C4B	5.68	1.49	1.38
82	E7	201	PEB	CHB-C4B	5.68	1.49	1.38
84	j3	1001	CYC	CHB-C1B	5.68	1.51	1.38
82	j1	203	PEB	C3B-C2B	5.68	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	O3	1001	CYC	CHB-C1B	5.68	1.51	1.38
82	x8	201	PEB	CHB-C4B	5.68	1.49	1.38
82	vC	202	PEB	CHB-C4B	5.68	1.49	1.38
82	WA	202	PEB	C3B-C2B	5.67	1.48	1.36
84	U3	1001	CYC	CHB-C1B	5.67	1.51	1.38
82	pK	202	PEB	CHB-C4B	5.67	1.49	1.38
82	sC	203	PEB	CHB-C4B	5.67	1.49	1.38
82	bF	202	PEB	CHB-C4B	5.67	1.49	1.38
82	iE	201	PEB	C3B-C2B	5.67	1.48	1.36
82	xF	304	PEB	C3B-C2B	5.67	1.48	1.36
84	f3	1001	CYC	CHB-C1B	5.67	1.51	1.38
82	U9	203	PEB	C3B-C2B	5.67	1.48	1.36
82	uC	202	PEB	CHB-C4B	5.67	1.49	1.38
82	VA	203	PEB	CHB-C4B	5.67	1.49	1.38
84	EG	1001	CYC	C3B-C2B	5.67	1.48	1.36
82	OH	202	PEB	C3B-C2B	5.67	1.48	1.36
82	H9	203	PEB	C3B-C2B	5.67	1.48	1.36
84	I3	1001	CYC	CHB-C1B	5.67	1.51	1.38
84	CG	1001	CYC	C3B-C2B	5.67	1.48	1.36
84	B3	1001	CYC	CHB-C1B	5.67	1.51	1.38
82	H7	203	PEB	CHB-C4B	5.66	1.49	1.38
84	n3	1001	CYC	CHB-C1B	5.66	1.51	1.38
82	HD	201	PEB	C3B-C2B	5.66	1.48	1.36
84	M3	1001	CYC	CHB-C1B	5.66	1.51	1.38
82	xK	303	PEB	C3B-C2B	5.66	1.48	1.36
84	KH	1001	CYC	C3B-C2B	5.66	1.48	1.36
91	A6	407	PHO	C3B-C4B	5.66	1.48	1.41
82	uF	202	PEB	C3B-C2B	5.66	1.48	1.36
84	DE	1001	CYC	C3B-C2B	5.66	1.48	1.36
84	DG	1001	CYC	C3B-C2B	5.66	1.48	1.36
82	tK	201	PEB	CHB-C4B	5.66	1.49	1.38
84	BE	1002	CYC	C3B-C2B	5.66	1.48	1.36
82	EA	201	PEB	CHB-C4B	5.65	1.49	1.38
82	nK	202	PEB	CHB-C4B	5.65	1.49	1.38
82	s8	203	PEB	CHB-C4B	5.65	1.49	1.38
82	YA	301	PEB	C3B-C2B	5.65	1.48	1.36
82	A7	202	PEB	C3B-C2B	5.65	1.48	1.36
84	S3	1001	CYC	CHB-C1B	5.65	1.51	1.38
82	bK	202	PEB	CHB-C4B	5.65	1.49	1.38
82	AH	302	PEB	C3B-C2B	5.65	1.48	1.36
83	Z5	302	PUB	CHB-C1C	5.65	1.49	1.38
82	AM	301	PEB	C3B-C2B	5.65	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A7	201	PEB	C3B-C2B	5.65	1.48	1.36
82	W7	202	PEB	C3B-C2B	5.65	1.48	1.36
91	a6	613	PHO	C3B-C4B	5.65	1.48	1.41
83	A4	302	PUB	C2C-C3C	5.65	1.48	1.36
84	LH	1002	CYC	CHA-C1A	5.65	1.49	1.38
82	gJ	201	PEB	C3B-C2B	5.65	1.48	1.36
82	sK	202	PEB	C3B-C2B	5.65	1.48	1.36
82	kK	203	PEB	CHB-C4B	5.65	1.49	1.38
82	D7	203	PEB	C3B-C2B	5.64	1.48	1.36
83	M5	302	PUB	CHB-C1C	5.64	1.49	1.38
84	D1	1001	CYC	C3B-C2B	5.64	1.48	1.36
82	UE	202	PEB	CHB-C4B	5.64	1.49	1.38
82	AH	305	PEB	C3B-C2B	5.64	1.48	1.36
82	tK	203	PEB	CHB-C4B	5.64	1.49	1.38
82	uK	201	PEB	C3B-C2B	5.64	1.48	1.36
82	pC	201	PEB	CHB-C4B	5.64	1.49	1.38
84	CH	1001	CYC	C3B-C2B	5.64	1.48	1.36
82	tC	201	PEB	C3B-C2B	5.64	1.48	1.36
82	jM	203	PEB	C3B-C2B	5.64	1.48	1.36
82	u8	202	PEB	CHB-C4B	5.64	1.49	1.38
82	PF	202	PEB	CHB-C4B	5.64	1.49	1.38
82	H7	201	PEB	CHB-C4B	5.64	1.49	1.38
82	pK	201	PEB	C3B-C2B	5.63	1.48	1.36
82	jM	201	PEB	C3B-C2B	5.63	1.48	1.36
82	v8	202	PEB	CHB-C4B	5.63	1.49	1.38
82	HQ	201	PEB	C3B-C2B	5.63	1.48	1.36
82	RQ	201	PEB	CHB-C4B	5.63	1.49	1.38
82	JP	201	PEB	CHB-C4B	5.63	1.49	1.38
82	U9	204	PEB	CHB-C4B	5.63	1.49	1.38
82	hG	201	PEB	C3B-C2B	5.63	1.48	1.36
82	WI	201	PEB	C3B-C2B	5.63	1.48	1.36
84	C1	1001	CYC	C3B-C2B	5.63	1.48	1.36
82	uC	203	PEB	C3B-C2B	5.63	1.48	1.36
82	HA	201	PEB	CHB-C4B	5.63	1.49	1.38
82	BI	203	PEB	CHB-C4B	5.63	1.49	1.38
82	tF	201	PEB	CHB-C4B	5.63	1.49	1.38
82	HH	1002	PEB	C3B-C2B	5.63	1.48	1.36
82	Z5	305	PEB	C3B-C2B	5.63	1.48	1.36
82	BA	202	PEB	CHB-C4B	5.62	1.49	1.38
84	H4	1001	CYC	C3B-C2B	5.62	1.48	1.36
82	ZH	203	PEB	C3B-C2B	5.62	1.48	1.36
84	K1	1001	CYC	C3B-C2B	5.62	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	GE	1001	CYC	C3B-C2B	5.62	1.48	1.36
84	GG	1001	CYC	C3B-C2B	5.62	1.48	1.36
82	lF	201	PEB	C3B-C2B	5.62	1.48	1.36
82	lM	203	PEB	C3B-C2B	5.62	1.48	1.36
82	lE	201	PEB	C3B-C2B	5.62	1.48	1.36
84	BG	1001	CYC	C3B-C2B	5.62	1.48	1.36
82	UG	202	PEB	CHB-C4B	5.62	1.49	1.38
82	DF	202	PEB	C3B-C2B	5.62	1.48	1.36
82	l4	202	PEB	CHB-C4B	5.62	1.49	1.38
82	DA	201	PEB	C3B-C2B	5.62	1.48	1.36
82	O1	202	PEB	C3B-C2B	5.62	1.48	1.36
82	JI	201	PEB	C3B-C2B	5.61	1.48	1.36
82	AA	201	PEB	C3B-C2B	5.61	1.48	1.36
82	vC	202	PEB	C3B-C2B	5.61	1.48	1.36
82	UI	201	PEB	C3B-C2B	5.61	1.48	1.36
84	LH	1002	CYC	C3B-C2B	5.61	1.48	1.36
82	XD	202	PEB	C3B-C2B	5.61	1.48	1.36
82	XA	203	PEB	CHB-C4B	5.61	1.49	1.38
82	YK	203	PEB	C3B-C2B	5.61	1.48	1.36
82	B9	201	PEB	CHB-C4B	5.61	1.49	1.38
82	sF	202	PEB	C3B-C2B	5.61	1.48	1.36
82	mG	201	PEB	C3B-C2B	5.61	1.48	1.36
82	HP	201	PEB	CHB-C4B	5.61	1.49	1.38
82	Z9	303	PEB	C3B-C2B	5.61	1.48	1.36
82	uC	202	PEB	C3B-C2B	5.60	1.48	1.36
82	M9	304	PEB	C3B-C2B	5.60	1.48	1.36
82	W5	202	PEB	CHB-C4B	5.60	1.49	1.38
82	YK	202	PEB	C3B-C2B	5.60	1.48	1.36
82	lK	201	PEB	C3B-C2B	5.60	1.48	1.36
82	H1	1002	PEB	C3B-C2B	5.60	1.48	1.36
82	M5	305	PEB	C3B-C2B	5.60	1.48	1.36
82	fG	203	PEB	C3B-C2B	5.60	1.48	1.36
82	ZI	401	PEB	CHB-C4B	5.60	1.49	1.38
82	Z1	203	PEB	C3B-C2B	5.60	1.48	1.36
82	eE	203	PEB	CHB-C4B	5.60	1.49	1.38
82	p8	201	PEB	CHB-C4B	5.60	1.49	1.38
82	YF	203	PEB	C3B-C2B	5.60	1.48	1.36
82	AO	304	PEB	C3B-C2B	5.60	1.48	1.36
82	A4	304	PEB	C3B-C2B	5.60	1.48	1.36
84	HO	1001	CYC	C3B-C2B	5.60	1.48	1.36
84	L1	1001	CYC	CHA-C1A	5.60	1.49	1.38
82	z8	202	PEB	CHB-C4B	5.59	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	ME	1001	CYC	C3B-C2B	5.59	1.48	1.36
82	eG	203	PEB	CHB-C4B	5.59	1.49	1.38
82	DK	202	PEB	C3B-C2B	5.59	1.48	1.36
82	mE	201	PEB	C3B-C2B	5.59	1.48	1.36
82	B7	202	PEB	CHB-C4B	5.59	1.49	1.38
84	DH	1003	CYC	C3B-C2B	5.59	1.48	1.36
82	lO	202	PEB	CHB-C4B	5.59	1.49	1.38
82	eE	203	PEB	C3B-C2B	5.59	1.48	1.36
82	OI	202	PEB	C3B-C2B	5.59	1.48	1.36
82	RD	202	PEB	C3B-C2B	5.59	1.48	1.36
82	g1	202	PEB	C3B-C2B	5.59	1.48	1.36
82	c4	202	PEB	C3B-C2B	5.59	1.48	1.36
84	FH	1001	CYC	C3B-C2B	5.59	1.48	1.36
82	RD	201	PEB	CHB-C4B	5.59	1.49	1.38
82	YF	202	PEB	C3B-C2B	5.58	1.48	1.36
82	MF	203	PEB	C3B-C2B	5.58	1.48	1.36
82	SF	201	PEB	C3B-C2B	5.58	1.48	1.36
82	R4	203	PEB	CHB-C4B	5.58	1.49	1.38
82	18	202	PEB	CHB-C4B	5.58	1.49	1.38
82	ZK	202	PEB	CHB-C4B	5.58	1.49	1.38
82	lG	201	PEB	C3B-C2B	5.58	1.48	1.36
82	FA	203	PEB	C3B-C2B	5.58	1.48	1.36
82	iG	201	PEB	C3B-C2B	5.58	1.48	1.36
82	gH	202	PEB	C3B-C2B	5.58	1.48	1.36
82	vK	202	PEB	CHB-C4B	5.58	1.49	1.38
84	GO	1001	CYC	C2A-C3A	5.57	1.48	1.36
82	dK	201	PEB	CHB-C4B	5.57	1.49	1.38
82	D7	202	PEB	C3B-C2B	5.57	1.48	1.36
83	AO	302	PUB	C2C-C3C	5.57	1.48	1.36
82	u8	203	PEB	C3B-C2B	5.57	1.48	1.36
82	BI	201	PEB	C3B-C2B	5.57	1.48	1.36
82	pF	201	PEB	C3B-C2B	5.57	1.48	1.36
82	F7	203	PEB	C3B-C2B	5.57	1.48	1.36
84	HO	1001	CYC	C2A-C3A	5.57	1.48	1.36
82	FP	201	PEB	CHB-C4B	5.57	1.49	1.38
82	eE	202	PEB	C3B-C2B	5.57	1.48	1.36
82	gE	202	PEB	C3B-C2B	5.57	1.48	1.36
82	wF	302	PEB	C3B-C2B	5.57	1.48	1.36
82	RD	201	PEB	C3B-C2B	5.57	1.48	1.36
82	WH	202	PEB	C3B-C2B	5.57	1.48	1.36
82	WI	202	PEB	C3B-C2B	5.57	1.48	1.36
82	HI	201	PEB	C3B-C2B	5.56	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	vF	202	PEB	CHB-C4B	5.56	1.49	1.38
82	u8	202	PEB	C3B-C2B	5.56	1.48	1.36
82	iM	202	PEB	C3B-C2B	5.56	1.48	1.36
84	L1	1001	CYC	C3B-C2B	5.56	1.48	1.36
82	t8	201	PEB	C3B-C2B	5.56	1.48	1.36
82	EM	201	PEB	C3B-C2B	5.55	1.48	1.36
82	XF	202	PEB	C3B-C2B	5.55	1.48	1.36
82	h1	201	PEB	C3B-C2B	5.55	1.48	1.36
82	a1	202	PEB	C3B-C2B	5.55	1.48	1.36
82	LA	203	PEB	CHB-C4B	5.55	1.49	1.38
82	dG	203	PEB	CHB-C4B	5.55	1.49	1.38
83	YA	302	PUB	CHB-C1C	5.55	1.49	1.38
82	SI	201	PEB	C3B-C2B	5.55	1.48	1.36
82	cO	202	PEB	C3B-C2B	5.55	1.48	1.36
84	MO	1001	CYC	C3B-C2B	5.55	1.48	1.36
84	M4	1001	CYC	C3B-C2B	5.55	1.48	1.36
82	HA	201	PEB	C3B-C2B	5.55	1.48	1.36
83	K7	203	PUB	C2C-C3C	5.55	1.48	1.36
82	q8	201	PEB	CHB-C4B	5.55	1.49	1.38
82	RQ	202	PEB	C3B-C2B	5.54	1.48	1.36
82	RO	203	PEB	CHB-C4B	5.54	1.49	1.38
82	oK	202	PEB	CHB-C4B	5.54	1.49	1.38
82	H7	201	PEB	C3B-C2B	5.54	1.48	1.36
82	dE	203	PEB	CHB-C4B	5.54	1.49	1.38
82	oF	202	PEB	CHB-C4B	5.54	1.49	1.38
82	v8	202	PEB	C3B-C2B	5.54	1.48	1.36
82	W1	202	PEB	C3B-C2B	5.54	1.48	1.36
82	OI	201	PEB	CHB-C4B	5.54	1.49	1.38
82	f1	201	PEB	C3B-C2B	5.54	1.48	1.36
82	B5	201	PEB	C3B-C2B	5.54	1.48	1.36
82	DA	202	PEB	C3B-C2B	5.54	1.48	1.36
82	lH	201	PEB	C3B-C2B	5.54	1.48	1.36
82	fH	201	PEB	CHB-C4B	5.54	1.49	1.38
84	FE	1002	CYC	C2A-C3A	5.54	1.48	1.36
82	AF	202	PEB	CHB-C4B	5.54	1.49	1.38
82	rF	201	PEB	C3B-C2B	5.54	1.48	1.36
82	OD	201	PEB	C3B-C2B	5.54	1.48	1.36
82	f1	201	PEB	CHB-C4B	5.54	1.49	1.38
82	IJ	203	PEB	C3B-C2B	5.54	1.48	1.36
82	CF	201	PEB	C3B-C2B	5.54	1.48	1.36
82	1C	202	PEB	CHB-C4B	5.53	1.49	1.38
82	kF	202	PEB	C3B-C2B	5.53	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hB	301	PEB	CHB-C4B	5.53	1.49	1.38
82	OQ	201	PEB	C3B-C2B	5.53	1.48	1.36
82	Y9	201	PEB	CHB-C4B	5.53	1.49	1.38
96	f6	101	HEM	FE-NB	5.53	2.12	1.94
82	XM	201	PEB	C3B-C2B	5.53	1.48	1.36
82	ZF	202	PEB	CHB-C4B	5.53	1.49	1.38
82	HD	203	PEB	C3B-C2B	5.53	1.48	1.36
82	aH	202	PEB	C3B-C2B	5.53	1.48	1.36
83	KA	203	PUB	C2C-C3C	5.53	1.48	1.36
82	U1	203	PEB	C3B-C2B	5.53	1.48	1.36
82	zC	202	PEB	CHB-C4B	5.53	1.49	1.38
82	fK	202	PEB	CHB-C4B	5.53	1.49	1.38
82	l1	202	PEB	C3B-C2B	5.53	1.48	1.36
82	qF	201	PEB	C3B-C2B	5.53	1.48	1.36
82	s8	202	PEB	CHB-C4B	5.53	1.49	1.38
82	qC	203	PEB	C3B-C2B	5.53	1.48	1.36
82	u8	201	PEB	CHB-C4B	5.53	1.49	1.38
82	kF	203	PEB	CHB-C4B	5.53	1.49	1.38
84	LH	1001	CYC	C3B-C2B	5.53	1.48	1.36
82	uC	201	PEB	CHB-C4B	5.53	1.49	1.38
82	YQ	201	PEB	C3B-C2B	5.53	1.48	1.36
82	eG	202	PEB	C3B-C2B	5.53	1.48	1.36
84	G4	1001	CYC	C2A-C3A	5.53	1.48	1.36
82	IJ	203	PEB	CHB-C4B	5.53	1.49	1.38
84	I1	1001	CYC	C3B-C2B	5.53	1.48	1.36
82	rK	201	PEB	C3B-C2B	5.52	1.48	1.36
82	SM	202	PEB	CHB-C4B	5.52	1.49	1.38
83	A1	303	PUB	CHB-C1C	5.52	1.49	1.38
82	RQ	201	PEB	C3B-C2B	5.52	1.48	1.36
82	f1	203	PEB	C3B-C2B	5.52	1.48	1.36
82	ND	204	PEB	C3B-C2B	5.52	1.48	1.36
82	hG	203	PEB	C3B-C2B	5.52	1.48	1.36
82	RH	202	PEB	CHB-C4B	5.52	1.49	1.38
82	R1	202	PEB	CHB-C4B	5.52	1.49	1.38
82	AP	202	PEB	C3B-C2B	5.52	1.48	1.36
82	mF	201	PEB	C3B-C2B	5.52	1.48	1.36
83	M9	303	PUB	C2C-C3C	5.52	1.48	1.36
82	bO	202	PEB	C3B-C2B	5.52	1.48	1.36
84	NH	1001	CYC	C2A-C3A	5.52	1.48	1.36
82	SK	201	PEB	C3B-C2B	5.52	1.48	1.36
82	xF	303	PEB	C3B-C2B	5.52	1.48	1.36
82	g1	202	PEB	CHB-C4B	5.52	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hF	201	PEB	C3B-C2B	5.52	1.48	1.36
84	F1	1001	CYC	C3B-C2B	5.52	1.48	1.36
84	J4	1001	CYC	C3B-C2B	5.52	1.48	1.36
83	Y7	302	PUB	CHB-C1C	5.52	1.49	1.38
82	gH	203	PEB	C3B-C2B	5.52	1.48	1.36
82	hK	201	PEB	C3B-C2B	5.52	1.48	1.36
96	E6	101	HEM	FE-NB	5.52	2.12	1.94
82	II	203	PEB	C3B-C2B	5.52	1.48	1.36
82	MP	202	PEB	C3B-C2B	5.52	1.48	1.36
82	1C	201	PEB	C3B-C2B	5.52	1.48	1.36
82	HA	203	PEB	C3B-C2B	5.52	1.48	1.36
82	yC	203	PEB	C3B-C2B	5.52	1.48	1.36
82	AK	202	PEB	CHB-C4B	5.51	1.49	1.38
82	TQ	202	PEB	CHB-C4B	5.51	1.49	1.38
82	y8	203	PEB	C3B-C2B	5.51	1.48	1.36
82	sC	203	PEB	C3B-C2B	5.51	1.48	1.36
82	RP	201	PEB	C3B-C2B	5.51	1.48	1.36
82	wK	302	PEB	C3B-C2B	5.51	1.48	1.36
82	rF	201	PEB	CHB-C4B	5.51	1.49	1.38
84	W3	1001	CYC	CHA-C1A	5.51	1.49	1.38
82	JD	202	PEB	C3B-C2B	5.51	1.48	1.36
82	wC	203	PEB	CHB-C4B	5.51	1.49	1.38
82	rK	201	PEB	CHB-C4B	5.51	1.49	1.38
82	TQ	201	PEB	C3B-C2B	5.51	1.48	1.36
82	fB	301	PEB	CHB-C4B	5.51	1.49	1.38
83	Z9	302	PUB	C2C-C3C	5.51	1.48	1.36
84	DH	1001	CYC	CHA-C1A	5.51	1.49	1.38
82	XP	202	PEB	C3B-C2B	5.51	1.48	1.36
84	H4	1001	CYC	C2A-C3A	5.51	1.48	1.36
82	w8	203	PEB	CHB-C4B	5.51	1.49	1.38
82	QJ	204	PEB	C3B-C2B	5.51	1.48	1.36
82	iH	202	PEB	CHB-C4B	5.50	1.49	1.38
82	KM	202	PEB	C3B-C2B	5.50	1.48	1.36
82	CK	201	PEB	C3B-C2B	5.50	1.48	1.36
82	S5	201	PEB	CHB-C4B	5.50	1.49	1.38
82	kG	201	PEB	CHB-C4B	5.50	1.49	1.38
82	q8	203	PEB	C3B-C2B	5.50	1.48	1.36
82	HQ	203	PEB	C3B-C2B	5.50	1.48	1.36
82	qC	201	PEB	CHB-C4B	5.50	1.49	1.38
82	JF	201	PEB	CHB-C4B	5.50	1.49	1.38
82	sC	202	PEB	CHB-C4B	5.50	1.49	1.38
84	V3	1001	CYC	C3B-C2B	5.50	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	yC	203	PEB	CHB-C4B	5.50	1.49	1.38
82	kK	203	PEB	C3B-C2B	5.50	1.48	1.36
82	QM	203	PEB	C3B-C2B	5.50	1.48	1.36
82	M5	304	PEB	C3B-C2B	5.50	1.48	1.36
82	wC	201	PEB	C3B-C2B	5.50	1.48	1.36
82	cM	201	PEB	C3B-C2B	5.50	1.48	1.36
82	WH	201	PEB	C3B-C2B	5.50	1.48	1.36
84	x3	1001	CYC	C3B-C2B	5.50	1.48	1.36
82	VI	203	PEB	C3B-C2B	5.50	1.48	1.36
82	PM	201	PEB	C3B-C2B	5.50	1.48	1.36
82	AA	201	PEB	CHB-C4B	5.50	1.49	1.38
82	kH	203	PEB	C3B-C2B	5.50	1.48	1.36
82	JQ	202	PEB	C3B-C2B	5.49	1.48	1.36
82	fK	201	PEB	CHB-C4B	5.49	1.49	1.38
82	B7	202	PEB	C3B-C2B	5.49	1.48	1.36
82	iE	202	PEB	CHB-C4B	5.49	1.49	1.38
84	D1	1001	CYC	CHA-C1A	5.49	1.49	1.38
82	HI	202	PEB	C3B-C2B	5.49	1.48	1.36
82	H5	201	PEB	C3B-C2B	5.49	1.48	1.36
82	s8	203	PEB	C3B-C2B	5.49	1.48	1.36
82	DD	201	PEB	C3B-C2B	5.49	1.48	1.36
82	TQ	203	PEB	C3B-C2B	5.49	1.48	1.36
82	TD	203	PEB	C3B-C2B	5.49	1.48	1.36
82	YD	201	PEB	C3B-C2B	5.49	1.48	1.36
84	LO	1001	CYC	C3B-C2B	5.49	1.48	1.36
82	oK	202	PEB	C3B-C2B	5.49	1.48	1.36
82	UD	201	PEB	CHB-C4B	5.49	1.49	1.38
83	AH	303	PUB	CHB-C1C	5.49	1.49	1.38
82	SE	202	PEB	C3B-C2B	5.49	1.48	1.36
82	LQ	202	PEB	C3B-C2B	5.49	1.48	1.36
82	VQ	201	PEB	C3B-C2B	5.49	1.48	1.36
82	QM	204	PEB	C3B-C2B	5.49	1.48	1.36
82	Q9	202	PEB	C3B-C2B	5.49	1.48	1.36
82	oF	202	PEB	C3B-C2B	5.49	1.48	1.36
84	y3	1001	CYC	CHA-C1A	5.49	1.49	1.38
82	l1	201	PEB	C3B-C2B	5.49	1.48	1.36
82	UH	203	PEB	C3B-C2B	5.49	1.48	1.36
82	L9	202	PEB	CHB-C4B	5.49	1.49	1.38
82	QH	202	PEB	C3B-C2B	5.49	1.48	1.36
82	U5	201	PEB	C3B-C2B	5.48	1.48	1.36
82	SG	203	PEB	C3B-C2B	5.48	1.48	1.36
82	fE	203	PEB	C3B-C2B	5.48	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jE	202	PEB	C3B-C2B	5.48	1.48	1.36
83	xF	305	PUB	C2C-C3C	5.48	1.48	1.36
82	V1	202	PEB	CHB-C4B	5.48	1.49	1.38
82	uF	201	PEB	CHB-C4B	5.48	1.49	1.38
82	M5	301	PEB	C3B-C2B	5.48	1.48	1.36
82	VP	201	PEB	CHB-C4B	5.48	1.49	1.38
82	mM	201	PEB	C3B-C2B	5.48	1.48	1.36
84	JO	1001	CYC	C3B-C2B	5.48	1.48	1.36
82	OM	202	PEB	C3B-C2B	5.48	1.48	1.36
82	dM	203	PEB	C3B-C2B	5.48	1.48	1.36
82	18	203	PEB	C3B-C2B	5.48	1.48	1.36
82	dF	201	PEB	CHB-C4B	5.48	1.49	1.38
82	gH	202	PEB	CHB-C4B	5.48	1.49	1.38
82	hE	203	PEB	C3B-C2B	5.48	1.48	1.36
82	CP	203	PEB	C3B-C2B	5.48	1.48	1.36
82	HP	202	PEB	C3B-C2B	5.48	1.48	1.36
82	18	201	PEB	C3B-C2B	5.48	1.48	1.36
82	mM	202	PEB	C3B-C2B	5.48	1.48	1.36
83	A1	303	PUB	C2C-C3C	5.48	1.48	1.36
82	ND	204	PEB	CHB-C4B	5.48	1.49	1.38
82	XK	202	PEB	C3B-C2B	5.48	1.48	1.36
82	kK	202	PEB	C3B-C2B	5.48	1.48	1.36
82	hM	202	PEB	C3B-C2B	5.48	1.48	1.36
82	Z5	301	PEB	C3B-C2B	5.48	1.48	1.36
82	VG	202	PEB	C3B-C2B	5.48	1.48	1.36
82	UD	202	PEB	CHB-C4B	5.48	1.49	1.38
82	CK	203	PEB	CHB-C4B	5.48	1.49	1.38
82	NQ	204	PEB	CHB-C4B	5.48	1.49	1.38
82	fH	203	PEB	C3B-C2B	5.48	1.48	1.36
82	Z5	304	PEB	C3B-C2B	5.47	1.48	1.36
82	VF	201	PEB	CHB-C4B	5.47	1.49	1.38
82	XF	203	PEB	CHB-C4B	5.47	1.49	1.38
82	fK	201	PEB	C3B-C2B	5.47	1.48	1.36
82	qK	201	PEB	C3B-C2B	5.47	1.48	1.36
82	YH	201	PEB	CHB-C4B	5.47	1.49	1.38
82	pK	202	PEB	C3B-C2B	5.47	1.48	1.36
82	UJ	203	PEB	CHB-C4B	5.47	1.49	1.38
82	iO	203	PEB	CHB-C4B	5.47	1.49	1.38
82	dK	201	PEB	C3B-C2B	5.47	1.48	1.36
82	GJ	202	PEB	C3B-C2B	5.47	1.48	1.36
82	DH	1002	PEB	C3B-C2B	5.47	1.48	1.36
82	AJ	301	PEB	C3B-C2B	5.47	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	IM	203	PEB	C3B-C2B	5.47	1.48	1.36
82	dE	201	PEB	C3B-C2B	5.47	1.48	1.36
82	YQ	201	PEB	CHB-C4B	5.47	1.49	1.38
82	y8	203	PEB	CHB-C4B	5.47	1.49	1.38
82	D1	1002	PEB	C3B-C2B	5.47	1.48	1.36
82	s8	201	PEB	C3B-C2B	5.47	1.48	1.36
82	uK	201	PEB	CHB-C4B	5.47	1.49	1.38
82	VG	202	PEB	CHB-C4B	5.47	1.49	1.38
82	cE	202	PEB	CHB-C4B	5.47	1.49	1.38
82	NQ	204	PEB	C3B-C2B	5.47	1.48	1.36
82	b4	202	PEB	C3B-C2B	5.47	1.48	1.36
82	w8	201	PEB	C3B-C2B	5.47	1.48	1.36
82	fM	202	PEB	C3B-C2B	5.47	1.48	1.36
82	pF	202	PEB	C3B-C2B	5.47	1.48	1.36
82	gG	202	PEB	C3B-C2B	5.47	1.48	1.36
82	vK	201	PEB	CHB-C4B	5.46	1.49	1.38
82	OD	202	PEB	C3B-C2B	5.46	1.48	1.36
82	iE	202	PEB	C3B-C2B	5.46	1.48	1.36
82	bH	202	PEB	CHB-C4B	5.46	1.49	1.38
82	kO	202	PEB	C3B-C2B	5.46	1.48	1.36
82	mE	203	PEB	CHB-C4B	5.46	1.49	1.38
82	FP	201	PEB	C3B-C2B	5.46	1.48	1.36
82	gK	203	PEB	C3B-C2B	5.46	1.48	1.36
82	XQ	203	PEB	C3B-C2B	5.46	1.48	1.36
82	J7	202	PEB	C3B-C2B	5.46	1.48	1.36
83	AH	303	PUB	C2C-C3C	5.46	1.48	1.36
82	fJ	202	PEB	CHB-C4B	5.46	1.49	1.38
82	MB	202	PEB	C3B-C2B	5.46	1.48	1.36
82	f1	203	PEB	CHB-C4B	5.46	1.49	1.38
82	c4	202	PEB	CHB-C4B	5.46	1.49	1.38
82	GM	202	PEB	C3B-C2B	5.46	1.48	1.36
82	W1	201	PEB	C3B-C2B	5.46	1.48	1.36
82	J7	201	PEB	C3B-C2B	5.46	1.48	1.36
82	aJ	201	PEB	C3B-C2B	5.46	1.48	1.36
82	YD	201	PEB	CHB-C4B	5.46	1.49	1.38
82	dD	401	PEB	C3B-C2B	5.46	1.48	1.36
82	1C	203	PEB	C3B-C2B	5.46	1.48	1.36
82	gF	203	PEB	C3B-C2B	5.46	1.48	1.36
84	N1	1001	CYC	C2A-C3A	5.46	1.48	1.36
82	ID	202	PEB	CHB-C4B	5.46	1.49	1.38
82	JA	202	PEB	C3B-C2B	5.45	1.48	1.36
82	XA	203	PEB	C3B-C2B	5.45	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q1	202	PEB	C3B-C2B	5.45	1.48	1.36
87	A2	828	CLA	C4B-NB	5.45	1.44	1.37
82	L9	202	PEB	C3B-C2B	5.45	1.48	1.36
82	hM	203	PEB	C3B-C2B	5.45	1.48	1.36
84	L4	1001	CYC	C3B-C2B	5.45	1.48	1.36
82	mG	203	PEB	CHB-C4B	5.45	1.49	1.38
82	TD	202	PEB	CHB-C4B	5.45	1.49	1.38
82	i4	203	PEB	CHB-C4B	5.45	1.49	1.38
82	Y1	201	PEB	CHB-C4B	5.45	1.49	1.38
83	xK	305	PUB	C2C-C3C	5.45	1.48	1.36
82	AD	304	PEB	CHB-C4B	5.45	1.49	1.38
82	AQ	304	PEB	CHB-C4B	5.45	1.49	1.38
82	Q9	202	PEB	CHB-C4B	5.45	1.49	1.38
82	ND	203	PEB	C3B-C2B	5.45	1.48	1.36
82	tK	201	PEB	C3B-C2B	5.45	1.48	1.36
82	fF	201	PEB	CHB-C4B	5.45	1.49	1.38
82	JA	201	PEB	C3B-C2B	5.45	1.48	1.36
82	m1	202	PEB	C2A-C1A	-5.45	1.47	1.52
82	lK	202	PEB	C3B-C2B	5.45	1.48	1.36
87	O2	202	CLA	C1D-ND	5.45	1.44	1.37
82	SH	203	PEB	CHB-C4B	5.45	1.49	1.38
82	VE	202	PEB	C3B-C2B	5.45	1.48	1.36
82	OJ	202	PEB	C3B-C2B	5.45	1.48	1.36
82	LD	202	PEB	C3B-C2B	5.45	1.48	1.36
82	YG	202	PEB	C3B-C2B	5.45	1.48	1.36
82	iF	203	PEB	C3B-C2B	5.45	1.48	1.36
82	jG	202	PEB	C3B-C2B	5.45	1.48	1.36
82	PQ	201	PEB	CHB-C4B	5.45	1.49	1.38
82	NQ	203	PEB	C3B-C2B	5.45	1.48	1.36
82	XQ	201	PEB	C3B-C2B	5.45	1.48	1.36
82	XD	201	PEB	C3B-C2B	5.45	1.48	1.36
82	fH	201	PEB	C3B-C2B	5.45	1.48	1.36
82	gK	202	PEB	C3B-C2B	5.44	1.48	1.36
82	SP	203	PEB	CHB-C4B	5.44	1.49	1.38
82	V7	201	PEB	C3B-C2B	5.44	1.48	1.36
82	AO	305	PEB	C3B-C2B	5.44	1.48	1.36
82	j1	203	PEB	CHB-C4B	5.44	1.49	1.38
82	SM	201	PEB	C3B-C2B	5.44	1.48	1.36
82	m4	202	PEB	C3B-C2B	5.44	1.48	1.36
82	R7	203	PEB	C3B-C2B	5.44	1.48	1.36
82	D9	202	PEB	CHB-C4B	5.44	1.49	1.38
82	UQ	202	PEB	CHB-C4B	5.44	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	TO	202	PEB	C3B-C2B	5.44	1.48	1.36
82	VK	201	PEB	CHB-C4B	5.44	1.49	1.38
82	hO	202	PEB	C3B-C2B	5.44	1.48	1.36
82	X7	203	PEB	C3B-C2B	5.44	1.48	1.36
82	UQ	201	PEB	CHB-C4B	5.44	1.49	1.38
82	tF	201	PEB	C3B-C2B	5.44	1.48	1.36
84	FG	1001	CYC	C2A-C3A	5.44	1.48	1.36
82	lE	203	PEB	CHB-C4B	5.44	1.49	1.38
82	XK	203	PEB	CHB-C4B	5.44	1.49	1.38
82	r8	201	PEB	C3B-C2B	5.44	1.48	1.36
82	cO	203	PEB	C3B-C2B	5.44	1.48	1.36
82	BP	201	PEB	CHB-C4B	5.44	1.49	1.38
83	AH	304	PUB	CHB-C1C	5.44	1.49	1.38
82	PG	202	PEB	C3B-C2B	5.44	1.48	1.36
82	lJ	203	PEB	C3B-C2B	5.44	1.48	1.36
82	mG	201	PEB	CHB-C4B	5.43	1.49	1.38
82	YE	202	PEB	C3B-C2B	5.43	1.48	1.36
82	L7	203	PEB	CHB-C4B	5.43	1.49	1.38
82	T4	202	PEB	C3B-C2B	5.43	1.48	1.36
82	vK	201	PEB	C3B-C2B	5.43	1.48	1.36
82	YK	201	PEB	C3B-C2B	5.43	1.48	1.36
82	CQ	202	PEB	CHB-C4B	5.43	1.49	1.38
82	VD	201	PEB	C3B-C2B	5.43	1.48	1.36
82	DK	203	PEB	CHB-C4B	5.43	1.49	1.38
82	QH	201	PEB	C3B-C2B	5.43	1.48	1.36
82	BI	202	PEB	C3B-C2B	5.43	1.48	1.36
82	dQ	401	PEB	C3B-C2B	5.43	1.48	1.36
82	gM	201	PEB	C3B-C2B	5.43	1.48	1.36
82	CD	202	PEB	CHB-C4B	5.43	1.49	1.38
82	lG	203	PEB	CHB-C4B	5.43	1.49	1.38
82	XD	203	PEB	C3B-C2B	5.43	1.48	1.36
82	F7	201	PEB	C3B-C2B	5.43	1.48	1.36
84	63	901	CYC	C2A-C3A	5.43	1.48	1.36
82	SJ	202	PEB	C3B-C2B	5.43	1.48	1.36
82	wC	204	PEB	C3B-C2B	5.43	1.48	1.36
82	AD	301	PEB	C3B-C2B	5.43	1.48	1.36
82	DJ	201	PEB	C3B-C2B	5.43	1.48	1.36
82	AQ	301	PEB	C3B-C2B	5.43	1.48	1.36
82	TD	201	PEB	C3B-C2B	5.43	1.48	1.36
82	VK	201	PEB	C3B-C2B	5.43	1.48	1.36
82	D9	202	PEB	C3B-C2B	5.43	1.48	1.36
82	mK	201	PEB	C3B-C2B	5.43	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BA	202	PEB	C3B-C2B	5.42	1.48	1.36
82	HD	202	PEB	C3B-C2B	5.42	1.48	1.36
82	KM	201	PEB	C3B-C2B	5.42	1.48	1.36
82	nK	202	PEB	C3B-C2B	5.42	1.48	1.36
82	DM	201	PEB	C3B-C2B	5.42	1.48	1.36
82	WQ	202	PEB	C3B-C2B	5.42	1.48	1.36
82	vF	201	PEB	C3B-C2B	5.42	1.48	1.36
83	AM	303	PUB	C2C-C3C	5.42	1.48	1.36
82	fF	202	PEB	CHB-C4B	5.42	1.49	1.38
82	iG	202	PEB	C3B-C2B	5.42	1.48	1.36
84	E1	1001	CYC	C3B-C2B	5.42	1.48	1.36
82	VI	202	PEB	C3B-C2B	5.42	1.48	1.36
82	OJ	202	PEB	CHB-C4B	5.42	1.49	1.38
82	e4	202	PEB	C3B-C2B	5.42	1.48	1.36
82	eF	203	PEB	C3B-C2B	5.42	1.48	1.36
82	eK	203	PEB	C3B-C2B	5.42	1.48	1.36
82	b1	202	PEB	CHB-C4B	5.42	1.49	1.38
82	VF	201	PEB	C3B-C2B	5.42	1.48	1.36
82	JM	202	PEB	C3B-C2B	5.42	1.48	1.36
82	wC	203	PEB	C3B-C2B	5.42	1.48	1.36
82	LG	1002	PEB	C3B-C2B	5.42	1.48	1.36
82	XQ	202	PEB	C3B-C2B	5.42	1.48	1.36
82	CB	202	PEB	C3B-C2B	5.42	1.48	1.36
82	JK	201	PEB	CHB-C4B	5.42	1.49	1.38
82	OQ	202	PEB	C3B-C2B	5.42	1.48	1.36
83	AE	302	PUB	C2C-C3C	5.41	1.48	1.36
82	hF	202	PEB	CHB-C4B	5.41	1.49	1.38
82	XI	202	PEB	C3B-C2B	5.41	1.48	1.36
82	GP	201	PEB	C3B-C2B	5.41	1.48	1.36
82	Q1	201	PEB	C3B-C2B	5.41	1.48	1.36
82	kE	201	PEB	CHB-C4B	5.41	1.49	1.38
82	mE	202	PEB	CHB-C4B	5.41	1.49	1.38
82	iE	201	PEB	CHB-C4B	5.41	1.49	1.38
82	FA	201	PEB	C3B-C2B	5.41	1.48	1.36
82	rC	201	PEB	C3B-C2B	5.41	1.48	1.36
82	IQ	202	PEB	CHB-C4B	5.41	1.49	1.38
82	w8	204	PEB	C3B-C2B	5.41	1.48	1.36
82	AM	302	PEB	C3B-C2B	5.41	1.48	1.36
82	j4	203	PEB	C3B-C2B	5.41	1.48	1.36
82	H7	203	PEB	C3B-C2B	5.41	1.48	1.36
82	H5	201	PEB	CHB-C4B	5.41	1.49	1.38
82	dF	201	PEB	C3B-C2B	5.41	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mO	202	PEB	C3B-C2B	5.41	1.48	1.36
82	GJ	202	PEB	CHB-C4B	5.41	1.49	1.38
82	AE	301	PEB	C3B-C2B	5.41	1.48	1.36
91	d6	404	PHO	C3B-C4B	5.41	1.47	1.41
82	EI	202	PEB	C3B-C2B	5.41	1.48	1.36
82	xK	303	PEB	CHB-C4B	5.41	1.49	1.38
82	WQ	201	PEB	CHB-C4B	5.40	1.49	1.38
82	OH	203	PEB	C3B-C2B	5.40	1.48	1.36
82	YI	201	PEB	CHB-C4B	5.40	1.49	1.38
82	RP	201	PEB	CHB-C4B	5.40	1.49	1.38
82	LE	1002	PEB	C3B-C2B	5.40	1.48	1.36
82	O1	203	PEB	C3B-C2B	5.40	1.48	1.36
82	aO	202	PEB	C3B-C2B	5.40	1.48	1.36
82	UP	202	PEB	CHB-C4B	5.40	1.49	1.38
82	jJ	201	PEB	C3B-C2B	5.40	1.48	1.36
82	NF	202	PEB	CHB-C4B	5.40	1.49	1.38
82	XJ	201	PEB	C3B-C2B	5.40	1.48	1.36
82	KI	203	PEB	C3B-C2B	5.40	1.48	1.36
82	vF	201	PEB	CHB-C4B	5.40	1.49	1.38
82	A4	305	PEB	C3B-C2B	5.40	1.48	1.36
82	YM	203	PEB	C3B-C2B	5.40	1.48	1.36
82	JQ	203	PEB	C3B-C2B	5.40	1.48	1.36
82	CF	203	PEB	CHB-C4B	5.40	1.49	1.38
82	jH	203	PEB	CHB-C4B	5.40	1.49	1.38
82	T4	203	PEB	CHB-C4B	5.40	1.49	1.38
82	iG	202	PEB	CHB-C4B	5.40	1.49	1.38
82	c4	203	PEB	C3B-C2B	5.40	1.48	1.36
82	RI	202	PEB	C3B-C2B	5.40	1.48	1.36
82	EB	501	PEB	C3B-C2B	5.39	1.48	1.36
82	aJ	203	PEB	C3B-C2B	5.39	1.48	1.36
82	dM	201	PEB	C3B-C2B	5.39	1.48	1.36
82	QE	202	PEB	CHB-C4B	5.39	1.49	1.38
82	VD	202	PEB	CHB-C4B	5.39	1.49	1.38
82	cO	202	PEB	CHB-C4B	5.39	1.49	1.38
82	L9	203	PEB	C3B-C2B	5.39	1.48	1.36
82	HQ	202	PEB	C3B-C2B	5.39	1.48	1.36
82	D9	203	PEB	CHB-C4B	5.39	1.49	1.38
82	TA	203	PEB	C3B-C2B	5.39	1.48	1.36
82	l4	202	PEB	C3B-C2B	5.39	1.48	1.36
82	gB	202	PEB	C3B-C2B	5.39	1.48	1.36
82	jM	202	PEB	C3B-C2B	5.39	1.48	1.36
82	mH	202	PEB	C2A-C1A	-5.39	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BI	203	PEB	C3B-C2B	5.39	1.48	1.36
82	NI	202	PEB	C3B-C2B	5.39	1.48	1.36
82	sC	201	PEB	C3B-C2B	5.39	1.48	1.36
84	JO	1001	CYC	C2A-C3A	5.39	1.48	1.36
82	h4	202	PEB	C3B-C2B	5.39	1.48	1.36
83	QM	201	PUB	C2C-C3C	5.39	1.48	1.36
82	PI	202	PEB	C3B-C2B	5.39	1.48	1.36
82	aM	201	PEB	C3B-C2B	5.39	1.48	1.36
82	mJ	201	PEB	C3B-C2B	5.39	1.48	1.36
87	B2	801	CLA	C1D-ND	5.39	1.44	1.37
82	CK	203	PEB	C3B-C2B	5.39	1.48	1.36
82	BK	201	PEB	CHB-C4B	5.39	1.49	1.38
82	kF	201	PEB	C3B-C2B	5.39	1.48	1.36
82	cO	203	PEB	CHB-C4B	5.39	1.49	1.38
82	T7	203	PEB	C3B-C2B	5.39	1.48	1.36
82	FK	202	PEB	CHB-C4B	5.39	1.49	1.38
82	VQ	202	PEB	CHB-C4B	5.39	1.49	1.38
82	VA	201	PEB	C3B-C2B	5.38	1.48	1.36
82	NP	201	PEB	C3B-C2B	5.38	1.48	1.36
82	hK	202	PEB	CHB-C4B	5.38	1.49	1.38
82	OK	201	PEB	C3B-C2B	5.38	1.48	1.36
83	wF	304	PUB	CHB-C1C	5.38	1.49	1.38
82	PE	202	PEB	C3B-C2B	5.38	1.48	1.36
82	CI	202	PEB	C3B-C2B	5.38	1.48	1.36
82	eG	201	PEB	C3B-C2B	5.38	1.48	1.36
82	wF	303	PEB	CHB-C4B	5.38	1.49	1.38
82	II	202	PEB	C3B-C2B	5.38	1.48	1.36
82	NP	202	PEB	C3B-C2B	5.38	1.48	1.36
82	a4	202	PEB	C3B-C2B	5.38	1.48	1.36
87	ON	202	CLA	C1D-ND	5.38	1.44	1.37
82	F7	201	PEB	CHB-C4B	5.38	1.49	1.38
82	H9	201	PEB	CHB-C4B	5.38	1.49	1.38
82	nF	201	PEB	CHB-C4B	5.38	1.49	1.38
82	cG	202	PEB	CHB-C4B	5.38	1.49	1.38
82	TI	201	PEB	C3B-C2B	5.38	1.48	1.36
82	mG	202	PEB	CHB-C4B	5.38	1.49	1.38
82	AI	202	PEB	C3B-C2B	5.38	1.48	1.36
82	GI	203	PEB	C3B-C2B	5.38	1.48	1.36
83	A1	304	PUB	CHB-C1C	5.38	1.49	1.38
82	PJ	202	PEB	C3B-C2B	5.38	1.48	1.36
82	UK	202	PEB	C3B-C2B	5.38	1.48	1.36
84	W3	1001	CYC	C3B-C2B	5.38	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MA	202	PEB	C3B-C2B	5.38	1.48	1.36
82	dG	201	PEB	C3B-C2B	5.38	1.48	1.36
82	w8	203	PEB	C3B-C2B	5.38	1.48	1.36
82	BF	201	PEB	CHB-C4B	5.38	1.49	1.38
82	kF	203	PEB	C3B-C2B	5.38	1.48	1.36
87	AN	828	CLA	C4B-NB	5.38	1.44	1.37
82	GM	201	PEB	C3B-C2B	5.38	1.48	1.36
82	hJ	201	PEB	C3B-C2B	5.38	1.48	1.36
82	i4	201	PEB	CHB-C4B	5.37	1.49	1.38
82	fF	201	PEB	C3B-C2B	5.37	1.48	1.36
82	fO	202	PEB	CHB-C4B	5.37	1.49	1.38
82	JD	203	PEB	C3B-C2B	5.37	1.48	1.36
82	W9	203	PEB	C3B-C2B	5.37	1.48	1.36
82	i1	202	PEB	CHB-C4B	5.37	1.49	1.38
82	QH	203	PEB	C3B-C2B	5.37	1.48	1.36
82	sF	201	PEB	C3B-C2B	5.37	1.48	1.36
82	WH	203	PEB	C3B-C2B	5.37	1.48	1.36
82	BP	202	PEB	C3B-C2B	5.37	1.48	1.36
82	DQ	201	PEB	C3B-C2B	5.37	1.48	1.36
82	UM	203	PEB	CHB-C4B	5.37	1.49	1.38
84	73	1002	CYC	CHA-C1A	5.37	1.49	1.38
82	iG	201	PEB	CHB-C4B	5.37	1.49	1.38
82	cK	202	PEB	C3B-C2B	5.37	1.48	1.36
82	XK	201	PEB	CHB-C4B	5.37	1.49	1.38
82	U5	201	PEB	CHB-C4B	5.37	1.49	1.38
82	MF	202	PEB	C3B-C2B	5.37	1.48	1.36
82	bF	202	PEB	C3B-C2B	5.37	1.48	1.36
82	WB	402	PEB	C3B-C2B	5.37	1.48	1.36
82	EJ	203	PEB	C3B-C2B	5.37	1.48	1.36
82	W9	202	PEB	C3B-C2B	5.37	1.48	1.36
82	nK	201	PEB	CHB-C4B	5.37	1.49	1.38
82	P1	202	PEB	C3B-C2B	5.37	1.48	1.36
82	kO	201	PEB	C3B-C2B	5.37	1.48	1.36
82	MD	201	PEB	CHB-C4B	5.37	1.49	1.38
82	aO	203	PEB	CHB-C4B	5.37	1.49	1.38
82	q8	202	PEB	C3B-C2B	5.37	1.48	1.36
83	Z9	305	PUB	C2C-C3C	5.37	1.48	1.36
82	PA	201	PEB	CHB-C4B	5.37	1.49	1.38
82	wC	202	PEB	C3B-C2B	5.37	1.48	1.36
82	GI	201	PEB	C3B-C2B	5.37	1.48	1.36
82	VE	202	PEB	CHB-C4B	5.37	1.49	1.38
82	lO	202	PEB	C3B-C2B	5.37	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DF	203	PEB	CHB-C4B	5.37	1.49	1.38
82	A7	201	PEB	CHB-C4B	5.37	1.49	1.38
82	BP	201	PEB	C3B-C2B	5.36	1.48	1.36
82	b1	201	PEB	C3B-C2B	5.36	1.48	1.36
82	fH	203	PEB	CHB-C4B	5.36	1.49	1.38
82	RI	203	PEB	C3B-C2B	5.36	1.48	1.36
82	dH	202	PEB	C3B-C2B	5.36	1.48	1.36
82	mH	201	PEB	CHB-C4B	5.36	1.49	1.38
82	H7	202	PEB	C3B-C2B	5.36	1.48	1.36
82	LQ	201	PEB	C3B-C2B	5.36	1.48	1.36
82	M7	202	PEB	C3B-C2B	5.36	1.48	1.36
82	lE	203	PEB	C3B-C2B	5.36	1.48	1.36
82	iK	203	PEB	C3B-C2B	5.36	1.48	1.36
82	T1	201	PEB	C3B-C2B	5.36	1.48	1.36
82	W1	203	PEB	C3B-C2B	5.36	1.48	1.36
82	dH	201	PEB	C3B-C2B	5.36	1.48	1.36
82	PH	202	PEB	C3B-C2B	5.36	1.48	1.36
82	LH	1003	PEB	C3B-C2B	5.36	1.48	1.36
82	OF	201	PEB	C3B-C2B	5.36	1.48	1.36
82	Q1	203	PEB	C3B-C2B	5.36	1.48	1.36
84	y3	1001	CYC	C3B-C2B	5.36	1.48	1.36
82	iF	201	PEB	CHB-C4B	5.36	1.49	1.38
82	YF	201	PEB	C3B-C2B	5.36	1.48	1.36
82	qC	202	PEB	C3B-C2B	5.36	1.48	1.36
82	jJ	202	PEB	C3B-C2B	5.36	1.48	1.36
82	HA	202	PEB	C3B-C2B	5.36	1.48	1.36
82	CD	202	PEB	C3B-C2B	5.36	1.48	1.36
82	NQ	202	PEB	CHB-C4B	5.36	1.49	1.38
82	TI	203	PEB	C3B-C2B	5.36	1.48	1.36
84	EH	1001	CYC	C3B-C2B	5.36	1.48	1.36
82	dB	201	PEB	C3B-C2B	5.36	1.48	1.36
82	DM	202	PEB	C3B-C2B	5.36	1.48	1.36
82	eO	202	PEB	C3B-C2B	5.36	1.48	1.36
82	FA	201	PEB	CHB-C4B	5.36	1.49	1.38
82	CQ	202	PEB	C3B-C2B	5.36	1.48	1.36
82	d1	202	PEB	C3B-C2B	5.36	1.48	1.36
82	K7	202	PEB	C3B-C2B	5.36	1.48	1.36
82	VG	201	PEB	CHB-C4B	5.36	1.49	1.38
82	IJ	201	PEB	C3B-C2B	5.35	1.48	1.36
82	B9	201	PEB	C3B-C2B	5.35	1.48	1.36
82	lF	202	PEB	C3B-C2B	5.35	1.48	1.36
82	JK	202	PEB	CHB-C4B	5.35	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	s8	201	PEB	CHB-C4B	5.35	1.49	1.38
82	CF	203	PEB	C3B-C2B	5.35	1.48	1.36
82	dM	202	PEB	C3B-C2B	5.35	1.48	1.36
82	NI	203	PEB	C3B-C2B	5.35	1.48	1.36
82	Q1	202	PEB	CHB-C4B	5.35	1.49	1.38
82	m1	201	PEB	CHB-C4B	5.35	1.49	1.38
82	bO	202	PEB	CHB-C4B	5.35	1.49	1.38
82	I5	202	PEB	C3B-C2B	5.35	1.48	1.36
82	XF	201	PEB	CHB-C4B	5.35	1.49	1.38
82	CM	202	PEB	C3B-C2B	5.35	1.48	1.36
82	O4	202	PEB	CHB-C4B	5.35	1.49	1.38
82	q8	203	PEB	CHB-C4B	5.35	1.49	1.38
82	BA	203	PEB	C3B-C2B	5.35	1.48	1.36
82	kO	201	PEB	CHB-C4B	5.35	1.49	1.38
82	hK	202	PEB	C3B-C2B	5.35	1.48	1.36
82	sK	201	PEB	C3B-C2B	5.35	1.48	1.36
82	GP	203	PEB	C3B-C2B	5.35	1.48	1.36
82	QB	202	PEB	CHB-C4B	5.35	1.49	1.38
82	QQ	202	PEB	CHB-C4B	5.35	1.49	1.38
82	KA	202	PEB	C3B-C2B	5.35	1.48	1.36
82	xF	304	PEB	CHB-C4B	5.35	1.49	1.38
82	TO	203	PEB	CHB-C4B	5.35	1.49	1.38
84	FH	1001	CYC	CHA-C1A	5.35	1.49	1.38
82	aF	203	PEB	C3B-C2B	5.35	1.48	1.36
82	mK	202	PEB	C3B-C2B	5.35	1.48	1.36
82	QG	202	PEB	CHB-C4B	5.35	1.49	1.38
82	TP	201	PEB	C3B-C2B	5.35	1.48	1.36
82	kK	201	PEB	C3B-C2B	5.34	1.48	1.36
82	fM	201	PEB	C3B-C2B	5.34	1.48	1.36
82	QF	202	PEB	CHB-C4B	5.34	1.49	1.38
82	EP	202	PEB	C3B-C2B	5.34	1.48	1.36
82	qK	203	PEB	C3B-C2B	5.34	1.48	1.36
82	qF	201	PEB	CHB-C4B	5.34	1.49	1.38
82	dE	202	PEB	CHB-C4B	5.34	1.49	1.38
82	FF	202	PEB	CHB-C4B	5.34	1.49	1.38
82	MK	202	PEB	CHB-C4B	5.34	1.49	1.38
82	jG	201	PEB	CHB-C4B	5.34	1.49	1.38
82	VP	202	PEB	C3B-C2B	5.34	1.48	1.36
82	V5	202	PEB	C3B-C2B	5.34	1.48	1.36
82	k4	201	PEB	CHB-C4B	5.34	1.49	1.38
82	WD	201	PEB	CHB-C4B	5.34	1.49	1.38
82	VF	202	PEB	CHB-C4B	5.34	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	iF	203	PEB	CHB-C4B	5.34	1.49	1.38
82	TH	201	PEB	C3B-C2B	5.34	1.48	1.36
82	BQ	201	PEB	C3B-C2B	5.34	1.48	1.36
82	V7	202	PEB	C3B-C2B	5.34	1.48	1.36
82	iK	203	PEB	CHB-C4B	5.34	1.49	1.38
82	MA	201	PEB	C3B-C2B	5.34	1.48	1.36
82	LK	201	PEB	C3B-C2B	5.34	1.48	1.36
82	gF	202	PEB	C3B-C2B	5.34	1.48	1.36
82	PA	203	PEB	CHB-C4B	5.34	1.49	1.38
82	PD	201	PEB	CHB-C4B	5.34	1.49	1.38
82	VA	202	PEB	C3B-C2B	5.34	1.48	1.36
82	l1	202	PEB	CHB-C4B	5.34	1.49	1.38
82	xK	304	PEB	CHB-C4B	5.34	1.49	1.38
82	k4	201	PEB	C3B-C2B	5.34	1.48	1.36
82	mE	201	PEB	CHB-C4B	5.34	1.49	1.38
82	dM	203	PEB	CHB-C4B	5.34	1.49	1.38
82	MQ	201	PEB	CHB-C4B	5.34	1.49	1.38
82	aK	203	PEB	C3B-C2B	5.34	1.48	1.36
82	iK	201	PEB	CHB-C4B	5.34	1.49	1.38
82	PQ	203	PEB	C3B-C2B	5.33	1.48	1.36
82	S1	202	PEB	C3B-C2B	5.33	1.48	1.36
82	JF	202	PEB	CHB-C4B	5.33	1.49	1.38
82	OM	203	PEB	C3B-C2B	5.33	1.48	1.36
82	bH	201	PEB	C3B-C2B	5.33	1.48	1.36
83	AG	302	PUB	C2C-C3C	5.33	1.48	1.36
82	RA	203	PEB	C3B-C2B	5.33	1.48	1.36
82	RH	201	PEB	CHB-C4B	5.33	1.49	1.38
82	C5	202	PEB	C3B-C2B	5.33	1.48	1.36
82	WB	401	PEB	C3B-C2B	5.33	1.48	1.36
82	T5	202	PEB	C3B-C2B	5.33	1.48	1.36
82	NP	201	PEB	CHB-C4B	5.33	1.49	1.38
82	qF	203	PEB	CHB-C4B	5.33	1.49	1.38
82	lH	201	PEB	CHB-C4B	5.33	1.49	1.38
82	fJ	203	PEB	CHB-C4B	5.33	1.49	1.38
84	F1	1001	CYC	CHA-C1A	5.33	1.49	1.38
82	HI	201	PEB	CHB-C4B	5.33	1.49	1.38
82	a1	201	PEB	CHB-C4B	5.33	1.49	1.38
82	P5	202	PEB	C3B-C2B	5.33	1.48	1.36
82	w8	202	PEB	C3B-C2B	5.33	1.48	1.36
82	gO	202	PEB	C3B-C2B	5.33	1.48	1.36
82	YO	201	PEB	CHB-C4B	5.33	1.49	1.38
82	uF	202	PEB	CHB-C4B	5.33	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NF	201	PEB	C3B-C2B	5.33	1.48	1.36
82	nF	202	PEB	C3B-C2B	5.33	1.48	1.36
82	KA	202	PEB	CHB-C4B	5.33	1.49	1.38
82	QJ	203	PEB	C3B-C2B	5.33	1.48	1.36
82	UI	201	PEB	CHB-C4B	5.33	1.49	1.38
82	VK	202	PEB	CHB-C4B	5.33	1.49	1.38
82	J9	202	PEB	CHB-C4B	5.33	1.49	1.38
82	U1	201	PEB	C3B-C2B	5.33	1.48	1.36
82	Y1	202	PEB	C3B-C2B	5.33	1.48	1.36
82	qK	203	PEB	CHB-C4B	5.33	1.49	1.38
82	B7	203	PEB	C3B-C2B	5.33	1.48	1.36
82	MM	203	PEB	C3B-C2B	5.33	1.48	1.36
82	B5	202	PEB	C3B-C2B	5.33	1.48	1.36
82	LF	201	PEB	C3B-C2B	5.33	1.48	1.36
82	h4	202	PEB	CHB-C4B	5.33	1.49	1.38
82	QP	203	PEB	C3B-C2B	5.33	1.48	1.36
82	BF	202	PEB	CHB-C4B	5.33	1.49	1.38
82	E5	202	PEB	C3B-C2B	5.33	1.48	1.36
82	cG	202	PEB	C3B-C2B	5.33	1.48	1.36
82	f4	202	PEB	CHB-C4B	5.33	1.49	1.38
82	WD	202	PEB	C3B-C2B	5.33	1.48	1.36
82	a4	203	PEB	CHB-C4B	5.33	1.49	1.38
82	jJ	202	PEB	CHB-C4B	5.32	1.49	1.38
82	N5	202	PEB	C3B-C2B	5.32	1.48	1.36
87	BN	802	CLA	C1D-ND	5.32	1.44	1.37
82	L1	1002	PEB	C3B-C2B	5.32	1.48	1.36
82	DE	1002	PEB	C3B-C2B	5.32	1.48	1.36
82	a4	203	PEB	C3B-C2B	5.32	1.48	1.36
83	AJ	304	PUB	C2C-C3C	5.32	1.48	1.36
82	NK	202	PEB	CHB-C4B	5.32	1.49	1.38
82	wK	303	PEB	CHB-C4B	5.32	1.49	1.38
82	fJ	201	PEB	C3B-C2B	5.32	1.48	1.36
82	cH	202	PEB	CHB-C4B	5.32	1.49	1.38
82	ND	202	PEB	CHB-C4B	5.32	1.49	1.38
82	PD	203	PEB	C3B-C2B	5.32	1.48	1.36
82	f4	202	PEB	C3B-C2B	5.32	1.48	1.36
82	TM	201	PEB	C3B-C2B	5.32	1.48	1.36
82	EA	202	PEB	CHB-C4B	5.32	1.49	1.38
82	eG	202	PEB	CHB-C4B	5.32	1.49	1.38
82	M9	302	PEB	C3B-C2B	5.32	1.48	1.36
82	JF	201	PEB	C3B-C2B	5.32	1.48	1.36
82	A4	301	PEB	C3B-C2B	5.32	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	LE	1001	CYC	C3B-C2B	5.32	1.48	1.36
84	CO	1001	CYC	C2A-C3A	5.32	1.48	1.36
82	DD	203	PEB	C3B-C2B	5.32	1.48	1.36
82	G5	202	PEB	C3B-C2B	5.32	1.48	1.36
82	P7	201	PEB	CHB-C4B	5.32	1.49	1.38
82	AG	301	PEB	C3B-C2B	5.32	1.48	1.36
82	UD	202	PEB	C3B-C2B	5.32	1.48	1.36
82	QH	202	PEB	CHB-C4B	5.32	1.49	1.38
82	qC	203	PEB	CHB-C4B	5.32	1.49	1.38
82	KM	203	PEB	C3B-C2B	5.32	1.48	1.36
82	YD	202	PEB	CHB-C4B	5.31	1.49	1.38
82	YQ	202	PEB	CHB-C4B	5.31	1.49	1.38
82	A5	202	PEB	C3B-C2B	5.31	1.48	1.36
82	18	203	PEB	CHB-C4B	5.31	1.49	1.38
82	BD	201	PEB	C3B-C2B	5.31	1.48	1.36
82	sC	201	PEB	CHB-C4B	5.31	1.49	1.38
84	NH	1001	CYC	CHA-C1A	5.31	1.49	1.38
82	mF	202	PEB	C3B-C2B	5.31	1.48	1.36
84	J1	1001	CYC	C3B-C2B	5.31	1.48	1.36
82	QD	202	PEB	CHB-C4B	5.31	1.49	1.38
82	TQ	201	PEB	CHB-C4B	5.31	1.49	1.38
82	QB	203	PEB	C3B-C2B	5.31	1.48	1.36
82	TP	202	PEB	C3B-C2B	5.31	1.48	1.36
82	AH	305	PEB	CHB-C4B	5.31	1.49	1.38
82	qK	201	PEB	CHB-C4B	5.31	1.49	1.38
82	EM	202	PEB	C3B-C2B	5.31	1.48	1.36
82	TF	201	PEB	C3B-C2B	5.31	1.48	1.36
82	rF	202	PEB	C3B-C2B	5.31	1.48	1.36
84	BG	1001	CYC	C2A-C3A	5.31	1.48	1.36
82	Y4	201	PEB	CHB-C4B	5.31	1.49	1.38
82	hO	201	PEB	CHB-C4B	5.31	1.49	1.38
82	UB	303	PEB	C3B-C2B	5.31	1.48	1.36
82	D5	203	PEB	C3B-C2B	5.31	1.48	1.36
82	bK	202	PEB	C3B-C2B	5.31	1.48	1.36
82	iM	201	PEB	C3B-C2B	5.31	1.48	1.36
82	SJ	201	PEB	C3B-C2B	5.31	1.48	1.36
84	KO	1001	CYC	C2A-C3A	5.31	1.48	1.36
82	PH	202	PEB	CHB-C4B	5.30	1.49	1.38
82	P7	203	PEB	CHB-C4B	5.30	1.49	1.38
82	fG	202	PEB	CHB-C4B	5.30	1.49	1.38
82	DI	201	PEB	C3B-C2B	5.30	1.48	1.36
82	UJ	203	PEB	C3B-C2B	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	R5	202	PEB	C3B-C2B	5.30	1.48	1.36
82	M7	201	PEB	C3B-C2B	5.30	1.48	1.36
84	J4	1001	CYC	C2A-C3A	5.30	1.48	1.36
82	UH	201	PEB	C3B-C2B	5.30	1.48	1.36
82	YP	503	PEB	C3B-C2B	5.30	1.48	1.36
82	d4	202	PEB	C3B-C2B	5.30	1.48	1.36
82	bK	201	PEB	C3B-C2B	5.30	1.48	1.36
82	Z9	301	PEB	C3B-C2B	5.30	1.48	1.36
82	E7	202	PEB	CHB-C4B	5.30	1.49	1.38
82	kM	202	PEB	C3B-C2B	5.30	1.48	1.36
84	LG	1001	CYC	C3B-C2B	5.30	1.48	1.36
82	YO	203	PEB	CHB-C4B	5.30	1.49	1.38
82	QM	204	PEB	CHB-C4B	5.30	1.49	1.38
82	OQ	202	PEB	CHB-C4B	5.30	1.49	1.38
82	ZB	202	PEB	C3B-C2B	5.30	1.48	1.36
82	FI	202	PEB	C3B-C2B	5.30	1.48	1.36
82	RM	201	PEB	C3B-C2B	5.30	1.48	1.36
82	SM	202	PEB	C3B-C2B	5.30	1.48	1.36
82	k1	201	PEB	C3B-C2B	5.30	1.48	1.36
82	OO	202	PEB	CHB-C4B	5.30	1.48	1.38
82	hB	301	PEB	C3B-C2B	5.30	1.48	1.36
82	R1	201	PEB	CHB-C4B	5.30	1.48	1.38
82	lF	201	PEB	CHB-C4B	5.30	1.48	1.38
82	ZM	201	PEB	C3B-C2B	5.30	1.48	1.36
82	UE	202	PEB	C3B-C2B	5.30	1.48	1.36
82	JP	201	PEB	C3B-C2B	5.30	1.48	1.36
82	e1	202	PEB	CHB-C4B	5.30	1.48	1.38
82	SP	202	PEB	CHB-C4B	5.30	1.48	1.38
82	YH	202	PEB	C3B-C2B	5.30	1.48	1.36
82	lG	203	PEB	C3B-C2B	5.30	1.48	1.36
82	xF	303	PEB	CHB-C4B	5.30	1.48	1.38
82	i4	201	PEB	C3B-C2B	5.30	1.48	1.36
82	cE	202	PEB	C3B-C2B	5.30	1.48	1.36
82	SD	202	PEB	C3B-C2B	5.30	1.48	1.36
82	EM	203	PEB	C3B-C2B	5.29	1.48	1.36
82	XM	202	PEB	C3B-C2B	5.29	1.48	1.36
82	eE	202	PEB	CHB-C4B	5.29	1.48	1.38
82	AI	203	PEB	C3B-C2B	5.29	1.48	1.36
82	iF	202	PEB	C3B-C2B	5.29	1.48	1.36
82	jK	202	PEB	CHB-C4B	5.29	1.48	1.38
82	kH	201	PEB	C3B-C2B	5.29	1.48	1.36
84	73	1002	CYC	C3B-C2B	5.29	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hO	202	PEB	CHB-C4B	5.29	1.48	1.38
82	gM	202	PEB	C3B-C2B	5.29	1.48	1.36
84	FE	1002	CYC	C3B-C2B	5.29	1.48	1.36
82	MJ	203	PEB	CHB-C4B	5.29	1.48	1.38
82	S5	201	PEB	C3B-C2B	5.29	1.48	1.36
82	X5	202	PEB	C3B-C2B	5.29	1.48	1.36
82	BB	201	PEB	C3B-C2B	5.29	1.48	1.36
82	A7	202	PEB	CHB-C4B	5.29	1.48	1.38
82	EQ	202	PEB	C3B-C2B	5.29	1.48	1.36
82	K7	202	PEB	CHB-C4B	5.29	1.48	1.38
82	PH	201	PEB	CHB-C4B	5.29	1.48	1.38
82	b4	202	PEB	CHB-C4B	5.29	1.48	1.38
82	L7	201	PEB	C3B-C2B	5.29	1.48	1.36
82	NB	202	PEB	C3B-C2B	5.29	1.48	1.36
82	eA	301	PEB	CHB-C4B	5.29	1.48	1.38
82	QD	201	PEB	CHB-C4B	5.29	1.48	1.38
82	TD	201	PEB	CHB-C4B	5.29	1.48	1.38
82	QQ	201	PEB	CHB-C4B	5.29	1.48	1.38
82	QJ	204	PEB	CHB-C4B	5.29	1.48	1.38
82	JK	201	PEB	C3B-C2B	5.29	1.48	1.36
82	DP	202	PEB	C3B-C2B	5.29	1.48	1.36
82	K5	202	PEB	C3B-C2B	5.29	1.48	1.36
82	aM	202	PEB	C3B-C2B	5.29	1.48	1.36
82	fE	202	PEB	C3B-C2B	5.29	1.48	1.36
82	LI	201	PEB	CHB-C4B	5.29	1.48	1.38
82	hM	201	PEB	C3B-C2B	5.29	1.48	1.36
82	W9	203	PEB	CHB-C4B	5.29	1.48	1.38
84	M3	1001	CYC	CHA-C1A	5.29	1.48	1.38
82	HJ	202	PEB	C3B-C2B	5.29	1.48	1.36
82	ZO	202	PEB	C3B-C2B	5.29	1.48	1.36
82	QQ	202	PEB	C3B-C2B	5.29	1.48	1.36
82	d1	201	PEB	C3B-C2B	5.29	1.48	1.36
82	DM	201	PEB	CHB-C4B	5.29	1.48	1.38
82	V1	201	PEB	CHB-C4B	5.29	1.48	1.38
82	l1	201	PEB	CHB-C4B	5.29	1.48	1.38
82	c4	203	PEB	CHB-C4B	5.29	1.48	1.38
82	OG	201	PEB	CHB-C4B	5.29	1.48	1.38
82	UH	201	PEB	CHB-C4B	5.28	1.48	1.38
82	LI	201	PEB	C3B-C2B	5.28	1.48	1.36
82	TH	202	PEB	C3B-C2B	5.28	1.48	1.36
82	fO	202	PEB	C3B-C2B	5.28	1.48	1.36
82	DG	1002	PEB	C3B-C2B	5.28	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OM	201	PEB	C3B-C2B	5.28	1.48	1.36
82	TK	201	PEB	C3B-C2B	5.28	1.48	1.36
82	HI	203	PEB	C3B-C2B	5.28	1.48	1.36
82	KB	302	PEB	CHB-C4B	5.28	1.48	1.38
82	QE	202	PEB	C3B-C2B	5.28	1.48	1.36
82	aO	203	PEB	C3B-C2B	5.28	1.48	1.36
84	BE	1001	CYC	C2A-C3A	5.28	1.48	1.36
84	CH	1001	CYC	C2A-C3A	5.28	1.48	1.36
82	m4	203	PEB	CHB-C4B	5.28	1.48	1.38
82	IA	202	PEB	C3B-C2B	5.28	1.48	1.36
82	eE	201	PEB	C3B-C2B	5.28	1.48	1.36
82	B5	202	PEB	CHB-C4B	5.28	1.48	1.38
82	PP	202	PEB	C3B-C2B	5.28	1.48	1.36
82	UQ	202	PEB	C3B-C2B	5.28	1.48	1.36
82	1C	203	PEB	CHB-C4B	5.28	1.48	1.38
82	OP	202	PEB	CHB-C4B	5.28	1.48	1.38
82	VM	202	PEB	C3B-C2B	5.28	1.47	1.36
82	BI	201	PEB	CHB-C4B	5.28	1.48	1.38
83	wK	304	PUB	CHB-C1C	5.28	1.48	1.38
82	SP	201	PEB	C3B-C2B	5.28	1.47	1.36
84	FG	1001	CYC	C3B-C2B	5.28	1.47	1.36
82	QF	203	PEB	CHB-C4B	5.28	1.48	1.38
84	H3	1001	CYC	CHA-C1A	5.28	1.48	1.38
82	k1	202	PEB	CHB-C4B	5.28	1.48	1.38
82	hF	202	PEB	C3B-C2B	5.28	1.47	1.36
82	RA	202	PEB	C3B-C2B	5.28	1.47	1.36
82	LM	201	PEB	CHB-C4B	5.27	1.48	1.38
91	dL	403	PHO	C3C-C2C	5.27	1.47	1.36
82	lH	202	PEB	CHB-C4B	5.27	1.48	1.38
82	J5	201	PEB	CHB-C4B	5.27	1.48	1.38
82	SG	201	PEB	C3B-C2B	5.27	1.47	1.36
82	eK	201	PEB	C3B-C2B	5.27	1.47	1.36
82	EA	202	PEB	C3B-C2B	5.27	1.47	1.36
82	wK	301	PEB	C3B-C2B	5.27	1.47	1.36
84	FH	1001	CYC	C2A-C3A	5.27	1.47	1.36
82	XA	201	PEB	C3B-C2B	5.27	1.47	1.36
82	R7	202	PEB	C3B-C2B	5.27	1.47	1.36
84	H3	1001	CYC	C3B-C2B	5.27	1.47	1.36
84	q3	1001	CYC	CHA-C1A	5.27	1.48	1.38
82	SI	202	PEB	C3B-C2B	5.27	1.47	1.36
82	lM	202	PEB	C3B-C2B	5.27	1.47	1.36
82	PM	202	PEB	C3B-C2B	5.27	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	cO	201	PEB	C3B-C2B	5.27	1.47	1.36
83	M5	302	PUB	C3B-C2B	5.27	1.52	1.38
82	iO	201	PEB	CHB-C4B	5.27	1.48	1.38
84	JH	1001	CYC	C2A-C3A	5.27	1.47	1.36
84	h3	1001	CYC	C3B-C2B	5.27	1.47	1.36
82	RG	202	PEB	CHB-C4B	5.27	1.48	1.38
83	Z5	302	PUB	C3B-C2B	5.27	1.52	1.38
82	SH	201	PEB	C3B-C2B	5.27	1.47	1.36
82	qF	203	PEB	C3B-C2B	5.27	1.47	1.36
82	QD	202	PEB	C3B-C2B	5.27	1.47	1.36
84	N1	1001	CYC	C3B-C2B	5.27	1.47	1.36
84	n3	1001	CYC	C3B-C2B	5.27	1.47	1.36
84	w3	1001	CYC	C3B-C2B	5.27	1.47	1.36
84	C4	1001	CYC	C2A-C3A	5.27	1.47	1.36
82	LQ	201	PEB	CHB-C4B	5.27	1.48	1.38
82	dO	202	PEB	C3B-C2B	5.27	1.47	1.36
82	YE	202	PEB	CHB-C4B	5.27	1.48	1.38
82	JQ	201	PEB	CHB-C4B	5.27	1.48	1.38
82	A1	305	PEB	CHB-C4B	5.27	1.48	1.38
82	AP	203	PEB	C3B-C2B	5.26	1.47	1.36
82	P4	201	PEB	C3B-C2B	5.26	1.47	1.36
84	f3	1001	CYC	C3B-C2B	5.26	1.47	1.36
84	u3	1001	CYC	C3B-C2B	5.26	1.47	1.36
82	LD	201	PEB	C3B-C2B	5.26	1.47	1.36
82	L9	201	PEB	C3B-C2B	5.26	1.47	1.36
84	N1	1001	CYC	CHA-C1A	5.26	1.48	1.38
82	NK	201	PEB	C3B-C2B	5.26	1.47	1.36
84	L3	1001	CYC	C3B-C2B	5.26	1.47	1.36
82	cB	402	PEB	C3B-C2B	5.26	1.47	1.36
82	dG	202	PEB	C3B-C2B	5.26	1.47	1.36
84	D3	1001	CYC	CHA-C1A	5.26	1.48	1.38
84	d3	1001	CYC	CHA-C1A	5.26	1.48	1.38
84	q3	1001	CYC	C3B-C2B	5.26	1.47	1.36
82	BK	202	PEB	CHB-C4B	5.26	1.48	1.38
82	JP	202	PEB	C3B-C2B	5.26	1.47	1.36
82	VE	201	PEB	CHB-C4B	5.26	1.48	1.38
84	B3	1001	CYC	CHA-C1A	5.26	1.48	1.38
82	D9	203	PEB	C3B-C2B	5.26	1.47	1.36
82	Y9	202	PEB	CHB-C4B	5.26	1.48	1.38
84	d3	1001	CYC	C3B-C2B	5.26	1.47	1.36
84	K4	1001	CYC	C2A-C3A	5.26	1.47	1.36
82	P1	201	PEB	CHB-C4B	5.26	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A9	201	PEB	CHB-C4B	5.26	1.48	1.38
82	VM	201	PEB	C3B-C2B	5.26	1.47	1.36
82	J9	202	PEB	C3B-C2B	5.26	1.47	1.36
82	wF	301	PEB	C3B-C2B	5.26	1.47	1.36
82	HQ	202	PEB	CHB-C4B	5.26	1.48	1.38
82	WQ	202	PEB	CHB-C4B	5.26	1.48	1.38
84	u3	1001	CYC	CHA-C1A	5.26	1.48	1.38
82	Y4	203	PEB	CHB-C4B	5.26	1.48	1.38
84	JH	1001	CYC	C3B-C2B	5.26	1.47	1.36
84	D3	1001	CYC	C3B-C2B	5.26	1.47	1.36
82	UG	203	PEB	CHB-C4B	5.26	1.48	1.38
82	PI	201	PEB	CHB-C4B	5.26	1.48	1.38
82	PB	201	PEB	C3B-C2B	5.26	1.47	1.36
82	V9	201	PEB	CHB-C4B	5.26	1.48	1.38
82	QG	203	PEB	C3B-C2B	5.26	1.47	1.36
82	T1	202	PEB	C3B-C2B	5.26	1.47	1.36
82	eJ	201	PEB	C3B-C2B	5.26	1.47	1.36
84	L3	1001	CYC	CHA-C1A	5.26	1.48	1.38
84	f3	1001	CYC	CHA-C1A	5.26	1.48	1.38
82	MJ	203	PEB	C3B-C2B	5.26	1.47	1.36
82	QK	202	PEB	CHB-C4B	5.25	1.48	1.38
82	W1	203	PEB	CHB-C4B	5.25	1.48	1.38
82	WD	202	PEB	CHB-C4B	5.25	1.48	1.38
82	G5	202	PEB	CHB-C4B	5.25	1.48	1.38
82	k1	202	PEB	C3B-C2B	5.25	1.47	1.36
82	SJ	203	PEB	C3B-C2B	5.25	1.47	1.36
82	DQ	203	PEB	C3B-C2B	5.25	1.47	1.36
82	bF	201	PEB	C3B-C2B	5.25	1.47	1.36
84	F1	1001	CYC	C2A-C3A	5.25	1.47	1.36
84	S3	1001	CYC	C3B-C2B	5.25	1.47	1.36
82	XB	201	PEB	C3B-C2B	5.25	1.47	1.36
82	UF	202	PEB	C3B-C2B	5.25	1.47	1.36
82	GD	202	PEB	CHB-C4B	5.25	1.48	1.38
82	LA	201	PEB	C3B-C2B	5.25	1.47	1.36
82	aH	201	PEB	CHB-C4B	5.25	1.48	1.38
82	OI	203	PEB	C3B-C2B	5.25	1.47	1.36
84	k3	1001	CYC	C3B-C2B	5.25	1.47	1.36
84	Q3	1001	CYC	CHA-C1A	5.25	1.48	1.38
84	o3	1001	CYC	CHA-C1A	5.25	1.48	1.38
82	kH	202	PEB	C3B-C2B	5.25	1.47	1.36
82	L5	203	PEB	C3B-C2B	5.25	1.47	1.36
82	eM	202	PEB	C3B-C2B	5.25	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	iM	202	PEB	CHB-C4B	5.25	1.48	1.38
82	I7	202	PEB	C3B-C2B	5.25	1.47	1.36
82	M9	305	PEB	C3B-C2B	5.25	1.47	1.36
82	GD	201	PEB	CHB-C4B	5.25	1.48	1.38
84	n3	1001	CYC	CHA-C1A	5.25	1.48	1.38
82	KB	304	PEB	C3B-C2B	5.25	1.47	1.36
82	YG	202	PEB	CHB-C4B	5.25	1.48	1.38
82	GD	202	PEB	C3B-C2B	5.25	1.47	1.36
82	QG	202	PEB	C3B-C2B	5.25	1.47	1.36
82	eH	202	PEB	CHB-C4B	5.25	1.48	1.38
82	PK	201	PEB	C3B-C2B	5.25	1.47	1.36
82	mO	203	PEB	CHB-C4B	5.25	1.48	1.38
82	IB	203	PEB	C3B-C2B	5.25	1.47	1.36
82	J9	201	PEB	CHB-C4B	5.25	1.48	1.38
82	e1	201	PEB	C3B-C2B	5.25	1.47	1.36
82	fG	202	PEB	C3B-C2B	5.25	1.47	1.36
82	jF	202	PEB	CHB-C4B	5.25	1.48	1.38
82	cB	401	PEB	C3B-C2B	5.25	1.47	1.36
82	XI	201	PEB	CHB-C4B	5.25	1.48	1.38
82	GQ	201	PEB	CHB-C4B	5.25	1.48	1.38
82	Y1	202	PEB	CHB-C4B	5.25	1.48	1.38
82	R9	201	PEB	CHB-C4B	5.25	1.48	1.38
82	jE	201	PEB	CHB-C4B	5.25	1.48	1.38
84	U3	1001	CYC	CHA-C1A	5.25	1.48	1.38
82	j4	202	PEB	C3B-C2B	5.25	1.47	1.36
82	T5	202	PEB	CHB-C4B	5.25	1.48	1.38
82	tF	202	PEB	C3B-C2B	5.25	1.47	1.36
82	qK	202	PEB	C3B-C2B	5.25	1.47	1.36
82	fB	301	PEB	C3B-C2B	5.25	1.47	1.36
84	J3	1001	CYC	C2A-C3A	5.25	1.47	1.36
82	RE	201	PEB	CHB-C4B	5.25	1.48	1.38
82	WG	202	PEB	CHB-C4B	5.25	1.48	1.38
82	ED	202	PEB	C3B-C2B	5.24	1.47	1.36
82	qF	202	PEB	C3B-C2B	5.24	1.47	1.36
82	eM	201	PEB	C3B-C2B	5.24	1.47	1.36
82	hM	202	PEB	CHB-C4B	5.24	1.48	1.38
82	J9	201	PEB	C3B-C2B	5.24	1.47	1.36
82	E9	201	PEB	CHB-C4B	5.24	1.48	1.38
82	mG	203	PEB	C3B-C2B	5.24	1.47	1.36
82	T9	201	PEB	CHB-C4B	5.24	1.48	1.38
82	DJ	202	PEB	C3B-C2B	5.24	1.47	1.36
84	F3	1001	CYC	C3B-C2B	5.24	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	I3	1001	CYC	C3B-C2B	5.24	1.47	1.36
84	F3	1001	CYC	CHA-C1A	5.24	1.48	1.38
82	kJ	201	PEB	C3B-C2B	5.24	1.47	1.36
84	l3	1001	CYC	C2A-C3A	5.24	1.47	1.36
82	TI	202	PEB	CHB-C4B	5.24	1.48	1.38
82	jE	202	PEB	CHB-C4B	5.24	1.48	1.38
84	B3	1001	CYC	C3B-C2B	5.24	1.47	1.36
82	KI	202	PEB	CHB-C4B	5.24	1.48	1.38
82	SH	202	PEB	C3B-C2B	5.24	1.47	1.36
82	RI	201	PEB	CHB-C4B	5.24	1.48	1.38
82	k1	201	PEB	CHB-C4B	5.24	1.48	1.38
84	S3	1001	CYC	CHA-C1A	5.24	1.48	1.38
84	h3	1001	CYC	CHA-C1A	5.24	1.48	1.38
82	GM	202	PEB	CHB-C4B	5.24	1.48	1.38
82	fM	203	PEB	C3B-C2B	5.24	1.47	1.36
82	c4	201	PEB	C3B-C2B	5.24	1.47	1.36
82	yC	202	PEB	C3B-C2B	5.24	1.47	1.36
84	o3	1001	CYC	C3B-C2B	5.24	1.47	1.36
82	UB	302	PEB	CHB-C4B	5.24	1.48	1.38
82	iK	202	PEB	C3B-C2B	5.24	1.47	1.36
82	MP	201	PEB	CHB-C4B	5.24	1.48	1.38
82	U9	203	PEB	CHB-C4B	5.24	1.48	1.38
82	AO	301	PEB	C3B-C2B	5.24	1.47	1.36
82	b1	203	PEB	C3B-C2B	5.24	1.47	1.36
82	OE	202	PEB	CHB-C4B	5.24	1.48	1.38
82	H5	203	PEB	C3B-C2B	5.24	1.47	1.36
82	G7	202	PEB	C3B-C2B	5.24	1.47	1.36
84	O3	1001	CYC	C3B-C2B	5.24	1.47	1.36
82	RE	202	PEB	CHB-C4B	5.24	1.48	1.38
82	Q9	203	PEB	CHB-C4B	5.24	1.48	1.38
82	OB	201	PEB	C3B-C2B	5.24	1.47	1.36
82	LP	202	PEB	C3B-C2B	5.24	1.47	1.36
82	S1	201	PEB	C3B-C2B	5.24	1.47	1.36
83	AE	303	PUB	C2C-C3C	5.24	1.47	1.36
84	M3	1001	CYC	C3B-C2B	5.24	1.47	1.36
82	C9	201	PEB	CHB-C4B	5.24	1.48	1.38
82	SM	203	PEB	C3B-C2B	5.24	1.47	1.36
82	AA	202	PEB	CHB-C4B	5.24	1.48	1.38
82	SO	202	PEB	CHB-C4B	5.24	1.48	1.38
82	hK	201	PEB	CHB-C4B	5.24	1.48	1.38
82	GI	202	PEB	CHB-C4B	5.23	1.48	1.38
82	mJ	202	PEB	C3B-C2B	5.23	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	NH	1001	CYC	C3B-C2B	5.23	1.47	1.36
82	X7	201	PEB	C3B-C2B	5.23	1.47	1.36
84	73	1001	CYC	C3B-C2B	5.23	1.47	1.36
82	mM	202	PEB	CHB-C4B	5.23	1.48	1.38
84	73	1001	CYC	CHA-C1A	5.23	1.48	1.38
82	QK	203	PEB	CHB-C4B	5.23	1.48	1.38
82	OO	202	PEB	C3B-C2B	5.23	1.47	1.36
82	YM	203	PEB	CHB-C4B	5.23	1.48	1.38
82	N5	202	PEB	CHB-C4B	5.23	1.48	1.38
82	X9	201	PEB	CHB-C4B	5.23	1.48	1.38
84	T3	1001	CYC	C3B-C2B	5.23	1.47	1.36
82	OP	201	PEB	C3B-C2B	5.23	1.47	1.36
82	Z4	202	PEB	C3B-C2B	5.23	1.47	1.36
84	e3	1001	CYC	C2A-C3A	5.23	1.47	1.36
82	HF	202	PEB	CHB-C4B	5.23	1.48	1.38
82	RH	201	PEB	C3B-C2B	5.23	1.47	1.36
84	E3	1001	CYC	C2A-C3A	5.23	1.47	1.36
83	AG	303	PUB	C2C-C3C	5.23	1.47	1.36
84	U3	1001	CYC	C3B-C2B	5.23	1.47	1.36
84	g3	1001	CYC	C2A-C3A	5.23	1.47	1.36
82	R7	203	PEB	CHB-C4B	5.23	1.48	1.38
82	PJ	201	PEB	C3B-C2B	5.23	1.47	1.36
82	eH	201	PEB	C3B-C2B	5.23	1.47	1.36
82	OI	203	PEB	CHB-C4B	5.23	1.48	1.38
82	h4	201	PEB	CHB-C4B	5.23	1.48	1.38
82	I9	201	PEB	CHB-C4B	5.23	1.48	1.38
82	K9	201	PEB	CHB-C4B	5.23	1.48	1.38
84	m3	1001	CYC	C2A-C3A	5.23	1.47	1.36
82	A5	202	PEB	CHB-C4B	5.23	1.48	1.38
82	P5	202	PEB	CHB-C4B	5.23	1.48	1.38
82	H7	202	PEB	CHB-C4B	5.23	1.48	1.38
82	sF	203	PEB	CHB-C4B	5.23	1.48	1.38
84	Q3	1001	CYC	C3B-C2B	5.23	1.47	1.36
82	OD	202	PEB	CHB-C4B	5.23	1.48	1.38
84	R3	1001	CYC	C2A-C3A	5.23	1.47	1.36
84	G3	1001	CYC	C2A-C3A	5.23	1.47	1.36
84	O3	1001	CYC	CHA-C1A	5.23	1.48	1.38
91	A6	407	PHO	C3D-C4D	-5.23	1.33	1.41
82	rK	202	PEB	C3B-C2B	5.23	1.47	1.36
82	BB	203	PEB	C3B-C2B	5.23	1.47	1.36
82	kM	201	PEB	C3B-C2B	5.23	1.47	1.36
82	CF	201	PEB	CHB-C4B	5.23	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	LF	201	PEB	CHB-C4B	5.23	1.48	1.38
82	E5	202	PEB	CHB-C4B	5.23	1.48	1.38
82	Z9	304	PEB	C3B-C2B	5.23	1.47	1.36
82	MF	202	PEB	CHB-C4B	5.23	1.48	1.38
82	A4	305	PEB	CHB-C4B	5.23	1.48	1.38
82	VJ	201	PEB	C3B-C2B	5.23	1.47	1.36
82	GF	203	PEB	CHB-C4B	5.22	1.48	1.38
82	X5	202	PEB	CHB-C4B	5.22	1.48	1.38
82	lF	202	PEB	CHB-C4B	5.22	1.48	1.38
82	S9	203	PEB	C3B-C2B	5.22	1.47	1.36
82	jO	202	PEB	C3B-C2B	5.22	1.47	1.36
84	J3	1001	CYC	C3B-C2B	5.22	1.47	1.36
82	RA	203	PEB	CHB-C4B	5.22	1.48	1.38
82	WH	203	PEB	CHB-C4B	5.22	1.48	1.38
82	P9	201	PEB	CHB-C4B	5.22	1.48	1.38
84	C3	1001	CYC	C2A-C3A	5.22	1.47	1.36
82	G9	201	PEB	CHB-C4B	5.22	1.48	1.38
82	fE	203	PEB	CHB-C4B	5.22	1.48	1.38
82	RM	202	PEB	C3B-C2B	5.22	1.47	1.36
82	c1	202	PEB	CHB-C4B	5.22	1.48	1.38
84	G4	1001	CYC	CHA-C1A	5.22	1.48	1.38
82	TK	202	PEB	CHB-C4B	5.22	1.48	1.38
84	p3	1001	CYC	C2A-C3A	5.22	1.47	1.36
84	m3	1001	CYC	C2C-C1C	-5.22	1.47	1.52
84	HH	1001	CYC	CHA-C1A	5.22	1.48	1.38
82	OG	203	PEB	C3B-C2B	5.22	1.47	1.36
82	AE	304	PEB	C3B-C2B	5.22	1.47	1.36
84	i3	1001	CYC	C2A-C3A	5.22	1.47	1.36
84	K3	1001	CYC	C2C-C1C	-5.22	1.47	1.52
82	AJ	302	PEB	C3B-C2B	5.22	1.47	1.36
82	LD	201	PEB	CHB-C4B	5.22	1.48	1.38
82	QH	201	PEB	CHB-C4B	5.22	1.48	1.38
82	AM	302	PEB	CHB-C4B	5.22	1.48	1.38
82	CP	203	PEB	CHB-C4B	5.22	1.48	1.38
82	hM	201	PEB	CHB-C4B	5.22	1.48	1.38
82	T1	201	PEB	CHB-C4B	5.22	1.48	1.38
82	K7	201	PEB	C3B-C2B	5.22	1.47	1.36
84	j3	1001	CYC	C3B-C2B	5.22	1.47	1.36
82	jJ	203	PEB	C3B-C2B	5.22	1.47	1.36
82	LA	203	PEB	C3B-C2B	5.22	1.47	1.36
82	M9	301	PEB	CHB-C4B	5.22	1.48	1.38
82	IM	201	PEB	C3B-C2B	5.22	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	fK	202	PEB	C3B-C2B	5.22	1.47	1.36
84	c3	1001	CYC	C2A-C3A	5.22	1.47	1.36
82	II	201	PEB	CHB-C4B	5.22	1.48	1.38
82	NI	201	PEB	CHB-C4B	5.22	1.48	1.38
84	GO	1001	CYC	CHA-C1A	5.22	1.48	1.38
82	UA	201	PEB	C3B-C2B	5.22	1.47	1.36
82	YB	201	PEB	C3B-C2B	5.22	1.47	1.36
82	U7	201	PEB	C3B-C2B	5.22	1.47	1.36
82	O9	203	PEB	CHB-C4B	5.22	1.48	1.38
82	RG	201	PEB	CHB-C4B	5.21	1.48	1.38
82	N9	201	PEB	CHB-C4B	5.21	1.48	1.38
82	dM	202	PEB	CHB-C4B	5.21	1.48	1.38
82	SB	203	PEB	C3B-C2B	5.21	1.47	1.36
82	VH	202	PEB	C3B-C2B	5.21	1.47	1.36
83	AJ	303	PUB	C2C-C3C	5.21	1.47	1.36
84	G3	1001	CYC	C3B-C2B	5.21	1.47	1.36
84	w3	1001	CYC	CHA-C1A	5.21	1.48	1.38
82	SE	201	PEB	C3B-C2B	5.21	1.47	1.36
82	y8	202	PEB	C3B-C2B	5.21	1.47	1.36
83	A4	303	PUB	C2C-C3C	5.21	1.47	1.36
82	GA	202	PEB	C3B-C2B	5.21	1.47	1.36
82	UD	201	PEB	C3B-C2B	5.21	1.47	1.36
82	RE	202	PEB	C3B-C2B	5.21	1.47	1.36
84	C3	1001	CYC	C3B-C2B	5.21	1.47	1.36
82	NM	202	PEB	C3B-C2B	5.21	1.47	1.36
82	UE	203	PEB	CHB-C4B	5.21	1.48	1.38
82	mF	202	PEB	CHB-C4B	5.21	1.48	1.38
82	dH	202	PEB	CHB-C4B	5.21	1.48	1.38
82	QE	203	PEB	C3B-C2B	5.21	1.47	1.36
84	J1	1001	CYC	C2A-C3A	5.21	1.47	1.36
82	gH	203	PEB	CHB-C4B	5.21	1.48	1.38
82	VA	203	PEB	C3B-C2B	5.21	1.47	1.36
82	SB	202	PEB	C3B-C2B	5.21	1.47	1.36
84	A3	1001	CYC	C2A-C3A	5.21	1.47	1.36
82	UG	202	PEB	C3B-C2B	5.21	1.47	1.36
82	QQ	201	PEB	C3B-C2B	5.21	1.47	1.36
82	OE	201	PEB	CHB-C4B	5.21	1.48	1.38
82	UM	201	PEB	C3B-C2B	5.21	1.47	1.36
82	V5	202	PEB	CHB-C4B	5.21	1.48	1.38
82	UG	203	PEB	C3B-C2B	5.21	1.47	1.36
84	e3	1001	CYC	C3B-C2B	5.21	1.47	1.36
84	73	1002	CYC	C2A-C3A	5.21	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	R5	202	PEB	CHB-C4B	5.21	1.48	1.38
84	DH	1001	CYC	C2A-C3A	5.21	1.47	1.36
82	VI	201	PEB	CHB-C4B	5.21	1.48	1.38
82	lK	201	PEB	CHB-C4B	5.21	1.48	1.38
84	k3	1001	CYC	CHA-C1A	5.21	1.48	1.38
82	LK	201	PEB	CHB-C4B	5.21	1.48	1.38
82	L9	203	PEB	CHB-C4B	5.21	1.48	1.38
82	PO	201	PEB	C3B-C2B	5.21	1.47	1.36
82	j4	201	PEB	CHB-C4B	5.21	1.48	1.38
82	JJ	201	PEB	C3B-C2B	5.21	1.47	1.36
82	tK	202	PEB	C3B-C2B	5.21	1.47	1.36
82	NE	202	PEB	CHB-C4B	5.21	1.48	1.38
82	NG	201	PEB	CHB-C4B	5.21	1.48	1.38
82	RK	202	PEB	CHB-C4B	5.21	1.48	1.38
84	i3	1001	CYC	C2C-C1C	-5.21	1.47	1.52
82	TJ	201	PEB	C3B-C2B	5.21	1.47	1.36
84	K3	1001	CYC	C2A-C3A	5.21	1.47	1.36
84	l3	1001	CYC	C3B-C2B	5.21	1.47	1.36
82	jM	203	PEB	CHB-C4B	5.21	1.48	1.38
84	H1	1001	CYC	CHA-C1A	5.21	1.48	1.38
82	CJ	202	PEB	C3B-C2B	5.21	1.47	1.36
84	v3	1001	CYC	C2A-C3A	5.21	1.47	1.36
82	ZJ	202	PEB	C3B-C2B	5.21	1.47	1.36
82	A4	301	PEB	CHB-C4B	5.21	1.48	1.38
82	RG	202	PEB	C3B-C2B	5.20	1.47	1.36
82	E7	202	PEB	C3B-C2B	5.20	1.47	1.36
84	HH	1001	CYC	C3B-C2B	5.20	1.47	1.36
82	L9	201	PEB	CHB-C4B	5.20	1.48	1.38
82	YH	202	PEB	CHB-C4B	5.20	1.48	1.38
82	dG	204	PEB	CHB-C4B	5.20	1.48	1.38
82	U5	203	PEB	C3B-C2B	5.20	1.47	1.36
82	VP	201	PEB	C3B-C2B	5.20	1.47	1.36
82	eH	201	PEB	CHB-C4B	5.20	1.48	1.38
84	I3	1001	CYC	CHA-C1A	5.20	1.48	1.38
82	dE	202	PEB	C3B-C2B	5.20	1.47	1.36
84	T3	1001	CYC	C2A-C3A	5.20	1.47	1.36
84	t3	1001	CYC	C2A-C3A	5.20	1.47	1.36
82	KA	201	PEB	C3B-C2B	5.20	1.47	1.36
82	kJ	202	PEB	C3B-C2B	5.20	1.47	1.36
82	KD	201	PEB	C3B-C2B	5.20	1.47	1.36
82	WF	201	PEB	C3B-C2B	5.20	1.47	1.36
82	KQ	201	PEB	C3B-C2B	5.20	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	N3	1001	CYC	C2A-C3A	5.20	1.47	1.36
82	AI	201	PEB	CHB-C4B	5.20	1.48	1.38
82	BQ	202	PEB	C3B-C2B	5.20	1.47	1.36
82	W5	203	PEB	C3B-C2B	5.20	1.47	1.36
84	j3	1001	CYC	CHA-C1A	5.20	1.48	1.38
82	kH	202	PEB	CHB-C4B	5.20	1.48	1.38
82	mO	201	PEB	CHB-C4B	5.20	1.48	1.38
82	IB	202	PEB	C3B-C2B	5.20	1.47	1.36
82	g4	202	PEB	C3B-C2B	5.20	1.47	1.36
84	t3	1001	CYC	C3B-C2B	5.20	1.47	1.36
82	fE	202	PEB	CHB-C4B	5.20	1.48	1.38
82	JM	201	PEB	C3B-C2B	5.20	1.47	1.36
82	QM	202	PEB	C3B-C2B	5.20	1.47	1.36
84	i3	1001	CYC	C3B-C2B	5.20	1.47	1.36
82	lJ	201	PEB	C3B-C2B	5.20	1.47	1.36
82	aM	203	PEB	C3B-C2B	5.20	1.47	1.36
84	K3	1001	CYC	C3B-C2B	5.20	1.47	1.36
82	SJ	202	PEB	CHB-C4B	5.20	1.48	1.38
82	GQ	202	PEB	CHB-C4B	5.20	1.48	1.38
82	QD	201	PEB	C3B-C2B	5.20	1.47	1.36
82	iJ	201	PEB	C3B-C2B	5.20	1.47	1.36
82	g4	202	PEB	CHB-C4B	5.20	1.48	1.38
82	FB	201	PEB	C3B-C2B	5.20	1.47	1.36
82	jO	202	PEB	CHB-C4B	5.20	1.48	1.38
82	UE	201	PEB	C3B-C2B	5.20	1.47	1.36
82	UG	201	PEB	C3B-C2B	5.20	1.47	1.36
84	NO	1001	CYC	CHB-C1B	5.20	1.50	1.38
82	lK	202	PEB	CHB-C4B	5.20	1.48	1.38
82	GB	203	PEB	C3B-C2B	5.20	1.47	1.36
82	H9	202	PEB	C3B-C2B	5.20	1.47	1.36
82	K5	202	PEB	CHB-C4B	5.20	1.48	1.38
82	N7	203	PEB	CHB-C4B	5.20	1.48	1.38
82	HE	1002	PEB	C3B-C2B	5.20	1.47	1.36
82	CI	201	PEB	CHB-C4B	5.20	1.48	1.38
82	CP	201	PEB	C3B-C2B	5.20	1.47	1.36
84	E3	1001	CYC	C3B-C2B	5.20	1.47	1.36
82	AO	304	PEB	CHB-C4B	5.19	1.48	1.38
84	P3	1001	CYC	C2A-C3A	5.19	1.47	1.36
84	R3	1001	CYC	C2C-C1C	-5.19	1.47	1.52
82	BD	202	PEB	C3B-C2B	5.19	1.47	1.36
82	a1	201	PEB	C3B-C2B	5.19	1.47	1.36
82	c1	202	PEB	C3B-C2B	5.19	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	F9	203	PEB	C3B-C2B	5.19	1.47	1.36
82	D7	201	PEB	CHB-C4B	5.19	1.48	1.38
82	GQ	202	PEB	C3B-C2B	5.19	1.47	1.36
82	aB	202	PEB	C3B-C2B	5.19	1.47	1.36
82	FO	1002	PEB	C3B-C2B	5.19	1.47	1.36
82	P1	202	PEB	CHB-C4B	5.19	1.48	1.38
82	gG	201	PEB	CHB-C4B	5.19	1.48	1.38
82	jG	202	PEB	CHB-C4B	5.19	1.48	1.38
82	VB	202	PEB	C3B-C2B	5.19	1.47	1.36
82	mE	203	PEB	C3B-C2B	5.19	1.47	1.36
82	PO	203	PEB	CHB-C4B	5.19	1.48	1.38
82	fJ	202	PEB	C3B-C2B	5.19	1.47	1.36
82	HQ	203	PEB	CHB-C4B	5.19	1.48	1.38
82	WE	202	PEB	C3B-C2B	5.19	1.47	1.36
82	I7	201	PEB	C3B-C2B	5.19	1.47	1.36
82	SB	202	PEB	CHB-C4B	5.19	1.48	1.38
84	DO	1001	CYC	C2A-C3A	5.19	1.47	1.36
84	H1	1001	CYC	C3B-C2B	5.19	1.47	1.36
82	J5	202	PEB	C3B-C2B	5.19	1.47	1.36
82	iJ	202	PEB	C3B-C2B	5.19	1.47	1.36
82	lM	201	PEB	C3B-C2B	5.19	1.47	1.36
84	N3	1001	CYC	C3B-C2B	5.19	1.47	1.36
82	U1	201	PEB	CHB-C4B	5.19	1.48	1.38
82	SQ	202	PEB	C3B-C2B	5.19	1.47	1.36
82	MB	201	PEB	C3B-C2B	5.19	1.47	1.36
82	L7	202	PEB	C3B-C2B	5.19	1.47	1.36
82	lJ	203	PEB	CHB-C4B	5.19	1.48	1.38
82	LA	202	PEB	C3B-C2B	5.19	1.47	1.36
82	LM	201	PEB	C3B-C2B	5.19	1.47	1.36
82	HK	202	PEB	CHB-C4B	5.19	1.48	1.38
82	I5	202	PEB	CHB-C4B	5.19	1.48	1.38
84	C1	1001	CYC	CHA-C1A	5.19	1.48	1.38
84	73	1002	CYC	C1C-NC	-5.19	1.30	1.37
82	MP	203	PEB	C3B-C2B	5.19	1.47	1.36
82	h1	201	PEB	CHB-C4B	5.19	1.48	1.38
82	cG	201	PEB	C3B-C2B	5.19	1.47	1.36
82	L7	201	PEB	CHB-C4B	5.19	1.48	1.38
82	fF	202	PEB	C3B-C2B	5.19	1.47	1.36
82	Q5	201	PEB	C3B-C2B	5.18	1.47	1.36
84	R3	1001	CYC	C3B-C2B	5.18	1.47	1.36
84	g3	1001	CYC	C3B-C2B	5.18	1.47	1.36
82	VH	201	PEB	CHB-C4B	5.18	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	TA	201	PEB	C3B-C2B	5.18	1.47	1.36
84	P3	1001	CYC	C3B-C2B	5.18	1.47	1.36
82	V7	201	PEB	CHB-C4B	5.18	1.48	1.38
82	YM	202	PEB	C3B-C2B	5.18	1.47	1.36
82	eH	203	PEB	C3B-C2B	5.18	1.47	1.36
82	UQ	201	PEB	C3B-C2B	5.18	1.47	1.36
84	m3	1001	CYC	C3B-C2B	5.18	1.47	1.36
82	MM	203	PEB	CHB-C4B	5.18	1.48	1.38
82	SM	201	PEB	CHB-C4B	5.18	1.48	1.38
82	cG	201	PEB	CHB-C4B	5.18	1.48	1.38
82	U9	202	PEB	C3B-C2B	5.18	1.47	1.36
82	HG	1002	PEB	C3B-C2B	5.18	1.47	1.36
82	TM	202	PEB	CHB-C4B	5.18	1.48	1.38
82	RP	202	PEB	CHB-C4B	5.18	1.48	1.38
82	C5	202	PEB	CHB-C4B	5.18	1.48	1.38
82	PF	201	PEB	C3B-C2B	5.18	1.47	1.36
82	fG	203	PEB	CHB-C4B	5.18	1.48	1.38
82	Y5	201	PEB	C3B-C2B	5.18	1.47	1.36
82	Y9	202	PEB	C3B-C2B	5.18	1.47	1.36
82	AO	305	PEB	CHB-C4B	5.18	1.48	1.38
82	T4	201	PEB	CHB-C4B	5.18	1.48	1.38
82	YF	202	PEB	CHB-C4B	5.18	1.48	1.38
82	LO	1002	PEB	CHB-C4B	5.18	1.48	1.38
82	EP	203	PEB	C3B-C2B	5.18	1.47	1.36
84	v3	1001	CYC	C3B-C2B	5.18	1.47	1.36
82	NE	202	PEB	C3B-C2B	5.18	1.47	1.36
82	YJ	203	PEB	C3B-C2B	5.18	1.47	1.36
82	IP	203	PEB	C3B-C2B	5.18	1.47	1.36
82	m4	201	PEB	CHB-C4B	5.18	1.48	1.38
82	UE	203	PEB	C3B-C2B	5.18	1.47	1.36
82	c4	201	PEB	CHB-C4B	5.18	1.48	1.38
82	ZB	201	PEB	CHB-C4B	5.18	1.48	1.38
84	FG	1001	CYC	CHA-C1A	5.18	1.48	1.38
82	cF	201	PEB	C3B-C2B	5.18	1.47	1.36
82	CM	203	PEB	C3B-C2B	5.18	1.47	1.36
82	dJ	202	PEB	C3B-C2B	5.18	1.47	1.36
82	fJ	203	PEB	C3B-C2B	5.18	1.47	1.36
82	RD	203	PEB	CHB-C4B	5.17	1.48	1.38
82	AQ	303	PEB	CHB-C4B	5.17	1.48	1.38
82	O9	201	PEB	CHB-C4B	5.17	1.48	1.38
82	BM	301	PEB	C3B-C2B	5.17	1.47	1.36
84	FO	1001	CYC	C2A-C3A	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dG	202	PEB	CHB-C4B	5.17	1.48	1.38
82	IA	201	PEB	C3B-C2B	5.17	1.47	1.36
82	jO	201	PEB	CHB-C4B	5.17	1.48	1.38
82	HF	201	PEB	C3B-C2B	5.17	1.47	1.36
84	L4	1001	CYC	C2A-C3A	5.17	1.47	1.36
82	AO	301	PEB	CHB-C4B	5.17	1.48	1.38
82	Y5	202	PEB	C3B-C2B	5.17	1.47	1.36
82	OG	202	PEB	CHB-C4B	5.17	1.48	1.38
82	gO	201	PEB	CHB-C4B	5.17	1.48	1.38
82	P4	202	PEB	C3B-C2B	5.17	1.47	1.36
82	HD	202	PEB	CHB-C4B	5.17	1.48	1.38
82	aB	201	PEB	C3B-C2B	5.17	1.47	1.36
84	A3	1001	CYC	C3B-C2B	5.17	1.47	1.36
82	HA	202	PEB	CHB-C4B	5.17	1.48	1.38
82	GA	201	PEB	C3B-C2B	5.17	1.47	1.36
82	WI	201	PEB	CHB-C4B	5.17	1.48	1.38
82	aH	202	PEB	CHB-C4B	5.17	1.48	1.38
91	aL	610	PHO	C3C-C2C	5.17	1.47	1.36
82	bP	502	PEB	CHB-C4B	5.17	1.48	1.38
82	EI	201	PEB	CHB-C4B	5.17	1.48	1.38
82	P7	202	PEB	C3B-C2B	5.17	1.47	1.36
82	O4	201	PEB	CHB-C4B	5.17	1.48	1.38
82	hM	203	PEB	CHB-C4B	5.17	1.48	1.38
82	gM	202	PEB	CHB-C4B	5.17	1.48	1.38
82	F4	1002	PEB	C3B-C2B	5.17	1.47	1.36
82	HD	203	PEB	CHB-C4B	5.17	1.48	1.38
82	U9	201	PEB	CHB-C4B	5.17	1.48	1.38
82	aM	204	PEB	CHB-C4B	5.17	1.48	1.38
84	e3	1001	CYC	C2C-C1C	-5.17	1.47	1.52
82	JI	201	PEB	CHB-C4B	5.17	1.48	1.38
82	MK	202	PEB	C3B-C2B	5.17	1.47	1.36
82	N7	203	PEB	C3B-C2B	5.17	1.47	1.36
82	TH	201	PEB	CHB-C4B	5.17	1.48	1.38
82	I7	202	PEB	CHB-C4B	5.17	1.48	1.38
82	QP	201	PEB	C3B-C2B	5.17	1.47	1.36
82	XD	203	PEB	CHB-C4B	5.17	1.48	1.38
82	jG	201	PEB	C3B-C2B	5.17	1.47	1.36
82	G7	201	PEB	C3B-C2B	5.16	1.47	1.36
82	VA	201	PEB	CHB-C4B	5.16	1.48	1.38
82	TF	202	PEB	CHB-C4B	5.16	1.48	1.38
82	Q1	201	PEB	CHB-C4B	5.16	1.48	1.38
82	cK	202	PEB	CHB-C4B	5.16	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	l3	1001	CYC	C2C-C1C	-5.16	1.47	1.52
82	FQ	202	PEB	CHB-C4B	5.16	1.48	1.38
82	mK	202	PEB	CHB-C4B	5.16	1.48	1.38
82	WG	202	PEB	C3B-C2B	5.16	1.47	1.36
82	TD	202	PEB	C3B-C2B	5.16	1.47	1.36
82	gJ	202	PEB	C3B-C2B	5.16	1.47	1.36
84	p3	1001	CYC	C3B-C2B	5.16	1.47	1.36
82	BB	201	PEB	CHB-C4B	5.16	1.48	1.38
82	GK	203	PEB	CHB-C4B	5.16	1.48	1.38
82	dE	204	PEB	CHB-C4B	5.16	1.48	1.38
84	LO	1001	CYC	C2A-C3A	5.16	1.47	1.36
82	IK	203	PEB	C3B-C2B	5.16	1.47	1.36
82	d1	202	PEB	CHB-C4B	5.16	1.48	1.38
82	TD	203	PEB	CHB-C4B	5.16	1.48	1.38
82	OG	202	PEB	C3B-C2B	5.16	1.47	1.36
82	VJ	202	PEB	C3B-C2B	5.16	1.47	1.36
82	V7	203	PEB	C3B-C2B	5.16	1.47	1.36
82	TG	201	PEB	CHB-C4B	5.16	1.48	1.38
82	WI	203	PEB	CHB-C4B	5.16	1.48	1.38
84	N4	1001	CYC	CHB-C1B	5.16	1.50	1.38
82	aH	201	PEB	C3B-C2B	5.16	1.47	1.36
82	PO	202	PEB	C3B-C2B	5.16	1.47	1.36
82	T7	201	PEB	C3B-C2B	5.16	1.47	1.36
82	g4	201	PEB	CHB-C4B	5.16	1.48	1.38
82	aG	202	PEB	CHB-C4B	5.16	1.48	1.38
82	F9	202	PEB	C3B-C2B	5.16	1.47	1.36
84	BG	1001	CYC	CHA-C1A	5.16	1.48	1.38
82	LJ	202	PEB	C3B-C2B	5.16	1.47	1.36
84	C1	1001	CYC	C2A-C3A	5.16	1.47	1.36
82	KD	202	PEB	CHB-C4B	5.16	1.48	1.38
82	JI	202	PEB	CHB-C4B	5.16	1.48	1.38
82	aJ	203	PEB	CHB-C4B	5.16	1.48	1.38
82	NG	201	PEB	C3B-C2B	5.16	1.47	1.36
82	gO	203	PEB	CHB-C4B	5.16	1.48	1.38
82	AB	501	PEB	C3B-C2B	5.15	1.47	1.36
82	WK	201	PEB	C3B-C2B	5.15	1.47	1.36
83	AQ	302	PUB	CHB-C1C	5.15	1.48	1.38
82	NA	203	PEB	CHB-C4B	5.15	1.48	1.38
82	DP	201	PEB	CHB-C4B	5.15	1.48	1.38
82	S9	202	PEB	C3B-C2B	5.15	1.47	1.36
82	PD	202	PEB	C3B-C2B	5.15	1.47	1.36
82	PQ	202	PEB	C3B-C2B	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	iO	201	PEB	C3B-C2B	5.15	1.47	1.36
82	gE	201	PEB	CHB-C4B	5.15	1.48	1.38
82	WA	202	PEB	CHB-C4B	5.15	1.48	1.38
82	H5	202	PEB	C3B-C2B	5.15	1.47	1.36
84	g3	1001	CYC	C1C-NC	-5.15	1.30	1.37
82	cE	201	PEB	C3B-C2B	5.15	1.47	1.36
82	eF	201	PEB	C3B-C2B	5.15	1.47	1.36
82	UA	202	PEB	C3B-C2B	5.15	1.47	1.36
83	QJ	201	PUB	C2C-C3C	5.15	1.47	1.36
82	FD	202	PEB	CHB-C4B	5.15	1.48	1.38
84	c3	1001	CYC	C2C-C1C	-5.15	1.47	1.52
82	RB	202	PEB	C3B-C2B	5.15	1.47	1.36
82	kE	202	PEB	C3B-C2B	5.15	1.47	1.36
82	AH	302	PEB	CHB-C4B	5.15	1.48	1.38
82	l1	203	PEB	CHB-C4B	5.15	1.48	1.38
82	a1	202	PEB	CHB-C4B	5.15	1.48	1.38
82	qK	202	PEB	CHB-C4B	5.15	1.48	1.38
82	aJ	204	PEB	C3B-C2B	5.15	1.47	1.36
82	GM	203	PEB	C3B-C2B	5.15	1.47	1.36
91	AL	410	PHO	C3D-C4D	-5.15	1.33	1.41
82	LA	201	PEB	CHB-C4B	5.15	1.48	1.38
84	P3	1001	CYC	C2C-C1C	-5.15	1.47	1.52
82	g4	203	PEB	CHB-C4B	5.15	1.48	1.38
82	aF	201	PEB	CHB-C4B	5.15	1.48	1.38
82	V1	203	PEB	C3B-C2B	5.15	1.47	1.36
82	L5	202	PEB	C3B-C2B	5.15	1.47	1.36
82	O9	203	PEB	C3B-C2B	5.15	1.47	1.36
82	kH	201	PEB	CHB-C4B	5.15	1.48	1.38
82	sK	203	PEB	CHB-C4B	5.15	1.48	1.38
82	QF	202	PEB	C3B-C2B	5.15	1.47	1.36
84	MO	1001	CYC	C2A-C3A	5.15	1.47	1.36
82	DA	201	PEB	CHB-C4B	5.15	1.48	1.38
82	gB	201	PEB	CHB-C4B	5.15	1.48	1.38
82	ZB	201	PEB	C3B-C2B	5.15	1.47	1.36
82	pC	201	PEB	C3B-C2B	5.15	1.47	1.36
82	e4	203	PEB	CHB-C4B	5.15	1.48	1.38
84	T3	1001	CYC	C1C-NC	-5.15	1.30	1.37
82	TP	202	PEB	CHB-C4B	5.15	1.48	1.38
83	yF	302	PUB	CHB-C1C	5.15	1.48	1.38
84	C3	1001	CYC	C2C-C1C	-5.15	1.47	1.52
82	IF	203	PEB	C3B-C2B	5.14	1.47	1.36
83	BM	302	PUB	C2C-C3C	5.14	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	C3	1001	CYC	C1C-NC	-5.14	1.30	1.37
82	b1	201	PEB	CHB-C4B	5.14	1.48	1.38
82	S4	202	PEB	CHB-C4B	5.14	1.48	1.38
82	SA	202	PEB	C3B-C2B	5.14	1.47	1.36
82	WE	202	PEB	CHB-C4B	5.14	1.48	1.38
82	lE	201	PEB	CHB-C4B	5.14	1.48	1.38
91	a6	613	PHO	C3C-C2C	5.14	1.47	1.36
82	eB	201	PEB	C3B-C2B	5.14	1.47	1.36
84	J3	1001	CYC	C2C-C1C	-5.14	1.47	1.52
82	gM	201	PEB	CHB-C4B	5.14	1.48	1.38
82	OE	203	PEB	C3B-C2B	5.14	1.47	1.36
82	R1	201	PEB	C3B-C2B	5.14	1.47	1.36
82	F5	201	PEB	C3B-C2B	5.14	1.47	1.36
82	NA	203	PEB	C3B-C2B	5.14	1.47	1.36
84	A3	1001	CYC	C2C-C1C	-5.14	1.47	1.52
82	FA	202	PEB	CHB-C4B	5.14	1.48	1.38
82	F7	202	PEB	CHB-C4B	5.14	1.48	1.38
82	SH	203	PEB	C3B-C2B	5.14	1.47	1.36
82	sK	202	PEB	CHB-C4B	5.14	1.48	1.38
82	XP	202	PEB	CHB-C4B	5.14	1.48	1.38
82	lG	202	PEB	CHB-C4B	5.14	1.48	1.38
82	m4	201	PEB	C3B-C2B	5.14	1.47	1.36
82	XD	201	PEB	CHB-C4B	5.14	1.48	1.38
82	CM	202	PEB	CHB-C4B	5.14	1.48	1.38
82	L4	1002	PEB	CHB-C4B	5.14	1.48	1.38
84	F4	1001	CYC	C2A-C3A	5.14	1.47	1.36
82	T4	202	PEB	CHB-C4B	5.14	1.48	1.38
84	c3	1001	CYC	C3B-C2B	5.14	1.47	1.36
82	U4	202	PEB	C3B-C2B	5.14	1.47	1.36
82	JO	1002	PEB	C3B-C2B	5.14	1.47	1.36
83	AM	304	PUB	C2C-C3C	5.14	1.47	1.36
82	e4	201	PEB	CHB-C4B	5.14	1.48	1.38
82	xC	202	PEB	CHB-C4B	5.14	1.48	1.38
83	AD	302	PUB	CHB-C1C	5.14	1.48	1.38
82	U7	202	PEB	C3B-C2B	5.14	1.47	1.36
82	QG	203	PEB	CHB-C4B	5.14	1.48	1.38
82	PA	202	PEB	C3B-C2B	5.14	1.47	1.36
84	D4	1001	CYC	C3B-C2B	5.14	1.47	1.36
82	WF	203	PEB	CHB-C4B	5.14	1.48	1.38
82	e1	201	PEB	CHB-C4B	5.14	1.48	1.38
82	S7	201	PEB	C1A-NA	-5.14	1.31	1.37
82	CK	201	PEB	CHB-C4B	5.14	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DM	202	PEB	CHB-C4B	5.14	1.48	1.38
82	A1	301	PEB	CHB-C4B	5.14	1.48	1.38
82	HK	201	PEB	C3B-C2B	5.13	1.47	1.36
82	OB	201	PEB	CHB-C4B	5.13	1.48	1.38
82	KD	201	PEB	CHB-C4B	5.13	1.48	1.38
82	bH	201	PEB	CHB-C4B	5.13	1.48	1.38
84	BE	1001	CYC	CHA-C1A	5.13	1.48	1.38
82	QG	201	PEB	C3B-C2B	5.13	1.47	1.36
82	XF	201	PEB	C3B-C2B	5.13	1.47	1.36
82	cH	202	PEB	C3B-C2B	5.13	1.47	1.36
82	PD	202	PEB	CHB-C4B	5.13	1.48	1.38
82	AE	301	PEB	CHB-C4B	5.13	1.48	1.38
82	qC	202	PEB	CHB-C4B	5.13	1.48	1.38
82	eG	201	PEB	CHB-C4B	5.13	1.48	1.38
84	F4	1001	CYC	CHA-C1A	5.13	1.48	1.38
82	gE	201	PEB	C3B-C2B	5.13	1.47	1.36
82	SO	201	PEB	CHB-C4B	5.13	1.48	1.38
82	L7	203	PEB	C3B-C2B	5.13	1.47	1.36
82	kG	202	PEB	C3B-C2B	5.13	1.47	1.36
82	VP	202	PEB	CHB-C4B	5.13	1.48	1.38
82	U5	202	PEB	CHB-C4B	5.13	1.48	1.38
82	XQ	201	PEB	CHB-C4B	5.13	1.48	1.38
82	UI	202	PEB	C3B-C2B	5.13	1.47	1.36
82	V1	202	PEB	C3B-C2B	5.13	1.47	1.36
84	G3	1001	CYC	C1C-NC	-5.13	1.31	1.37
82	UO	202	PEB	CHB-C4B	5.13	1.48	1.38
82	GP	203	PEB	CHB-C4B	5.13	1.48	1.38
82	BB	202	PEB	C3B-C2B	5.13	1.47	1.36
82	uC	201	PEB	C3B-C2B	5.13	1.47	1.36
82	RF	202	PEB	CHB-C4B	5.13	1.48	1.38
82	i4	202	PEB	C3B-C2B	5.13	1.47	1.36
82	H4	1002	PEB	C3B-C2B	5.13	1.47	1.36
82	PJ	201	PEB	CHB-C4B	5.13	1.48	1.38
82	KK	202	PEB	C3B-C2B	5.13	1.47	1.36
82	P9	201	PEB	C3B-C2B	5.13	1.47	1.36
83	AO	303	PUB	C2C-C3C	5.13	1.47	1.36
82	MB	202	PEB	CHA-C1B	5.13	1.52	1.40
82	lM	203	PEB	CHB-C4B	5.13	1.48	1.38
82	QI	201	PEB	C3B-C2B	5.13	1.47	1.36
82	OD	201	PEB	CHB-C4B	5.13	1.48	1.38
82	yF	301	PEB	C3B-C2B	5.13	1.47	1.36
82	x8	201	PEB	C3B-C2B	5.12	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FB	201	PEB	CHB-C4B	5.12	1.48	1.38
82	CP	202	PEB	C3B-C2B	5.12	1.47	1.36
82	bP	502	PEB	C3B-C2B	5.12	1.47	1.36
82	PQ	202	PEB	CHB-C4B	5.12	1.48	1.38
82	aE	202	PEB	CHB-C4B	5.12	1.48	1.38
84	P3	1001	CYC	C1C-NC	-5.12	1.31	1.37
82	PE	201	PEB	CHB-C4B	5.12	1.48	1.38
82	KM	201	PEB	CHB-C4B	5.12	1.48	1.38
82	B9	203	PEB	CHB-C4B	5.12	1.48	1.38
82	hF	201	PEB	CHB-C4B	5.12	1.48	1.38
82	NF	201	PEB	CHB-C4B	5.12	1.48	1.38
82	WK	203	PEB	CHB-C4B	5.12	1.48	1.38
82	UO	202	PEB	C3B-C2B	5.12	1.47	1.36
84	t3	1001	CYC	C2C-C1C	-5.12	1.47	1.52
82	b4	201	PEB	CHB-C4B	5.12	1.48	1.38
82	G7	202	PEB	CHB-C4B	5.12	1.48	1.38
82	lM	201	PEB	CHB-C4B	5.12	1.48	1.38
82	KB	301	PEB	C3B-C2B	5.12	1.47	1.36
82	JD	201	PEB	CHB-C4B	5.12	1.48	1.38
82	x8	202	PEB	CHB-C4B	5.12	1.48	1.38
82	O4	202	PEB	C3B-C2B	5.12	1.47	1.36
82	IA	202	PEB	CHB-C4B	5.12	1.48	1.38
82	e4	202	PEB	CHB-C4B	5.12	1.48	1.38
82	EF	202	PEB	C3B-C2B	5.12	1.47	1.36
82	X9	201	PEB	C3B-C2B	5.12	1.47	1.36
82	BK	201	PEB	C3B-C2B	5.12	1.47	1.36
82	LP	201	PEB	C3B-C2B	5.12	1.47	1.36
82	OJ	203	PEB	C3B-C2B	5.12	1.47	1.36
82	LQ	203	PEB	C3B-C2B	5.12	1.47	1.36
82	iO	202	PEB	C3B-C2B	5.12	1.47	1.36
82	bE	201	PEB	C3B-C2B	5.12	1.47	1.36
82	OE	202	PEB	C3B-C2B	5.12	1.47	1.36
82	TQ	203	PEB	CHB-C4B	5.12	1.48	1.38
82	hH	201	PEB	CHB-C4B	5.12	1.48	1.38
82	VO	202	PEB	C3B-C2B	5.12	1.47	1.36
84	N3	1001	CYC	C2C-C1C	-5.12	1.47	1.52
82	T4	203	PEB	C3B-C2B	5.12	1.47	1.36
82	I9	201	PEB	C3B-C2B	5.12	1.47	1.36
82	UB	302	PEB	C3B-C2B	5.12	1.47	1.36
82	gG	201	PEB	C3B-C2B	5.12	1.47	1.36
82	AD	303	PEB	CHB-C4B	5.12	1.48	1.38
82	QE	203	PEB	CHB-C4B	5.12	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WM	201	PEB	CHB-C4B	5.12	1.48	1.38
82	EK	202	PEB	C3B-C2B	5.11	1.47	1.36
84	D1	1001	CYC	C2A-C3A	5.11	1.47	1.36
84	M4	1001	CYC	C2A-C3A	5.11	1.47	1.36
82	QE	201	PEB	C3B-C2B	5.11	1.47	1.36
82	eJ	202	PEB	C3B-C2B	5.11	1.47	1.36
82	cO	201	PEB	CHB-C4B	5.11	1.48	1.38
82	XP	201	PEB	C3B-C2B	5.11	1.47	1.36
82	VB	201	PEB	C3B-C2B	5.11	1.47	1.36
82	ZM	202	PEB	C3B-C2B	5.11	1.47	1.36
82	EK	202	PEB	CHB-C4B	5.11	1.48	1.38
82	BM	301	PEB	CHB-C4B	5.11	1.48	1.38
82	VO	201	PEB	CHB-C4B	5.11	1.48	1.38
82	FF	201	PEB	C3B-C2B	5.11	1.47	1.36
82	J5	201	PEB	C3B-C2B	5.11	1.47	1.36
82	kH	203	PEB	CHB-C4B	5.11	1.48	1.38
82	KF	202	PEB	C3B-C2B	5.11	1.47	1.36
82	LP	201	PEB	CHB-C4B	5.11	1.48	1.38
82	AG	304	PEB	C3B-C2B	5.11	1.47	1.36
82	YF	203	PEB	CHB-C4B	5.11	1.48	1.38
82	KM	202	PEB	CHB-C4B	5.11	1.48	1.38
82	S5	202	PEB	C3B-C2B	5.11	1.47	1.36
82	xC	201	PEB	C3B-C2B	5.11	1.47	1.36
84	DO	1001	CYC	C3B-C2B	5.11	1.47	1.36
82	AH	301	PEB	CHB-C4B	5.11	1.48	1.38
83	AD	302	PUB	C2C-C3C	5.11	1.47	1.36
82	sF	202	PEB	CHB-C4B	5.11	1.48	1.38
84	y3	1001	CYC	C1C-NC	-5.11	1.31	1.37
82	LP	202	PEB	CHB-C4B	5.11	1.48	1.38
82	KQ	202	PEB	CHB-C4B	5.11	1.48	1.38
82	q8	202	PEB	CHB-C4B	5.11	1.48	1.38
84	JH	1003	CYC	CHA-C1A	5.11	1.48	1.38
82	JB	202	PEB	C3B-C2B	5.11	1.47	1.36
82	DI	202	PEB	C3B-C2B	5.11	1.47	1.36
82	NP	202	PEB	CHB-C4B	5.11	1.48	1.38
82	XQ	203	PEB	CHB-C4B	5.11	1.48	1.38
82	bF	201	PEB	CHB-C4B	5.11	1.48	1.38
82	cE	201	PEB	CHB-C4B	5.11	1.48	1.38
82	V9	201	PEB	C3B-C2B	5.11	1.47	1.36
84	GE	1001	CYC	C2A-C3A	5.11	1.47	1.36
84	I4	1001	CYC	C2A-C3A	5.11	1.47	1.36
84	E3	1001	CYC	C2C-C1C	-5.10	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	P4	201	PEB	CHB-C4B	5.10	1.48	1.38
84	FE	1002	CYC	CHA-C1A	5.10	1.48	1.38
82	hE	202	PEB	C3B-C2B	5.10	1.47	1.36
84	e3	1001	CYC	C1C-NC	-5.10	1.31	1.37
82	W7	202	PEB	CHB-C4B	5.10	1.48	1.38
82	Q7	202	PEB	C3B-C2B	5.10	1.47	1.36
82	dB	201	PEB	CHB-C4B	5.10	1.48	1.38
83	AQ	302	PUB	C2C-C3C	5.10	1.47	1.36
82	LQ	202	PEB	CHB-C4B	5.10	1.48	1.38
82	TQ	202	PEB	C3B-C2B	5.10	1.47	1.36
82	E9	201	PEB	C3B-C2B	5.10	1.47	1.36
82	gB	203	PEB	C3B-C2B	5.10	1.47	1.36
96	VL	201	HEM	FE-NB	5.10	2.10	1.94
82	RB	201	PEB	CHB-C4B	5.10	1.48	1.38
82	OF	201	PEB	CHB-C4B	5.10	1.48	1.38
82	qF	202	PEB	CHB-C4B	5.10	1.48	1.38
82	KB	304	PEB	CHB-C4B	5.10	1.48	1.38
82	DP	202	PEB	CHB-C4B	5.10	1.48	1.38
82	mK	201	PEB	CHB-C4B	5.10	1.48	1.38
82	YO	202	PEB	C3B-C2B	5.10	1.47	1.36
82	S4	202	PEB	C3B-C2B	5.10	1.47	1.36
84	m3	1001	CYC	C1C-NC	-5.10	1.31	1.37
82	I7	201	PEB	CHB-C4B	5.10	1.48	1.38
82	hJ	201	PEB	CHB-C4B	5.10	1.48	1.38
82	hG	202	PEB	C3B-C2B	5.10	1.47	1.36
84	K3	1001	CYC	C1C-NC	-5.10	1.31	1.37
82	cM	202	PEB	CHB-C4B	5.10	1.48	1.38
84	CH	1001	CYC	CHA-C1A	5.10	1.48	1.38
82	RJ	202	PEB	C3B-C2B	5.10	1.47	1.36
82	vK	202	PEB	C3B-C2B	5.10	1.47	1.36
82	NA	201	PEB	C3B-C2B	5.10	1.47	1.36
82	AG	301	PEB	CHB-C4B	5.10	1.48	1.38
82	OK	203	PEB	C3B-C2B	5.10	1.47	1.36
82	Y4	202	PEB	C3B-C2B	5.10	1.47	1.36
84	g3	1001	CYC	C2C-C1C	-5.10	1.47	1.52
82	H1	1002	PEB	CHB-C4B	5.10	1.48	1.38
84	FO	1001	CYC	CHA-C1A	5.10	1.48	1.38
82	TB	202	PEB	C3B-C2B	5.10	1.47	1.36
82	LJ	201	PEB	C3B-C2B	5.10	1.47	1.36
82	hJ	202	PEB	C3B-C2B	5.10	1.47	1.36
82	bG	201	PEB	C3B-C2B	5.10	1.47	1.36
82	rF	202	PEB	CHB-C4B	5.10	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	fM	201	PEB	CHB-C4B	5.10	1.48	1.38
82	DB	202	PEB	C3B-C2B	5.10	1.47	1.36
82	RJ	201	PEB	C3B-C2B	5.10	1.47	1.36
82	CJ	202	PEB	CHB-C4B	5.10	1.48	1.38
82	eO	202	PEB	CHB-C4B	5.10	1.48	1.38
82	QK	202	PEB	C3B-C2B	5.10	1.47	1.36
82	C9	201	PEB	C3B-C2B	5.10	1.47	1.36
82	OO	201	PEB	CHB-C4B	5.10	1.48	1.38
83	A4	302	PUB	CHB-C1C	5.10	1.48	1.38
82	u8	201	PEB	C3B-C2B	5.10	1.47	1.36
82	dK	202	PEB	C3B-C2B	5.10	1.47	1.36
82	TJ	202	PEB	C3B-C2B	5.09	1.47	1.36
84	F3	1001	CYC	C2A-C3A	5.09	1.47	1.36
82	OF	203	PEB	C3B-C2B	5.09	1.47	1.36
82	YI	201	PEB	C3B-C2B	5.09	1.47	1.36
82	LM	202	PEB	C3B-C2B	5.09	1.47	1.36
83	ND	201	PUB	C2C-C3C	5.09	1.47	1.36
82	h1	202	PEB	CHB-C4B	5.09	1.48	1.38
82	A9	201	PEB	C3B-C2B	5.09	1.47	1.36
84	EH	1001	CYC	C2A-C3A	5.09	1.47	1.36
82	H5	203	PEB	CHB-C4B	5.09	1.48	1.38
82	bK	201	PEB	CHB-C4B	5.09	1.48	1.38
82	TO	203	PEB	C3B-C2B	5.09	1.47	1.36
82	SD	201	PEB	CHB-C4B	5.09	1.48	1.38
82	ZB	203	PEB	C3B-C2B	5.09	1.47	1.36
82	XK	201	PEB	C3B-C2B	5.09	1.47	1.36
82	N9	201	PEB	C3B-C2B	5.09	1.47	1.36
82	U4	202	PEB	CHB-C4B	5.09	1.48	1.38
84	R3	1001	CYC	C1C-NC	-5.09	1.31	1.37
82	cJ	201	PEB	C3B-C2B	5.09	1.47	1.36
82	gO	201	PEB	C3B-C2B	5.09	1.47	1.36
82	v8	201	PEB	C3B-C2B	5.09	1.47	1.36
82	DJ	201	PEB	CHB-C4B	5.09	1.48	1.38
83	AO	303	PUB	CHB-C1C	5.09	1.48	1.38
82	RK	201	PEB	C3B-C2B	5.09	1.47	1.36
82	Y1	201	PEB	C3B-C2B	5.09	1.47	1.36
82	T9	201	PEB	C3B-C2B	5.09	1.47	1.36
82	MD	202	PEB	CHB-C4B	5.09	1.48	1.38
82	Q5	202	PEB	CHB-C4B	5.09	1.48	1.38
84	p3	1001	CYC	C2C-C1C	-5.09	1.47	1.52
82	cJ	202	PEB	C3B-C2B	5.09	1.47	1.36
83	NQ	201	PUB	C2C-C3C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	E1	1001	CYC	C2A-C3A	5.09	1.47	1.36
83	BJ	302	PUB	C2C-C3C	5.09	1.47	1.36
82	OA	201	PEB	C1A-NA	-5.09	1.31	1.37
82	eO	201	PEB	CHB-C4B	5.09	1.48	1.38
82	g4	201	PEB	C3B-C2B	5.09	1.47	1.36
84	GG	1001	CYC	C2A-C3A	5.09	1.47	1.36
82	NK	201	PEB	CHB-C4B	5.09	1.48	1.38
82	IB	201	PEB	C3B-C2B	5.09	1.47	1.36
82	iH	201	PEB	C3B-C2B	5.09	1.47	1.36
84	t3	1001	CYC	C1C-NC	-5.09	1.31	1.37
82	YK	202	PEB	CHB-C4B	5.08	1.48	1.38
82	UH	202	PEB	C3B-C2B	5.08	1.47	1.36
82	S7	202	PEB	C3B-C2B	5.08	1.47	1.36
91	A6	407	PHO	C3C-C2C	5.08	1.47	1.36
82	UP	203	PEB	C3B-C2B	5.08	1.47	1.36
82	YB	202	PEB	CHB-C4B	5.08	1.48	1.38
82	R9	201	PEB	C3B-C2B	5.08	1.47	1.36
84	l3	1001	CYC	C1C-NC	-5.08	1.31	1.37
82	U5	202	PEB	C3B-C2B	5.08	1.47	1.36
82	N7	201	PEB	C3B-C2B	5.08	1.47	1.36
84	HE	1001	CYC	C3B-C2B	5.08	1.47	1.36
82	WG	201	PEB	CHB-C4B	5.08	1.48	1.38
82	lG	201	PEB	CHB-C4B	5.08	1.48	1.38
82	J5	203	PEB	C3B-C2B	5.08	1.47	1.36
82	WM	202	PEB	C3B-C2B	5.08	1.47	1.36
82	GB	201	PEB	C3B-C2B	5.08	1.47	1.36
82	aM	204	PEB	C3B-C2B	5.08	1.47	1.36
84	IO	1001	CYC	C2A-C3A	5.08	1.47	1.36
82	PP	202	PEB	CHB-C4B	5.08	1.48	1.38
96	vL	201	HEM	FE-NB	5.08	2.10	1.94
84	v3	1001	CYC	C2C-C1C	-5.08	1.47	1.52
82	YA	303	PEB	CHB-C4B	5.08	1.48	1.38
82	V4	202	PEB	C3B-C2B	5.08	1.47	1.36
96	V6	201	HEM	FE-NB	5.08	2.10	1.94
84	T3	1001	CYC	C2C-C1C	-5.08	1.47	1.52
82	NQ	202	PEB	C3B-C2B	5.08	1.47	1.36
82	mE	202	PEB	C3B-C2B	5.08	1.47	1.36
82	DH	1002	PEB	CHB-C4B	5.08	1.48	1.38
82	OM	202	PEB	CHB-C4B	5.08	1.48	1.38
82	OQ	201	PEB	CHB-C4B	5.08	1.48	1.38
82	PF	201	PEB	CHB-C4B	5.08	1.48	1.38
82	YJ	201	PEB	C3B-C2B	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kE	201	PEB	C3B-C2B	5.08	1.47	1.36
84	NH	1001	CYC	CHB-C1B	5.08	1.50	1.38
82	eF	201	PEB	CHB-C4B	5.08	1.48	1.38
84	E3	1001	CYC	C1C-NC	-5.08	1.31	1.37
84	J3	1001	CYC	C1C-NC	-5.08	1.31	1.37
82	dJ	201	PEB	C3B-C2B	5.08	1.47	1.36
82	FA	202	PEB	C3B-C2B	5.08	1.47	1.36
84	N1	1001	CYC	CHB-C1B	5.08	1.50	1.38
82	TF	201	PEB	CHB-C4B	5.08	1.48	1.38
82	ND	202	PEB	C3B-C2B	5.08	1.47	1.36
84	c3	1001	CYC	C1C-NC	-5.08	1.31	1.37
82	fE	201	PEB	CHB-C4B	5.08	1.48	1.38
91	dL	403	PHO	C3B-C2B	5.07	1.47	1.40
82	SD	201	PEB	C3B-C2B	5.07	1.47	1.36
82	SQ	201	PEB	C3B-C2B	5.07	1.47	1.36
82	EF	202	PEB	CHB-C4B	5.07	1.48	1.38
82	L5	201	PEB	CHB-C4B	5.07	1.48	1.38
82	gJ	202	PEB	CHB-C4B	5.07	1.48	1.38
82	KQ	201	PEB	CHB-C4B	5.07	1.48	1.38
84	W3	1001	CYC	C1C-NC	-5.07	1.31	1.37
82	K9	201	PEB	C3B-C2B	5.07	1.47	1.36
82	MK	203	PEB	CHB-C4B	5.07	1.48	1.38
82	H9	203	PEB	CHB-C4B	5.07	1.48	1.38
82	SO	202	PEB	C3B-C2B	5.07	1.47	1.36
82	TO	202	PEB	CHB-C4B	5.07	1.48	1.38
82	A4	304	PEB	CHB-C4B	5.07	1.48	1.38
82	J7	203	PEB	CHB-C4B	5.07	1.48	1.38
82	fG	201	PEB	CHB-C4B	5.07	1.48	1.38
82	KP	201	PEB	C3B-C2B	5.07	1.47	1.36
82	A1	302	PEB	CHB-C4B	5.07	1.48	1.38
82	dE	201	PEB	CHB-C4B	5.07	1.48	1.38
82	PG	201	PEB	CHB-C4B	5.07	1.48	1.38
82	HM	202	PEB	CHB-C4B	5.07	1.48	1.38
82	gG	202	PEB	CHB-C4B	5.07	1.48	1.38
82	kK	201	PEB	CHB-C4B	5.07	1.48	1.38
82	RQ	203	PEB	CHB-C4B	5.07	1.48	1.38
82	WP	201	PEB	C3B-C2B	5.07	1.47	1.36
82	G9	201	PEB	C3B-C2B	5.07	1.47	1.36
82	cB	403	PEB	C3B-C2B	5.07	1.47	1.36
82	XA	201	PEB	C2A-C1A	-5.07	1.47	1.52
82	WM	201	PEB	C3B-C2B	5.07	1.47	1.36
82	vC	201	PEB	C3B-C2B	5.07	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PO	201	PEB	CHB-C4B	5.07	1.48	1.38
82	SA	201	PEB	C1A-NA	-5.07	1.31	1.37
91	d6	404	PHO	C3C-C2C	5.07	1.47	1.36
82	U5	203	PEB	CHB-C4B	5.07	1.48	1.38
84	v3	1001	CYC	C1C-NC	-5.07	1.31	1.37
82	B9	203	PEB	C3B-C2B	5.07	1.47	1.36
84	M1	201	CYC	CHA-C1A	5.07	1.48	1.38
84	G3	1001	CYC	C2C-C1C	-5.07	1.47	1.52
96	v6	201	HEM	FE-NB	5.07	2.10	1.94
83	xK	306	PUB	C2C-C3C	5.07	1.47	1.36
84	j3	1001	CYC	C2A-C3A	5.07	1.47	1.36
82	mG	202	PEB	C3B-C2B	5.06	1.47	1.36
82	lO	201	PEB	CHB-C4B	5.06	1.48	1.38
82	TO	201	PEB	CHB-C4B	5.06	1.48	1.38
82	U1	202	PEB	C3B-C2B	5.06	1.47	1.36
82	mF	201	PEB	CHB-C4B	5.06	1.48	1.38
83	AG	303	PUB	CHB-C1C	5.06	1.48	1.38
84	A3	1001	CYC	C1C-NC	-5.06	1.31	1.37
82	QA	202	PEB	C3B-C2B	5.06	1.47	1.36
82	M7	202	PEB	CHB-C4B	5.06	1.48	1.38
82	VH	201	PEB	C3B-C2B	5.06	1.47	1.36
83	A4	303	PUB	CHB-C1C	5.06	1.48	1.38
84	D4	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	OK	201	PEB	CHB-C4B	5.06	1.48	1.38
82	B5	201	PEB	CHB-C4B	5.06	1.48	1.38
82	bO	201	PEB	CHB-C4B	5.06	1.48	1.38
84	B3	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	U9	201	PEB	C3B-C2B	5.06	1.47	1.36
82	ZF	201	PEB	CHB-C4B	5.06	1.48	1.38
84	NO	1001	CYC	CHA-C1A	5.06	1.48	1.38
82	DQ	202	PEB	C3B-C2B	5.06	1.47	1.36
84	k3	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	dM	201	PEB	CHB-C4B	5.06	1.48	1.38
82	aO	201	PEB	CHB-C4B	5.06	1.48	1.38
84	I3	1001	CYC	C2A-C3A	5.06	1.47	1.36
84	73	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	U7	201	PEB	C1A-NA	-5.06	1.31	1.37
82	V4	201	PEB	CHB-C4B	5.06	1.48	1.38
82	uF	203	PEB	CHB-C4B	5.06	1.48	1.38
82	eO	203	PEB	CHB-C4B	5.06	1.48	1.38
84	h3	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	ZE	203	PEB	C3B-C2B	5.06	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	F7	202	PEB	C3B-C2B	5.06	1.47	1.36
82	EJ	201	PEB	C3B-C2B	5.06	1.47	1.36
82	IP	202	PEB	C3B-C2B	5.06	1.47	1.36
84	o3	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	aK	201	PEB	CHB-C4B	5.06	1.48	1.38
84	EE	1001	CYC	CHB-C1B	5.06	1.50	1.38
82	jE	201	PEB	C3B-C2B	5.06	1.47	1.36
84	U3	1001	CYC	C2A-C3A	5.06	1.47	1.36
82	YP	501	PEB	CHB-C4B	5.06	1.48	1.38
82	aM	203	PEB	CHB-C4B	5.06	1.48	1.38
82	GB	202	PEB	C3B-C2B	5.06	1.47	1.36
82	lG	202	PEB	C3B-C2B	5.06	1.47	1.36
84	N3	1001	CYC	C1C-NC	-5.06	1.31	1.37
82	MA	202	PEB	CHB-C4B	5.06	1.48	1.38
82	WJ	202	PEB	CHB-C4B	5.06	1.48	1.38
83	yK	302	PUB	CHB-C1C	5.06	1.48	1.38
82	ZK	202	PEB	C3B-C2B	5.06	1.47	1.36
84	DG	1001	CYC	C2A-C3A	5.05	1.47	1.36
82	ZK	201	PEB	CHB-C4B	5.05	1.48	1.38
82	dE	203	PEB	C3B-C2B	5.05	1.47	1.36
91	D6	404	PHO	C3C-C2C	5.05	1.47	1.36
82	TE	201	PEB	CHB-C4B	5.05	1.48	1.38
82	Y9	203	PEB	CHB-C4B	5.05	1.48	1.38
82	bG	201	PEB	CHB-C4B	5.05	1.48	1.38
84	HG	1001	CYC	C3B-C2B	5.05	1.47	1.36
82	KG	201	PEB	C3B-C2B	5.05	1.47	1.36
82	NM	201	PEB	C3B-C2B	5.05	1.47	1.36
82	hG	202	PEB	CHB-C4B	5.05	1.48	1.38
91	AL	410	PHO	C3C-C2C	5.05	1.47	1.36
82	CA	201	PEB	C3B-C2B	5.05	1.47	1.36
82	fG	201	PEB	C3B-C2B	5.05	1.47	1.36
82	DG	1002	PEB	CHB-C4B	5.05	1.48	1.38
82	HH	1002	PEB	CHB-C4B	5.05	1.48	1.38
82	LI	202	PEB	C3B-C2B	5.05	1.47	1.36
82	FM	202	PEB	C3B-C2B	5.05	1.47	1.36
82	DP	201	PEB	C3B-C2B	5.05	1.47	1.36
82	R4	202	PEB	C3B-C2B	5.05	1.47	1.36
82	NQ	203	PEB	CHB-C4B	5.05	1.48	1.38
84	IG	1001	CYC	CHB-C1B	5.05	1.50	1.38
82	dF	202	PEB	C3B-C2B	5.05	1.47	1.36
82	ZG	202	PEB	CHB-C4B	5.05	1.48	1.38
84	DH	1003	CYC	C2A-C3A	5.05	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	d3	1001	CYC	C2A-C3A	5.05	1.47	1.36
82	pK	201	PEB	CHB-C4B	5.05	1.48	1.38
84	EG	1001	CYC	CHB-C1B	5.05	1.50	1.38
82	QJ	202	PEB	C3B-C2B	5.05	1.47	1.36
82	SP	201	PEB	CHB-C4B	5.05	1.48	1.38
82	J9	203	PEB	C3B-C2B	5.05	1.47	1.36
82	TJ	202	PEB	CHB-C4B	5.05	1.48	1.38
82	MQ	202	PEB	CHB-C4B	5.05	1.48	1.38
82	CJ	201	PEB	C3B-C2B	5.05	1.47	1.36
82	HO	1002	PEB	C3B-C2B	5.05	1.47	1.36
82	MF	203	PEB	CHB-C4B	5.05	1.48	1.38
84	Q3	1001	CYC	C2A-C3A	5.05	1.47	1.36
84	f3	1001	CYC	C2A-C3A	5.05	1.47	1.36
82	LD	202	PEB	CHB-C4B	5.05	1.48	1.38
82	RK	201	PEB	CHB-C4B	5.05	1.48	1.38
83	yK	303	PUB	C2C-C3C	5.05	1.47	1.36
82	UP	201	PEB	CHB-C4B	5.05	1.48	1.38
82	yF	301	PEB	CHB-C4B	5.05	1.48	1.38
82	eA	301	PEB	C3B-C2B	5.04	1.47	1.36
82	SQ	201	PEB	CHB-C4B	5.04	1.48	1.38
82	YP	501	PEB	C3B-C2B	5.04	1.47	1.36
84	M3	1001	CYC	C2A-C3A	5.04	1.47	1.36
82	YK	203	PEB	CHB-C4B	5.04	1.48	1.38
82	H9	201	PEB	C3B-C2B	5.04	1.47	1.36
84	n3	1001	CYC	C2A-C3A	5.04	1.47	1.36
91	d6	404	PHO	C3D-C4D	-5.04	1.34	1.41
83	AO	302	PUB	CHB-C1C	5.04	1.48	1.38
84	KO	1001	CYC	CHA-C1A	5.04	1.48	1.38
82	OP	203	PEB	C3B-C2B	5.04	1.47	1.36
82	V1	201	PEB	C3B-C2B	5.04	1.47	1.36
82	Y5	203	PEB	C3B-C2B	5.04	1.47	1.36
84	H3	1001	CYC	C2A-C3A	5.04	1.47	1.36
82	p8	201	PEB	C3B-C2B	5.04	1.47	1.36
82	yK	301	PEB	C3B-C2B	5.04	1.47	1.36
82	YP	503	PEB	CHB-C4B	5.04	1.48	1.38
84	N4	1001	CYC	CHA-C1A	5.04	1.48	1.38
82	XJ	202	PEB	C3B-C2B	5.04	1.47	1.36
82	rK	202	PEB	CHB-C4B	5.04	1.48	1.38
82	ND	203	PEB	CHB-C4B	5.04	1.48	1.38
84	D3	1001	CYC	C2A-C3A	5.04	1.47	1.36
82	RM	202	PEB	CHB-C4B	5.04	1.48	1.38
82	aM	202	PEB	CHB-C4B	5.04	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HP	201	PEB	C3B-C2B	5.04	1.47	1.36
82	Z1	202	PEB	C3B-C2B	5.04	1.47	1.36
82	MD	202	PEB	C3B-C2B	5.04	1.47	1.36
82	RP	202	PEB	C3B-C2B	5.04	1.47	1.36
82	i1	201	PEB	C3B-C2B	5.04	1.47	1.36
82	WE	201	PEB	CHB-C4B	5.03	1.48	1.38
82	fM	202	PEB	CHB-C4B	5.03	1.48	1.38
82	LD	203	PEB	CHB-C4B	5.03	1.48	1.38
84	q3	1001	CYC	C2A-C3A	5.03	1.47	1.36
82	jF	201	PEB	CHB-C4B	5.03	1.48	1.38
84	L3	1001	CYC	C2A-C3A	5.03	1.47	1.36
84	p3	1001	CYC	C1C-NC	-5.03	1.31	1.37
82	Y7	303	PEB	CHB-C4B	5.03	1.48	1.38
82	eK	201	PEB	CHB-C4B	5.03	1.48	1.38
82	Y4	203	PEB	C3B-C2B	5.03	1.47	1.36
82	gH	201	PEB	C3B-C2B	5.03	1.47	1.36
82	BP	202	PEB	CHB-C4B	5.03	1.48	1.38
82	CP	202	PEB	CHB-C4B	5.03	1.48	1.38
91	aL	610	PHO	C3D-C4D	-5.03	1.34	1.41
82	HB	202	PEB	C3B-C2B	5.03	1.47	1.36
82	Q5	203	PEB	C3B-C2B	5.03	1.47	1.36
82	aK	202	PEB	C3B-C2B	5.03	1.47	1.36
83	YA	302	PUB	C2C-C3C	5.03	1.47	1.36
82	SQ	202	PEB	CHB-C4B	5.03	1.48	1.38
84	K4	1001	CYC	CHA-C1A	5.03	1.48	1.38
82	kG	201	PEB	C3B-C2B	5.03	1.47	1.36
84	u3	1001	CYC	C2A-C3A	5.03	1.47	1.36
82	O1	201	PEB	CHB-C4B	5.03	1.48	1.38
82	S4	201	PEB	CHB-C4B	5.03	1.48	1.38
82	kF	201	PEB	CHB-C4B	5.03	1.48	1.38
82	ZG	203	PEB	C3B-C2B	5.03	1.47	1.36
84	w3	1001	CYC	C2A-C3A	5.03	1.47	1.36
82	WM	202	PEB	CHB-C4B	5.03	1.48	1.38
82	fM	203	PEB	CHB-C4B	5.03	1.48	1.38
84	FE	1001	CYC	CHB-C1B	5.03	1.50	1.38
84	S3	1001	CYC	C2A-C3A	5.03	1.47	1.36
83	Y7	302	PUB	C2C-C3C	5.02	1.47	1.36
82	gE	202	PEB	CHB-C4B	5.02	1.48	1.38
82	eE	201	PEB	CHB-C4B	5.02	1.48	1.38
82	YH	201	PEB	C3B-C2B	5.02	1.47	1.36
82	RF	201	PEB	CHB-C4B	5.02	1.48	1.38
82	PQ	203	PEB	CHB-C4B	5.02	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hJ	202	PEB	CHB-C4B	5.02	1.48	1.38
82	Z4	202	PEB	CHB-C4B	5.02	1.48	1.38
82	BD	202	PEB	CHB-C4B	5.02	1.48	1.38
82	bP	501	PEB	CHB-C4B	5.02	1.48	1.38
82	UA	201	PEB	C1A-NA	-5.02	1.31	1.37
82	YO	203	PEB	C3B-C2B	5.02	1.47	1.36
82	hE	202	PEB	CHB-C4B	5.02	1.48	1.38
82	gO	202	PEB	CHB-C4B	5.02	1.48	1.38
82	WF	202	PEB	C3B-C2B	5.02	1.47	1.36
82	S5	203	PEB	C3B-C2B	5.02	1.47	1.36
82	Z4	201	PEB	CHB-C4B	5.02	1.48	1.38
82	J7	202	PEB	CHB-C4B	5.02	1.48	1.38
82	PH	201	PEB	C3B-C2B	5.02	1.47	1.36
82	aF	202	PEB	C3B-C2B	5.02	1.47	1.36
82	vF	202	PEB	C3B-C2B	5.02	1.47	1.36
82	BQ	202	PEB	CHB-C4B	5.02	1.48	1.38
82	QM	202	PEB	CHB-C4B	5.02	1.48	1.38
82	QM	203	PEB	CHB-C4B	5.02	1.48	1.38
82	RO	202	PEB	C3B-C2B	5.02	1.47	1.36
82	FQ	201	PEB	C3B-C2B	5.02	1.47	1.36
82	QI	201	PEB	CHB-C4B	5.02	1.48	1.38
82	dG	201	PEB	CHB-C4B	5.02	1.48	1.38
84	K3	1001	CYC	CHD-C1D	5.01	1.52	1.40
82	RB	202	PEB	CHB-C4B	5.01	1.48	1.38
82	FH	1002	PEB	CHB-C4B	5.01	1.48	1.38
82	MQ	202	PEB	C3B-C2B	5.01	1.47	1.36
82	cK	201	PEB	C3B-C2B	5.01	1.47	1.36
82	LD	203	PEB	C3B-C2B	5.01	1.47	1.36
82	J4	1002	PEB	C3B-C2B	5.01	1.47	1.36
84	O3	1001	CYC	C2A-C3A	5.01	1.47	1.36
84	DE	1001	CYC	C2A-C3A	5.01	1.47	1.36
84	i3	1001	CYC	C1C-NC	-5.01	1.31	1.37
82	JA	203	PEB	CHB-C4B	5.01	1.48	1.38
82	D4	1002	PEB	CHB-C4B	5.01	1.48	1.38
82	FK	201	PEB	C3B-C2B	5.01	1.47	1.36
82	C7	201	PEB	C3B-C2B	5.01	1.47	1.36
82	SM	203	PEB	CHB-C4B	5.01	1.48	1.38
82	LQ	203	PEB	CHB-C4B	5.01	1.48	1.38
82	V1	203	PEB	CHB-C4B	5.01	1.48	1.38
82	J9	203	PEB	CHB-C4B	5.01	1.48	1.38
83	yF	302	PUB	C2C-C3C	5.01	1.47	1.36
91	a6	613	PHO	C3D-C4D	-5.01	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	j4	202	PEB	CHB-C4B	5.01	1.48	1.38
82	DO	1002	PEB	C3B-C2B	5.01	1.47	1.36
82	D4	1002	PEB	C3B-C2B	5.01	1.47	1.36
82	KJ	202	PEB	C3B-C2B	5.01	1.47	1.36
82	WJ	202	PEB	C3B-C2B	5.01	1.47	1.36
82	eB	202	PEB	CHB-C4B	5.01	1.48	1.38
82	yC	202	PEB	CHB-C4B	5.01	1.48	1.38
84	K1	1001	CYC	CHA-C1A	5.01	1.48	1.38
84	T3	1001	CYC	CHD-C1D	5.01	1.52	1.40
82	VJ	202	PEB	CHB-C4B	5.01	1.48	1.38
82	Q9	201	PEB	C3B-C2B	5.01	1.47	1.36
82	SG	201	PEB	CHB-C4B	5.01	1.48	1.38
82	mO	201	PEB	C3B-C2B	5.01	1.47	1.36
82	PM	201	PEB	CHB-C4B	5.01	1.48	1.38
82	ZE	202	PEB	CHB-C4B	5.01	1.48	1.38
82	AP	202	PEB	CHB-C4B	5.01	1.48	1.38
82	D1	1002	PEB	CHB-C4B	5.01	1.48	1.38
82	KE	201	PEB	C3B-C2B	5.01	1.47	1.36
82	O5	202	PEB	C3B-C2B	5.01	1.47	1.36
82	IA	201	PEB	CHB-C4B	5.00	1.48	1.38
84	CG	1001	CYC	CHB-C1B	5.00	1.49	1.38
82	gJ	201	PEB	CHB-C4B	5.00	1.48	1.38
82	MP	202	PEB	CHB-C4B	5.00	1.48	1.38
82	kO	202	PEB	CHB-C4B	5.00	1.48	1.38
82	CJ	203	PEB	C3B-C2B	5.00	1.47	1.36
82	VE	201	PEB	C3B-C2B	5.00	1.47	1.36
82	bP	501	PEB	C3B-C2B	5.00	1.47	1.36
82	PG	202	PEB	CHB-C4B	5.00	1.48	1.38
82	IP	201	PEB	CHB-C4B	5.00	1.48	1.38
82	d1	203	PEB	CHB-C4B	5.00	1.48	1.38
84	MG	1001	CYC	C2A-C3A	5.00	1.47	1.36
84	KH	1001	CYC	CHA-C1A	5.00	1.48	1.38
84	BE	1001	CYC	CHB-C1B	5.00	1.49	1.38
82	L5	202	PEB	CHB-C4B	5.00	1.48	1.38
82	DF	201	PEB	CHB-C4B	5.00	1.48	1.38
82	HG	1002	PEB	CHB-C4B	5.00	1.48	1.38
82	kJ	202	PEB	CHB-C4B	5.00	1.48	1.38
82	bE	201	PEB	CHB-C4B	5.00	1.48	1.38
82	QP	202	PEB	C3B-C2B	5.00	1.47	1.36
84	D1	1003	CYC	C2A-C3A	5.00	1.47	1.36
84	N3	1001	CYC	CHD-C1D	5.00	1.52	1.40
82	SD	202	PEB	CHB-C4B	5.00	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kM	202	PEB	CHB-C4B	5.00	1.48	1.38
83	AE	303	PUB	CHB-C1C	5.00	1.48	1.38
82	GA	202	PEB	CHB-C4B	5.00	1.48	1.38
82	UB	303	PEB	CHB-C4B	5.00	1.48	1.38
82	PD	203	PEB	CHB-C4B	5.00	1.48	1.38
82	WH	202	PEB	CHB-C4B	5.00	1.48	1.38
82	EM	203	PEB	CHB-C4B	5.00	1.48	1.38
82	YJ	203	PEB	CHB-C4B	5.00	1.48	1.38
82	FF	201	PEB	C2A-C1A	-5.00	1.47	1.52
82	dO	202	PEB	CHB-C4B	5.00	1.48	1.38
84	t3	1001	CYC	CHD-C1D	5.00	1.52	1.40
82	YO	201	PEB	C3B-C2B	5.00	1.47	1.36
84	IE	1001	CYC	CHB-C1B	5.00	1.49	1.38
82	NF	202	PEB	C3B-C2B	5.00	1.47	1.36
84	P3	1001	CYC	CHD-C1D	5.00	1.52	1.40
82	BJ	301	PEB	C3B-C2B	5.00	1.47	1.36
82	DF	201	PEB	C3B-C2B	5.00	1.47	1.36
82	IM	202	PEB	C3B-C2B	5.00	1.47	1.36
82	O5	203	PEB	C3B-C2B	5.00	1.47	1.36
82	IB	202	PEB	CHB-C4B	4.99	1.48	1.38
82	RF	201	PEB	C3B-C2B	4.99	1.47	1.36
82	LO	1002	PEB	C3B-C2B	4.99	1.47	1.36
82	dG	203	PEB	C3B-C2B	4.99	1.47	1.36
82	QB	201	PEB	C3B-C2B	4.99	1.47	1.36
82	d4	202	PEB	CHB-C4B	4.99	1.48	1.38
91	DL	405	PHO	C3D-C4D	-4.99	1.34	1.41
84	CG	1001	CYC	CHA-C1A	4.99	1.48	1.38
91	D6	404	PHO	C3D-C4D	-4.99	1.34	1.41
82	TH	202	PEB	CHB-C4B	4.99	1.48	1.38
82	W1	202	PEB	CHB-C4B	4.99	1.48	1.38
84	BG	1001	CYC	CHB-C1B	4.99	1.49	1.38
84	E3	1001	CYC	CHD-C1D	4.99	1.52	1.40
82	j4	203	PEB	CHB-C4B	4.99	1.48	1.38
84	i3	1001	CYC	CHD-C1D	4.99	1.52	1.40
82	UM	202	PEB	C3B-C2B	4.99	1.47	1.36
82	eB	201	PEB	CHB-C4B	4.99	1.48	1.38
84	m3	1001	CYC	CHD-C1D	4.99	1.52	1.40
82	SB	201	PEB	C3B-C2B	4.99	1.47	1.36
82	wC	204	PEB	CHB-C4B	4.99	1.48	1.38
82	jK	201	PEB	CHB-C4B	4.99	1.48	1.38
84	l3	1001	CYC	CHD-C1D	4.99	1.52	1.40
82	EP	201	PEB	C3B-C2B	4.99	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	H5	202	PEB	CHB-C4B	4.99	1.48	1.38
82	FD	201	PEB	C3B-C2B	4.99	1.47	1.36
82	BF	201	PEB	C3B-C2B	4.99	1.47	1.36
96	fL	102	HEM	FE-NB	4.99	2.10	1.94
82	PK	201	PEB	CHB-C4B	4.99	1.48	1.38
82	O9	201	PEB	C3B-C2B	4.99	1.47	1.36
82	ZH	202	PEB	C3B-C2B	4.99	1.47	1.36
82	FP	202	PEB	C3B-C2B	4.99	1.47	1.36
82	U9	202	PEB	CHB-C4B	4.99	1.48	1.38
82	N1	1002	PEB	C3B-C2B	4.98	1.47	1.36
82	VG	201	PEB	C3B-C2B	4.98	1.47	1.36
84	v3	1001	CYC	CHD-C1D	4.98	1.52	1.40
82	PP	201	PEB	CHB-C4B	4.98	1.48	1.38
84	EG	1001	CYC	C2A-C3A	4.98	1.47	1.36
82	N4	1002	PEB	CHB-C4B	4.98	1.48	1.38
82	y8	202	PEB	CHB-C4B	4.98	1.48	1.38
82	oF	203	PEB	CHB-C4B	4.98	1.48	1.38
82	dB	202	PEB	C3B-C2B	4.98	1.47	1.36
84	HH	1001	CYC	CHB-C1B	4.98	1.49	1.38
84	p3	1001	CYC	CHD-C1D	4.98	1.52	1.40
82	KB	301	PEB	CHB-C4B	4.98	1.48	1.38
82	TK	201	PEB	CHB-C4B	4.98	1.48	1.38
82	uK	202	PEB	CHB-C4B	4.98	1.48	1.38
84	R3	1001	CYC	CHD-C1D	4.98	1.52	1.40
82	pF	201	PEB	CHB-C4B	4.98	1.48	1.38
84	63	901	CYC	CHB-C1B	4.98	1.49	1.38
82	eF	203	PEB	CHB-C4B	4.98	1.48	1.38
82	RB	201	PEB	C3B-C2B	4.98	1.47	1.36
84	G3	1001	CYC	CHD-C1D	4.98	1.52	1.40
82	cF	203	PEB	CHB-C4B	4.98	1.48	1.38
82	GJ	201	PEB	C3B-C2B	4.97	1.47	1.36
82	eO	201	PEB	C3B-C2B	4.97	1.47	1.36
83	xF	306	PUB	C2C-C3C	4.97	1.47	1.36
82	gK	202	PEB	CHB-C4B	4.97	1.48	1.38
82	w8	204	PEB	CHB-C4B	4.97	1.48	1.38
82	TG	201	PEB	C3B-C2B	4.97	1.47	1.36
82	O1	203	PEB	CHB-C4B	4.97	1.48	1.38
82	ZG	201	PEB	C3B-C2B	4.97	1.47	1.36
82	ZB	202	PEB	CHB-C4B	4.97	1.48	1.38
82	F1	1002	PEB	CHB-C4B	4.97	1.48	1.38
82	HJ	201	PEB	C3B-C2B	4.97	1.47	1.36
82	NJ	202	PEB	C3B-C2B	4.97	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ZE	203	PEB	CHB-C4B	4.97	1.48	1.38
82	dH	203	PEB	CHB-C4B	4.97	1.48	1.38
84	EE	1001	CYC	C2A-C3A	4.97	1.47	1.36
82	NK	202	PEB	C3B-C2B	4.97	1.47	1.36
82	KG	201	PEB	CHB-C4B	4.97	1.48	1.38
82	DA	203	PEB	CHB-C4B	4.97	1.48	1.38
82	DK	201	PEB	CHB-C4B	4.97	1.48	1.38
83	QM	201	PUB	CHB-C1C	4.97	1.48	1.38
82	TB	201	PEB	C2A-C1A	-4.97	1.47	1.52
82	yK	301	PEB	CHB-C4B	4.97	1.48	1.38
82	QA	201	PEB	C3B-C2B	4.97	1.47	1.36
82	FJ	202	PEB	C3B-C2B	4.97	1.47	1.36
84	FE	1001	CYC	C2A-C3A	4.97	1.47	1.36
84	e3	1001	CYC	CHD-C1D	4.97	1.52	1.40
84	C3	1001	CYC	CHD-C1D	4.97	1.52	1.40
82	a4	201	PEB	CHB-C4B	4.97	1.48	1.38
82	oK	203	PEB	CHB-C4B	4.97	1.48	1.38
84	ME	1001	CYC	C2A-C3A	4.97	1.47	1.36
82	EJ	203	PEB	CHB-C4B	4.97	1.48	1.38
82	T1	202	PEB	CHB-C4B	4.97	1.48	1.38
83	xK	301	PUB	C2C-C3C	4.97	1.47	1.36
82	eM	202	PEB	CHB-C4B	4.96	1.48	1.38
82	ZG	203	PEB	CHB-C4B	4.96	1.48	1.38
82	DO	1002	PEB	CHB-C4B	4.96	1.48	1.38
82	FJ	201	PEB	C3B-C2B	4.96	1.47	1.36
82	FM	201	PEB	C3B-C2B	4.96	1.47	1.36
84	g3	1001	CYC	CHD-C1D	4.96	1.52	1.40
82	BD	203	PEB	C3B-C2B	4.96	1.47	1.36
82	JB	201	PEB	C2A-C1A	-4.96	1.47	1.52
82	SF	203	PEB	C3B-C2B	4.96	1.47	1.36
82	b1	203	PEB	CHB-C4B	4.96	1.48	1.38
82	SK	203	PEB	C3B-C2B	4.96	1.47	1.36
82	Y9	203	PEB	C3B-C2B	4.96	1.47	1.36
82	N4	1002	PEB	C3B-C2B	4.96	1.47	1.36
84	A3	1001	CYC	CHD-C1D	4.96	1.52	1.40
82	lF	203	PEB	CHB-C4B	4.96	1.48	1.38
82	Z9	303	PEB	CHB-C4B	4.96	1.48	1.38
82	P1	201	PEB	C3B-C2B	4.96	1.47	1.36
82	AQ	301	PEB	CHB-C4B	4.96	1.48	1.38
82	d4	201	PEB	CHB-C4B	4.96	1.48	1.38
82	II	201	PEB	C3B-C2B	4.96	1.47	1.36
82	Y9	201	PEB	C3B-C2B	4.96	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PE	202	PEB	CHB-C4B	4.96	1.48	1.38
82	kE	202	PEB	CHB-C4B	4.96	1.48	1.38
82	YM	202	PEB	CHB-C4B	4.96	1.48	1.38
82	aO	202	PEB	CHB-C4B	4.96	1.48	1.38
82	QB	203	PEB	CHB-C4B	4.96	1.48	1.38
82	VH	202	PEB	CHB-C4B	4.96	1.48	1.38
82	TM	202	PEB	C3B-C2B	4.96	1.47	1.36
82	D7	203	PEB	CHB-C4B	4.96	1.48	1.38
82	NH	1002	PEB	C3B-C2B	4.96	1.47	1.36
82	aB	202	PEB	CHB-C4B	4.96	1.48	1.38
82	f4	201	PEB	CHB-C4B	4.96	1.48	1.38
84	63	901	CYC	CHA-C1A	4.96	1.48	1.38
82	B5	203	PEB	C3B-C2B	4.95	1.47	1.36
82	XM	201	PEB	CHB-C4B	4.95	1.48	1.38
84	JH	1003	CYC	CHB-C1B	4.95	1.49	1.38
82	CI	201	PEB	C3B-C2B	4.95	1.47	1.36
82	F9	201	PEB	CHB-C4B	4.95	1.48	1.38
82	wF	302	PEB	CHB-C4B	4.95	1.48	1.38
82	M9	301	PEB	C3B-C2B	4.95	1.47	1.36
91	DL	405	PHO	O2D-CGD	4.95	1.45	1.33
82	eH	203	PEB	CHB-C4B	4.95	1.48	1.38
82	SF	202	PEB	C2A-C1A	-4.95	1.47	1.52
82	ZE	201	PEB	C3B-C2B	4.95	1.47	1.36
82	F1	1002	PEB	C3B-C2B	4.95	1.47	1.36
91	DL	405	PHO	C3C-C2C	4.95	1.47	1.36
82	VM	201	PEB	CHB-C4B	4.95	1.48	1.38
82	mM	201	PEB	CHB-C4B	4.95	1.48	1.38
82	U7	202	PEB	CHB-C4B	4.95	1.48	1.38
83	wK	304	PUB	C2C-C3C	4.95	1.47	1.36
82	SP	202	PEB	C3B-C2B	4.95	1.47	1.36
82	fE	201	PEB	C3B-C2B	4.95	1.47	1.36
91	d6	404	PHO	O2D-CGD	4.95	1.45	1.33
82	DK	201	PEB	C3B-C2B	4.95	1.47	1.36
82	gK	203	PEB	CHB-C4B	4.95	1.48	1.38
84	c3	1001	CYC	CHD-C1D	4.95	1.52	1.40
82	JA	202	PEB	CHB-C4B	4.95	1.48	1.38
82	SJ	203	PEB	CHB-C4B	4.95	1.48	1.38
82	Q7	201	PEB	C3B-C2B	4.95	1.47	1.36
82	QP	203	PEB	CHB-C4B	4.95	1.48	1.38
82	aJ	202	PEB	C3B-C2B	4.95	1.47	1.36
82	SI	202	PEB	CHB-C4B	4.95	1.48	1.38
82	dJ	201	PEB	CHB-C4B	4.95	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	iJ	201	PEB	CHB-C4B	4.95	1.48	1.38
83	QJ	201	PUB	CHB-C1C	4.95	1.48	1.38
82	ZO	202	PEB	CHB-C4B	4.95	1.48	1.38
82	HB	201	PEB	C3B-C2B	4.95	1.47	1.36
82	PP	201	PEB	C3B-C2B	4.95	1.47	1.36
82	O7	201	PEB	C1A-NA	-4.95	1.31	1.37
82	LB	201	PEB	C3B-C2B	4.95	1.47	1.36
82	HO	1002	PEB	CHB-C4B	4.94	1.48	1.38
82	O5	201	PEB	CHB-C4B	4.94	1.48	1.38
82	X7	201	PEB	C2A-C1A	-4.94	1.47	1.52
82	l4	201	PEB	CHB-C4B	4.94	1.48	1.38
82	VJ	201	PEB	CHB-C4B	4.94	1.48	1.38
82	dO	201	PEB	CHB-C4B	4.94	1.48	1.38
84	M1	201	CYC	CHB-C1B	4.94	1.49	1.38
82	e4	201	PEB	C3B-C2B	4.94	1.47	1.36
82	DE	1002	PEB	CHB-C4B	4.94	1.48	1.38
82	JM	202	PEB	CHB-C4B	4.94	1.48	1.38
84	J3	1001	CYC	CHD-C1D	4.94	1.52	1.40
82	RQ	202	PEB	CHB-C4B	4.94	1.48	1.38
82	EP	201	PEB	CHB-C4B	4.94	1.48	1.38
82	g1	201	PEB	C3B-C2B	4.94	1.47	1.36
82	HE	1002	PEB	CHB-C4B	4.94	1.48	1.38
82	lK	203	PEB	CHB-C4B	4.94	1.48	1.38
82	aM	201	PEB	CHB-C4B	4.94	1.48	1.38
82	KK	203	PEB	CHB-C4B	4.94	1.48	1.38
82	KI	202	PEB	C3B-C2B	4.94	1.47	1.36
82	W7	201	PEB	C3B-C2B	4.94	1.47	1.36
82	BA	203	PEB	CHB-C4B	4.94	1.48	1.38
82	OM	203	PEB	CHB-C4B	4.94	1.48	1.38
82	GI	202	PEB	C3B-C2B	4.94	1.47	1.36
82	KB	302	PEB	C3B-C2B	4.94	1.47	1.36
82	ZG	202	PEB	C3B-C2B	4.94	1.47	1.36
82	OH	201	PEB	CHB-C4B	4.94	1.48	1.38
82	M9	304	PEB	CHB-C4B	4.94	1.48	1.38
82	Y4	201	PEB	C3B-C2B	4.94	1.47	1.36
82	ZO	201	PEB	CHB-C4B	4.94	1.48	1.38
82	VI	201	PEB	C3B-C2B	4.94	1.47	1.36
82	KE	201	PEB	CHB-C4B	4.93	1.48	1.38
82	IM	203	PEB	CHB-C4B	4.93	1.48	1.38
84	FH	1001	CYC	CHB-C1B	4.93	1.49	1.38
82	SE	201	PEB	CHB-C4B	4.93	1.48	1.38
84	63	901	CYC	C3B-C2B	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NO	1002	PEB	CHB-C4B	4.93	1.48	1.38
82	HP	202	PEB	CHB-C4B	4.93	1.48	1.38
82	PO	203	PEB	C3B-C2B	4.93	1.47	1.36
84	CG	1001	CYC	C2A-C3A	4.93	1.47	1.36
82	EI	201	PEB	C3B-C2B	4.93	1.47	1.36
82	UM	201	PEB	CHB-C4B	4.93	1.48	1.38
83	xF	301	PUB	C2C-C3C	4.93	1.47	1.36
82	JJ	202	PEB	C3B-C2B	4.93	1.47	1.36
82	AD	301	PEB	CHB-C4B	4.93	1.48	1.38
82	EP	202	PEB	CHB-C4B	4.93	1.48	1.38
82	OM	201	PEB	CHB-C4B	4.93	1.48	1.38
82	RO	203	PEB	C3B-C2B	4.93	1.47	1.36
82	j1	201	PEB	C3B-C2B	4.93	1.47	1.36
82	eB	202	PEB	C3B-C2B	4.93	1.47	1.36
82	aF	202	PEB	CHB-C4B	4.93	1.48	1.38
82	gF	202	PEB	CHB-C4B	4.93	1.48	1.38
82	NO	1002	PEB	C3B-C2B	4.93	1.47	1.36
87	2N	303	CLA	C1D-C2D	4.93	1.55	1.45
83	BM	302	PUB	CHB-C1C	4.93	1.48	1.38
82	ZE	202	PEB	C3B-C2B	4.93	1.47	1.36
91	D6	404	PHO	O2D-CGD	4.93	1.45	1.33
84	FE	1001	CYC	CHA-C1A	4.93	1.48	1.38
82	WJ	201	PEB	C3B-C2B	4.93	1.47	1.36
82	JI	202	PEB	C3B-C2B	4.93	1.47	1.36
82	FK	201	PEB	C2A-C1A	-4.93	1.47	1.52
82	MB	201	PEB	CHB-C4B	4.93	1.48	1.38
82	XF	202	PEB	CHB-C4B	4.93	1.48	1.38
82	j1	202	PEB	CHB-C4B	4.93	1.48	1.38
84	JH	1001	CYC	CHB-C1B	4.93	1.49	1.38
82	GB	203	PEB	CHB-C4B	4.93	1.48	1.38
84	M1	201	CYC	C2A-C3A	4.93	1.47	1.36
87	32	302	CLA	C1D-ND	4.93	1.43	1.37
82	RA	201	PEB	CHB-C4B	4.93	1.48	1.38
82	TO	201	PEB	C3B-C2B	4.92	1.47	1.36
83	yF	303	PUB	C2C-C3C	4.92	1.47	1.36
82	lJ	202	PEB	C2A-C1A	-4.92	1.47	1.52
82	WK	202	PEB	C3B-C2B	4.92	1.47	1.36
82	D5	202	PEB	C3B-C2B	4.92	1.47	1.36
84	LG	1001	CYC	C2A-C3A	4.92	1.47	1.36
91	a6	613	PHO	O2D-CGD	4.92	1.45	1.33
87	22	602	CLA	C1D-C2D	4.92	1.55	1.45
82	BB	202	PEB	CHB-C4B	4.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	cB	401	PEB	CHB-C4B	4.92	1.48	1.38
82	EJ	202	PEB	C3B-C2B	4.92	1.47	1.36
82	MF	201	PEB	CHB-C4B	4.92	1.48	1.38
82	B7	203	PEB	CHB-C4B	4.92	1.48	1.38
82	xK	302	PEB	CHB-C4B	4.92	1.48	1.38
82	YI	202	PEB	CHB-C4B	4.92	1.48	1.38
82	OJ	201	PEB	C3B-C2B	4.92	1.47	1.36
82	LE	1002	PEB	CHB-C4B	4.92	1.48	1.38
83	yK	302	PUB	C2C-C3C	4.92	1.47	1.36
82	LJ	201	PEB	CHB-C4B	4.92	1.48	1.38
82	V4	201	PEB	C3B-C2B	4.92	1.47	1.36
82	Q5	202	PEB	C3B-C2B	4.92	1.47	1.36
82	WG	203	PEB	C3B-C2B	4.92	1.47	1.36
84	HO	1001	CYC	CHA-C1A	4.92	1.48	1.38
82	cM	201	PEB	CHB-C4B	4.92	1.48	1.38
82	ZF	202	PEB	C3B-C2B	4.92	1.47	1.36
82	KJ	203	PEB	C3B-C2B	4.92	1.47	1.36
82	UA	202	PEB	CHB-C4B	4.92	1.48	1.38
82	XP	201	PEB	CHB-C4B	4.92	1.48	1.38
82	PI	201	PEB	C3B-C2B	4.92	1.47	1.36
82	J5	202	PEB	CHB-C4B	4.91	1.48	1.38
82	FI	201	PEB	CHB-C4B	4.91	1.48	1.38
82	BK	202	PEB	C3B-C2B	4.91	1.47	1.36
84	K1	1001	CYC	C2A-C3A	4.91	1.47	1.36
82	RI	201	PEB	C3B-C2B	4.91	1.47	1.36
82	a4	202	PEB	CHB-C4B	4.91	1.48	1.38
84	C4	1001	CYC	CHA-C1A	4.91	1.48	1.38
82	WA	201	PEB	C3B-C2B	4.91	1.47	1.36
82	JM	201	PEB	CHB-C4B	4.91	1.48	1.38
82	BB	203	PEB	CHB-C4B	4.91	1.48	1.38
82	cK	203	PEB	CHB-C4B	4.91	1.48	1.38
82	fO	201	PEB	CHB-C4B	4.91	1.48	1.38
82	XI	201	PEB	C3B-C2B	4.91	1.47	1.36
82	GJ	203	PEB	C3B-C2B	4.91	1.47	1.36
84	F1	1001	CYC	CHB-C1B	4.91	1.49	1.38
82	XB	201	PEB	CHB-C4B	4.91	1.48	1.38
82	S9	202	PEB	CHB-C4B	4.91	1.48	1.38
82	iM	201	PEB	CHB-C4B	4.91	1.48	1.38
82	JQ	203	PEB	CHB-C4B	4.90	1.48	1.38
82	W9	201	PEB	CHB-C4B	4.90	1.48	1.38
82	R4	201	PEB	CHB-C4B	4.90	1.48	1.38
82	TI	202	PEB	C3B-C2B	4.90	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DD	202	PEB	C3B-C2B	4.90	1.47	1.36
84	73	1002	CYC	CHB-C1B	4.90	1.49	1.38
82	P4	202	PEB	CHB-C4B	4.90	1.48	1.38
82	YM	201	PEB	C3B-C2B	4.90	1.47	1.36
84	JH	1001	CYC	CHA-C1A	4.90	1.48	1.38
82	NA	201	PEB	CHB-C4B	4.90	1.48	1.38
82	HI	203	PEB	CHB-C4B	4.90	1.48	1.38
82	UB	301	PEB	C3B-C2B	4.90	1.47	1.36
82	AI	201	PEB	C3B-C2B	4.90	1.47	1.36
82	XK	202	PEB	CHB-C4B	4.90	1.48	1.38
82	VM	202	PEB	CHB-C4B	4.90	1.48	1.38
82	HM	201	PEB	C3B-C2B	4.90	1.47	1.36
82	IQ	202	PEB	C3B-C2B	4.90	1.47	1.36
83	wF	304	PUB	C2C-C3C	4.90	1.47	1.36
84	LE	1001	CYC	C2A-C3A	4.90	1.47	1.36
82	mJ	202	PEB	CHB-C4B	4.90	1.48	1.38
84	C1	1001	CYC	CHB-C1B	4.90	1.49	1.38
83	AE	302	PUB	CHB-C1C	4.90	1.48	1.38
83	AG	302	PUB	CHB-C1C	4.90	1.48	1.38
82	PM	202	PEB	CHB-C4B	4.90	1.48	1.38
96	FL	102	HEM	FE-NB	4.89	2.10	1.94
82	YB	202	PEB	C3B-C2B	4.89	1.47	1.36
82	ZM	201	PEB	CHB-C4B	4.89	1.48	1.38
82	EM	201	PEB	CHB-C4B	4.89	1.48	1.38
82	O7	202	PEB	CHB-C4B	4.89	1.48	1.38
82	jJ	203	PEB	CHB-C4B	4.89	1.48	1.38
82	ED	201	PEB	CHB-C4B	4.89	1.48	1.38
82	dQ	401	PEB	CHB-C4B	4.89	1.48	1.38
82	WO	201	PEB	CHB-C4B	4.89	1.48	1.38
82	JO	1002	PEB	CHB-C4B	4.89	1.48	1.38
82	kG	202	PEB	CHB-C4B	4.89	1.48	1.38
84	H1	1001	CYC	CHB-C1B	4.89	1.49	1.38
82	IB	201	PEB	CHB-C4B	4.89	1.48	1.38
82	wK	302	PEB	CHB-C4B	4.89	1.48	1.38
82	TE	201	PEB	C3B-C2B	4.89	1.47	1.36
82	NI	201	PEB	C3B-C2B	4.89	1.47	1.36
82	J4	1002	PEB	CHB-C4B	4.89	1.48	1.38
82	B7	201	PEB	CHB-C4B	4.89	1.48	1.38
82	FJ	202	PEB	CHB-C4B	4.89	1.48	1.38
82	F9	202	PEB	CHB-C4B	4.89	1.48	1.38
82	c1	201	PEB	C3B-C2B	4.89	1.47	1.36
82	e4	203	PEB	C3B-C2B	4.89	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NB	203	PEB	CHB-C4B	4.89	1.48	1.38
82	F9	201	PEB	C3B-C2B	4.88	1.47	1.36
82	MA	201	PEB	CHB-C4B	4.88	1.48	1.38
82	cB	403	PEB	CHB-C4B	4.88	1.48	1.38
82	WJ	203	PEB	C3B-C2B	4.88	1.47	1.36
82	NA	202	PEB	C3B-C2B	4.88	1.47	1.36
82	YB	201	PEB	CHB-C4B	4.88	1.48	1.38
82	GQ	201	PEB	C3B-C2B	4.88	1.47	1.36
82	ED	201	PEB	C3B-C2B	4.88	1.47	1.36
82	R4	203	PEB	C3B-C2B	4.88	1.47	1.36
82	R7	201	PEB	CHB-C4B	4.88	1.48	1.38
82	JD	203	PEB	CHB-C4B	4.88	1.48	1.38
82	WE	203	PEB	C3B-C2B	4.88	1.47	1.36
82	mO	202	PEB	CHB-C4B	4.88	1.48	1.38
83	AJ	304	PUB	CHB-C1C	4.88	1.48	1.38
82	CB	201	PEB	C3B-C2B	4.88	1.47	1.36
82	JH	1002	PEB	C3B-C2B	4.88	1.47	1.36
82	LG	1002	PEB	CHB-C4B	4.88	1.48	1.38
82	QO	201	PEB	CHB-C4B	4.88	1.48	1.38
82	L4	1002	PEB	C3B-C2B	4.88	1.47	1.36
82	BF	202	PEB	C3B-C2B	4.88	1.47	1.36
82	cH	201	PEB	C3B-C2B	4.88	1.47	1.36
82	S9	203	PEB	CHB-C4B	4.88	1.48	1.38
82	YI	202	PEB	C3B-C2B	4.88	1.47	1.36
82	LM	202	PEB	CHB-C4B	4.88	1.48	1.38
84	JH	1003	CYC	C2A-C3A	4.88	1.47	1.36
84	H1	1001	CYC	C2A-C3A	4.87	1.47	1.36
82	RO	201	PEB	CHB-C4B	4.87	1.48	1.38
82	N7	202	PEB	C3B-C2B	4.87	1.47	1.36
82	FH	1002	PEB	C3B-C2B	4.87	1.47	1.36
82	T4	201	PEB	C3B-C2B	4.87	1.47	1.36
84	I4	1001	CYC	CHA-C1A	4.87	1.48	1.38
82	EQ	201	PEB	C3B-C2B	4.87	1.47	1.36
82	c1	201	PEB	CHB-C4B	4.87	1.48	1.38
82	hE	203	PEB	CHB-C4B	4.87	1.48	1.38
82	hG	203	PEB	CHB-C4B	4.87	1.48	1.38
82	P7	203	PEB	C3B-C2B	4.87	1.47	1.36
82	lJ	202	PEB	C3B-C2B	4.87	1.47	1.36
84	J1	1001	CYC	CHB-C1B	4.87	1.49	1.38
82	YP	502	PEB	C3B-C2B	4.87	1.47	1.36
84	BG	1001	CYC	C2C-C1C	-4.87	1.47	1.52
82	ID	202	PEB	C3B-C2B	4.87	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UJ	201	PEB	C3B-C2B	4.87	1.47	1.36
82	i1	201	PEB	CHB-C4B	4.87	1.48	1.38
82	V7	202	PEB	CHB-C4B	4.87	1.48	1.38
84	IO	1001	CYC	CHA-C1A	4.87	1.48	1.38
82	W5	202	PEB	C3B-C2B	4.87	1.47	1.36
82	kJ	201	PEB	CHB-C4B	4.87	1.48	1.38
82	BQ	203	PEB	C3B-C2B	4.87	1.47	1.36
82	DB	201	PEB	CHB-C4B	4.87	1.48	1.38
82	BJ	301	PEB	CHB-C4B	4.87	1.48	1.38
82	GB	202	PEB	CHB-C4B	4.87	1.48	1.38
82	PO	202	PEB	CHB-C4B	4.87	1.48	1.38
82	OP	202	PEB	C3B-C2B	4.86	1.47	1.36
91	DL	405	PHO	C3B-C2B	4.86	1.47	1.40
82	AG	304	PEB	CHB-C4B	4.86	1.48	1.38
91	dL	403	PHO	C3D-C4D	-4.86	1.34	1.41
82	xF	302	PEB	CHB-C4B	4.86	1.48	1.38
82	QH	203	PEB	CHB-C4B	4.86	1.48	1.38
82	NM	202	PEB	CHB-C4B	4.86	1.48	1.38
84	D1	1003	CYC	CHA-C1A	4.86	1.48	1.38
82	ZB	203	PEB	CHB-C4B	4.86	1.48	1.38
82	GD	201	PEB	C3B-C2B	4.86	1.47	1.36
82	WB	402	PEB	CHB-C4B	4.86	1.48	1.38
84	K4	1001	CYC	CHB-C1B	4.86	1.49	1.38
87	3N	303	CLA	C1D-ND	4.86	1.43	1.37
84	J1	1001	CYC	CHA-C1A	4.86	1.48	1.38
82	PA	203	PEB	C3B-C2B	4.85	1.47	1.36
82	JJ	202	PEB	CHB-C4B	4.85	1.48	1.38
82	jH	202	PEB	CHB-C4B	4.85	1.48	1.38
84	NE	201	CYC	CHB-C1B	4.85	1.49	1.38
82	WI	203	PEB	C3B-C2B	4.85	1.47	1.36
82	FD	201	PEB	CHB-C4B	4.85	1.48	1.38
82	L5	201	PEB	C3B-C2B	4.85	1.47	1.36
84	GG	1001	CYC	CHB-C1B	4.85	1.49	1.38
82	ZJ	201	PEB	C3B-C2B	4.85	1.47	1.36
82	FP	202	PEB	CHB-C4B	4.85	1.48	1.38
84	MO	1001	CYC	CHA-C1A	4.85	1.48	1.38
84	KG	202	CYC	CHB-C1B	4.85	1.49	1.38
82	KJ	202	PEB	CHB-C4B	4.85	1.48	1.38
82	UG	201	PEB	CHB-C4B	4.85	1.48	1.38
82	JP	202	PEB	CHB-C4B	4.85	1.48	1.38
82	gF	203	PEB	CHB-C4B	4.85	1.48	1.38
82	iH	201	PEB	CHB-C4B	4.85	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GP	202	PEB	C3B-C2B	4.85	1.47	1.36
82	eK	203	PEB	CHB-C4B	4.85	1.48	1.38
83	AM	304	PUB	CHB-C1C	4.85	1.48	1.38
82	QB	204	PEB	C3B-C2B	4.85	1.47	1.36
82	m1	201	PEB	C3B-C2B	4.85	1.47	1.36
82	PJ	202	PEB	CHB-C4B	4.85	1.48	1.38
82	CP	201	PEB	CHB-C4B	4.85	1.48	1.38
82	LJ	202	PEB	CHB-C4B	4.85	1.48	1.38
82	Y5	203	PEB	CHB-C4B	4.85	1.48	1.38
84	CO	1001	CYC	CHA-C1A	4.85	1.48	1.38
84	BE	1002	CYC	C2A-C3A	4.85	1.47	1.36
91	A6	407	PHO	O2D-CGD	4.84	1.45	1.33
82	FD	203	PEB	CHB-C4B	4.84	1.48	1.38
82	EQ	201	PEB	CHB-C4B	4.84	1.48	1.38
82	F5	202	PEB	CHB-C4B	4.84	1.48	1.38
84	BE	1001	CYC	C2C-C1C	-4.84	1.47	1.52
82	LI	202	PEB	CHB-C4B	4.84	1.48	1.38
82	mH	201	PEB	C3B-C2B	4.84	1.47	1.36
82	OK	203	PEB	CHB-C4B	4.84	1.48	1.38
82	F5	203	PEB	C3B-C2B	4.84	1.47	1.36
82	aF	203	PEB	CHB-C4B	4.84	1.48	1.38
82	FM	202	PEB	CHB-C4B	4.84	1.48	1.38
82	S5	202	PEB	CHB-C4B	4.84	1.48	1.38
82	cH	201	PEB	CHB-C4B	4.84	1.48	1.38
82	BA	201	PEB	CHB-C4B	4.84	1.48	1.38
82	XM	202	PEB	CHB-C4B	4.84	1.48	1.38
82	N7	201	PEB	CHB-C4B	4.84	1.48	1.38
82	RD	202	PEB	CHB-C4B	4.84	1.48	1.38
82	Y7	304	PEB	CHB-C4B	4.84	1.48	1.38
82	XB	202	PEB	CHB-C4B	4.84	1.48	1.38
84	HG	1001	CYC	C2A-C3A	4.83	1.47	1.36
82	D5	202	PEB	CHB-C4B	4.83	1.48	1.38
82	KJ	201	PEB	C3B-C2B	4.83	1.47	1.36
82	gB	202	PEB	CHB-C4B	4.83	1.48	1.38
82	ED	202	PEB	CHB-C4B	4.83	1.48	1.38
82	OH	203	PEB	CHB-C4B	4.83	1.48	1.38
82	AE	304	PEB	CHB-C4B	4.83	1.48	1.38
82	M7	201	PEB	CHB-C4B	4.83	1.48	1.38
82	jM	202	PEB	CHB-C4B	4.83	1.48	1.38
84	KH	1001	CYC	C2A-C3A	4.83	1.47	1.36
82	CM	201	PEB	C3B-C2B	4.83	1.47	1.36
82	KF	203	PEB	CHB-C4B	4.83	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NB	202	PEB	CHB-C4B	4.83	1.48	1.38
82	dD	401	PEB	CHB-C4B	4.83	1.48	1.38
82	HB	203	PEB	C3B-C2B	4.83	1.47	1.36
82	O5	202	PEB	CHB-C4B	4.83	1.48	1.38
84	I1	1001	CYC	C2A-C3A	4.83	1.47	1.36
84	CH	1001	CYC	CHB-C1B	4.83	1.49	1.38
84	W3	1001	CYC	C2A-C3A	4.83	1.47	1.36
82	RG	201	PEB	C3B-C2B	4.83	1.47	1.36
82	CB	202	PEB	CHB-C4B	4.83	1.48	1.38
84	KO	1001	CYC	CHB-C1B	4.82	1.49	1.38
84	M4	1001	CYC	CHA-C1A	4.82	1.48	1.38
84	y3	1001	CYC	C2A-C3A	4.82	1.47	1.36
82	cJ	202	PEB	CHB-C4B	4.82	1.48	1.38
91	dL	403	PHO	O2D-CGD	4.82	1.45	1.33
82	PQ	202	PEB	C1A-NA	-4.82	1.31	1.37
82	EB	501	PEB	CHB-C4B	4.82	1.48	1.38
82	EP	203	PEB	CHB-C4B	4.82	1.48	1.38
83	yK	303	PUB	CHB-C1C	4.82	1.48	1.38
84	HE	1001	CYC	C2A-C3A	4.82	1.47	1.36
82	AM	301	PEB	CHB-C4B	4.82	1.48	1.38
82	JJ	201	PEB	CHB-C4B	4.82	1.48	1.38
82	QB	202	PEB	C3B-C2B	4.82	1.47	1.36
82	SH	201	PEB	CHB-C4B	4.82	1.48	1.38
82	W4	201	PEB	CHB-C4B	4.82	1.48	1.38
82	RE	201	PEB	C3B-C2B	4.82	1.47	1.36
82	WA	201	PEB	CHB-C4B	4.82	1.48	1.38
82	UB	301	PEB	CHB-C4B	4.82	1.48	1.38
82	D7	202	PEB	CHB-C4B	4.82	1.48	1.38
82	DB	201	PEB	C3B-C2B	4.82	1.47	1.36
82	NB	201	PEB	CHB-C4B	4.82	1.48	1.38
84	DH	1003	CYC	CHA-C1A	4.82	1.48	1.38
82	VA	202	PEB	CHB-C4B	4.81	1.48	1.38
82	KK	202	PEB	CHB-C4B	4.81	1.48	1.38
82	MJ	201	PEB	C3B-C2B	4.81	1.47	1.36
82	Q4	201	PEB	CHB-C4B	4.81	1.48	1.38
82	J1	1002	PEB	C3B-C2B	4.81	1.47	1.36
82	O7	202	PEB	C3B-C2B	4.81	1.47	1.36
82	GM	201	PEB	CHB-C4B	4.81	1.48	1.38
82	ZH	203	PEB	CHB-C4B	4.81	1.48	1.38
82	dJ	202	PEB	CHB-C4B	4.81	1.48	1.38
82	QJ	202	PEB	CHB-C4B	4.81	1.48	1.38
82	eO	203	PEB	C3B-C2B	4.81	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VB	202	PEB	CHB-C4B	4.81	1.48	1.38
82	YJ	201	PEB	CHB-C4B	4.81	1.48	1.38
82	FQ	203	PEB	CHB-C4B	4.81	1.48	1.38
82	DI	202	PEB	CHB-C4B	4.81	1.48	1.38
82	F5	203	PEB	CHB-C4B	4.81	1.48	1.38
82	ZM	202	PEB	CHB-C4B	4.80	1.48	1.38
82	KF	203	PEB	C3B-C2B	4.80	1.46	1.36
82	EQ	202	PEB	CHB-C4B	4.80	1.48	1.38
84	EO	1001	CYC	CHA-C1A	4.80	1.48	1.38
84	HH	1001	CYC	C2A-C3A	4.80	1.46	1.36
82	DA	202	PEB	CHB-C4B	4.80	1.48	1.38
82	YA	304	PEB	CHB-C4B	4.80	1.48	1.38
84	LG	1001	CYC	CHA-C1A	4.80	1.48	1.38
82	VO	201	PEB	C3B-C2B	4.80	1.46	1.36
82	OP	201	PEB	CHB-C4B	4.80	1.48	1.38
84	63	901	CYC	C1C-NC	-4.80	1.31	1.37
82	lM	202	PEB	CHB-C4B	4.80	1.48	1.38
84	EO	1001	CYC	C2A-C3A	4.80	1.46	1.36
82	IM	201	PEB	CHB-C4B	4.80	1.48	1.38
82	S1	201	PEB	CHB-C4B	4.80	1.48	1.38
82	rC	201	PEB	CHB-C4B	4.80	1.48	1.38
84	IE	1001	CYC	C2A-C3A	4.80	1.46	1.36
82	QJ	203	PEB	CHB-C4B	4.80	1.48	1.38
82	GP	201	PEB	CHB-C4B	4.80	1.48	1.38
84	CO	1001	CYC	CHB-C1B	4.80	1.49	1.38
82	O1	202	PEB	CHB-C4B	4.79	1.48	1.38
82	jH	201	PEB	C3B-C2B	4.79	1.46	1.36
82	OA	202	PEB	C3B-C2B	4.79	1.46	1.36
82	CQ	201	PEB	C3B-C2B	4.79	1.46	1.36
82	aJ	201	PEB	CHB-C4B	4.79	1.48	1.38
84	GE	1001	CYC	C2C-C1C	-4.79	1.47	1.52
82	m4	202	PEB	CHB-C4B	4.79	1.48	1.38
82	aJ	204	PEB	CHB-C4B	4.79	1.48	1.38
84	DG	1001	CYC	CHA-C1A	4.79	1.48	1.38
84	GE	1001	CYC	CHB-C1B	4.79	1.49	1.38
82	FQ	201	PEB	CHB-C4B	4.79	1.48	1.38
82	GM	203	PEB	CHB-C4B	4.79	1.48	1.38
82	S5	203	PEB	CHB-C4B	4.79	1.48	1.38
82	SF	202	PEB	C3B-C2B	4.79	1.46	1.36
82	Z1	203	PEB	CHB-C4B	4.79	1.48	1.38
84	H4	1001	CYC	CHA-C1A	4.78	1.48	1.38
82	QP	201	PEB	CHB-C4B	4.78	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	iO	202	PEB	CHB-C4B	4.78	1.48	1.38
82	X5	201	PEB	C3B-C2B	4.78	1.46	1.36
82	cJ	201	PEB	CHB-C4B	4.78	1.48	1.38
84	V3	1001	CYC	C2A-C3A	4.78	1.46	1.36
82	i4	202	PEB	CHB-C4B	4.78	1.48	1.38
82	KK	203	PEB	C3B-C2B	4.78	1.46	1.36
84	LH	1001	CYC	C2A-C3A	4.78	1.46	1.36
82	WP	202	PEB	CHB-C4B	4.78	1.48	1.38
82	MK	201	PEB	CHB-C4B	4.78	1.47	1.38
82	W7	201	PEB	CHB-C4B	4.78	1.47	1.38
82	R5	201	PEB	C3B-C2B	4.78	1.46	1.36
82	UE	201	PEB	CHB-C4B	4.78	1.47	1.38
82	WJ	201	PEB	CHB-C4B	4.78	1.47	1.38
84	E4	1001	CYC	C2A-C3A	4.78	1.46	1.36
84	I1	1001	CYC	C2C-C1C	-4.78	1.47	1.52
82	B5	203	PEB	CHB-C4B	4.78	1.47	1.38
82	aE	201	PEB	CHB-C4B	4.78	1.47	1.38
82	aG	201	PEB	CHB-C4B	4.78	1.47	1.38
82	CM	201	PEB	CHB-C4B	4.78	1.47	1.38
84	G4	1001	CYC	CHB-C1B	4.78	1.49	1.38
84	LE	1001	CYC	CHA-C1A	4.78	1.47	1.38
82	XB	202	PEB	C3B-C2B	4.78	1.46	1.36
82	FI	202	PEB	CHB-C4B	4.78	1.47	1.38
82	OF	203	PEB	CHB-C4B	4.78	1.47	1.38
84	C4	1001	CYC	CHB-C1B	4.78	1.49	1.38
82	WF	201	PEB	CHB-C4B	4.77	1.47	1.38
82	DB	202	PEB	CHB-C4B	4.77	1.47	1.38
82	ZJ	201	PEB	CHB-C4B	4.77	1.47	1.38
84	MG	1001	CYC	CHB-C1B	4.77	1.49	1.38
82	OA	202	PEB	CHB-C4B	4.77	1.47	1.38
82	ZI	401	PEB	CHA-C1B	4.77	1.51	1.40
82	IP	201	PEB	C3B-C2B	4.77	1.46	1.36
83	yF	303	PUB	CHB-C1C	4.77	1.47	1.38
82	GP	202	PEB	CHB-C4B	4.77	1.47	1.38
82	YP	502	PEB	CHB-C4B	4.77	1.47	1.38
82	aB	201	PEB	CHB-C4B	4.77	1.47	1.38
82	cB	402	PEB	CHB-C4B	4.77	1.47	1.38
82	GB	201	PEB	CHB-C4B	4.77	1.47	1.38
82	IB	203	PEB	CHB-C4B	4.77	1.47	1.38
84	KG	202	CYC	CHA-C1A	4.77	1.47	1.38
82	E5	201	PEB	C3B-C2B	4.77	1.46	1.36
84	ME	1001	CYC	CHB-C1B	4.77	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	cM	202	PEB	C3B-C2B	4.77	1.46	1.36
82	KF	202	PEB	CHB-C4B	4.77	1.47	1.38
82	Z1	202	PEB	CHB-C4B	4.76	1.47	1.38
82	AJ	302	PEB	CHB-C4B	4.76	1.47	1.38
82	DJ	202	PEB	CHB-C4B	4.76	1.47	1.38
84	x3	1001	CYC	C2A-C3A	4.76	1.46	1.36
82	YA	301	PEB	CHB-C4B	4.76	1.47	1.38
82	eM	201	PEB	CHB-C4B	4.76	1.47	1.38
82	bB	201	PEB	C3B-C2B	4.76	1.46	1.36
82	CA	201	PEB	CHB-C4B	4.76	1.47	1.38
82	aO	201	PEB	C3B-C2B	4.76	1.46	1.36
82	BD	201	PEB	CHB-C4B	4.76	1.47	1.38
82	ZJ	202	PEB	CHB-C4B	4.76	1.47	1.38
82	f1	202	PEB	CHB-C4B	4.76	1.47	1.38
82	Q1	203	PEB	CHB-C4B	4.76	1.47	1.38
83	KA	203	PUB	CHB-C1C	4.76	1.47	1.38
82	I5	201	PEB	C3B-C2B	4.76	1.46	1.36
82	K5	201	PEB	C3B-C2B	4.76	1.46	1.36
82	aJ	202	PEB	CHB-C4B	4.76	1.47	1.38
82	N5	201	PEB	C3B-C2B	4.76	1.46	1.36
82	EM	202	PEB	CHB-C4B	4.76	1.47	1.38
84	DE	1001	CYC	CHA-C1A	4.76	1.47	1.38
82	MM	201	PEB	C3B-C2B	4.76	1.46	1.36
82	r8	201	PEB	CHB-C4B	4.76	1.47	1.38
82	D5	201	PEB	C3B-C2B	4.75	1.46	1.36
82	SI	201	PEB	CHB-C4B	4.75	1.47	1.38
82	F4	1002	PEB	CHB-C4B	4.75	1.47	1.38
82	F5	202	PEB	C3B-C2B	4.75	1.46	1.36
82	ZH	202	PEB	CHB-C4B	4.75	1.47	1.38
82	RF	202	PEB	C3B-C2B	4.75	1.46	1.36
84	HO	1001	CYC	CHB-C1B	4.75	1.49	1.38
84	BG	1002	CYC	C2A-C3A	4.75	1.46	1.36
84	IG	1001	CYC	C2A-C3A	4.75	1.46	1.36
82	CJ	201	PEB	CHB-C4B	4.75	1.47	1.38
82	AP	203	PEB	CHB-C4B	4.75	1.47	1.38
82	N1	1002	PEB	CHB-C4B	4.75	1.47	1.38
84	NE	201	CYC	CHA-C1A	4.75	1.47	1.38
82	aK	203	PEB	CHB-C4B	4.75	1.47	1.38
82	aE	201	PEB	C3B-C2B	4.75	1.46	1.36
84	I1	1001	CYC	CHB-C1B	4.75	1.49	1.38
82	mJ	201	PEB	CHB-C4B	4.75	1.47	1.38
82	IM	202	PEB	CHB-C4B	4.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kM	201	PEB	CHB-C4B	4.75	1.47	1.38
82	P5	201	PEB	C3B-C2B	4.74	1.46	1.36
91	aL	610	PHO	C3B-C2B	4.74	1.47	1.40
82	fJ	201	PEB	CHB-C4B	4.74	1.47	1.38
82	G5	201	PEB	C3B-C2B	4.74	1.46	1.36
82	XJ	201	PEB	CHB-C4B	4.74	1.47	1.38
82	O5	201	PEB	C3B-C2B	4.74	1.46	1.36
82	OH	202	PEB	CHB-C4B	4.74	1.47	1.38
82	S7	202	PEB	CHB-C4B	4.74	1.47	1.38
82	V5	201	PEB	C3B-C2B	4.74	1.46	1.36
82	H4	1002	PEB	CHB-C4B	4.74	1.47	1.38
82	DD	201	PEB	CHB-C4B	4.74	1.47	1.38
82	NJ	202	PEB	CHB-C4B	4.74	1.47	1.38
82	A5	201	PEB	C3B-C2B	4.74	1.46	1.36
82	AP	201	PEB	CHB-C4B	4.74	1.47	1.38
82	JB	201	PEB	C1A-NA	-4.73	1.31	1.37
82	oF	201	PEB	C1A-NA	-4.73	1.31	1.37
82	RK	202	PEB	C3B-C2B	4.73	1.46	1.36
82	T5	201	PEB	C3B-C2B	4.73	1.46	1.36
82	W5	201	PEB	C3B-C2B	4.73	1.46	1.36
82	fH	202	PEB	CHB-C4B	4.73	1.47	1.38
82	aK	202	PEB	CHB-C4B	4.73	1.47	1.38
82	sK	202	PEB	CHA-C1B	4.73	1.51	1.40
84	I4	1001	CYC	CHB-C1B	4.73	1.49	1.38
82	SB	203	PEB	CHB-C4B	4.73	1.47	1.38
82	iJ	202	PEB	CHB-C4B	4.73	1.47	1.38
84	LG	1001	CYC	C2C-C1C	-4.73	1.47	1.52
82	YJ	202	PEB	C3B-C2B	4.73	1.46	1.36
82	R4	201	PEB	C3B-C2B	4.73	1.46	1.36
82	E5	201	PEB	CHB-C4B	4.73	1.47	1.38
82	CD	201	PEB	C3B-C2B	4.72	1.46	1.36
82	SK	202	PEB	C3B-C2B	4.72	1.46	1.36
82	UJ	202	PEB	C2A-C1A	-4.72	1.47	1.52
82	d1	201	PEB	CHB-C4B	4.72	1.47	1.38
82	CB	201	PEB	CHB-C4B	4.72	1.47	1.38
82	P7	202	PEB	CHB-C4B	4.72	1.47	1.38
84	KG	202	CYC	C2A-C3A	4.72	1.46	1.36
82	Q5	201	PEB	CHB-C4B	4.72	1.47	1.38
82	WK	201	PEB	CHB-C4B	4.72	1.47	1.38
82	S1	202	PEB	CHB-C4B	4.72	1.47	1.38
82	a4	201	PEB	C3B-C2B	4.72	1.46	1.36
82	X7	202	PEB	C3B-C2B	4.72	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SH	202	PEB	CHB-C4B	4.72	1.47	1.38
83	K7	203	PUB	CHB-C1C	4.72	1.47	1.38
82	P5	201	PEB	CHB-C4B	4.72	1.47	1.38
82	QP	202	PEB	CHB-C4B	4.72	1.47	1.38
82	hO	201	PEB	C3B-C2B	4.72	1.46	1.36
82	OA	201	PEB	C3B-C2B	4.72	1.46	1.36
82	jF	202	PEB	C3B-C2B	4.72	1.46	1.36
82	MM	202	PEB	C3B-C2B	4.72	1.46	1.36
84	EE	1001	CYC	CHA-C1A	4.72	1.47	1.38
82	NH	1002	PEB	CHB-C4B	4.71	1.47	1.38
82	aG	201	PEB	C3B-C2B	4.71	1.46	1.36
82	dO	201	PEB	C3B-C2B	4.71	1.46	1.36
84	NE	201	CYC	C2A-C3A	4.71	1.46	1.36
82	fO	201	PEB	C3B-C2B	4.71	1.46	1.36
82	RO	201	PEB	C3B-C2B	4.71	1.46	1.36
84	B3	1001	CYC	C2C-C1C	-4.71	1.47	1.52
84	EG	1001	CYC	CHA-C1A	4.71	1.47	1.38
84	LH	1001	CYC	C2C-C1C	-4.71	1.47	1.52
84	IO	1001	CYC	CHB-C1B	4.71	1.49	1.38
84	DO	1001	CYC	CHA-C1A	4.71	1.47	1.38
84	D4	1001	CYC	CHA-C1A	4.71	1.47	1.38
82	C5	201	PEB	C3B-C2B	4.71	1.46	1.36
82	HB	202	PEB	CHB-C4B	4.71	1.47	1.38
82	SA	202	PEB	CHB-C4B	4.71	1.47	1.38
82	hE	201	PEB	CHB-C1C	4.71	1.51	1.40
82	TB	201	PEB	C1A-NA	-4.71	1.31	1.37
82	S9	201	PEB	C3B-C2B	4.71	1.46	1.36
82	TA	203	PEB	CHB-C4B	4.71	1.47	1.38
82	SE	202	PEB	CHB-C4B	4.71	1.47	1.38
82	f4	201	PEB	C3B-C2B	4.71	1.46	1.36
82	T7	203	PEB	C1A-NA	-4.71	1.31	1.37
82	BQ	201	PEB	CHB-C4B	4.71	1.47	1.38
82	jJ	201	PEB	CHB-C4B	4.71	1.47	1.38
82	OE	203	PEB	CHB-C4B	4.71	1.47	1.38
82	lJ	201	PEB	CHB-C4B	4.70	1.47	1.38
84	O3	1001	CYC	C2C-C1C	-4.70	1.47	1.52
82	GG	1002	PEB	CHB-C4B	4.70	1.47	1.38
82	WP	202	PEB	C3B-C2B	4.70	1.46	1.36
82	WM	203	PEB	C3B-C2B	4.70	1.46	1.36
84	W3	1001	CYC	CHD-C1D	4.70	1.51	1.40
82	JA	201	PEB	CHB-C4B	4.70	1.47	1.38
82	TI	203	PEB	CHB-C4B	4.70	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MM	201	PEB	CHB-C4B	4.70	1.47	1.38
82	h4	201	PEB	C3B-C2B	4.70	1.46	1.36
84	H4	1001	CYC	CHB-C1B	4.70	1.49	1.38
82	SA	201	PEB	C3B-C2B	4.70	1.46	1.36
82	GE	1002	PEB	CHB-C4B	4.70	1.47	1.38
82	T5	201	PEB	CHB-C4B	4.70	1.47	1.38
84	y3	1001	CYC	CHD-C1D	4.70	1.51	1.40
82	QB	201	PEB	CHB-C4B	4.70	1.47	1.38
82	C5	201	PEB	CHB-C4B	4.70	1.47	1.38
82	II	202	PEB	CHB-C4B	4.70	1.47	1.38
82	VI	202	PEB	CHB-C4B	4.70	1.47	1.38
84	E4	1001	CYC	CHA-C1A	4.70	1.47	1.38
82	PF	202	PEB	C3B-C2B	4.70	1.46	1.36
82	PK	202	PEB	C3B-C2B	4.70	1.46	1.36
82	VB	201	PEB	CHB-C4B	4.70	1.47	1.38
82	T7	203	PEB	CHB-C4B	4.69	1.47	1.38
84	GO	1001	CYC	CHB-C1B	4.69	1.49	1.38
82	LB	201	PEB	CHB-C4B	4.69	1.47	1.38
82	QF	203	PEB	CHB-C1C	4.69	1.51	1.40
82	FD	203	PEB	CHB-C1C	4.69	1.51	1.40
82	J5	203	PEB	CHB-C4B	4.69	1.47	1.38
82	S9	201	PEB	CHB-C4B	4.69	1.47	1.38
83	AM	303	PUB	CHB-C1C	4.69	1.47	1.38
82	KI	203	PEB	CHB-C4B	4.69	1.47	1.38
82	Y7	301	PEB	CHB-C4B	4.69	1.47	1.38
82	QA	201	PEB	CHB-C4B	4.69	1.47	1.38
82	WK	202	PEB	CHB-C4B	4.69	1.47	1.38
82	JF	202	PEB	C3B-C2B	4.69	1.46	1.36
82	dB	202	PEB	CHB-C4B	4.69	1.47	1.38
84	LH	1001	CYC	CHB-C1B	4.69	1.49	1.38
82	N5	201	PEB	CHB-C4B	4.69	1.47	1.38
82	Y5	202	PEB	CHB-C4B	4.69	1.47	1.38
82	GI	203	PEB	CHB-C4B	4.69	1.47	1.38
82	DQ	201	PEB	CHB-C4B	4.69	1.47	1.38
84	q3	1001	CYC	C2C-C1C	-4.69	1.47	1.52
82	AB	501	PEB	CHB-C4B	4.69	1.47	1.38
83	xK	305	PUB	CHB-C1C	4.69	1.47	1.38
84	MG	1001	CYC	CHA-C1A	4.69	1.47	1.38
82	hG	201	PEB	CHB-C1C	4.68	1.51	1.40
82	AI	202	PEB	CHB-C4B	4.68	1.47	1.38
84	I1	1001	CYC	CHA-C1A	4.68	1.47	1.38
82	QK	203	PEB	CHB-C1C	4.68	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	XI	202	PEB	CHB-C4B	4.68	1.47	1.38
82	FO	1002	PEB	CHB-C4B	4.68	1.47	1.38
82	C7	201	PEB	CHB-C4B	4.68	1.47	1.38
82	I5	201	PEB	CHB-C4B	4.68	1.47	1.38
82	L7	202	PEB	CHB-C4B	4.68	1.47	1.38
82	IP	203	PEB	CHB-C4B	4.68	1.47	1.38
82	eJ	202	PEB	CHB-C4B	4.68	1.47	1.38
82	TB	201	PEB	CHB-C4B	4.68	1.47	1.38
82	V5	201	PEB	CHB-C4B	4.68	1.47	1.38
82	Q4	201	PEB	C2A-C1A	-4.67	1.47	1.52
82	R5	201	PEB	CHB-C4B	4.67	1.47	1.38
82	O7	201	PEB	C3B-C2B	4.67	1.46	1.36
82	NI	202	PEB	CHB-C4B	4.67	1.47	1.38
82	UI	202	PEB	CHB-C4B	4.67	1.47	1.38
82	RM	201	PEB	CHB-C4B	4.67	1.47	1.38
82	UK	202	PEB	CHB-C4B	4.67	1.47	1.38
82	U1	202	PEB	CHB-C4B	4.67	1.47	1.38
82	jM	201	PEB	CHB-C4B	4.67	1.47	1.38
82	G5	201	PEB	CHB-C4B	4.67	1.47	1.38
82	UH	203	PEB	CHB-C4B	4.67	1.47	1.38
82	K5	201	PEB	CHB-C4B	4.67	1.47	1.38
82	dH	201	PEB	CHB-C4B	4.67	1.47	1.38
82	EI	202	PEB	CHB-C4B	4.67	1.47	1.38
82	HJ	202	PEB	CHB-C4B	4.67	1.47	1.38
82	RJ	201	PEB	CHB-C4B	4.67	1.47	1.38
82	PI	202	PEB	CHB-C4B	4.67	1.47	1.38
82	FJ	201	PEB	CHB-C4B	4.67	1.47	1.38
82	eJ	201	PEB	CHB-C4B	4.67	1.47	1.38
82	wF	301	PEB	CHB-C4B	4.67	1.47	1.38
82	TM	201	PEB	CHB-C4B	4.67	1.47	1.38
82	PB	201	PEB	CHB-C4B	4.67	1.47	1.38
84	y3	1001	CYC	C1D-C2D	4.67	1.52	1.41
84	HG	1001	CYC	CHA-C1A	4.67	1.47	1.38
82	NF	201	PEB	C2A-C1A	-4.67	1.47	1.52
82	jK	202	PEB	C3B-C2B	4.66	1.46	1.36
84	K1	1001	CYC	CHB-C1B	4.66	1.49	1.38
84	EH	1001	CYC	CHB-C1B	4.66	1.49	1.38
82	JB	201	PEB	CHB-C4B	4.66	1.47	1.38
82	VQ	201	PEB	CHB-C4B	4.66	1.47	1.38
82	JK	202	PEB	C3B-C2B	4.66	1.46	1.36
82	Q7	201	PEB	C1A-NA	-4.66	1.31	1.37
82	ZH	201	PEB	CHB-C4B	4.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SK	202	PEB	C2A-C1A	-4.66	1.47	1.52
84	L3	1001	CYC	C2C-C1C	-4.66	1.47	1.52
84	W3	1001	CYC	C1D-C2D	4.66	1.52	1.41
82	PD	202	PEB	C1A-NA	-4.66	1.31	1.37
82	X5	201	PEB	CHB-C4B	4.66	1.47	1.38
84	S3	1001	CYC	C2C-C1C	-4.66	1.47	1.52
82	LA	202	PEB	CHB-C4B	4.66	1.47	1.38
82	CI	202	PEB	CHB-C4B	4.66	1.47	1.38
82	SK	203	PEB	CHB-C4B	4.66	1.47	1.38
82	S7	201	PEB	C3B-C2B	4.66	1.46	1.36
82	SG	203	PEB	CHB-C4B	4.66	1.47	1.38
82	YG	201	PEB	C3B-C2B	4.66	1.46	1.36
82	UO	201	PEB	CHB-C4B	4.66	1.47	1.38
82	MB	202	PEB	C2A-C1A	-4.66	1.47	1.52
82	WJ	201	PEB	C2A-C1A	-4.66	1.47	1.52
82	sF	202	PEB	CHA-C1B	4.66	1.51	1.40
82	RI	202	PEB	CHB-C4B	4.66	1.47	1.38
82	KP	202	PEB	CHB-C4B	4.66	1.47	1.38
82	W1	201	PEB	CHB-C4B	4.65	1.47	1.38
82	XA	202	PEB	C3B-C2B	4.65	1.46	1.36
84	U3	1001	CYC	C2C-C1C	-4.65	1.47	1.52
82	Z1	201	PEB	CHB-C4B	4.65	1.47	1.38
84	D1	1001	CYC	CHB-C1B	4.65	1.49	1.38
83	BJ	302	PUB	CHB-C1C	4.65	1.47	1.38
82	MJ	202	PEB	C1A-NA	-4.65	1.31	1.37
82	SF	201	PEB	CHB-C4B	4.65	1.47	1.38
84	E1	1001	CYC	CHB-C1B	4.65	1.49	1.38
82	YE	201	PEB	C3B-C2B	4.65	1.46	1.36
82	IP	202	PEB	CHB-C4B	4.65	1.47	1.38
82	oF	201	PEB	CHB-C4B	4.65	1.47	1.38
82	d4	201	PEB	C3B-C2B	4.65	1.46	1.36
82	NM	201	PEB	CHB-C4B	4.65	1.47	1.38
87	F2	205	CLA	C1D-ND	4.65	1.43	1.37
82	OF	202	PEB	CHA-C1B	4.65	1.51	1.40
82	A5	201	PEB	CHB-C4B	4.65	1.47	1.38
82	TA	203	PEB	C1A-NA	-4.65	1.31	1.37
82	J7	201	PEB	CHB-C4B	4.64	1.47	1.38
82	UH	202	PEB	CHB-C4B	4.64	1.47	1.38
82	iF	202	PEB	CHB-C4B	4.64	1.47	1.38
82	QO	201	PEB	C2A-C1A	-4.64	1.47	1.52
82	GF	203	PEB	C3B-C2B	4.64	1.46	1.36
92	XL	601	LMG	O7-C10	4.64	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WH	201	PEB	CHB-C4B	4.64	1.47	1.38
82	HQ	201	PEB	CHB-C4B	4.64	1.47	1.38
84	HE	1001	CYC	CHA-C1A	4.64	1.47	1.38
84	KH	1001	CYC	CHB-C1B	4.64	1.49	1.38
82	IJ	201	PEB	CHB-C4B	4.64	1.47	1.38
84	GG	1001	CYC	C2C-C1C	-4.64	1.48	1.52
84	w3	1001	CYC	C2C-C1C	-4.64	1.48	1.52
84	MO	1001	CYC	CHB-C1B	4.64	1.49	1.38
84	o3	1001	CYC	C2C-C1C	-4.64	1.48	1.52
91	aL	610	PHO	O2D-CGD	4.63	1.44	1.33
82	FQ	203	PEB	CHB-C1C	4.63	1.51	1.40
82	PA	202	PEB	CHB-C4B	4.63	1.47	1.38
82	U4	201	PEB	CHB-C4B	4.63	1.47	1.38
84	ME	1001	CYC	CHA-C1A	4.63	1.47	1.38
84	LH	1001	CYC	CHA-C1A	4.63	1.47	1.38
82	GK	203	PEB	C3B-C2B	4.63	1.46	1.36
82	MD	201	PEB	C3B-C2B	4.63	1.46	1.36
84	E4	1001	CYC	CHB-C1B	4.63	1.49	1.38
84	k3	1001	CYC	C2C-C1C	-4.63	1.48	1.52
82	D5	203	PEB	CHB-C4B	4.63	1.47	1.38
84	73	1001	CYC	C2C-C1C	-4.63	1.48	1.52
84	EO	1001	CYC	CHB-C1B	4.63	1.49	1.38
84	h3	1001	CYC	C2C-C1C	-4.63	1.48	1.52
82	OK	202	PEB	CHA-C1B	4.62	1.51	1.40
84	H3	1001	CYC	C2C-C1C	-4.62	1.48	1.52
82	UJ	202	PEB	C3B-C2B	4.62	1.46	1.36
82	M5	304	PEB	CHB-C4B	4.62	1.47	1.38
82	DB	203	PEB	C3B-C2B	4.62	1.46	1.36
82	AF	201	PEB	CHB-C4B	4.62	1.47	1.38
82	U1	203	PEB	CHB-C4B	4.62	1.47	1.38
84	F3	1001	CYC	C2C-C1C	-4.62	1.48	1.52
82	D9	201	PEB	CHB-C4B	4.62	1.47	1.38
82	VK	202	PEB	C3B-C2B	4.62	1.46	1.36
82	YO	202	PEB	CHB-C4B	4.62	1.47	1.38
84	BG	1002	CYC	CHB-C1B	4.61	1.49	1.38
87	FN	205	CLA	C1D-ND	4.61	1.43	1.37
82	IJ	202	PEB	C1A-NA	-4.61	1.31	1.37
82	OG	201	PEB	C3B-C2B	4.61	1.46	1.36
82	Z1	201	PEB	C3B-C2B	4.61	1.46	1.36
82	QA	202	PEB	CHB-C4B	4.61	1.47	1.38
82	wK	301	PEB	CHB-C4B	4.61	1.47	1.38
82	AK	201	PEB	CHB-C4B	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	RJ	202	PEB	CHB-C4B	4.61	1.47	1.38
82	AP	201	PEB	C3B-C2B	4.61	1.46	1.36
82	Y5	201	PEB	CHB-C4B	4.61	1.47	1.38
82	HB	201	PEB	CHB-C4B	4.60	1.47	1.38
84	GE	1001	CYC	CHA-C1A	4.60	1.47	1.38
84	DH	1001	CYC	CHB-C1B	4.60	1.49	1.38
82	KJ	201	PEB	C2A-C1A	-4.60	1.48	1.52
84	DH	1003	CYC	CHB-C1B	4.60	1.49	1.38
84	BE	1002	CYC	CHA-C1A	4.60	1.47	1.38
82	KK	202	PEB	C1A-NA	-4.60	1.31	1.37
82	MQ	201	PEB	C3B-C2B	4.60	1.46	1.36
82	SF	203	PEB	CHB-C4B	4.60	1.47	1.38
82	AJ	301	PEB	CHB-C4B	4.60	1.47	1.38
84	BG	1002	CYC	CHA-C1A	4.60	1.47	1.38
82	NB	203	PEB	C3B-C2B	4.60	1.46	1.36
82	HD	201	PEB	CHB-C4B	4.60	1.47	1.38
82	YK	201	PEB	CHB-C4B	4.60	1.47	1.38
82	HK	202	PEB	C3B-C2B	4.60	1.46	1.36
82	SK	202	PEB	CHB-C4B	4.59	1.47	1.38
82	F9	203	PEB	CHB-C4B	4.59	1.47	1.38
82	S4	201	PEB	C1A-NA	-4.59	1.31	1.37
82	SO	201	PEB	C1A-NA	-4.59	1.31	1.37
82	QB	204	PEB	CHB-C4B	4.59	1.47	1.38
82	UM	202	PEB	CHB-C4B	4.59	1.47	1.38
82	FM	201	PEB	CHB-C4B	4.59	1.47	1.38
82	ZO	201	PEB	C2A-C1A	-4.59	1.48	1.52
84	D1	1003	CYC	CHB-C1B	4.59	1.48	1.38
84	D3	1001	CYC	C2C-C1C	-4.59	1.48	1.52
82	oK	201	PEB	C1A-NA	-4.59	1.31	1.37
82	RA	201	PEB	C3B-C2B	4.59	1.46	1.36
82	Q7	202	PEB	CHB-C4B	4.59	1.47	1.38
82	MB	202	PEB	CHB-C4B	4.59	1.47	1.38
82	CM	203	PEB	CHB-C4B	4.59	1.47	1.38
82	iK	202	PEB	CHB-C4B	4.59	1.47	1.38
91	a6	613	PHO	OBD-CAD	4.59	1.28	1.22
82	Q7	201	PEB	CHB-C4B	4.59	1.47	1.38
84	J4	1001	CYC	CHA-C1A	4.59	1.47	1.38
92	b6	624	LMG	O7-C10	4.58	1.47	1.34
82	DD	203	PEB	CHB-C4B	4.58	1.47	1.38
82	WB	401	PEB	CHB-C4B	4.58	1.47	1.38
82	JH	1002	PEB	CHB-C4B	4.58	1.47	1.38
82	KP	202	PEB	C3B-C2B	4.58	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SK	201	PEB	CHB-C4B	4.58	1.47	1.38
82	W5	203	PEB	CHB-C4B	4.58	1.47	1.38
83	xF	305	PUB	CHB-C1C	4.58	1.47	1.38
84	Q3	1001	CYC	C2C-C1C	-4.58	1.48	1.52
82	DQ	203	PEB	CHB-C4B	4.58	1.47	1.38
82	NB	201	PEB	C3B-C2B	4.58	1.46	1.36
84	N4	1001	CYC	C2C-C1C	-4.58	1.48	1.52
82	VD	201	PEB	CHB-C4B	4.58	1.47	1.38
82	LD	202	PEB	C1A-NA	-4.58	1.31	1.37
84	M4	1001	CYC	CHB-C1B	4.58	1.48	1.38
91	A6	407	PHO	C3B-C2B	4.58	1.46	1.40
84	L1	1001	CYC	C2A-C3A	4.58	1.46	1.36
82	UF	202	PEB	CHB-C4B	4.58	1.47	1.38
82	GJ	203	PEB	CHB-C4B	4.58	1.47	1.38
84	M3	1001	CYC	C2C-C1C	-4.58	1.48	1.52
82	W5	201	PEB	CHB-C4B	4.58	1.47	1.38
82	SF	202	PEB	CHB-C4B	4.58	1.47	1.38
82	OG	203	PEB	CHB-C4B	4.58	1.47	1.38
84	u3	1001	CYC	C2C-C1C	-4.57	1.48	1.52
82	TF	202	PEB	C3B-C2B	4.57	1.46	1.36
82	TK	202	PEB	C3B-C2B	4.57	1.46	1.36
82	YF	201	PEB	CHB-C4B	4.57	1.47	1.38
82	NK	201	PEB	C2A-C1A	-4.57	1.48	1.52
82	ZJ	202	PEB	C1A-NA	-4.57	1.31	1.37
82	J1	1002	PEB	CHB-C4B	4.57	1.47	1.38
84	IE	1001	CYC	CHA-C1A	4.57	1.47	1.38
82	MP	203	PEB	CHB-C4B	4.57	1.47	1.38
82	Z5	304	PEB	CHB-C4B	4.57	1.47	1.38
82	D9	201	PEB	C3B-C2B	4.57	1.46	1.36
82	SK	202	PEB	C1A-NA	-4.57	1.31	1.37
84	BE	1002	CYC	CHB-C1B	4.57	1.48	1.38
82	ZH	201	PEB	C3B-C2B	4.57	1.46	1.36
82	z8	201	PEB	C3B-C2B	4.57	1.46	1.36
82	DK	203	PEB	C3B-C2B	4.56	1.46	1.36
82	sF	201	PEB	CHB-C4B	4.56	1.47	1.38
82	j4	201	PEB	C3B-C2B	4.56	1.46	1.36
84	j3	1001	CYC	C2C-C1C	-4.56	1.48	1.52
82	Y4	202	PEB	CHB-C4B	4.56	1.47	1.38
84	x3	1001	CYC	C1C-NC	-4.56	1.31	1.37
82	TB	202	PEB	CHB-C4B	4.56	1.47	1.38
82	JQ	202	PEB	CHB-C4B	4.56	1.47	1.38
82	UP	203	PEB	CHB-C4B	4.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	RO	202	PEB	CHB-C4B	4.56	1.47	1.38
82	X7	201	PEB	CHA-C1B	4.56	1.51	1.40
82	ZO	201	PEB	C1A-NA	-4.55	1.31	1.37
82	OE	201	PEB	C3B-C2B	4.55	1.46	1.36
82	PE	201	PEB	C3B-C2B	4.55	1.46	1.36
82	R7	201	PEB	C3B-C2B	4.55	1.46	1.36
82	UA	201	PEB	CHB-C4B	4.55	1.47	1.38
82	UJ	202	PEB	C1A-NA	-4.55	1.31	1.37
91	D6	404	PHO	C3B-C2B	4.55	1.46	1.40
82	TB	201	PEB	C3B-C2B	4.55	1.46	1.36
82	PG	201	PEB	C3B-C2B	4.55	1.46	1.36
82	oK	201	PEB	CHB-C4B	4.55	1.47	1.38
82	XK	203	PEB	C3B-C2B	4.55	1.46	1.36
82	SB	201	PEB	CHB-C4B	4.55	1.47	1.38
82	bB	201	PEB	CHB-C4B	4.55	1.47	1.38
82	KF	202	PEB	C1A-NA	-4.54	1.31	1.37
82	U7	201	PEB	CHB-C4B	4.54	1.47	1.38
84	f3	1001	CYC	C2C-C1C	-4.54	1.48	1.52
82	ZI	401	PEB	C2A-C1A	-4.54	1.48	1.52
84	LH	1002	CYC	C2A-C3A	4.54	1.46	1.36
82	KJ	201	PEB	CHB-C4B	4.54	1.47	1.38
82	W9	201	PEB	C3B-C2B	4.54	1.46	1.36
82	OJ	203	PEB	CHB-C4B	4.54	1.47	1.38
82	SJ	201	PEB	CHB-C4B	4.54	1.47	1.38
84	GG	1001	CYC	CHA-C1A	4.54	1.47	1.38
82	P7	201	PEB	C3B-C2B	4.54	1.46	1.36
82	XA	201	PEB	CHA-C1B	4.54	1.51	1.40
82	KM	203	PEB	CHB-C4B	4.53	1.47	1.38
84	d3	1001	CYC	C2C-C1C	-4.53	1.48	1.52
82	WF	202	PEB	CHB-C4B	4.53	1.47	1.38
82	KP	201	PEB	CHB-C4B	4.53	1.47	1.38
82	zC	201	PEB	C3B-C2B	4.53	1.46	1.36
82	HF	202	PEB	C3B-C2B	4.53	1.46	1.36
91	AL	410	PHO	O2D-CGD	4.53	1.44	1.33
82	SF	202	PEB	C1A-NA	-4.53	1.31	1.37
82	DF	202	PEB	CHB-C4B	4.53	1.47	1.38
84	LG	1001	CYC	CHB-C1B	4.53	1.48	1.38
84	IG	1001	CYC	CHA-C1A	4.53	1.47	1.38
84	NO	1001	CYC	C2C-C1C	-4.53	1.48	1.52
82	OJ	201	PEB	CHB-C4B	4.53	1.47	1.38
87	1N	608	CLA	C1D-ND	4.53	1.43	1.37
82	WE	201	PEB	C3B-C2B	4.53	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	sK	201	PEB	CHB-C4B	4.53	1.47	1.38
82	MJ	202	PEB	C2A-C1A	-4.53	1.48	1.52
82	KK	201	PEB	C3B-C2B	4.53	1.46	1.36
82	Z4	201	PEB	C2A-C1A	-4.53	1.48	1.52
83	AJ	303	PUB	CHB-C1C	4.52	1.47	1.38
84	LE	1001	CYC	C2C-C1C	-4.52	1.48	1.52
82	WM	203	PEB	CHB-C4B	4.52	1.47	1.38
82	WP	201	PEB	CHB-C4B	4.52	1.47	1.38
82	KF	201	PEB	C3B-C2B	4.52	1.46	1.36
98	A2	842	PQN	C10-C5	4.52	1.48	1.40
82	KI	201	PEB	CHB-C4B	4.52	1.47	1.38
91	d6	404	PHO	C3B-C2B	4.52	1.46	1.40
82	Z4	201	PEB	C1A-NA	-4.52	1.31	1.37
84	I3	1001	CYC	C2C-C1C	-4.52	1.48	1.52
84	D4	1001	CYC	CHB-C1B	4.52	1.48	1.38
84	S3	1001	CYC	C1C-NC	-4.51	1.31	1.37
82	jO	201	PEB	C3B-C2B	4.51	1.46	1.36
84	n3	1001	CYC	C2C-C1C	-4.51	1.48	1.52
82	JB	201	PEB	C3B-C2B	4.51	1.46	1.36
82	DF	203	PEB	C3B-C2B	4.51	1.46	1.36
82	R4	202	PEB	CHB-C4B	4.51	1.47	1.38
82	F5	201	PEB	CHB-C4B	4.51	1.47	1.38
82	H9	202	PEB	CHB-C4B	4.51	1.47	1.38
82	mH	202	PEB	CHA-C1B	4.51	1.51	1.40
82	m1	202	PEB	CHA-C1B	4.51	1.51	1.40
82	L5	203	PEB	CHB-C4B	4.51	1.47	1.38
82	VD	203	PEB	CHB-C4B	4.51	1.47	1.38
82	JD	202	PEB	CHB-C4B	4.51	1.47	1.38
98	AN	842	PQN	C10-C5	4.51	1.48	1.40
92	bL	611	LMG	O7-C10	4.51	1.47	1.34
84	L4	1001	CYC	CHB-C1B	4.50	1.48	1.38
82	AF	201	PEB	C3B-C2B	4.50	1.46	1.36
82	MM	202	PEB	CHB-C4B	4.50	1.47	1.38
82	NJ	201	PEB	C3B-C2B	4.50	1.46	1.36
82	AK	201	PEB	C3B-C2B	4.50	1.46	1.36
82	c1	202	PEB	CHA-C1B	4.50	1.51	1.40
84	LE	1001	CYC	CHB-C1B	4.50	1.48	1.38
82	QA	201	PEB	C1A-NA	-4.50	1.31	1.37
84	w3	1001	CYC	C1C-NC	-4.50	1.31	1.37
82	HB	203	PEB	CHB-C4B	4.50	1.47	1.38
82	WJ	203	PEB	CHB-C4B	4.50	1.47	1.38
84	LH	1002	CYC	C1C-NC	-4.50	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WE	203	PEB	CHB-C4B	4.49	1.47	1.38
82	VF	202	PEB	C3B-C2B	4.49	1.46	1.36
82	WG	201	PEB	C3B-C2B	4.49	1.46	1.36
84	DO	1001	CYC	CHB-C1B	4.49	1.48	1.38
82	PA	201	PEB	C3B-C2B	4.49	1.46	1.36
84	I3	1001	CYC	C1C-NC	-4.49	1.31	1.37
91	AL	410	PHO	C3B-C2B	4.49	1.46	1.40
82	JB	202	PEB	CHB-C4B	4.49	1.47	1.38
82	YM	201	PEB	CHB-C4B	4.49	1.47	1.38
82	Z1	203	PEB	CHA-C1B	4.49	1.50	1.40
84	U3	1001	CYC	C1C-NC	-4.49	1.31	1.37
82	VQ	203	PEB	CHB-C4B	4.49	1.47	1.38
84	u3	1001	CYC	C1C-NC	-4.48	1.31	1.37
84	F3	1001	CYC	C1C-NC	-4.48	1.31	1.37
82	TA	202	PEB	C3B-C2B	4.48	1.46	1.36
87	12	608	CLA	C1D-ND	4.48	1.43	1.37
84	f3	1001	CYC	C1C-NC	-4.48	1.31	1.37
82	HK	201	PEB	CHB-C4B	4.48	1.47	1.38
84	J4	1001	CYC	CHB-C1B	4.48	1.48	1.38
82	gF	201	PEB	CHA-C1B	4.48	1.50	1.40
82	O5	203	PEB	CHB-C4B	4.48	1.47	1.38
82	TJ	201	PEB	CHB-C4B	4.48	1.47	1.38
84	n3	1001	CYC	C1C-NC	-4.48	1.31	1.37
84	d3	1001	CYC	C1C-NC	-4.47	1.31	1.37
82	UO	201	PEB	C1A-NA	-4.47	1.31	1.37
82	WQ	201	PEB	C3B-C2B	4.47	1.46	1.36
82	UJ	201	PEB	CHB-C4B	4.47	1.47	1.38
84	H3	1001	CYC	C1C-NC	-4.47	1.31	1.37
82	EJ	202	PEB	CHB-C4B	4.47	1.47	1.38
91	dL	403	PHO	OBD-CAD	4.47	1.28	1.22
82	GF	201	PEB	C1A-NA	-4.47	1.31	1.37
82	cK	201	PEB	CHB-C4B	4.47	1.47	1.38
84	JO	1001	CYC	CHA-C1A	4.47	1.47	1.38
84	D3	1001	CYC	C1C-NC	-4.47	1.31	1.37
84	73	1001	CYC	C1C-NC	-4.47	1.31	1.37
84	B3	1001	CYC	C1C-NC	-4.47	1.31	1.37
91	d6	404	PHO	OBD-CAD	4.46	1.28	1.22
84	IG	1001	CYC	C2C-C1C	-4.46	1.48	1.52
88	iL	101	LHG	O7-C7	4.46	1.46	1.34
84	LO	1001	CYC	CHB-C1B	4.46	1.48	1.38
82	DK	202	PEB	CHB-C4B	4.46	1.47	1.38
84	k3	1001	CYC	C1C-NC	-4.46	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	LH	1003	PEB	CHB-C4B	4.46	1.47	1.38
82	L1	1002	PEB	CHB-C4B	4.46	1.47	1.38
82	J9	203	PEB	CHA-C1B	4.46	1.50	1.40
84	O3	1001	CYC	C1C-NC	-4.46	1.31	1.37
84	V3	1001	CYC	C1C-NC	-4.46	1.31	1.37
84	JO	1001	CYC	CHB-C1B	4.46	1.48	1.38
84	j3	1001	CYC	C1C-NC	-4.45	1.31	1.37
82	WG	203	PEB	CHB-C4B	4.45	1.47	1.38
82	XJ	202	PEB	CHB-C4B	4.45	1.47	1.38
82	MF	201	PEB	C3B-C2B	4.45	1.46	1.36
82	U4	201	PEB	C1A-NA	-4.45	1.31	1.37
84	M3	1001	CYC	C1C-NC	-4.45	1.31	1.37
82	GF	201	PEB	CHB-C4B	4.45	1.47	1.38
84	L3	1001	CYC	C1C-NC	-4.45	1.31	1.37
84	FG	1001	CYC	CHB-C1B	4.45	1.48	1.38
84	L4	1001	CYC	CHA-C1A	4.45	1.47	1.38
82	ZM	202	PEB	C1A-NA	-4.45	1.31	1.37
84	Q3	1001	CYC	C1C-NC	-4.45	1.31	1.37
82	T7	201	PEB	C2A-C1A	-4.45	1.48	1.52
82	O9	203	PEB	CHA-C1B	4.44	1.50	1.40
82	T7	202	PEB	C3B-C2B	4.44	1.46	1.36
84	LO	1001	CYC	CHA-C1A	4.44	1.47	1.38
82	kH	202	PEB	CHA-C1B	4.44	1.50	1.40
82	k1	202	PEB	CHA-C1B	4.44	1.50	1.40
84	h3	1001	CYC	C1C-NC	-4.44	1.31	1.37
82	GJ	201	PEB	CHB-C4B	4.44	1.47	1.38
82	BF	201	PEB	C2A-C1A	-4.44	1.48	1.52
82	GK	201	PEB	CHB-C4B	4.44	1.47	1.38
82	yC	203	PEB	C1A-NA	-4.44	1.31	1.37
82	cH	202	PEB	CHA-C1B	4.44	1.50	1.40
82	y8	203	PEB	C1A-NA	-4.44	1.31	1.37
82	BI	202	PEB	CHB-C4B	4.44	1.47	1.38
82	CJ	203	PEB	CHB-C4B	4.44	1.47	1.38
82	HF	201	PEB	CHB-C4B	4.44	1.47	1.38
84	IE	1001	CYC	C2C-C1C	-4.44	1.48	1.52
82	ID	201	PEB	C3B-C2B	4.44	1.46	1.36
84	V3	1001	CYC	C1D-C2D	4.44	1.52	1.41
82	Y1	202	PEB	CHA-C1B	4.43	1.50	1.40
82	OE	201	PEB	C2A-C1A	-4.43	1.48	1.52
84	o3	1001	CYC	C1C-NC	-4.42	1.31	1.37
82	KF	201	PEB	CHB-C4B	4.42	1.47	1.38
82	D5	201	PEB	CHB-C4B	4.42	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	ON	203	CLA	C1D-ND	4.42	1.43	1.37
84	x3	1001	CYC	C1D-C2D	4.42	1.52	1.41
82	IQ	201	PEB	C3B-C2B	4.42	1.46	1.36
82	QF	201	PEB	CHB-C4B	4.42	1.47	1.38
82	EJ	201	PEB	CHB-C4B	4.42	1.47	1.38
82	YH	202	PEB	CHA-C1B	4.42	1.50	1.40
87	O2	203	CLA	C1D-ND	4.42	1.43	1.37
82	WP	202	PEB	C1A-NA	-4.42	1.31	1.37
82	JJ	202	PEB	C1A-NA	-4.42	1.31	1.37
82	kF	201	PEB	CHA-C1B	4.42	1.50	1.40
82	WD	201	PEB	C3B-C2B	4.42	1.46	1.36
84	E3	1001	CYC	CHB-C4A	4.41	1.50	1.40
87	aL	606	CLA	O2D-CGD	4.41	1.44	1.33
82	FF	202	PEB	C3B-C2B	4.41	1.46	1.36
82	FK	202	PEB	C3B-C2B	4.41	1.46	1.36
82	QK	201	PEB	CHB-C4B	4.41	1.47	1.38
84	K3	1001	CYC	CHB-C4A	4.41	1.50	1.40
82	kG	202	PEB	C1A-NA	-4.41	1.31	1.37
84	q3	1001	CYC	C1C-NC	-4.41	1.31	1.37
82	gB	203	PEB	CHB-C4B	4.41	1.47	1.38
82	XK	201	PEB	C2A-C1A	-4.41	1.48	1.52
84	l3	1001	CYC	CHB-C4A	4.41	1.50	1.40
84	FO	1001	CYC	CHB-C1B	4.41	1.48	1.38
84	p3	1001	CYC	CHB-C4A	4.41	1.50	1.40
82	KK	201	PEB	CHB-C4B	4.41	1.47	1.38
82	S5	201	PEB	C2C-C3C	4.41	1.50	1.38
84	m3	1001	CYC	CHB-C4A	4.40	1.50	1.40
82	ZH	203	PEB	CHA-C1B	4.40	1.50	1.40
82	KA	201	PEB	CHB-C4B	4.40	1.47	1.38
82	WO	201	PEB	C1A-NA	-4.40	1.31	1.37
84	i3	1001	CYC	CHB-C4A	4.40	1.50	1.40
84	FE	1002	CYC	CHB-C1B	4.40	1.48	1.38
82	LJ	202	PEB	CHA-C1B	4.40	1.50	1.40
84	N3	1001	CYC	CHB-C4A	4.40	1.50	1.40
84	e3	1001	CYC	CHB-C4A	4.40	1.50	1.40
82	LQ	202	PEB	C1A-NA	-4.40	1.31	1.37
84	R3	1001	CYC	CHB-C4A	4.40	1.50	1.40
84	c3	1001	CYC	CHB-C4A	4.40	1.50	1.40
84	A3	1001	CYC	CHB-C4A	4.40	1.50	1.40
82	gK	201	PEB	CHA-C1B	4.40	1.50	1.40
82	DB	203	PEB	CHB-C4B	4.40	1.47	1.38
84	g3	1001	CYC	CHB-C4A	4.39	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	YJ	202	PEB	CHB-C4B	4.39	1.47	1.38
82	AP	201	PEB	C1A-NA	-4.39	1.31	1.37
84	v3	1001	CYC	CHB-C4A	4.39	1.50	1.40
82	CB	202	PEB	C1A-NA	-4.39	1.31	1.37
82	XF	203	PEB	C3B-C2B	4.39	1.46	1.36
82	HJ	201	PEB	CHB-C4B	4.39	1.47	1.38
82	eF	202	PEB	CHA-C1B	4.39	1.50	1.40
82	DB	201	PEB	C1A-NA	-4.39	1.31	1.37
84	T3	1001	CYC	CHB-C4A	4.39	1.50	1.40
82	K7	201	PEB	CHB-C4B	4.39	1.47	1.38
84	F4	1001	CYC	CHB-C1B	4.39	1.48	1.38
92	D6	409	LMG	O8-C28	4.39	1.46	1.33
84	P3	1001	CYC	CHB-C4A	4.39	1.50	1.40
91	DL	405	PHO	OBD-CAD	4.38	1.28	1.22
82	WJ	201	PEB	C1A-NA	-4.38	1.31	1.37
82	PQ	202	PEB	CHA-C1B	4.38	1.50	1.40
84	t3	1001	CYC	CHB-C4A	4.38	1.50	1.40
84	J3	1001	CYC	CHB-C4A	4.38	1.50	1.40
92	dL	407	LMG	O8-C28	4.38	1.46	1.33
103	8N	310	ZEX	C21-C26	-4.38	1.47	1.53
82	PD	202	PEB	CHA-C1B	4.38	1.50	1.40
84	G3	1001	CYC	CHB-C4A	4.37	1.50	1.40
84	L1	1001	CYC	CHB-C4A	4.37	1.50	1.40
84	C3	1001	CYC	CHB-C4A	4.37	1.50	1.40
84	LE	1001	CYC	C1C-NC	-4.37	1.31	1.37
82	IA	202	PEB	C1A-NA	-4.37	1.31	1.37
84	CO	1001	CYC	C2C-C1C	-4.37	1.48	1.52
84	n3	1001	CYC	CHB-C4A	4.37	1.50	1.40
82	R7	202	PEB	CHB-C4B	4.37	1.47	1.38
82	IJ	202	PEB	C2A-C1A	-4.36	1.48	1.52
84	G4	1001	CYC	CHD-C1D	4.36	1.50	1.40
82	MK	201	PEB	C3B-C2B	4.36	1.46	1.36
82	IJ	202	PEB	C3B-C2B	4.36	1.46	1.36
91	a6	613	PHO	C3B-C2B	4.36	1.46	1.40
84	q3	1001	CYC	CHB-C4A	4.36	1.50	1.40
82	cM	202	PEB	CHA-C1B	4.36	1.50	1.40
82	F5	203	PEB	C1A-NA	-4.36	1.32	1.37
82	PK	201	PEB	C2A-C1A	-4.36	1.48	1.52
82	u8	202	PEB	CHB-C1C	4.36	1.50	1.40
82	cF	201	PEB	CHB-C4B	4.36	1.47	1.38
95	h6	101	DGD	O2G-C1B	4.35	1.46	1.34
84	B3	1001	CYC	CHB-C4A	4.35	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WI	203	PEB	CHA-C1B	4.35	1.50	1.40
82	RA	203	PEB	C1A-NA	-4.35	1.32	1.37
84	GO	1001	CYC	CHD-C1D	4.35	1.50	1.40
82	YJ	202	PEB	C1A-NA	-4.35	1.32	1.37
84	LG	1001	CYC	C1C-NC	-4.35	1.32	1.37
84	DE	1001	CYC	C2C-C1C	-4.35	1.48	1.52
84	U3	1001	CYC	CHB-C4A	4.35	1.50	1.40
82	W4	201	PEB	C1A-NA	-4.35	1.32	1.37
84	Q3	1001	CYC	CHB-C4A	4.35	1.50	1.40
84	d3	1001	CYC	CHB-C4A	4.35	1.50	1.40
82	BK	201	PEB	C2A-C1A	-4.35	1.48	1.52
82	IJ	202	PEB	CHB-C4B	4.35	1.47	1.38
84	I3	1001	CYC	CHB-C4A	4.35	1.50	1.40
84	O3	1001	CYC	CHB-C4A	4.35	1.50	1.40
82	S4	201	PEB	C2A-C1A	-4.35	1.48	1.52
84	M3	1001	CYC	CHB-C4A	4.35	1.50	1.40
82	TA	201	PEB	C2A-C1A	-4.35	1.48	1.52
87	7N	608	CLA	C1D-ND	4.35	1.43	1.37
82	NI	203	PEB	CHB-C4B	4.35	1.47	1.38
91	D6	404	PHO	OBD-CAD	4.35	1.28	1.22
84	u3	1001	CYC	CHB-C4A	4.34	1.50	1.40
84	S3	1001	CYC	CHB-C4A	4.34	1.50	1.40
103	82	310	ZEX	C21-C26	-4.34	1.47	1.53
83	xK	301	PUB	CHB-C1C	4.34	1.47	1.38
84	H3	1001	CYC	CHB-C4A	4.34	1.50	1.40
84	LH	1002	CYC	CHB-C4A	4.34	1.50	1.40
84	k3	1001	CYC	CHB-C4A	4.34	1.50	1.40
82	M5	305	PEB	CHB-C4B	4.34	1.47	1.38
83	xF	301	PUB	CHB-C1C	4.34	1.47	1.38
92	d6	409	LMG	O8-C28	4.34	1.46	1.33
82	LF	201	PEB	C2A-C1A	-4.34	1.48	1.52
82	l4	201	PEB	C3B-C2B	4.34	1.45	1.36
84	D3	1001	CYC	CHB-C4A	4.34	1.50	1.40
82	I7	202	PEB	C1A-NA	-4.34	1.32	1.37
82	kK	201	PEB	CHA-C1B	4.34	1.50	1.40
82	MJ	202	PEB	C3B-C2B	4.34	1.45	1.36
84	w3	1001	CYC	CHB-C4A	4.34	1.50	1.40
82	Z5	305	PEB	CHB-C4B	4.34	1.47	1.38
82	DM	202	PEB	CHA-C1B	4.34	1.50	1.40
84	F3	1001	CYC	CHB-C4A	4.34	1.50	1.40
84	j3	1001	CYC	CHB-C4A	4.34	1.50	1.40
82	MP	201	PEB	C1A-NA	-4.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	L3	1001	CYC	CHB-C4A	4.33	1.50	1.40
82	GK	201	PEB	C1A-NA	-4.33	1.32	1.37
82	EK	201	PEB	CHB-C4B	4.33	1.47	1.38
84	h3	1001	CYC	CHB-C4A	4.33	1.50	1.40
92	DL	402	LMG	O8-C28	4.33	1.46	1.33
82	B9	202	PEB	CHB-C4B	4.33	1.47	1.38
84	NO	1001	CYC	C1C-NC	-4.33	1.32	1.37
84	N4	1001	CYC	C1C-NC	-4.33	1.32	1.37
82	PF	201	PEB	C2A-C1A	-4.33	1.48	1.52
82	G7	201	PEB	CHB-C4B	4.33	1.47	1.38
82	LI	201	PEB	C1A-NA	-4.33	1.32	1.37
82	aB	202	PEB	C1A-NA	-4.33	1.32	1.37
84	H4	1001	CYC	C1C-NC	-4.33	1.32	1.37
82	uC	202	PEB	CHB-C1C	4.33	1.50	1.40
82	RA	202	PEB	CHB-C4B	4.33	1.47	1.38
84	f3	1001	CYC	CHB-C4A	4.33	1.50	1.40
82	DD	202	PEB	CHB-C4B	4.33	1.47	1.38
82	KJ	203	PEB	C1A-NA	-4.32	1.32	1.37
84	L1	1001	CYC	C1C-NC	-4.32	1.32	1.37
82	D9	203	PEB	CHA-C1B	4.32	1.50	1.40
84	K1	1001	CYC	CHD-C1D	4.32	1.50	1.40
82	QF	201	PEB	CHA-C1B	4.32	1.50	1.40
82	eK	202	PEB	CHA-C1B	4.32	1.50	1.40
87	cL	515	CLA	C1D-ND	4.32	1.43	1.37
82	QG	201	PEB	CHB-C4B	4.32	1.47	1.38
82	Q5	203	PEB	CHB-C4B	4.32	1.47	1.38
82	bO	201	PEB	C3B-C2B	4.32	1.45	1.36
84	73	1001	CYC	CHB-C4A	4.32	1.50	1.40
82	OG	201	PEB	C2A-C1A	-4.32	1.48	1.52
84	BE	1002	CYC	C2C-C1C	-4.32	1.48	1.52
82	b4	201	PEB	C3B-C2B	4.32	1.45	1.36
82	HM	201	PEB	CHB-C4B	4.32	1.47	1.38
92	bL	611	LMG	O8-C28	4.32	1.46	1.33
84	E1	1001	CYC	C1C-NC	-4.32	1.32	1.37
82	WM	201	PEB	C1A-NA	-4.32	1.32	1.37
82	LF	202	PEB	C2C-C3C	4.32	1.50	1.38
82	GA	201	PEB	CHB-C4B	4.31	1.47	1.38
82	R7	203	PEB	C1A-NA	-4.31	1.32	1.37
83	Z5	302	PUB	C2C-C3C	4.31	1.45	1.36
82	TM	202	PEB	CHA-C1B	4.31	1.50	1.40
84	FG	1001	CYC	CHD-C1D	4.31	1.50	1.40
82	cJ	202	PEB	CHA-C1B	4.31	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	HG	1001	CYC	C2C-C1C	-4.31	1.48	1.52
84	HO	1001	CYC	C1C-NC	-4.31	1.32	1.37
82	N7	202	PEB	CHB-C4B	4.31	1.47	1.38
91	A6	407	PHO	OBD-CAD	4.31	1.28	1.22
82	eK	202	PEB	C3B-C2B	4.31	1.45	1.36
84	o3	1001	CYC	CHB-C4A	4.31	1.50	1.40
82	WF	202	PEB	CHA-C1B	4.31	1.50	1.40
92	A6	408	LMG	O8-C28	4.31	1.45	1.33
84	HG	1001	CYC	CHB-C1B	4.31	1.48	1.38
84	LH	1001	CYC	CHD-C1D	4.31	1.50	1.40
82	tK	202	PEB	C2C-C3C	4.31	1.50	1.38
82	x8	202	PEB	C2C-C3C	4.31	1.50	1.38
82	QK	201	PEB	CHA-C1B	4.31	1.50	1.40
82	DB	203	PEB	C1A-NA	-4.31	1.32	1.37
82	DQ	202	PEB	CHB-C4B	4.30	1.47	1.38
82	WK	201	PEB	C1A-NA	-4.30	1.32	1.37
84	DE	1001	CYC	C1C-NC	-4.30	1.32	1.37
87	72	608	CLA	C1D-ND	4.30	1.43	1.37
82	eF	202	PEB	C3B-C2B	4.30	1.45	1.36
82	j1	203	PEB	CHB-C1C	4.30	1.50	1.40
82	SA	201	PEB	CHB-C4B	4.30	1.47	1.38
88	CL	521	LHG	O7-C7	4.30	1.46	1.34
82	WK	202	PEB	CHA-C1B	4.30	1.50	1.40
82	jH	201	PEB	CHB-C4B	4.30	1.47	1.38
82	LK	202	PEB	C2C-C3C	4.30	1.50	1.38
91	aL	610	PHO	OBD-CAD	4.30	1.28	1.22
95	B2	844	DGD	O1G-C1A	4.30	1.45	1.33
92	a6	614	LMG	O8-C28	4.30	1.45	1.33
82	j1	201	PEB	CHB-C4B	4.30	1.47	1.38
95	BN	844	DGD	O1G-C1A	4.30	1.45	1.33
83	Z9	305	PUB	O1C-CGC	4.30	1.36	1.22
82	jH	203	PEB	CHB-C1C	4.30	1.50	1.40
82	V4	202	PEB	C1A-NA	-4.30	1.32	1.37
82	V1	203	PEB	CHA-C1B	4.30	1.50	1.40
82	aH	202	PEB	CHA-C1B	4.30	1.50	1.40
83	M5	302	PUB	C2C-C3C	4.30	1.45	1.36
95	b6	621	DGD	O1G-C1A	4.29	1.45	1.33
87	72	606	CLA	C1D-ND	4.29	1.43	1.37
82	QE	201	PEB	CHB-C4B	4.29	1.47	1.38
82	YP	501	PEB	C2A-C1A	-4.29	1.48	1.52
82	lO	201	PEB	C3B-C2B	4.29	1.45	1.36
84	73	1002	CYC	CHD-C1D	4.29	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CK	202	PEB	CHA-C1B	4.29	1.50	1.40
87	b6	605	CLA	C1D-ND	4.29	1.43	1.37
82	CB	202	PEB	CHA-C1B	4.29	1.50	1.40
82	ZG	201	PEB	CHB-C4B	4.29	1.47	1.38
82	JJ	202	PEB	CHA-C1B	4.29	1.50	1.40
84	HE	1001	CYC	CHB-C1B	4.29	1.48	1.38
87	62	303	CLA	C1D-ND	4.29	1.43	1.37
82	M5	301	PEB	CHB-C4B	4.29	1.47	1.38
82	eJ	202	PEB	C1A-NA	-4.29	1.32	1.37
84	EH	1001	CYC	C1C-NC	-4.29	1.32	1.37
82	XK	202	PEB	C1A-NA	-4.29	1.32	1.37
82	WG	201	PEB	C1A-NA	-4.29	1.32	1.37
82	J5	201	PEB	C1A-NA	-4.29	1.32	1.37
82	eG	203	PEB	C2C-C3C	4.29	1.50	1.38
82	VH	202	PEB	CHA-C1B	4.28	1.50	1.40
82	zF	501	PEB	CHA-C1B	4.28	1.50	1.40
87	7N	606	CLA	C1D-ND	4.28	1.43	1.37
84	HE	1001	CYC	C1C-NC	-4.28	1.32	1.37
82	zK	501	PEB	CHA-C1B	4.28	1.50	1.40
84	FE	1002	CYC	CHD-C1D	4.28	1.50	1.40
82	bG	201	PEB	C1A-NA	-4.28	1.32	1.37
82	LJ	202	PEB	C1A-NA	-4.28	1.32	1.37
82	Q5	201	PEB	C1A-NA	-4.28	1.32	1.37
82	W5	202	PEB	C1A-NA	-4.28	1.32	1.37
82	B9	203	PEB	CHA-C1B	4.28	1.50	1.40
82	sK	203	PEB	CHB-C1C	4.27	1.50	1.40
82	FJ	202	PEB	CHA-C1B	4.27	1.50	1.40
82	WO	201	PEB	C2A-C1A	-4.27	1.48	1.52
82	gF	201	PEB	C3B-C2B	4.27	1.45	1.36
82	KK	202	PEB	C2A-C1A	-4.27	1.48	1.52
82	DD	202	PEB	C1A-NA	-4.27	1.32	1.37
82	eE	203	PEB	C2C-C3C	4.27	1.50	1.38
82	MJ	201	PEB	CHB-C4B	4.27	1.47	1.38
84	BG	1002	CYC	C1C-NC	-4.27	1.32	1.37
82	ZE	201	PEB	C1A-NA	-4.27	1.32	1.37
82	LF	202	PEB	C3B-C2B	4.27	1.45	1.36
82	MB	202	PEB	C1A-NA	-4.27	1.32	1.37
84	KH	1001	CYC	CHD-C1D	4.27	1.50	1.40
82	RM	202	PEB	CHA-C1B	4.27	1.50	1.40
82	S7	201	PEB	CHB-C4B	4.27	1.47	1.38
82	MQ	201	PEB	C1A-NA	-4.26	1.32	1.37
92	CL	519	LMG	O7-C10	4.26	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VM	202	PEB	CHA-C1B	4.26	1.50	1.40
92	bL	624	LMG	O7-C10	4.26	1.46	1.34
82	xC	202	PEB	C2C-C3C	4.26	1.50	1.38
84	BE	1002	CYC	CHB-C4A	4.26	1.50	1.40
82	MB	201	PEB	C1A-NA	-4.26	1.32	1.37
87	7N	602	CLA	C1D-ND	4.26	1.43	1.37
82	OF	202	PEB	CHB-C4B	4.26	1.46	1.38
82	T1	202	PEB	CHA-C1B	4.26	1.50	1.40
88	i6	101	LHG	O7-C7	4.26	1.46	1.34
82	MK	201	PEB	C1A-NA	-4.26	1.32	1.37
82	VO	202	PEB	C1A-NA	-4.26	1.32	1.37
84	DG	1001	CYC	C1C-NC	-4.26	1.32	1.37
82	gK	201	PEB	C3B-C2B	4.26	1.45	1.36
92	BL	612	LMG	O7-C10	4.26	1.46	1.34
95	a6	603	DGD	O1G-C1A	4.25	1.45	1.33
82	OK	202	PEB	CHB-C4B	4.25	1.46	1.38
82	OO	201	PEB	C3B-C2B	4.25	1.45	1.36
82	VO	202	PEB	CHB-C4B	4.25	1.46	1.38
82	s8	201	PEB	CHA-C1B	4.25	1.50	1.40
91	d6	404	PHO	O2A-CGA	4.25	1.45	1.33
82	oF	202	PEB	CHA-C1B	4.25	1.50	1.40
82	18	202	PEB	CHB-C1C	4.25	1.50	1.40
82	LK	202	PEB	C3B-C2B	4.25	1.45	1.36
95	B2	844	DGD	O2G-C1B	4.25	1.46	1.34
82	WF	202	PEB	C1A-NA	-4.25	1.32	1.37
82	UP	201	PEB	C3B-C2B	4.25	1.45	1.36
82	ZE	201	PEB	CHB-C4B	4.25	1.46	1.38
82	AK	201	PEB	CHA-C1B	4.25	1.50	1.40
82	U9	201	PEB	CHA-C1B	4.25	1.50	1.40
82	O7	201	PEB	C2A-C1A	-4.25	1.48	1.52
92	k6	101	LMG	O8-C28	4.25	1.45	1.33
82	lJ	202	PEB	CHB-C4B	4.25	1.46	1.38
83	Z9	302	PUB	CHB-C1C	4.25	1.46	1.38
82	FF	202	PEB	C1A-NA	-4.25	1.32	1.37
82	tF	202	PEB	C2C-C3C	4.25	1.50	1.38
82	EF	201	PEB	CHB-C4B	4.25	1.46	1.38
88	C6	505	LHG	O7-C7	4.25	1.46	1.34
82	zF	501	PEB	CHB-C4B	4.25	1.46	1.38
82	1C	202	PEB	CHB-C1C	4.24	1.50	1.40
95	BN	844	DGD	O2G-C1B	4.24	1.46	1.34
82	UB	302	PEB	C2C-C3C	4.24	1.50	1.38
82	NJ	201	PEB	CHB-C4B	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6N	607	CLA	C1D-ND	4.24	1.43	1.37
82	RB	201	PEB	CHA-C1B	4.24	1.50	1.40
82	WE	201	PEB	C1A-NA	-4.24	1.32	1.37
82	Q5	202	PEB	C1A-NA	-4.24	1.32	1.37
84	O3	1001	CYC	CHD-C1D	4.24	1.50	1.40
92	b6	624	LMG	O8-C28	4.24	1.45	1.33
82	DM	201	PEB	CHA-C1B	4.24	1.50	1.40
82	RJ	202	PEB	CHA-C1B	4.24	1.50	1.40
82	VJ	202	PEB	CHA-C1B	4.24	1.50	1.40
82	Z5	301	PEB	CHB-C4B	4.24	1.46	1.38
84	S3	1001	CYC	CHD-C1D	4.23	1.50	1.40
82	F5	201	PEB	C2C-C3C	4.23	1.50	1.38
88	iL	101	LHG	O8-C23	4.23	1.45	1.33
82	MM	202	PEB	C1A-NA	-4.23	1.32	1.37
92	XL	601	LMG	O8-C28	4.23	1.45	1.33
96	E6	101	HEM	FE-NC	4.23	2.09	1.95
84	I1	1001	CYC	CHD-C1D	4.23	1.50	1.40
96	f6	101	HEM	FE-NC	4.23	2.09	1.95
88	A2	844	LHG	O7-C7	4.23	1.46	1.34
84	L3	1001	CYC	CHD-C1D	4.23	1.50	1.40
84	73	1002	CYC	C2C-C1C	-4.23	1.48	1.52
82	sF	203	PEB	CHB-C1C	4.23	1.50	1.40
82	IF	203	PEB	C1A-NA	-4.23	1.32	1.37
84	d3	1001	CYC	CHD-C1D	4.23	1.50	1.40
84	o3	1001	CYC	CHD-C1D	4.23	1.50	1.40
84	BG	1002	CYC	C2C-C1C	-4.23	1.48	1.52
82	NJ	202	PEB	C1A-NA	-4.23	1.32	1.37
82	eK	202	PEB	CHB-C4B	4.23	1.46	1.38
82	AF	201	PEB	CHA-C1B	4.23	1.50	1.40
84	I3	1001	CYC	CHD-C1D	4.22	1.50	1.40
92	ML	101	LMG	O7-C10	4.22	1.46	1.34
82	PM	202	PEB	CHA-C1B	4.22	1.50	1.40
82	VF	202	PEB	CHA-C1B	4.22	1.50	1.40
82	gM	202	PEB	CHA-C1B	4.22	1.50	1.40
82	V4	202	PEB	CHB-C4B	4.22	1.46	1.38
82	P1	202	PEB	CHA-C1B	4.22	1.50	1.40
82	sC	201	PEB	CHA-C1B	4.22	1.50	1.40
82	KP	202	PEB	C1A-NA	-4.22	1.32	1.37
82	MD	201	PEB	C1A-NA	-4.22	1.32	1.37
84	B3	1001	CYC	CHD-C1D	4.22	1.50	1.40
84	HE	1001	CYC	C2C-C1C	-4.22	1.48	1.52
82	H5	201	PEB	C1A-NA	-4.22	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	RA	203	PEB	CHA-C1B	4.22	1.50	1.40
82	T7	201	PEB	C1A-NA	-4.22	1.32	1.37
84	FE	1001	CYC	CHB-C4A	4.22	1.50	1.40
84	f3	1001	CYC	CHD-C1D	4.22	1.50	1.40
88	mL	102	LHG	O8-C23	4.22	1.45	1.33
96	GN	201	HEM	FE-ND	4.22	2.07	1.94
87	72	602	CLA	C1D-ND	4.22	1.43	1.37
82	OF	202	PEB	C3B-C2B	4.22	1.45	1.36
84	FO	1001	CYC	CHD-C1D	4.22	1.50	1.40
87	CL	513	CLA	C1D-ND	4.22	1.43	1.37
84	u3	1001	CYC	CHD-C1D	4.22	1.50	1.40
82	M9	305	PEB	CHB-C4B	4.22	1.46	1.38
82	uK	201	PEB	CHA-C1B	4.22	1.50	1.40
83	M9	303	PUB	CHB-C1C	4.22	1.46	1.38
82	lJ	202	PEB	C1A-NA	-4.22	1.32	1.37
82	MF	201	PEB	C1A-NA	-4.22	1.32	1.37
87	62	308	CLA	C1D-ND	4.22	1.43	1.37
87	72	607	CLA	C1D-ND	4.22	1.43	1.37
92	jL	101	LMG	O7-C10	4.22	1.46	1.34
82	CK	202	PEB	CHB-C4B	4.22	1.46	1.38
82	EA	201	PEB	CHB-C1C	4.22	1.50	1.40
82	E7	201	PEB	CHB-C1C	4.22	1.50	1.40
84	w3	1001	CYC	CHD-C1D	4.22	1.50	1.40
95	CL	520	DGD	O1G-C1A	4.22	1.45	1.33
84	CG	1001	CYC	CHB-C4A	4.21	1.50	1.40
82	P7	201	PEB	CHA-C1B	4.21	1.50	1.40
82	NA	202	PEB	CHB-C4B	4.21	1.46	1.38
84	73	1001	CYC	CHD-C1D	4.21	1.50	1.40
87	3N	305	CLA	C1D-ND	4.21	1.43	1.37
84	h3	1001	CYC	CHD-C1D	4.21	1.50	1.40
82	U5	202	PEB	C1A-NA	-4.21	1.32	1.37
82	PA	201	PEB	CHA-C1B	4.21	1.50	1.40
82	uF	202	PEB	CHA-C1B	4.21	1.50	1.40
82	RE	201	PEB	C2A-C1A	-4.21	1.48	1.52
82	TH	202	PEB	CHA-C1B	4.21	1.50	1.40
95	DL	408	DGD	O1G-C1A	4.21	1.45	1.33
84	F4	1001	CYC	CHD-C1D	4.21	1.50	1.40
92	BL	611	LMG	O8-C28	4.21	1.45	1.33
82	qF	203	PEB	CHA-C1B	4.21	1.50	1.40
82	V5	201	PEB	C1A-NA	-4.21	1.32	1.37
95	h6	101	DGD	O1G-C1A	4.21	1.45	1.33
84	W3	1001	CYC	CHB-C4A	4.21	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	M5	303	PUB	C2C-C3C	4.21	1.45	1.36
95	BL	613	DGD	O1G-C1A	4.20	1.45	1.33
84	EH	1001	CYC	C2C-C1C	-4.20	1.48	1.52
84	F3	1001	CYC	CHD-C1D	4.20	1.50	1.40
82	O4	201	PEB	C1A-NA	-4.20	1.32	1.37
88	bL	612	LHG	O8-C23	4.20	1.45	1.33
82	MP	201	PEB	C3B-C2B	4.20	1.45	1.36
82	fH	203	PEB	CHB-C1C	4.20	1.50	1.40
84	Q3	1001	CYC	CHD-C1D	4.20	1.50	1.40
92	b6	619	LMG	O8-C28	4.20	1.45	1.33
92	aL	611	LMG	O7-C10	4.20	1.46	1.34
84	M3	1001	CYC	CHD-C1D	4.20	1.50	1.40
88	BL	610	LHG	O8-C23	4.20	1.45	1.33
84	D3	1001	CYC	CHD-C1D	4.20	1.50	1.40
82	SD	201	PEB	CHA-C1B	4.20	1.50	1.40
82	bK	202	PEB	CHA-C1B	4.20	1.50	1.40
84	NO	1001	CYC	CHB-C4A	4.20	1.50	1.40
82	H5	201	PEB	CHB-C1C	4.20	1.50	1.40
82	QQ	201	PEB	CHA-C1B	4.20	1.50	1.40
82	V1	201	PEB	CHA-C1B	4.20	1.50	1.40
82	VK	201	PEB	C2A-C1A	-4.20	1.48	1.52
84	HO	1001	CYC	CHD-C1D	4.20	1.50	1.40
84	H4	1001	CYC	CHD-C1D	4.20	1.50	1.40
84	C1	1001	CYC	CHD-C1D	4.20	1.50	1.40
84	H3	1001	CYC	CHD-C1D	4.20	1.50	1.40
84	U3	1001	CYC	CHD-C1D	4.20	1.50	1.40
82	SO	201	PEB	C2A-C1A	-4.20	1.48	1.52
92	jL	101	LMG	O8-C28	4.20	1.45	1.33
84	k3	1001	CYC	CHD-C1D	4.20	1.50	1.40
82	zK	501	PEB	CHB-C4B	4.20	1.46	1.38
82	WF	201	PEB	C1A-NA	-4.20	1.32	1.37
82	T5	201	PEB	C1A-NA	-4.20	1.32	1.37
84	j3	1001	CYC	CHD-C1D	4.20	1.50	1.40
82	QD	201	PEB	CHA-C1B	4.19	1.50	1.40
82	NM	202	PEB	CHA-C1B	4.19	1.50	1.40
82	E5	201	PEB	C1A-NA	-4.19	1.32	1.37
84	C4	1001	CYC	C2C-C1C	-4.19	1.48	1.52
84	n3	1001	CYC	CHD-C1D	4.19	1.50	1.40
83	Z5	303	PUB	C2C-C3C	4.19	1.45	1.36
83	AH	303	PUB	CHB-C4B	4.19	1.50	1.40
92	JL	103	LMG	O8-C28	4.19	1.45	1.33
96	G2	201	HEM	FE-ND	4.19	2.07	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OJ	201	PEB	C1A-NA	-4.19	1.32	1.37
82	HD	202	PEB	CHA-C1B	4.19	1.50	1.40
84	BG	1001	CYC	C1C-NC	-4.19	1.32	1.37
82	DI	201	PEB	CHA-C1B	4.19	1.50	1.40
87	7N	607	CLA	C1D-ND	4.19	1.42	1.37
84	BE	1002	CYC	C1C-NC	-4.19	1.32	1.37
82	mM	202	PEB	CHA-C1B	4.19	1.50	1.40
95	D6	410	DGD	O1G-C1A	4.19	1.45	1.33
82	R4	202	PEB	C1A-NA	-4.19	1.32	1.37
84	x3	1001	CYC	CHD-C1D	4.19	1.50	1.40
95	AL	415	DGD	O1G-C1A	4.19	1.45	1.33
84	HH	1001	CYC	C1C-NC	-4.19	1.32	1.37
88	AN	844	LHG	O7-C7	4.19	1.46	1.34
82	dH	202	PEB	C1A-NA	-4.19	1.32	1.37
87	32	304	CLA	C1D-ND	4.18	1.42	1.37
82	ZM	201	PEB	CHA-C1B	4.18	1.50	1.40
82	IK	203	PEB	C1A-NA	-4.18	1.32	1.37
92	B6	619	LMG	O8-C28	4.18	1.45	1.33
87	aL	606	CLA	O2A-CGA	4.18	1.45	1.33
92	k6	101	LMG	O7-C10	4.18	1.46	1.34
92	B6	618	LMG	O8-C28	4.18	1.45	1.33
82	O4	201	PEB	C3B-C2B	4.18	1.45	1.36
84	y3	1001	CYC	CHB-C4A	4.18	1.50	1.40
82	VK	202	PEB	CHA-C1B	4.18	1.50	1.40
82	Z9	301	PEB	C1A-NA	-4.18	1.32	1.37
87	6N	602	CLA	C1D-ND	4.18	1.42	1.37
84	N4	1001	CYC	CHB-C4A	4.18	1.50	1.40
82	qK	203	PEB	CHA-C1B	4.18	1.50	1.40
82	OH	201	PEB	CHB-C1C	4.18	1.50	1.40
82	LM	202	PEB	CHA-C1B	4.18	1.50	1.40
82	DQ	202	PEB	C1A-NA	-4.18	1.32	1.37
82	CF	202	PEB	C3B-C2B	4.18	1.45	1.36
82	tC	201	PEB	CHA-C1B	4.18	1.50	1.40
84	N1	1001	CYC	CHB-C4A	4.18	1.50	1.40
88	M6	101	LHG	O8-C23	4.18	1.45	1.33
91	AL	410	PHO	OBD-CAD	4.18	1.28	1.22
82	Z9	304	PEB	CHB-C4B	4.18	1.46	1.38
82	ZG	201	PEB	C1A-NA	-4.18	1.32	1.37
82	LI	202	PEB	C1A-NA	-4.18	1.32	1.37
95	AL	416	DGD	O1G-C1A	4.18	1.45	1.33
84	NH	1001	CYC	CHB-C4A	4.18	1.50	1.40
82	D5	201	PEB	C1A-NA	-4.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	bE	201	PEB	C1A-NA	-4.18	1.32	1.37
82	XF	201	PEB	C2A-C1A	-4.18	1.48	1.52
87	F2	205	CLA	C4B-NB	4.18	1.42	1.37
84	V3	1001	CYC	CHD-C1D	4.18	1.50	1.40
82	NB	203	PEB	CHA-C1B	4.18	1.50	1.40
82	C5	201	PEB	C1A-NA	-4.17	1.32	1.37
92	DL	402	LMG	O7-C10	4.17	1.46	1.34
92	B6	622	LMG	O8-C28	4.17	1.45	1.33
92	mL	101	LMG	O7-C10	4.17	1.46	1.34
82	CB	201	PEB	C1A-NA	-4.17	1.32	1.37
88	BL	615	LHG	O8-C23	4.17	1.45	1.33
82	d1	202	PEB	C1A-NA	-4.17	1.32	1.37
82	W9	202	PEB	CHB-C1C	4.17	1.50	1.40
84	CH	1001	CYC	CHB-C4A	4.17	1.50	1.40
87	FN	205	CLA	C4B-NB	4.17	1.42	1.37
82	UJ	202	PEB	CHB-C4B	4.17	1.46	1.38
82	a1	202	PEB	CHA-C1B	4.17	1.50	1.40
82	YI	201	PEB	C1A-NA	-4.17	1.32	1.37
84	DO	1001	CYC	CHD-C1D	4.17	1.50	1.40
82	GG	1002	PEB	C1A-NA	-4.17	1.32	1.37
82	R7	203	PEB	CHA-C1B	4.17	1.50	1.40
82	OK	202	PEB	C3B-C2B	4.17	1.45	1.36
95	lL	101	DGD	O1G-C1A	4.17	1.45	1.33
82	PH	202	PEB	CHA-C1B	4.17	1.50	1.40
82	ED	201	PEB	C1A-NA	-4.17	1.32	1.37
84	J1	1001	CYC	C1C-NC	-4.17	1.32	1.37
82	SQ	201	PEB	CHA-C1B	4.17	1.50	1.40
95	b6	622	DGD	O1G-C1A	4.17	1.45	1.33
82	YE	201	PEB	C1A-NA	-4.16	1.32	1.37
95	BL	613	DGD	O2G-C1B	4.16	1.46	1.34
84	q3	1001	CYC	CHD-C1D	4.16	1.50	1.40
82	zF	501	PEB	C3B-C2B	4.16	1.45	1.36
82	U5	201	PEB	CHB-C1C	4.16	1.50	1.40
82	PJ	202	PEB	CHA-C1B	4.16	1.50	1.40
84	D4	1001	CYC	C1C-NC	-4.16	1.32	1.37
82	kM	202	PEB	CHA-C1B	4.16	1.50	1.40
84	BE	1001	CYC	C1C-NC	-4.16	1.32	1.37
82	wC	202	PEB	CHB-C1C	4.16	1.50	1.40
84	DH	1001	CYC	CHD-C1D	4.16	1.50	1.40
88	ML	102	LHG	O8-C23	4.16	1.45	1.33
82	H5	201	PEB	OD-C4D	4.16	1.31	1.23
82	I5	201	PEB	C1A-NA	-4.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	H4	1001	CYC	C2C-C1C	-4.16	1.48	1.52
92	D6	407	LMG	O8-C28	4.16	1.45	1.33
84	J1	1001	CYC	CHB-C4A	4.16	1.50	1.40
82	X5	201	PEB	C1A-NA	-4.16	1.32	1.37
82	F9	201	PEB	C1A-NA	-4.16	1.32	1.37
88	A2	844	LHG	O8-C23	4.16	1.45	1.33
82	XA	202	PEB	CHB-C4B	4.16	1.46	1.38
82	XJ	202	PEB	C1A-NA	-4.16	1.32	1.37
82	XP	202	PEB	C1A-NA	-4.16	1.32	1.37
84	DG	1001	CYC	C2C-C1C	-4.16	1.48	1.52
82	VK	201	PEB	CHA-C1B	4.16	1.50	1.40
82	CF	202	PEB	CHA-C1B	4.16	1.50	1.40
92	b6	620	LMG	O8-C28	4.16	1.45	1.33
82	TA	201	PEB	C1A-NA	-4.16	1.32	1.37
82	A5	201	PEB	C1A-NA	-4.16	1.32	1.37
82	KJ	203	PEB	CHB-C4B	4.16	1.46	1.38
92	AL	411	LMG	O8-C28	4.15	1.45	1.33
82	oK	202	PEB	CHA-C1B	4.15	1.50	1.40
84	E1	1001	CYC	CHA-C1A	4.15	1.46	1.38
82	zK	501	PEB	C3B-C2B	4.15	1.45	1.36
88	dL	408	LHG	O8-C23	4.15	1.45	1.33
91	a6	613	PHO	O2A-CGA	4.15	1.45	1.33
84	L1	1001	CYC	C2C-C1C	-4.15	1.48	1.52
82	LD	201	PEB	CHB-C1C	4.15	1.50	1.40
82	lF	203	PEB	CHB-C1C	4.15	1.50	1.40
82	EQ	201	PEB	C1A-NA	-4.15	1.32	1.37
82	R5	201	PEB	C1A-NA	-4.15	1.32	1.37
88	d6	402	LHG	O8-C23	4.15	1.45	1.33
82	N7	201	PEB	C2A-C1A	-4.15	1.48	1.52
82	U5	201	PEB	OD-C4D	4.15	1.31	1.23
82	R7	201	PEB	C1A-NA	-4.15	1.32	1.37
82	HM	202	PEB	CHA-C1B	4.15	1.50	1.40
88	mL	102	LHG	O7-C7	4.15	1.46	1.34
88	m6	102	LHG	O7-C7	4.15	1.46	1.34
82	P5	201	PEB	C1A-NA	-4.15	1.32	1.37
84	H1	1001	CYC	C1C-NC	-4.15	1.32	1.37
82	TM	202	PEB	C1A-NA	-4.14	1.32	1.37
95	B6	620	DGD	O1G-C1A	4.14	1.45	1.33
88	AN	844	LHG	O8-C23	4.14	1.45	1.33
95	BL	614	DGD	O1G-C1A	4.14	1.45	1.33
82	uK	202	PEB	CHA-C1B	4.14	1.50	1.40
82	YP	501	PEB	C1A-NA	-4.14	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BD	203	PEB	CHB-C4B	4.14	1.46	1.38
88	AN	843	LHG	O8-C23	4.14	1.45	1.33
82	iH	202	PEB	CHA-C1B	4.14	1.50	1.40
82	d1	202	PEB	CHB-C1C	4.14	1.50	1.40
95	O6	301	DGD	O1G-C1A	4.14	1.45	1.33
95	b6	621	DGD	O2G-C1B	4.14	1.46	1.34
82	LJ	201	PEB	CHA-C1B	4.14	1.50	1.40
82	eG	203	PEB	CHA-C1B	4.14	1.50	1.40
88	A2	843	LHG	O8-C23	4.14	1.45	1.33
92	CL	519	LMG	O8-C28	4.14	1.45	1.33
82	G5	201	PEB	C1A-NA	-4.14	1.32	1.37
92	j6	102	LMG	O8-C28	4.14	1.45	1.33
82	Q4	201	PEB	C1A-NA	-4.14	1.32	1.37
91	d6	404	PHO	C3A-C2A	-4.14	1.50	1.54
82	BQ	203	PEB	CHB-C4B	4.14	1.46	1.38
82	WK	202	PEB	C1A-NA	-4.14	1.32	1.37
88	m6	102	LHG	O8-C23	4.14	1.45	1.33
82	CK	202	PEB	C3B-C2B	4.14	1.45	1.36
82	MJ	202	PEB	CHB-C4B	4.14	1.46	1.38
82	DJ	202	PEB	CHA-C1B	4.14	1.50	1.40
82	TJ	202	PEB	CHA-C1B	4.14	1.50	1.40
82	X7	202	PEB	CHB-C4B	4.14	1.46	1.38
82	Q9	201	PEB	CHA-C1B	4.14	1.50	1.40
88	aL	607	LHG	O7-C7	4.14	1.46	1.34
88	AL	406	LHG	O8-C23	4.14	1.45	1.33
82	uF	203	PEB	CHA-C1B	4.14	1.50	1.40
87	RN	201	CLA	C1D-ND	4.14	1.42	1.37
95	J6	101	DGD	O1G-C1A	4.13	1.45	1.33
82	DA	203	PEB	CHA-C1B	4.13	1.50	1.40
82	i1	202	PEB	CHA-C1B	4.13	1.50	1.40
82	N5	201	PEB	C1A-NA	-4.13	1.32	1.37
82	RI	203	PEB	CHB-C4B	4.13	1.46	1.38
95	C6	521	DGD	O1G-C1A	4.13	1.45	1.33
87	5N	608	CLA	C1D-ND	4.13	1.42	1.37
82	IP	201	PEB	C1A-NA	-4.13	1.32	1.37
82	h1	202	PEB	C1A-NA	-4.13	1.32	1.37
92	JL	103	LMG	O7-C10	4.13	1.46	1.34
82	UB	301	PEB	CHA-C1B	4.13	1.50	1.40
82	KJ	201	PEB	C1A-NA	-4.13	1.32	1.37
82	QO	201	PEB	C1A-NA	-4.13	1.32	1.37
82	K5	201	PEB	C1A-NA	-4.13	1.32	1.37
82	eM	202	PEB	C1A-NA	-4.13	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OO	201	PEB	C1A-NA	-4.13	1.32	1.37
84	ME	1001	CYC	C2C-C1C	-4.13	1.48	1.52
82	UF	201	PEB	C1A-NA	-4.13	1.32	1.37
95	c6	618	DGD	O1G-C1A	4.13	1.45	1.33
82	bF	202	PEB	CHA-C1B	4.13	1.50	1.40
95	C6	523	DGD	O1G-C1A	4.13	1.45	1.33
84	BG	1002	CYC	CHB-C4A	4.13	1.50	1.40
82	iM	202	PEB	CHA-C1B	4.13	1.50	1.40
84	A3	1001	CYC	C1D-C2D	4.13	1.51	1.41
82	M9	302	PEB	C1A-NA	-4.12	1.32	1.37
84	DO	1001	CYC	C1C-NC	-4.12	1.32	1.37
95	a6	603	DGD	O2G-C1B	4.12	1.45	1.34
82	tF	202	PEB	CHA-C1B	4.12	1.50	1.40
82	NQ	204	PEB	CHB-C1C	4.12	1.50	1.40
82	F5	202	PEB	C1A-NA	-4.12	1.32	1.37
88	i6	101	LHG	O8-C23	4.12	1.45	1.33
88	B6	617	LHG	O8-C23	4.12	1.45	1.33
84	C3	1001	CYC	C1D-C2D	4.12	1.51	1.41
82	gH	202	PEB	CHA-C1B	4.12	1.50	1.40
84	J3	1001	CYC	C1D-C2D	4.12	1.51	1.41
84	l3	1001	CYC	C1D-C2D	4.12	1.51	1.41
82	B7	202	PEB	CHB-C1C	4.12	1.50	1.40
84	CH	1001	CYC	CHD-C1D	4.12	1.50	1.40
95	c6	620	DGD	O1G-C1A	4.12	1.45	1.33
83	A1	303	PUB	CHB-C4B	4.12	1.50	1.40
82	YE	201	PEB	C2A-C1A	-4.12	1.48	1.52
82	YJ	202	PEB	C2A-C1A	-4.12	1.48	1.52
95	AL	415	DGD	O2G-C1B	4.12	1.45	1.34
82	YG	201	PEB	C1A-NA	-4.12	1.32	1.37
84	g3	1001	CYC	C1D-C2D	4.12	1.51	1.41
84	EE	1001	CYC	CHB-C4A	4.12	1.50	1.40
82	HQ	202	PEB	CHA-C1B	4.12	1.50	1.40
82	f1	203	PEB	CHB-C1C	4.12	1.50	1.40
87	R2	201	CLA	C1D-ND	4.12	1.42	1.37
82	W1	203	PEB	CHB-C1C	4.12	1.50	1.40
82	KQ	201	PEB	C1A-NA	-4.12	1.32	1.37
92	AL	411	LMG	O7-C10	4.12	1.45	1.34
82	N7	201	PEB	CHA-C1B	4.12	1.50	1.40
82	YE	201	PEB	CHB-C4B	4.12	1.46	1.38
84	N1	1001	CYC	CHD-C1D	4.12	1.50	1.40
84	HG	1001	CYC	C1C-NC	-4.12	1.32	1.37
84	N3	1001	CYC	C1D-C2D	4.12	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	P3	1001	CYC	C1D-C2D	4.12	1.51	1.41
82	YG	201	PEB	CHB-C4B	4.12	1.46	1.38
95	BL	607	DGD	O2G-C1B	4.12	1.45	1.34
82	KF	202	PEB	C2A-C1A	-4.12	1.48	1.52
82	LE	1002	PEB	CHC-C4C	4.12	1.54	1.49
92	dL	407	LMG	O7-C10	4.11	1.45	1.34
82	eF	201	PEB	C1A-NA	-4.11	1.32	1.37
82	hF	201	PEB	CHA-C1B	4.11	1.50	1.40
82	RA	201	PEB	C1A-NA	-4.11	1.32	1.37
84	D4	1001	CYC	CHD-C1D	4.11	1.50	1.40
84	EE	1001	CYC	CHD-C1D	4.11	1.50	1.40
84	v3	1001	CYC	C1D-C2D	4.11	1.51	1.41
82	OE	201	PEB	C1A-NA	-4.11	1.32	1.37
82	NA	201	PEB	C2A-C1A	-4.11	1.48	1.52
82	PA	203	PEB	C1A-NA	-4.11	1.32	1.37
82	t8	201	PEB	CHA-C1B	4.11	1.50	1.40
84	J4	1001	CYC	C1C-NC	-4.11	1.32	1.37
88	d6	407	LHG	O8-C23	4.11	1.45	1.33
82	VF	201	PEB	C2A-C1A	-4.11	1.48	1.52
92	bL	624	LMG	O8-C28	4.11	1.45	1.33
95	BL	607	DGD	O1G-C1A	4.11	1.45	1.33
84	EH	1001	CYC	CHA-C1A	4.11	1.46	1.38
82	L9	201	PEB	C1A-NA	-4.11	1.32	1.37
82	hK	201	PEB	CHA-C1B	4.11	1.50	1.40
82	fK	202	PEB	CHC-C4C	4.11	1.54	1.49
88	CL	521	LHG	O8-C23	4.11	1.45	1.33
92	x6	601	LMG	O8-C28	4.11	1.45	1.33
82	pK	202	PEB	CHA-C1B	4.11	1.50	1.40
84	T3	1001	CYC	C1D-C2D	4.11	1.51	1.41
82	RD	201	PEB	CHB-C1C	4.11	1.50	1.40
82	VJ	201	PEB	CHA-C1B	4.10	1.50	1.40
84	JH	1001	CYC	CHB-C4A	4.10	1.50	1.40
82	MM	202	PEB	CHA-C1B	4.10	1.50	1.40
84	EG	1001	CYC	CHB-C4A	4.10	1.50	1.40
82	Q1	201	PEB	CHB-C1C	4.10	1.50	1.40
95	B6	620	DGD	O2G-C1B	4.10	1.45	1.34
84	E3	1001	CYC	C1D-C2D	4.10	1.51	1.41
84	c3	1001	CYC	C1D-C2D	4.10	1.51	1.41
82	VH	201	PEB	CHA-C1B	4.10	1.50	1.40
84	C1	1001	CYC	CHB-C4A	4.10	1.50	1.40
88	C6	522	LHG	O8-C23	4.10	1.45	1.33
84	R3	1001	CYC	C1D-C2D	4.10	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dH	202	PEB	CHB-C1C	4.10	1.50	1.40
82	HJ	202	PEB	CHA-C1B	4.10	1.50	1.40
84	e3	1001	CYC	C1D-C2D	4.10	1.51	1.41
92	b6	619	LMG	O7-C10	4.10	1.45	1.34
82	DA	201	PEB	CHA-C1B	4.10	1.50	1.40
82	jO	201	PEB	C1A-NA	-4.10	1.32	1.37
82	CF	202	PEB	CHB-C4B	4.10	1.46	1.38
84	DG	1001	CYC	CHB-C1B	4.10	1.47	1.38
82	LQ	201	PEB	CHB-C1C	4.10	1.50	1.40
82	mJ	202	PEB	CHA-C1B	4.10	1.50	1.40
95	aL	603	DGD	O1G-C1A	4.10	1.45	1.33
92	BL	612	LMG	O8-C28	4.10	1.45	1.33
87	52	608	CLA	C1D-ND	4.10	1.42	1.37
95	CL	517	DGD	O1G-C1A	4.10	1.45	1.33
95	BL	614	DGD	O2G-C1B	4.10	1.45	1.34
88	L6	101	LHG	O8-C23	4.10	1.45	1.33
88	l6	101	LHG	O8-C23	4.10	1.45	1.33
82	aF	201	PEB	CHB-C1C	4.10	1.50	1.40
92	C6	501	LMG	O8-C28	4.10	1.45	1.33
95	JL	101	DGD	O1G-C1A	4.10	1.45	1.33
82	aK	201	PEB	CHB-C1C	4.09	1.50	1.40
92	a6	614	LMG	O7-C10	4.09	1.45	1.34
84	G3	1001	CYC	C1D-C2D	4.09	1.51	1.41
82	QB	202	PEB	CHA-C1B	4.09	1.50	1.40
88	bL	612	LHG	O7-C7	4.09	1.45	1.34
82	QB	201	PEB	C1A-NA	-4.09	1.32	1.37
82	tK	202	PEB	CHA-C1B	4.09	1.50	1.40
82	LG	1002	PEB	CHC-C4C	4.09	1.54	1.49
82	BA	202	PEB	CHB-C1C	4.09	1.50	1.40
84	p3	1001	CYC	C1D-C2D	4.09	1.51	1.41
82	S4	201	PEB	C3B-C2B	4.09	1.45	1.36
95	CL	523	DGD	O1G-C1A	4.09	1.45	1.33
82	iM	201	PEB	CHA-C1B	4.09	1.50	1.40
82	eK	201	PEB	C1A-NA	-4.09	1.32	1.37
95	a6	602	DGD	O1G-C1A	4.09	1.45	1.33
82	EK	201	PEB	C3B-C2B	4.09	1.45	1.36
82	lO	201	PEB	C1A-NA	-4.09	1.32	1.37
82	BB	203	PEB	C1A-NA	-4.09	1.32	1.37
82	P7	201	PEB	C1A-NA	-4.09	1.32	1.37
82	qF	201	PEB	CHA-C1B	4.09	1.50	1.40
92	m6	101	LMG	O8-C28	4.09	1.45	1.33
84	t3	1001	CYC	C1D-C2D	4.09	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	pF	202	PEB	CHA-C1B	4.09	1.50	1.40
87	B2	824	CLA	C4B-NB	4.09	1.42	1.37
82	EK	201	PEB	CHA-C1B	4.09	1.50	1.40
82	aG	201	PEB	C1A-NA	-4.09	1.32	1.37
95	cL	520	DGD	O1G-C1A	4.09	1.45	1.33
82	TD	201	PEB	CHB-C1C	4.09	1.50	1.40
82	NJ	201	PEB	C1A-NA	-4.09	1.32	1.37
82	W4	201	PEB	C2A-C1A	-4.09	1.48	1.52
87	A2	809	CLA	C1D-ND	4.09	1.42	1.37
83	Z5	303	PUB	OD-C4D	4.09	1.31	1.23
82	PA	201	PEB	C1A-NA	-4.09	1.32	1.37
91	D6	404	PHO	O2A-CGA	4.09	1.45	1.33
84	NH	1001	CYC	CHD-C1D	4.09	1.50	1.40
82	kE	202	PEB	C1A-NA	-4.09	1.32	1.37
82	FK	202	PEB	C1A-NA	-4.08	1.32	1.37
84	i3	1001	CYC	CHA-C4D	4.08	1.50	1.40
92	j6	102	LMG	O7-C10	4.08	1.45	1.34
92	A6	408	LMG	O7-C10	4.08	1.45	1.34
82	CP	202	PEB	CHA-C1B	4.08	1.50	1.40
82	eF	202	PEB	CHB-C4B	4.08	1.46	1.38
84	i3	1001	CYC	C1D-C2D	4.08	1.51	1.41
84	m3	1001	CYC	C1D-C2D	4.08	1.51	1.41
82	VF	201	PEB	CHA-C1B	4.08	1.50	1.40
88	AL	406	LHG	O7-C7	4.08	1.45	1.34
96	VL	201	HEM	FE-NC	4.08	2.09	1.95
82	dK	202	PEB	CHA-C1B	4.08	1.50	1.40
82	PB	201	PEB	C1A-NA	-4.08	1.32	1.37
95	CL	520	DGD	O2G-C1B	4.08	1.45	1.34
84	FH	1001	CYC	CHD-C1D	4.08	1.50	1.40
95	AL	416	DGD	O2G-C1B	4.08	1.45	1.34
84	HO	1001	CYC	C2C-C1C	-4.08	1.48	1.52
95	a6	604	DGD	O1G-C1A	4.08	1.45	1.33
84	L4	1001	CYC	CHD-C1D	4.08	1.50	1.40
82	FM	201	PEB	C1A-NA	-4.08	1.32	1.37
88	AN	843	LHG	O7-C7	4.08	1.45	1.34
82	eE	203	PEB	CHA-C1B	4.08	1.50	1.40
84	t3	1001	CYC	CHA-C4D	4.08	1.50	1.40
82	pC	202	PEB	CHA-C1B	4.08	1.50	1.40
82	O1	201	PEB	CHB-C1C	4.08	1.50	1.40
87	42	607	CLA	C1D-ND	4.08	1.42	1.37
82	LM	201	PEB	CHA-C1B	4.08	1.50	1.40
96	vL	201	HEM	FE-NC	4.08	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	JJ	202	PEB	C2A-C1A	-4.08	1.48	1.52
82	jK	202	PEB	C1A-NA	-4.08	1.32	1.37
82	cG	202	PEB	CHA-C1B	4.08	1.50	1.40
82	dF	202	PEB	CHA-C1B	4.08	1.50	1.40
82	IF	203	PEB	CHB-C4B	4.07	1.46	1.38
82	cB	403	PEB	C2C-C3C	4.07	1.49	1.38
82	SO	201	PEB	C3B-C2B	4.07	1.45	1.36
82	RO	202	PEB	C1A-NA	-4.07	1.32	1.37
95	L6	102	DGD	O1G-C1A	4.07	1.45	1.33
88	A2	843	LHG	O7-C7	4.07	1.45	1.34
82	EF	201	PEB	CHA-C1B	4.07	1.50	1.40
82	OO	201	PEB	C2A-C1A	-4.07	1.48	1.52
84	F1	1001	CYC	CHD-C1D	4.07	1.50	1.40
92	m6	103	LMG	O8-C28	4.07	1.45	1.33
82	ID	201	PEB	C1A-NA	-4.07	1.32	1.37
82	bF	202	PEB	CHC-C4C	4.07	1.54	1.49
84	A3	1001	CYC	CHA-C4D	4.07	1.50	1.40
84	C3	1001	CYC	CHA-C4D	4.07	1.50	1.40
82	UF	201	PEB	CHA-C1B	4.07	1.49	1.40
88	D6	401	LHG	O8-C23	4.07	1.45	1.33
84	K3	1001	CYC	C1D-C2D	4.07	1.51	1.41
92	bL	623	LMG	O8-C28	4.07	1.45	1.33
88	d6	402	LHG	O7-C7	4.07	1.45	1.34
91	A6	407	PHO	O2A-CGA	4.07	1.45	1.33
82	FJ	201	PEB	C2A-C1A	-4.07	1.48	1.52
84	L4	1001	CYC	C2C-C1C	-4.07	1.48	1.52
82	TJ	202	PEB	C1A-NA	-4.07	1.32	1.37
82	L9	202	PEB	CHB-C1C	4.07	1.50	1.40
84	KG	202	CYC	CHD-C1D	4.07	1.50	1.40
87	4N	607	CLA	C1D-ND	4.07	1.42	1.37
82	GB	203	PEB	C1A-NA	-4.07	1.32	1.37
82	RM	201	PEB	CHA-C1B	4.07	1.49	1.40
95	AL	414	DGD	O1G-C1A	4.07	1.45	1.33
82	g1	202	PEB	CHB-C1C	4.07	1.50	1.40
82	ZG	202	PEB	C1A-NA	-4.07	1.32	1.37
82	O9	202	PEB	C1A-NA	-4.07	1.32	1.37
82	fF	202	PEB	CHC-C4C	4.07	1.54	1.49
82	bK	202	PEB	CHC-C4C	4.07	1.54	1.49
82	S5	201	PEB	C1A-NA	-4.07	1.32	1.37
82	IM	202	PEB	C1A-NA	-4.06	1.32	1.37
84	P3	1001	CYC	CHA-C4D	4.06	1.50	1.40
82	W5	202	PEB	CHB-C1C	4.06	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	M5	303	PUB	OD-C4D	4.06	1.31	1.23
88	c6	619	LHG	O8-C23	4.06	1.45	1.33
82	UJ	202	PEB	CHA-C1B	4.06	1.49	1.40
82	UK	201	PEB	CHA-C1B	4.06	1.49	1.40
82	LJ	202	PEB	C2A-C1A	-4.06	1.48	1.52
84	MG	1001	CYC	C2C-C1C	-4.06	1.48	1.52
82	HA	202	PEB	CHB-C1C	4.06	1.49	1.40
82	H7	202	PEB	CHB-C1C	4.06	1.49	1.40
82	FJ	202	PEB	C1A-NA	-4.06	1.32	1.37
82	w8	202	PEB	CHB-C1C	4.06	1.49	1.40
82	gH	202	PEB	CHB-C1C	4.06	1.49	1.40
82	UB	302	PEB	CHA-C1B	4.06	1.49	1.40
82	L7	201	PEB	CHA-C1B	4.06	1.49	1.40
82	s8	203	PEB	CHA-C1B	4.06	1.49	1.40
82	FK	201	PEB	CHB-C1C	4.06	1.49	1.40
82	P7	203	PEB	C1A-NA	-4.06	1.32	1.37
82	gK	201	PEB	C1A-NA	-4.06	1.32	1.37
84	JO	1001	CYC	C1C-NC	-4.06	1.32	1.37
82	TF	202	PEB	C1A-NA	-4.06	1.32	1.37
84	J4	1001	CYC	CHD-C1D	4.06	1.49	1.40
92	aL	611	LMG	O8-C28	4.06	1.45	1.33
84	NE	201	CYC	CHD-C1D	4.06	1.49	1.40
84	LO	1001	CYC	CHD-C1D	4.06	1.49	1.40
87	A2	852	CLA	C1D-C2D	4.06	1.53	1.45
82	g1	202	PEB	CHA-C1B	4.06	1.49	1.40
82	D7	203	PEB	CHA-C1B	4.06	1.49	1.40
82	JK	201	PEB	CHA-C1B	4.06	1.49	1.40
84	l3	1001	CYC	CHA-C4D	4.06	1.49	1.40
84	v3	1001	CYC	CHA-C4D	4.06	1.49	1.40
95	lL	101	DGD	O2G-C1B	4.06	1.45	1.34
92	d6	409	LMG	O7-C10	4.06	1.45	1.34
82	NB	203	PEB	C1A-NA	-4.05	1.32	1.37
92	qL	301	LMG	O8-C28	4.05	1.45	1.33
82	FM	202	PEB	CHA-C1B	4.05	1.49	1.40
95	CL	517	DGD	O2G-C1B	4.05	1.45	1.34
82	IQ	202	PEB	CHA-C1B	4.05	1.49	1.40
82	SH	201	PEB	C1A-NA	-4.05	1.32	1.37
82	HJ	202	PEB	C1A-NA	-4.05	1.32	1.37
82	gM	201	PEB	CHA-C1B	4.05	1.49	1.40
82	h1	201	PEB	CHB-C1C	4.05	1.49	1.40
82	KD	201	PEB	C1A-NA	-4.05	1.32	1.37
82	TQ	201	PEB	CHB-C1C	4.05	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	D9	201	PEB	C1A-NA	-4.05	1.32	1.37
82	IQ	201	PEB	CHA-C1B	4.05	1.49	1.40
84	T3	1001	CYC	CHA-C4D	4.05	1.49	1.40
82	Q9	201	PEB	CHB-C1C	4.05	1.49	1.40
82	MP	201	PEB	C2A-C1A	-4.05	1.48	1.52
82	CD	201	PEB	CHB-C4B	4.05	1.46	1.38
84	K3	1001	CYC	CHA-C4D	4.05	1.49	1.40
82	FM	201	PEB	CHA-C1B	4.05	1.49	1.40
95	O6	301	DGD	O2G-C1B	4.05	1.45	1.34
82	XM	202	PEB	CHA-C1B	4.05	1.49	1.40
88	CL	522	LHG	O8-C23	4.05	1.45	1.33
82	IJ	202	PEB	CHA-C1B	4.05	1.49	1.40
82	bK	201	PEB	CHA-C1B	4.05	1.49	1.40
82	lK	203	PEB	CHB-C1C	4.05	1.49	1.40
82	p8	202	PEB	CHA-C1B	4.05	1.49	1.40
84	E1	1001	CYC	C2C-C1C	-4.05	1.48	1.52
84	N3	1001	CYC	CHA-C4D	4.05	1.49	1.40
88	cL	501	LHG	O8-C23	4.05	1.45	1.33
82	RQ	201	PEB	CHB-C1C	4.05	1.49	1.40
84	p3	1001	CYC	CHA-C4D	4.05	1.49	1.40
82	Q5	203	PEB	CHA-C1B	4.05	1.49	1.40
82	U1	201	PEB	CHB-C1C	4.05	1.49	1.40
82	mE	203	PEB	CHA-C1B	4.05	1.49	1.40
87	BN	825	CLA	C4B-NB	4.05	1.42	1.37
88	ML	102	LHG	O7-C7	4.04	1.45	1.34
95	a6	604	DGD	O2G-C1B	4.04	1.45	1.34
82	H9	201	PEB	CHA-C1B	4.04	1.49	1.40
82	mF	201	PEB	CHA-C1B	4.04	1.49	1.40
82	mJ	201	PEB	CHA-C1B	4.04	1.49	1.40
82	EF	201	PEB	C3B-C2B	4.04	1.45	1.36
82	TQ	202	PEB	CHA-C1B	4.04	1.49	1.40
84	G3	1001	CYC	CHA-C4D	4.04	1.49	1.40
84	g3	1001	CYC	CHA-C4D	4.04	1.49	1.40
82	T7	201	PEB	CHB-C1C	4.04	1.49	1.40
84	EE	1001	CYC	C1C-NC	-4.04	1.32	1.37
84	LO	1001	CYC	C1C-NC	-4.04	1.32	1.37
82	mG	203	PEB	CHA-C1B	4.04	1.49	1.40
82	D9	202	PEB	CHB-C1C	4.04	1.49	1.40
92	m6	103	LMG	O7-C10	4.04	1.45	1.34
82	NA	201	PEB	CHA-C1B	4.04	1.49	1.40
82	dF	202	PEB	C2C-C3C	4.04	1.49	1.38
82	HM	201	PEB	CHA-C1B	4.04	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WM	201	PEB	C2A-C1A	-4.04	1.48	1.52
84	E3	1001	CYC	CHA-C4D	4.04	1.49	1.40
84	e3	1001	CYC	CHA-C4D	4.04	1.49	1.40
84	m3	1001	CYC	CHA-C4D	4.04	1.49	1.40
96	FL	102	HEM	C4D-ND	-4.04	1.33	1.40
82	QH	201	PEB	CHB-C1C	4.04	1.49	1.40
82	kK	202	PEB	CHB-C1C	4.04	1.49	1.40
87	3N	304	CLA	C1D-ND	4.04	1.42	1.37
82	GB	201	PEB	C1A-NA	-4.04	1.32	1.37
82	YB	202	PEB	C1A-NA	-4.04	1.32	1.37
95	cL	519	DGD	O1G-C1A	4.04	1.45	1.33
84	JH	1001	CYC	C1C-NC	-4.04	1.32	1.37
82	KA	202	PEB	CHA-C1B	4.04	1.49	1.40
82	NJ	202	PEB	CHA-C1B	4.04	1.49	1.40
82	TK	202	PEB	C1A-NA	-4.04	1.32	1.37
88	a6	610	LHG	O8-C23	4.04	1.45	1.33
82	uF	201	PEB	CHB-C1C	4.03	1.49	1.40
82	U9	204	PEB	CHB-C1C	4.03	1.49	1.40
82	RK	201	PEB	C2A-C1A	-4.03	1.48	1.52
84	EG	1001	CYC	CHD-C1D	4.03	1.49	1.40
82	ND	204	PEB	CHB-C1C	4.03	1.49	1.40
84	D1	1001	CYC	CHD-C1D	4.03	1.49	1.40
82	hH	201	PEB	C1A-NA	-4.03	1.32	1.37
82	JI	201	PEB	C1A-NA	-4.03	1.32	1.37
88	dL	405	LHG	O7-C7	4.03	1.45	1.34
95	hL	101	DGD	O1G-C1A	4.03	1.45	1.33
82	S9	201	PEB	CHA-C1B	4.03	1.49	1.40
82	eM	202	PEB	CHA-C1B	4.03	1.49	1.40
82	ZJ	201	PEB	C1A-NA	-4.03	1.32	1.37
82	jM	203	PEB	CHB-C1C	4.03	1.49	1.40
82	aO	202	PEB	CHB-C1C	4.03	1.49	1.40
82	O4	201	PEB	C2A-C1A	-4.03	1.48	1.52
88	DL	407	LHG	O8-C23	4.03	1.45	1.33
82	gH	203	PEB	CHB-C1C	4.03	1.49	1.40
82	ZB	203	PEB	C1A-NA	-4.03	1.32	1.37
82	cE	202	PEB	CHA-C1B	4.02	1.49	1.40
82	jF	202	PEB	C1A-NA	-4.02	1.32	1.37
84	J3	1001	CYC	CHA-C4D	4.02	1.49	1.40
84	c3	1001	CYC	CHA-C4D	4.02	1.49	1.40
82	ZI	401	PEB	C2C-C3C	4.02	1.49	1.38
82	LD	202	PEB	CHA-C1B	4.02	1.49	1.40
82	LQ	202	PEB	CHA-C1B	4.02	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FQ	203	PEB	C4B-NB	-4.02	1.30	1.38
82	QB	202	PEB	C1A-NA	-4.02	1.32	1.37
95	cL	502	DGD	O1G-C1A	4.02	1.45	1.33
82	FF	201	PEB	CHB-C1C	4.02	1.49	1.40
84	GG	1001	CYC	CHD-C1D	4.02	1.49	1.40
84	GO	1001	CYC	C2C-C1C	-4.02	1.48	1.52
82	sC	203	PEB	CHA-C1B	4.02	1.49	1.40
82	WH	203	PEB	CHB-C1C	4.02	1.49	1.40
87	32	303	CLA	C1D-ND	4.02	1.42	1.37
92	B6	618	LMG	O7-C10	4.02	1.45	1.34
95	aL	603	DGD	O2G-C1B	4.02	1.45	1.34
82	ID	202	PEB	CHA-C1B	4.02	1.49	1.40
82	aH	201	PEB	CHA-C1B	4.02	1.49	1.40
82	dK	202	PEB	C2C-C3C	4.02	1.49	1.38
82	TD	202	PEB	CHA-C1B	4.02	1.49	1.40
82	j4	201	PEB	C1A-NA	-4.02	1.32	1.37
82	BM	301	PEB	CHA-C1B	4.02	1.49	1.40
82	JM	202	PEB	CHA-C1B	4.02	1.49	1.40
82	a4	203	PEB	CHA-C1B	4.02	1.49	1.40
87	AN	809	CLA	C1D-ND	4.02	1.42	1.37
82	LA	201	PEB	CHA-C1B	4.02	1.49	1.40
82	JF	201	PEB	CHA-C1B	4.02	1.49	1.40
82	RO	203	PEB	CHB-C1C	4.02	1.49	1.40
82	CM	201	PEB	C1A-NA	-4.02	1.32	1.37
82	a1	201	PEB	CHA-C1B	4.02	1.49	1.40
87	AN	852	CLA	C1D-C2D	4.02	1.53	1.45
82	s8	202	PEB	CHB-C1C	4.02	1.49	1.40
82	RF	201	PEB	C2A-C1A	-4.01	1.48	1.52
92	D6	409	LMG	O7-C10	4.01	1.45	1.34
82	i4	203	PEB	CHA-C1B	4.01	1.49	1.40
82	QQ	202	PEB	C1A-NA	-4.01	1.32	1.37
82	jF	202	PEB	CHA-C1B	4.01	1.49	1.40
82	FQ	201	PEB	C1A-NA	-4.01	1.32	1.37
82	W5	201	PEB	C1A-NA	-4.01	1.32	1.37
82	fK	202	PEB	C1A-NA	-4.01	1.32	1.37
88	a6	610	LHG	O7-C7	4.01	1.45	1.34
82	mH	201	PEB	C1A-NA	-4.01	1.32	1.37
84	EG	1001	CYC	C1C-NC	-4.01	1.32	1.37
82	YG	201	PEB	C2A-C1A	-4.01	1.48	1.52
84	BG	1001	CYC	CHD-C1D	4.01	1.49	1.40
82	WM	201	PEB	CHA-C1B	4.01	1.49	1.40
82	OA	201	PEB	C2A-C1A	-4.01	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	fF	202	PEB	C1A-NA	-4.01	1.32	1.37
95	a6	602	DGD	O2G-C1B	4.01	1.45	1.34
88	aL	607	LHG	O8-C23	4.01	1.45	1.33
91	D6	404	PHO	C3A-C2A	-4.01	1.51	1.54
82	GP	202	PEB	C1A-NA	-4.01	1.32	1.37
82	B5	201	PEB	C1A-NA	-4.01	1.32	1.37
82	H5	203	PEB	C1A-NA	-4.01	1.32	1.37
82	dJ	202	PEB	C1A-NA	-4.01	1.32	1.37
82	RF	202	PEB	C1A-NA	-4.01	1.32	1.37
82	S1	201	PEB	C1A-NA	-4.01	1.32	1.37
82	hO	201	PEB	C1A-NA	-4.01	1.32	1.37
82	ZJ	202	PEB	CHA-C1B	4.00	1.49	1.40
82	D7	201	PEB	CHA-C1B	4.00	1.49	1.40
82	eO	201	PEB	CHA-C1B	4.00	1.49	1.40
82	W4	201	PEB	C3B-C2B	4.00	1.45	1.36
82	sC	202	PEB	CHB-C1C	4.00	1.49	1.40
84	R3	1001	CYC	CHA-C4D	4.00	1.49	1.40
88	AL	407	LHG	O8-C23	4.00	1.45	1.33
84	IE	1001	CYC	C1C-NC	-4.00	1.32	1.37
84	73	1002	CYC	CHB-C4A	4.00	1.49	1.40
82	NB	201	PEB	C1A-NA	-4.00	1.32	1.37
82	e1	201	PEB	C1A-NA	-4.00	1.32	1.37
82	fJ	203	PEB	CHB-C1C	4.00	1.49	1.40
84	GE	1001	CYC	CHD-C1D	4.00	1.49	1.40
82	AI	203	PEB	CHB-C4B	4.00	1.46	1.38
82	Y9	203	PEB	CHA-C1B	4.00	1.49	1.40
88	I6	101	LHG	O8-C23	4.00	1.45	1.33
84	EO	1001	CYC	CHD-C1D	4.00	1.49	1.40
82	ID	201	PEB	CHA-C1B	4.00	1.49	1.40
82	T7	201	PEB	CHA-C1B	4.00	1.49	1.40
82	SH	201	PEB	CHB-C1C	4.00	1.49	1.40
82	WE	201	PEB	C2A-C1A	-4.00	1.48	1.52
82	WB	402	PEB	C2C-C3C	4.00	1.49	1.38
82	LA	203	PEB	CHA-C1B	4.00	1.49	1.40
82	P7	201	PEB	C2A-C1A	-4.00	1.48	1.52
82	LK	201	PEB	C2A-C1A	-4.00	1.48	1.52
82	H5	202	PEB	C1A-NA	-4.00	1.32	1.37
82	kF	202	PEB	CHB-C1C	4.00	1.49	1.40
82	ZM	202	PEB	CHA-C1B	4.00	1.49	1.40
96	fL	102	HEM	FE-NC	4.00	2.08	1.95
82	iO	203	PEB	CHA-C1B	4.00	1.49	1.40
82	tK	203	PEB	CHB-C1C	3.99	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	M5	305	PEB	C1A-NA	-3.99	1.32	1.37
92	m6	101	LMG	O7-C10	3.99	1.45	1.34
82	gF	201	PEB	CHB-C4B	3.99	1.46	1.38
88	d6	407	LHG	O7-C7	3.99	1.45	1.34
82	SA	201	PEB	C2A-C1A	-3.99	1.48	1.52
82	MJ	201	PEB	C2A-C1A	-3.99	1.48	1.52
82	SP	203	PEB	CHB-C1C	3.99	1.49	1.40
82	WJ	203	PEB	C1A-NA	-3.99	1.32	1.37
88	AL	407	LHG	O7-C7	3.99	1.45	1.34
82	jK	202	PEB	CHA-C1B	3.99	1.49	1.40
84	EO	1001	CYC	C2C-C1C	-3.99	1.48	1.52
84	E4	1001	CYC	C2C-C1C	-3.99	1.48	1.52
82	aJ	202	PEB	C1A-NA	-3.99	1.32	1.37
84	BE	1001	CYC	CHD-C1D	3.99	1.49	1.40
82	PA	201	PEB	C2A-C1A	-3.99	1.48	1.52
82	m1	201	PEB	C1A-NA	-3.99	1.32	1.37
82	fE	203	PEB	CHB-C1C	3.99	1.49	1.40
84	I1	1001	CYC	C1C-NC	-3.99	1.32	1.37
82	TA	201	PEB	CHB-C1C	3.99	1.49	1.40
82	UK	201	PEB	C1A-NA	-3.99	1.32	1.37
82	aO	203	PEB	CHA-C1B	3.99	1.49	1.40
82	nF	201	PEB	CHB-C1C	3.99	1.49	1.40
84	LO	1001	CYC	C2C-C1C	-3.99	1.48	1.52
84	F1	1001	CYC	CHB-C4A	3.99	1.49	1.40
82	L5	201	PEB	C1A-NA	-3.99	1.32	1.37
82	YM	202	PEB	CHA-C1B	3.98	1.49	1.40
82	T4	203	PEB	CHB-C1C	3.98	1.49	1.40
82	R4	203	PEB	CHB-C1C	3.98	1.49	1.40
82	HK	201	PEB	C1A-NA	-3.98	1.32	1.37
82	WJ	203	PEB	C2A-C1A	-3.98	1.48	1.52
82	UP	201	PEB	C1A-NA	-3.98	1.32	1.37
82	aE	201	PEB	C1A-NA	-3.98	1.32	1.37
82	GQ	202	PEB	C2C-C3C	3.98	1.49	1.38
82	CQ	201	PEB	CHB-C4B	3.98	1.46	1.38
87	62	307	CLA	C1D-ND	3.98	1.42	1.37
82	ZG	202	PEB	CHA-C1B	3.98	1.49	1.40
82	IQ	201	PEB	C1A-NA	-3.98	1.32	1.37
82	eB	202	PEB	C1A-NA	-3.98	1.32	1.37
84	LG	1001	CYC	CHD-C1D	3.98	1.49	1.40
82	z8	202	PEB	C2C-C3C	3.98	1.49	1.38
82	RM	201	PEB	C1A-NA	-3.98	1.32	1.37
84	E4	1001	CYC	CHD-C1D	3.98	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	QP	201	PEB	C1A-NA	-3.98	1.32	1.37
82	GF	202	PEB	C1A-NA	-3.98	1.32	1.37
82	cO	202	PEB	CHB-C1C	3.98	1.49	1.40
82	HB	201	PEB	C1A-NA	-3.98	1.32	1.37
82	ED	201	PEB	CHA-C1B	3.98	1.49	1.40
82	A1	305	PEB	C2C-C3C	3.98	1.49	1.38
82	aF	203	PEB	CHA-C1B	3.98	1.49	1.40
82	HK	202	PEB	C1A-NA	-3.98	1.32	1.37
82	DJ	201	PEB	CHA-C1B	3.98	1.49	1.40
82	aK	203	PEB	CHA-C1B	3.98	1.49	1.40
92	JL	102	LMG	O7-C10	3.98	1.45	1.34
82	eJ	202	PEB	CHA-C1B	3.97	1.49	1.40
82	XD	202	PEB	CHB-C1C	3.97	1.49	1.40
82	UJ	201	PEB	C1A-NA	-3.97	1.32	1.37
82	U5	201	PEB	C1A-NA	-3.97	1.32	1.37
82	a4	202	PEB	CHB-C1C	3.97	1.49	1.40
82	IM	202	PEB	CHA-C1B	3.97	1.49	1.40
82	GK	201	PEB	CHB-C1C	3.97	1.49	1.40
82	DB	201	PEB	C2A-C1A	-3.97	1.48	1.52
84	BG	1001	CYC	CHB-C4A	3.97	1.49	1.40
82	S1	201	PEB	CHB-C1C	3.97	1.49	1.40
82	QQ	202	PEB	CHA-C1B	3.97	1.49	1.40
82	PP	201	PEB	C1A-NA	-3.97	1.32	1.37
95	L6	102	DGD	O2G-C1B	3.97	1.45	1.34
82	UM	202	PEB	C1A-NA	-3.97	1.32	1.37
82	YM	202	PEB	C1A-NA	-3.97	1.32	1.37
95	cL	502	DGD	O2G-C1B	3.97	1.45	1.34
82	TA	201	PEB	CHA-C1B	3.97	1.49	1.40
88	I6	101	LHG	O7-C7	3.97	1.45	1.34
82	VD	203	PEB	CHB-C1C	3.97	1.49	1.40
82	G9	202	PEB	CHA-C1B	3.97	1.49	1.40
82	GE	1002	PEB	C1A-NA	-3.97	1.32	1.37
88	B6	617	LHG	O7-C7	3.97	1.45	1.34
82	EJ	202	PEB	C1A-NA	-3.97	1.32	1.37
84	FE	1002	CYC	C1C-NC	-3.97	1.32	1.37
92	qL	301	LMG	O7-C10	3.97	1.45	1.34
84	KG	202	CYC	CHB-C4A	3.97	1.49	1.40
82	ZE	202	PEB	CHA-C1B	3.97	1.49	1.40
82	fG	203	PEB	CHB-C1C	3.97	1.49	1.40
88	D6	406	LHG	O8-C23	3.97	1.44	1.33
82	hH	201	PEB	CHB-C1C	3.97	1.49	1.40
84	IG	1001	CYC	C1C-NC	-3.97	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	D6	401	LHG	O7-C7	3.97	1.45	1.34
82	L7	203	PEB	CHA-C1B	3.97	1.49	1.40
82	LF	202	PEB	C2A-C1A	-3.97	1.48	1.52
82	AG	304	PEB	C1A-NA	-3.97	1.32	1.37
82	GD	202	PEB	C2C-C3C	3.96	1.49	1.38
82	UQ	201	PEB	CHA-C1B	3.96	1.49	1.40
82	xC	201	PEB	CHA-C1B	3.96	1.49	1.40
82	CD	201	PEB	C1A-NA	-3.96	1.32	1.37
95	cL	520	DGD	O2G-C1B	3.96	1.45	1.34
95	b6	622	DGD	O2G-C1B	3.96	1.45	1.34
82	UH	201	PEB	CHB-C1C	3.96	1.49	1.40
82	GJ	201	PEB	C1A-NA	-3.96	1.32	1.37
82	FD	203	PEB	C4B-NB	-3.96	1.30	1.38
82	SF	202	PEB	CHA-C1B	3.96	1.49	1.40
82	lH	202	PEB	CHB-C1C	3.96	1.49	1.40
82	QD	202	PEB	C1A-NA	-3.96	1.32	1.37
82	TG	201	PEB	C1A-NA	-3.96	1.32	1.37
82	IK	203	PEB	CHB-C4B	3.96	1.46	1.38
92	C6	501	LMG	O7-C10	3.96	1.45	1.34
82	KA	201	PEB	C1A-NA	-3.96	1.32	1.37
82	GF	201	PEB	CHB-C1C	3.96	1.49	1.40
84	M1	201	CYC	CHB-C4A	3.96	1.49	1.40
92	J6	102	LMG	O7-C10	3.96	1.45	1.34
82	K7	202	PEB	CHA-C1B	3.96	1.49	1.40
82	wF	303	PEB	CHA-C1B	3.96	1.49	1.40
82	Q9	202	PEB	CHB-C1C	3.96	1.49	1.40
84	JO	1001	CYC	CHD-C1D	3.96	1.49	1.40
84	GG	1001	CYC	CHB-C4A	3.96	1.49	1.40
82	HJ	201	PEB	C1A-NA	-3.96	1.32	1.37
82	IQ	202	PEB	C1A-NA	-3.96	1.32	1.37
82	ID	202	PEB	C1A-NA	-3.96	1.32	1.37
84	L4	1001	CYC	C1C-NC	-3.96	1.32	1.37
82	OJ	203	PEB	C1A-NA	-3.95	1.32	1.37
82	SP	202	PEB	C1A-NA	-3.95	1.32	1.37
82	f1	201	PEB	C1A-NA	-3.95	1.32	1.37
84	G4	1001	CYC	CHA-C4D	3.95	1.49	1.40
82	B7	203	PEB	CHA-C1B	3.95	1.49	1.40
82	BI	203	PEB	CHB-C1C	3.95	1.49	1.40
96	FL	102	HEM	FE-NC	3.95	2.08	1.95
82	dK	201	PEB	CHA-C1B	3.95	1.49	1.40
82	JM	201	PEB	CHA-C1B	3.95	1.49	1.40
82	qK	201	PEB	CHA-C1B	3.95	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	BE	1001	CYC	CHB-C4A	3.95	1.49	1.40
84	DE	1001	CYC	CHB-C1B	3.95	1.47	1.38
82	MJ	201	PEB	C1A-NA	-3.95	1.32	1.37
82	JJ	201	PEB	CHA-C1B	3.95	1.49	1.40
82	R9	202	PEB	CHA-C1B	3.95	1.49	1.40
82	pC	202	PEB	C2C-C3C	3.95	1.49	1.38
84	E1	1001	CYC	CHD-C1D	3.95	1.49	1.40
82	YI	202	PEB	C1A-NA	-3.95	1.32	1.37
82	CQ	202	PEB	CHA-C1B	3.95	1.49	1.40
82	HF	202	PEB	CHA-C1B	3.95	1.49	1.40
82	HK	202	PEB	CHA-C1B	3.95	1.49	1.40
82	gK	201	PEB	CHB-C4B	3.95	1.46	1.38
82	E9	202	PEB	CHA-C1B	3.95	1.49	1.40
82	I9	202	PEB	CHA-C1B	3.95	1.49	1.40
82	h1	202	PEB	CHB-C1C	3.95	1.49	1.40
82	BA	201	PEB	CHA-C1B	3.95	1.49	1.40
84	GO	1001	CYC	CHA-C4D	3.95	1.49	1.40
82	DJ	201	PEB	C1A-NA	-3.95	1.32	1.37
82	tF	202	PEB	CHB-C1C	3.95	1.49	1.40
82	F7	201	PEB	CHA-C1B	3.95	1.49	1.40
87	6N	606	CLA	C1D-ND	3.95	1.42	1.37
82	dF	201	PEB	CHA-C1B	3.95	1.49	1.40
82	TP	202	PEB	CHA-C1B	3.95	1.49	1.40
82	UQ	202	PEB	CHA-C1B	3.95	1.49	1.40
82	RD	203	PEB	CHB-C1C	3.95	1.49	1.40
82	WI	202	PEB	CHB-C4B	3.95	1.46	1.38
82	eH	201	PEB	C1A-NA	-3.95	1.32	1.37
82	SK	202	PEB	CHA-C1B	3.95	1.49	1.40
82	VQ	203	PEB	CHB-C1C	3.95	1.49	1.40
82	N7	203	PEB	CHA-C1B	3.95	1.49	1.40
82	fG	202	PEB	CHA-C1B	3.95	1.49	1.40
82	FJ	201	PEB	CHC-C4C	3.95	1.54	1.49
82	JD	203	PEB	CHB-C1C	3.95	1.49	1.40
82	OG	201	PEB	C1A-NA	-3.95	1.32	1.37
82	HQ	202	PEB	C1A-NA	-3.95	1.32	1.37
82	X9	202	PEB	CHA-C1B	3.95	1.49	1.40
88	dL	408	LHG	O7-C7	3.95	1.45	1.34
82	P9	202	PEB	CHA-C1B	3.95	1.49	1.40
82	iK	201	PEB	CHB-C1C	3.95	1.49	1.40
82	UB	301	PEB	C1A-NA	-3.95	1.32	1.37
82	fH	201	PEB	C1A-NA	-3.95	1.32	1.37
82	hJ	202	PEB	C1A-NA	-3.95	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	NE	201	CYC	CHB-C4A	3.95	1.49	1.40
82	OG	201	PEB	CHA-C1B	3.95	1.49	1.40
82	Y7	303	PEB	C2C-C3C	3.95	1.49	1.38
88	DL	407	LHG	O7-C7	3.95	1.45	1.34
82	OD	202	PEB	CHA-C1B	3.95	1.49	1.40
82	l1	203	PEB	CHB-C1C	3.94	1.49	1.40
82	c4	202	PEB	CHB-C1C	3.94	1.49	1.40
92	mL	101	LMG	O8-C28	3.94	1.44	1.33
82	D5	202	PEB	C1A-NA	-3.94	1.32	1.37
82	K9	202	PEB	CHA-C1B	3.94	1.49	1.40
82	wK	303	PEB	CHA-C1B	3.94	1.49	1.40
82	iJ	202	PEB	CHA-C1B	3.94	1.49	1.40
82	l4	201	PEB	C1A-NA	-3.94	1.32	1.37
82	nK	201	PEB	CHB-C1C	3.94	1.49	1.40
88	dL	405	LHG	O8-C23	3.94	1.44	1.33
82	fK	201	PEB	C2A-C1A	-3.94	1.48	1.52
82	OP	202	PEB	C1A-NA	-3.94	1.32	1.37
82	T7	203	PEB	CHA-C1B	3.94	1.49	1.40
96	vL	201	HEM	C1B-NB	-3.94	1.33	1.40
82	fH	202	PEB	C1A-NA	-3.94	1.32	1.37
82	p8	202	PEB	C2C-C3C	3.94	1.49	1.38
82	T9	202	PEB	CHA-C1B	3.94	1.49	1.40
82	V9	202	PEB	CHA-C1B	3.94	1.49	1.40
82	A9	202	PEB	CHA-C1B	3.94	1.49	1.40
82	IK	201	PEB	C1A-NA	-3.94	1.32	1.37
82	YM	201	PEB	C1A-NA	-3.94	1.32	1.37
82	tK	202	PEB	CHB-C1C	3.94	1.49	1.40
82	S7	201	PEB	C2A-C1A	-3.94	1.48	1.52
84	N1	1001	CYC	C2C-C1C	-3.94	1.48	1.52
82	bB	201	PEB	C1A-NA	-3.94	1.32	1.37
82	FA	201	PEB	CHA-C1B	3.94	1.49	1.40
82	PA	203	PEB	CHA-C1B	3.94	1.49	1.40
95	C6	521	DGD	O2G-C1B	3.94	1.45	1.34
82	m4	201	PEB	CHA-C1B	3.94	1.49	1.40
82	iF	201	PEB	CHB-C1C	3.94	1.49	1.40
82	XF	202	PEB	C1A-NA	-3.94	1.32	1.37
82	XP	202	PEB	CHA-C1B	3.94	1.49	1.40
82	fK	201	PEB	CHA-C1B	3.94	1.49	1.40
82	BB	201	PEB	C1A-NA	-3.94	1.32	1.37
82	OM	201	PEB	C1A-NA	-3.94	1.32	1.37
84	KH	1001	CYC	C1D-C2D	3.94	1.51	1.41
82	Q1	202	PEB	CHA-C1B	3.94	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	XJ	201	PEB	CHA-C1B	3.94	1.49	1.40
82	OM	201	PEB	CHA-C1B	3.94	1.49	1.40
82	gO	203	PEB	CHA-C1B	3.94	1.49	1.40
82	SF	201	PEB	C1A-NA	-3.94	1.32	1.37
82	U5	203	PEB	C1A-NA	-3.94	1.32	1.37
82	YG	202	PEB	CHA-C1B	3.94	1.49	1.40
82	r8	202	PEB	CHA-C1B	3.94	1.49	1.40
92	x6	601	LMG	O7-C10	3.94	1.45	1.34
82	FF	201	PEB	CHA-C1B	3.94	1.49	1.40
82	mH	201	PEB	CHA-C1B	3.94	1.49	1.40
82	B7	201	PEB	CHA-C1B	3.94	1.49	1.40
82	RO	201	PEB	C1A-NA	-3.93	1.32	1.37
82	CQ	201	PEB	C1A-NA	-3.93	1.32	1.37
82	lM	202	PEB	CHA-C1B	3.93	1.49	1.40
84	HG	1001	CYC	CHD-C1D	3.93	1.49	1.40
82	YK	203	PEB	CHB-C1C	3.93	1.49	1.40
82	cB	401	PEB	CHA-C1B	3.93	1.49	1.40
82	HE	1002	PEB	C1A-NA	-3.93	1.32	1.37
84	EE	1001	CYC	C2C-C1C	-3.93	1.48	1.52
82	BI	201	PEB	CHB-C1C	3.93	1.49	1.40
82	N9	202	PEB	CHA-C1B	3.93	1.49	1.40
84	MO	1001	CYC	CHD-C1D	3.93	1.49	1.40
82	H1	1002	PEB	C1A-NA	-3.93	1.32	1.37
82	f4	201	PEB	C1A-NA	-3.93	1.32	1.37
82	MM	202	PEB	C2A-C1A	-3.93	1.48	1.52
82	UD	202	PEB	CHA-C1B	3.93	1.49	1.40
82	LK	201	PEB	CHA-C1B	3.93	1.49	1.40
82	MK	201	PEB	CHA-C1B	3.93	1.49	1.40
82	OI	201	PEB	CHA-C1B	3.93	1.49	1.40
84	K1	1001	CYC	C1D-C2D	3.93	1.51	1.41
82	Z9	301	PEB	CHB-C4B	3.93	1.46	1.38
82	M9	302	PEB	CHB-C4B	3.93	1.46	1.38
82	QE	202	PEB	C1A-NA	-3.93	1.32	1.37
84	LH	1002	CYC	CHD-C1D	3.93	1.49	1.40
82	CD	202	PEB	CHA-C1B	3.93	1.49	1.40
82	hB	301	PEB	CHA-C1B	3.93	1.49	1.40
95	cL	519	DGD	O2G-C1B	3.93	1.45	1.34
82	XA	203	PEB	C1A-NA	-3.93	1.32	1.37
82	iK	203	PEB	C1A-NA	-3.93	1.32	1.37
87	O2	202	CLA	C4B-NB	3.93	1.42	1.37
84	GE	1001	CYC	CHB-C4A	3.93	1.49	1.40
82	gF	201	PEB	C1A-NA	-3.93	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PG	202	PEB	C2C-C3C	3.93	1.49	1.38
82	ZB	201	PEB	CHA-C1B	3.93	1.49	1.40
82	e4	201	PEB	CHA-C1B	3.93	1.49	1.40
82	lF	201	PEB	CHB-C1C	3.93	1.49	1.40
84	LE	1001	CYC	CHD-C1D	3.93	1.49	1.40
82	Q7	201	PEB	CHA-C1B	3.93	1.49	1.40
82	rK	202	PEB	CHA-C1B	3.93	1.49	1.40
82	PE	202	PEB	C2C-C3C	3.93	1.49	1.38
82	EQ	201	PEB	CHA-C1B	3.93	1.49	1.40
82	HF	202	PEB	C1A-NA	-3.92	1.32	1.37
82	L5	203	PEB	CHA-C1B	3.92	1.49	1.40
84	FH	1001	CYC	CHB-C4A	3.92	1.49	1.40
95	C6	523	DGD	O2G-C1B	3.92	1.45	1.34
82	TO	203	PEB	CHB-C1C	3.92	1.49	1.40
87	ON	202	CLA	C4B-NB	3.92	1.42	1.37
82	W5	203	PEB	C1A-NA	-3.92	1.32	1.37
82	PF	202	PEB	C2C-C3C	3.92	1.49	1.38
82	B5	203	PEB	CHA-C1B	3.92	1.49	1.40
82	PF	202	PEB	CHA-C1B	3.92	1.49	1.40
82	mO	201	PEB	CHA-C1B	3.92	1.49	1.40
82	h4	201	PEB	C1A-NA	-3.92	1.32	1.37
82	N7	201	PEB	C1A-NA	-3.92	1.32	1.37
82	RQ	203	PEB	CHB-C1C	3.92	1.49	1.40
82	A1	301	PEB	C2C-C3C	3.92	1.49	1.38
82	QP	201	PEB	CHA-C1B	3.92	1.49	1.40
82	OM	202	PEB	C2C-C3C	3.92	1.49	1.38
82	cF	203	PEB	CHA-C1B	3.92	1.49	1.40
82	AE	304	PEB	C1A-NA	-3.92	1.32	1.37
84	GE	1001	CYC	C1C-NC	-3.92	1.32	1.37
92	j6	101	LMG	O7-C10	3.92	1.45	1.34
82	P7	203	PEB	CHA-C1B	3.92	1.49	1.40
82	cK	203	PEB	CHA-C1B	3.92	1.49	1.40
95	CL	523	DGD	O2G-C1B	3.92	1.45	1.34
84	IG	1001	CYC	CHD-C1D	3.92	1.49	1.40
82	X7	203	PEB	C1A-NA	-3.92	1.32	1.37
82	OK	201	PEB	CHB-C1C	3.92	1.49	1.40
84	K4	1001	CYC	CHD-C1D	3.92	1.49	1.40
87	AN	802	CLA	C1D-ND	3.92	1.42	1.37
84	G4	1001	CYC	C2C-C1C	-3.92	1.48	1.52
84	GG	1001	CYC	C1C-NC	-3.92	1.32	1.37
82	C9	202	PEB	CHA-C1B	3.92	1.49	1.40
84	L1	1001	CYC	CHD-C1D	3.92	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SB	203	PEB	C1A-NA	-3.92	1.32	1.37
82	bF	201	PEB	CHA-C1B	3.92	1.49	1.40
88	M6	101	LHG	O7-C7	3.92	1.45	1.34
82	DK	203	PEB	C1A-NA	-3.91	1.32	1.37
82	KM	203	PEB	C1A-NA	-3.91	1.32	1.37
82	DP	201	PEB	C1A-NA	-3.91	1.32	1.37
82	x8	201	PEB	CHA-C1B	3.91	1.49	1.40
82	18	201	PEB	CHB-C1C	3.91	1.49	1.40
96	V6	201	HEM	FE-NC	3.91	2.08	1.95
82	IF	201	PEB	C1A-NA	-3.91	1.32	1.37
82	AH	301	PEB	C2C-C3C	3.91	1.49	1.38
84	J4	1001	CYC	CHB-C4A	3.91	1.49	1.40
84	LO	1001	CYC	CHB-C4A	3.91	1.49	1.40
82	J9	202	PEB	CHB-C1C	3.91	1.49	1.40
82	QH	202	PEB	CHA-C1B	3.91	1.49	1.40
82	CP	202	PEB	C1A-NA	-3.91	1.32	1.37
84	LH	1001	CYC	C1C-NC	-3.91	1.32	1.37
82	zC	202	PEB	C2C-C3C	3.91	1.49	1.38
82	YE	202	PEB	CHA-C1B	3.91	1.49	1.40
82	QA	201	PEB	CHA-C1B	3.91	1.49	1.40
82	TA	203	PEB	CHA-C1B	3.91	1.49	1.40
82	RE	201	PEB	CHA-C1B	3.91	1.49	1.40
82	B5	201	PEB	CHA-C1B	3.91	1.49	1.40
82	PJ	202	PEB	C1A-NA	-3.91	1.32	1.37
82	RG	201	PEB	CHA-C1B	3.91	1.49	1.40
82	hJ	203	PEB	CHB-C1C	3.91	1.49	1.40
82	VB	202	PEB	C1A-NA	-3.91	1.32	1.37
82	Z5	305	PEB	C1A-NA	-3.91	1.32	1.37
82	RA	201	PEB	CHA-C1B	3.91	1.49	1.40
82	LK	202	PEB	CHA-C1B	3.91	1.49	1.40
82	mK	201	PEB	CHA-C1B	3.91	1.49	1.40
82	YF	203	PEB	CHB-C1C	3.91	1.49	1.40
95	hL	101	DGD	O2G-C1B	3.91	1.45	1.34
82	m1	201	PEB	CHA-C1B	3.91	1.49	1.40
95	c6	618	DGD	O2G-C1B	3.91	1.45	1.34
92	JL	102	LMG	O8-C28	3.91	1.44	1.33
87	7N	609	CLA	C1D-ND	3.91	1.42	1.37
82	a4	201	PEB	C2A-C1A	-3.90	1.48	1.52
82	EM	202	PEB	C1A-NA	-3.90	1.32	1.37
82	fO	201	PEB	C1A-NA	-3.90	1.32	1.37
88	c6	619	LHG	O7-C7	3.90	1.45	1.34
82	AH	305	PEB	C2C-C3C	3.90	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VJ	201	PEB	C1A-NA	-3.90	1.32	1.37
82	lM	201	PEB	CHB-C1C	3.90	1.49	1.40
82	WH	202	PEB	CHA-C1B	3.90	1.49	1.40
82	rC	202	PEB	C2C-C3C	3.90	1.49	1.38
82	b1	202	PEB	CHB-C1C	3.90	1.49	1.40
82	xK	304	PEB	CHB-C1C	3.90	1.49	1.40
82	1C	201	PEB	C2C-C3C	3.90	1.49	1.38
82	DE	1002	PEB	CHB-C1C	3.90	1.49	1.40
82	f1	201	PEB	CHB-C1C	3.90	1.49	1.40
82	bH	202	PEB	CHB-C1C	3.90	1.49	1.40
84	EH	1001	CYC	CHD-C1D	3.90	1.49	1.40
82	OF	201	PEB	CHB-C1C	3.90	1.49	1.40
82	NB	203	PEB	C2A-C1A	-3.90	1.48	1.52
84	LH	1002	CYC	C2C-C1C	-3.90	1.48	1.52
82	EJ	201	PEB	C1A-NA	-3.90	1.32	1.37
82	XQ	202	PEB	CHB-C1C	3.90	1.49	1.40
82	X7	201	PEB	CHB-C1C	3.90	1.49	1.40
82	vF	201	PEB	CHB-C1C	3.90	1.49	1.40
82	OM	203	PEB	C1A-NA	-3.90	1.32	1.37
83	AD	302	PUB	CHB-C4B	3.90	1.49	1.40
82	jK	201	PEB	CHA-C1B	3.90	1.49	1.40
82	P1	202	PEB	C1A-NA	-3.90	1.32	1.37
82	tC	201	PEB	CHB-C1C	3.90	1.49	1.40
82	eE	202	PEB	CHB-C1C	3.90	1.49	1.40
82	SI	201	PEB	C1A-NA	-3.90	1.32	1.37
87	A2	801	CLA	C1D-ND	3.90	1.42	1.37
82	HA	201	PEB	CHB-C1C	3.90	1.49	1.40
82	SP	203	PEB	CHA-C1B	3.90	1.49	1.40
82	nK	202	PEB	CHA-C1B	3.89	1.49	1.40
84	FG	1001	CYC	C1C-NC	-3.89	1.32	1.37
84	F4	1001	CYC	C1C-NC	-3.89	1.32	1.37
82	BA	203	PEB	CHA-C1B	3.89	1.49	1.40
82	KK	202	PEB	CHA-C1B	3.89	1.49	1.40
82	WQ	202	PEB	CHA-C1B	3.89	1.49	1.40
82	g4	203	PEB	CHA-C1B	3.89	1.49	1.40
96	VL	201	HEM	C1B-NB	-3.89	1.33	1.40
84	N1	1001	CYC	C1C-NC	-3.89	1.32	1.37
84	NO	1001	CYC	CHD-C1D	3.89	1.49	1.40
87	5N	607	CLA	C1D-ND	3.89	1.42	1.37
82	ED	202	PEB	CHA-C1B	3.89	1.49	1.40
82	EQ	202	PEB	CHA-C1B	3.89	1.49	1.40
82	l4	202	PEB	CHA-C1B	3.89	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	801	CLA	C4B-NB	3.89	1.42	1.37
82	mG	202	PEB	CHB-C1C	3.89	1.49	1.40
82	OA	202	PEB	C1A-NA	-3.89	1.32	1.37
95	c6	620	DGD	O2G-C1B	3.89	1.45	1.34
82	iJ	201	PEB	CHA-C1B	3.89	1.49	1.40
84	CO	1001	CYC	CHB-C4A	3.89	1.49	1.40
82	Y1	201	PEB	CHA-C1B	3.89	1.49	1.40
87	42	605	CLA	C1D-ND	3.89	1.42	1.37
82	RJ	201	PEB	C1A-NA	-3.89	1.32	1.37
82	JQ	203	PEB	CHB-C1C	3.89	1.49	1.40
82	PK	202	PEB	C2C-C3C	3.89	1.49	1.38
82	YB	201	PEB	C1A-NA	-3.89	1.32	1.37
82	uC	203	PEB	CHB-C1C	3.89	1.49	1.40
82	eG	202	PEB	CHB-C1C	3.89	1.49	1.40
84	BG	1002	CYC	CHD-C1D	3.89	1.49	1.40
92	ML	101	LMG	O8-C28	3.89	1.44	1.33
82	eM	201	PEB	CHA-C1B	3.89	1.49	1.40
87	22	605	CLA	C4D-ND	-3.89	1.32	1.37
84	N4	1001	CYC	CHD-C1D	3.89	1.49	1.40
82	RG	201	PEB	C2A-C1A	-3.89	1.48	1.52
82	kH	203	PEB	CHB-C1C	3.89	1.49	1.40
82	IK	201	PEB	CHA-C1B	3.89	1.49	1.40
82	KF	201	PEB	C1A-NA	-3.89	1.32	1.37
82	PH	202	PEB	C1A-NA	-3.89	1.32	1.37
82	WO	201	PEB	C3B-C2B	3.89	1.45	1.36
82	UD	201	PEB	CHA-C1B	3.89	1.49	1.40
82	RH	202	PEB	CHA-C1B	3.89	1.49	1.40
82	fE	202	PEB	CHA-C1B	3.89	1.49	1.40
82	hJ	201	PEB	CHB-C1C	3.89	1.49	1.40
82	NA	201	PEB	C1A-NA	-3.88	1.32	1.37
82	RB	201	PEB	C1A-NA	-3.88	1.32	1.37
82	ZH	202	PEB	C1A-NA	-3.88	1.32	1.37
82	WI	201	PEB	C1A-NA	-3.88	1.32	1.37
82	QJ	203	PEB	C1A-NA	-3.88	1.32	1.37
87	LN	202	CLA	C1D-ND	3.88	1.42	1.37
82	NA	203	PEB	CHA-C1B	3.88	1.49	1.40
82	MF	201	PEB	CHA-C1B	3.88	1.49	1.40
82	Q9	202	PEB	CHA-C1B	3.88	1.49	1.40
84	JH	1003	CYC	CHB-C4A	3.88	1.49	1.40
82	u8	203	PEB	CHB-C1C	3.88	1.49	1.40
82	KF	202	PEB	CHA-C1B	3.88	1.49	1.40
82	eF	202	PEB	C1A-NA	-3.88	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WB	402	PEB	CHA-C1B	3.88	1.49	1.40
82	q8	202	PEB	CHB-C1C	3.88	1.49	1.40
82	YA	303	PEB	C2C-C3C	3.88	1.49	1.38
95	JL	101	DGD	O2G-C1B	3.88	1.45	1.34
87	2N	302	CLA	C1D-ND	3.88	1.42	1.37
82	V1	202	PEB	CHB-C1C	3.88	1.49	1.40
82	mE	202	PEB	CHB-C1C	3.88	1.49	1.40
82	XJ	202	PEB	CHA-C1B	3.88	1.49	1.40
82	nK	202	PEB	C2C-C3C	3.88	1.49	1.38
87	7N	604	CLA	C1D-ND	3.88	1.42	1.37
82	lK	201	PEB	CHB-C1C	3.88	1.49	1.40
82	A7	201	PEB	CHB-C1C	3.88	1.49	1.40
82	IF	201	PEB	CHA-C1B	3.88	1.49	1.40
82	JI	202	PEB	CHA-C1B	3.88	1.49	1.40
82	fF	201	PEB	CHA-C1B	3.88	1.49	1.40
84	JO	1001	CYC	CHB-C4A	3.88	1.49	1.40
82	18	201	PEB	C2C-C3C	3.88	1.49	1.38
82	EQ	202	PEB	C1A-NA	-3.88	1.32	1.37
82	WG	201	PEB	C2A-C1A	-3.88	1.48	1.52
82	SQ	202	PEB	CHA-C1B	3.88	1.49	1.40
82	UD	202	PEB	C1A-NA	-3.88	1.32	1.37
82	R7	201	PEB	CHA-C1B	3.88	1.49	1.40
87	72	609	CLA	C1D-ND	3.88	1.42	1.37
82	GK	203	PEB	CHA-C1B	3.88	1.49	1.40
82	SK	201	PEB	C1A-NA	-3.88	1.32	1.37
82	F5	201	PEB	C1A-NA	-3.88	1.32	1.37
82	s8	203	PEB	CHB-C1C	3.88	1.49	1.40
82	rK	201	PEB	CHB-C1C	3.88	1.49	1.40
82	SH	203	PEB	CHB-C1C	3.88	1.49	1.40
82	rC	202	PEB	CHA-C1B	3.88	1.49	1.40
82	TD	203	PEB	C2C-C3C	3.87	1.49	1.38
92	B6	622	LMG	O7-C10	3.87	1.45	1.34
96	v6	201	HEM	FE-NC	3.87	2.08	1.95
82	Z1	202	PEB	C1A-NA	-3.87	1.32	1.37
82	MJ	202	PEB	CHA-C1B	3.87	1.49	1.40
82	NM	201	PEB	CHA-C1B	3.87	1.49	1.40
82	TQ	203	PEB	C2C-C3C	3.87	1.49	1.38
82	NM	202	PEB	C1A-NA	-3.87	1.32	1.37
82	QF	201	PEB	C3B-C2B	3.87	1.45	1.36
84	IE	1001	CYC	CHD-C1D	3.87	1.49	1.40
92	D6	407	LMG	O7-C10	3.87	1.45	1.34
84	DG	1001	CYC	CHD-C1D	3.87	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	e1	202	PEB	CHA-C1B	3.87	1.49	1.40
82	OQ	202	PEB	CHA-C1B	3.87	1.49	1.40
82	TM	202	PEB	C2A-C1A	-3.87	1.48	1.52
82	dE	203	PEB	CHA-C1B	3.87	1.49	1.40
82	jF	201	PEB	CHA-C1B	3.87	1.49	1.40
82	R4	201	PEB	C1A-NA	-3.87	1.32	1.37
82	sC	203	PEB	CHB-C1C	3.87	1.49	1.40
92	b6	620	LMG	O7-C10	3.87	1.45	1.34
82	XM	201	PEB	CHA-C1B	3.87	1.49	1.40
82	nF	202	PEB	CHA-C1B	3.87	1.49	1.40
82	HG	1002	PEB	C1A-NA	-3.87	1.32	1.37
82	Q5	203	PEB	C1A-NA	-3.87	1.32	1.37
84	HH	1001	CYC	C2C-C1C	-3.87	1.48	1.52
82	O9	202	PEB	CHB-C4B	3.87	1.46	1.38
82	WD	202	PEB	C1A-NA	-3.87	1.32	1.37
84	MG	1001	CYC	CHD-C1D	3.87	1.49	1.40
82	IQ	201	PEB	C1C-C2C	3.87	1.51	1.42
82	VJ	202	PEB	C1A-NA	-3.87	1.32	1.37
82	JM	202	PEB	C1A-NA	-3.87	1.32	1.37
82	TG	201	PEB	CHA-C1B	3.87	1.49	1.40
82	XF	203	PEB	C2C-C3C	3.87	1.49	1.38
82	eK	201	PEB	CHB-C1C	3.87	1.49	1.40
82	j1	202	PEB	CHB-C1C	3.87	1.49	1.40
82	SB	201	PEB	C1A-NA	-3.87	1.32	1.37
82	QE	202	PEB	CHA-C1B	3.87	1.49	1.40
82	NK	202	PEB	CHA-C1B	3.87	1.49	1.40
82	XQ	201	PEB	CHB-C1C	3.87	1.49	1.40
82	QD	202	PEB	CHA-C1B	3.87	1.49	1.40
82	J9	202	PEB	C1A-NA	-3.87	1.32	1.37
82	tC	202	PEB	C2C-C3C	3.87	1.49	1.38
82	QE	203	PEB	CHA-C1B	3.86	1.49	1.40
82	1C	201	PEB	CHB-C1C	3.86	1.49	1.40
84	C4	1001	CYC	CHB-C4A	3.86	1.49	1.40
82	IF	203	PEB	C2A-C1A	-3.86	1.48	1.52
82	t8	201	PEB	CHB-C1C	3.86	1.49	1.40
87	B6	616	CLA	C1B-C2B	3.86	1.52	1.43
82	l1	202	PEB	CHA-C1B	3.86	1.49	1.40
82	JA	202	PEB	CHB-C1C	3.86	1.49	1.40
82	SD	202	PEB	CHA-C1B	3.86	1.49	1.40
82	QG	202	PEB	CHA-C1B	3.86	1.49	1.40
82	QG	202	PEB	C1A-NA	-3.86	1.32	1.37
82	f1	202	PEB	C1A-NA	-3.86	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	FO	1001	CYC	C1C-NC	-3.86	1.32	1.37
82	wC	203	PEB	CHA-C1B	3.86	1.49	1.40
82	R4	201	PEB	C2A-C1A	-3.86	1.48	1.52
88	C6	522	LHG	O7-C7	3.86	1.45	1.34
87	2N	301	CLA	C4D-ND	-3.86	1.32	1.37
82	O7	201	PEB	CHB-C4B	3.86	1.46	1.38
84	H1	1001	CYC	C2C-C1C	-3.86	1.48	1.52
82	TF	201	PEB	CHA-C1B	3.86	1.49	1.40
82	H5	201	PEB	CHA-C1B	3.86	1.49	1.40
82	J9	201	PEB	CHA-C1B	3.86	1.49	1.40
82	J5	203	PEB	C1A-NA	-3.86	1.32	1.37
82	O5	202	PEB	C1A-NA	-3.86	1.32	1.37
82	vK	201	PEB	CHB-C1C	3.86	1.49	1.40
82	FD	201	PEB	C1A-NA	-3.86	1.32	1.37
82	QD	201	PEB	C2A-C1A	-3.86	1.48	1.52
82	r8	202	PEB	C2C-C3C	3.86	1.49	1.38
82	jG	202	PEB	CHA-C1B	3.86	1.49	1.40
82	OE	201	PEB	CHA-C1B	3.86	1.49	1.40
84	L4	1001	CYC	CHB-C4A	3.86	1.49	1.40
82	K7	201	PEB	C1A-NA	-3.86	1.32	1.37
82	I9	202	PEB	C2C-C3C	3.86	1.49	1.38
82	TQ	202	PEB	CHB-C1C	3.86	1.49	1.40
82	P9	202	PEB	C2C-C3C	3.86	1.49	1.38
87	72	604	CLA	C1D-ND	3.86	1.42	1.37
82	TF	201	PEB	C2A-C1A	-3.86	1.48	1.52
82	fM	203	PEB	CHB-C1C	3.86	1.49	1.40
84	BE	1002	CYC	CHD-C1D	3.85	1.49	1.40
82	HP	201	PEB	C1A-NA	-3.85	1.32	1.37
82	VP	201	PEB	C1A-NA	-3.85	1.32	1.37
82	GF	203	PEB	CHA-C1B	3.85	1.49	1.40
82	PK	202	PEB	CHA-C1B	3.85	1.49	1.40
87	4N	605	CLA	C1D-ND	3.85	1.42	1.37
82	IB	203	PEB	C1A-NA	-3.85	1.32	1.37
82	mM	201	PEB	CHA-C1B	3.85	1.49	1.40
82	eF	201	PEB	CHB-C1C	3.85	1.49	1.40
82	dM	201	PEB	CHB-C1C	3.85	1.49	1.40
82	RO	201	PEB	C2A-C1A	-3.85	1.48	1.52
84	IE	1001	CYC	CHB-C4A	3.85	1.49	1.40
84	CG	1001	CYC	C1C-NC	-3.85	1.32	1.37
87	52	609	CLA	C1D-ND	3.85	1.42	1.37
84	63	901	CYC	CHD-C1D	3.85	1.49	1.40
82	QE	201	PEB	C1A-NA	-3.85	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HI	201	PEB	C1A-NA	-3.85	1.32	1.37
84	EO	1001	CYC	CHB-C4A	3.85	1.49	1.40
82	K9	202	PEB	C2C-C3C	3.85	1.49	1.38
82	l1	201	PEB	CHB-C1C	3.85	1.49	1.40
82	NF	202	PEB	CHA-C1B	3.85	1.49	1.40
82	D1	1002	PEB	CHA-C1B	3.85	1.49	1.40
82	fG	202	PEB	C1A-NA	-3.85	1.32	1.37
82	WD	202	PEB	CHA-C1B	3.85	1.49	1.40
82	rF	202	PEB	CHA-C1B	3.85	1.49	1.40
84	M4	1001	CYC	C2C-C1C	-3.85	1.48	1.52
82	LF	202	PEB	CHA-C1B	3.85	1.49	1.40
82	PO	201	PEB	CHA-C1B	3.85	1.49	1.40
82	JI	202	PEB	C1A-NA	-3.85	1.32	1.37
82	B5	203	PEB	C1A-NA	-3.85	1.32	1.37
82	S5	203	PEB	C1A-NA	-3.85	1.32	1.37
82	aK	202	PEB	C1A-NA	-3.85	1.32	1.37
84	HE	1001	CYC	CHD-C1D	3.85	1.49	1.40
82	IF	201	PEB	C1C-NC	-3.85	1.31	1.37
82	HH	1002	PEB	C1A-NA	-3.85	1.32	1.37
82	O5	201	PEB	C1A-NA	-3.85	1.32	1.37
82	fE	202	PEB	C1A-NA	-3.85	1.32	1.37
84	H1	1001	CYC	CHB-C4A	3.85	1.49	1.40
82	Z4	201	PEB	C3B-C2B	3.85	1.44	1.36
82	EP	201	PEB	C1A-NA	-3.85	1.32	1.37
82	aO	201	PEB	C2A-C1A	-3.85	1.48	1.52
82	W1	203	PEB	C1A-NA	-3.85	1.32	1.37
82	NF	201	PEB	CHA-C1B	3.85	1.49	1.40
82	qF	201	PEB	CHB-C1C	3.85	1.49	1.40
84	EG	1001	CYC	C2C-C1C	-3.85	1.48	1.52
82	SM	202	PEB	CHB-C1C	3.85	1.49	1.40
91	a6	613	PHO	C3A-C2A	-3.84	1.51	1.54
82	R9	202	PEB	C2C-C3C	3.84	1.49	1.38
82	P4	201	PEB	CHA-C1B	3.84	1.49	1.40
82	B9	201	PEB	CHA-C1B	3.84	1.49	1.40
82	T4	202	PEB	CHB-C1C	3.84	1.49	1.40
82	dD	401	PEB	C2A-C1A	-3.84	1.48	1.52
82	ZE	203	PEB	CHA-C1B	3.84	1.49	1.40
84	MG	1001	CYC	CHB-C4A	3.84	1.49	1.40
82	KK	203	PEB	C1A-NA	-3.84	1.32	1.37
84	KG	202	CYC	C1C-NC	-3.84	1.32	1.37
83	AQ	302	PUB	CHB-C4B	3.84	1.49	1.40
84	ME	1001	CYC	CHD-C1D	3.84	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	M4	1001	CYC	CHD-C1D	3.84	1.49	1.40
82	wC	201	PEB	CHB-C1C	3.84	1.49	1.40
82	jH	202	PEB	CHB-C1C	3.84	1.49	1.40
84	KO	1001	CYC	CHD-C1D	3.84	1.49	1.40
82	vF	201	PEB	CHA-C1B	3.84	1.49	1.40
82	qC	202	PEB	CHB-C1C	3.84	1.49	1.40
82	CJ	203	PEB	C1A-NA	-3.84	1.32	1.37
82	fF	201	PEB	C2A-C1A	-3.84	1.48	1.52
82	DG	1002	PEB	CHB-C1C	3.84	1.49	1.40
82	HH	1002	PEB	CHB-C1C	3.84	1.49	1.40
82	B5	202	PEB	CHB-C1C	3.84	1.49	1.40
82	BJ	301	PEB	C1A-NA	-3.84	1.32	1.37
82	KK	201	PEB	C1A-NA	-3.84	1.32	1.37
82	YP	501	PEB	CHA-C1B	3.84	1.49	1.40
82	OA	201	PEB	CHB-C4B	3.84	1.46	1.38
87	82	305	CLA	C1D-ND	3.84	1.42	1.37
87	1N	602	CLA	C1D-ND	3.84	1.42	1.37
82	GK	202	PEB	C1A-NA	-3.84	1.32	1.37
82	E9	202	PEB	C2C-C3C	3.84	1.49	1.38
82	GG	1002	PEB	C2A-C1A	-3.84	1.48	1.52
82	cE	202	PEB	C1A-NA	-3.84	1.32	1.37
87	2N	308	CLA	C1D-ND	3.84	1.42	1.37
82	Q1	202	PEB	CHB-C1C	3.84	1.49	1.40
82	VG	202	PEB	CHA-C1B	3.84	1.49	1.40
82	XK	203	PEB	CHA-C1B	3.84	1.49	1.40
82	UG	203	PEB	C1A-NA	-3.84	1.32	1.37
82	RK	201	PEB	CHB-C1C	3.84	1.49	1.40
82	AQ	304	PEB	C2C-C3C	3.84	1.49	1.38
82	HQ	202	PEB	CHB-C1C	3.84	1.49	1.40
84	CH	1001	CYC	C1D-C2D	3.84	1.50	1.41
84	C1	1001	CYC	C1D-C2D	3.84	1.50	1.41
82	A9	202	PEB	C2C-C3C	3.84	1.49	1.38
82	N9	202	PEB	C2C-C3C	3.84	1.49	1.38
82	t8	202	PEB	CHA-C1B	3.84	1.49	1.40
92	B6	619	LMG	O7-C10	3.84	1.45	1.34
82	UE	203	PEB	C1A-NA	-3.84	1.32	1.37
82	XD	201	PEB	CHB-C1C	3.84	1.49	1.40
87	L2	202	CLA	C1D-ND	3.84	1.42	1.37
82	NK	201	PEB	CHA-C1B	3.83	1.49	1.40
82	dG	203	PEB	CHA-C1B	3.83	1.49	1.40
82	QH	202	PEB	CHB-C1C	3.83	1.49	1.40
82	GJ	201	PEB	C2A-C1A	-3.83	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B9	202	PEB	C1A-NA	-3.83	1.32	1.37
82	1C	201	PEB	C1A-NA	-3.83	1.32	1.37
82	CM	201	PEB	CHA-C1B	3.83	1.49	1.40
84	I1	1001	CYC	C1D-C2D	3.83	1.50	1.41
82	GF	203	PEB	C2A-C1A	-3.83	1.48	1.52
82	FJ	201	PEB	C1A-NA	-3.83	1.32	1.37
82	XA	203	PEB	CHA-C1B	3.83	1.49	1.40
82	JK	202	PEB	CHA-C1B	3.83	1.49	1.40
82	t8	202	PEB	C2C-C3C	3.83	1.49	1.38
82	CQ	202	PEB	C1A-NA	-3.83	1.32	1.37
88	BL	610	LHG	O7-C7	3.83	1.45	1.34
87	8N	306	CLA	C1D-ND	3.83	1.42	1.37
82	dK	202	PEB	C2A-C1A	-3.83	1.48	1.52
87	BN	802	CLA	C4B-NB	3.83	1.42	1.37
82	V9	202	PEB	C2C-C3C	3.83	1.49	1.38
82	U9	201	PEB	C1A-NA	-3.83	1.32	1.37
82	m1	202	PEB	CHB-C1C	3.83	1.49	1.40
82	fH	201	PEB	CHB-C1C	3.83	1.49	1.40
88	D6	406	LHG	O7-C7	3.83	1.45	1.34
82	xF	302	PEB	C2C-C3C	3.83	1.49	1.38
82	ID	201	PEB	C1C-C2C	3.83	1.51	1.42
82	FM	202	PEB	C1A-NA	-3.83	1.32	1.37
84	NE	201	CYC	C1C-NC	-3.83	1.32	1.37
82	VA	203	PEB	CHB-C1C	3.83	1.49	1.40
82	ZG	202	PEB	C2A-C1A	-3.83	1.48	1.52
82	IK	203	PEB	C2A-C1A	-3.83	1.48	1.52
82	s8	202	PEB	CHA-C1B	3.83	1.49	1.40
82	J9	201	PEB	C1A-NA	-3.83	1.32	1.37
82	zC	202	PEB	C1A-NA	-3.83	1.32	1.37
82	vK	202	PEB	C1A-NA	-3.83	1.32	1.37
82	fK	201	PEB	CHB-C1C	3.83	1.49	1.40
82	ZE	202	PEB	C1A-NA	-3.83	1.32	1.37
82	QG	201	PEB	C1A-NA	-3.83	1.32	1.37
82	ID	201	PEB	C2C-C3C	3.83	1.49	1.38
82	J7	202	PEB	CHB-C1C	3.83	1.49	1.40
82	IP	202	PEB	CHA-C1B	3.83	1.49	1.40
91	aL	610	PHO	O2A-CGA	3.83	1.44	1.33
82	JJ	201	PEB	C1A-NA	-3.83	1.32	1.37
82	a4	201	PEB	C1A-NA	-3.83	1.32	1.37
84	H4	1001	CYC	CHB-C4A	3.83	1.49	1.40
82	nF	202	PEB	C2C-C3C	3.83	1.49	1.38
84	NH	1001	CYC	CHA-C4D	3.83	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	12	602	CLA	C1D-ND	3.83	1.42	1.37
82	Y5	202	PEB	C1A-NA	-3.83	1.32	1.37
82	T1	201	PEB	CHA-C1B	3.83	1.49	1.40
82	JK	201	PEB	CHB-C1C	3.83	1.49	1.40
84	DE	1001	CYC	CHD-C1D	3.83	1.49	1.40
87	A2	816	CLA	C1D-ND	3.83	1.42	1.37
82	mG	201	PEB	CHA-C1B	3.83	1.49	1.40
82	HD	202	PEB	CHB-C1C	3.83	1.49	1.40
82	G9	202	PEB	C2C-C3C	3.83	1.49	1.38
82	AD	303	PEB	CHA-C1B	3.83	1.49	1.40
82	FK	201	PEB	CHA-C1B	3.83	1.49	1.40
82	LM	202	PEB	C1A-NA	-3.83	1.32	1.37
82	MM	201	PEB	C1A-NA	-3.83	1.32	1.37
84	CO	1001	CYC	C1C-NC	-3.83	1.32	1.37
82	YH	201	PEB	CHA-C1B	3.82	1.49	1.40
82	a4	203	PEB	CHB-C1C	3.82	1.49	1.40
82	dE	204	PEB	CHB-C1C	3.82	1.49	1.40
82	HM	201	PEB	C1A-NA	-3.82	1.32	1.37
82	JP	202	PEB	C1A-NA	-3.82	1.32	1.37
82	TK	201	PEB	CHA-C1B	3.82	1.49	1.40
82	TD	202	PEB	CHB-C1C	3.82	1.49	1.40
82	YK	202	PEB	CHB-C1C	3.82	1.49	1.40
82	w8	201	PEB	CHB-C1C	3.82	1.49	1.40
82	II	203	PEB	CHB-C4B	3.82	1.46	1.38
82	R1	202	PEB	CHA-C1B	3.82	1.49	1.40
91	AL	410	PHO	O2A-CGA	3.82	1.44	1.33
82	HF	201	PEB	C1A-NA	-3.82	1.32	1.37
82	C9	202	PEB	C2C-C3C	3.82	1.49	1.38
82	KD	202	PEB	CHA-C1B	3.82	1.49	1.40
82	fB	301	PEB	CHA-C1B	3.82	1.49	1.40
82	mH	202	PEB	CHB-C1C	3.82	1.49	1.40
82	Y9	201	PEB	C1A-NA	-3.82	1.32	1.37
87	22	608	CLA	C1D-ND	3.82	1.42	1.37
82	TK	201	PEB	C2A-C1A	-3.82	1.48	1.52
82	TE	201	PEB	CHA-C1B	3.82	1.49	1.40
82	XA	201	PEB	CHB-C1C	3.82	1.49	1.40
83	AE	302	PUB	CHB-C4B	3.82	1.49	1.40
82	iF	202	PEB	C1A-NA	-3.82	1.32	1.37
82	NB	201	PEB	CHA-C1B	3.82	1.49	1.40
82	RE	202	PEB	CHA-C1B	3.82	1.49	1.40
82	dJ	201	PEB	CHB-C1C	3.82	1.49	1.40
82	HD	202	PEB	C1A-NA	-3.82	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AD	304	PEB	C2C-C3C	3.82	1.49	1.38
87	5N	609	CLA	C1D-ND	3.82	1.42	1.37
82	O9	202	PEB	CHC-C4C	3.82	1.54	1.49
82	T9	202	PEB	C2C-C3C	3.82	1.49	1.38
82	ZE	202	PEB	C2A-C1A	-3.82	1.48	1.52
82	GK	203	PEB	C2A-C1A	-3.82	1.48	1.52
82	XA	201	PEB	C1A-NA	-3.82	1.32	1.37
82	cG	201	PEB	CHA-C1B	3.82	1.49	1.40
82	aB	201	PEB	C1A-NA	-3.82	1.32	1.37
82	QO	201	PEB	C3B-C2B	3.82	1.44	1.36
82	PF	202	PEB	C1A-NA	-3.82	1.32	1.37
82	H9	202	PEB	C1A-NA	-3.82	1.32	1.37
82	aF	202	PEB	C1A-NA	-3.82	1.32	1.37
84	KO	1001	CYC	CHB-C4A	3.82	1.49	1.40
82	H7	201	PEB	CHB-C1C	3.82	1.49	1.40
82	VB	201	PEB	CHA-C1B	3.82	1.49	1.40
82	ZJ	201	PEB	C2A-C1A	-3.82	1.48	1.52
87	FN	201	CLA	C1D-ND	3.82	1.42	1.37
82	xC	201	PEB	C2C-C3C	3.82	1.49	1.38
82	TO	202	PEB	CHB-C1C	3.82	1.49	1.40
82	KB	301	PEB	C1A-NA	-3.82	1.32	1.37
82	ED	202	PEB	C1A-NA	-3.82	1.32	1.37
82	xC	201	PEB	CHB-C1C	3.82	1.49	1.40
82	AQ	303	PEB	CHA-C1B	3.82	1.49	1.40
82	kF	203	PEB	CHB-C1C	3.82	1.49	1.40
84	DH	1003	CYC	CHD-C1D	3.82	1.49	1.40
82	m4	202	PEB	C1A-NA	-3.82	1.32	1.37
82	mO	202	PEB	C1A-NA	-3.82	1.32	1.37
82	kE	201	PEB	CHA-C1B	3.82	1.49	1.40
82	x8	201	PEB	C2C-C3C	3.82	1.49	1.38
82	eH	202	PEB	CHA-C1B	3.82	1.49	1.40
84	NH	1001	CYC	C1C-NC	-3.82	1.32	1.37
82	zC	201	PEB	CHA-C1B	3.82	1.49	1.40
82	tC	202	PEB	CHA-C1B	3.81	1.49	1.40
87	62	311	CLA	C1D-ND	3.81	1.42	1.37
82	QK	202	PEB	CHB-C1C	3.81	1.49	1.40
82	AP	201	PEB	C2A-C1A	-3.81	1.48	1.52
82	ZJ	201	PEB	CHA-C1B	3.81	1.49	1.40
82	KQ	202	PEB	CHA-C1B	3.81	1.49	1.40
82	nK	201	PEB	CHA-C1B	3.81	1.49	1.40
82	TO	202	PEB	C1A-NA	-3.81	1.32	1.37
82	U9	204	PEB	C2C-C3C	3.81	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jE	201	PEB	CHB-C1C	3.81	1.49	1.40
82	GD	201	PEB	CHA-C1B	3.81	1.49	1.40
82	X7	203	PEB	CHA-C1B	3.81	1.49	1.40
82	rF	201	PEB	CHB-C1C	3.81	1.49	1.40
82	hM	201	PEB	CHB-C1C	3.81	1.49	1.40
82	aO	203	PEB	CHB-C1C	3.81	1.49	1.40
82	Y9	202	PEB	C1A-NA	-3.81	1.32	1.37
82	aO	201	PEB	C1A-NA	-3.81	1.32	1.37
82	WD	201	PEB	CHA-C1B	3.81	1.49	1.40
95	DL	408	DGD	O2G-C1B	3.81	1.45	1.34
82	lH	201	PEB	CHA-C1B	3.81	1.49	1.40
82	LF	202	PEB	C1A-NA	-3.81	1.32	1.37
82	mF	202	PEB	CHA-C1B	3.81	1.49	1.40
87	6N	610	CLA	C1D-ND	3.81	1.42	1.37
82	H7	203	PEB	C1A-NA	-3.81	1.32	1.37
82	X9	202	PEB	C2C-C3C	3.81	1.49	1.38
82	uC	203	PEB	CHA-C1B	3.81	1.49	1.40
82	HB	202	PEB	C1A-NA	-3.81	1.32	1.37
82	tF	201	PEB	CHB-C1C	3.81	1.49	1.40
82	NA	203	PEB	C1A-NA	-3.81	1.32	1.37
88	BL	615	LHG	O7-C7	3.81	1.45	1.34
84	IO	1001	CYC	CHB-C4A	3.81	1.49	1.40
82	XK	203	PEB	C2C-C3C	3.81	1.49	1.38
82	IK	201	PEB	C1C-NC	-3.81	1.31	1.37
82	Y7	303	PEB	CHA-C1B	3.81	1.49	1.40
82	QB	204	PEB	C1A-NA	-3.81	1.32	1.37
82	SE	201	PEB	C1A-NA	-3.81	1.32	1.37
82	LK	202	PEB	C1A-NA	-3.81	1.32	1.37
82	AA	201	PEB	CHB-C1C	3.81	1.49	1.40
82	HE	1002	PEB	CHB-C1C	3.81	1.49	1.40
82	FP	201	PEB	CHB-C1C	3.81	1.49	1.40
82	CJ	201	PEB	C1A-NA	-3.81	1.32	1.37
82	eE	201	PEB	C1A-NA	-3.81	1.32	1.37
87	52	607	CLA	C1D-ND	3.81	1.42	1.37
82	Y9	202	PEB	CHB-C1C	3.81	1.49	1.40
82	J7	201	PEB	CHA-C1B	3.81	1.49	1.40
82	vK	202	PEB	CHA-C1B	3.81	1.49	1.40
82	cK	203	PEB	CHB-C1C	3.81	1.49	1.40
87	AN	820	CLA	C1D-ND	3.81	1.42	1.37
82	w8	203	PEB	CHA-C1B	3.81	1.49	1.40
82	jE	202	PEB	CHA-C1B	3.81	1.49	1.40
91	A6	407	PHO	C3A-C2A	-3.81	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	lO	202	PEB	CHA-C1B	3.81	1.49	1.40
82	LJ	201	PEB	C1A-NA	-3.80	1.32	1.37
82	JF	202	PEB	CHA-C1B	3.80	1.49	1.40
82	FB	201	PEB	CHB-C1C	3.80	1.49	1.40
82	cO	203	PEB	CHA-C1B	3.80	1.49	1.40
82	NB	201	PEB	C2A-C1A	-3.80	1.48	1.52
82	LK	202	PEB	C2A-C1A	-3.80	1.48	1.52
83	QJ	201	PUB	C3B-C2B	3.80	1.49	1.38
83	ND	201	PUB	C3B-C2B	3.80	1.49	1.38
83	NQ	201	PUB	C3B-C2B	3.80	1.49	1.38
87	AN	834	CLA	C1D-ND	3.80	1.42	1.37
82	YG	202	PEB	C2C-C3C	3.80	1.49	1.38
83	AG	302	PUB	CHB-C4B	3.80	1.49	1.40
82	kG	201	PEB	CHA-C1B	3.80	1.49	1.40
82	hK	202	PEB	CHA-C1B	3.80	1.49	1.40
82	eO	203	PEB	CHA-C1B	3.80	1.49	1.40
87	22	601	CLA	C1D-ND	3.80	1.42	1.37
82	VE	202	PEB	CHA-C1B	3.80	1.49	1.40
82	MF	203	PEB	CHB-C1C	3.80	1.49	1.40
82	XB	201	PEB	C1A-NA	-3.80	1.32	1.37
82	GD	201	PEB	C1A-NA	-3.80	1.32	1.37
82	Y5	201	PEB	C1A-NA	-3.80	1.32	1.37
82	eB	202	PEB	CHA-C1B	3.80	1.49	1.40
84	ME	1001	CYC	CHB-C4A	3.80	1.49	1.40
82	OI	201	PEB	CHB-C1C	3.80	1.49	1.40
82	R4	203	PEB	CHA-C1B	3.80	1.49	1.40
82	RO	201	PEB	CHA-C1B	3.80	1.49	1.40
84	HO	1001	CYC	CHB-C4A	3.80	1.49	1.40
82	JB	201	PEB	C1B-C2B	3.80	1.54	1.45
82	GJ	203	PEB	C1A-NA	-3.80	1.32	1.37
95	J6	101	DGD	O2G-C1B	3.80	1.45	1.34
82	V4	201	PEB	CHA-C1B	3.80	1.49	1.40
82	S5	203	PEB	CHA-C1B	3.80	1.49	1.40
82	gB	201	PEB	CHA-C1B	3.80	1.49	1.40
82	FA	203	PEB	C1A-NA	-3.80	1.32	1.37
82	WG	203	PEB	C1A-NA	-3.80	1.32	1.37
82	t8	201	PEB	C2C-C3C	3.80	1.49	1.38
87	F2	202	CLA	C1D-ND	3.80	1.42	1.37
82	18	201	PEB	C1A-NA	-3.80	1.32	1.37
82	iH	201	PEB	C1A-NA	-3.80	1.32	1.37
82	W1	202	PEB	CHA-C1B	3.80	1.49	1.40
84	K4	1001	CYC	CHB-C4A	3.80	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ZB	201	PEB	C1A-NA	-3.80	1.32	1.37
82	WI	203	PEB	C1A-NA	-3.80	1.32	1.37
82	DJ	202	PEB	C1A-NA	-3.80	1.32	1.37
82	YP	503	PEB	C1A-NA	-3.80	1.32	1.37
82	iJ	201	PEB	C1A-NA	-3.80	1.32	1.37
84	DH	1003	CYC	C1C-NC	-3.80	1.32	1.37
82	m4	203	PEB	CHA-C1B	3.80	1.49	1.40
82	R4	201	PEB	CHA-C1B	3.80	1.49	1.40
87	B2	824	CLA	C1D-ND	3.80	1.42	1.37
82	eA	301	PEB	CHA-C1B	3.79	1.49	1.40
91	dL	403	PHO	O2A-CGA	3.79	1.44	1.33
82	Q4	201	PEB	C3B-C2B	3.79	1.44	1.36
82	WQ	201	PEB	CHA-C1B	3.79	1.49	1.40
82	kK	202	PEB	CHA-C1B	3.79	1.49	1.40
82	TE	201	PEB	C2A-C1A	-3.79	1.48	1.52
82	YF	203	PEB	C2A-C1A	-3.79	1.48	1.52
82	H1	1002	PEB	CHB-C1C	3.79	1.49	1.40
82	IQ	201	PEB	C2C-C3C	3.79	1.49	1.38
82	MQ	201	PEB	CHA-C1B	3.79	1.49	1.40
82	sC	202	PEB	CHA-C1B	3.79	1.49	1.40
82	lF	202	PEB	CHA-C1B	3.79	1.49	1.40
82	jJ	201	PEB	C1A-NA	-3.79	1.32	1.37
87	62	301	CLA	C1D-ND	3.79	1.42	1.37
82	mE	201	PEB	CHA-C1B	3.79	1.49	1.40
84	LH	1001	CYC	CHB-C4A	3.79	1.49	1.40
82	HA	201	PEB	CHA-C1B	3.79	1.49	1.40
82	BQ	201	PEB	C1A-NA	-3.79	1.32	1.37
87	RN	202	CLA	C1D-ND	3.79	1.42	1.37
82	YA	304	PEB	C2C-C3C	3.79	1.49	1.38
82	HG	1002	PEB	CHB-C1C	3.79	1.49	1.40
82	JI	201	PEB	CHA-C1B	3.79	1.49	1.40
82	iG	202	PEB	CHA-C1B	3.79	1.49	1.40
84	E4	1001	CYC	CHB-C4A	3.79	1.49	1.40
82	FJ	202	PEB	C2A-C1A	-3.79	1.48	1.52
87	7N	603	CLA	C1D-ND	3.79	1.42	1.37
82	GB	201	PEB	CHA-C1B	3.79	1.49	1.40
82	RK	202	PEB	C1A-NA	-3.79	1.32	1.37
82	TP	201	PEB	C1A-NA	-3.79	1.32	1.37
87	72	603	CLA	C1D-ND	3.79	1.42	1.37
82	FP	201	PEB	CHA-C1B	3.79	1.49	1.40
84	DH	1001	CYC	CHA-C4D	3.79	1.49	1.40
84	NH	1001	CYC	C2C-C1C	-3.79	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	xK	302	PEB	C2C-C3C	3.79	1.49	1.38
84	LH	1001	CYC	C1D-C2D	3.79	1.50	1.41
82	T4	202	PEB	C1A-NA	-3.79	1.32	1.37
82	sK	203	PEB	C1A-NA	-3.79	1.32	1.37
95	D6	410	DGD	O2G-C1B	3.79	1.45	1.34
82	DB	201	PEB	CHA-C1B	3.79	1.49	1.40
82	FJ	201	PEB	CHA-C1B	3.79	1.49	1.40
82	FA	202	PEB	CHB-C1C	3.79	1.49	1.40
84	FG	1001	CYC	C1D-C2D	3.79	1.50	1.41
82	KB	302	PEB	C1A-NA	-3.79	1.32	1.37
82	XJ	201	PEB	C1A-NA	-3.79	1.32	1.37
82	RO	203	PEB	CHA-C1B	3.79	1.49	1.40
82	JF	201	PEB	CHB-C1C	3.79	1.49	1.40
82	V7	203	PEB	CHB-C1C	3.79	1.49	1.40
84	E4	1001	CYC	C1C-NC	-3.79	1.32	1.37
82	AK	202	PEB	CHB-C1C	3.79	1.49	1.40
82	bH	201	PEB	CHB-C1C	3.79	1.49	1.40
82	WH	202	PEB	C2C-C3C	3.79	1.49	1.38
82	gB	202	PEB	CHA-C1B	3.79	1.49	1.40
82	XD	203	PEB	CHA-C1B	3.79	1.49	1.40
82	XF	203	PEB	CHA-C1B	3.79	1.49	1.40
87	32	304	CLA	C4B-NB	3.79	1.42	1.37
82	tC	201	PEB	C2C-C3C	3.79	1.49	1.38
82	UB	302	PEB	OD-C4D	3.79	1.30	1.23
82	W9	201	PEB	CHA-C1B	3.79	1.49	1.40
82	TB	201	PEB	C1B-C2B	3.79	1.54	1.45
87	1N	606	CLA	C1D-ND	3.79	1.42	1.37
84	IG	1001	CYC	CHB-C4A	3.79	1.49	1.40
82	cE	201	PEB	CHA-C1B	3.79	1.49	1.40
84	MO	1001	CYC	C2C-C1C	-3.78	1.48	1.52
87	62	306	CLA	C1D-ND	3.78	1.42	1.37
87	72	610	CLA	C1D-ND	3.78	1.42	1.37
82	mK	202	PEB	CHA-C1B	3.78	1.49	1.40
82	YB	201	PEB	CHA-C1B	3.78	1.49	1.40
87	A2	827	CLA	C4D-ND	-3.78	1.32	1.37
82	fF	201	PEB	CHB-C1C	3.78	1.49	1.40
87	BN	825	CLA	C1D-ND	3.78	1.42	1.37
87	3N	305	CLA	C4B-NB	3.78	1.42	1.37
82	A1	302	PEB	CHA-C1B	3.78	1.49	1.40
83	AM	303	PUB	OD-C4D	3.78	1.30	1.23
82	ZK	202	PEB	C2C-C3C	3.78	1.48	1.38
82	YJ	201	PEB	C1A-NA	-3.78	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CM	203	PEB	C1A-NA	-3.78	1.32	1.37
82	DQ	201	PEB	C1A-NA	-3.78	1.32	1.37
82	F7	203	PEB	C1A-NA	-3.78	1.32	1.37
84	GO	1001	CYC	CHB-C4A	3.78	1.49	1.40
103	82	310	ZEX	C5-C6	-3.78	1.27	1.34
82	F7	202	PEB	CHB-C1C	3.78	1.49	1.40
82	fB	301	PEB	CHB-C1C	3.78	1.49	1.40
82	GK	203	PEB	C1A-NA	-3.78	1.32	1.37
84	FE	1002	CYC	C1D-C2D	3.78	1.50	1.41
82	cB	403	PEB	CHA-C1B	3.78	1.49	1.40
87	A2	834	CLA	C1D-ND	3.78	1.42	1.37
82	b4	201	PEB	C1A-NA	-3.78	1.32	1.37
82	xF	304	PEB	CHB-C1C	3.78	1.49	1.40
82	D5	203	PEB	CHA-C1B	3.78	1.49	1.40
82	J5	203	PEB	CHA-C1B	3.78	1.49	1.40
82	L5	202	PEB	C1A-NA	-3.78	1.32	1.37
82	uK	202	PEB	C2C-C3C	3.78	1.48	1.38
82	BD	203	PEB	C1A-NA	-3.78	1.32	1.37
82	GF	202	PEB	C4A-NA	-3.78	1.29	1.37
82	VK	201	PEB	CHB-C1C	3.78	1.49	1.40
82	M9	304	PEB	CHA-C1B	3.78	1.49	1.40
84	I4	1001	CYC	CHB-C4A	3.78	1.49	1.40
87	c6	614	CLA	C1D-ND	3.78	1.42	1.37
87	6N	605	CLA	C1D-ND	3.78	1.42	1.37
82	YF	202	PEB	CHB-C1C	3.78	1.49	1.40
82	NK	202	PEB	C1A-NA	-3.78	1.32	1.37
82	hB	301	PEB	CHB-C1C	3.78	1.49	1.40
88	CL	522	LHG	O7-C7	3.78	1.45	1.34
82	vK	201	PEB	CHA-C1B	3.78	1.49	1.40
82	MD	201	PEB	CHA-C1B	3.78	1.49	1.40
87	7N	610	CLA	C1D-ND	3.77	1.42	1.37
82	u8	203	PEB	CHA-C1B	3.77	1.49	1.40
82	QJ	202	PEB	C1A-NA	-3.77	1.32	1.37
82	tC	202	PEB	C1A-NA	-3.77	1.32	1.37
82	mO	203	PEB	CHA-C1B	3.77	1.49	1.40
82	r8	201	PEB	C2C-C3C	3.77	1.48	1.38
82	S5	202	PEB	C1A-NA	-3.77	1.32	1.37
82	YA	303	PEB	CHA-C1B	3.77	1.49	1.40
87	52	605	CLA	C1D-ND	3.77	1.42	1.37
82	U1	201	PEB	CHA-C1B	3.77	1.49	1.40
82	EB	501	PEB	C1A-NA	-3.77	1.32	1.37
82	AH	301	PEB	CHA-C1B	3.77	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	tK	201	PEB	CHB-C1C	3.77	1.49	1.40
82	z8	202	PEB	CHA-C1B	3.77	1.49	1.40
82	bP	501	PEB	C1A-NA	-3.77	1.32	1.37
82	Z9	304	PEB	CHA-C1B	3.77	1.49	1.40
82	BD	202	PEB	C1A-NA	-3.77	1.32	1.37
82	RE	202	PEB	C1A-NA	-3.77	1.32	1.37
82	WH	203	PEB	C1A-NA	-3.77	1.32	1.37
82	ZE	203	PEB	C1A-NA	-3.77	1.32	1.37
82	eG	201	PEB	C1A-NA	-3.77	1.32	1.37
82	RF	201	PEB	CHB-C1C	3.77	1.49	1.40
82	w8	203	PEB	CHB-C1C	3.77	1.49	1.40
82	DH	1002	PEB	CHA-C1B	3.77	1.49	1.40
82	OI	203	PEB	CHA-C1B	3.77	1.49	1.40
82	NP	201	PEB	C1A-NA	-3.77	1.32	1.37
82	UM	201	PEB	CHB-C1C	3.77	1.49	1.40
82	VO	201	PEB	CHA-C1B	3.77	1.49	1.40
82	F7	203	PEB	CHB-C1C	3.77	1.49	1.40
82	U9	203	PEB	CHB-C1C	3.77	1.49	1.40
82	SB	202	PEB	C1A-NA	-3.77	1.32	1.37
82	RG	202	PEB	C1A-NA	-3.77	1.32	1.37
82	VQ	202	PEB	C1A-NA	-3.77	1.32	1.37
82	hF	202	PEB	CHA-C1B	3.77	1.49	1.40
82	b1	203	PEB	CHB-C1C	3.77	1.49	1.40
82	JM	201	PEB	C1A-NA	-3.77	1.32	1.37
84	DH	1001	CYC	CHB-C4A	3.77	1.49	1.40
95	AL	414	DGD	O2G-C1B	3.77	1.44	1.34
82	EP	201	PEB	CHA-C1B	3.77	1.49	1.40
82	c4	203	PEB	CHA-C1B	3.77	1.49	1.40
82	eB	201	PEB	CHA-C1B	3.77	1.49	1.40
82	FI	201	PEB	C1A-NA	-3.77	1.32	1.37
82	cG	202	PEB	C1A-NA	-3.77	1.32	1.37
82	cJ	201	PEB	C1A-NA	-3.77	1.32	1.37
82	x8	201	PEB	CHB-C1C	3.77	1.49	1.40
82	jJ	203	PEB	CHB-C1C	3.77	1.49	1.40
82	gJ	201	PEB	CHA-C1B	3.77	1.49	1.40
82	CJ	201	PEB	C2A-C1A	-3.77	1.48	1.52
88	cL	501	LHG	O7-C7	3.77	1.44	1.34
82	BQ	202	PEB	C1A-NA	-3.77	1.32	1.37
82	mO	203	PEB	CHB-C1C	3.76	1.49	1.40
82	RG	202	PEB	CHA-C1B	3.76	1.49	1.40
82	W9	201	PEB	C1A-NA	-3.76	1.32	1.37
82	b1	201	PEB	CHB-C1C	3.76	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	FE	1001	CYC	C1C-NC	-3.76	1.32	1.37
82	ZO	201	PEB	C3B-C2B	3.76	1.44	1.36
82	FD	201	PEB	C2A-C1A	-3.76	1.48	1.52
82	UM	202	PEB	C2A-C1A	-3.76	1.48	1.52
82	lG	201	PEB	CHB-C1C	3.76	1.49	1.40
82	GQ	201	PEB	CHA-C1B	3.76	1.49	1.40
82	nF	201	PEB	CHA-C1B	3.76	1.49	1.40
82	TE	201	PEB	C1A-NA	-3.76	1.32	1.37
84	D1	1003	CYC	CHD-C1D	3.76	1.49	1.40
82	lO	202	PEB	CHB-C1C	3.76	1.49	1.40
82	XM	202	PEB	C1A-NA	-3.76	1.32	1.37
82	BI	203	PEB	CHA-C1B	3.76	1.49	1.40
82	xC	202	PEB	CHA-C1B	3.76	1.49	1.40
82	YM	202	PEB	C2A-C1A	-3.76	1.48	1.52
82	eG	203	PEB	CHB-C1C	3.76	1.49	1.40
82	OP	203	PEB	CHB-C4B	3.76	1.46	1.38
84	G4	1001	CYC	CHB-C4A	3.76	1.49	1.40
82	VD	202	PEB	CHB-C1C	3.76	1.49	1.40
82	SF	203	PEB	CHA-C1B	3.76	1.49	1.40
82	VE	202	PEB	C2C-C3C	3.76	1.48	1.38
82	PJ	201	PEB	CHA-C1B	3.76	1.49	1.40
82	iE	202	PEB	CHA-C1B	3.76	1.49	1.40
82	L7	201	PEB	C1A-NA	-3.76	1.32	1.37
87	B2	815	CLA	C1D-ND	3.76	1.42	1.37
82	BK	201	PEB	CHA-C1B	3.76	1.49	1.40
82	OH	203	PEB	CHB-C1C	3.76	1.49	1.40
82	MK	203	PEB	CHB-C1C	3.76	1.49	1.40
82	eE	203	PEB	CHB-C1C	3.76	1.49	1.40
82	gO	202	PEB	CHB-C1C	3.76	1.49	1.40
91	DL	405	PHO	O2A-CGA	3.76	1.44	1.33
87	AN	816	CLA	C1D-ND	3.76	1.42	1.37
82	AH	302	PEB	CHA-C1B	3.76	1.49	1.40
82	fJ	203	PEB	C1A-NA	-3.76	1.32	1.37
87	5N	605	CLA	C1D-ND	3.76	1.42	1.37
82	JA	201	PEB	CHA-C1B	3.76	1.49	1.40
82	QG	203	PEB	CHA-C1B	3.76	1.49	1.40
82	tK	201	PEB	CHA-C1B	3.76	1.49	1.40
82	SG	201	PEB	C1A-NA	-3.76	1.32	1.37
82	t8	202	PEB	CHB-C1C	3.76	1.49	1.40
82	CP	203	PEB	CHA-C1B	3.76	1.49	1.40
82	QK	201	PEB	C3B-C2B	3.76	1.44	1.36
82	O5	203	PEB	C1A-NA	-3.76	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jG	201	PEB	CHB-C1C	3.76	1.49	1.40
87	BN	816	CLA	C1D-ND	3.76	1.42	1.37
87	2N	308	CLA	C4B-NB	3.76	1.42	1.37
87	3N	311	CLA	C1D-ND	3.76	1.42	1.37
82	cF	203	PEB	CHB-C1C	3.76	1.49	1.40
82	XP	201	PEB	C1A-NA	-3.76	1.32	1.37
82	X7	201	PEB	C1A-NA	-3.76	1.32	1.37
87	62	302	CLA	C1D-ND	3.75	1.42	1.37
87	R2	202	CLA	C1D-ND	3.75	1.42	1.37
82	XQ	203	PEB	CHA-C1B	3.75	1.49	1.40
82	BD	201	PEB	C1A-NA	-3.75	1.32	1.37
82	NF	201	PEB	CHB-C1C	3.75	1.49	1.40
82	Z9	303	PEB	CHA-C1B	3.75	1.49	1.40
82	tC	202	PEB	CHB-C1C	3.75	1.49	1.40
82	RQ	202	PEB	CHB-C1C	3.75	1.49	1.40
82	sF	203	PEB	C1A-NA	-3.75	1.32	1.37
84	D4	1001	CYC	C2C-C1C	-3.75	1.48	1.52
84	HH	1001	CYC	CHB-C4A	3.75	1.49	1.40
82	W1	202	PEB	C2C-C3C	3.75	1.48	1.38
84	C4	1001	CYC	C1C-NC	-3.75	1.32	1.37
82	UP	202	PEB	CHA-C1B	3.75	1.49	1.40
82	WI	201	PEB	CHB-C1C	3.75	1.49	1.40
82	NQ	202	PEB	CHB-C1C	3.75	1.49	1.40
82	Y4	203	PEB	CHB-C1C	3.75	1.49	1.40
84	D1	1001	CYC	CHA-C4D	3.75	1.49	1.40
82	SI	202	PEB	C1A-NA	-3.75	1.32	1.37
82	kF	203	PEB	CHA-C1B	3.75	1.49	1.40
82	UG	201	PEB	C1A-NA	-3.75	1.32	1.37
82	HB	202	PEB	CHA-C1B	3.75	1.49	1.40
87	CL	505	CLA	C1D-ND	3.75	1.42	1.37
87	12	606	CLA	C1D-ND	3.75	1.42	1.37
82	UE	201	PEB	C1A-NA	-3.75	1.32	1.37
83	QM	201	PUB	C3B-C2B	3.75	1.48	1.38
82	aB	201	PEB	CHA-C1B	3.75	1.49	1.40
82	TJ	201	PEB	CHA-C1B	3.75	1.49	1.40
82	VG	201	PEB	C1A-NA	-3.75	1.32	1.37
82	wC	203	PEB	CHB-C1C	3.75	1.49	1.40
82	HA	203	PEB	C1A-NA	-3.75	1.32	1.37
82	AB	501	PEB	C1A-NA	-3.75	1.32	1.37
82	BQ	203	PEB	C1A-NA	-3.75	1.32	1.37
82	dF	202	PEB	C1A-NA	-3.75	1.32	1.37
87	A2	820	CLA	C1D-ND	3.75	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6N	601	CLA	C1D-ND	3.75	1.42	1.37
82	LF	201	PEB	CHA-C1B	3.75	1.49	1.40
82	ZG	203	PEB	CHA-C1B	3.75	1.49	1.40
88	l6	101	LHG	O7-C7	3.75	1.44	1.34
82	UF	202	PEB	C1A-NA	-3.75	1.32	1.37
82	UO	201	PEB	C3B-C2B	3.75	1.44	1.36
82	U4	201	PEB	C3B-C2B	3.75	1.44	1.36
82	z8	201	PEB	CHA-C1B	3.75	1.49	1.40
82	PE	201	PEB	C1A-NA	-3.75	1.32	1.37
82	eJ	201	PEB	C1A-NA	-3.75	1.32	1.37
82	TP	201	PEB	CHA-C1B	3.75	1.49	1.40
82	QQ	201	PEB	CHB-C1C	3.75	1.49	1.40
82	fE	201	PEB	C1A-NA	-3.74	1.32	1.37
82	L9	201	PEB	CHA-C1B	3.74	1.49	1.40
82	MK	202	PEB	CHB-C1C	3.74	1.49	1.40
87	c6	604	CLA	C1D-ND	3.74	1.42	1.37
82	ZB	202	PEB	CHA-C1B	3.74	1.49	1.40
82	RM	202	PEB	C1A-NA	-3.74	1.32	1.37
82	z8	202	PEB	C1A-NA	-3.74	1.32	1.37
82	eK	202	PEB	C1A-NA	-3.74	1.32	1.37
82	qK	201	PEB	CHB-C1C	3.74	1.49	1.40
82	PD	201	PEB	CHA-C1B	3.74	1.49	1.40
82	KB	302	PEB	CHA-C1B	3.74	1.49	1.40
82	UH	202	PEB	C1A-NA	-3.74	1.32	1.37
82	d1	203	PEB	CHB-C1C	3.74	1.49	1.40
82	CB	201	PEB	CHA-C1B	3.74	1.49	1.40
82	u8	201	PEB	CHB-C1C	3.74	1.49	1.40
82	e4	203	PEB	CHA-C1B	3.74	1.49	1.40
82	kJ	202	PEB	CHA-C1B	3.74	1.49	1.40
82	UQ	202	PEB	C1A-NA	-3.74	1.32	1.37
87	6N	613	CLA	C1D-ND	3.74	1.42	1.37
82	hM	203	PEB	CHA-C1B	3.74	1.49	1.40
82	HI	202	PEB	CHB-C4B	3.74	1.46	1.38
82	Y7	304	PEB	C2C-C3C	3.74	1.48	1.38
82	lG	203	PEB	CHA-C1B	3.74	1.49	1.40
82	JP	201	PEB	C1A-NA	-3.74	1.32	1.37
82	mJ	202	PEB	C1A-NA	-3.74	1.32	1.37
82	c4	202	PEB	CHA-C1B	3.74	1.49	1.40
82	cO	202	PEB	CHA-C1B	3.74	1.49	1.40
87	32	311	CLA	C1D-ND	3.74	1.42	1.37
82	RP	201	PEB	CHA-C1B	3.74	1.49	1.40
87	32	303	CLA	C3B-C4B	3.74	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BA	203	PEB	C1A-NA	-3.74	1.32	1.37
82	LD	201	PEB	C1A-NA	-3.74	1.32	1.37
82	pC	202	PEB	C4B-C3B	3.74	1.51	1.45
82	FA	203	PEB	CHB-C1C	3.74	1.49	1.40
82	UH	201	PEB	CHA-C1B	3.74	1.49	1.40
82	GQ	201	PEB	C1A-NA	-3.74	1.32	1.37
82	LQ	203	PEB	CHA-C1B	3.74	1.49	1.40
82	VQ	202	PEB	CHA-C1B	3.74	1.49	1.40
82	kF	202	PEB	CHA-C1B	3.74	1.49	1.40
87	22	608	CLA	C4B-NB	3.74	1.42	1.37
82	dF	201	PEB	CHB-C1C	3.74	1.49	1.40
82	FK	202	PEB	C2C-C3C	3.74	1.48	1.38
82	UM	202	PEB	CHA-C1B	3.74	1.49	1.40
82	q8	203	PEB	CHA-C1B	3.74	1.49	1.40
82	dH	203	PEB	CHB-C1C	3.74	1.49	1.40
82	VB	201	PEB	C1A-NA	-3.74	1.32	1.37
82	qK	202	PEB	CHA-C1B	3.74	1.49	1.40
83	AH	303	PUB	C3B-C2B	3.74	1.48	1.38
82	mH	202	PEB	C2C-C3C	3.74	1.48	1.38
87	O2	203	CLA	C4D-ND	-3.74	1.32	1.37
82	GK	202	PEB	C4A-NA	-3.74	1.29	1.37
82	iF	203	PEB	C1A-NA	-3.74	1.32	1.37
82	hG	202	PEB	C1A-NA	-3.74	1.32	1.37
82	dG	204	PEB	CHB-C1C	3.74	1.49	1.40
82	OB	201	PEB	CHA-C1B	3.74	1.49	1.40
87	4N	610	CLA	C1D-ND	3.74	1.42	1.37
82	U1	202	PEB	C1A-NA	-3.73	1.32	1.37
82	W1	202	PEB	C1A-NA	-3.73	1.32	1.37
82	OQ	201	PEB	CHA-C1B	3.73	1.49	1.40
82	NM	201	PEB	C1A-NA	-3.73	1.32	1.37
84	FE	1001	CYC	CHD-C1D	3.73	1.49	1.40
84	CG	1001	CYC	CHD-C1D	3.73	1.49	1.40
82	DF	203	PEB	C1A-NA	-3.73	1.32	1.37
82	eJ	201	PEB	CHA-C1B	3.73	1.49	1.40
82	RD	202	PEB	CHB-C1C	3.73	1.49	1.40
82	V7	201	PEB	C1A-NA	-3.73	1.32	1.37
82	VG	202	PEB	C2C-C3C	3.73	1.48	1.38
82	m4	203	PEB	CHB-C1C	3.73	1.49	1.40
82	L7	201	PEB	CHB-C1C	3.73	1.49	1.40
82	DG	1002	PEB	C1A-NA	-3.73	1.32	1.37
82	P1	201	PEB	C1A-NA	-3.73	1.32	1.37
82	N7	203	PEB	C1A-NA	-3.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	qC	203	PEB	CHA-C1B	3.73	1.49	1.40
82	vF	202	PEB	CHA-C1B	3.73	1.49	1.40
82	YE	202	PEB	C2C-C3C	3.73	1.48	1.38
82	XF	203	PEB	C1A-NA	-3.73	1.32	1.37
84	I1	1001	CYC	CHB-C4A	3.73	1.49	1.40
82	cB	403	PEB	C1A-NA	-3.73	1.32	1.37
84	K4	1001	CYC	C1C-NC	-3.73	1.32	1.37
82	kG	201	PEB	CHB-C1C	3.73	1.49	1.40
82	GB	202	PEB	CHA-C1B	3.73	1.49	1.40
82	NJ	201	PEB	C2A-C1A	-3.73	1.48	1.52
87	42	607	CLA	C4D-ND	-3.73	1.32	1.37
82	Y9	201	PEB	C2C-C3C	3.73	1.48	1.38
82	JP	201	PEB	CHA-C1B	3.73	1.49	1.40
82	P4	202	PEB	C1A-NA	-3.73	1.32	1.37
82	WP	202	PEB	C2A-C1A	-3.73	1.48	1.52
87	1N	609	CLA	C1D-ND	3.73	1.42	1.37
87	7N	601	CLA	C1D-ND	3.73	1.42	1.37
82	tF	201	PEB	CHA-C1B	3.73	1.49	1.40
82	GM	201	PEB	C1A-NA	-3.73	1.32	1.37
82	VO	201	PEB	C1A-NA	-3.73	1.32	1.37
82	SQ	202	PEB	C1A-NA	-3.73	1.32	1.37
82	WM	202	PEB	C2C-C3C	3.73	1.48	1.38
82	M9	305	PEB	CHA-C1B	3.73	1.49	1.40
87	AN	827	CLA	C4D-ND	-3.73	1.32	1.37
82	ZF	202	PEB	C2C-C3C	3.73	1.48	1.38
82	kE	201	PEB	CHB-C1C	3.73	1.49	1.40
82	QM	203	PEB	C1A-NA	-3.73	1.32	1.37
82	Z5	301	PEB	C1A-NA	-3.73	1.32	1.37
82	jM	202	PEB	C2C-C3C	3.73	1.48	1.38
82	SJ	203	PEB	C1A-NA	-3.73	1.32	1.37
84	EO	1001	CYC	C1C-NC	-3.73	1.32	1.37
82	NJ	202	PEB	C2A-C1A	-3.73	1.48	1.52
82	VQ	202	PEB	CHB-C1C	3.73	1.49	1.40
82	fF	202	PEB	CHB-C1C	3.73	1.49	1.40
82	IM	201	PEB	C1A-NA	-3.72	1.32	1.37
82	DI	201	PEB	C2C-C3C	3.72	1.48	1.38
87	AN	831	CLA	CMB-C2B	-3.72	1.42	1.50
82	rC	201	PEB	C2C-C3C	3.72	1.48	1.38
84	LE	1001	CYC	CHB-C4A	3.72	1.49	1.40
87	AN	820	CLA	C4D-ND	-3.72	1.32	1.37
82	PD	202	PEB	C2A-C1A	-3.72	1.48	1.52
82	yC	203	PEB	C2C-C3C	3.72	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dQ	401	PEB	CHA-C1B	3.72	1.49	1.40
82	IM	201	PEB	CHB-C1C	3.72	1.49	1.40
84	C4	1001	CYC	CHD-C1D	3.72	1.49	1.40
82	VP	202	PEB	CHA-C1B	3.72	1.49	1.40
82	e1	201	PEB	CHA-C1B	3.72	1.49	1.40
82	F5	203	PEB	CHA-C1B	3.72	1.49	1.40
82	x8	202	PEB	CHA-C1B	3.72	1.49	1.40
82	GA	201	PEB	C1A-NA	-3.72	1.32	1.37
82	PO	202	PEB	C1A-NA	-3.72	1.32	1.37
84	K4	1001	CYC	C2C-C1C	-3.72	1.48	1.52
92	BL	611	LMG	O7-C10	3.72	1.44	1.34
82	HM	202	PEB	C1A-NA	-3.72	1.32	1.37
82	dQ	401	PEB	C2A-C1A	-3.72	1.48	1.52
84	D1	1001	CYC	C2C-C1C	-3.72	1.48	1.52
82	aM	204	PEB	CHB-C1C	3.72	1.49	1.40
82	H7	201	PEB	CHA-C1B	3.72	1.49	1.40
82	AH	305	PEB	CHA-C1B	3.72	1.49	1.40
82	OE	203	PEB	C1A-NA	-3.72	1.32	1.37
82	PD	201	PEB	CHB-C1C	3.72	1.49	1.40
82	TJ	201	PEB	C1A-NA	-3.72	1.32	1.37
82	UK	202	PEB	C1A-NA	-3.72	1.32	1.37
82	BP	202	PEB	C1A-NA	-3.72	1.32	1.37
82	gJ	202	PEB	CHA-C1B	3.72	1.49	1.40
82	u8	201	PEB	CHA-C1B	3.72	1.49	1.40
82	vC	202	PEB	CHA-C1B	3.72	1.49	1.40
82	KF	203	PEB	C1A-NA	-3.72	1.32	1.37
82	ZF	201	PEB	C1A-NA	-3.72	1.32	1.37
82	WM	202	PEB	CHB-C1C	3.72	1.49	1.40
83	A1	303	PUB	C3B-C2B	3.72	1.48	1.38
87	3N	304	CLA	C3B-C4B	3.72	1.51	1.42
82	WQ	202	PEB	C1A-NA	-3.72	1.32	1.37
82	N1	1002	PEB	C1A-NA	-3.72	1.32	1.37
82	YA	301	PEB	C2C-C3C	3.72	1.48	1.38
103	8N	310	ZEX	C5-C6	-3.72	1.28	1.34
82	vC	202	PEB	C2C-C3C	3.72	1.48	1.38
82	Y4	202	PEB	C1A-NA	-3.72	1.32	1.37
82	uC	201	PEB	CHB-C1C	3.72	1.49	1.40
82	v8	201	PEB	CHA-C1B	3.72	1.49	1.40
82	SP	203	PEB	C2C-C3C	3.72	1.48	1.38
82	iE	201	PEB	CHA-C1B	3.72	1.49	1.40
82	PK	202	PEB	C1A-NA	-3.72	1.32	1.37
87	42	610	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	72	602	CLA	C4D-ND	-3.72	1.32	1.37
82	XF	202	PEB	CHB-C1C	3.72	1.49	1.40
84	EH	1001	CYC	CHB-C4A	3.72	1.49	1.40
82	bG	201	PEB	C2A-C1A	-3.72	1.48	1.52
82	QH	202	PEB	C1A-NA	-3.71	1.32	1.37
82	M5	301	PEB	C1A-NA	-3.71	1.32	1.37
82	M7	201	PEB	C1A-NA	-3.71	1.32	1.37
82	QF	202	PEB	CHB-C1C	3.71	1.49	1.40
92	bL	623	LMG	O7-C10	3.71	1.44	1.34
82	VH	201	PEB	CHB-C1C	3.71	1.49	1.40
82	SM	203	PEB	CHB-C1C	3.71	1.49	1.40
82	RJ	202	PEB	C1A-NA	-3.71	1.32	1.37
82	aK	201	PEB	C1A-NA	-3.71	1.32	1.37
82	IJ	203	PEB	CHA-C1B	3.71	1.49	1.40
82	YP	502	PEB	CHA-C1B	3.71	1.49	1.40
82	eH	201	PEB	CHA-C1B	3.71	1.49	1.40
82	tK	203	PEB	CHA-C1B	3.71	1.49	1.40
82	jK	201	PEB	CHB-C1C	3.71	1.49	1.40
82	kK	203	PEB	CHB-C1C	3.71	1.49	1.40
82	FF	202	PEB	C2C-C3C	3.71	1.48	1.38
87	FN	203	CLA	C4D-ND	-3.71	1.32	1.37
82	uF	203	PEB	C2C-C3C	3.71	1.48	1.38
82	DA	201	PEB	CHB-C1C	3.71	1.49	1.40
82	D7	201	PEB	CHB-C1C	3.71	1.49	1.40
84	KO	1001	CYC	C2C-C1C	-3.71	1.48	1.52
82	hE	202	PEB	C1A-NA	-3.71	1.32	1.37
82	v8	202	PEB	C2C-C3C	3.71	1.48	1.38
84	D4	1001	CYC	CHB-C4A	3.71	1.49	1.40
82	aF	202	PEB	CHA-C1B	3.71	1.49	1.40
82	eH	203	PEB	CHB-C1C	3.71	1.49	1.40
82	WB	402	PEB	C1A-NA	-3.71	1.32	1.37
82	YJ	201	PEB	CHB-C1C	3.71	1.49	1.40
87	4N	607	CLA	C4D-ND	-3.71	1.32	1.37
82	UM	203	PEB	CHB-C1C	3.71	1.49	1.40
82	m4	202	PEB	CHB-C1C	3.71	1.49	1.40
82	XB	202	PEB	CHA-C1B	3.71	1.49	1.40
84	F4	1001	CYC	C2C-C1C	-3.71	1.48	1.52
82	TH	201	PEB	CHA-C1B	3.71	1.49	1.40
82	PH	201	PEB	C1A-NA	-3.71	1.32	1.37
82	jJ	203	PEB	C1A-NA	-3.71	1.32	1.37
82	PF	201	PEB	CHA-C1B	3.71	1.49	1.40
88	C6	505	LHG	O8-C23	3.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BF	201	PEB	CHA-C1B	3.71	1.49	1.40
82	i4	201	PEB	CHA-C1B	3.71	1.49	1.40
82	zC	202	PEB	CHA-C1B	3.71	1.49	1.40
82	iO	201	PEB	CHA-C1B	3.71	1.49	1.40
82	PQ	201	PEB	CHB-C1C	3.71	1.49	1.40
82	kM	201	PEB	CHA-C1B	3.71	1.49	1.40
84	D1	1001	CYC	CHB-C4A	3.71	1.49	1.40
84	EH	1001	CYC	C1D-C2D	3.71	1.50	1.41
82	K7	202	PEB	C2C-C3C	3.71	1.48	1.38
87	cL	517	CLA	C1D-ND	3.71	1.42	1.37
82	lE	203	PEB	CHA-C1B	3.71	1.49	1.40
82	i1	201	PEB	C1A-NA	-3.71	1.32	1.37
82	dD	401	PEB	C1A-NA	-3.71	1.32	1.37
84	ME	1001	CYC	C1C-NC	-3.71	1.32	1.37
82	YQ	201	PEB	CHA-C1B	3.71	1.49	1.40
87	K2	103	CLA	C4D-ND	-3.71	1.32	1.37
87	A2	831	CLA	CMB-C2B	-3.71	1.42	1.50
82	BM	301	PEB	C1A-NA	-3.71	1.32	1.37
82	aK	203	PEB	C1A-NA	-3.71	1.32	1.37
82	QQ	201	PEB	C2A-C1A	-3.71	1.48	1.52
82	iG	201	PEB	CHA-C1B	3.71	1.49	1.40
87	F2	201	CLA	C4D-ND	-3.71	1.32	1.37
82	KM	201	PEB	C1A-NA	-3.71	1.32	1.37
87	KN	102	CLA	C4D-ND	-3.71	1.32	1.37
82	YD	201	PEB	CHA-C1B	3.71	1.49	1.40
82	XB	202	PEB	C1A-NA	-3.70	1.32	1.37
82	iE	202	PEB	C2C-C3C	3.70	1.48	1.38
82	bG	201	PEB	CHA-C1B	3.70	1.49	1.40
87	6N	604	CLA	C4B-NB	3.70	1.42	1.37
84	DO	1001	CYC	C2C-C1C	-3.70	1.48	1.52
82	OD	201	PEB	CHA-C1B	3.70	1.49	1.40
82	JP	202	PEB	CHA-C1B	3.70	1.49	1.40
82	D9	201	PEB	CHA-C1B	3.70	1.49	1.40
82	oK	202	PEB	C2C-C3C	3.70	1.48	1.38
82	J5	201	PEB	CHA-C1B	3.70	1.49	1.40
82	HB	203	PEB	C1A-NA	-3.70	1.32	1.37
82	YQ	201	PEB	C2C-C3C	3.70	1.48	1.38
82	g4	202	PEB	CHB-C1C	3.70	1.49	1.40
82	oF	203	PEB	CHA-C1B	3.70	1.49	1.40
84	N1	1001	CYC	CHA-C4D	3.70	1.49	1.40
82	CJ	201	PEB	CHA-C1B	3.70	1.49	1.40
87	ON	201	CLA	C1D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	bE	201	PEB	CHA-C1B	3.70	1.49	1.40
82	VA	201	PEB	C1A-NA	-3.70	1.32	1.37
82	IB	202	PEB	C1A-NA	-3.70	1.32	1.37
82	CD	202	PEB	C1A-NA	-3.70	1.32	1.37
82	xK	302	PEB	C1A-NA	-3.70	1.32	1.37
82	BF	202	PEB	CHA-C1B	3.70	1.49	1.40
82	NQ	202	PEB	CHA-C1B	3.70	1.49	1.40
82	d1	203	PEB	CHA-C1B	3.70	1.49	1.40
84	DH	1001	CYC	C2C-C1C	-3.70	1.48	1.52
82	KB	301	PEB	CHA-C1B	3.70	1.49	1.40
82	PK	201	PEB	CHA-C1B	3.70	1.49	1.40
82	O1	203	PEB	CHB-C1C	3.70	1.49	1.40
82	L7	203	PEB	CHB-C1C	3.70	1.49	1.40
82	yC	203	PEB	CHB-C1C	3.70	1.49	1.40
82	UP	202	PEB	CHB-C1C	3.70	1.49	1.40
82	WI	201	PEB	CHA-C1B	3.70	1.49	1.40
82	g1	201	PEB	CHA-C1B	3.70	1.49	1.40
84	E1	1001	CYC	CHB-C4A	3.70	1.49	1.40
82	IQ	201	PEB	CHB-C1C	3.70	1.49	1.40
84	63	901	CYC	CHA-C4D	3.70	1.49	1.40
82	cJ	201	PEB	CHA-C1B	3.70	1.49	1.40
82	SD	202	PEB	C1A-NA	-3.70	1.32	1.37
82	YG	202	PEB	C1A-NA	-3.70	1.32	1.37
82	BI	201	PEB	C1A-NA	-3.70	1.32	1.37
82	H9	201	PEB	C1A-NA	-3.70	1.32	1.37
82	GJ	202	PEB	CHA-C1B	3.70	1.49	1.40
82	A1	305	PEB	CHA-C1B	3.70	1.49	1.40
82	YD	201	PEB	C2C-C3C	3.70	1.48	1.38
82	wC	201	PEB	CHA-C1B	3.70	1.49	1.40
82	IB	201	PEB	C1A-NA	-3.70	1.32	1.37
87	62	305	CLA	C4B-NB	3.70	1.42	1.37
87	72	601	CLA	C1D-ND	3.70	1.42	1.37
82	L9	203	PEB	CHB-C1C	3.70	1.49	1.40
82	VM	202	PEB	C1A-NA	-3.70	1.32	1.37
82	R1	202	PEB	CHB-C1C	3.70	1.49	1.40
82	fJ	202	PEB	C2C-C3C	3.70	1.48	1.38
82	SM	201	PEB	CHA-C1B	3.70	1.49	1.40
84	V3	1001	CYC	C2C-C1C	-3.70	1.48	1.52
82	BK	201	PEB	CHB-C1C	3.70	1.49	1.40
82	LM	201	PEB	C1A-NA	-3.70	1.32	1.37
82	HB	201	PEB	CHA-C1B	3.70	1.49	1.40
82	QK	202	PEB	CHA-C1B	3.70	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	fK	202	PEB	CHB-C1C	3.70	1.49	1.40
82	p8	202	PEB	C4B-C3B	3.70	1.51	1.45
96	v6	201	HEM	C1B-NB	-3.70	1.33	1.40
82	zC	201	PEB	C2C-C3C	3.70	1.48	1.38
82	dD	401	PEB	C2C-C3C	3.70	1.48	1.38
82	W1	201	PEB	CHB-C1C	3.70	1.49	1.40
82	GK	202	PEB	CHA-C1B	3.70	1.49	1.40
82	uC	201	PEB	CHA-C1B	3.70	1.49	1.40
82	RD	202	PEB	C1A-NA	-3.70	1.32	1.37
82	QJ	202	PEB	CHB-C1C	3.70	1.49	1.40
82	q8	201	PEB	CHA-C1B	3.70	1.49	1.40
82	y8	203	PEB	C2C-C3C	3.70	1.48	1.38
82	jM	201	PEB	C2C-C3C	3.70	1.48	1.38
84	x3	1001	CYC	C2C-C1C	-3.69	1.48	1.52
82	qC	201	PEB	CHA-C1B	3.69	1.49	1.40
82	NK	201	PEB	CHB-C1C	3.69	1.49	1.40
82	kE	202	PEB	C2C-C3C	3.69	1.48	1.38
82	y8	202	PEB	C1A-NA	-3.69	1.32	1.37
82	YO	203	PEB	CHB-C1C	3.69	1.49	1.40
87	bL	604	CLA	C1D-ND	3.69	1.42	1.37
82	F9	203	PEB	CHA-C1B	3.69	1.49	1.40
96	f6	101	HEM	C1B-NB	-3.69	1.33	1.40
82	UJ	203	PEB	CHA-C1B	3.69	1.49	1.40
82	SK	203	PEB	CHA-C1B	3.69	1.49	1.40
82	xF	303	PEB	C2C-C3C	3.69	1.48	1.38
82	a4	201	PEB	CHA-C1B	3.69	1.49	1.40
82	gH	201	PEB	CHA-C1B	3.69	1.49	1.40
82	WF	203	PEB	CHB-C1C	3.69	1.49	1.40
82	a1	201	PEB	CHB-C1C	3.69	1.49	1.40
82	X7	201	PEB	C2C-C3C	3.69	1.48	1.38
82	XK	202	PEB	CHA-C1B	3.69	1.49	1.40
82	PM	202	PEB	C1A-NA	-3.69	1.32	1.37
82	i4	202	PEB	C1A-NA	-3.69	1.32	1.37
82	kJ	202	PEB	C1A-NA	-3.69	1.32	1.37
82	BP	201	PEB	CHB-C1C	3.69	1.49	1.40
82	f1	202	PEB	C2C-C3C	3.69	1.48	1.38
82	EI	201	PEB	C1A-NA	-3.69	1.32	1.37
82	bO	201	PEB	C1A-NA	-3.69	1.32	1.37
82	U1	202	PEB	CHB-C1C	3.69	1.49	1.40
87	c6	605	CLA	C1D-ND	3.69	1.42	1.37
82	NF	202	PEB	C1A-NA	-3.69	1.32	1.37
82	M7	201	PEB	CHB-C1C	3.69	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	y8	203	PEB	CHB-C1C	3.69	1.49	1.40
91	a6	613	PHO	C3D-C2D	3.69	1.46	1.39
87	1N	605	CLA	C1D-ND	3.69	1.42	1.37
82	MB	201	PEB	CHA-C1B	3.69	1.49	1.40
82	v8	202	PEB	CHA-C1B	3.69	1.49	1.40
82	mE	203	PEB	C2C-C3C	3.69	1.48	1.38
82	mG	203	PEB	C2C-C3C	3.69	1.48	1.38
82	QK	203	PEB	C1A-NA	-3.69	1.32	1.37
84	MG	1001	CYC	C1C-NC	-3.69	1.32	1.37
82	W9	203	PEB	CHB-C1C	3.69	1.49	1.40
82	bH	202	PEB	C2C-C3C	3.69	1.48	1.38
82	PM	201	PEB	CHA-C1B	3.69	1.49	1.40
82	FA	201	PEB	CHB-C1C	3.69	1.49	1.40
82	ZK	202	PEB	CHB-C1C	3.69	1.49	1.40
82	z8	201	PEB	C2C-C3C	3.69	1.48	1.38
82	VM	201	PEB	CHA-C1B	3.69	1.49	1.40
82	vC	201	PEB	CHA-C1B	3.69	1.49	1.40
82	lE	201	PEB	CHB-C1C	3.69	1.49	1.40
82	EA	201	PEB	C1A-NA	-3.69	1.32	1.37
82	eB	201	PEB	C1A-NA	-3.69	1.32	1.37
82	dK	202	PEB	C1A-NA	-3.69	1.32	1.37
88	L6	101	LHG	O7-C7	3.69	1.44	1.34
82	UB	302	PEB	C1A-NA	-3.69	1.32	1.37
87	62	310	CLA	C1D-ND	3.69	1.42	1.37
96	fL	102	HEM	C4D-ND	-3.69	1.34	1.40
82	iM	202	PEB	CHB-C1C	3.69	1.49	1.40
82	HJ	201	PEB	CHA-C1B	3.69	1.49	1.40
82	TB	202	PEB	C1A-NA	-3.68	1.32	1.37
82	eM	201	PEB	C1A-NA	-3.68	1.32	1.37
82	FD	202	PEB	CHB-C1C	3.68	1.49	1.40
82	OM	203	PEB	CHB-C1C	3.68	1.49	1.40
82	aH	201	PEB	CHB-C1C	3.68	1.49	1.40
82	MF	202	PEB	CHB-C1C	3.68	1.49	1.40
82	Y7	301	PEB	C2C-C3C	3.68	1.48	1.38
82	lH	201	PEB	CHB-C1C	3.68	1.49	1.40
82	uF	201	PEB	CHA-C1B	3.68	1.49	1.40
82	DJ	201	PEB	C2A-C1A	-3.68	1.48	1.52
87	3N	312	CLA	C1D-ND	3.68	1.42	1.37
82	LP	202	PEB	CHA-C1B	3.68	1.49	1.40
84	LG	1001	CYC	CHB-C4A	3.68	1.49	1.40
82	FP	201	PEB	C1A-NA	-3.68	1.32	1.37
82	iK	202	PEB	C1A-NA	-3.68	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	bP	502	PEB	C1A-NA	-3.68	1.32	1.37
82	BA	202	PEB	CHA-C1B	3.68	1.49	1.40
82	rC	201	PEB	CHA-C1B	3.68	1.49	1.40
87	ON	203	CLA	C4D-ND	-3.68	1.32	1.37
82	GP	203	PEB	C2C-C3C	3.68	1.48	1.38
82	lM	202	PEB	C1A-NA	-3.68	1.32	1.37
82	KA	202	PEB	C2C-C3C	3.68	1.48	1.38
82	cG	202	PEB	CHB-C1C	3.68	1.49	1.40
82	ND	202	PEB	CHA-C1B	3.68	1.49	1.40
82	jE	202	PEB	CHB-C1C	3.68	1.49	1.40
82	L9	201	PEB	C2C-C3C	3.68	1.48	1.38
82	ZO	202	PEB	CHA-C1B	3.68	1.49	1.40
82	XQ	202	PEB	CHA-C1B	3.68	1.49	1.40
82	aH	202	PEB	C2C-C3C	3.68	1.48	1.38
82	RP	202	PEB	C1A-NA	-3.68	1.32	1.37
82	LA	201	PEB	CHB-C1C	3.68	1.49	1.40
82	kJ	201	PEB	CHB-C1C	3.68	1.49	1.40
82	OB	201	PEB	C1A-NA	-3.68	1.32	1.37
82	DE	1002	PEB	C1A-NA	-3.68	1.32	1.37
82	RG	201	PEB	C1A-NA	-3.68	1.32	1.37
82	YJ	202	PEB	CHA-C1B	3.68	1.49	1.40
87	7N	605	CLA	C1D-ND	3.68	1.42	1.37
82	QA	202	PEB	C1A-NA	-3.68	1.32	1.37
82	DB	202	PEB	CHA-C1B	3.68	1.49	1.40
82	DB	203	PEB	CHA-C1B	3.68	1.49	1.40
82	XF	201	PEB	CHB-C1C	3.68	1.49	1.40
82	jM	202	PEB	CHB-C1C	3.68	1.49	1.40
82	P4	201	PEB	C1A-NA	-3.68	1.32	1.37
82	m1	202	PEB	C2C-C3C	3.68	1.48	1.38
83	Z9	305	PUB	CHB-C1C	3.68	1.45	1.38
87	AN	828	CLA	C1D-ND	3.68	1.42	1.37
82	DP	202	PEB	CHA-C1B	3.68	1.49	1.40
82	LE	1002	PEB	C1A-NA	-3.68	1.32	1.37
82	OP	201	PEB	C1A-NA	-3.68	1.32	1.37
82	g4	201	PEB	CHA-C1B	3.68	1.49	1.40
82	YK	203	PEB	C2A-C1A	-3.68	1.48	1.52
82	bE	201	PEB	C2A-C1A	-3.68	1.48	1.52
82	UH	202	PEB	CHB-C1C	3.68	1.49	1.40
82	ZI	401	PEB	CHB-C1C	3.68	1.49	1.40
82	z8	201	PEB	CHB-C1C	3.68	1.49	1.40
82	WE	203	PEB	C1A-NA	-3.68	1.32	1.37
84	FH	1001	CYC	CHA-C4D	3.68	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FQ	202	PEB	CHB-C1C	3.67	1.49	1.40
82	FF	202	PEB	C2A-C1A	-3.67	1.48	1.52
82	UP	201	PEB	C2A-C1A	-3.67	1.48	1.52
82	S9	202	PEB	CHB-C1C	3.67	1.49	1.40
82	zC	201	PEB	CHB-C1C	3.67	1.49	1.40
82	iG	201	PEB	CHB-C1C	3.67	1.49	1.40
82	wK	303	PEB	CHB-C1C	3.67	1.49	1.40
87	82	302	CLA	C4D-ND	-3.67	1.32	1.37
82	V1	201	PEB	CHB-C1C	3.67	1.49	1.40
82	PE	202	PEB	C1A-NA	-3.67	1.32	1.37
82	VE	201	PEB	C1A-NA	-3.67	1.32	1.37
82	gE	202	PEB	C1A-NA	-3.67	1.32	1.37
82	PQ	203	PEB	CHA-C1B	3.67	1.49	1.40
82	XA	201	PEB	C2C-C3C	3.67	1.48	1.38
82	A1	301	PEB	CHA-C1B	3.67	1.49	1.40
82	JF	201	PEB	C2A-C1A	-3.67	1.48	1.52
82	LF	201	PEB	CHB-C1C	3.67	1.49	1.40
84	F1	1001	CYC	CHA-C4D	3.67	1.49	1.40
87	12	609	CLA	C1D-ND	3.67	1.42	1.37
82	B7	202	PEB	CHA-C1B	3.67	1.49	1.40
82	SK	201	PEB	CHB-C1C	3.67	1.49	1.40
82	l1	202	PEB	CHB-C1C	3.67	1.49	1.40
84	J1	1001	CYC	CHD-C1D	3.67	1.49	1.40
82	FD	202	PEB	CHA-C1B	3.67	1.49	1.40
82	YP	502	PEB	C1A-NA	-3.67	1.32	1.37
82	cM	201	PEB	C1A-NA	-3.67	1.32	1.37
87	A2	820	CLA	C4D-ND	-3.67	1.32	1.37
82	CF	203	PEB	CHB-C1C	3.67	1.49	1.40
82	DK	203	PEB	CHA-C1B	3.67	1.49	1.40
82	M9	301	PEB	CHA-C1B	3.67	1.49	1.40
82	ZG	203	PEB	C1A-NA	-3.67	1.32	1.37
82	IJ	201	PEB	C1A-NA	-3.67	1.32	1.37
82	BK	202	PEB	CHA-C1B	3.67	1.49	1.40
82	F7	201	PEB	CHB-C1C	3.67	1.49	1.40
82	AA	202	PEB	C1A-NA	-3.67	1.32	1.37
82	UM	201	PEB	C1A-NA	-3.67	1.32	1.37
82	yF	301	PEB	C1A-NA	-3.67	1.32	1.37
82	a1	202	PEB	C2C-C3C	3.67	1.48	1.38
82	j4	202	PEB	C2C-C3C	3.67	1.48	1.38
83	M5	303	PUB	C3B-C2B	3.67	1.48	1.38
82	AJ	302	PEB	CHA-C1B	3.67	1.49	1.40
87	A2	828	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	3N	304	CLA	C1B-C2B	3.67	1.51	1.43
82	YB	202	PEB	CHA-C1B	3.67	1.49	1.40
82	k4	201	PEB	CHB-C1C	3.67	1.49	1.40
82	cE	202	PEB	CHB-C1C	3.67	1.49	1.40
82	VD	202	PEB	C2C-C3C	3.67	1.48	1.38
82	UB	303	PEB	C1A-NA	-3.67	1.32	1.37
82	QI	201	PEB	C1A-NA	-3.67	1.32	1.37
82	RP	201	PEB	C1A-NA	-3.67	1.32	1.37
82	LD	203	PEB	CHA-C1B	3.67	1.49	1.40
87	A2	836	CLA	C1D-ND	3.67	1.42	1.37
82	AO	304	PEB	CHA-C1B	3.67	1.49	1.40
82	HI	201	PEB	CHB-C1C	3.67	1.49	1.40
82	TP	201	PEB	CHB-C1C	3.67	1.49	1.40
82	FQ	201	PEB	C2A-C1A	-3.67	1.48	1.52
82	RH	202	PEB	CHB-C1C	3.67	1.49	1.40
82	WJ	202	PEB	C1A-NA	-3.67	1.32	1.37
82	PQ	201	PEB	CHA-C1B	3.67	1.49	1.40
82	SI	202	PEB	CHA-C1B	3.67	1.49	1.40
82	L5	203	PEB	C1A-NA	-3.67	1.32	1.37
82	sF	202	PEB	CHB-C1C	3.67	1.49	1.40
82	XK	201	PEB	CHB-C1C	3.67	1.49	1.40
82	gF	203	PEB	CHB-C1C	3.67	1.49	1.40
82	LG	1002	PEB	C1A-NA	-3.67	1.32	1.37
82	PG	201	PEB	C1A-NA	-3.67	1.32	1.37
82	DI	201	PEB	C1A-NA	-3.67	1.32	1.37
82	KI	202	PEB	C1A-NA	-3.67	1.32	1.37
82	ZM	201	PEB	C1A-NA	-3.67	1.32	1.37
82	iJ	202	PEB	C1A-NA	-3.67	1.32	1.37
82	PG	202	PEB	CHA-C1B	3.67	1.49	1.40
82	WJ	201	PEB	CHA-C1B	3.67	1.49	1.40
84	DH	1001	CYC	C1D-C2D	3.67	1.50	1.41
82	FQ	202	PEB	CHA-C1B	3.66	1.49	1.40
87	8N	301	CLA	C4D-ND	-3.66	1.32	1.37
82	qC	203	PEB	C2C-C3C	3.66	1.48	1.38
82	uC	201	PEB	C2C-C3C	3.66	1.48	1.38
82	UB	301	PEB	C2A-C1A	-3.66	1.48	1.52
82	DA	202	PEB	CHB-C1C	3.66	1.49	1.40
82	iK	201	PEB	CHA-C1B	3.66	1.49	1.40
82	NH	1002	PEB	C1A-NA	-3.66	1.32	1.37
82	j1	203	PEB	C1A-NA	-3.66	1.32	1.37
87	cL	510	CLA	C1D-ND	3.66	1.42	1.37
87	6N	604	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	lJ	201	PEB	CHB-C1C	3.66	1.49	1.40
82	VP	202	PEB	C1A-NA	-3.66	1.32	1.37
82	G7	201	PEB	C1A-NA	-3.66	1.32	1.37
82	cH	201	PEB	C1A-NA	-3.66	1.32	1.37
82	TM	201	PEB	CHA-C1B	3.66	1.49	1.40
82	F9	201	PEB	CHA-C1B	3.66	1.49	1.40
84	63	901	CYC	CHB-C4A	3.66	1.49	1.40
82	J5	202	PEB	C1A-NA	-3.66	1.32	1.37
87	A2	839	CLA	C1D-ND	3.66	1.42	1.37
82	OJ	202	PEB	C1A-NA	-3.66	1.32	1.37
82	JP	201	PEB	CHB-C1C	3.66	1.49	1.40
82	dH	203	PEB	CHA-C1B	3.66	1.49	1.40
82	KM	203	PEB	C2A-C1A	-3.66	1.48	1.52
82	VF	201	PEB	CHB-C1C	3.66	1.49	1.40
82	F9	202	PEB	CHB-C1C	3.66	1.49	1.40
82	oF	202	PEB	C2C-C3C	3.66	1.48	1.38
87	BN	821	CLA	C1D-ND	3.66	1.42	1.37
87	O2	201	CLA	C1D-ND	3.66	1.42	1.37
82	Q1	202	PEB	C1A-NA	-3.66	1.32	1.37
82	dQ	401	PEB	C2C-C3C	3.66	1.48	1.38
82	NB	202	PEB	CHA-C1B	3.66	1.49	1.40
82	aG	202	PEB	CHA-C1B	3.66	1.49	1.40
82	QP	202	PEB	OD-C4D	3.66	1.30	1.23
82	xF	303	PEB	CHB-C1C	3.66	1.49	1.40
82	OP	202	PEB	CHA-C1B	3.66	1.49	1.40
82	r8	201	PEB	CHA-C1B	3.66	1.49	1.40
82	NI	201	PEB	C1A-NA	-3.66	1.32	1.37
82	BK	202	PEB	C1A-NA	-3.66	1.32	1.37
82	AM	302	PEB	CHA-C1B	3.66	1.49	1.40
82	QB	202	PEB	C2A-C1A	-3.66	1.48	1.52
82	PE	202	PEB	CHA-C1B	3.66	1.49	1.40
103	82	310	ZEX	C2-C3	-3.66	1.47	1.52
82	EM	201	PEB	CHB-C1C	3.66	1.49	1.40
82	ZK	201	PEB	C1A-NA	-3.66	1.32	1.37
82	O7	202	PEB	C1A-NA	-3.66	1.32	1.37
82	HF	201	PEB	CHB-C1C	3.66	1.49	1.40
82	L5	202	PEB	CHB-C1C	3.66	1.49	1.40
82	aK	202	PEB	CHA-C1B	3.66	1.49	1.40
82	kK	203	PEB	CHA-C1B	3.66	1.49	1.40
82	BB	202	PEB	CHA-C1B	3.66	1.49	1.40
87	cL	516	CLA	C1D-ND	3.66	1.42	1.37
82	XD	202	PEB	CHA-C1B	3.66	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	C7	201	PEB	CHA-C1B	3.66	1.49	1.40
82	LB	201	PEB	CHA-C1B	3.66	1.49	1.40
82	H7	203	PEB	CHA-C1B	3.66	1.49	1.40
82	b1	202	PEB	C2C-C3C	3.66	1.48	1.38
82	DM	201	PEB	C1A-NA	-3.66	1.32	1.37
87	BL	622	CLA	C1D-ND	3.66	1.42	1.37
96	V6	201	HEM	C1B-NB	-3.66	1.34	1.40
82	qK	203	PEB	OD-C4D	3.66	1.30	1.23
87	12	605	CLA	C1D-ND	3.66	1.42	1.37
87	M2	101	CLA	C1D-ND	3.66	1.42	1.37
82	e1	202	PEB	CHB-C1C	3.66	1.49	1.40
82	dJ	202	PEB	CHB-C1C	3.66	1.49	1.40
82	AO	305	PEB	CHA-C1B	3.66	1.49	1.40
82	S9	203	PEB	CHA-C1B	3.66	1.49	1.40
82	c4	203	PEB	CHB-C1C	3.65	1.49	1.40
84	D1	1001	CYC	C1D-C2D	3.65	1.50	1.41
82	V4	201	PEB	C2A-C1A	-3.65	1.48	1.52
82	XK	202	PEB	CHB-C1C	3.65	1.49	1.40
83	Z5	303	PUB	C3B-C2B	3.65	1.48	1.38
83	AJ	303	PUB	OD-C4D	3.65	1.30	1.23
82	LD	203	PEB	C1A-NA	-3.65	1.32	1.37
82	PP	202	PEB	CHA-C1B	3.65	1.49	1.40
87	C6	511	CLA	C1D-ND	3.65	1.42	1.37
82	HQ	203	PEB	C2C-C3C	3.65	1.48	1.38
82	XI	201	PEB	C1A-NA	-3.65	1.32	1.37
82	C7	201	PEB	C1A-NA	-3.65	1.32	1.37
82	dQ	401	PEB	C1A-NA	-3.65	1.32	1.37
82	SE	201	PEB	CHA-C1B	3.65	1.49	1.40
82	I5	202	PEB	CHA-C1B	3.65	1.49	1.40
82	dD	401	PEB	CHA-C1B	3.65	1.49	1.40
82	ND	204	PEB	CHA-C1B	3.65	1.49	1.40
82	kE	202	PEB	CHA-C1B	3.65	1.49	1.40
82	sF	201	PEB	CHA-C1B	3.65	1.49	1.40
82	NK	202	PEB	C2C-C3C	3.65	1.48	1.38
82	AI	201	PEB	C1A-NA	-3.65	1.32	1.37
82	GM	203	PEB	C1A-NA	-3.65	1.32	1.37
82	YO	202	PEB	C1A-NA	-3.65	1.32	1.37
82	jH	201	PEB	C1A-NA	-3.65	1.32	1.37
84	I4	1001	CYC	C2C-C1C	-3.65	1.48	1.52
82	KG	201	PEB	CHB-C1C	3.65	1.49	1.40
82	i4	203	PEB	CHB-C1C	3.65	1.49	1.40
82	YK	201	PEB	C2C-C3C	3.65	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	KA	203	PUB	C3B-C2B	3.65	1.48	1.38
82	W7	201	PEB	C1A-NA	-3.65	1.32	1.37
82	SG	201	PEB	CHA-C1B	3.65	1.49	1.40
82	E5	202	PEB	CHA-C1B	3.65	1.49	1.40
84	FG	1001	CYC	C2C-C1C	-3.65	1.48	1.52
82	OB	201	PEB	CHB-C1C	3.65	1.49	1.40
82	kO	202	PEB	CHB-C1C	3.65	1.49	1.40
82	BB	201	PEB	CHA-C1B	3.65	1.49	1.40
82	LQ	201	PEB	C1A-NA	-3.65	1.32	1.37
82	ZF	202	PEB	CHB-C1C	3.65	1.49	1.40
82	FI	201	PEB	CHB-C1C	3.65	1.49	1.40
82	nK	202	PEB	CHB-C1C	3.65	1.49	1.40
87	62	312	CLA	C1D-ND	3.65	1.42	1.37
82	JB	202	PEB	C1A-NA	-3.65	1.32	1.37
82	fH	202	PEB	C2C-C3C	3.65	1.48	1.38
82	AF	202	PEB	CHB-C1C	3.65	1.49	1.40
82	eO	202	PEB	CHB-C1C	3.65	1.49	1.40
82	A7	202	PEB	C2C-C3C	3.65	1.48	1.38
82	W7	202	PEB	CHB-C1C	3.65	1.49	1.40
87	2N	304	CLA	C1D-ND	3.65	1.42	1.37
87	A2	819	CLA	C4D-ND	-3.65	1.32	1.37
82	B7	201	PEB	C2C-C3C	3.65	1.48	1.38
82	jG	202	PEB	CHB-C1C	3.65	1.49	1.40
82	SF	203	PEB	C1A-NA	-3.65	1.32	1.37
82	SK	203	PEB	C1A-NA	-3.65	1.32	1.37
82	c4	201	PEB	C1A-NA	-3.65	1.32	1.37
82	VQ	202	PEB	C2C-C3C	3.65	1.48	1.38
82	iF	201	PEB	CHA-C1B	3.65	1.49	1.40
84	CO	1001	CYC	CHD-C1D	3.65	1.49	1.40
82	YK	201	PEB	C1A-NA	-3.65	1.32	1.37
87	7N	602	CLA	C4D-ND	-3.65	1.32	1.37
83	xF	306	PUB	C3B-C2B	3.65	1.48	1.38
82	YE	202	PEB	C1A-NA	-3.65	1.32	1.37
82	TG	201	PEB	C2A-C1A	-3.65	1.48	1.52
82	R7	201	PEB	C2A-C1A	-3.65	1.48	1.52
87	AN	819	CLA	C4D-ND	-3.65	1.32	1.37
82	sK	201	PEB	CHA-C1B	3.65	1.49	1.40
82	WH	201	PEB	CHB-C1C	3.65	1.49	1.40
82	vK	201	PEB	C2C-C3C	3.65	1.48	1.38
87	c6	606	CLA	C1D-ND	3.65	1.42	1.37
82	gE	201	PEB	C1A-NA	-3.65	1.32	1.37
82	vC	201	PEB	CHB-C1C	3.65	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	aM	203	PEB	CHB-C1C	3.65	1.49	1.40
82	KM	201	PEB	CHA-C1B	3.65	1.49	1.40
82	U9	204	PEB	CHA-C1B	3.65	1.49	1.40
82	VD	202	PEB	C1A-NA	-3.65	1.32	1.37
82	QF	203	PEB	C1A-NA	-3.65	1.32	1.37
82	WM	202	PEB	C1A-NA	-3.65	1.32	1.37
82	z8	201	PEB	C1A-NA	-3.65	1.32	1.37
82	YI	202	PEB	CHA-C1B	3.65	1.49	1.40
82	P5	202	PEB	CHA-C1B	3.65	1.49	1.40
84	DO	1001	CYC	CHB-C4A	3.65	1.49	1.40
82	vC	201	PEB	C2C-C3C	3.65	1.48	1.38
82	B9	201	PEB	CHB-C1C	3.64	1.49	1.40
82	oK	203	PEB	CHA-C1B	3.64	1.49	1.40
87	BN	809	CLA	C1D-ND	3.64	1.42	1.37
82	BA	201	PEB	C2C-C3C	3.64	1.48	1.38
82	PO	202	PEB	CHA-C1B	3.64	1.49	1.40
82	V5	201	PEB	CHA-C1B	3.64	1.49	1.40
87	72	605	CLA	C1D-ND	3.64	1.42	1.37
87	c6	616	CLA	C1D-ND	3.64	1.42	1.37
82	WA	201	PEB	C1A-NA	-3.64	1.32	1.37
82	V4	201	PEB	C1A-NA	-3.64	1.32	1.37
82	mM	201	PEB	C1A-NA	-3.64	1.32	1.37
87	32	303	CLA	C1B-C2B	3.64	1.51	1.43
82	ND	202	PEB	CHB-C1C	3.64	1.48	1.40
82	gK	203	PEB	CHB-C1C	3.64	1.48	1.40
82	hM	202	PEB	CHB-C1C	3.64	1.48	1.40
82	CA	201	PEB	CHA-C1B	3.64	1.49	1.40
82	aB	201	PEB	C2A-C1A	-3.64	1.48	1.52
82	SJ	201	PEB	C1A-NA	-3.64	1.32	1.37
82	l4	202	PEB	C1A-NA	-3.64	1.32	1.37
82	GF	202	PEB	CHA-C1B	3.64	1.48	1.40
82	UI	202	PEB	CHA-C1B	3.64	1.48	1.40
82	YD	202	PEB	CHB-C1C	3.64	1.48	1.40
82	D5	202	PEB	CHB-C1C	3.64	1.48	1.40
82	c4	202	PEB	C1A-NA	-3.64	1.32	1.37
82	gM	202	PEB	C1A-NA	-3.64	1.32	1.37
84	E1	1001	CYC	C1D-C2D	3.64	1.50	1.41
82	GP	203	PEB	CHA-C1B	3.64	1.48	1.40
82	NQ	203	PEB	CHA-C1B	3.64	1.48	1.40
82	Z1	201	PEB	C2A-C1A	-3.64	1.48	1.52
82	RP	201	PEB	CHB-C1C	3.64	1.48	1.40
82	aE	202	PEB	CHA-C1B	3.64	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kG	202	PEB	C2C-C3C	3.64	1.48	1.38
87	2N	307	CLA	C1D-ND	3.64	1.42	1.37
82	B7	203	PEB	C1A-NA	-3.64	1.32	1.37
82	fJ	202	PEB	C1A-NA	-3.64	1.32	1.37
82	wF	303	PEB	CHB-C1C	3.64	1.48	1.40
82	R5	202	PEB	CHA-C1B	3.64	1.48	1.40
82	xK	303	PEB	C2C-C3C	3.64	1.48	1.38
82	UI	201	PEB	CHB-C1C	3.64	1.48	1.40
82	OB	201	PEB	C2A-C1A	-3.64	1.48	1.52
82	NP	202	PEB	CHA-C1B	3.64	1.48	1.40
82	D5	203	PEB	C1A-NA	-3.64	1.32	1.37
82	aJ	204	PEB	C1A-NA	-3.64	1.32	1.37
82	K5	202	PEB	CHA-C1B	3.64	1.48	1.40
82	PO	203	PEB	CHA-C1B	3.64	1.48	1.40
87	MN	101	CLA	C1D-ND	3.64	1.42	1.37
82	FP	202	PEB	CHA-C1B	3.64	1.48	1.40
82	N5	202	PEB	CHA-C1B	3.64	1.48	1.40
82	Q9	203	PEB	CHA-C1B	3.64	1.48	1.40
82	HD	203	PEB	C2C-C3C	3.64	1.48	1.38
82	J7	201	PEB	C2C-C3C	3.64	1.48	1.38
82	WF	201	PEB	CHB-C1C	3.64	1.48	1.40
82	HA	203	PEB	CHA-C1B	3.64	1.48	1.40
82	HH	1002	PEB	CHA-C1B	3.64	1.48	1.40
82	GM	201	PEB	CHA-C1B	3.64	1.48	1.40
82	w8	201	PEB	CHA-C1B	3.64	1.48	1.40
82	jO	202	PEB	C2C-C3C	3.64	1.48	1.38
82	GM	203	PEB	CHB-C1C	3.64	1.48	1.40
82	iK	203	PEB	CHB-C1C	3.64	1.48	1.40
87	82	306	CLA	C4D-ND	-3.64	1.32	1.37
82	mK	202	PEB	C1A-NA	-3.64	1.32	1.37
82	lO	202	PEB	C1A-NA	-3.64	1.32	1.37
84	D1	1003	CYC	C1C-NC	-3.64	1.32	1.37
82	SI	201	PEB	CHA-C1B	3.64	1.48	1.40
82	D4	1002	PEB	CHA-C1B	3.64	1.48	1.40
87	32	310	CLA	C1D-ND	3.64	1.42	1.37
82	U9	202	PEB	CHB-C1C	3.64	1.48	1.40
84	FE	1002	CYC	CHA-C4D	3.64	1.48	1.40
82	Q9	201	PEB	C4B-C3B	3.64	1.51	1.45
82	CB	202	PEB	C2A-C1A	-3.64	1.48	1.52
82	VI	201	PEB	C1A-NA	-3.64	1.32	1.37
82	KM	201	PEB	CHB-C1C	3.64	1.48	1.40
82	jF	201	PEB	CHB-C1C	3.64	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AA	202	PEB	C2C-C3C	3.64	1.48	1.38
82	iG	202	PEB	C2C-C3C	3.64	1.48	1.38
82	VD	202	PEB	CHA-C1B	3.64	1.48	1.40
82	BB	201	PEB	CHB-C1C	3.64	1.48	1.40
82	HP	201	PEB	CHA-C1B	3.64	1.48	1.40
87	22	611	CLA	C1D-ND	3.64	1.42	1.37
82	u8	201	PEB	C2C-C3C	3.64	1.48	1.38
82	kO	202	PEB	C1A-NA	-3.64	1.32	1.37
87	5N	601	CLA	C1D-ND	3.64	1.42	1.37
82	C5	202	PEB	CHA-C1B	3.64	1.48	1.40
82	D7	202	PEB	CHB-C1C	3.64	1.48	1.40
82	p8	201	PEB	C2C-C3C	3.64	1.48	1.38
82	Q9	201	PEB	C2C-C3C	3.64	1.48	1.38
82	UA	201	PEB	C2A-C1A	-3.64	1.48	1.52
82	YK	201	PEB	CHA-C1B	3.64	1.48	1.40
82	qF	202	PEB	CHA-C1B	3.64	1.48	1.40
82	t8	202	PEB	C1A-NA	-3.64	1.32	1.37
82	O4	202	PEB	CHA-C1B	3.64	1.48	1.40
82	CK	203	PEB	CHB-C1C	3.63	1.48	1.40
82	qC	201	PEB	CHB-C1C	3.63	1.48	1.40
82	dE	203	PEB	CHB-C1C	3.63	1.48	1.40
87	6N	611	CLA	C1D-ND	3.63	1.42	1.37
82	RB	202	PEB	C1A-NA	-3.63	1.32	1.37
82	EM	203	PEB	C1A-NA	-3.63	1.32	1.37
84	M1	201	CYC	CHA-C4D	3.63	1.48	1.40
96	FL	102	HEM	C1B-NB	-3.63	1.34	1.40
87	8N	303	CLA	C4D-ND	-3.63	1.32	1.37
82	Z4	202	PEB	CHA-C1B	3.63	1.48	1.40
82	kG	202	PEB	CHA-C1B	3.63	1.48	1.40
82	aO	201	PEB	CHA-C1B	3.63	1.48	1.40
82	OJ	203	PEB	CHB-C1C	3.63	1.48	1.40
82	gJ	202	PEB	CHB-C1C	3.63	1.48	1.40
82	CP	203	PEB	C2C-C3C	3.63	1.48	1.38
82	A5	202	PEB	CHA-C1B	3.63	1.48	1.40
82	K5	201	PEB	CHA-C1B	3.63	1.48	1.40
82	lK	202	PEB	CHA-C1B	3.63	1.48	1.40
82	VF	202	PEB	C2C-C3C	3.63	1.48	1.38
87	cL	509	CLA	C1D-ND	3.63	1.42	1.37
82	X5	202	PEB	CHA-C1B	3.63	1.48	1.40
82	WM	203	PEB	C1A-NA	-3.63	1.32	1.37
82	eH	202	PEB	CHB-C1C	3.63	1.48	1.40
82	CF	201	PEB	CHA-C1B	3.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DF	203	PEB	C2C-C3C	3.63	1.48	1.38
82	AQ	303	PEB	C2C-C3C	3.63	1.48	1.38
82	q8	201	PEB	C2C-C3C	3.63	1.48	1.38
82	Q7	202	PEB	C1A-NA	-3.63	1.32	1.37
82	nF	202	PEB	C1A-NA	-3.63	1.32	1.37
82	mO	202	PEB	CHB-C1C	3.63	1.48	1.40
82	bB	201	PEB	CHA-C1B	3.63	1.48	1.40
82	dG	201	PEB	CHA-C1B	3.63	1.48	1.40
82	xK	304	PEB	C2C-C3C	3.63	1.48	1.38
82	OG	203	PEB	C1A-NA	-3.63	1.32	1.37
82	TM	201	PEB	C1A-NA	-3.63	1.32	1.37
82	BP	202	PEB	CHA-C1B	3.63	1.48	1.40
82	hJ	203	PEB	CHA-C1B	3.63	1.48	1.40
82	bO	202	PEB	CHA-C1B	3.63	1.48	1.40
84	F4	1001	CYC	CHA-C4D	3.63	1.48	1.40
87	82	305	CLA	C4D-ND	-3.63	1.32	1.37
87	dL	404	CLA	C1D-ND	3.63	1.42	1.37
82	JQ	201	PEB	CHA-C1B	3.63	1.48	1.40
82	RQ	202	PEB	CHA-C1B	3.63	1.48	1.40
82	A4	304	PEB	CHA-C1B	3.63	1.48	1.40
83	A1	304	PUB	C3B-C2B	3.63	1.48	1.38
82	QP	202	PEB	CHA-C1B	3.63	1.48	1.40
82	IA	201	PEB	C1A-NA	-3.63	1.32	1.37
82	PD	203	PEB	CHA-C1B	3.63	1.48	1.40
82	JH	1002	PEB	CHA-C1B	3.63	1.48	1.40
82	aB	202	PEB	CHA-C1B	3.63	1.48	1.40
82	aJ	202	PEB	CHA-C1B	3.63	1.48	1.40
82	YF	201	PEB	C2C-C3C	3.63	1.48	1.38
82	QD	201	PEB	CHB-C1C	3.63	1.48	1.40
83	xK	306	PUB	C3B-C2B	3.63	1.48	1.38
87	A2	826	CLA	C1D-ND	3.63	1.42	1.37
87	5N	606	CLA	C1D-ND	3.63	1.42	1.37
82	BB	202	PEB	C1A-NA	-3.63	1.32	1.37
84	FO	1001	CYC	C2C-C1C	-3.63	1.48	1.52
82	pC	201	PEB	C2C-C3C	3.63	1.48	1.38
82	FI	201	PEB	CHA-C1B	3.63	1.48	1.40
82	KQ	201	PEB	CHA-C1B	3.63	1.48	1.40
82	EJ	201	PEB	CHB-C1C	3.63	1.48	1.40
82	qC	201	PEB	C2C-C3C	3.63	1.48	1.38
87	62	304	CLA	C1D-ND	3.63	1.42	1.37
82	QF	202	PEB	CHA-C1B	3.63	1.48	1.40
82	LK	201	PEB	CHB-C1C	3.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GI	202	PEB	C1A-NA	-3.63	1.32	1.37
82	YH	201	PEB	C2C-C3C	3.63	1.48	1.38
82	YM	203	PEB	CHB-C1C	3.63	1.48	1.40
82	xK	303	PEB	CHB-C1C	3.63	1.48	1.40
82	G5	202	PEB	CHA-C1B	3.63	1.48	1.40
82	S5	201	PEB	CHA-C1B	3.63	1.48	1.40
82	DP	202	PEB	C1A-NA	-3.63	1.32	1.37
87	5N	603	CLA	C1D-ND	3.63	1.42	1.37
82	FI	202	PEB	CHA-C1B	3.63	1.48	1.40
82	jM	201	PEB	CHA-C1B	3.63	1.48	1.40
82	RB	202	PEB	CHA-C1B	3.62	1.48	1.40
82	ND	203	PEB	CHA-C1B	3.62	1.48	1.40
82	SP	202	PEB	CHA-C1B	3.62	1.48	1.40
82	dG	203	PEB	C1A-NA	-3.62	1.32	1.37
87	32	309	CLA	C1D-ND	3.62	1.42	1.37
82	iF	203	PEB	CHB-C1C	3.62	1.48	1.40
82	W9	203	PEB	CHA-C1B	3.62	1.48	1.40
82	OJ	201	PEB	C2A-C1A	-3.62	1.48	1.52
82	NQ	203	PEB	C2C-C3C	3.62	1.48	1.38
82	WK	203	PEB	CHB-C1C	3.62	1.48	1.40
82	GQ	202	PEB	CHB-C1C	3.62	1.48	1.40
82	FK	202	PEB	CHA-C1B	3.62	1.48	1.40
82	Q9	202	PEB	C1A-NA	-3.62	1.32	1.37
87	1N	611	CLA	C1D-ND	3.62	1.42	1.37
82	A4	305	PEB	CHA-C1B	3.62	1.48	1.40
82	eG	201	PEB	CHA-C1B	3.62	1.48	1.40
82	aM	202	PEB	CHA-C1B	3.62	1.48	1.40
82	MA	201	PEB	C1A-NA	-3.62	1.32	1.37
82	TI	202	PEB	C1A-NA	-3.62	1.32	1.37
91	d6	404	PHO	C3D-C2D	3.62	1.45	1.39
82	YI	201	PEB	CHB-C1C	3.62	1.48	1.40
82	NP	202	PEB	CHB-C1C	3.62	1.48	1.40
84	JH	1001	CYC	CHD-C1D	3.62	1.48	1.40
82	c1	201	PEB	C1A-NA	-3.62	1.32	1.37
82	lJ	201	PEB	C1A-NA	-3.62	1.32	1.37
82	RP	202	PEB	CHA-C1B	3.62	1.48	1.40
82	P1	201	PEB	CHA-C1B	3.62	1.48	1.40
82	V5	202	PEB	CHA-C1B	3.62	1.48	1.40
87	K2	101	CLA	C1D-ND	3.62	1.42	1.37
82	dE	201	PEB	CHA-C1B	3.62	1.48	1.40
82	PO	203	PEB	CHB-C1C	3.62	1.48	1.40
82	DF	203	PEB	CHA-C1B	3.62	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	ND	201	PUB	CHB-C4B	3.62	1.48	1.40
83	NQ	201	PUB	CHB-C4B	3.62	1.48	1.40
82	OO	202	PEB	CHA-C1B	3.62	1.48	1.40
82	dB	202	PEB	CHA-C1B	3.62	1.48	1.40
82	LP	202	PEB	C1A-NA	-3.62	1.32	1.37
82	HK	202	PEB	C2C-C3C	3.62	1.48	1.38
87	6N	603	CLA	C1D-ND	3.62	1.42	1.37
82	NI	201	PEB	CHA-C1B	3.62	1.48	1.40
82	eF	203	PEB	OD-C4D	3.62	1.30	1.23
82	ID	201	PEB	CHB-C1C	3.62	1.48	1.40
82	lM	202	PEB	C2A-C1A	-3.62	1.48	1.52
82	VB	202	PEB	CHA-C1B	3.62	1.48	1.40
87	32	312	CLA	C1D-ND	3.62	1.42	1.37
87	B2	816	CLA	C1D-ND	3.62	1.42	1.37
87	B2	820	CLA	C1D-ND	3.62	1.42	1.37
82	W7	202	PEB	CHA-C1B	3.62	1.48	1.40
82	iF	203	PEB	C2C-C3C	3.62	1.48	1.38
82	JA	201	PEB	C2C-C3C	3.62	1.48	1.38
87	62	305	CLA	C1D-ND	3.62	1.42	1.37
82	M9	301	PEB	CHB-C1C	3.62	1.48	1.40
82	jH	203	PEB	C1A-NA	-3.62	1.32	1.37
82	iO	203	PEB	CHB-C1C	3.62	1.48	1.40
82	O9	201	PEB	C2C-C3C	3.62	1.48	1.38
87	2N	311	CLA	C1D-ND	3.62	1.42	1.37
84	EG	1001	CYC	C1D-C2D	3.62	1.50	1.41
96	E6	101	HEM	C4D-ND	-3.62	1.34	1.40
82	aJ	203	PEB	CHB-C1C	3.62	1.48	1.40
82	gJ	202	PEB	C1A-NA	-3.62	1.32	1.37
82	kK	201	PEB	C1A-NA	-3.62	1.32	1.37
82	ZH	203	PEB	CHB-C1C	3.62	1.48	1.40
82	D4	1002	PEB	CHB-C1C	3.62	1.48	1.40
82	DA	203	PEB	C1A-NA	-3.62	1.32	1.37
82	MD	202	PEB	CHB-C1C	3.62	1.48	1.40
82	TI	201	PEB	CHB-C4B	3.62	1.45	1.38
82	OQ	202	PEB	C2C-C3C	3.62	1.48	1.38
82	vF	202	PEB	C1A-NA	-3.62	1.32	1.37
82	CK	201	PEB	CHA-C1B	3.61	1.48	1.40
82	OH	201	PEB	C1A-NA	-3.61	1.32	1.37
82	II	201	PEB	C1A-NA	-3.61	1.32	1.37
84	KO	1001	CYC	C1C-NC	-3.61	1.32	1.37
82	R5	201	PEB	CHA-C1B	3.61	1.48	1.40
82	iK	202	PEB	CHA-C1B	3.61	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SM	201	PEB	CHB-C1C	3.61	1.48	1.40
82	A4	301	PEB	CHB-C1C	3.61	1.48	1.40
87	bL	605	CLA	C1D-ND	3.61	1.42	1.37
82	QB	204	PEB	CHA-C1B	3.61	1.48	1.40
82	KE	201	PEB	CHB-C1C	3.61	1.48	1.40
87	AN	808	CLA	C1D-ND	3.61	1.42	1.37
87	BL	608	CLA	C4D-ND	-3.61	1.32	1.37
82	VP	201	PEB	CHA-C1B	3.61	1.48	1.40
82	Y9	201	PEB	CHA-C1B	3.61	1.48	1.40
87	b6	606	CLA	C1D-ND	3.61	1.42	1.37
87	c6	612	CLA	C1D-ND	3.61	1.42	1.37
82	Y5	202	PEB	CHB-C1C	3.61	1.48	1.40
84	JH	1003	CYC	CHA-C4D	3.61	1.48	1.40
87	BN	805	CLA	C4D-ND	-3.61	1.32	1.37
82	KE	201	PEB	C1A-NA	-3.61	1.32	1.37
82	N1	1002	PEB	CHA-C1B	3.61	1.48	1.40
82	C5	201	PEB	CHA-C1B	3.61	1.48	1.40
82	yC	203	PEB	CHA-C1B	3.61	1.48	1.40
82	JF	202	PEB	C1A-NA	-3.61	1.32	1.37
82	RI	201	PEB	C1A-NA	-3.61	1.32	1.37
82	dK	201	PEB	CHB-C1C	3.61	1.48	1.40
84	MG	1001	CYC	C1D-C2D	3.61	1.50	1.41
82	NH	1002	PEB	CHA-C1B	3.61	1.48	1.40
103	8N	310	ZEX	C2-C3	-3.61	1.47	1.52
82	OQ	202	PEB	C1A-NA	-3.61	1.32	1.37
82	cB	402	PEB	CHA-C1B	3.61	1.48	1.40
82	dG	203	PEB	CHB-C1C	3.61	1.48	1.40
82	KE	201	PEB	CHA-C1B	3.61	1.48	1.40
82	TO	201	PEB	CHA-C1B	3.61	1.48	1.40
82	T4	201	PEB	CHA-C1B	3.61	1.48	1.40
82	MQ	202	PEB	C2C-C3C	3.61	1.48	1.38
82	HK	201	PEB	CHB-C1C	3.61	1.48	1.40
82	PD	201	PEB	C1A-NA	-3.61	1.32	1.37
82	SO	202	PEB	C1A-NA	-3.61	1.32	1.37
82	UQ	201	PEB	C1A-NA	-3.61	1.32	1.37
82	qK	202	PEB	C1A-NA	-3.61	1.32	1.37
82	dM	202	PEB	C1A-NA	-3.61	1.32	1.37
82	lJ	202	PEB	CHA-C1B	3.61	1.48	1.40
82	UB	303	PEB	CHA-C1B	3.61	1.48	1.40
82	FF	202	PEB	CHA-C1B	3.61	1.48	1.40
82	UG	202	PEB	CHA-C1B	3.61	1.48	1.40
84	FE	1002	CYC	CHB-C4A	3.61	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	H7	203	PEB	CHB-C1C	3.61	1.48	1.40
96	vL	201	HEM	C4D-ND	-3.61	1.34	1.40
82	EI	201	PEB	CHA-C1B	3.61	1.48	1.40
82	iE	201	PEB	CHB-C1C	3.61	1.48	1.40
82	mF	202	PEB	C2C-C3C	3.61	1.48	1.38
84	HH	1001	CYC	CHD-C1D	3.61	1.48	1.40
82	FQ	201	PEB	CHA-C1B	3.61	1.48	1.40
82	1C	202	PEB	CHA-C1B	3.61	1.48	1.40
82	v8	201	PEB	CHB-C1C	3.61	1.48	1.40
84	CO	1001	CYC	CHA-C4D	3.61	1.48	1.40
82	H1	1002	PEB	CHA-C1B	3.61	1.48	1.40
82	ID	201	PEB	C2A-C1A	-3.61	1.48	1.52
87	42	606	CLA	C1D-ND	3.61	1.42	1.37
96	VL	201	HEM	C4D-ND	-3.61	1.34	1.40
82	UO	202	PEB	CHA-C1B	3.61	1.48	1.40
82	AM	302	PEB	C2C-C3C	3.61	1.48	1.38
82	QP	203	PEB	CHB-C1C	3.61	1.48	1.40
87	AN	811	CLA	C1D-ND	3.61	1.42	1.37
87	B2	808	CLA	C1D-ND	3.61	1.42	1.37
82	q8	203	PEB	C2C-C3C	3.61	1.48	1.38
82	q8	201	PEB	CHB-C1C	3.61	1.48	1.40
82	N5	201	PEB	CHA-C1B	3.61	1.48	1.40
82	ND	203	PEB	C2C-C3C	3.61	1.48	1.38
82	LA	201	PEB	C1A-NA	-3.61	1.32	1.37
82	wF	301	PEB	C1A-NA	-3.61	1.32	1.37
82	G5	201	PEB	CHA-C1B	3.61	1.48	1.40
96	fL	102	HEM	C1B-NB	-3.61	1.34	1.40
82	MA	201	PEB	CHB-C1C	3.61	1.48	1.40
82	NJ	201	PEB	CHA-C1B	3.61	1.48	1.40
82	a4	201	PEB	C2C-C3C	3.61	1.48	1.38
82	CA	201	PEB	C1A-NA	-3.61	1.32	1.37
82	LB	201	PEB	C1A-NA	-3.61	1.32	1.37
82	iO	202	PEB	C1A-NA	-3.61	1.32	1.37
82	NP	201	PEB	CHA-C1B	3.61	1.48	1.40
82	jJ	202	PEB	CHA-C1B	3.61	1.48	1.40
87	AN	836	CLA	C1D-ND	3.60	1.42	1.37
87	52	606	CLA	C1D-ND	3.60	1.42	1.37
87	3N	307	CLA	C1D-ND	3.60	1.42	1.37
82	uK	201	PEB	CHB-C1C	3.60	1.48	1.40
82	A5	201	PEB	CHA-C1B	3.60	1.48	1.40
87	cL	506	CLA	C1D-ND	3.60	1.42	1.37
82	PI	201	PEB	CHA-C1B	3.60	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UI	201	PEB	C1A-NA	-3.60	1.32	1.37
82	yC	202	PEB	C1A-NA	-3.60	1.32	1.37
82	LM	202	PEB	CHB-C1C	3.60	1.48	1.40
82	AI	201	PEB	CHA-C1B	3.60	1.48	1.40
87	4N	609	CLA	C1D-ND	3.60	1.42	1.37
82	I5	201	PEB	CHA-C1B	3.60	1.48	1.40
82	CM	203	PEB	CHB-C1C	3.60	1.48	1.40
87	22	607	CLA	C1D-ND	3.60	1.42	1.37
84	LH	1002	CYC	C1D-C2D	3.60	1.50	1.41
82	CP	201	PEB	CHB-C1C	3.60	1.48	1.40
83	yK	302	PUB	CHB-C4B	3.60	1.48	1.40
82	NB	202	PEB	C1A-NA	-3.60	1.32	1.37
82	BF	202	PEB	C1A-NA	-3.60	1.32	1.37
82	NP	202	PEB	C1A-NA	-3.60	1.32	1.37
82	V1	201	PEB	C1A-NA	-3.60	1.32	1.37
82	tF	201	PEB	C2C-C3C	3.60	1.48	1.38
82	dG	201	PEB	C2C-C3C	3.60	1.48	1.38
87	32	306	CLA	C1D-ND	3.60	1.42	1.37
82	ZB	203	PEB	CHA-C1B	3.60	1.48	1.40
82	UG	202	PEB	CHB-C1C	3.60	1.48	1.40
82	QM	202	PEB	CHA-C1B	3.60	1.48	1.40
82	WK	201	PEB	CHB-C1C	3.60	1.48	1.40
82	AO	301	PEB	CHB-C1C	3.60	1.48	1.40
82	UD	201	PEB	C1A-NA	-3.60	1.32	1.37
84	K1	1001	CYC	C1C-NC	-3.60	1.32	1.37
82	OI	202	PEB	CHB-C4B	3.60	1.45	1.38
82	nF	202	PEB	CHB-C1C	3.60	1.48	1.40
82	aJ	202	PEB	C2A-C1A	-3.60	1.48	1.52
82	WA	202	PEB	CHB-C1C	3.60	1.48	1.40
82	HQ	203	PEB	CHB-C1C	3.60	1.48	1.40
82	oF	203	PEB	CHB-C1C	3.60	1.48	1.40
82	xF	302	PEB	C1A-NA	-3.60	1.32	1.37
82	mJ	201	PEB	C1A-NA	-3.60	1.32	1.37
82	ZH	202	PEB	CHB-C1C	3.60	1.48	1.40
82	f4	202	PEB	CHA-C1B	3.60	1.48	1.40
82	P5	201	PEB	CHA-C1B	3.60	1.48	1.40
82	OD	202	PEB	C2C-C3C	3.60	1.48	1.38
87	52	601	CLA	C1D-ND	3.60	1.42	1.37
82	YJ	201	PEB	C2A-C1A	-3.60	1.48	1.52
82	fM	201	PEB	CHA-C1B	3.60	1.48	1.40
82	XQ	202	PEB	C2C-C3C	3.60	1.48	1.38
82	iK	203	PEB	C2C-C3C	3.60	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	r8	202	PEB	CHB-C1C	3.60	1.48	1.40
82	dM	202	PEB	CHB-C1C	3.60	1.48	1.40
82	vF	201	PEB	C2C-C3C	3.60	1.48	1.38
82	KI	202	PEB	CHA-C1B	3.60	1.48	1.40
82	P4	202	PEB	CHA-C1B	3.60	1.48	1.40
82	BF	201	PEB	CHB-C1C	3.60	1.48	1.40
87	8N	306	CLA	C4D-ND	-3.60	1.32	1.37
82	DD	201	PEB	C1A-NA	-3.60	1.32	1.37
82	PP	202	PEB	C1A-NA	-3.60	1.32	1.37
82	lF	201	PEB	C2C-C3C	3.60	1.48	1.38
82	II	201	PEB	CHA-C1B	3.60	1.48	1.40
82	JJ	201	PEB	C2A-C1A	-3.60	1.48	1.52
82	RE	202	PEB	C2C-C3C	3.60	1.48	1.38
82	RG	202	PEB	C2C-C3C	3.60	1.48	1.38
82	J9	201	PEB	C2C-C3C	3.60	1.48	1.38
83	AH	304	PUB	C3B-C2B	3.60	1.48	1.38
82	aM	204	PEB	CHA-C1B	3.60	1.48	1.40
82	DB	202	PEB	C1A-NA	-3.60	1.32	1.37
82	CI	201	PEB	C1A-NA	-3.60	1.32	1.37
82	kM	202	PEB	C1A-NA	-3.60	1.32	1.37
82	SF	201	PEB	CHB-C1C	3.60	1.48	1.40
82	HF	202	PEB	C2C-C3C	3.60	1.48	1.38
82	SB	202	PEB	C2A-C1A	-3.60	1.48	1.52
87	A2	811	CLA	C1D-ND	3.60	1.42	1.37
82	YF	202	PEB	C1A-NA	-3.60	1.32	1.37
82	jE	202	PEB	C1A-NA	-3.60	1.32	1.37
82	gJ	201	PEB	C2C-C3C	3.60	1.48	1.38
82	Z1	202	PEB	CHB-C1C	3.60	1.48	1.40
82	R4	201	PEB	C2C-C3C	3.60	1.48	1.38
82	GF	203	PEB	C1A-NA	-3.60	1.32	1.37
82	A7	201	PEB	C1A-NA	-3.60	1.32	1.37
82	MD	202	PEB	C2C-C3C	3.60	1.48	1.38
87	JN	101	CLA	C1D-ND	3.60	1.42	1.37
87	3N	309	CLA	C1D-ND	3.60	1.42	1.37
82	e4	202	PEB	CHB-C1C	3.60	1.48	1.40
82	rC	202	PEB	CHB-C1C	3.60	1.48	1.40
82	CK	201	PEB	CHB-C1C	3.59	1.48	1.40
82	AK	201	PEB	C1A-NA	-3.59	1.32	1.37
82	iM	201	PEB	C1A-NA	-3.59	1.32	1.37
82	Y1	201	PEB	C2C-C3C	3.59	1.48	1.38
82	qF	203	PEB	CHB-C1C	3.59	1.48	1.40
83	xF	305	PUB	CHB-C4B	3.59	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	K4	1001	CYC	CHA-C4D	3.59	1.48	1.40
82	AD	303	PEB	C2C-C3C	3.59	1.48	1.38
82	1C	203	PEB	C1A-NA	-3.59	1.32	1.37
82	QM	203	PEB	CHA-C1B	3.59	1.48	1.40
82	QJ	203	PEB	CHB-C1C	3.59	1.48	1.40
83	NQ	201	PUB	C4B-NB	-3.59	1.31	1.37
82	RI	201	PEB	CHA-C1B	3.59	1.48	1.40
82	l4	202	PEB	CHB-C1C	3.59	1.48	1.40
82	KB	301	PEB	C2C-C3C	3.59	1.48	1.38
82	UI	202	PEB	C1A-NA	-3.59	1.32	1.37
82	F1	1002	PEB	C1A-NA	-3.59	1.32	1.37
82	U7	202	PEB	C1A-NA	-3.59	1.32	1.37
84	FE	1002	CYC	C2C-C1C	-3.59	1.48	1.52
87	DL	406	CLA	C1D-ND	3.59	1.42	1.37
87	B2	813	CLA	C1D-ND	3.59	1.42	1.37
82	QI	201	PEB	CHA-C1B	3.59	1.48	1.40
82	yC	202	PEB	CHB-C1C	3.59	1.48	1.40
82	d4	202	PEB	CHA-C1B	3.59	1.48	1.40
82	eE	201	PEB	CHA-C1B	3.59	1.48	1.40
82	y8	202	PEB	CHB-C1C	3.59	1.48	1.40
82	D7	203	PEB	C1A-NA	-3.59	1.33	1.37
82	SM	202	PEB	C2C-C3C	3.59	1.48	1.38
82	v8	201	PEB	C2C-C3C	3.59	1.48	1.38
82	WA	202	PEB	CHA-C1B	3.59	1.48	1.40
82	HP	202	PEB	CHA-C1B	3.59	1.48	1.40
82	E5	201	PEB	CHA-C1B	3.59	1.48	1.40
82	OE	202	PEB	CHA-C1B	3.59	1.48	1.40
82	f4	202	PEB	C2C-C3C	3.59	1.48	1.38
84	M4	1001	CYC	C1D-C2D	3.59	1.50	1.41
82	PI	201	PEB	C1A-NA	-3.59	1.33	1.37
82	a4	202	PEB	C1A-NA	-3.59	1.33	1.37
82	mE	201	PEB	C1A-NA	-3.59	1.33	1.37
82	bP	502	PEB	CHA-C1B	3.59	1.48	1.40
82	LA	203	PEB	CHB-C1C	3.59	1.48	1.40
82	kK	201	PEB	CHB-C1C	3.59	1.48	1.40
87	52	604	CLA	C1D-ND	3.59	1.42	1.37
87	4N	606	CLA	C1D-ND	3.59	1.42	1.37
82	XF	202	PEB	CHA-C1B	3.59	1.48	1.40
82	YD	201	PEB	CHB-C1C	3.59	1.48	1.40
82	k1	201	PEB	CHB-C1C	3.59	1.48	1.40
82	JD	201	PEB	C1A-NA	-3.59	1.33	1.37
82	A4	301	PEB	C1A-NA	-3.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VI	201	PEB	CHA-C1B	3.59	1.48	1.40
82	YK	202	PEB	CHA-C1B	3.59	1.48	1.40
82	T5	202	PEB	CHA-C1B	3.59	1.48	1.40
82	V7	203	PEB	CHA-C1B	3.59	1.48	1.40
82	wK	302	PEB	CHA-C1B	3.59	1.48	1.40
82	kM	202	PEB	CHB-C1C	3.59	1.48	1.40
87	1N	603	CLA	C1D-ND	3.59	1.42	1.37
82	18	202	PEB	C1A-NA	-3.59	1.33	1.37
82	DP	201	PEB	CHA-C1B	3.59	1.48	1.40
82	DK	203	PEB	C2C-C3C	3.59	1.48	1.38
82	CI	201	PEB	CHA-C1B	3.59	1.48	1.40
82	SO	201	PEB	CHA-C1B	3.59	1.48	1.40
82	18	201	PEB	CHA-C1B	3.59	1.48	1.40
82	FM	201	PEB	C2A-C1A	-3.59	1.48	1.52
82	R1	202	PEB	C2A-C1A	-3.59	1.48	1.52
82	DM	202	PEB	C1A-NA	-3.59	1.33	1.37
82	S9	202	PEB	C1A-NA	-3.59	1.33	1.37
82	fG	201	PEB	C1A-NA	-3.59	1.33	1.37
82	DI	202	PEB	CHA-C1B	3.59	1.48	1.40
82	hE	202	PEB	CHA-C1B	3.59	1.48	1.40
82	hJ	202	PEB	CHB-C1C	3.59	1.48	1.40
82	IB	201	PEB	CHA-C1B	3.59	1.48	1.40
82	cK	201	PEB	CHB-C1C	3.59	1.48	1.40
82	kO	201	PEB	CHB-C1C	3.59	1.48	1.40
82	JD	201	PEB	CHA-C1B	3.59	1.48	1.40
82	T5	201	PEB	CHA-C1B	3.59	1.48	1.40
82	cO	203	PEB	CHB-C1C	3.59	1.48	1.40
82	QB	201	PEB	CHA-C1B	3.59	1.48	1.40
83	K7	203	PUB	C3B-C2B	3.59	1.48	1.38
82	S5	201	PEB	CHB-C1C	3.59	1.48	1.40
87	22	612	CLA	C1D-ND	3.59	1.42	1.37
82	FK	202	PEB	C2A-C1A	-3.59	1.48	1.52
82	K5	201	PEB	C2A-C1A	-3.59	1.48	1.52
84	L1	1001	CYC	C1D-C2D	3.59	1.50	1.41
82	YQ	202	PEB	CHB-C1C	3.59	1.48	1.40
82	WG	201	PEB	CHA-C1B	3.59	1.48	1.40
82	X5	201	PEB	CHA-C1B	3.59	1.48	1.40
82	cF	203	PEB	C1A-NA	-3.59	1.33	1.37
82	kF	201	PEB	C1A-NA	-3.59	1.33	1.37
82	hG	201	PEB	C1A-NA	-3.59	1.33	1.37
82	aM	202	PEB	C1A-NA	-3.59	1.33	1.37
82	NQ	204	PEB	CHA-C1B	3.58	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gO	201	PEB	CHA-C1B	3.58	1.48	1.40
82	qF	203	PEB	OD-C4D	3.58	1.30	1.23
82	TI	202	PEB	CHA-C1B	3.58	1.48	1.40
82	XI	201	PEB	CHA-C1B	3.58	1.48	1.40
82	gB	203	PEB	C1A-NA	-3.58	1.33	1.37
82	gF	203	PEB	C1A-NA	-3.58	1.33	1.37
82	VA	202	PEB	CHB-C1C	3.58	1.48	1.40
84	IO	1001	CYC	CHD-C1D	3.58	1.48	1.40
82	BJ	301	PEB	CHA-C1B	3.58	1.48	1.40
82	WF	202	PEB	C2C-C3C	3.58	1.48	1.38
82	YE	202	PEB	C2A-C1A	-3.58	1.48	1.52
82	KP	202	PEB	C2A-C1A	-3.58	1.48	1.52
82	UG	202	PEB	C1A-NA	-3.58	1.33	1.37
82	PO	201	PEB	C1A-NA	-3.58	1.33	1.37
82	O5	203	PEB	CHA-C1B	3.58	1.48	1.40
82	CP	203	PEB	CHB-C1C	3.58	1.48	1.40
82	NP	201	PEB	CHB-C1C	3.58	1.48	1.40
82	YD	202	PEB	C1A-NA	-3.58	1.33	1.37
82	gO	202	PEB	C1A-NA	-3.58	1.33	1.37
82	JP	201	PEB	C2C-C3C	3.58	1.48	1.38
82	YQ	202	PEB	C2C-C3C	3.58	1.48	1.38
82	gM	202	PEB	C2C-C3C	3.58	1.48	1.38
82	aO	201	PEB	C2C-C3C	3.58	1.48	1.38
82	dM	203	PEB	CHB-C1C	3.58	1.48	1.40
82	RD	202	PEB	CHA-C1B	3.58	1.48	1.40
87	AL	405	CLA	C1D-ND	3.58	1.42	1.37
82	S9	203	PEB	C1A-NA	-3.58	1.33	1.37
82	lE	203	PEB	C1A-NA	-3.58	1.33	1.37
82	dM	203	PEB	C2C-C3C	3.58	1.48	1.38
82	GI	202	PEB	CHA-C1B	3.58	1.48	1.40
82	U5	203	PEB	CHA-C1B	3.58	1.48	1.40
82	tK	201	PEB	C2C-C3C	3.58	1.48	1.38
87	42	609	CLA	C1D-ND	3.58	1.42	1.37
82	YF	202	PEB	CHA-C1B	3.58	1.48	1.40
84	EE	1001	CYC	C1D-C2D	3.58	1.50	1.41
82	VK	202	PEB	C2C-C3C	3.58	1.48	1.38
82	pK	201	PEB	C2C-C3C	3.58	1.48	1.38
82	D1	1002	PEB	CHB-C1C	3.58	1.48	1.40
82	E7	202	PEB	CHB-C1C	3.58	1.48	1.40
84	FO	1001	CYC	CHA-C4D	3.58	1.48	1.40
87	B6	609	CLA	C1D-ND	3.58	1.42	1.37
82	bO	202	PEB	CHB-C1C	3.58	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	JA	203	PEB	CHA-C1B	3.58	1.48	1.40
82	F7	203	PEB	CHA-C1B	3.58	1.48	1.40
82	fM	202	PEB	C1A-NA	-3.58	1.33	1.37
87	52	603	CLA	C1D-ND	3.58	1.42	1.37
95	C6	502	DGD	O1G-C1A	3.58	1.43	1.33
82	TM	202	PEB	CHB-C1C	3.58	1.48	1.40
82	fO	202	PEB	C2C-C3C	3.58	1.48	1.38
82	MF	203	PEB	C1A-NA	-3.58	1.33	1.37
82	UH	203	PEB	C1A-NA	-3.58	1.33	1.37
82	S9	201	PEB	C1A-NA	-3.58	1.33	1.37
82	SH	203	PEB	CHA-C1B	3.58	1.48	1.40
82	HA	203	PEB	CHB-C1C	3.58	1.48	1.40
82	FD	201	PEB	CHA-C1B	3.58	1.48	1.40
82	UE	202	PEB	CHA-C1B	3.58	1.48	1.40
82	V1	202	PEB	CHA-C1B	3.58	1.48	1.40
82	aJ	204	PEB	CHB-C1C	3.58	1.48	1.40
82	PG	202	PEB	C1A-NA	-3.58	1.33	1.37
82	gE	202	PEB	CHA-C1B	3.58	1.48	1.40
82	jO	202	PEB	CHA-C1B	3.58	1.48	1.40
82	kF	201	PEB	CHB-C1C	3.58	1.48	1.40
82	PQ	203	PEB	C2C-C3C	3.58	1.48	1.38
82	Q9	203	PEB	CHB-C1C	3.58	1.48	1.40
87	AN	839	CLA	C1D-ND	3.58	1.42	1.37
82	dB	201	PEB	C1A-NA	-3.58	1.33	1.37
82	H7	203	PEB	C4B-C3B	3.58	1.51	1.45
82	d4	202	PEB	C2C-C3C	3.58	1.48	1.38
82	JQ	201	PEB	C1A-NA	-3.58	1.33	1.37
82	T1	201	PEB	C1A-NA	-3.58	1.33	1.37
82	qF	202	PEB	C1A-NA	-3.58	1.33	1.37
82	J1	1002	PEB	CHA-C1B	3.58	1.48	1.40
82	L7	202	PEB	CHB-C1C	3.57	1.48	1.40
83	yF	302	PUB	CHB-C4B	3.57	1.48	1.40
87	AN	826	CLA	C1D-ND	3.57	1.42	1.37
87	BN	814	CLA	C1D-ND	3.57	1.42	1.37
82	dF	202	PEB	C2A-C1A	-3.57	1.48	1.52
82	18	202	PEB	CHA-C1B	3.57	1.48	1.40
82	L9	202	PEB	CHA-C1B	3.57	1.48	1.40
82	hG	202	PEB	CHA-C1B	3.57	1.48	1.40
82	GD	202	PEB	CHB-C1C	3.57	1.48	1.40
82	XK	203	PEB	C1A-NA	-3.57	1.33	1.37
87	bL	614	CLA	C1D-ND	3.57	1.42	1.37
82	VP	201	PEB	C2C-C3C	3.57	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	JK	201	PEB	C2A-C1A	-3.57	1.48	1.52
82	lE	203	PEB	CHB-C1C	3.57	1.48	1.40
82	VM	201	PEB	C1A-NA	-3.57	1.33	1.37
82	WP	201	PEB	C1A-NA	-3.57	1.33	1.37
82	fM	203	PEB	C1A-NA	-3.57	1.33	1.37
82	mK	202	PEB	C2C-C3C	3.57	1.48	1.38
82	OG	202	PEB	CHA-C1B	3.57	1.48	1.40
82	GK	202	PEB	C1C-NC	-3.57	1.31	1.37
87	82	303	CLA	C1D-ND	3.57	1.42	1.37
87	A2	808	CLA	C1D-ND	3.57	1.42	1.37
82	DO	1002	PEB	CHA-C1B	3.57	1.48	1.40
82	g4	201	PEB	C1A-NA	-3.57	1.33	1.37
82	PK	201	PEB	CHB-C1C	3.57	1.48	1.40
82	PD	203	PEB	C2C-C3C	3.57	1.48	1.38
82	T4	202	PEB	CHA-C1B	3.57	1.48	1.40
82	OI	201	PEB	C1A-NA	-3.57	1.33	1.37
82	xK	303	PEB	C1A-NA	-3.57	1.33	1.37
82	dB	201	PEB	CHB-C1C	3.57	1.48	1.40
82	UH	202	PEB	C2C-C3C	3.57	1.48	1.38
82	xF	304	PEB	C2C-C3C	3.57	1.48	1.38
82	HP	201	PEB	CHB-C1C	3.57	1.48	1.40
82	WH	202	PEB	C1A-NA	-3.57	1.33	1.37
82	Q9	203	PEB	C2C-C3C	3.57	1.48	1.38
82	QM	204	PEB	CHB-C1C	3.57	1.48	1.40
84	KO	1001	CYC	CHA-C4D	3.57	1.48	1.40
82	WE	201	PEB	CHA-C1B	3.57	1.48	1.40
82	UG	203	PEB	CHA-C1B	3.57	1.48	1.40
82	U9	203	PEB	C2C-C3C	3.57	1.48	1.38
82	dG	202	PEB	CHB-C1C	3.57	1.48	1.40
87	J2	101	CLA	C1D-ND	3.57	1.42	1.37
82	IQ	201	PEB	C2A-C1A	-3.57	1.48	1.52
82	TO	202	PEB	CHA-C1B	3.57	1.48	1.40
82	UE	202	PEB	CHB-C1C	3.57	1.48	1.40
82	DQ	201	PEB	CHB-C1C	3.57	1.48	1.40
82	Y7	303	PEB	CHB-C1C	3.57	1.48	1.40
82	QE	202	PEB	CHB-C1C	3.57	1.48	1.40
82	A4	304	PEB	CHB-C1C	3.57	1.48	1.40
82	b4	202	PEB	CHB-C1C	3.57	1.48	1.40
82	UP	202	PEB	C2C-C3C	3.57	1.48	1.38
95	C6	502	DGD	O2G-C1B	3.57	1.44	1.34
82	AA	201	PEB	C1A-NA	-3.57	1.33	1.37
82	Z1	203	PEB	CHB-C1C	3.57	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B9	201	PEB	C2C-C3C	3.57	1.48	1.38
87	BN	817	CLA	C1D-ND	3.57	1.42	1.37
82	YA	303	PEB	CHB-C1C	3.57	1.48	1.40
82	zC	201	PEB	C1A-NA	-3.57	1.33	1.37
82	GE	1002	PEB	C2A-C1A	-3.57	1.48	1.52
82	N1	1002	PEB	CHB-C1C	3.57	1.48	1.40
82	1C	202	PEB	C2C-C3C	3.57	1.48	1.38
82	xF	303	PEB	C1A-NA	-3.57	1.33	1.37
82	dE	201	PEB	C2C-C3C	3.57	1.48	1.38
82	gO	201	PEB	CHB-C1C	3.57	1.48	1.40
82	fO	202	PEB	CHA-C1B	3.57	1.48	1.40
87	3N	313	CLA	C1D-ND	3.57	1.42	1.37
82	MK	203	PEB	C1A-NA	-3.57	1.33	1.37
82	W9	202	PEB	C1A-NA	-3.57	1.33	1.37
82	DO	1002	PEB	CHB-C1C	3.57	1.48	1.40
87	3N	310	CLA	C1D-ND	3.57	1.42	1.37
82	HI	203	PEB	C1A-NA	-3.57	1.33	1.37
82	l1	202	PEB	C1A-NA	-3.57	1.33	1.37
82	e4	201	PEB	C1A-NA	-3.57	1.33	1.37
82	E7	202	PEB	C1A-NA	-3.57	1.33	1.37
82	HI	201	PEB	CHA-C1B	3.57	1.48	1.40
82	X5	201	PEB	C2A-C1A	-3.56	1.48	1.52
84	IO	1001	CYC	C2C-C1C	-3.56	1.48	1.52
82	FF	201	PEB	C2C-C3C	3.56	1.48	1.38
82	LQ	203	PEB	C1A-NA	-3.56	1.33	1.37
82	O1	201	PEB	C1A-NA	-3.56	1.33	1.37
82	HA	203	PEB	C4B-C3B	3.56	1.51	1.45
87	CL	504	CLA	C4D-ND	-3.56	1.32	1.37
82	ZH	201	PEB	C2A-C1A	-3.56	1.48	1.52
82	PH	201	PEB	CHA-C1B	3.56	1.48	1.40
82	MM	203	PEB	CHA-C1B	3.56	1.48	1.40
82	OM	202	PEB	C1A-NA	-3.56	1.33	1.37
84	KG	202	CYC	C1D-C2D	3.56	1.50	1.41
82	QG	202	PEB	CHB-C1C	3.56	1.48	1.40
82	J9	201	PEB	CHB-C1C	3.56	1.48	1.40
87	B2	804	CLA	C4D-ND	-3.56	1.32	1.37
82	NF	202	PEB	C2C-C3C	3.56	1.48	1.38
82	PF	201	PEB	CHB-C1C	3.56	1.48	1.40
82	VJ	202	PEB	C2A-C1A	-3.56	1.48	1.52
84	DO	1001	CYC	C1D-C2D	3.56	1.50	1.41
82	LG	1002	PEB	CHB-C1C	3.56	1.48	1.40
82	GB	203	PEB	CHA-C1B	3.56	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	KG	201	PEB	C1A-NA	-3.56	1.33	1.37
84	IO	1001	CYC	C1C-NC	-3.56	1.33	1.37
87	22	603	CLA	C1D-ND	3.56	1.42	1.37
82	oK	203	PEB	CHB-C1C	3.56	1.48	1.40
84	I4	1001	CYC	CHD-C1D	3.56	1.48	1.40
82	VA	203	PEB	CHA-C1B	3.56	1.48	1.40
82	J7	203	PEB	CHA-C1B	3.56	1.48	1.40
82	OP	203	PEB	C1A-NA	-3.56	1.33	1.37
84	CH	1001	CYC	CHA-C4D	3.56	1.48	1.40
82	YO	202	PEB	CHA-C1B	3.56	1.48	1.40
82	Y4	202	PEB	CHA-C1B	3.56	1.48	1.40
82	gG	202	PEB	CHA-C1B	3.56	1.48	1.40
82	HO	1002	PEB	C1A-NA	-3.56	1.33	1.37
82	1C	202	PEB	C1A-NA	-3.56	1.33	1.37
87	cL	507	CLA	C1D-ND	3.56	1.42	1.37
82	aE	202	PEB	C2C-C3C	3.56	1.48	1.38
82	HD	203	PEB	CHB-C1C	3.56	1.48	1.40
82	BJ	301	PEB	CHB-C1C	3.56	1.48	1.40
82	XQ	203	PEB	CHB-C1C	3.56	1.48	1.40
82	EP	202	PEB	CHA-C1B	3.56	1.48	1.40
87	12	611	CLA	C1D-ND	3.56	1.42	1.37
87	c6	615	CLA	C1D-ND	3.56	1.42	1.37
87	2N	312	CLA	C1D-ND	3.56	1.42	1.37
82	AP	202	PEB	C2C-C3C	3.56	1.48	1.38
82	RA	201	PEB	C2A-C1A	-3.56	1.48	1.52
82	sK	202	PEB	CHB-C1C	3.56	1.48	1.40
82	aO	202	PEB	C1A-NA	-3.56	1.33	1.37
82	TF	202	PEB	CHA-C1B	3.56	1.48	1.40
82	mM	202	PEB	CHB-C1C	3.56	1.48	1.40
82	D7	201	PEB	C2C-C3C	3.56	1.48	1.38
82	1C	201	PEB	CHA-C1B	3.56	1.48	1.40
82	jJ	201	PEB	CHA-C1B	3.56	1.48	1.40
82	DD	201	PEB	CHB-C1C	3.56	1.48	1.40
82	d1	201	PEB	CHB-C1C	3.56	1.48	1.40
82	NO	1002	PEB	C1A-NA	-3.56	1.33	1.37
82	eO	202	PEB	C1A-NA	-3.56	1.33	1.37
82	W9	201	PEB	C2C-C3C	3.56	1.48	1.38
82	FM	202	PEB	C2A-C1A	-3.56	1.48	1.52
82	RQ	202	PEB	C1A-NA	-3.56	1.33	1.37
87	BN	831	CLA	C4D-ND	-3.56	1.32	1.37
82	MQ	202	PEB	CHB-C1C	3.56	1.48	1.40
82	bK	202	PEB	CHB-C1C	3.56	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	815	CLA	C1D-ND	3.56	1.42	1.37
87	dL	409	CLA	C1D-ND	3.56	1.42	1.37
87	6N	609	CLA	C1D-ND	3.56	1.42	1.37
82	BP	201	PEB	CHA-C1B	3.56	1.48	1.40
82	dB	201	PEB	CHA-C1B	3.56	1.48	1.40
82	EM	201	PEB	C1A-NA	-3.56	1.33	1.37
82	GP	203	PEB	C1A-NA	-3.56	1.33	1.37
82	L4	1002	PEB	C2A-C1A	-3.56	1.48	1.52
82	R5	201	PEB	C2A-C1A	-3.56	1.48	1.52
82	KQ	201	PEB	CHB-C1C	3.56	1.48	1.40
82	gO	203	PEB	CHB-C1C	3.56	1.48	1.40
82	PD	202	PEB	C2C-C3C	3.56	1.48	1.38
82	Y4	201	PEB	CHA-C1B	3.56	1.48	1.40
82	j1	201	PEB	C1A-NA	-3.56	1.33	1.37
82	JM	202	PEB	CHB-C1C	3.55	1.48	1.40
82	QM	202	PEB	CHB-C1C	3.55	1.48	1.40
82	U9	201	PEB	CHB-C1C	3.55	1.48	1.40
82	18	202	PEB	C2C-C3C	3.55	1.48	1.38
87	cL	513	CLA	C1D-ND	3.55	1.42	1.37
87	4N	611	CLA	C1D-ND	3.55	1.42	1.37
87	B2	831	CLA	C4D-ND	-3.55	1.32	1.37
82	MF	202	PEB	C1A-NA	-3.55	1.33	1.37
82	wF	302	PEB	CHA-C1B	3.55	1.48	1.40
84	D4	1001	CYC	C1D-C2D	3.55	1.50	1.41
82	FA	203	PEB	CHA-C1B	3.55	1.48	1.40
82	S4	201	PEB	CHA-C1B	3.55	1.48	1.40
82	eE	201	PEB	CHB-C1C	3.55	1.48	1.40
82	aM	203	PEB	C2C-C3C	3.55	1.48	1.38
82	ZF	202	PEB	C1A-NA	-3.55	1.33	1.37
82	MK	202	PEB	C1A-NA	-3.55	1.33	1.37
82	T4	201	PEB	C2A-C1A	-3.55	1.48	1.52
82	jK	202	PEB	C2C-C3C	3.55	1.48	1.38
82	DH	1002	PEB	CHB-C1C	3.55	1.48	1.40
84	FG	1001	CYC	CHA-C4D	3.55	1.48	1.40
82	YF	201	PEB	CHA-C1B	3.55	1.48	1.40
82	YO	203	PEB	CHA-C1B	3.55	1.48	1.40
82	Y4	203	PEB	CHA-C1B	3.55	1.48	1.40
82	gJ	202	PEB	C2C-C3C	3.55	1.48	1.38
82	QJ	204	PEB	CHA-C1B	3.55	1.48	1.40
82	OM	203	PEB	CHA-C1B	3.55	1.48	1.40
82	MP	202	PEB	CHA-C1B	3.55	1.48	1.40
82	D9	202	PEB	CHA-C1B	3.55	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	lG	203	PEB	CHB-C1C	3.55	1.48	1.40
82	wC	202	PEB	C2C-C3C	3.55	1.48	1.38
82	iM	202	PEB	C2C-C3C	3.55	1.48	1.38
87	B6	608	CLA	C1D-ND	3.55	1.42	1.37
82	YO	201	PEB	CHA-C1B	3.55	1.48	1.40
84	FG	1001	CYC	CHB-C4A	3.55	1.48	1.40
82	U1	201	PEB	C1A-NA	-3.55	1.33	1.37
82	JI	201	PEB	C2C-C3C	3.55	1.48	1.38
84	N3	1001	CYC	C3D-C2D	3.55	1.48	1.38
82	h4	202	PEB	C2C-C3C	3.55	1.48	1.38
84	LG	1001	CYC	C3D-C2D	3.55	1.48	1.38
82	H4	1002	PEB	C1A-NA	-3.55	1.33	1.37
82	GQ	202	PEB	CHA-C1B	3.55	1.48	1.40
82	fH	202	PEB	CHA-C1B	3.55	1.48	1.40
82	j4	203	PEB	CHB-C1C	3.55	1.48	1.40
82	Y9	201	PEB	CHB-C1C	3.55	1.48	1.40
84	63	901	CYC	C2C-C1C	-3.55	1.48	1.52
82	AP	202	PEB	CHA-C1B	3.55	1.48	1.40
82	K9	201	PEB	C2C-C3C	3.55	1.48	1.38
84	GO	1001	CYC	C1C-NC	-3.55	1.33	1.37
84	C1	1001	CYC	C1C-NC	-3.55	1.33	1.37
87	8N	307	CLA	C1D-ND	3.55	1.42	1.37
84	K3	1001	CYC	C3D-C2D	3.55	1.48	1.38
82	YQ	201	PEB	CHB-C1C	3.55	1.48	1.40
82	CD	201	PEB	C2C-C3C	3.55	1.48	1.38
87	c6	610	CLA	C1D-ND	3.55	1.42	1.37
84	e3	1001	CYC	C3D-C2D	3.55	1.48	1.38
82	UI	201	PEB	CHA-C1B	3.55	1.48	1.40
82	JO	1002	PEB	CHA-C1B	3.55	1.48	1.40
82	JD	201	PEB	CHB-C1C	3.55	1.48	1.40
91	aL	610	PHO	C3D-C2D	3.55	1.45	1.39
82	WG	202	PEB	CHA-C1B	3.55	1.48	1.40
82	OD	202	PEB	C1A-NA	-3.55	1.33	1.37
82	qK	203	PEB	C1A-NA	-3.55	1.33	1.37
82	O4	202	PEB	C2C-C3C	3.55	1.48	1.38
82	cO	201	PEB	C1A-NA	-3.55	1.33	1.37
82	wK	303	PEB	C2C-C3C	3.55	1.48	1.38
84	E3	1001	CYC	C3D-C2D	3.55	1.48	1.38
82	18	203	PEB	CHB-C1C	3.55	1.48	1.40
84	D1	1003	CYC	CHB-C4A	3.55	1.48	1.40
82	MQ	201	PEB	CHB-C1C	3.55	1.48	1.40
82	X9	201	PEB	C2C-C3C	3.55	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	814	CLA	C1D-ND	3.55	1.42	1.37
82	h4	202	PEB	CHB-C1C	3.55	1.48	1.40
82	D9	203	PEB	CHB-C1C	3.55	1.48	1.40
82	hO	202	PEB	CHB-C1C	3.55	1.48	1.40
82	kJ	201	PEB	C1A-NA	-3.55	1.33	1.37
82	fM	201	PEB	CHB-C1C	3.55	1.48	1.40
84	73	1002	CYC	CHA-C4D	3.55	1.48	1.40
82	ED	201	PEB	C2A-C1A	-3.55	1.48	1.52
82	x8	202	PEB	C1C-NC	-3.55	1.31	1.37
82	PE	201	PEB	CHA-C1B	3.55	1.48	1.40
82	BP	201	PEB	C1A-NA	-3.55	1.33	1.37
82	uK	202	PEB	CHB-C1C	3.54	1.48	1.40
82	pF	201	PEB	C2C-C3C	3.54	1.48	1.38
82	MM	201	PEB	CHB-C1C	3.54	1.48	1.40
82	OM	202	PEB	CHB-C1C	3.54	1.48	1.40
82	rF	201	PEB	CHA-C1B	3.54	1.48	1.40
82	eG	201	PEB	CHB-C1C	3.54	1.48	1.40
84	C4	1001	CYC	CHA-C4D	3.54	1.48	1.40
82	lK	201	PEB	C2C-C3C	3.54	1.48	1.38
82	e4	202	PEB	C1A-NA	-3.54	1.33	1.37
87	C6	512	CLA	C1D-ND	3.54	1.42	1.37
82	DQ	202	PEB	CHA-C1B	3.54	1.48	1.40
95	c6	601	DGD	O2G-C1B	3.54	1.44	1.34
82	oF	202	PEB	CHB-C1C	3.54	1.48	1.40
84	p3	1001	CYC	C3D-C2D	3.54	1.48	1.38
82	A7	202	PEB	C1A-NA	-3.54	1.33	1.37
82	U9	202	PEB	C1A-NA	-3.54	1.33	1.37
82	P9	201	PEB	C2C-C3C	3.54	1.48	1.38
87	CL	508	CLA	C1D-ND	3.54	1.42	1.37
87	4N	610	CLA	C4B-NB	3.54	1.42	1.37
82	D9	203	PEB	C2C-C3C	3.54	1.48	1.38
82	E9	201	PEB	C2C-C3C	3.54	1.48	1.38
84	ME	1001	CYC	C1D-C2D	3.54	1.50	1.41
82	lM	203	PEB	C2C-C3C	3.54	1.48	1.38
87	BN	834	CLA	C4D-ND	-3.54	1.32	1.37
82	PI	202	PEB	C1A-NA	-3.54	1.33	1.37
82	qK	203	PEB	CHB-C1C	3.54	1.48	1.40
82	hO	202	PEB	C2C-C3C	3.54	1.48	1.38
82	uF	202	PEB	CHB-C1C	3.54	1.48	1.40
82	kF	202	PEB	C2C-C3C	3.54	1.48	1.38
82	AF	201	PEB	C1A-NA	-3.54	1.33	1.37
82	NI	202	PEB	C1A-NA	-3.54	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PJ	201	PEB	C1A-NA	-3.54	1.33	1.37
82	MP	202	PEB	C1A-NA	-3.54	1.33	1.37
82	cF	201	PEB	CHB-C1C	3.54	1.48	1.40
82	hG	202	PEB	CHB-C1C	3.54	1.48	1.40
84	E4	1001	CYC	CHA-C4D	3.54	1.48	1.40
82	p8	201	PEB	CHA-C1B	3.54	1.48	1.40
82	H5	202	PEB	CHB-C1C	3.54	1.48	1.40
82	IP	201	PEB	CHA-C1B	3.54	1.48	1.40
87	62	310	CLA	C4B-NB	3.54	1.42	1.37
82	OP	201	PEB	CHB-C1C	3.54	1.48	1.40
82	i1	202	PEB	CHB-C1C	3.54	1.48	1.40
82	I5	201	PEB	C2A-C1A	-3.54	1.48	1.52
82	T5	201	PEB	C2A-C1A	-3.54	1.48	1.52
82	yK	301	PEB	C1A-NA	-3.54	1.33	1.37
82	AK	202	PEB	CHA-C1B	3.54	1.48	1.40
82	YM	202	PEB	CHB-C1C	3.54	1.48	1.40
84	H1	1001	CYC	CHD-C1D	3.54	1.48	1.40
82	LI	201	PEB	CHA-C1B	3.54	1.48	1.40
82	GP	203	PEB	CHB-C1C	3.54	1.48	1.40
82	g1	201	PEB	CHB-C1C	3.54	1.48	1.40
82	NE	202	PEB	C1A-NA	-3.54	1.33	1.37
82	KD	201	PEB	CHA-C1B	3.54	1.48	1.40
82	LA	202	PEB	CHB-C1C	3.54	1.48	1.40
82	lG	202	PEB	C2C-C3C	3.54	1.48	1.38
82	wK	302	PEB	C2C-C3C	3.54	1.48	1.38
82	B9	202	PEB	CHB-C1C	3.54	1.48	1.40
82	kH	202	PEB	CHB-C1C	3.54	1.48	1.40
82	OH	203	PEB	C1A-NA	-3.54	1.33	1.37
82	FO	1002	PEB	CHA-C1B	3.54	1.48	1.40
82	WQ	202	PEB	CHB-C1C	3.54	1.48	1.40
87	B2	833	CLA	C4D-ND	-3.54	1.32	1.37
82	H9	203	PEB	CHA-C1B	3.54	1.48	1.40
87	C6	510	CLA	C1D-ND	3.54	1.42	1.37
84	KH	1001	CYC	C1C-NC	-3.54	1.33	1.37
82	EA	202	PEB	CHB-C1C	3.54	1.48	1.40
82	H9	201	PEB	CHB-C1C	3.54	1.48	1.40
82	cG	202	PEB	C2C-C3C	3.54	1.48	1.38
82	b4	202	PEB	CHA-C1B	3.54	1.48	1.40
82	kK	202	PEB	C2C-C3C	3.54	1.48	1.38
84	R3	1001	CYC	C3D-C2D	3.54	1.48	1.38
82	MD	202	PEB	CHA-C1B	3.54	1.48	1.40
82	MQ	202	PEB	CHA-C1B	3.54	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dO	202	PEB	CHA-C1B	3.54	1.48	1.40
82	SM	201	PEB	C1A-NA	-3.54	1.33	1.37
82	a4	203	PEB	C1A-NA	-3.54	1.33	1.37
84	G4	1001	CYC	C1C-NC	-3.54	1.33	1.37
82	YA	304	PEB	CHA-C1B	3.54	1.48	1.40
82	j4	202	PEB	CHA-C1B	3.54	1.48	1.40
82	cM	201	PEB	CHA-C1B	3.54	1.48	1.40
84	G3	1001	CYC	C3D-C2D	3.54	1.48	1.38
82	cO	202	PEB	C1A-NA	-3.54	1.33	1.37
87	IN	103	CLA	C1D-ND	3.54	1.42	1.37
83	AQ	302	PUB	C3B-C2B	3.53	1.48	1.38
84	i3	1001	CYC	C3D-C2D	3.53	1.48	1.38
82	SP	201	PEB	CHB-C1C	3.53	1.48	1.40
82	JQ	201	PEB	CHB-C1C	3.53	1.48	1.40
82	18	203	PEB	CHA-C1B	3.53	1.48	1.40
82	SM	203	PEB	C1A-NA	-3.53	1.33	1.37
82	TP	202	PEB	C1A-NA	-3.53	1.33	1.37
82	S1	202	PEB	C1A-NA	-3.53	1.33	1.37
82	gK	203	PEB	C1A-NA	-3.53	1.33	1.37
87	I2	103	CLA	C1D-ND	3.53	1.42	1.37
82	i4	203	PEB	C2C-C3C	3.53	1.48	1.38
82	CB	202	PEB	OD-C4D	3.53	1.30	1.23
82	MD	201	PEB	CHB-C1C	3.53	1.48	1.40
82	SQ	201	PEB	C1A-NA	-3.53	1.33	1.37
87	BL	608	CLA	C1D-ND	3.53	1.42	1.37
87	CL	515	CLA	C1D-ND	3.53	1.42	1.37
82	KD	201	PEB	CHB-C1C	3.53	1.48	1.40
82	IA	201	PEB	CHB-C1C	3.53	1.48	1.40
82	UP	203	PEB	C1A-NA	-3.53	1.33	1.37
82	u8	201	PEB	C1A-NA	-3.53	1.33	1.37
82	aF	203	PEB	C1A-NA	-3.53	1.33	1.37
82	aM	204	PEB	C1A-NA	-3.53	1.33	1.37
82	cM	202	PEB	C1A-NA	-3.53	1.33	1.37
82	gG	202	PEB	C2C-C3C	3.53	1.48	1.38
87	AN	850	CLA	C1D-ND	3.53	1.42	1.37
87	bL	607	CLA	C1D-ND	3.53	1.42	1.37
82	O9	201	PEB	CHA-C1B	3.53	1.48	1.40
82	V7	202	PEB	CHB-C1C	3.53	1.48	1.40
82	GQ	201	PEB	C2C-C3C	3.53	1.48	1.38
82	V9	201	PEB	C2C-C3C	3.53	1.48	1.38
82	KP	201	PEB	CHA-C1B	3.53	1.48	1.40
84	t3	1001	CYC	C3D-C2D	3.53	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	G7	202	PEB	CHB-C1C	3.53	1.48	1.40
96	V6	201	HEM	C4D-ND	-3.53	1.34	1.40
82	w8	203	PEB	C2C-C3C	3.53	1.48	1.38
82	aG	202	PEB	C2C-C3C	3.53	1.48	1.38
82	DK	201	PEB	CHA-C1B	3.53	1.48	1.40
82	YP	503	PEB	CHA-C1B	3.53	1.48	1.40
82	R9	201	PEB	C2C-C3C	3.53	1.48	1.38
82	UE	202	PEB	C1A-NA	-3.53	1.33	1.37
84	KG	202	CYC	C2C-C1C	-3.53	1.48	1.52
82	HJ	202	PEB	CHB-C1C	3.53	1.48	1.40
82	I7	202	PEB	CHB-C1C	3.53	1.48	1.40
82	LP	201	PEB	CHA-C1B	3.53	1.48	1.40
82	UB	302	PEB	CHB-C1C	3.53	1.48	1.40
82	G9	201	PEB	C2C-C3C	3.53	1.48	1.38
82	O4	202	PEB	C1A-NA	-3.53	1.33	1.37
82	c4	203	PEB	C1A-NA	-3.53	1.33	1.37
82	B5	202	PEB	C1A-NA	-3.53	1.33	1.37
87	12	603	CLA	C1D-ND	3.53	1.42	1.37
82	hF	202	PEB	C2C-C3C	3.53	1.48	1.38
82	SJ	202	PEB	CHA-C1B	3.53	1.48	1.40
84	DH	1003	CYC	CHB-C4A	3.53	1.48	1.40
82	fG	201	PEB	CHB-C1C	3.53	1.48	1.40
82	GB	202	PEB	C1A-NA	-3.53	1.33	1.37
82	RE	201	PEB	C1A-NA	-3.53	1.33	1.37
82	E7	201	PEB	C1A-NA	-3.53	1.33	1.37
82	cK	202	PEB	C1A-NA	-3.53	1.33	1.37
96	v6	201	HEM	C4D-ND	-3.53	1.34	1.40
82	UM	203	PEB	CHA-C1B	3.53	1.48	1.40
82	kH	201	PEB	CHA-C1B	3.53	1.48	1.40
87	BN	829	CLA	C1D-ND	3.53	1.42	1.37
87	42	611	CLA	C1D-ND	3.53	1.42	1.37
87	1N	604	CLA	C1D-ND	3.53	1.42	1.37
82	LE	1002	PEB	CHB-C1C	3.53	1.48	1.40
82	uF	203	PEB	CHB-C1C	3.53	1.48	1.40
84	C1	1001	CYC	CHA-C4D	3.53	1.48	1.40
82	SD	201	PEB	C2C-C3C	3.53	1.48	1.38
82	dM	203	PEB	C1A-NA	-3.53	1.33	1.37
82	sC	201	PEB	CHB-C1C	3.53	1.48	1.40
82	w8	202	PEB	C2C-C3C	3.53	1.48	1.38
82	h4	201	PEB	CHB-C1C	3.53	1.48	1.40
82	SB	201	PEB	CHA-C1B	3.53	1.48	1.40
82	iO	203	PEB	C1A-NA	-3.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	CH	1001	CYC	C1C-NC	-3.53	1.33	1.37
82	RH	202	PEB	C2A-C1A	-3.53	1.48	1.52
87	42	604	CLA	C4B-NB	3.53	1.42	1.37
82	QD	202	PEB	C2C-C3C	3.53	1.48	1.38
82	RD	201	PEB	C2C-C3C	3.53	1.48	1.38
84	C3	1001	CYC	C3D-C2D	3.53	1.48	1.38
82	YF	203	PEB	C1A-NA	-3.53	1.33	1.37
82	IJ	203	PEB	C1A-NA	-3.53	1.33	1.37
82	H7	201	PEB	C1A-NA	-3.53	1.33	1.37
82	kH	201	PEB	CHB-C1C	3.53	1.48	1.40
91	AL	410	PHO	C3A-C2A	-3.53	1.51	1.54
82	FB	201	PEB	CHA-C1B	3.53	1.48	1.40
83	ND	201	PUB	C4B-NB	-3.53	1.31	1.37
82	C5	201	PEB	C2A-C1A	-3.53	1.48	1.52
82	gG	202	PEB	C1A-NA	-3.53	1.33	1.37
82	cJ	202	PEB	C1A-NA	-3.53	1.33	1.37
82	cO	203	PEB	C1A-NA	-3.53	1.33	1.37
95	c6	601	DGD	O1G-C1A	3.53	1.43	1.33
87	5N	604	CLA	C1D-ND	3.53	1.42	1.37
82	YM	203	PEB	CHA-C1B	3.53	1.48	1.40
82	QQ	202	PEB	C2C-C3C	3.53	1.48	1.38
82	KM	203	PEB	CHB-C1C	3.53	1.48	1.40
82	WP	202	PEB	CHA-C1B	3.53	1.48	1.40
82	DJ	202	PEB	CHB-C1C	3.53	1.48	1.40
82	1C	203	PEB	CHB-C1C	3.53	1.48	1.40
82	NQ	204	PEB	C1A-NA	-3.52	1.33	1.37
82	i4	201	PEB	C1A-NA	-3.52	1.33	1.37
82	aF	201	PEB	C1A-NA	-3.52	1.33	1.37
82	dJ	201	PEB	C1A-NA	-3.52	1.33	1.37
82	eK	203	PEB	OD-C4D	3.52	1.30	1.23
84	J3	1001	CYC	C3D-C2D	3.52	1.48	1.38
82	eO	203	PEB	CHB-C1C	3.52	1.48	1.40
87	AN	801	CLA	C1D-ND	3.52	1.42	1.37
87	A2	822	CLA	C1D-ND	3.52	1.42	1.37
84	m3	1001	CYC	C3D-C2D	3.52	1.48	1.38
87	BN	833	CLA	C4D-ND	-3.52	1.32	1.37
82	LA	201	PEB	C2A-C1A	-3.52	1.48	1.52
82	dM	202	PEB	CHA-C1B	3.52	1.48	1.40
84	M4	1001	CYC	CHB-C4A	3.52	1.48	1.40
82	YQ	202	PEB	C1A-NA	-3.52	1.33	1.37
82	RQ	201	PEB	C2C-C3C	3.52	1.48	1.38
82	OD	201	PEB	CHB-C1C	3.52	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SG	203	PEB	CHB-C1C	3.52	1.48	1.40
82	H9	201	PEB	C2C-C3C	3.52	1.48	1.38
87	B2	830	CLA	C1D-ND	3.52	1.42	1.37
87	D6	405	CLA	C1D-ND	3.52	1.42	1.37
84	LE	1001	CYC	C3D-C2D	3.52	1.48	1.38
82	GI	201	PEB	CHB-C4B	3.52	1.45	1.38
82	O4	202	PEB	CHB-C1C	3.52	1.48	1.40
82	EA	202	PEB	C1A-NA	-3.52	1.33	1.37
82	ZO	202	PEB	C1A-NA	-3.52	1.33	1.37
82	j4	203	PEB	CHA-C1B	3.52	1.48	1.40
82	QB	203	PEB	C1A-NA	-3.52	1.33	1.37
82	LP	201	PEB	C1A-NA	-3.52	1.33	1.37
82	lG	203	PEB	C1A-NA	-3.52	1.33	1.37
82	k1	202	PEB	CHB-C1C	3.52	1.48	1.40
82	P1	201	PEB	C2C-C3C	3.52	1.48	1.38
82	AG	304	PEB	CHA-C1B	3.52	1.48	1.40
82	U1	202	PEB	C2C-C3C	3.52	1.48	1.38
82	CP	201	PEB	C1A-NA	-3.52	1.33	1.37
82	V7	203	PEB	C1A-NA	-3.52	1.33	1.37
82	PH	201	PEB	C2C-C3C	3.52	1.48	1.38
82	dO	202	PEB	C2C-C3C	3.52	1.48	1.38
82	RE	202	PEB	CHB-C1C	3.52	1.48	1.40
82	T7	203	PEB	C2A-C1A	-3.52	1.48	1.52
82	FQ	201	PEB	CHB-C1C	3.52	1.48	1.40
82	KG	201	PEB	CHA-C1B	3.52	1.48	1.40
87	5N	610	CLA	C1D-ND	3.52	1.42	1.37
82	dG	202	PEB	C1A-NA	-3.52	1.33	1.37
82	E7	202	PEB	C2C-C3C	3.52	1.48	1.38
82	AA	202	PEB	CHA-C1B	3.52	1.48	1.40
82	Z1	203	PEB	C1A-NA	-3.52	1.33	1.37
82	WE	202	PEB	CHA-C1B	3.52	1.48	1.40
87	22	604	CLA	C1D-ND	3.52	1.42	1.37
82	hJ	203	PEB	C2C-C3C	3.52	1.48	1.38
83	AD	302	PUB	C3B-C2B	3.52	1.48	1.38
82	UK	202	PEB	CHB-C1C	3.52	1.48	1.40
82	fF	202	PEB	CHA-C1B	3.52	1.48	1.40
82	AD	304	PEB	CHB-C1C	3.52	1.48	1.40
82	YG	202	PEB	C2A-C1A	-3.52	1.48	1.52
87	52	602	CLA	C1D-ND	3.52	1.42	1.37
87	5N	602	CLA	C1D-ND	3.52	1.42	1.37
82	d1	203	PEB	C2C-C3C	3.52	1.48	1.38
87	4N	604	CLA	C3D-CAD	3.52	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	IA	202	PEB	CHB-C1C	3.52	1.48	1.40
82	EP	202	PEB	C2C-C3C	3.52	1.48	1.38
82	T9	201	PEB	C2C-C3C	3.52	1.48	1.38
82	FH	1002	PEB	C1A-NA	-3.52	1.33	1.37
82	g4	202	PEB	C1A-NA	-3.52	1.33	1.37
87	B6	604	CLA	C1D-ND	3.52	1.42	1.37
87	d6	406	CLA	C1D-ND	3.52	1.42	1.37
82	y8	203	PEB	CHA-C1B	3.52	1.48	1.40
82	XD	202	PEB	C2C-C3C	3.52	1.48	1.38
82	N9	201	PEB	C2C-C3C	3.52	1.48	1.38
82	FA	203	PEB	C2C-C3C	3.52	1.48	1.38
82	QM	203	PEB	C2C-C3C	3.52	1.48	1.38
82	fJ	201	PEB	C1A-NA	-3.52	1.33	1.37
82	WM	201	PEB	CHB-C1C	3.52	1.48	1.40
82	dE	202	PEB	CHB-C1C	3.52	1.48	1.40
82	TK	202	PEB	CHA-C1B	3.52	1.48	1.40
82	C9	201	PEB	C2C-C3C	3.52	1.48	1.38
82	VG	201	PEB	CHA-C1B	3.52	1.48	1.40
82	iJ	201	PEB	C2C-C3C	3.52	1.48	1.38
82	WD	202	PEB	CHB-C1C	3.52	1.48	1.40
87	A2	802	CLA	C1D-ND	3.52	1.42	1.37
82	GM	202	PEB	CHA-C1B	3.52	1.48	1.40
82	cB	402	PEB	C2C-C3C	3.52	1.48	1.38
82	sC	203	PEB	C2C-C3C	3.52	1.48	1.38
82	eH	201	PEB	C2C-C3C	3.52	1.48	1.38
82	QH	203	PEB	CHA-C1B	3.52	1.48	1.40
82	QM	203	PEB	CHB-C1C	3.52	1.48	1.40
87	A2	818	CLA	C1D-ND	3.52	1.42	1.37
82	U7	201	PEB	C2A-C1A	-3.52	1.49	1.52
84	T3	1001	CYC	C3D-C2D	3.52	1.48	1.38
82	g1	201	PEB	C1A-NA	-3.51	1.33	1.37
82	m4	201	PEB	C1A-NA	-3.51	1.33	1.37
82	I7	201	PEB	C1A-NA	-3.51	1.33	1.37
82	cO	201	PEB	CHA-C1B	3.51	1.48	1.40
82	SJ	203	PEB	CHB-C1C	3.51	1.48	1.40
82	YD	202	PEB	C2C-C3C	3.51	1.48	1.38
82	PG	201	PEB	CHA-C1B	3.51	1.48	1.40
82	jJ	202	PEB	CHB-C1C	3.51	1.48	1.40
83	wK	304	PUB	CHB-C4B	3.51	1.48	1.40
82	TA	203	PEB	C2A-C1A	-3.51	1.49	1.52
84	NE	201	CYC	C1D-C2D	3.51	1.50	1.41
82	LG	1002	PEB	CHA-C1B	3.51	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	HG	1001	CYC	CHB-C4A	3.51	1.48	1.40
87	32	313	CLA	C1D-ND	3.51	1.42	1.37
82	KB	302	PEB	CHB-C1C	3.51	1.48	1.40
87	B2	834	CLA	C4D-ND	-3.51	1.32	1.37
82	T4	201	PEB	C1A-NA	-3.51	1.33	1.37
82	Q9	201	PEB	C1A-NA	-3.51	1.33	1.37
82	OK	203	PEB	C2C-C3C	3.51	1.48	1.38
82	A9	201	PEB	C2C-C3C	3.51	1.48	1.38
82	GD	202	PEB	CHA-C1B	3.51	1.48	1.40
84	P3	1001	CYC	C3D-C2D	3.51	1.48	1.38
84	c3	1001	CYC	C3D-C2D	3.51	1.48	1.38
82	NE	202	PEB	CHA-C1B	3.51	1.48	1.40
82	KP	202	PEB	CHA-C1B	3.51	1.48	1.40
82	AA	202	PEB	OD-C4D	3.51	1.30	1.23
82	dH	203	PEB	C2C-C3C	3.51	1.48	1.38
82	NH	1002	PEB	CHB-C1C	3.51	1.48	1.40
82	fM	202	PEB	CHB-C1C	3.51	1.48	1.40
84	A3	1001	CYC	C3D-C2D	3.51	1.48	1.38
82	r8	201	PEB	CHB-C1C	3.51	1.48	1.40
82	hK	202	PEB	C2C-C3C	3.51	1.48	1.38
84	G4	1001	CYC	C1D-C2D	3.51	1.50	1.41
87	BL	619	CLA	C1D-ND	3.51	1.42	1.37
82	CF	201	PEB	CHB-C1C	3.51	1.48	1.40
82	WJ	201	PEB	CHB-C1C	3.51	1.48	1.40
82	ZH	203	PEB	C2C-C3C	3.51	1.48	1.38
82	e1	202	PEB	C2C-C3C	3.51	1.48	1.38
82	jF	202	PEB	C2C-C3C	3.51	1.48	1.38
82	eH	202	PEB	C2C-C3C	3.51	1.48	1.38
84	v3	1001	CYC	C3D-C2D	3.51	1.48	1.38
82	UA	202	PEB	C1A-NA	-3.51	1.33	1.37
82	RI	202	PEB	C1A-NA	-3.51	1.33	1.37
82	AP	203	PEB	C1A-NA	-3.51	1.33	1.37
82	dH	202	PEB	CHA-C1B	3.51	1.48	1.40
82	mO	202	PEB	CHA-C1B	3.51	1.48	1.40
82	ND	203	PEB	CHB-C1C	3.51	1.48	1.40
82	m4	201	PEB	C2C-C3C	3.51	1.48	1.38
82	N5	201	PEB	C2A-C1A	-3.51	1.49	1.52
82	P5	201	PEB	C2A-C1A	-3.51	1.49	1.52
82	g4	202	PEB	CHA-C1B	3.51	1.48	1.40
82	CQ	201	PEB	C2C-C3C	3.51	1.48	1.38
82	AO	301	PEB	C1A-NA	-3.51	1.33	1.37
82	I7	202	PEB	C2C-C3C	3.51	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B9	203	PEB	C2C-C3C	3.51	1.48	1.38
82	I9	201	PEB	C2C-C3C	3.51	1.48	1.38
82	U4	202	PEB	CHA-C1B	3.51	1.48	1.40
82	V7	201	PEB	CHB-C1C	3.51	1.48	1.40
82	H9	203	PEB	CHB-C1C	3.51	1.48	1.40
82	mG	201	PEB	CHB-C1C	3.51	1.48	1.40
82	F4	1002	PEB	C2A-C1A	-3.51	1.49	1.52
82	FH	1002	PEB	CHA-C1B	3.51	1.48	1.40
82	kO	202	PEB	CHA-C1B	3.51	1.48	1.40
82	SI	201	PEB	CHB-C1C	3.51	1.48	1.40
82	GI	203	PEB	C1A-NA	-3.51	1.33	1.37
82	s8	201	PEB	C1A-NA	-3.51	1.33	1.37
82	xC	202	PEB	C1C-NC	-3.51	1.31	1.37
82	AA	201	PEB	C2C-C3C	3.51	1.48	1.38
82	ZF	201	PEB	CHA-C1B	3.51	1.48	1.40
82	FD	201	PEB	CHB-C1C	3.51	1.48	1.40
82	pK	202	PEB	CHB-C1C	3.51	1.48	1.40
82	gE	202	PEB	C2C-C3C	3.51	1.48	1.38
87	b6	615	CLA	C1D-ND	3.51	1.42	1.37
82	ZK	201	PEB	CHB-C1C	3.51	1.48	1.40
82	gB	201	PEB	CHB-C1C	3.51	1.48	1.40
82	d1	202	PEB	CHA-C1B	3.51	1.48	1.40
82	W9	202	PEB	CHA-C1B	3.51	1.48	1.40
82	hO	202	PEB	CHA-C1B	3.51	1.48	1.40
82	wC	203	PEB	C2C-C3C	3.51	1.48	1.38
82	oK	201	PEB	C2C-C3C	3.51	1.48	1.38
82	kO	201	PEB	C2C-C3C	3.51	1.48	1.38
82	qC	202	PEB	CHA-C1B	3.51	1.48	1.40
82	CI	202	PEB	C1A-NA	-3.51	1.33	1.37
82	aO	203	PEB	C1A-NA	-3.51	1.33	1.37
82	Q1	203	PEB	CHA-C1B	3.51	1.48	1.40
82	k4	201	PEB	CHA-C1B	3.51	1.48	1.40
82	A5	201	PEB	C2A-C1A	-3.51	1.49	1.52
87	CL	504	CLA	C1D-ND	3.51	1.42	1.37
87	B2	829	CLA	C1D-ND	3.51	1.42	1.37
82	OE	202	PEB	C1A-NA	-3.51	1.33	1.37
82	gH	201	PEB	C1A-NA	-3.51	1.33	1.37
82	UG	202	PEB	C2C-C3C	3.51	1.48	1.38
82	Z1	203	PEB	C2C-C3C	3.51	1.48	1.38
87	62	313	CLA	C1D-C2D	3.51	1.52	1.45
82	BQ	202	PEB	CHA-C1B	3.51	1.48	1.40
82	UD	201	PEB	CHB-C1C	3.51	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AB	501	PEB	CHA-C1B	3.51	1.48	1.40
87	82	304	CLA	C1D-ND	3.51	1.42	1.37
82	GD	201	PEB	C2C-C3C	3.51	1.48	1.38
82	iO	203	PEB	C2C-C3C	3.51	1.48	1.38
82	l1	203	PEB	CHA-C1B	3.51	1.48	1.40
82	dG	203	PEB	C2C-C3C	3.51	1.48	1.38
84	l3	1001	CYC	C3D-C2D	3.51	1.48	1.38
82	z8	202	PEB	CHB-C1C	3.51	1.48	1.40
84	BG	1002	CYC	C1B-NB	-3.51	1.31	1.37
87	AN	814	CLA	C1D-ND	3.51	1.42	1.37
87	5N	611	CLA	C1D-ND	3.51	1.42	1.37
82	U9	201	PEB	C2C-C3C	3.51	1.48	1.38
82	sF	201	PEB	C2C-C3C	3.51	1.48	1.38
82	OG	202	PEB	C1A-NA	-3.51	1.33	1.37
82	rC	201	PEB	C1A-NA	-3.51	1.33	1.37
82	kH	201	PEB	C1A-NA	-3.51	1.33	1.37
82	H4	1002	PEB	CHB-C1C	3.51	1.48	1.40
82	F1	1002	PEB	CHA-C1B	3.51	1.48	1.40
82	UK	201	PEB	C1C-NC	-3.51	1.31	1.37
82	gH	201	PEB	CHB-C1C	3.51	1.48	1.40
82	W9	203	PEB	C2C-C3C	3.50	1.48	1.38
87	cL	505	CLA	C1D-ND	3.50	1.42	1.37
82	DD	202	PEB	CHA-C1B	3.50	1.48	1.40
82	F5	202	PEB	CHA-C1B	3.50	1.48	1.40
82	oF	203	PEB	C2C-C3C	3.50	1.48	1.38
82	fM	202	PEB	C2C-C3C	3.50	1.48	1.38
84	IO	1001	CYC	CHA-C4D	3.50	1.48	1.40
82	bH	202	PEB	CHA-C1B	3.50	1.48	1.40
82	bP	501	PEB	CHA-C1B	3.50	1.48	1.40
82	LI	201	PEB	CHB-C1C	3.50	1.48	1.40
82	hE	202	PEB	CHB-C1C	3.50	1.48	1.40
82	XD	203	PEB	C2C-C3C	3.50	1.48	1.38
82	EM	202	PEB	C2C-C3C	3.50	1.48	1.38
82	GM	202	PEB	CHB-C1C	3.50	1.48	1.40
82	dM	201	PEB	C1A-NA	-3.50	1.33	1.37
82	SM	201	PEB	C2C-C3C	3.50	1.48	1.38
82	ZF	202	PEB	CHA-C1B	3.50	1.48	1.40
82	XQ	203	PEB	C2C-C3C	3.50	1.48	1.38
82	QA	201	PEB	CHB-C1C	3.50	1.48	1.40
82	Q7	201	PEB	CHB-C1C	3.50	1.48	1.40
82	uC	201	PEB	C1A-NA	-3.50	1.33	1.37
84	M1	201	CYC	C1C-NC	-3.50	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	12	604	CLA	C1D-ND	3.50	1.42	1.37
82	J4	1002	PEB	CHA-C1B	3.50	1.48	1.40
82	h4	202	PEB	CHA-C1B	3.50	1.48	1.40
82	oF	201	PEB	CHB-C1C	3.50	1.48	1.40
82	RK	202	PEB	CHA-C1B	3.50	1.48	1.40
84	EE	1001	CYC	CHA-C4D	3.50	1.48	1.40
87	BL	601	CLA	C1D-ND	3.50	1.42	1.37
84	MO	1001	CYC	CHB-C4A	3.50	1.48	1.40
82	UQ	201	PEB	C2C-C3C	3.50	1.48	1.38
82	A4	304	PEB	C2C-C3C	3.50	1.48	1.38
82	jH	202	PEB	C2C-C3C	3.50	1.48	1.38
82	AF	202	PEB	CHA-C1B	3.50	1.48	1.40
82	I7	201	PEB	CHB-C1C	3.50	1.48	1.40
82	mK	201	PEB	CHB-C1C	3.50	1.48	1.40
84	M1	201	CYC	CHD-C1D	3.50	1.48	1.40
82	UE	202	PEB	C2C-C3C	3.50	1.48	1.38
82	E5	201	PEB	C2A-C1A	-3.50	1.49	1.52
82	G5	201	PEB	C2A-C1A	-3.50	1.49	1.52
82	f1	202	PEB	CHA-C1B	3.50	1.48	1.40
84	HE	1001	CYC	CHB-C4A	3.50	1.48	1.40
87	6N	612	CLA	C1D-C2D	3.50	1.52	1.45
82	EK	202	PEB	C1A-NA	-3.50	1.33	1.37
82	WK	203	PEB	C1A-NA	-3.50	1.33	1.37
82	gG	201	PEB	C1A-NA	-3.50	1.33	1.37
82	AO	304	PEB	C2C-C3C	3.50	1.48	1.38
82	uK	201	PEB	C2C-C3C	3.50	1.48	1.38
87	BN	813	CLA	C1D-ND	3.50	1.42	1.37
87	A2	815	CLA	C1D-ND	3.50	1.42	1.37
82	BD	202	PEB	CHA-C1B	3.50	1.48	1.40
83	AO	302	PUB	C3B-C2B	3.50	1.48	1.38
83	A4	302	PUB	C3B-C2B	3.50	1.48	1.38
84	g3	1001	CYC	C3D-C2D	3.50	1.48	1.38
82	bF	202	PEB	CHB-C1C	3.50	1.48	1.40
82	EJ	202	PEB	CHA-C1B	3.50	1.48	1.40
82	RO	201	PEB	C2C-C3C	3.50	1.48	1.38
82	wC	204	PEB	C2C-C3C	3.50	1.48	1.38
87	6N	609	CLA	C4B-NB	3.50	1.42	1.37
87	42	604	CLA	C3D-CAD	3.50	1.57	1.45
82	SD	201	PEB	C1A-NA	-3.50	1.33	1.37
82	WH	201	PEB	C1A-NA	-3.50	1.33	1.37
82	dE	202	PEB	C1A-NA	-3.50	1.33	1.37
82	LO	1002	PEB	CHB-C1C	3.50	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AA	201	PEB	CHA-C1B	3.50	1.48	1.40
87	CL	511	CLA	C4D-ND	-3.50	1.32	1.37
82	OH	202	PEB	CHB-C1C	3.50	1.48	1.40
82	TI	203	PEB	C1A-NA	-3.50	1.33	1.37
82	QK	202	PEB	C1A-NA	-3.50	1.33	1.37
82	hE	201	PEB	C1A-NA	-3.50	1.33	1.37
96	f6	101	HEM	C4D-ND	-3.50	1.34	1.40
87	AN	818	CLA	C1D-ND	3.50	1.42	1.37
87	42	610	CLA	C4B-NB	3.50	1.42	1.37
87	c6	607	CLA	C1D-ND	3.50	1.42	1.37
82	AO	304	PEB	CHB-C1C	3.50	1.48	1.40
87	BL	602	CLA	C4D-ND	-3.50	1.32	1.37
82	AI	202	PEB	C1A-NA	-3.50	1.33	1.37
82	k1	201	PEB	C1A-NA	-3.50	1.33	1.37
82	OM	201	PEB	CHB-C1C	3.50	1.48	1.40
82	SQ	201	PEB	C2C-C3C	3.50	1.48	1.38
87	R2	204	CLA	C1D-ND	3.50	1.42	1.37
82	g4	201	PEB	CHB-C1C	3.50	1.48	1.40
82	OO	202	PEB	C2C-C3C	3.50	1.48	1.38
82	H1	1002	PEB	C2C-C3C	3.50	1.48	1.38
82	FP	202	PEB	C1A-NA	-3.50	1.33	1.37
82	cF	201	PEB	C1A-NA	-3.50	1.33	1.37
82	F7	203	PEB	C2C-C3C	3.50	1.48	1.38
82	A4	305	PEB	CHB-C1C	3.50	1.48	1.40
82	oK	201	PEB	CHB-C1C	3.50	1.48	1.40
82	GF	202	PEB	C1C-NC	-3.50	1.32	1.37
82	fJ	201	PEB	CHA-C1B	3.50	1.48	1.40
87	a6	607	CLA	C1D-ND	3.50	1.42	1.37
82	TQ	202	PEB	C2C-C3C	3.50	1.48	1.38
82	mM	202	PEB	C2C-C3C	3.50	1.48	1.38
87	A2	841	CLA	C4D-ND	-3.50	1.32	1.37
82	EP	202	PEB	C1A-NA	-3.50	1.33	1.37
82	f4	202	PEB	C1A-NA	-3.50	1.33	1.37
82	lH	201	PEB	C1A-NA	-3.50	1.33	1.37
82	L9	203	PEB	C2C-C3C	3.50	1.48	1.38
82	mO	201	PEB	C2C-C3C	3.50	1.48	1.38
82	NG	201	PEB	CHA-C1B	3.50	1.48	1.40
82	m4	202	PEB	CHA-C1B	3.50	1.48	1.40
82	H5	201	PEB	C2A-C1A	-3.50	1.49	1.52
82	J5	202	PEB	CHB-C1C	3.50	1.48	1.40
82	PQ	201	PEB	C1A-NA	-3.49	1.33	1.37
82	aG	202	PEB	C1A-NA	-3.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	j1	202	PEB	C2C-C3C	3.49	1.48	1.38
82	iH	202	PEB	CHB-C1C	3.49	1.48	1.40
82	kM	202	PEB	C2C-C3C	3.49	1.48	1.38
87	A2	807	CLA	C4D-ND	-3.49	1.32	1.37
82	AO	305	PEB	CHB-C1C	3.49	1.48	1.40
82	K7	201	PEB	CHB-C1C	3.49	1.48	1.40
82	mE	203	PEB	CHB-C1C	3.49	1.48	1.40
96	E6	101	HEM	C1B-NB	-3.49	1.34	1.40
82	JD	203	PEB	C1A-NA	-3.49	1.33	1.37
82	XI	202	PEB	C1A-NA	-3.49	1.33	1.37
82	OO	202	PEB	C1A-NA	-3.49	1.33	1.37
82	wF	303	PEB	C2C-C3C	3.49	1.48	1.38
82	VO	201	PEB	C2A-C1A	-3.49	1.49	1.52
82	aH	202	PEB	CHB-C1C	3.49	1.48	1.40
87	a6	609	CLA	C1D-ND	3.49	1.42	1.37
82	HD	203	PEB	CHA-C1B	3.49	1.48	1.40
83	AO	302	PUB	CHB-C4B	3.49	1.48	1.40
82	bF	201	PEB	C2C-C3C	3.49	1.48	1.38
82	TO	201	PEB	C1A-NA	-3.49	1.33	1.37
82	mF	202	PEB	C1A-NA	-3.49	1.33	1.37
82	aJ	203	PEB	CHA-C1B	3.49	1.48	1.40
82	kJ	201	PEB	C2C-C3C	3.49	1.48	1.38
87	b6	609	CLA	C4D-ND	-3.49	1.32	1.37
82	Q5	202	PEB	CHA-C1B	3.49	1.48	1.40
82	EA	202	PEB	C2C-C3C	3.49	1.48	1.38
82	RF	202	PEB	CHA-C1B	3.49	1.48	1.40
82	mG	202	PEB	C1A-NA	-3.49	1.33	1.37
82	jG	201	PEB	CHA-C1B	3.49	1.48	1.40
82	HM	202	PEB	CHB-C1C	3.49	1.48	1.40
82	mE	201	PEB	CHB-C1C	3.49	1.48	1.40
83	Y7	302	PUB	CHB-C4B	3.49	1.48	1.40
84	I4	1001	CYC	CHA-C4D	3.49	1.48	1.40
82	SO	202	PEB	CHA-C1B	3.49	1.48	1.40
82	RM	202	PEB	CHB-C1C	3.49	1.48	1.40
87	4N	602	CLA	C1D-ND	3.49	1.42	1.37
82	DA	201	PEB	C2C-C3C	3.49	1.48	1.38
82	wK	301	PEB	C1A-NA	-3.49	1.33	1.37
82	AQ	304	PEB	CHB-C1C	3.49	1.48	1.40
82	cE	202	PEB	C2C-C3C	3.49	1.48	1.38
82	s8	203	PEB	C2C-C3C	3.49	1.48	1.38
87	A6	402	CLA	C1D-ND	3.49	1.42	1.37
82	iM	202	PEB	C1A-NA	-3.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UE	201	PEB	CHB-C1C	3.49	1.48	1.40
82	RG	202	PEB	CHB-C1C	3.49	1.48	1.40
82	c4	201	PEB	CHA-C1B	3.49	1.48	1.40
82	iF	202	PEB	CHA-C1B	3.49	1.48	1.40
82	MP	202	PEB	CHB-C1C	3.49	1.48	1.40
82	s8	201	PEB	CHB-C1C	3.49	1.48	1.40
82	EI	202	PEB	C1A-NA	-3.49	1.33	1.37
82	hJ	203	PEB	C1A-NA	-3.49	1.33	1.37
82	iO	201	PEB	C1A-NA	-3.49	1.33	1.37
82	UG	201	PEB	CHB-C1C	3.49	1.48	1.40
82	WK	203	PEB	C2C-C3C	3.49	1.48	1.38
82	GA	202	PEB	CHB-C1C	3.49	1.48	1.40
82	S4	202	PEB	CHA-C1B	3.49	1.48	1.40
82	hE	203	PEB	C1A-NA	-3.49	1.33	1.37
82	g4	203	PEB	CHB-C1C	3.49	1.48	1.40
82	NG	201	PEB	C1A-NA	-3.49	1.33	1.37
82	HB	203	PEB	CHA-C1B	3.49	1.48	1.40
82	YI	201	PEB	CHA-C1B	3.49	1.48	1.40
82	WJ	202	PEB	CHA-C1B	3.49	1.48	1.40
82	QG	203	PEB	C1A-NA	-3.49	1.33	1.37
82	ZH	203	PEB	C1A-NA	-3.49	1.33	1.37
82	OK	202	PEB	C1A-NA	-3.49	1.33	1.37
82	cB	401	PEB	C1A-NA	-3.49	1.33	1.37
82	aJ	203	PEB	C1A-NA	-3.49	1.33	1.37
82	IJ	203	PEB	CHB-C1C	3.49	1.48	1.40
82	WH	203	PEB	CHA-C1B	3.49	1.48	1.40
82	L9	203	PEB	CHA-C1B	3.49	1.48	1.40
82	UD	201	PEB	C2C-C3C	3.49	1.48	1.38
82	dH	201	PEB	CHB-C1C	3.49	1.48	1.40
82	UM	203	PEB	C2C-C3C	3.49	1.48	1.38
87	52	611	CLA	C1D-ND	3.49	1.42	1.37
87	C6	519	CLA	C1D-ND	3.49	1.42	1.37
82	F4	1002	PEB	CHA-C1B	3.49	1.48	1.40
82	sC	203	PEB	C1A-NA	-3.49	1.33	1.37
87	BN	824	CLA	C4D-ND	-3.49	1.32	1.37
82	VE	201	PEB	CHA-C1B	3.48	1.48	1.40
82	J7	201	PEB	C1A-NA	-3.48	1.33	1.37
82	hK	201	PEB	CHB-C1C	3.48	1.48	1.40
84	EG	1001	CYC	CHA-C4D	3.48	1.48	1.40
82	1C	203	PEB	CHA-C1B	3.48	1.48	1.40
84	V3	1001	CYC	CHB-C4A	3.48	1.48	1.40
95	C6	503	DGD	O1G-C1A	3.48	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	EE	1001	CYC	C3D-C2D	3.48	1.48	1.38
82	fE	201	PEB	CHB-C1C	3.48	1.48	1.40
82	pF	202	PEB	CHB-C1C	3.48	1.48	1.40
82	AO	301	PEB	CHA-C1B	3.48	1.48	1.40
82	gO	202	PEB	CHA-C1B	3.48	1.48	1.40
82	RG	201	PEB	C2C-C3C	3.48	1.48	1.38
84	FE	1001	CYC	CHA-C4D	3.48	1.48	1.40
87	AN	822	CLA	C1D-ND	3.48	1.42	1.37
87	d6	403	CLA	C1D-ND	3.48	1.42	1.37
82	UE	203	PEB	CHA-C1B	3.48	1.48	1.40
91	D6	404	PHO	C3D-C2D	3.48	1.45	1.39
82	AK	202	PEB	C1A-NA	-3.48	1.33	1.37
82	r8	201	PEB	C1A-NA	-3.48	1.33	1.37
82	gH	202	PEB	C2C-C3C	3.48	1.48	1.38
82	OJ	201	PEB	CHA-C1B	3.48	1.48	1.40
82	aE	201	PEB	CHA-C1B	3.48	1.48	1.40
87	4N	604	CLA	C4B-NB	3.48	1.42	1.37
82	w8	204	PEB	C2C-C3C	3.48	1.48	1.38
82	wF	302	PEB	C2C-C3C	3.48	1.48	1.38
82	eG	201	PEB	C2C-C3C	3.48	1.48	1.38
84	D1	1003	CYC	C3D-C2D	3.48	1.48	1.38
82	VE	202	PEB	CHB-C1C	3.48	1.48	1.40
82	CM	202	PEB	CHA-C1B	3.48	1.48	1.40
82	EM	202	PEB	CHA-C1B	3.48	1.48	1.40
82	kO	201	PEB	CHA-C1B	3.48	1.48	1.40
82	RE	201	PEB	C2C-C3C	3.48	1.48	1.38
82	xK	303	PEB	CHA-C1B	3.48	1.48	1.40
82	cG	201	PEB	C1A-NA	-3.48	1.33	1.37
82	IA	202	PEB	C2C-C3C	3.48	1.48	1.38
82	E7	202	PEB	CHA-C1B	3.48	1.48	1.40
82	lH	202	PEB	C1A-NA	-3.48	1.33	1.37
82	PA	201	PEB	CHB-C1C	3.48	1.48	1.40
82	P7	201	PEB	CHB-C1C	3.48	1.48	1.40
82	U9	203	PEB	CHA-C1B	3.48	1.48	1.40
82	PO	201	PEB	C2C-C3C	3.48	1.48	1.38
82	PQ	202	PEB	C2C-C3C	3.48	1.48	1.38
82	A7	201	PEB	C2C-C3C	3.48	1.48	1.38
82	cJ	201	PEB	C2C-C3C	3.48	1.48	1.38
82	dE	203	PEB	C1A-NA	-3.48	1.33	1.37
82	mG	201	PEB	C1A-NA	-3.48	1.33	1.37
83	xK	305	PUB	CHB-C4B	3.48	1.48	1.40
82	TM	201	PEB	C2C-C3C	3.48	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MF	203	PEB	CHA-C1B	3.48	1.48	1.40
82	YK	203	PEB	CHA-C1B	3.48	1.48	1.40
87	AN	840	CLA	C4D-ND	-3.48	1.32	1.37
82	PE	201	PEB	C2A-C1A	-3.48	1.49	1.52
82	PH	201	PEB	C2A-C1A	-3.48	1.49	1.52
87	B6	616	CLA	C1D-ND	3.48	1.42	1.37
82	A1	302	PEB	CHB-C1C	3.48	1.48	1.40
82	aF	202	PEB	CHB-C1C	3.48	1.48	1.40
84	KH	1001	CYC	CHA-C4D	3.48	1.48	1.40
82	OG	202	PEB	C2C-C3C	3.48	1.48	1.38
82	II	202	PEB	C1A-NA	-3.48	1.33	1.37
82	c1	202	PEB	C1A-NA	-3.48	1.33	1.37
82	KQ	202	PEB	C2C-C3C	3.48	1.48	1.38
82	lM	203	PEB	CHB-C1C	3.48	1.48	1.40
87	B2	805	CLA	C4D-ND	-3.48	1.32	1.37
87	HL	101	CLA	C1D-ND	3.48	1.42	1.37
82	VG	202	PEB	CHB-C1C	3.48	1.48	1.40
82	QJ	204	PEB	CHB-C1C	3.48	1.48	1.40
82	aK	202	PEB	CHB-C1C	3.48	1.48	1.40
82	B7	201	PEB	C1A-NA	-3.48	1.33	1.37
82	QB	203	PEB	CHA-C1B	3.48	1.48	1.40
82	TA	201	PEB	C2C-C3C	3.48	1.48	1.38
82	T7	201	PEB	C2C-C3C	3.48	1.48	1.38
87	C6	516	CLA	C1D-ND	3.48	1.42	1.37
87	2N	305	CLA	C1D-ND	3.48	1.42	1.37
82	xF	304	PEB	CHA-C1B	3.48	1.48	1.40
82	g1	202	PEB	C2C-C3C	3.48	1.48	1.38
82	FB	201	PEB	C2A-C1A	-3.48	1.49	1.52
82	gM	201	PEB	C1A-NA	-3.48	1.33	1.37
87	BN	806	CLA	C4D-ND	-3.48	1.32	1.37
82	CF	203	PEB	CHA-C1B	3.48	1.48	1.40
82	A4	301	PEB	CHA-C1B	3.48	1.48	1.40
82	UQ	201	PEB	CHB-C1C	3.48	1.48	1.40
87	82	301	CLA	C1D-ND	3.48	1.42	1.37
82	A7	202	PEB	CHA-C1B	3.48	1.48	1.40
82	kM	201	PEB	C2C-C3C	3.48	1.48	1.38
87	42	603	CLA	C1D-ND	3.48	1.42	1.37
87	B6	615	CLA	C1D-ND	3.48	1.42	1.37
87	8N	302	CLA	C1D-ND	3.48	1.42	1.37
82	QE	203	PEB	C1A-NA	-3.48	1.33	1.37
82	kG	201	PEB	C1A-NA	-3.48	1.33	1.37
82	OI	203	PEB	CHB-C1C	3.48	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Y1	201	PEB	CHB-C1C	3.48	1.48	1.40
82	oK	203	PEB	C2C-C3C	3.48	1.48	1.38
82	lE	201	PEB	CHA-C1B	3.48	1.48	1.40
82	OO	202	PEB	CHB-C1C	3.47	1.48	1.40
82	PD	203	PEB	C1A-NA	-3.47	1.33	1.37
82	dB	202	PEB	C1A-NA	-3.47	1.33	1.37
82	wK	303	PEB	C1A-NA	-3.47	1.33	1.37
87	B2	823	CLA	C4D-ND	-3.47	1.32	1.37
82	AG	301	PEB	CHA-C1B	3.47	1.48	1.40
82	k1	201	PEB	CHA-C1B	3.47	1.48	1.40
82	jJ	202	PEB	C2C-C3C	3.47	1.48	1.38
82	EF	201	PEB	C1A-NA	-3.47	1.33	1.37
82	sC	201	PEB	C1A-NA	-3.47	1.33	1.37
82	nK	202	PEB	C1A-NA	-3.47	1.33	1.37
82	hM	202	PEB	C1A-NA	-3.47	1.33	1.37
87	B2	835	CLA	C1D-ND	3.47	1.42	1.37
82	WK	202	PEB	C2C-C3C	3.47	1.48	1.38
82	XM	201	PEB	C2C-C3C	3.47	1.48	1.38
82	PG	201	PEB	C2A-C1A	-3.47	1.49	1.52
82	k4	201	PEB	C2C-C3C	3.47	1.48	1.38
82	SP	201	PEB	CHA-C1B	3.47	1.48	1.40
82	HA	201	PEB	C1A-NA	-3.47	1.33	1.37
82	VG	202	PEB	C1A-NA	-3.47	1.33	1.37
82	S4	202	PEB	C1A-NA	-3.47	1.33	1.37
82	dG	201	PEB	CHB-C1C	3.47	1.48	1.40
82	P4	201	PEB	C2C-C3C	3.47	1.48	1.38
82	vK	201	PEB	C2A-C1A	-3.47	1.49	1.52
84	NE	201	CYC	C2C-C1C	-3.47	1.49	1.52
82	pC	201	PEB	CHA-C1B	3.47	1.48	1.40
82	hM	202	PEB	CHA-C1B	3.47	1.48	1.40
82	EF	202	PEB	C1A-NA	-3.47	1.33	1.37
82	e4	203	PEB	CHB-C1C	3.47	1.48	1.40
82	oK	202	PEB	CHB-C1C	3.47	1.48	1.40
87	CL	518	CLA	C1D-ND	3.47	1.42	1.37
87	RN	204	CLA	C1D-ND	3.47	1.42	1.37
87	a6	608	CLA	C1D-ND	3.47	1.42	1.37
87	b6	616	CLA	C1D-ND	3.47	1.42	1.37
82	SE	202	PEB	C1A-NA	-3.47	1.33	1.37
82	UP	202	PEB	C1A-NA	-3.47	1.33	1.37
87	AL	405	CLA	C4D-ND	-3.47	1.32	1.37
82	GJ	201	PEB	CHA-C1B	3.47	1.48	1.40
82	YP	501	PEB	CHB-C1C	3.47	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q5	202	PEB	CHB-C1C	3.47	1.48	1.40
87	8N	304	CLA	C1D-ND	3.47	1.42	1.37
82	w8	201	PEB	C2C-C3C	3.47	1.48	1.38
82	eE	201	PEB	C2C-C3C	3.47	1.48	1.38
82	f4	202	PEB	CHB-C1C	3.47	1.48	1.40
82	H9	202	PEB	CHB-C1C	3.47	1.48	1.40
87	B6	607	CLA	C1D-ND	3.47	1.42	1.37
82	A7	202	PEB	OD-C4D	3.47	1.30	1.23
82	EQ	201	PEB	C2A-C1A	-3.47	1.49	1.52
82	WM	202	PEB	CHA-C1B	3.47	1.48	1.40
82	EK	201	PEB	C1A-NA	-3.47	1.33	1.37
82	F1	1002	PEB	C2C-C3C	3.47	1.48	1.38
82	IP	201	PEB	CHB-C1C	3.47	1.48	1.40
87	42	602	CLA	C1D-ND	3.47	1.42	1.37
87	4N	601	CLA	C1D-ND	3.47	1.42	1.37
82	OQ	201	PEB	CHB-C1C	3.47	1.48	1.40
82	O1	202	PEB	CHB-C1C	3.47	1.48	1.40
82	fK	202	PEB	CHA-C1B	3.47	1.48	1.40
82	s8	203	PEB	C1A-NA	-3.47	1.33	1.37
87	A2	809	CLA	C4B-NB	3.47	1.42	1.37
82	YF	202	PEB	C2C-C3C	3.47	1.48	1.38
82	eK	203	PEB	CHB-C1C	3.47	1.48	1.40
82	iE	201	PEB	C1A-NA	-3.47	1.33	1.37
82	MA	202	PEB	C2C-C3C	3.47	1.48	1.38
87	CL	512	CLA	C1D-ND	3.47	1.42	1.37
87	52	610	CLA	C1D-ND	3.47	1.42	1.37
82	KD	202	PEB	C2C-C3C	3.47	1.48	1.38
82	TG	201	PEB	C2C-C3C	3.47	1.48	1.38
82	gB	202	PEB	C2C-C3C	3.47	1.48	1.38
83	AH	303	PUB	C4B-C3B	3.47	1.51	1.42
87	CL	509	CLA	C4D-ND	-3.47	1.32	1.37
82	YH	201	PEB	CHB-C1C	3.47	1.48	1.40
82	AM	302	PEB	CHB-C1C	3.47	1.48	1.40
82	fE	202	PEB	C2C-C3C	3.47	1.48	1.38
82	jG	202	PEB	C1A-NA	-3.47	1.33	1.37
87	8N	305	CLA	C1D-ND	3.47	1.42	1.37
82	rC	201	PEB	CHB-C1C	3.47	1.48	1.40
82	AD	304	PEB	CHA-C1B	3.47	1.48	1.40
82	DF	201	PEB	CHA-C1B	3.47	1.48	1.40
82	SP	202	PEB	CHB-C1C	3.47	1.48	1.40
87	B2	809	CLA	C1D-ND	3.47	1.42	1.37
82	XD	203	PEB	CHB-C1C	3.47	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	aG	201	PEB	CHA-C1B	3.47	1.48	1.40
82	gM	201	PEB	C2C-C3C	3.47	1.48	1.38
82	DF	202	PEB	CHB-C1C	3.47	1.48	1.40
82	OG	203	PEB	CHB-C1C	3.47	1.48	1.40
82	pF	201	PEB	CHB-C1C	3.47	1.48	1.40
82	oF	201	PEB	C2C-C3C	3.47	1.48	1.38
87	c6	613	CLA	C1D-ND	3.47	1.42	1.37
84	DE	1001	CYC	CHA-C4D	3.47	1.48	1.40
82	lF	203	PEB	CHA-C1B	3.47	1.48	1.40
82	hG	203	PEB	C1A-NA	-3.47	1.33	1.37
82	a1	202	PEB	CHB-C1C	3.47	1.48	1.40
87	B2	812	CLA	C1D-ND	3.47	1.42	1.37
82	PM	202	PEB	CHB-C1C	3.46	1.48	1.40
82	EB	501	PEB	CHA-C1B	3.46	1.48	1.40
82	SM	202	PEB	C1A-NA	-3.46	1.33	1.37
82	pC	202	PEB	C1A-NA	-3.46	1.33	1.37
82	dE	204	PEB	C1A-NA	-3.46	1.33	1.37
82	F5	201	PEB	C1C-NC	-3.46	1.32	1.37
82	g1	201	PEB	C2C-C3C	3.46	1.48	1.38
82	dG	202	PEB	CHA-C1B	3.46	1.48	1.40
82	QK	203	PEB	C4B-NB	-3.46	1.31	1.38
82	R1	201	PEB	C2C-C3C	3.46	1.48	1.38
82	P7	202	PEB	CHB-C1C	3.46	1.48	1.40
82	AO	304	PEB	C1A-NA	-3.46	1.33	1.37
82	mM	202	PEB	C1A-NA	-3.46	1.33	1.37
82	q8	202	PEB	CHA-C1B	3.46	1.48	1.40
82	FK	201	PEB	C2C-C3C	3.46	1.48	1.38
87	BN	830	CLA	C1D-ND	3.46	1.42	1.37
82	IK	201	PEB	CMB-C2B	-3.46	1.43	1.50
82	GJ	202	PEB	CHB-C1C	3.46	1.48	1.40
82	HI	203	PEB	CHA-C1B	3.46	1.48	1.40
82	lH	202	PEB	CHA-C1B	3.46	1.48	1.40
82	Y4	201	PEB	C2C-C3C	3.46	1.48	1.38
82	sK	201	PEB	C2C-C3C	3.46	1.48	1.38
82	MB	201	PEB	CHB-C1C	3.46	1.48	1.40
82	PD	202	PEB	CHB-C1C	3.46	1.48	1.40
82	ZF	201	PEB	CHB-C1C	3.46	1.48	1.40
82	hF	201	PEB	CHB-C1C	3.46	1.48	1.40
82	QD	201	PEB	C2C-C3C	3.46	1.48	1.38
82	XB	201	PEB	CHA-C1B	3.46	1.48	1.40
87	B2	821	CLA	C1D-ND	3.46	1.42	1.37
82	zC	202	PEB	CHB-C1C	3.46	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dK	201	PEB	C2C-C3C	3.46	1.48	1.38
84	C1	1001	CYC	C3D-C2D	3.46	1.48	1.38
82	L4	1002	PEB	CHB-C1C	3.46	1.48	1.40
87	RN	203	CLA	C1D-ND	3.46	1.42	1.37
87	B2	819	CLA	C1D-ND	3.46	1.42	1.37
82	HP	202	PEB	C1A-NA	-3.46	1.33	1.37
82	LM	201	PEB	C2C-C3C	3.46	1.48	1.38
82	cH	201	PEB	C2C-C3C	3.46	1.48	1.38
82	AE	304	PEB	CHA-C1B	3.46	1.48	1.40
82	KJ	203	PEB	CHB-C1C	3.46	1.48	1.40
87	BL	604	CLA	C1D-ND	3.46	1.42	1.37
87	82	306	CLA	C1D-ND	3.46	1.42	1.37
82	JO	1002	PEB	C1A-NA	-3.46	1.33	1.37
82	AP	202	PEB	C1A-NA	-3.46	1.33	1.37
84	F4	1001	CYC	CHB-C4A	3.46	1.48	1.40
82	KA	201	PEB	CHB-C1C	3.46	1.48	1.40
84	JH	1003	CYC	CHD-C1D	3.46	1.48	1.40
82	J9	201	PEB	C4B-C3B	3.46	1.51	1.45
82	cM	201	PEB	C2C-C3C	3.46	1.48	1.38
82	IJ	201	PEB	CHB-C1C	3.46	1.48	1.40
87	C6	514	CLA	C1D-ND	3.46	1.42	1.37
87	AN	825	CLA	C4D-ND	-3.46	1.32	1.37
82	JF	202	PEB	C2C-C3C	3.46	1.48	1.38
82	iO	201	PEB	CHB-C1C	3.46	1.48	1.40
82	VI	202	PEB	C1A-NA	-3.46	1.33	1.37
82	v8	202	PEB	C1A-NA	-3.46	1.33	1.37
82	vC	202	PEB	C1A-NA	-3.46	1.33	1.37
87	42	601	CLA	C1D-ND	3.46	1.42	1.37
82	BI	201	PEB	C2C-C3C	3.46	1.48	1.38
82	TQ	203	PEB	CHA-C1B	3.46	1.48	1.40
82	Y7	304	PEB	CHA-C1B	3.46	1.48	1.40
82	OE	203	PEB	CHB-C1C	3.46	1.48	1.40
82	K5	202	PEB	CHB-C1C	3.46	1.48	1.40
82	sF	202	PEB	C2C-C3C	3.46	1.48	1.38
82	fK	202	PEB	C2C-C3C	3.46	1.48	1.38
82	mE	202	PEB	CHA-C1B	3.46	1.48	1.40
82	lG	201	PEB	CHA-C1B	3.46	1.48	1.40
84	BE	1002	CYC	C1D-C2D	3.46	1.49	1.41
82	JQ	203	PEB	C1A-NA	-3.46	1.33	1.37
82	j4	203	PEB	C1A-NA	-3.46	1.33	1.37
87	AN	812	CLA	C1D-ND	3.46	1.42	1.37
82	gB	201	PEB	C2C-C3C	3.46	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mO	203	PEB	C2C-C3C	3.46	1.48	1.38
82	PO	203	PEB	C1A-NA	-3.46	1.33	1.37
82	EP	203	PEB	C1A-NA	-3.46	1.33	1.37
82	d4	202	PEB	C1A-NA	-3.46	1.33	1.37
87	BN	808	CLA	C4D-ND	-3.46	1.32	1.37
82	L7	201	PEB	C2A-C1A	-3.46	1.49	1.52
82	dG	204	PEB	C2C-C3C	3.46	1.48	1.38
82	NG	201	PEB	CHB-C1C	3.46	1.48	1.40
82	NQ	203	PEB	CHB-C1C	3.46	1.48	1.40
96	GN	201	HEM	CAC-C3C	3.46	1.56	1.47
82	CF	202	PEB	C2C-C3C	3.46	1.48	1.38
82	dF	201	PEB	C2C-C3C	3.46	1.48	1.38
82	lG	203	PEB	C2C-C3C	3.46	1.48	1.38
82	QI	201	PEB	CHB-C1C	3.46	1.48	1.40
82	i4	202	PEB	CHB-C1C	3.46	1.48	1.40
82	X5	202	PEB	CHB-C1C	3.46	1.48	1.40
87	A2	825	CLA	C4D-ND	-3.46	1.32	1.37
82	OH	202	PEB	C2C-C3C	3.46	1.48	1.38
83	xK	301	PUB	CHB-C4B	3.46	1.48	1.40
82	HH	1002	PEB	C2C-C3C	3.46	1.48	1.38
82	IM	203	PEB	CHA-C1B	3.46	1.48	1.40
82	M7	202	PEB	CHB-C1C	3.46	1.48	1.40
87	B2	812	CLA	C4D-ND	-3.46	1.32	1.37
82	KP	201	PEB	C1A-NA	-3.46	1.33	1.37
82	b1	202	PEB	CHA-C1B	3.45	1.48	1.40
84	x3	1001	CYC	CHB-C4A	3.45	1.48	1.40
84	GO	1001	CYC	C1D-C2D	3.45	1.49	1.41
84	JH	1003	CYC	C1C-NC	-3.45	1.33	1.37
87	B6	613	CLA	C1D-ND	3.45	1.42	1.37
82	M9	304	PEB	C2C-C3C	3.45	1.48	1.38
87	DL	403	CLA	C4D-ND	-3.45	1.32	1.37
84	EO	1001	CYC	CHA-C4D	3.45	1.48	1.40
82	18	203	PEB	C1A-NA	-3.45	1.33	1.37
87	A2	806	CLA	C1D-ND	3.45	1.42	1.37
82	mF	201	PEB	CHB-C1C	3.45	1.48	1.40
82	aM	202	PEB	CHB-C1C	3.45	1.48	1.40
82	OI	201	PEB	C2C-C3C	3.45	1.48	1.38
87	AN	807	CLA	C4D-ND	-3.45	1.32	1.37
82	TE	201	PEB	C2C-C3C	3.45	1.48	1.38
82	RA	202	PEB	CHB-C1C	3.45	1.48	1.40
82	eK	203	PEB	C1A-NA	-3.45	1.33	1.37
82	FM	201	PEB	C2C-C3C	3.45	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	wC	201	PEB	C2C-C3C	3.45	1.48	1.38
84	IG	1001	CYC	C3D-C2D	3.45	1.48	1.38
87	AN	809	CLA	C4B-NB	3.45	1.42	1.37
87	2N	306	CLA	C1D-ND	3.45	1.42	1.37
82	cK	203	PEB	C1A-NA	-3.45	1.33	1.37
87	4N	608	CLA	C1D-ND	3.45	1.42	1.37
82	MK	202	PEB	CHA-C1B	3.45	1.48	1.40
82	UA	201	PEB	CHB-C1C	3.45	1.48	1.40
87	B6	616	CLA	C3B-C4B	3.45	1.50	1.42
82	qF	203	PEB	C1A-NA	-3.45	1.33	1.37
82	w8	204	PEB	CHA-C1B	3.45	1.48	1.40
82	xF	302	PEB	CHA-C1B	3.45	1.48	1.40
82	YB	201	PEB	C2A-C1A	-3.45	1.49	1.52
82	TO	201	PEB	C2A-C1A	-3.45	1.49	1.52
82	AE	304	PEB	C2C-C3C	3.45	1.48	1.38
82	jG	202	PEB	C2C-C3C	3.45	1.48	1.38
82	iJ	202	PEB	C2C-C3C	3.45	1.48	1.38
87	1N	601	CLA	C1D-ND	3.45	1.42	1.37
82	BM	301	PEB	CHB-C1C	3.45	1.48	1.40
82	VA	203	PEB	C1A-NA	-3.45	1.33	1.37
82	J4	1002	PEB	C1A-NA	-3.45	1.33	1.37
82	UJ	201	PEB	CHB-C1C	3.45	1.48	1.40
82	fO	202	PEB	CHB-C1C	3.45	1.48	1.40
82	sC	201	PEB	C2C-C3C	3.45	1.48	1.38
82	UF	202	PEB	CHB-C1C	3.45	1.48	1.40
82	BB	203	PEB	CHA-C1B	3.45	1.48	1.40
82	xK	304	PEB	CHA-C1B	3.45	1.48	1.40
82	A4	305	PEB	C2C-C3C	3.45	1.48	1.38
87	A2	852	CLA	C4C-C3C	3.45	1.51	1.45
82	VD	203	PEB	C1A-NA	-3.45	1.33	1.37
82	QH	203	PEB	C1A-NA	-3.45	1.33	1.37
82	V5	202	PEB	CHB-C1C	3.45	1.48	1.40
82	qK	202	PEB	CHB-C1C	3.45	1.48	1.40
82	LE	1002	PEB	CHA-C1B	3.45	1.48	1.40
87	dL	401	CLA	C4D-ND	-3.45	1.33	1.37
87	12	607	CLA	C1D-ND	3.45	1.42	1.37
87	bL	619	CLA	C1D-ND	3.45	1.42	1.37
83	AM	304	PUB	C3B-C2B	3.45	1.48	1.38
82	K7	202	PEB	CHB-C1C	3.45	1.48	1.40
82	QM	204	PEB	CHA-C1B	3.45	1.48	1.40
82	J9	202	PEB	CHA-C1B	3.45	1.48	1.40
82	c1	201	PEB	C2C-C3C	3.45	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	Z9	302	PUB	OD-C4D	3.45	1.30	1.23
87	BL	603	CLA	C4D-ND	-3.45	1.33	1.37
87	B6	611	CLA	C1D-ND	3.45	1.42	1.37
82	cJ	202	PEB	C2C-C3C	3.45	1.48	1.38
82	AJ	302	PEB	C1A-NA	-3.45	1.33	1.37
82	VQ	203	PEB	C1A-NA	-3.45	1.33	1.37
82	fF	202	PEB	C2C-C3C	3.45	1.48	1.38
87	32	306	CLA	C4D-ND	-3.45	1.33	1.37
87	BN	835	CLA	C1D-ND	3.45	1.42	1.37
82	dE	201	PEB	CHB-C1C	3.45	1.48	1.40
82	KM	202	PEB	CHB-C1C	3.45	1.48	1.40
82	A1	305	PEB	CHB-C1C	3.45	1.48	1.40
82	hO	201	PEB	CHB-C1C	3.45	1.48	1.40
82	AE	301	PEB	CHA-C1B	3.45	1.48	1.40
82	GM	202	PEB	C2C-C3C	3.45	1.48	1.38
82	aB	201	PEB	C2C-C3C	3.45	1.48	1.38
82	O1	203	PEB	C1A-NA	-3.45	1.33	1.37
82	YG	202	PEB	CHB-C1C	3.45	1.48	1.40
82	fH	202	PEB	CHB-C1C	3.45	1.48	1.40
82	OD	201	PEB	C2C-C3C	3.45	1.48	1.38
82	e1	201	PEB	C2C-C3C	3.45	1.48	1.38
82	XP	202	PEB	CHB-C1C	3.45	1.48	1.40
82	S1	202	PEB	CHA-C1B	3.45	1.48	1.40
82	OM	201	PEB	C2A-C1A	-3.45	1.49	1.52
82	M7	202	PEB	C2C-C3C	3.45	1.48	1.38
82	R5	202	PEB	CHB-C1C	3.45	1.48	1.40
87	A2	850	CLA	C1D-ND	3.45	1.42	1.37
82	eO	201	PEB	C1A-NA	-3.45	1.33	1.37
82	U5	202	PEB	CHB-C1C	3.45	1.48	1.40
82	uF	202	PEB	C2C-C3C	3.45	1.48	1.38
84	GO	1001	CYC	C3D-C2D	3.45	1.48	1.38
82	lJ	203	PEB	C1A-NA	-3.44	1.33	1.37
82	DF	201	PEB	C2A-C1A	-3.44	1.49	1.52
82	V5	201	PEB	C2A-C1A	-3.44	1.49	1.52
87	DL	404	CLA	C4D-ND	-3.44	1.33	1.37
82	SO	202	PEB	CHB-C1C	3.44	1.48	1.40
82	OQ	201	PEB	C1A-NA	-3.44	1.33	1.37
82	mO	201	PEB	C1A-NA	-3.44	1.33	1.37
84	M4	1001	CYC	C1C-NC	-3.44	1.33	1.37
82	VI	203	PEB	CHB-C4B	3.44	1.45	1.38
82	qF	202	PEB	CHB-C1C	3.44	1.48	1.40
96	G2	201	HEM	CAC-C3C	3.44	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	O9	203	PEB	C2C-C3C	3.44	1.48	1.38
82	hM	203	PEB	C2C-C3C	3.44	1.48	1.38
87	82	307	CLA	C1D-ND	3.44	1.42	1.37
87	A6	403	CLA	C1D-ND	3.44	1.42	1.37
82	HQ	203	PEB	CHA-C1B	3.44	1.48	1.40
82	jM	202	PEB	CHA-C1B	3.44	1.48	1.40
82	Z9	303	PEB	C2C-C3C	3.44	1.48	1.38
82	TF	201	PEB	CHB-C1C	3.44	1.48	1.40
82	TO	203	PEB	CHA-C1B	3.44	1.48	1.40
82	PQ	202	PEB	C2A-C1A	-3.44	1.49	1.52
82	MP	202	PEB	C2C-C3C	3.44	1.48	1.38
91	DL	405	PHO	C3A-C2A	-3.44	1.51	1.54
82	KB	304	PEB	CHB-C1C	3.44	1.48	1.40
82	NE	202	PEB	CHB-C1C	3.44	1.48	1.40
82	VJ	202	PEB	CHB-C1C	3.44	1.48	1.40
82	TP	202	PEB	CHB-C1C	3.44	1.48	1.40
82	V1	203	PEB	CHB-C1C	3.44	1.48	1.40
82	iG	202	PEB	CHB-C1C	3.44	1.48	1.40
87	BN	822	CLA	C1D-ND	3.44	1.42	1.37
87	62	313	CLA	C4B-NB	3.44	1.42	1.37
82	GP	201	PEB	CHA-C1B	3.44	1.48	1.40
87	3N	307	CLA	C4D-ND	-3.44	1.33	1.37
82	KI	203	PEB	C1A-NA	-3.44	1.33	1.37
82	QM	204	PEB	C2C-C3C	3.44	1.48	1.38
84	DH	1003	CYC	C3D-C2D	3.44	1.48	1.38
82	UF	201	PEB	C1C-NC	-3.44	1.32	1.37
82	PA	202	PEB	CHB-C1C	3.44	1.48	1.40
82	U7	201	PEB	CHB-C1C	3.44	1.48	1.40
87	22	610	CLA	C1D-ND	3.44	1.42	1.37
82	CM	202	PEB	C2C-C3C	3.44	1.48	1.38
82	cM	202	PEB	C2C-C3C	3.44	1.48	1.38
82	TD	203	PEB	CHA-C1B	3.44	1.48	1.40
82	rK	201	PEB	CHA-C1B	3.44	1.48	1.40
83	YA	302	PUB	CHB-C4B	3.44	1.48	1.40
87	BN	813	CLA	C4D-ND	-3.44	1.33	1.37
82	YO	201	PEB	C2C-C3C	3.44	1.48	1.38
84	EG	1001	CYC	C3D-C2D	3.44	1.48	1.38
82	UH	201	PEB	C1A-NA	-3.44	1.33	1.37
82	XM	201	PEB	C1A-NA	-3.44	1.33	1.37
82	SJ	201	PEB	CHB-C1C	3.44	1.48	1.40
82	E9	202	PEB	CHB-C1C	3.44	1.48	1.40
82	TK	202	PEB	C2C-C3C	3.44	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	P5	202	PEB	CHB-C1C	3.44	1.48	1.40
82	dM	202	PEB	C2C-C3C	3.44	1.48	1.38
84	CH	1001	CYC	C3D-C2D	3.44	1.48	1.38
82	jM	203	PEB	C1A-NA	-3.44	1.33	1.37
82	V9	202	PEB	CHB-C1C	3.44	1.48	1.40
82	hE	203	PEB	CHB-C1C	3.44	1.48	1.40
82	cJ	202	PEB	CHB-C1C	3.44	1.48	1.40
82	AJ	301	PEB	C1A-NA	-3.44	1.33	1.37
82	cB	402	PEB	C1A-NA	-3.44	1.33	1.37
82	cE	201	PEB	C1A-NA	-3.44	1.33	1.37
82	eE	203	PEB	C1A-NA	-3.44	1.33	1.37
84	MO	1001	CYC	C1D-C2D	3.44	1.49	1.41
82	LI	202	PEB	CHA-C1B	3.44	1.48	1.40
87	3N	311	CLA	C4B-NB	3.44	1.42	1.37
82	ZJ	202	PEB	CHB-C1C	3.44	1.48	1.40
82	BP	202	PEB	CHB-C1C	3.44	1.48	1.40
82	jE	201	PEB	CHA-C1B	3.44	1.48	1.40
82	OI	203	PEB	C1A-NA	-3.44	1.33	1.37
82	U9	203	PEB	C1A-NA	-3.44	1.33	1.37
82	DM	202	PEB	CHB-C1C	3.44	1.48	1.40
82	bK	201	PEB	CHB-C1C	3.44	1.48	1.40
82	PF	202	PEB	CHC-C4C	3.44	1.53	1.49
82	WF	203	PEB	C2C-C3C	3.44	1.48	1.38
82	m4	203	PEB	C2C-C3C	3.44	1.48	1.38
82	IP	203	PEB	C1A-NA	-3.44	1.33	1.37
82	EJ	202	PEB	C2A-C1A	-3.44	1.49	1.52
87	72	602	CLA	C1D-C2D	3.44	1.52	1.45
87	cL	517	CLA	C4B-NB	3.44	1.42	1.37
82	VA	201	PEB	CHB-C1C	3.44	1.48	1.40
82	YO	202	PEB	CHB-C1C	3.44	1.48	1.40
82	fM	201	PEB	C2C-C3C	3.44	1.48	1.38
82	SH	202	PEB	CHA-C1B	3.44	1.48	1.40
82	iF	203	PEB	CHA-C1B	3.44	1.48	1.40
83	A1	304	PUB	CHB-C4B	3.44	1.48	1.40
83	Z9	305	PUB	CHB-C4B	3.44	1.48	1.40
82	CB	202	PEB	C2C-C3C	3.44	1.48	1.38
87	BN	824	CLA	C1D-ND	3.44	1.42	1.37
82	Q1	203	PEB	CHB-C1C	3.44	1.48	1.40
82	WB	401	PEB	CHA-C1B	3.44	1.48	1.40
82	KJ	202	PEB	CHA-C1B	3.44	1.48	1.40
82	hG	203	PEB	CHB-C1C	3.44	1.48	1.40
82	cK	202	PEB	CHB-C1C	3.44	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	814	CLA	C1D-ND	3.43	1.42	1.37
82	iO	202	PEB	CHB-C1C	3.43	1.48	1.40
82	WI	201	PEB	C2C-C3C	3.43	1.48	1.38
82	SJ	202	PEB	C2C-C3C	3.43	1.48	1.38
82	bK	201	PEB	C2C-C3C	3.43	1.48	1.38
82	UA	201	PEB	CHA-C1B	3.43	1.48	1.40
82	O5	201	PEB	CHA-C1B	3.43	1.48	1.40
82	VP	201	PEB	CHB-C1C	3.43	1.48	1.40
82	QF	203	PEB	C4B-NB	-3.43	1.31	1.38
87	6N	612	CLA	C4B-NB	3.43	1.42	1.37
82	kM	201	PEB	C1A-NA	-3.43	1.33	1.37
82	QQ	201	PEB	C2C-C3C	3.43	1.48	1.38
82	1C	203	PEB	C2C-C3C	3.43	1.48	1.38
82	dE	204	PEB	C2C-C3C	3.43	1.48	1.38
84	IE	1001	CYC	C3D-C2D	3.43	1.48	1.38
87	CL	510	CLA	C4D-ND	-3.43	1.33	1.37
82	lK	203	PEB	CHA-C1B	3.43	1.48	1.40
82	AE	301	PEB	C2C-C3C	3.43	1.48	1.38
87	C6	520	CLA	C1D-ND	3.43	1.42	1.37
83	AH	304	PUB	CHB-C4B	3.43	1.48	1.40
82	JA	201	PEB	C1A-NA	-3.43	1.33	1.37
82	ZB	202	PEB	C1A-NA	-3.43	1.33	1.37
82	VH	201	PEB	C2C-C3C	3.43	1.48	1.38
82	XM	202	PEB	C2C-C3C	3.43	1.48	1.38
82	iE	201	PEB	C2C-C3C	3.43	1.48	1.38
83	AJ	304	PUB	C3B-C2B	3.43	1.48	1.38
87	BL	623	CLA	C1D-ND	3.43	1.42	1.37
87	8N	301	CLA	C1D-ND	3.43	1.42	1.37
82	O9	201	PEB	CHB-C1C	3.43	1.48	1.40
82	kE	202	PEB	CHB-C1C	3.43	1.48	1.40
83	AE	303	PUB	CHB-C4B	3.43	1.48	1.40
82	TB	202	PEB	CHC-C4C	3.43	1.53	1.49
82	d1	202	PEB	C2C-C3C	3.43	1.48	1.38
82	v8	201	PEB	C1A-NA	-3.43	1.33	1.37
82	fO	202	PEB	C1A-NA	-3.43	1.33	1.37
82	PM	202	PEB	C2C-C3C	3.43	1.48	1.38
82	A1	302	PEB	C2C-C3C	3.43	1.48	1.38
82	ZK	201	PEB	CHA-C1B	3.43	1.48	1.40
82	wC	204	PEB	CHA-C1B	3.43	1.48	1.40
82	OJ	202	PEB	CHB-C1C	3.43	1.48	1.40
84	K1	1001	CYC	CHA-C4D	3.43	1.48	1.40
82	KB	301	PEB	C2A-C1A	-3.43	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NE	202	PEB	C2C-C3C	3.43	1.48	1.38
82	GI	203	PEB	C2C-C3C	3.43	1.48	1.38
82	W7	201	PEB	CHB-C1C	3.43	1.48	1.40
87	AN	824	CLA	C1D-ND	3.43	1.42	1.37
82	cG	201	PEB	C2C-C3C	3.43	1.48	1.38
82	SE	202	PEB	CHB-C1C	3.43	1.48	1.40
82	CK	203	PEB	CHA-C1B	3.43	1.48	1.40
82	CP	201	PEB	C2C-C3C	3.43	1.48	1.38
82	DF	202	PEB	C2A-C1A	-3.43	1.49	1.52
82	D7	203	PEB	C2C-C3C	3.43	1.48	1.38
82	LJ	202	PEB	CHB-C1C	3.43	1.48	1.40
82	EA	201	PEB	CHA-C1B	3.43	1.48	1.40
82	jJ	201	PEB	C2C-C3C	3.43	1.48	1.38
87	12	601	CLA	C1D-ND	3.43	1.42	1.37
82	QB	203	PEB	CHB-C1C	3.43	1.48	1.40
82	C5	202	PEB	CHB-C1C	3.43	1.48	1.40
82	AM	301	PEB	C2C-C3C	3.43	1.48	1.38
82	i1	201	PEB	CHA-C1B	3.43	1.48	1.40
82	AP	202	PEB	CHB-C1C	3.43	1.48	1.40
84	MO	1001	CYC	CHA-C4D	3.43	1.48	1.40
87	LN	203	CLA	C4D-ND	-3.43	1.33	1.37
82	UO	202	PEB	C1A-NA	-3.43	1.33	1.37
82	U4	202	PEB	C1A-NA	-3.43	1.33	1.37
82	Z9	303	PEB	C1A-NA	-3.43	1.33	1.37
87	AN	833	CLA	C1D-ND	3.43	1.42	1.37
87	b6	610	CLA	C1D-ND	3.43	1.42	1.37
82	VI	202	PEB	C2C-C3C	3.43	1.48	1.38
82	N5	202	PEB	CHB-C1C	3.43	1.48	1.40
82	eB	201	PEB	CHB-C1C	3.43	1.48	1.40
82	DA	203	PEB	C2C-C3C	3.43	1.48	1.38
82	DJ	202	PEB	C2C-C3C	3.43	1.48	1.38
82	cG	201	PEB	CHB-C1C	3.43	1.48	1.40
82	dK	202	PEB	CHB-C1C	3.43	1.48	1.40
83	A4	302	PUB	CHB-C4B	3.43	1.48	1.40
82	XF	201	PEB	CHA-C1B	3.43	1.48	1.40
82	pK	202	PEB	C2C-C3C	3.43	1.48	1.38
87	B2	836	CLA	C4D-ND	-3.43	1.33	1.37
82	EP	203	PEB	CHB-C1C	3.43	1.48	1.40
82	fO	201	PEB	CHB-C1C	3.43	1.48	1.40
82	RO	202	PEB	CHA-C1B	3.43	1.48	1.40
82	a4	202	PEB	CHA-C1B	3.43	1.48	1.40
82	H9	202	PEB	CHA-C1B	3.43	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	rK	201	PEB	C2C-C3C	3.43	1.48	1.38
82	PQ	202	PEB	CHB-C1C	3.43	1.48	1.40
84	BE	1002	CYC	C1B-NB	-3.43	1.32	1.37
82	dE	202	PEB	CHA-C1B	3.43	1.48	1.40
82	xF	303	PEB	CHA-C1B	3.43	1.48	1.40
82	hK	201	PEB	C2C-C3C	3.43	1.48	1.38
82	AF	202	PEB	C1A-NA	-3.43	1.33	1.37
82	YQ	201	PEB	C1A-NA	-3.43	1.33	1.37
82	eA	301	PEB	C1A-NA	-3.43	1.33	1.37
83	wF	304	PUB	CHB-C4B	3.43	1.48	1.40
84	LE	1001	CYC	CHA-C4D	3.43	1.48	1.40
84	LG	1001	CYC	CHA-C4D	3.43	1.48	1.40
87	B6	603	CLA	C1D-ND	3.43	1.42	1.37
87	C6	517	CLA	C1D-ND	3.43	1.42	1.37
87	b6	604	CLA	C1D-ND	3.43	1.42	1.37
82	CJ	202	PEB	CHA-C1B	3.43	1.48	1.40
82	hJ	202	PEB	CHA-C1B	3.43	1.48	1.40
82	DM	201	PEB	C2C-C3C	3.43	1.48	1.38
82	JM	202	PEB	C2C-C3C	3.43	1.48	1.38
82	AO	305	PEB	C2C-C3C	3.43	1.48	1.38
82	RD	203	PEB	C1A-NA	-3.43	1.33	1.37
82	MP	203	PEB	C1A-NA	-3.43	1.33	1.37
82	PQ	203	PEB	C1A-NA	-3.43	1.33	1.37
87	AN	806	CLA	C1D-ND	3.43	1.42	1.37
87	C6	518	CLA	C1D-ND	3.43	1.42	1.37
87	c6	609	CLA	C1D-ND	3.43	1.42	1.37
82	OP	202	PEB	CHB-C1C	3.43	1.48	1.40
82	MD	201	PEB	C2C-C3C	3.43	1.48	1.38
82	hM	202	PEB	C2C-C3C	3.43	1.48	1.38
84	BG	1002	CYC	C1D-C2D	3.42	1.49	1.41
82	JI	201	PEB	CHB-C1C	3.42	1.48	1.40
82	P9	202	PEB	CHB-C1C	3.42	1.48	1.40
82	ND	204	PEB	C1A-NA	-3.42	1.33	1.37
87	3N	303	CLA	C4B-NB	3.42	1.42	1.37
82	cO	201	PEB	CHB-C1C	3.42	1.48	1.40
82	18	203	PEB	C2C-C3C	3.42	1.48	1.38
82	W1	201	PEB	C1A-NA	-3.42	1.33	1.37
82	c1	201	PEB	CHA-C1B	3.42	1.48	1.40
82	fJ	201	PEB	CHB-C1C	3.42	1.48	1.40
82	E7	201	PEB	CHA-C1B	3.42	1.48	1.40
82	u8	202	PEB	CHA-C1B	3.42	1.48	1.40
82	NI	202	PEB	C2C-C3C	3.42	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DK	202	PEB	CHB-C1C	3.42	1.48	1.40
82	TQ	203	PEB	CHB-C1C	3.42	1.48	1.40
83	QM	201	PUB	CHB-C4B	3.42	1.48	1.40
82	b1	202	PEB	C1A-NA	-3.42	1.33	1.37
84	DG	1001	CYC	CHA-C4D	3.42	1.48	1.40
82	RI	202	PEB	C2C-C3C	3.42	1.48	1.38
82	HM	201	PEB	C2C-C3C	3.42	1.48	1.38
82	EA	202	PEB	CHA-C1B	3.42	1.48	1.40
84	E4	1001	CYC	C1D-C2D	3.42	1.49	1.41
82	KB	304	PEB	C1A-NA	-3.42	1.33	1.37
82	M9	301	PEB	C1A-NA	-3.42	1.33	1.37
82	f4	201	PEB	CHB-C1C	3.42	1.48	1.40
82	BB	202	PEB	C2A-C1A	-3.42	1.49	1.52
82	CK	202	PEB	C2C-C3C	3.42	1.48	1.38
82	iM	201	PEB	C2C-C3C	3.42	1.48	1.38
82	wC	202	PEB	CHA-C1B	3.42	1.48	1.40
82	dE	204	PEB	CHA-C1B	3.42	1.48	1.40
87	A2	812	CLA	C1D-ND	3.42	1.42	1.37
84	DH	1003	CYC	CHA-C4D	3.42	1.48	1.40
82	DG	1002	PEB	CHA-C1B	3.42	1.48	1.40
82	A7	201	PEB	CHA-C1B	3.42	1.48	1.40
84	Q3	1001	CYC	O1D-CGD	3.42	1.33	1.22
82	QF	202	PEB	C1A-NA	-3.42	1.33	1.37
82	jO	202	PEB	C1A-NA	-3.42	1.33	1.37
82	FH	1002	PEB	C2A-C1A	-3.42	1.49	1.52
82	AH	302	PEB	C2C-C3C	3.42	1.48	1.38
84	H1	1001	CYC	CHA-C4D	3.42	1.48	1.40
82	PK	202	PEB	CHC-C4C	3.42	1.53	1.49
82	MK	203	PEB	CHA-C1B	3.42	1.48	1.40
82	HO	1002	PEB	CHA-C1B	3.42	1.48	1.40
82	xK	302	PEB	CHA-C1B	3.42	1.48	1.40
82	g4	201	PEB	C2C-C3C	3.42	1.48	1.38
84	HO	1001	CYC	C1D-C2D	3.42	1.49	1.41
82	AH	305	PEB	CHB-C1C	3.42	1.48	1.40
87	RN	203	CLA	C4D-ND	-3.42	1.33	1.37
82	NM	202	PEB	C2C-C3C	3.42	1.48	1.38
82	YP	501	PEB	C2C-C3C	3.42	1.48	1.38
82	lK	202	PEB	C2C-C3C	3.42	1.48	1.38
82	AE	301	PEB	CHB-C1C	3.42	1.48	1.40
82	DK	202	PEB	C1A-NA	-3.42	1.33	1.37
82	RO	202	PEB	C2A-C1A	-3.42	1.49	1.52
82	pK	201	PEB	CHA-C1B	3.42	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WB	401	PEB	C2C-C3C	3.42	1.48	1.38
82	mE	202	PEB	C1A-NA	-3.42	1.33	1.37
82	EI	202	PEB	C2C-C3C	3.42	1.48	1.38
87	C6	517	CLA	C4D-ND	-3.42	1.33	1.37
82	ZB	201	PEB	CHB-C1C	3.42	1.48	1.40
87	A6	404	CLA	C1D-ND	3.42	1.42	1.37
82	W1	203	PEB	CHA-C1B	3.42	1.48	1.40
82	CJ	203	PEB	CHB-C1C	3.42	1.48	1.40
82	A5	202	PEB	CHB-C1C	3.42	1.48	1.40
82	SH	202	PEB	C1A-NA	-3.42	1.33	1.37
82	p8	202	PEB	C1A-NA	-3.42	1.33	1.37
82	ZB	203	PEB	C2C-C3C	3.42	1.48	1.38
82	JD	201	PEB	C2C-C3C	3.42	1.48	1.38
82	OM	202	PEB	CHA-C1B	3.42	1.48	1.40
82	RB	202	PEB	CHB-C1C	3.42	1.48	1.40
82	HO	1002	PEB	CHB-C1C	3.42	1.48	1.40
82	NG	201	PEB	C2C-C3C	3.42	1.48	1.38
82	LM	201	PEB	C1C-NC	-3.42	1.32	1.37
87	A2	833	CLA	C1D-ND	3.42	1.42	1.37
82	AJ	301	PEB	C2C-C3C	3.42	1.48	1.38
82	YK	203	PEB	C1A-NA	-3.42	1.33	1.37
82	OE	202	PEB	CHB-C1C	3.42	1.48	1.40
82	AG	301	PEB	CHB-C1C	3.42	1.48	1.40
82	BI	202	PEB	CHB-C1C	3.42	1.48	1.40
87	bL	618	CLA	C4D-ND	-3.42	1.33	1.37
82	TD	202	PEB	C2C-C3C	3.42	1.48	1.38
82	QD	202	PEB	CHB-C1C	3.42	1.48	1.40
82	eF	203	PEB	CHB-C1C	3.42	1.48	1.40
87	42	608	CLA	C1D-ND	3.42	1.42	1.37
87	C6	509	CLA	C1D-ND	3.42	1.42	1.37
87	2N	310	CLA	C1D-ND	3.42	1.42	1.37
82	cK	201	PEB	C1A-NA	-3.42	1.33	1.37
82	FJ	202	PEB	CHB-C1C	3.42	1.48	1.40
82	I5	202	PEB	CHB-C1C	3.42	1.48	1.40
82	C9	202	PEB	CHB-C1C	3.42	1.48	1.40
82	AK	202	PEB	C2C-C3C	3.42	1.48	1.38
82	T5	202	PEB	CHB-C1C	3.42	1.48	1.40
82	aK	203	PEB	CHB-C1C	3.42	1.48	1.40
82	XI	202	PEB	C2C-C3C	3.42	1.48	1.38
82	RM	201	PEB	CHB-C1C	3.42	1.48	1.40
82	eM	202	PEB	CHB-C1C	3.42	1.48	1.40
82	dJ	202	PEB	C2C-C3C	3.42	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NB	202	PEB	CHB-C1C	3.42	1.48	1.40
82	FH	1002	PEB	C2C-C3C	3.42	1.48	1.38
82	VE	202	PEB	C1A-NA	-3.42	1.33	1.37
82	w8	204	PEB	C1A-NA	-3.42	1.33	1.37
82	O9	201	PEB	C1A-NA	-3.42	1.33	1.37
87	AN	837	CLA	C4D-ND	-3.42	1.33	1.37
82	TK	201	PEB	CHB-C1C	3.42	1.48	1.40
82	YP	503	PEB	CHB-C1C	3.42	1.48	1.40
82	CI	202	PEB	C2C-C3C	3.42	1.48	1.38
82	O1	202	PEB	C2C-C3C	3.42	1.48	1.38
82	eM	202	PEB	C2C-C3C	3.42	1.48	1.38
82	SB	202	PEB	CHA-C1B	3.41	1.48	1.40
82	MP	203	PEB	CHA-C1B	3.41	1.48	1.40
82	WA	201	PEB	CHB-C1C	3.41	1.48	1.40
87	62	312	CLA	C4B-NB	3.41	1.42	1.37
82	FB	201	PEB	C1A-NA	-3.41	1.33	1.37
82	HD	201	PEB	C1A-NA	-3.41	1.33	1.37
84	H4	1001	CYC	C1D-C2D	3.41	1.49	1.41
82	aJ	201	PEB	CHA-C1B	3.41	1.48	1.40
82	SQ	202	PEB	C2C-C3C	3.41	1.48	1.38
82	g4	203	PEB	C2C-C3C	3.41	1.48	1.38
82	E5	202	PEB	CHB-C1C	3.41	1.48	1.40
82	gK	203	PEB	CHA-C1B	3.41	1.48	1.40
82	ZE	203	PEB	C2C-C3C	3.41	1.48	1.38
87	BN	810	CLA	C1D-ND	3.41	1.42	1.37
87	4N	604	CLA	CMD-C2D	3.41	1.58	1.50
82	RM	202	PEB	C2C-C3C	3.41	1.48	1.38
83	AG	303	PUB	C3B-C2B	3.41	1.48	1.38
82	eA	301	PEB	CHB-C1C	3.41	1.48	1.40
84	h3	1001	CYC	O1D-CGD	3.41	1.33	1.22
82	NA	201	PEB	CHB-C1C	3.41	1.48	1.40
82	f1	202	PEB	CHB-C1C	3.41	1.48	1.40
84	I3	1001	CYC	O1D-CGD	3.41	1.33	1.22
82	PB	201	PEB	CHA-C1B	3.41	1.48	1.40
82	AD	301	PEB	C2C-C3C	3.41	1.48	1.38
87	a6	609	CLA	C4D-ND	-3.41	1.33	1.37
82	iG	202	PEB	C1A-NA	-3.41	1.33	1.37
82	EM	203	PEB	CHA-C1B	3.41	1.48	1.40
82	W5	203	PEB	CHA-C1B	3.41	1.48	1.40
82	aF	203	PEB	CHB-C1C	3.41	1.48	1.40
82	pK	201	PEB	CHB-C1C	3.41	1.48	1.40
87	BN	819	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	P1	201	PEB	C2A-C1A	-3.41	1.49	1.52
82	KA	201	PEB	C2C-C3C	3.41	1.48	1.38
82	iO	202	PEB	CHA-C1B	3.41	1.48	1.40
82	MM	203	PEB	CHB-C1C	3.41	1.48	1.40
91	DL	405	PHO	C3D-C2D	3.41	1.45	1.39
82	Y1	202	PEB	C1A-NA	-3.41	1.33	1.37
82	R5	202	PEB	C1A-NA	-3.41	1.33	1.37
82	O9	203	PEB	C1A-NA	-3.41	1.33	1.37
87	4N	602	CLA	C4B-NB	3.41	1.42	1.37
87	4N	603	CLA	C1D-ND	3.41	1.42	1.37
83	YA	302	PUB	C3B-C2B	3.41	1.47	1.38
82	PP	202	PEB	CHB-C1C	3.41	1.48	1.40
82	AM	301	PEB	CHA-C1B	3.41	1.48	1.40
82	JK	202	PEB	C2C-C3C	3.41	1.47	1.38
82	hF	201	PEB	C2C-C3C	3.41	1.47	1.38
87	KN	103	CLA	C1D-ND	3.41	1.42	1.37
82	I9	202	PEB	CHB-C1C	3.41	1.48	1.40
87	B2	807	CLA	C4D-ND	-3.41	1.33	1.37
82	AH	302	PEB	CHB-C1C	3.41	1.48	1.40
87	BN	820	CLA	C1D-ND	3.41	1.42	1.37
82	PJ	202	PEB	CHB-C1C	3.41	1.48	1.40
82	WF	203	PEB	CHA-C1B	3.41	1.48	1.40
82	WK	203	PEB	CHA-C1B	3.41	1.48	1.40
82	iG	201	PEB	C1A-NA	-3.41	1.33	1.37
82	JM	201	PEB	C2C-C3C	3.41	1.47	1.38
87	AN	852	CLA	C4C-C3C	3.41	1.50	1.45
82	JB	202	PEB	CHC-C4C	3.41	1.53	1.49
84	H3	1001	CYC	O1D-CGD	3.41	1.33	1.22
82	C7	201	PEB	CHB-C1C	3.41	1.48	1.40
82	ZK	202	PEB	CHA-C1B	3.41	1.48	1.40
82	dG	204	PEB	CHA-C1B	3.41	1.48	1.40
82	lF	202	PEB	C2C-C3C	3.41	1.47	1.38
82	gO	203	PEB	C2C-C3C	3.41	1.47	1.38
82	X9	202	PEB	CHB-C1C	3.41	1.48	1.40
82	CP	203	PEB	C1A-NA	-3.41	1.33	1.37
82	U1	203	PEB	C1A-NA	-3.41	1.33	1.37
82	dO	202	PEB	C1A-NA	-3.41	1.33	1.37
84	FO	1001	CYC	CHB-C4A	3.41	1.48	1.40
84	73	1001	CYC	O1D-CGD	3.41	1.33	1.22
84	LE	1001	CYC	C1D-C2D	3.41	1.49	1.41
84	HO	1001	CYC	CHA-C4D	3.41	1.48	1.40
82	AP	201	PEB	CHA-C1B	3.41	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SP	201	PEB	C2C-C3C	3.41	1.47	1.38
82	gO	201	PEB	C2C-C3C	3.41	1.47	1.38
103	8N	310	ZEX	C1-C6	-3.41	1.49	1.53
82	dG	204	PEB	C1A-NA	-3.41	1.33	1.37
84	I4	1001	CYC	C1C-NC	-3.41	1.33	1.37
82	DK	202	PEB	C2A-C1A	-3.41	1.49	1.52
82	zF	501	PEB	C2C-C3C	3.41	1.47	1.38
87	L2	203	CLA	C1D-ND	3.41	1.42	1.37
82	P4	201	PEB	CHB-C1C	3.41	1.48	1.40
82	MF	202	PEB	CHA-C1B	3.41	1.48	1.40
82	l1	203	PEB	C1A-NA	-3.41	1.33	1.37
82	TI	203	PEB	C2C-C3C	3.41	1.47	1.38
84	B3	1001	CYC	O1D-CGD	3.41	1.33	1.22
82	SQ	202	PEB	CHB-C1C	3.41	1.48	1.40
82	AQ	304	PEB	CHA-C1B	3.41	1.48	1.40
82	S1	201	PEB	CHA-C1B	3.41	1.48	1.40
84	N4	1001	CYC	C1D-C2D	3.41	1.49	1.41
87	42	602	CLA	C4B-NB	3.41	1.42	1.37
87	d6	401	CLA	C1D-ND	3.41	1.42	1.37
87	aL	606	CLA	C1D-ND	3.41	1.42	1.37
84	q3	1001	CYC	O1D-CGD	3.41	1.33	1.22
82	s8	201	PEB	C2C-C3C	3.41	1.47	1.38
82	VH	202	PEB	CHB-C1C	3.41	1.48	1.40
82	IM	203	PEB	CHB-C1C	3.41	1.48	1.40
82	LO	1002	PEB	CHA-C1B	3.41	1.48	1.40
82	U7	201	PEB	CHA-C1B	3.41	1.48	1.40
82	YF	201	PEB	C1A-NA	-3.41	1.33	1.37
82	CA	201	PEB	CHB-C1C	3.41	1.48	1.40
82	GF	203	PEB	CHB-C1C	3.41	1.48	1.40
82	eE	202	PEB	CHA-C1B	3.41	1.48	1.40
87	B2	828	CLA	C1D-ND	3.41	1.42	1.37
84	f3	1001	CYC	O1D-CGD	3.41	1.33	1.22
82	OD	202	PEB	CHB-C1C	3.41	1.48	1.40
82	GP	201	PEB	CHB-C1C	3.41	1.48	1.40
82	R7	202	PEB	CHB-C1C	3.41	1.48	1.40
82	mG	202	PEB	CHA-C1B	3.41	1.48	1.40
82	DM	202	PEB	C2C-C3C	3.41	1.47	1.38
82	iH	201	PEB	C2C-C3C	3.41	1.47	1.38
84	j3	1001	CYC	O1D-CGD	3.40	1.33	1.22
82	AG	304	PEB	C2C-C3C	3.40	1.47	1.38
82	I7	201	PEB	CHA-C1B	3.40	1.48	1.40
87	AN	841	CLA	C4D-ND	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	H4	1001	CYC	CHA-C4D	3.40	1.48	1.40
82	PI	202	PEB	C2C-C3C	3.40	1.47	1.38
82	aM	201	PEB	CHA-C1B	3.40	1.48	1.40
82	H5	203	PEB	CHB-C1C	3.40	1.48	1.40
82	JQ	201	PEB	C2C-C3C	3.40	1.47	1.38
82	bG	201	PEB	C2C-C3C	3.40	1.47	1.38
82	OK	203	PEB	C1A-NA	-3.40	1.33	1.37
82	dE	201	PEB	C1A-NA	-3.40	1.33	1.37
82	YF	203	PEB	CHA-C1B	3.40	1.48	1.40
83	AO	303	PUB	CHB-C4B	3.40	1.48	1.40
83	A1	303	PUB	C4B-C3B	3.40	1.50	1.42
82	AQ	301	PEB	C2C-C3C	3.40	1.47	1.38
82	b4	202	PEB	C2C-C3C	3.40	1.47	1.38
82	kH	201	PEB	C2C-C3C	3.40	1.47	1.38
82	GP	201	PEB	C1A-NA	-3.40	1.33	1.37
84	EO	1001	CYC	C1D-C2D	3.40	1.49	1.41
82	II	202	PEB	C2C-C3C	3.40	1.47	1.38
84	G4	1001	CYC	C3D-C2D	3.40	1.47	1.38
87	BN	828	CLA	C1D-ND	3.40	1.42	1.37
87	B2	823	CLA	C1D-ND	3.40	1.42	1.37
87	B6	614	CLA	C1D-ND	3.40	1.42	1.37
82	T4	203	PEB	CHA-C1B	3.40	1.48	1.40
82	rK	202	PEB	C1A-NA	-3.40	1.33	1.37
82	MJ	203	PEB	CHB-C1C	3.40	1.48	1.40
87	L2	203	CLA	C4D-ND	-3.40	1.33	1.37
82	uC	202	PEB	CHA-C1B	3.40	1.48	1.40
82	l1	203	PEB	C2C-C3C	3.40	1.47	1.38
82	KA	202	PEB	CHB-C1C	3.40	1.48	1.40
82	VM	202	PEB	CHB-C1C	3.40	1.48	1.40
82	QQ	202	PEB	CHB-C1C	3.40	1.48	1.40
82	DH	1002	PEB	C2C-C3C	3.40	1.47	1.38
82	GM	202	PEB	C1A-NA	-3.40	1.33	1.37
82	cH	202	PEB	C1A-NA	-3.40	1.33	1.37
84	FH	1001	CYC	C1C-NC	-3.40	1.33	1.37
87	A2	815	CLA	C4D-ND	-3.40	1.33	1.37
82	CD	202	PEB	CHB-C1C	3.40	1.48	1.40
82	fE	202	PEB	CHB-C1C	3.40	1.48	1.40
82	N7	201	PEB	CHB-C1C	3.40	1.48	1.40
84	CG	1001	CYC	CHA-C4D	3.40	1.48	1.40
82	jE	202	PEB	C2C-C3C	3.40	1.47	1.38
84	IG	1001	CYC	C1D-C2D	3.40	1.49	1.41
83	M9	303	PUB	OD-C4D	3.40	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OD	201	PEB	C1A-NA	-3.40	1.33	1.37
82	M9	304	PEB	C1A-NA	-3.40	1.33	1.37
84	F1	1001	CYC	C1C-NC	-3.40	1.33	1.37
82	PA	203	PEB	C2C-C3C	3.40	1.47	1.38
82	c4	203	PEB	C2C-C3C	3.40	1.47	1.38
82	gB	203	PEB	C2C-C3C	3.40	1.47	1.38
82	zK	501	PEB	C2C-C3C	3.40	1.47	1.38
82	R4	202	PEB	CHA-C1B	3.40	1.48	1.40
82	ZB	202	PEB	C2C-C3C	3.40	1.47	1.38
82	VH	201	PEB	C1A-NA	-3.40	1.33	1.37
82	gO	201	PEB	C1A-NA	-3.40	1.33	1.37
82	S5	202	PEB	CHB-C1C	3.40	1.48	1.40
84	EH	1001	CYC	CHA-C4D	3.40	1.48	1.40
82	dO	201	PEB	CHA-C1B	3.40	1.48	1.40
82	fG	202	PEB	C2C-C3C	3.40	1.47	1.38
82	gH	201	PEB	C2C-C3C	3.40	1.47	1.38
84	w3	1001	CYC	O1D-CGD	3.40	1.33	1.22
87	5N	602	CLA	C4D-ND	-3.40	1.33	1.37
82	oK	202	PEB	OD-C4D	3.40	1.30	1.23
82	iE	202	PEB	CHB-C1C	3.40	1.48	1.40
82	dH	202	PEB	C2C-C3C	3.40	1.47	1.38
84	V3	1001	CYC	CHA-C4D	3.40	1.48	1.40
87	FN	203	CLA	C1D-ND	3.40	1.42	1.37
103	82	310	ZEX	C1-C6	-3.40	1.49	1.53
82	C9	201	PEB	CHB-C1C	3.40	1.48	1.40
87	AN	838	CLA	C4D-ND	-3.40	1.33	1.37
87	C6	515	CLA	C4D-ND	-3.40	1.33	1.37
82	w8	202	PEB	CHA-C1B	3.40	1.48	1.40
82	mJ	202	PEB	CHB-C1C	3.40	1.48	1.40
87	bL	613	CLA	C1D-ND	3.40	1.42	1.37
82	c4	201	PEB	CHB-C1C	3.40	1.48	1.40
82	OF	203	PEB	C2C-C3C	3.40	1.47	1.38
82	bE	201	PEB	C2C-C3C	3.40	1.47	1.38
82	UP	201	PEB	C2C-C3C	3.40	1.47	1.38
82	fJ	202	PEB	CHA-C1B	3.40	1.48	1.40
82	FO	1002	PEB	C2A-C1A	-3.40	1.49	1.52
82	AI	202	PEB	C2C-C3C	3.40	1.47	1.38
82	LM	202	PEB	C2C-C3C	3.40	1.47	1.38
84	x3	1001	CYC	CHA-C4D	3.40	1.48	1.40
82	iE	202	PEB	C1A-NA	-3.40	1.33	1.37
91	AL	410	PHO	C3D-C2D	3.40	1.45	1.39
82	b4	201	PEB	CHA-C1B	3.40	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	311	CLA	C4B-NB	3.40	1.42	1.37
87	b6	614	CLA	C1D-ND	3.40	1.42	1.37
87	aL	605	CLA	C1D-ND	3.40	1.42	1.37
82	UK	201	PEB	C3B-C2B	3.40	1.43	1.36
84	S3	1001	CYC	O1D-CGD	3.40	1.33	1.22
82	VE	201	PEB	C2C-C3C	3.40	1.47	1.38
82	BF	202	PEB	C2C-C3C	3.40	1.47	1.38
82	RK	201	PEB	CHA-C1B	3.40	1.48	1.40
82	OG	202	PEB	CHB-C1C	3.40	1.48	1.40
82	SJ	202	PEB	CHB-C1C	3.40	1.48	1.40
82	MP	201	PEB	CHB-C1C	3.40	1.48	1.40
82	YJ	203	PEB	C1A-NA	-3.40	1.33	1.37
82	N4	1002	PEB	C1A-NA	-3.40	1.33	1.37
82	jM	201	PEB	C1A-NA	-3.40	1.33	1.37
82	DJ	201	PEB	C2C-C3C	3.40	1.47	1.38
87	A2	831	CLA	C4D-ND	-3.39	1.33	1.37
82	i4	203	PEB	C1A-NA	-3.39	1.33	1.37
82	kJ	202	PEB	C2C-C3C	3.39	1.47	1.38
84	k3	1001	CYC	O1D-CGD	3.39	1.33	1.22
82	T1	202	PEB	CHB-C1C	3.39	1.48	1.40
82	kM	201	PEB	CHB-C1C	3.39	1.48	1.40
87	b6	611	CLA	C4D-ND	-3.39	1.33	1.37
87	b6	617	CLA	C4D-ND	-3.39	1.33	1.37
82	V1	203	PEB	C2C-C3C	3.39	1.47	1.38
82	iG	201	PEB	C2C-C3C	3.39	1.47	1.38
82	GQ	201	PEB	CHB-C1C	3.39	1.48	1.40
82	V1	201	PEB	C2C-C3C	3.39	1.47	1.38
84	o3	1001	CYC	O1D-CGD	3.39	1.33	1.22
87	BN	815	CLA	C1D-ND	3.39	1.42	1.37
82	mG	203	PEB	CHB-C1C	3.39	1.48	1.40
82	OQ	201	PEB	C2C-C3C	3.39	1.47	1.38
82	iH	202	PEB	C2C-C3C	3.39	1.47	1.38
82	IB	203	PEB	C2A-C1A	-3.39	1.49	1.52
82	IF	201	PEB	CMB-C2B	-3.39	1.43	1.50
82	FD	203	PEB	C1A-NA	-3.39	1.33	1.37
82	IM	203	PEB	C1A-NA	-3.39	1.33	1.37
82	UM	203	PEB	C1A-NA	-3.39	1.33	1.37
82	vC	201	PEB	C1A-NA	-3.39	1.33	1.37
82	wC	204	PEB	C1A-NA	-3.39	1.33	1.37
82	aE	202	PEB	C1A-NA	-3.39	1.33	1.37
82	N9	202	PEB	CHB-C1C	3.39	1.48	1.40
84	D1	1003	CYC	CHA-C4D	3.39	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BL	606	CLA	C1D-ND	3.39	1.42	1.37
87	CL	506	CLA	C1D-ND	3.39	1.42	1.37
82	j1	203	PEB	CHA-C1B	3.39	1.48	1.40
82	JD	202	PEB	CHB-C1C	3.39	1.48	1.40
82	i4	201	PEB	CHB-C1C	3.39	1.48	1.40
82	R9	202	PEB	CHB-C1C	3.39	1.48	1.40
82	TH	201	PEB	C1A-NA	-3.39	1.33	1.37
82	Y5	203	PEB	CHA-C1B	3.39	1.48	1.40
82	QB	202	PEB	CHB-C1C	3.39	1.48	1.40
82	UO	201	PEB	C2A-C1A	-3.39	1.49	1.52
87	A2	825	CLA	C1D-ND	3.39	1.42	1.37
82	ZM	201	PEB	C2C-C3C	3.39	1.47	1.38
82	SA	201	PEB	CHA-C1B	3.39	1.48	1.40
82	fJ	202	PEB	CHB-C1C	3.39	1.48	1.40
82	SG	203	PEB	C1A-NA	-3.39	1.33	1.37
82	SD	202	PEB	CHB-C1C	3.39	1.48	1.40
82	QH	203	PEB	CHB-C1C	3.39	1.48	1.40
82	P4	202	PEB	CHB-C1C	3.39	1.48	1.40
82	S9	203	PEB	CHB-C1C	3.39	1.48	1.40
84	HH	1001	CYC	CHA-C4D	3.39	1.48	1.40
87	AN	815	CLA	C4D-ND	-3.39	1.33	1.37
87	AN	850	CLA	C4D-ND	-3.39	1.33	1.37
82	UB	301	PEB	C2C-C3C	3.39	1.47	1.38
82	WG	202	PEB	C2C-C3C	3.39	1.47	1.38
82	S7	201	PEB	CHA-C1B	3.39	1.48	1.40
82	cH	201	PEB	CHA-C1B	3.39	1.48	1.40
82	QM	204	PEB	C1A-NA	-3.39	1.33	1.37
82	kO	201	PEB	C1A-NA	-3.39	1.33	1.37
87	7N	602	CLA	C1D-C2D	3.39	1.52	1.45
82	T9	202	PEB	CHB-C1C	3.39	1.48	1.40
87	AN	839	CLA	C4D-ND	-3.39	1.33	1.37
82	cO	203	PEB	C2C-C3C	3.39	1.47	1.38
82	q8	203	PEB	CHB-C1C	3.39	1.48	1.40
82	N9	201	PEB	CHB-C1C	3.39	1.48	1.40
82	MP	203	PEB	CHB-C1C	3.39	1.48	1.40
82	G9	201	PEB	CHB-C1C	3.39	1.48	1.40
82	G9	202	PEB	CHB-C1C	3.39	1.48	1.40
82	K9	202	PEB	CHB-C1C	3.39	1.48	1.40
82	A4	301	PEB	C2C-C3C	3.39	1.47	1.38
82	lE	203	PEB	C2C-C3C	3.39	1.47	1.38
82	M5	301	PEB	CHA-C1B	3.39	1.48	1.40
84	O3	1001	CYC	O1D-CGD	3.39	1.33	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	b6	612	CLA	C1D-ND	3.39	1.42	1.37
82	GJ	202	PEB	C2C-C3C	3.39	1.47	1.38
82	G5	202	PEB	CHB-C1C	3.39	1.48	1.40
84	M4	1001	CYC	CHA-C4D	3.39	1.48	1.40
82	FQ	203	PEB	C1A-NA	-3.39	1.33	1.37
82	s8	202	PEB	C2C-C3C	3.39	1.47	1.38
84	IE	1001	CYC	C1D-C2D	3.39	1.49	1.41
82	iJ	202	PEB	CHB-C1C	3.39	1.48	1.40
82	L4	1002	PEB	CHA-C1B	3.39	1.48	1.40
84	D3	1001	CYC	O1D-CGD	3.39	1.33	1.22
84	JO	1001	CYC	C2C-C1C	-3.39	1.49	1.52
82	bO	202	PEB	C2C-C3C	3.39	1.47	1.38
82	P9	201	PEB	CHB-C1C	3.39	1.48	1.40
83	AG	303	PUB	CHB-C4B	3.39	1.48	1.40
82	d4	201	PEB	C1A-NA	-3.39	1.33	1.37
82	bH	202	PEB	C1A-NA	-3.39	1.33	1.37
82	gH	203	PEB	CHA-C1B	3.39	1.48	1.40
82	aO	202	PEB	CHA-C1B	3.39	1.48	1.40
82	R9	201	PEB	CHB-C1C	3.39	1.48	1.40
87	K6	101	CLA	C1D-ND	3.39	1.41	1.37
87	3N	306	CLA	C1D-ND	3.39	1.41	1.37
82	rF	202	PEB	C2C-C3C	3.39	1.47	1.38
82	E5	202	PEB	C1A-NA	-3.39	1.33	1.37
87	b6	604	CLA	C4D-ND	-3.39	1.33	1.37
82	oK	201	PEB	CHA-C1B	3.39	1.48	1.40
84	d3	1001	CYC	O1D-CGD	3.39	1.33	1.22
82	PJ	201	PEB	CHB-C1C	3.39	1.48	1.40
82	uC	203	PEB	C2C-C3C	3.39	1.47	1.38
82	aM	201	PEB	C2C-C3C	3.39	1.47	1.38
82	F9	203	PEB	C1A-NA	-3.39	1.33	1.37
82	V9	201	PEB	CHB-C1C	3.39	1.48	1.40
82	RE	202	PEB	C2A-C1A	-3.39	1.49	1.52
82	A9	202	PEB	CHB-C1C	3.39	1.48	1.40
84	I1	1001	CYC	CHA-C4D	3.39	1.48	1.40
82	XI	201	PEB	C2C-C3C	3.39	1.47	1.38
87	dL	402	CLA	C4B-NB	3.39	1.41	1.37
82	YD	202	PEB	CHA-C1B	3.39	1.48	1.40
87	BN	836	CLA	C4D-ND	-3.39	1.33	1.37
82	j4	202	PEB	C1A-NA	-3.39	1.33	1.37
87	42	604	CLA	CMD-C2D	3.39	1.58	1.50
82	TF	202	PEB	C2C-C3C	3.39	1.47	1.38
82	KI	203	PEB	C2C-C3C	3.39	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	sC	202	PEB	C2C-C3C	3.39	1.47	1.38
82	AP	203	PEB	CHA-C1B	3.39	1.48	1.40
82	AM	301	PEB	CHB-C1C	3.39	1.48	1.40
82	EM	203	PEB	CHB-C1C	3.39	1.48	1.40
87	B6	606	CLA	C1D-ND	3.39	1.41	1.37
87	1N	607	CLA	C1D-ND	3.39	1.41	1.37
82	IA	201	PEB	CHA-C1B	3.39	1.48	1.40
82	g4	203	PEB	C1A-NA	-3.39	1.33	1.37
82	BD	201	PEB	C2A-C1A	-3.39	1.49	1.52
82	MJ	203	PEB	CHA-C1B	3.38	1.48	1.40
82	PP	201	PEB	CHA-C1B	3.38	1.48	1.40
82	KF	202	PEB	C2C-C3C	3.38	1.47	1.38
82	EI	201	PEB	C2C-C3C	3.38	1.47	1.38
82	AE	301	PEB	C1A-NA	-3.38	1.33	1.37
82	F9	203	PEB	C2C-C3C	3.38	1.47	1.38
82	UA	202	PEB	CHB-C1C	3.38	1.48	1.40
82	j4	202	PEB	CHB-C1C	3.38	1.48	1.40
84	u3	1001	CYC	O1D-CGD	3.38	1.33	1.22
82	N4	1002	PEB	CHA-C1B	3.38	1.48	1.40
82	YK	202	PEB	C2C-C3C	3.38	1.47	1.38
82	cE	201	PEB	C2C-C3C	3.38	1.47	1.38
82	mM	201	PEB	C2C-C3C	3.38	1.47	1.38
82	gE	201	PEB	CHB-C1C	3.38	1.48	1.40
87	BL	605	CLA	C1D-ND	3.38	1.41	1.37
87	BN	818	CLA	C1D-ND	3.38	1.41	1.37
87	52	609	CLA	C4B-NB	3.38	1.41	1.37
87	B2	831	CLA	C1D-ND	3.38	1.41	1.37
82	TI	201	PEB	C1A-NA	-3.38	1.33	1.37
82	SD	202	PEB	C2C-C3C	3.38	1.47	1.38
82	LP	202	PEB	CHB-C1C	3.38	1.48	1.40
82	CQ	202	PEB	CHB-C1C	3.38	1.48	1.40
87	A2	840	CLA	C4D-ND	-3.38	1.33	1.37
82	ZJ	202	PEB	C2A-C1A	-3.38	1.49	1.52
82	BA	201	PEB	C1A-NA	-3.38	1.33	1.37
82	T5	202	PEB	C1A-NA	-3.38	1.33	1.37
82	ZM	202	PEB	CHB-C1C	3.38	1.48	1.40
87	LN	203	CLA	C1D-ND	3.38	1.41	1.37
87	K2	106	CLA	C4B-NB	3.38	1.41	1.37
87	5N	609	CLA	C4B-NB	3.38	1.41	1.37
82	eO	202	PEB	CHA-C1B	3.38	1.48	1.40
82	SJ	201	PEB	C2C-C3C	3.38	1.47	1.38
87	AN	831	CLA	C4D-ND	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	F3	1001	CYC	O1D-CGD	3.38	1.33	1.22
82	PM	201	PEB	C1A-NA	-3.38	1.33	1.37
82	BK	202	PEB	C2C-C3C	3.38	1.47	1.38
87	c6	608	CLA	C1D-ND	3.38	1.41	1.37
83	A4	303	PUB	CHB-C4B	3.38	1.48	1.40
82	O4	201	PEB	CHA-C1B	3.38	1.48	1.40
82	k1	201	PEB	C2C-C3C	3.38	1.47	1.38
82	lH	201	PEB	C2C-C3C	3.38	1.47	1.38
83	xF	301	PUB	CHB-C4B	3.38	1.48	1.40
82	OK	203	PEB	CHA-C1B	3.38	1.48	1.40
82	NI	201	PEB	C2C-C3C	3.38	1.47	1.38
87	B2	832	CLA	C1D-ND	3.38	1.41	1.37
82	K9	201	PEB	CHB-C1C	3.38	1.48	1.40
84	BE	1002	CYC	C4B-NB	-3.38	1.30	1.38
87	bL	617	CLA	C4D-ND	-3.38	1.33	1.37
82	GJ	203	PEB	CHB-C1C	3.38	1.48	1.40
82	OE	202	PEB	C2C-C3C	3.38	1.47	1.38
84	U3	1001	CYC	O1D-CGD	3.38	1.33	1.22
87	2N	303	CLA	C4B-NB	3.38	1.41	1.37
82	dE	203	PEB	C2C-C3C	3.38	1.47	1.38
82	gM	202	PEB	CHB-C1C	3.38	1.48	1.40
82	UD	202	PEB	C2C-C3C	3.38	1.47	1.38
82	O5	202	PEB	CHA-C1B	3.38	1.48	1.40
82	YE	202	PEB	CHB-C1C	3.38	1.48	1.40
82	N4	1002	PEB	CHB-C1C	3.38	1.48	1.40
82	s8	202	PEB	C2A-C1A	-3.38	1.49	1.52
82	FJ	201	PEB	C2C-C3C	3.38	1.47	1.38
82	YM	202	PEB	C2C-C3C	3.38	1.47	1.38
82	MA	202	PEB	CHB-C1C	3.38	1.48	1.40
82	PO	202	PEB	CHB-C1C	3.38	1.48	1.40
82	cB	402	PEB	CHB-C1C	3.38	1.48	1.40
82	aG	201	PEB	CHB-C1C	3.38	1.48	1.40
82	F4	1002	PEB	C1A-NA	-3.38	1.33	1.37
82	kJ	201	PEB	CHA-C1B	3.38	1.48	1.40
82	dM	203	PEB	CHA-C1B	3.38	1.48	1.40
87	B2	817	CLA	C1D-ND	3.38	1.41	1.37
82	PO	201	PEB	CHB-C1C	3.38	1.48	1.40
82	i1	202	PEB	C2C-C3C	3.38	1.47	1.38
84	M3	1001	CYC	O1D-CGD	3.38	1.33	1.22
84	GE	1001	CYC	C1D-C2D	3.38	1.49	1.41
82	UA	202	PEB	C2C-C3C	3.38	1.47	1.38
82	KI	201	PEB	CHB-C1C	3.38	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	BM	302	PUB	CHB-C4B	3.38	1.48	1.40
82	JK	202	PEB	C1A-NA	-3.38	1.33	1.37
82	pK	202	PEB	C1A-NA	-3.38	1.33	1.37
84	KO	1001	CYC	C1D-C2D	3.38	1.49	1.41
82	m1	201	PEB	C2C-C3C	3.38	1.47	1.38
82	LJ	201	PEB	C1C-NC	-3.38	1.32	1.37
82	CJ	202	PEB	CHB-C1C	3.38	1.48	1.40
82	JO	1002	PEB	CHB-C1C	3.38	1.48	1.40
84	n3	1001	CYC	O1D-CGD	3.38	1.33	1.22
84	BG	1002	CYC	C4B-NB	-3.38	1.30	1.38
82	lH	202	PEB	OD-C4D	3.38	1.30	1.23
82	EJ	202	PEB	C2C-C3C	3.38	1.47	1.38
82	RP	201	PEB	C2C-C3C	3.38	1.47	1.38
82	f1	201	PEB	C2C-C3C	3.38	1.47	1.38
82	RJ	201	PEB	CHA-C1B	3.38	1.48	1.40
82	P5	202	PEB	C1A-NA	-3.38	1.33	1.37
82	T9	201	PEB	CHB-C1C	3.38	1.48	1.40
82	vF	202	PEB	CHB-C1C	3.38	1.48	1.40
83	AM	303	PUB	C3B-C2B	3.38	1.47	1.38
82	eK	203	PEB	CHA-C1B	3.38	1.48	1.40
82	GD	201	PEB	CHB-C1C	3.38	1.48	1.40
82	AP	203	PEB	CHB-C1C	3.38	1.48	1.40
82	F7	201	PEB	C1A-NA	-3.38	1.33	1.37
84	GE	1001	CYC	CHA-C4D	3.38	1.48	1.40
82	MB	202	PEB	C2C-C3C	3.38	1.47	1.38
82	fJ	201	PEB	C2C-C3C	3.38	1.47	1.38
87	32	305	CLA	C1D-ND	3.38	1.41	1.37
82	Y5	201	PEB	CHA-C1B	3.38	1.48	1.40
82	YF	201	PEB	CHB-C1C	3.38	1.48	1.40
82	YM	201	PEB	CHB-C1C	3.38	1.48	1.40
82	A9	201	PEB	CHB-C1C	3.38	1.48	1.40
82	fG	202	PEB	CHB-C1C	3.38	1.48	1.40
82	LQ	203	PEB	C2C-C3C	3.38	1.47	1.38
82	GA	201	PEB	CHB-C1C	3.38	1.48	1.40
82	I9	201	PEB	CHB-C1C	3.38	1.48	1.40
82	PJ	202	PEB	C2C-C3C	3.38	1.47	1.38
82	C5	202	PEB	C1A-NA	-3.38	1.33	1.37
83	AE	303	PUB	C3B-C2B	3.37	1.47	1.38
82	cE	201	PEB	CHB-C1C	3.37	1.48	1.40
82	kG	202	PEB	CHB-C1C	3.37	1.48	1.40
83	M5	303	PUB	CHB-C4B	3.37	1.48	1.40
87	AN	825	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	22	602	CLA	C4B-NB	3.37	1.41	1.37
87	32	302	CLA	C4B-NB	3.37	1.41	1.37
82	GI	202	PEB	C2C-C3C	3.37	1.47	1.38
82	bF	201	PEB	CHB-C1C	3.37	1.48	1.40
82	mJ	201	PEB	CHB-C1C	3.37	1.48	1.40
84	W3	1001	CYC	CHA-C4D	3.37	1.48	1.40
82	SP	201	PEB	C1A-NA	-3.37	1.33	1.37
87	D6	403	CLA	C4D-ND	-3.37	1.33	1.37
87	8N	302	CLA	C4D-ND	-3.37	1.33	1.37
82	MB	201	PEB	C2A-C1A	-3.37	1.49	1.52
82	J5	201	PEB	C2A-C1A	-3.37	1.49	1.52
82	HP	201	PEB	C2C-C3C	3.37	1.47	1.38
84	L3	1001	CYC	O1D-CGD	3.37	1.33	1.22
82	WA	201	PEB	CHA-C1B	3.37	1.48	1.40
87	LN	204	CLA	C4D-ND	-3.37	1.33	1.37
82	EF	202	PEB	C2C-C3C	3.37	1.47	1.38
82	IM	202	PEB	CHB-C1C	3.37	1.48	1.40
82	HP	202	PEB	CHB-C1C	3.37	1.48	1.40
87	B6	612	CLA	C1D-ND	3.37	1.41	1.37
82	Z5	301	PEB	CHA-C1B	3.37	1.48	1.40
82	WE	202	PEB	C1A-NA	-3.37	1.33	1.37
82	HQ	201	PEB	C1A-NA	-3.37	1.33	1.37
82	K5	202	PEB	C1A-NA	-3.37	1.33	1.37
82	UB	303	PEB	CHB-C1C	3.37	1.48	1.40
82	GK	203	PEB	CHB-C1C	3.37	1.48	1.40
82	XM	202	PEB	CHB-C1C	3.37	1.48	1.40
82	X9	201	PEB	CHB-C1C	3.37	1.48	1.40
87	O2	201	CLA	C4D-ND	-3.37	1.33	1.37
82	eG	202	PEB	CHA-C1B	3.37	1.48	1.40
82	vK	202	PEB	C2C-C3C	3.37	1.47	1.38
82	V5	202	PEB	C1A-NA	-3.37	1.33	1.37
82	i4	202	PEB	CHA-C1B	3.37	1.48	1.40
82	gG	201	PEB	CHB-C1C	3.37	1.48	1.40
82	PI	201	PEB	C2C-C3C	3.37	1.47	1.38
82	rF	201	PEB	C2C-C3C	3.37	1.47	1.38
82	AQ	304	PEB	C1A-NA	-3.37	1.33	1.37
82	jM	202	PEB	C1A-NA	-3.37	1.33	1.37
82	RH	201	PEB	C2C-C3C	3.37	1.47	1.38
82	TH	202	PEB	CHB-C1C	3.37	1.48	1.40
82	Y4	202	PEB	CHB-C1C	3.37	1.48	1.40
84	GG	1001	CYC	C1D-C2D	3.37	1.49	1.41
82	Y9	203	PEB	C2C-C3C	3.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S4	202	PEB	CHB-C1C	3.37	1.48	1.40
82	AD	304	PEB	C1A-NA	-3.37	1.33	1.37
82	fE	201	PEB	C2C-C3C	3.37	1.47	1.38
84	I3	1001	CYC	CHA-C4D	3.37	1.48	1.40
82	SP	202	PEB	C2C-C3C	3.37	1.47	1.38
82	O5	201	PEB	C2C-C3C	3.37	1.47	1.38
82	JQ	202	PEB	CHB-C1C	3.37	1.48	1.40
82	Y1	202	PEB	CHB-C1C	3.37	1.48	1.40
87	A2	833	CLA	C4D-ND	-3.37	1.33	1.37
82	EF	202	PEB	CHA-C1B	3.37	1.48	1.40
82	XK	201	PEB	CHA-C1B	3.37	1.48	1.40
82	WF	203	PEB	C1A-NA	-3.37	1.33	1.37
82	LO	1002	PEB	C1A-NA	-3.37	1.33	1.37
82	G5	202	PEB	C1A-NA	-3.37	1.33	1.37
84	CO	1001	CYC	C1D-C2D	3.37	1.49	1.41
82	QA	202	PEB	CHA-C1B	3.37	1.48	1.40
82	cJ	202	PEB	C2A-C1A	-3.37	1.49	1.52
82	LD	203	PEB	C2C-C3C	3.37	1.47	1.38
82	AF	201	PEB	C2C-C3C	3.37	1.47	1.38
82	QP	203	PEB	C2C-C3C	3.37	1.47	1.38
87	A2	838	CLA	C4D-ND	-3.37	1.33	1.37
84	L3	1001	CYC	CHA-C4D	3.37	1.48	1.40
87	A2	824	CLA	C1D-ND	3.37	1.41	1.37
87	b6	617	CLA	C1D-ND	3.37	1.41	1.37
82	HG	1002	PEB	CHA-C1B	3.37	1.48	1.40
82	KJ	201	PEB	CHA-C1B	3.37	1.48	1.40
82	jH	202	PEB	CHA-C1B	3.37	1.48	1.40
82	AI	201	PEB	C2C-C3C	3.37	1.47	1.38
82	WM	201	PEB	C2C-C3C	3.37	1.47	1.38
87	dL	409	CLA	C4D-ND	-3.37	1.33	1.37
82	E9	201	PEB	CHB-C1C	3.37	1.48	1.40
82	h1	202	PEB	C2C-C3C	3.37	1.47	1.38
82	RH	201	PEB	CHA-C1B	3.37	1.48	1.40
82	d4	201	PEB	CHA-C1B	3.37	1.48	1.40
95	C6	504	DGD	O2G-C1B	3.37	1.43	1.34
83	Y7	302	PUB	C3B-C2B	3.37	1.47	1.38
82	VP	202	PEB	CHB-C1C	3.37	1.48	1.40
82	P1	202	PEB	CHB-C1C	3.37	1.48	1.40
82	KB	304	PEB	CHA-C1B	3.37	1.48	1.40
82	KM	202	PEB	CHA-C1B	3.37	1.48	1.40
82	gF	203	PEB	CHA-C1B	3.37	1.48	1.40
82	WE	202	PEB	C2C-C3C	3.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	608	CLA	C1D-ND	3.37	1.41	1.37
82	UJ	203	PEB	CHB-C1C	3.37	1.48	1.40
82	H5	203	PEB	CHA-C1B	3.37	1.48	1.40
82	LH	1003	PEB	C2A-C1A	-3.37	1.49	1.52
82	N7	203	PEB	C2A-C1A	-3.37	1.49	1.52
82	NF	201	PEB	C2C-C3C	3.37	1.47	1.38
82	qC	203	PEB	CHB-C1C	3.37	1.48	1.40
87	52	602	CLA	C4D-ND	-3.37	1.33	1.37
82	TP	201	PEB	C2C-C3C	3.37	1.47	1.38
82	VF	202	PEB	C1A-NA	-3.37	1.33	1.37
82	DO	1002	PEB	C1A-NA	-3.37	1.33	1.37
82	hE	203	PEB	CHA-C1B	3.37	1.48	1.40
82	iH	201	PEB	CHA-C1B	3.37	1.48	1.40
84	KH	1001	CYC	CHB-C4A	3.37	1.48	1.40
84	w3	1001	CYC	CHA-C4D	3.37	1.48	1.40
82	TF	202	PEB	C2A-C1A	-3.37	1.49	1.52
82	gG	201	PEB	CHA-C1B	3.37	1.48	1.40
82	gM	201	PEB	CHB-C1C	3.37	1.48	1.40
87	L2	204	CLA	C4D-ND	-3.37	1.33	1.37
82	j1	202	PEB	CHA-C1B	3.37	1.48	1.40
82	dG	201	PEB	C1A-NA	-3.37	1.33	1.37
82	DB	203	PEB	C2A-C1A	-3.36	1.49	1.52
82	YK	201	PEB	CHB-C1C	3.36	1.48	1.40
82	w8	204	PEB	CHB-C1C	3.36	1.48	1.40
82	aE	201	PEB	CHB-C1C	3.36	1.48	1.40
82	Y5	201	PEB	C2C-C3C	3.36	1.47	1.38
82	S9	202	PEB	CHA-C1B	3.36	1.48	1.40
82	h1	201	PEB	C2C-C3C	3.36	1.47	1.38
82	YK	202	PEB	C1A-NA	-3.36	1.33	1.37
82	QB	202	PEB	C2C-C3C	3.36	1.47	1.38
82	U4	202	PEB	C2C-C3C	3.36	1.47	1.38
82	XM	201	PEB	CHB-C1C	3.36	1.48	1.40
87	b6	613	CLA	C4D-ND	-3.36	1.33	1.37
82	DE	1002	PEB	CHA-C1B	3.36	1.48	1.40
82	D4	1002	PEB	C2A-C1A	-3.36	1.49	1.52
82	DK	201	PEB	CHB-C1C	3.36	1.48	1.40
82	CF	201	PEB	C1A-NA	-3.36	1.33	1.37
87	BN	812	CLA	C1D-ND	3.36	1.41	1.37
82	NB	202	PEB	C2C-C3C	3.36	1.47	1.38
82	P7	203	PEB	C2C-C3C	3.36	1.47	1.38
82	SI	202	PEB	CHB-C1C	3.36	1.48	1.40
82	U7	202	PEB	CHB-C1C	3.36	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	fG	201	PEB	CHA-C1B	3.36	1.48	1.40
82	CI	201	PEB	C2C-C3C	3.36	1.47	1.38
82	I5	202	PEB	C1A-NA	-3.36	1.33	1.37
82	X5	202	PEB	C1A-NA	-3.36	1.33	1.37
82	G7	201	PEB	CHB-C1C	3.36	1.48	1.40
82	QP	201	PEB	CHB-C1C	3.36	1.48	1.40
84	NO	1001	CYC	C1D-C2D	3.36	1.49	1.41
82	e4	203	PEB	C2C-C3C	3.36	1.47	1.38
82	S9	203	PEB	C2C-C3C	3.36	1.47	1.38
82	HE	1002	PEB	CHA-C1B	3.36	1.48	1.40
82	Z9	303	PEB	CHB-C1C	3.36	1.48	1.40
87	K6	101	CLA	C4D-ND	-3.36	1.33	1.37
82	a1	201	PEB	C2C-C3C	3.36	1.47	1.38
87	b6	611	CLA	C1D-ND	3.36	1.41	1.37
82	RJ	202	PEB	C2C-C3C	3.36	1.47	1.38
82	YP	503	PEB	C2C-C3C	3.36	1.47	1.38
82	W5	202	PEB	C2C-C3C	3.36	1.47	1.38
82	L9	202	PEB	C1A-NA	-3.36	1.33	1.37
82	mE	203	PEB	C1A-NA	-3.36	1.33	1.37
87	nL	101	CLA	C4D-ND	-3.36	1.33	1.37
84	d3	1001	CYC	CHA-C4D	3.36	1.48	1.40
82	VM	202	PEB	C2C-C3C	3.36	1.47	1.38
82	kF	201	PEB	C2C-C3C	3.36	1.47	1.38
87	F2	201	CLA	C1D-ND	3.36	1.41	1.37
82	RI	201	PEB	C2C-C3C	3.36	1.47	1.38
82	OA	202	PEB	CHA-C1B	3.36	1.48	1.40
82	TM	202	PEB	C2C-C3C	3.36	1.47	1.38
87	A2	837	CLA	C1D-ND	3.36	1.41	1.37
82	VF	201	PEB	C2C-C3C	3.36	1.47	1.38
82	KI	202	PEB	C2C-C3C	3.36	1.47	1.38
82	IP	203	PEB	CHB-C1C	3.36	1.48	1.40
82	AO	305	PEB	C1A-NA	-3.36	1.33	1.37
82	Y1	201	PEB	C1A-NA	-3.36	1.33	1.37
82	A4	305	PEB	C1A-NA	-3.36	1.33	1.37
82	eH	203	PEB	C1A-NA	-3.36	1.33	1.37
82	RF	201	PEB	CHA-C1B	3.36	1.48	1.40
82	OP	201	PEB	CHA-C1B	3.36	1.48	1.40
84	LH	1001	CYC	CHA-C4D	3.36	1.48	1.40
82	JO	1002	PEB	C2A-C1A	-3.36	1.49	1.52
82	HG	1002	PEB	C2C-C3C	3.36	1.47	1.38
82	oF	202	PEB	OD-C4D	3.36	1.30	1.23
82	CM	202	PEB	CHB-C1C	3.36	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q1	203	PEB	C1A-NA	-3.36	1.33	1.37
82	LJ	201	PEB	C2C-C3C	3.36	1.47	1.38
82	H7	201	PEB	C2C-C3C	3.36	1.47	1.38
82	YE	201	PEB	CHA-C1B	3.36	1.48	1.40
87	BN	832	CLA	C1D-ND	3.36	1.41	1.37
82	GG	1002	PEB	CHA-C1B	3.36	1.48	1.40
82	gK	202	PEB	CHB-C1C	3.36	1.48	1.40
82	kK	201	PEB	C2C-C3C	3.36	1.47	1.38
82	eO	203	PEB	C2C-C3C	3.36	1.47	1.38
83	AO	303	PUB	C3B-C2B	3.36	1.47	1.38
82	gF	202	PEB	CHB-C1C	3.36	1.48	1.40
84	k3	1001	CYC	CHA-C4D	3.36	1.48	1.40
82	iK	203	PEB	CHA-C1B	3.36	1.48	1.40
82	AA	202	PEB	CHB-C1C	3.36	1.48	1.40
82	AG	301	PEB	C2C-C3C	3.36	1.47	1.38
82	VI	201	PEB	C2C-C3C	3.36	1.47	1.38
82	aH	201	PEB	C2C-C3C	3.36	1.47	1.38
82	lO	202	PEB	C2C-C3C	3.36	1.47	1.38
82	R4	202	PEB	C2A-C1A	-3.36	1.49	1.52
82	D1	1002	PEB	C2C-C3C	3.36	1.47	1.38
87	HL	102	CLA	C1D-ND	3.36	1.41	1.37
87	6N	611	CLA	C4B-NB	3.36	1.41	1.37
82	VD	201	PEB	C1A-NA	-3.36	1.33	1.37
82	VQ	201	PEB	C1A-NA	-3.36	1.33	1.37
82	kE	201	PEB	C1A-NA	-3.36	1.33	1.37
82	lM	201	PEB	C1A-NA	-3.36	1.33	1.37
82	PE	202	PEB	CHB-C1C	3.36	1.48	1.40
82	eO	201	PEB	C2C-C3C	3.36	1.47	1.38
82	Z1	201	PEB	CHA-C1B	3.36	1.48	1.40
84	j3	1001	CYC	CHA-C4D	3.36	1.48	1.40
87	A2	839	CLA	C4D-ND	-3.36	1.33	1.37
82	LJ	201	PEB	C2A-C1A	-3.36	1.49	1.52
82	fH	201	PEB	CHA-C1B	3.36	1.48	1.40
82	UO	202	PEB	C2C-C3C	3.36	1.47	1.38
82	aG	201	PEB	C2C-C3C	3.36	1.47	1.38
82	AD	301	PEB	CHA-C1B	3.36	1.48	1.40
82	LD	202	PEB	CHB-C1C	3.36	1.48	1.40
82	A1	301	PEB	CHB-C1C	3.36	1.48	1.40
87	1N	607	CLA	C4B-NB	3.36	1.41	1.37
82	d1	203	PEB	C1A-NA	-3.36	1.33	1.37
82	sK	202	PEB	C2C-C3C	3.36	1.47	1.38
82	M9	305	PEB	C2C-C3C	3.36	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	LE	1002	PEB	C2C-C3C	3.35	1.47	1.38
82	u8	203	PEB	C2C-C3C	3.35	1.47	1.38
87	R2	203	CLA	C4D-ND	-3.35	1.33	1.37
82	R1	201	PEB	CHA-C1B	3.35	1.48	1.40
87	LN	206	CLA	C1D-ND	3.35	1.41	1.37
87	22	606	CLA	C1D-ND	3.35	1.41	1.37
82	fH	203	PEB	C2C-C3C	3.35	1.47	1.38
82	YD	201	PEB	C1A-NA	-3.35	1.33	1.37
82	CK	201	PEB	C1A-NA	-3.35	1.33	1.37
82	G7	202	PEB	CHA-C1B	3.35	1.48	1.40
82	W7	201	PEB	CHA-C1B	3.35	1.48	1.40
83	Z5	303	PUB	CHB-C4B	3.35	1.48	1.40
82	IP	201	PEB	C2C-C3C	3.35	1.47	1.38
82	K5	202	PEB	C2C-C3C	3.35	1.47	1.38
82	AF	202	PEB	C2C-C3C	3.35	1.47	1.38
82	ZG	203	PEB	C2C-C3C	3.35	1.47	1.38
82	SO	202	PEB	C2C-C3C	3.35	1.47	1.38
82	MQ	201	PEB	C2C-C3C	3.35	1.47	1.38
82	aE	201	PEB	C2C-C3C	3.35	1.47	1.38
82	PH	202	PEB	CHB-C1C	3.35	1.48	1.40
82	RP	202	PEB	CHB-C1C	3.35	1.48	1.40
82	eG	203	PEB	C1A-NA	-3.35	1.33	1.37
82	II	201	PEB	C2C-C3C	3.35	1.47	1.38
82	TI	202	PEB	C2C-C3C	3.35	1.47	1.38
82	DF	201	PEB	CHB-C1C	3.35	1.48	1.40
91	A6	407	PHO	C3D-C2D	3.35	1.45	1.39
87	BN	801	CLA	C4D-ND	-3.35	1.33	1.37
82	HE	1002	PEB	C2C-C3C	3.35	1.47	1.38
82	VH	202	PEB	C2C-C3C	3.35	1.47	1.38
87	B2	811	CLA	C1D-ND	3.35	1.41	1.37
87	bL	621	CLA	C1D-ND	3.35	1.41	1.37
82	LD	203	PEB	CHB-C1C	3.35	1.48	1.40
82	BQ	201	PEB	CHB-C1C	3.35	1.48	1.40
84	u3	1001	CYC	CHA-C4D	3.35	1.48	1.40
82	QP	201	PEB	C2A-C1A	-3.35	1.49	1.52
82	EM	203	PEB	C2C-C3C	3.35	1.47	1.38
82	OP	201	PEB	C2C-C3C	3.35	1.47	1.38
82	QP	201	PEB	C2C-C3C	3.35	1.47	1.38
82	V5	202	PEB	C2C-C3C	3.35	1.47	1.38
87	A2	850	CLA	C4D-ND	-3.35	1.33	1.37
82	B5	201	PEB	C2C-C3C	3.35	1.47	1.38
82	rF	202	PEB	C1A-NA	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	cL	514	CLA	C1D-ND	3.35	1.41	1.37
84	S3	1001	CYC	CHA-C4D	3.35	1.48	1.40
87	KN	103	CLA	C4D-ND	-3.35	1.33	1.37
82	VQ	201	PEB	CHB-C1C	3.35	1.48	1.40
82	RF	202	PEB	C2A-C1A	-3.35	1.49	1.52
82	ZK	202	PEB	C1A-NA	-3.35	1.33	1.37
87	K2	104	CLA	C1D-ND	3.35	1.41	1.37
82	DD	201	PEB	CHA-C1B	3.35	1.48	1.40
82	jH	203	PEB	CHA-C1B	3.35	1.48	1.40
87	A2	837	CLA	C4D-ND	-3.35	1.33	1.37
84	IO	1001	CYC	C1D-C2D	3.35	1.49	1.41
82	ZB	203	PEB	CHB-C1C	3.35	1.48	1.40
82	CP	202	PEB	C2A-C1A	-3.35	1.49	1.52
87	AL	403	CLA	C1D-ND	3.35	1.41	1.37
82	B5	201	PEB	CHB-C1C	3.35	1.48	1.40
82	SM	203	PEB	CHA-C1B	3.35	1.48	1.40
87	B2	816	CLA	C4D-ND	-3.35	1.33	1.37
84	JH	1003	CYC	C1D-C2D	3.35	1.49	1.41
82	Y7	303	PEB	C1A-NA	-3.35	1.33	1.37
87	cL	508	CLA	C1D-ND	3.35	1.41	1.37
82	ZM	202	PEB	C2C-C3C	3.35	1.47	1.38
82	b4	201	PEB	CHB-C1C	3.35	1.48	1.40
82	bO	201	PEB	CHB-C1C	3.35	1.48	1.40
82	GE	1002	PEB	CHA-C1B	3.35	1.48	1.40
82	rK	202	PEB	C2C-C3C	3.35	1.47	1.38
84	f3	1001	CYC	CHA-C4D	3.35	1.48	1.40
82	QJ	204	PEB	C1A-NA	-3.35	1.33	1.37
82	RQ	203	PEB	C1A-NA	-3.35	1.33	1.37
82	RH	202	PEB	C2C-C3C	3.35	1.47	1.38
82	e4	201	PEB	C2C-C3C	3.35	1.47	1.38
82	aM	203	PEB	C1A-NA	-3.35	1.33	1.37
82	eB	202	PEB	CHB-C1C	3.35	1.48	1.40
82	RK	202	PEB	C2A-C1A	-3.35	1.49	1.52
82	Q7	202	PEB	CHA-C1B	3.35	1.48	1.40
82	f1	203	PEB	C2C-C3C	3.35	1.47	1.38
82	GK	203	PEB	C2C-C3C	3.35	1.47	1.38
82	OH	202	PEB	C1A-NA	-3.35	1.33	1.37
82	jJ	201	PEB	CHB-C1C	3.35	1.48	1.40
87	K2	104	CLA	C4D-ND	-3.35	1.33	1.37
82	QJ	203	PEB	CHA-C1B	3.35	1.48	1.40
87	AL	403	CLA	C4D-ND	-3.35	1.33	1.37
82	j4	201	PEB	C2C-C3C	3.35	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	73	1001	CYC	CHA-C4D	3.35	1.48	1.40
95	C6	504	DGD	O1G-C1A	3.35	1.43	1.33
91	AL	410	PHO	CBD-CGD	-3.35	1.47	1.52
82	IP	201	PEB	C2A-C1A	-3.35	1.49	1.52
82	k1	202	PEB	C2A-C1A	-3.35	1.49	1.52
82	QD	201	PEB	C1A-NA	-3.35	1.33	1.37
82	wF	303	PEB	C1A-NA	-3.35	1.33	1.37
87	AN	829	CLA	C4D-ND	-3.35	1.33	1.37
82	VM	201	PEB	C2C-C3C	3.35	1.47	1.38
82	BD	202	PEB	CHB-C1C	3.35	1.48	1.40
82	XP	201	PEB	CHA-C1B	3.35	1.48	1.40
82	G7	201	PEB	CHA-C1B	3.35	1.48	1.40
82	OM	201	PEB	C2C-C3C	3.35	1.47	1.38
82	DF	203	PEB	CHB-C1C	3.35	1.48	1.40
82	AH	301	PEB	CHB-C1C	3.35	1.48	1.40
82	N5	202	PEB	C1A-NA	-3.35	1.33	1.37
82	Y5	203	PEB	C1A-NA	-3.35	1.33	1.37
82	fM	201	PEB	C1A-NA	-3.35	1.33	1.37
87	82	301	CLA	C4D-ND	-3.35	1.33	1.37
82	aB	202	PEB	CHB-C1C	3.34	1.48	1.40
84	O3	1001	CYC	CHA-C4D	3.34	1.48	1.40
87	B2	827	CLA	CMB-C2B	-3.34	1.43	1.50
87	BN	831	CLA	C1D-ND	3.34	1.41	1.37
82	OK	202	PEB	C2C-C3C	3.34	1.47	1.38
82	MP	201	PEB	C2C-C3C	3.34	1.47	1.38
82	j1	202	PEB	OD-C4D	3.34	1.29	1.23
82	WB	401	PEB	CHB-C1C	3.34	1.48	1.40
82	pC	201	PEB	CHB-C1C	3.34	1.48	1.40
84	h3	1001	CYC	CHA-C4D	3.34	1.48	1.40
82	GM	201	PEB	C2C-C3C	3.34	1.47	1.38
82	aJ	202	PEB	C2C-C3C	3.34	1.47	1.38
82	SH	201	PEB	CHA-C1B	3.34	1.48	1.40
82	TQ	201	PEB	CHA-C1B	3.34	1.48	1.40
82	pF	201	PEB	CHA-C1B	3.34	1.48	1.40
84	U3	1001	CYC	CHA-C4D	3.34	1.48	1.40
87	bL	616	CLA	C1D-ND	3.34	1.41	1.37
82	SQ	201	PEB	CHB-C1C	3.34	1.48	1.40
82	cM	202	PEB	CHB-C1C	3.34	1.48	1.40
84	H3	1001	CYC	CHA-C4D	3.34	1.48	1.40
82	VG	201	PEB	C2C-C3C	3.34	1.47	1.38
82	FM	202	PEB	C2C-C3C	3.34	1.47	1.38
82	JI	202	PEB	C2C-C3C	3.34	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	CG	1001	CYC	C3D-C2D	3.34	1.47	1.38
82	fM	202	PEB	CHA-C1B	3.34	1.48	1.40
84	FE	1001	CYC	C1D-C2D	3.34	1.49	1.41
82	AO	301	PEB	C2C-C3C	3.34	1.47	1.38
82	FP	202	PEB	CHB-C1C	3.34	1.48	1.40
82	mO	201	PEB	CHB-C1C	3.34	1.48	1.40
82	GA	202	PEB	C2C-C3C	3.34	1.47	1.38
82	i1	201	PEB	C2C-C3C	3.34	1.47	1.38
82	lH	202	PEB	C2C-C3C	3.34	1.47	1.38
82	wC	204	PEB	CHB-C1C	3.34	1.48	1.40
84	q3	1001	CYC	CHA-C4D	3.34	1.48	1.40
87	D6	402	CLA	C1D-ND	3.34	1.41	1.37
82	OF	203	PEB	CHA-C1B	3.34	1.48	1.40
84	K1	1001	CYC	CHB-C4A	3.34	1.48	1.40
82	YH	202	PEB	C1A-NA	-3.34	1.33	1.37
82	qF	201	PEB	C1A-NA	-3.34	1.33	1.37
82	PG	202	PEB	CHB-C1C	3.34	1.48	1.40
82	JM	201	PEB	CHB-C1C	3.34	1.48	1.40
82	eB	201	PEB	C2C-C3C	3.34	1.47	1.38
84	W3	1001	CYC	C3D-C2D	3.34	1.47	1.38
87	CL	511	CLA	C1D-ND	3.34	1.41	1.37
82	M5	301	PEB	C2C-C3C	3.34	1.47	1.38
82	WE	203	PEB	CHB-C1C	3.34	1.48	1.40
82	GM	201	PEB	CHB-C1C	3.34	1.48	1.40
84	GG	1001	CYC	CHA-C4D	3.34	1.48	1.40
87	R2	202	CLA	C4B-NB	3.34	1.41	1.37
82	jO	201	PEB	C2C-C3C	3.34	1.47	1.38
82	b1	203	PEB	C1A-NA	-3.34	1.33	1.37
84	MO	1001	CYC	C1C-NC	-3.34	1.33	1.37
82	cM	201	PEB	CHB-C1C	3.34	1.48	1.40
84	y3	1001	CYC	CHA-C4D	3.34	1.48	1.40
82	ZH	201	PEB	CHA-C1B	3.34	1.48	1.40
82	aM	201	PEB	CHB-C1C	3.34	1.48	1.40
82	AQ	301	PEB	C1A-NA	-3.34	1.33	1.37
82	BD	201	PEB	CHA-C1B	3.34	1.48	1.40
82	DQ	201	PEB	CHA-C1B	3.34	1.48	1.40
82	RF	202	PEB	C2C-C3C	3.34	1.47	1.38
87	52	608	CLA	C4B-NB	3.34	1.41	1.37
83	AM	304	PUB	CHB-C4B	3.34	1.48	1.40
82	WB	401	PEB	C1A-NA	-3.34	1.33	1.37
84	LG	1001	CYC	C1D-C2D	3.34	1.49	1.41
82	M7	202	PEB	CHA-C1B	3.34	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FA	201	PEB	C2C-C3C	3.34	1.47	1.38
87	2N	312	CLA	C4D-ND	-3.34	1.33	1.37
82	oF	201	PEB	CHA-C1B	3.34	1.48	1.40
82	FI	202	PEB	C1A-NA	-3.34	1.33	1.37
82	lJ	203	PEB	CHB-C1C	3.34	1.48	1.40
82	NK	201	PEB	C2C-C3C	3.34	1.47	1.38
82	mH	201	PEB	C2C-C3C	3.34	1.47	1.38
82	gE	201	PEB	CHA-C1B	3.34	1.48	1.40
87	AN	834	CLA	C4D-ND	-3.34	1.33	1.37
82	SA	202	PEB	OD-C4D	3.34	1.29	1.23
82	fH	201	PEB	C2C-C3C	3.34	1.47	1.38
82	KA	201	PEB	CHA-C1B	3.34	1.48	1.40
82	Y7	304	PEB	C1A-NA	-3.34	1.33	1.37
82	lG	202	PEB	CHA-C1B	3.34	1.48	1.40
82	Y1	202	PEB	C2A-C1A	-3.34	1.49	1.52
82	YA	303	PEB	C1A-NA	-3.34	1.33	1.37
82	bF	201	PEB	C1A-NA	-3.34	1.33	1.37
82	J1	1002	PEB	C2C-C3C	3.34	1.47	1.38
82	PG	201	PEB	C2C-C3C	3.34	1.47	1.38
82	cF	201	PEB	C2C-C3C	3.34	1.47	1.38
82	YA	304	PEB	C1A-NA	-3.34	1.33	1.37
82	L1	1002	PEB	C1A-NA	-3.34	1.33	1.37
82	IB	203	PEB	CHA-C1B	3.34	1.48	1.40
84	B3	1001	CYC	CHA-C4D	3.34	1.48	1.40
87	BN	819	CLA	C4D-ND	-3.34	1.33	1.37
82	ZE	203	PEB	CHB-C1C	3.34	1.48	1.40
82	p8	201	PEB	CHB-C1C	3.34	1.48	1.40
84	LH	1002	CYC	CHA-C4D	3.34	1.48	1.40
87	CL	514	CLA	C1D-ND	3.33	1.41	1.37
82	aJ	201	PEB	CHB-C1C	3.33	1.48	1.40
82	KJ	203	PEB	C2A-C1A	-3.33	1.49	1.52
82	vF	201	PEB	C2A-C1A	-3.33	1.49	1.52
82	vF	202	PEB	C2C-C3C	3.33	1.47	1.38
83	AJ	303	PUB	C3B-C2B	3.33	1.47	1.38
82	f1	201	PEB	CHA-C1B	3.33	1.48	1.40
82	NM	202	PEB	CHB-C1C	3.33	1.48	1.40
82	VK	201	PEB	C2C-C3C	3.33	1.47	1.38
82	FP	201	PEB	C2C-C3C	3.33	1.47	1.38
82	MP	203	PEB	C2C-C3C	3.33	1.47	1.38
82	h1	201	PEB	CHA-C1B	3.33	1.48	1.40
82	TD	203	PEB	CHB-C1C	3.33	1.48	1.40
87	BN	827	CLA	CMB-C2B	-3.33	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	eA	301	PEB	C2C-C3C	3.33	1.47	1.38
82	GA	201	PEB	CHA-C1B	3.33	1.48	1.40
82	M9	304	PEB	CHB-C1C	3.33	1.48	1.40
84	Q3	1001	CYC	CHA-C4D	3.33	1.48	1.40
82	gB	203	PEB	CHA-C1B	3.33	1.48	1.40
84	J4	1001	CYC	CHA-C4D	3.33	1.48	1.40
82	ZH	202	PEB	C2C-C3C	3.33	1.47	1.38
82	C5	202	PEB	C2C-C3C	3.33	1.47	1.38
82	hE	202	PEB	C2C-C3C	3.33	1.47	1.38
82	hG	202	PEB	C2C-C3C	3.33	1.47	1.38
82	lO	201	PEB	C2C-C3C	3.33	1.47	1.38
82	OF	202	PEB	C1A-NA	-3.33	1.33	1.37
82	b1	201	PEB	C1A-NA	-3.33	1.33	1.37
82	MJ	201	PEB	CHB-C1C	3.33	1.48	1.40
82	lG	202	PEB	CHB-C1C	3.33	1.48	1.40
84	M3	1001	CYC	CHA-C4D	3.33	1.48	1.40
82	T5	202	PEB	C2C-C3C	3.33	1.47	1.38
84	y3	1001	CYC	C3D-C2D	3.33	1.47	1.38
87	62	302	CLA	C4B-NB	3.33	1.41	1.37
87	L2	206	CLA	C1D-ND	3.33	1.41	1.37
82	LO	1002	PEB	C2A-C1A	-3.33	1.49	1.52
82	LF	202	PEB	CHB-C1C	3.33	1.48	1.40
84	L4	1001	CYC	CHA-C4D	3.33	1.48	1.40
82	S7	202	PEB	C2C-C3C	3.33	1.47	1.38
82	bP	502	PEB	CHB-C1C	3.33	1.48	1.40
84	K4	1001	CYC	C1D-C2D	3.33	1.49	1.41
82	WE	201	PEB	C2C-C3C	3.33	1.47	1.38
82	A5	202	PEB	C2C-C3C	3.33	1.47	1.38
82	Y9	202	PEB	CHA-C1B	3.33	1.48	1.40
82	lF	201	PEB	CHA-C1B	3.33	1.48	1.40
82	PO	201	PEB	C2A-C1A	-3.33	1.49	1.52
82	jF	201	PEB	C2A-C1A	-3.33	1.49	1.52
82	kE	201	PEB	C2C-C3C	3.33	1.47	1.38
87	B2	808	CLA	C4D-ND	-3.33	1.33	1.37
87	H6	103	CLA	C4D-ND	-3.33	1.33	1.37
82	WP	201	PEB	CHA-C1B	3.33	1.48	1.40
82	fE	201	PEB	CHA-C1B	3.33	1.48	1.40
87	AN	821	CLA	C1D-ND	3.33	1.41	1.37
87	B6	605	CLA	C1D-ND	3.33	1.41	1.37
82	LG	1002	PEB	C2C-C3C	3.33	1.47	1.38
82	dF	202	PEB	CHB-C1C	3.33	1.48	1.40
82	FO	1002	PEB	C1A-NA	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	H9	203	PEB	C1A-NA	-3.33	1.33	1.37
82	I5	202	PEB	C2C-C3C	3.33	1.47	1.38
82	J5	201	PEB	C2C-C3C	3.33	1.47	1.38
82	lM	203	PEB	CHA-C1B	3.33	1.48	1.40
82	HJ	201	PEB	C2C-C3C	3.33	1.47	1.38
82	TK	201	PEB	C2C-C3C	3.33	1.47	1.38
82	F1	1002	PEB	CHB-C1C	3.33	1.48	1.40
87	C6	512	CLA	C4D-ND	-3.33	1.33	1.37
82	CF	203	PEB	C1A-NA	-3.33	1.33	1.37
82	OO	201	PEB	CHA-C1B	3.33	1.48	1.40
82	hG	203	PEB	CHA-C1B	3.33	1.48	1.40
87	R2	203	CLA	C1D-ND	3.33	1.41	1.37
82	GB	203	PEB	C2A-C1A	-3.33	1.49	1.52
82	KF	202	PEB	CHB-C1C	3.33	1.48	1.40
82	hJ	202	PEB	C2C-C3C	3.33	1.47	1.38
82	QP	202	PEB	C1A-NA	-3.33	1.33	1.37
82	AQ	303	PEB	C1A-NA	-3.33	1.33	1.37
82	R1	202	PEB	C2C-C3C	3.33	1.47	1.38
82	d4	202	PEB	CHB-C1C	3.33	1.48	1.40
82	cH	202	PEB	CHB-C1C	3.33	1.48	1.40
84	JO	1001	CYC	CHA-C4D	3.33	1.48	1.40
82	D9	203	PEB	C1A-NA	-3.33	1.33	1.37
82	gO	203	PEB	C1A-NA	-3.33	1.33	1.37
82	DD	203	PEB	CHB-C1C	3.33	1.48	1.40
82	V7	201	PEB	CHA-C1B	3.33	1.48	1.40
82	OF	202	PEB	C2C-C3C	3.33	1.47	1.38
82	bF	202	PEB	C2C-C3C	3.33	1.47	1.38
82	NJ	202	PEB	CHB-C1C	3.33	1.48	1.40
84	D3	1001	CYC	CHA-C4D	3.33	1.48	1.40
82	bO	201	PEB	CHA-C1B	3.33	1.48	1.40
87	D6	402	CLA	C4D-ND	-3.33	1.33	1.37
82	IJ	203	PEB	C2C-C3C	3.33	1.47	1.38
82	G5	202	PEB	C2C-C3C	3.33	1.47	1.38
82	NO	1002	PEB	CHA-C1B	3.33	1.48	1.40
82	bP	501	PEB	CHB-C1C	3.33	1.48	1.40
82	DQ	202	PEB	C2A-C1A	-3.33	1.49	1.52
87	CL	513	CLA	C4B-NB	3.33	1.41	1.37
82	O1	202	PEB	C1A-NA	-3.33	1.33	1.37
82	A5	202	PEB	C1A-NA	-3.33	1.33	1.37
82	E9	201	PEB	C1A-NA	-3.33	1.33	1.37
82	R9	201	PEB	C1A-NA	-3.33	1.33	1.37
82	K7	201	PEB	C1C-C2C	3.33	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	KD	201	PEB	C2C-C3C	3.33	1.47	1.38
82	GF	203	PEB	C2C-C3C	3.33	1.47	1.38
82	j1	201	PEB	C2C-C3C	3.33	1.47	1.38
82	U7	202	PEB	C2C-C3C	3.33	1.47	1.38
82	aM	202	PEB	C2C-C3C	3.33	1.47	1.38
84	FE	1001	CYC	C3D-C2D	3.33	1.47	1.38
82	O9	203	PEB	CHB-C1C	3.33	1.48	1.40
82	R5	202	PEB	C2C-C3C	3.33	1.47	1.38
82	KM	202	PEB	C1A-NA	-3.33	1.33	1.37
82	bH	201	PEB	C1A-NA	-3.33	1.33	1.37
82	XB	201	PEB	CHB-C1C	3.33	1.48	1.40
82	DP	202	PEB	CHB-C1C	3.33	1.48	1.40
82	U9	202	PEB	CHA-C1B	3.33	1.48	1.40
87	B2	819	CLA	C4D-ND	-3.33	1.33	1.37
82	Y4	203	PEB	C2C-C3C	3.33	1.47	1.38
87	JN	101	CLA	C4B-NB	3.33	1.41	1.37
87	H6	103	CLA	C1D-ND	3.33	1.41	1.37
82	cO	201	PEB	C2C-C3C	3.32	1.47	1.38
82	HD	201	PEB	CHB-C1C	3.32	1.48	1.40
82	LK	202	PEB	CHB-C1C	3.32	1.48	1.40
82	EP	202	PEB	CHB-C1C	3.32	1.48	1.40
82	bH	201	PEB	CHA-C1B	3.32	1.48	1.40
82	S7	202	PEB	OD-C4D	3.32	1.29	1.23
82	OH	201	PEB	C2C-C3C	3.32	1.47	1.38
82	K7	201	PEB	C2C-C3C	3.32	1.47	1.38
84	o3	1001	CYC	CHA-C4D	3.32	1.48	1.40
82	d1	201	PEB	C1A-NA	-3.32	1.33	1.37
82	b4	202	PEB	C1A-NA	-3.32	1.33	1.37
82	OG	201	PEB	C2C-C3C	3.32	1.47	1.38
82	AJ	302	PEB	C2C-C3C	3.32	1.47	1.38
82	O7	202	PEB	OD-C4D	3.32	1.29	1.23
82	gB	202	PEB	CHB-C1C	3.32	1.48	1.40
83	xF	306	PUB	CHB-C4B	3.32	1.48	1.40
84	F3	1001	CYC	CHA-C4D	3.32	1.48	1.40
82	VM	201	PEB	CHB-C1C	3.32	1.48	1.40
84	F4	1001	CYC	C1D-C2D	3.32	1.49	1.41
82	YO	201	PEB	C1A-NA	-3.32	1.33	1.37
82	SJ	201	PEB	CHA-C1B	3.32	1.48	1.40
82	UQ	202	PEB	C2C-C3C	3.32	1.47	1.38
82	Z9	304	PEB	C2C-C3C	3.32	1.47	1.38
87	B6	614	CLA	C4D-ND	-3.32	1.33	1.37
87	8N	308	CLA	C4D-ND	-3.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PJ	201	PEB	C2C-C3C	3.32	1.47	1.38
82	FQ	203	PEB	CHA-C1B	3.32	1.48	1.40
82	RH	202	PEB	C1A-NA	-3.32	1.33	1.37
87	ON	201	CLA	C4B-NB	3.32	1.41	1.37
82	FH	1002	PEB	CHB-C1C	3.32	1.48	1.40
84	NO	1001	CYC	CHA-C4D	3.32	1.48	1.40
84	N4	1001	CYC	CHA-C4D	3.32	1.48	1.40
82	KK	202	PEB	C2C-C3C	3.32	1.47	1.38
87	IN	103	CLA	C4D-ND	-3.32	1.33	1.37
82	CM	201	PEB	C2A-C1A	-3.32	1.49	1.52
82	QJ	203	PEB	C2C-C3C	3.32	1.47	1.38
82	LA	203	PEB	C1A-NA	-3.32	1.33	1.37
82	jJ	202	PEB	C1A-NA	-3.32	1.33	1.37
87	BN	811	CLA	C1D-ND	3.32	1.41	1.37
82	J4	1002	PEB	CHB-C1C	3.32	1.48	1.40
82	F9	201	PEB	C2C-C3C	3.32	1.47	1.38
87	22	612	CLA	C4D-ND	-3.32	1.33	1.37
87	I2	103	CLA	C4D-ND	-3.32	1.33	1.37
87	cL	511	CLA	C4D-ND	-3.32	1.33	1.37
82	W1	201	PEB	C2C-C3C	3.32	1.47	1.38
82	WM	203	PEB	CHA-C1B	3.32	1.48	1.40
82	Y7	301	PEB	CHA-C1B	3.32	1.48	1.40
87	AN	817	CLA	C1D-ND	3.32	1.41	1.37
82	LQ	202	PEB	CHB-C1C	3.32	1.48	1.40
87	d6	403	CLA	C4D-ND	-3.32	1.33	1.37
82	ZO	201	PEB	CHA-C1B	3.32	1.48	1.40
84	HE	1001	CYC	CHA-C4D	3.32	1.48	1.40
84	n3	1001	CYC	CHA-C4D	3.32	1.48	1.40
82	OI	201	PEB	C4B-C3B	3.32	1.51	1.45
82	N5	202	PEB	C2C-C3C	3.32	1.47	1.38
87	cL	513	CLA	C4B-NB	3.32	1.41	1.37
82	PF	202	PEB	CHB-C1C	3.32	1.48	1.40
82	A7	202	PEB	CHB-C1C	3.32	1.48	1.40
82	RM	202	PEB	C2A-C1A	-3.32	1.49	1.52
82	J4	1002	PEB	C2A-C1A	-3.32	1.49	1.52
82	VO	201	PEB	C2C-C3C	3.32	1.47	1.38
82	jH	202	PEB	OD-C4D	3.32	1.29	1.23
82	lF	202	PEB	CHB-C1C	3.32	1.48	1.40
82	DD	203	PEB	C1A-NA	-3.32	1.33	1.37
82	P5	202	PEB	C2C-C3C	3.32	1.47	1.38
82	AG	301	PEB	C1A-NA	-3.32	1.33	1.37
82	u8	203	PEB	C1A-NA	-3.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	eF	203	PEB	CHA-C1B	3.32	1.48	1.40
82	Y9	201	PEB	C4B-C3B	3.32	1.51	1.45
82	RD	202	PEB	C2C-C3C	3.32	1.47	1.38
82	c4	201	PEB	C2C-C3C	3.32	1.47	1.38
82	DK	201	PEB	C2A-C1A	-3.32	1.49	1.52
82	hE	201	PEB	CHA-C1B	3.32	1.48	1.40
82	NQ	204	PEB	C2C-C3C	3.32	1.47	1.38
82	lG	201	PEB	C2C-C3C	3.32	1.47	1.38
82	NI	203	PEB	CHB-C1C	3.32	1.48	1.40
82	OF	203	PEB	C1A-NA	-3.32	1.33	1.37
82	E5	202	PEB	C2C-C3C	3.32	1.47	1.38
82	SG	203	PEB	CHA-C1B	3.32	1.48	1.40
82	JQ	202	PEB	C2C-C3C	3.32	1.47	1.38
87	B2	806	CLA	C4D-ND	-3.32	1.33	1.37
82	DI	201	PEB	C1C-NC	-3.32	1.32	1.37
82	gH	203	PEB	C2C-C3C	3.32	1.47	1.38
87	BN	809	CLA	C4D-ND	-3.32	1.33	1.37
82	AQ	301	PEB	CHA-C1B	3.32	1.48	1.40
82	HJ	202	PEB	C2A-C1A	-3.32	1.49	1.52
83	QJ	201	PUB	CHB-C4B	3.32	1.48	1.40
82	ZB	201	PEB	C2C-C3C	3.32	1.47	1.38
82	Z5	301	PEB	C2C-C3C	3.32	1.47	1.38
87	B2	827	CLA	C4B-NB	3.32	1.41	1.37
82	YI	202	PEB	CHB-C1C	3.32	1.48	1.40
87	A2	834	CLA	C4D-ND	-3.32	1.33	1.37
82	CM	202	PEB	C1A-NA	-3.31	1.33	1.37
82	V9	201	PEB	C1A-NA	-3.31	1.33	1.37
82	XP	201	PEB	CHB-C1C	3.31	1.48	1.40
82	jH	201	PEB	C2C-C3C	3.31	1.47	1.38
87	A2	821	CLA	C1D-ND	3.31	1.41	1.37
82	JO	1002	PEB	C2C-C3C	3.31	1.47	1.38
82	F7	201	PEB	C2C-C3C	3.31	1.47	1.38
82	ZB	202	PEB	CHB-C1C	3.31	1.48	1.40
82	aB	201	PEB	CHB-C1C	3.31	1.48	1.40
82	YH	201	PEB	C1A-NA	-3.31	1.33	1.37
82	DP	201	PEB	CHB-C1C	3.31	1.48	1.40
82	KJ	201	PEB	CHB-C1C	3.31	1.48	1.40
82	RJ	202	PEB	CHB-C1C	3.31	1.48	1.40
82	T4	203	PEB	C1A-NA	-3.31	1.33	1.37
82	D9	202	PEB	C1A-NA	-3.31	1.33	1.37
84	CG	1001	CYC	C1D-C2D	3.31	1.49	1.41
82	BQ	202	PEB	CHB-C1C	3.31	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mG	203	PEB	C1A-NA	-3.31	1.33	1.37
82	OQ	202	PEB	CHB-C1C	3.31	1.48	1.40
82	SB	203	PEB	CHA-C1B	3.31	1.48	1.40
82	X5	202	PEB	C2C-C3C	3.31	1.47	1.38
82	IA	202	PEB	OD-C4D	3.31	1.29	1.23
82	QP	203	PEB	CHA-C1B	3.31	1.48	1.40
82	CJ	202	PEB	C1A-NA	-3.31	1.33	1.37
82	oF	202	PEB	C1A-NA	-3.31	1.33	1.37
82	lG	202	PEB	C1A-NA	-3.31	1.33	1.37
82	I7	202	PEB	OD-C4D	3.31	1.29	1.23
87	B2	818	CLA	C1D-ND	3.31	1.41	1.37
84	D1	1001	CYC	C3D-C2D	3.31	1.47	1.38
82	BQ	201	PEB	C2A-C1A	-3.31	1.49	1.52
82	XP	202	PEB	C2C-C3C	3.31	1.47	1.38
82	BF	201	PEB	OD-C4D	3.31	1.29	1.23
82	M9	301	PEB	C2C-C3C	3.31	1.47	1.38
82	EM	202	PEB	CHB-C1C	3.31	1.48	1.40
82	WG	203	PEB	CHB-C1C	3.31	1.48	1.40
82	ZG	203	PEB	CHB-C1C	3.31	1.48	1.40
87	B2	818	CLA	C4D-ND	-3.31	1.33	1.37
82	IP	203	PEB	C2C-C3C	3.31	1.47	1.38
82	LP	201	PEB	C2C-C3C	3.31	1.47	1.38
82	L9	201	PEB	CHB-C1C	3.31	1.48	1.40
82	UE	203	PEB	C2C-C3C	3.31	1.47	1.38
82	YH	202	PEB	CHB-C1C	3.31	1.48	1.40
87	IN	102	CLA	C4D-ND	-3.31	1.33	1.37
82	gK	202	PEB	CHA-C1B	3.31	1.48	1.40
82	JA	203	PEB	C1A-NA	-3.31	1.33	1.37
82	HM	202	PEB	C2C-C3C	3.31	1.47	1.38
82	Z1	202	PEB	C2C-C3C	3.31	1.47	1.38
87	c6	611	CLA	C4D-ND	-3.31	1.33	1.37
82	pF	202	PEB	C2C-C3C	3.31	1.47	1.38
87	H6	102	CLA	C1D-ND	3.31	1.41	1.37
82	G7	202	PEB	C1A-NA	-3.31	1.33	1.37
82	pF	202	PEB	C1A-NA	-3.31	1.33	1.37
82	fG	201	PEB	C2C-C3C	3.31	1.47	1.38
82	GA	202	PEB	CHA-C1B	3.31	1.48	1.40
82	PH	202	PEB	C2A-C1A	-3.31	1.49	1.52
82	CJ	203	PEB	C2A-C1A	-3.31	1.49	1.52
82	OJ	203	PEB	C2A-C1A	-3.31	1.49	1.52
87	BN	822	CLA	C4D-ND	-3.31	1.33	1.37
87	B2	825	CLA	C4D-ND	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BD	201	PEB	CHB-C1C	3.31	1.48	1.40
82	EP	203	PEB	CHA-C1B	3.31	1.48	1.40
87	c6	611	CLA	C1D-ND	3.31	1.41	1.37
87	BN	823	CLA	C4D-ND	-3.31	1.33	1.37
82	EJ	203	PEB	C2C-C3C	3.31	1.47	1.38
84	E1	1001	CYC	CHA-C4D	3.31	1.48	1.40
82	yC	202	PEB	CHA-C1B	3.31	1.48	1.40
82	gJ	201	PEB	C1A-NA	-3.31	1.33	1.37
87	82	308	CLA	C4D-ND	-3.31	1.33	1.37
82	KB	301	PEB	CHB-C1C	3.31	1.48	1.40
82	TB	202	PEB	CHB-C1C	3.31	1.48	1.40
82	LP	201	PEB	CHB-C1C	3.31	1.48	1.40
82	QP	203	PEB	C1A-NA	-3.30	1.33	1.37
82	JB	202	PEB	CHB-C1C	3.30	1.48	1.40
82	Q5	201	PEB	CHA-C1B	3.30	1.48	1.40
82	wK	301	PEB	CHA-C1B	3.30	1.48	1.40
82	T7	202	PEB	CHB-C4B	3.30	1.45	1.38
82	bH	201	PEB	C2C-C3C	3.30	1.47	1.38
87	1N	601	CLA	C4D-ND	-3.30	1.33	1.37
87	2N	305	CLA	C4D-ND	-3.30	1.33	1.37
82	fH	203	PEB	CHA-C1B	3.30	1.48	1.40
82	D5	202	PEB	C2C-C3C	3.30	1.47	1.38
82	WA	202	PEB	OD-C4D	3.30	1.29	1.23
82	XD	201	PEB	C1A-NA	-3.30	1.33	1.37
82	dH	201	PEB	C1A-NA	-3.30	1.33	1.37
87	B2	822	CLA	C4D-ND	-3.30	1.33	1.37
84	JO	1001	CYC	C1D-C2D	3.30	1.49	1.41
82	TD	201	PEB	CHA-C1B	3.30	1.48	1.40
87	KN	105	CLA	C4B-NB	3.30	1.41	1.37
82	EK	202	PEB	C2C-C3C	3.30	1.47	1.38
91	dL	403	PHO	C3D-C2D	3.30	1.45	1.39
82	b1	201	PEB	C2C-C3C	3.30	1.47	1.38
82	I7	201	PEB	C2C-C3C	3.30	1.47	1.38
87	BL	604	CLA	C4D-ND	-3.30	1.33	1.37
87	22	604	CLA	C4D-ND	-3.30	1.33	1.37
87	bL	606	CLA	C4D-ND	-3.30	1.33	1.37
87	42	601	CLA	C4B-NB	3.30	1.41	1.37
82	aJ	201	PEB	C2C-C3C	3.30	1.47	1.38
82	WJ	203	PEB	CHB-C1C	3.30	1.48	1.40
82	HA	201	PEB	C2C-C3C	3.30	1.47	1.38
82	W9	202	PEB	C2C-C3C	3.30	1.47	1.38
82	QQ	201	PEB	C1A-NA	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	L4	1002	PEB	C1A-NA	-3.30	1.33	1.37
87	BN	817	CLA	C4D-ND	-3.30	1.33	1.37
82	FI	202	PEB	C2C-C3C	3.30	1.47	1.38
82	e4	202	PEB	CHA-C1B	3.30	1.48	1.40
87	DL	404	CLA	C4B-NB	3.30	1.41	1.37
87	b6	608	CLA	C1D-ND	3.30	1.41	1.37
82	gB	202	PEB	C1A-NA	-3.30	1.33	1.37
82	bK	201	PEB	C1A-NA	-3.30	1.33	1.37
82	aM	203	PEB	CHA-C1B	3.30	1.48	1.40
82	LO	1002	PEB	C2C-C3C	3.30	1.47	1.38
82	PK	202	PEB	CHB-C1C	3.30	1.48	1.40
82	sC	202	PEB	C2A-C1A	-3.30	1.49	1.52
82	GP	202	PEB	CHA-C1B	3.30	1.48	1.40
82	U1	203	PEB	C2C-C3C	3.30	1.47	1.38
84	MO	1001	CYC	C3D-C2D	3.30	1.47	1.38
82	FD	202	PEB	C1A-NA	-3.30	1.33	1.37
82	QF	202	PEB	OD-C4D	3.30	1.29	1.23
82	WJ	202	PEB	CHB-C1C	3.30	1.48	1.40
82	aE	202	PEB	CHB-C1C	3.30	1.48	1.40
87	12	607	CLA	C4B-NB	3.30	1.41	1.37
87	5N	608	CLA	C4B-NB	3.30	1.41	1.37
82	VJ	202	PEB	C2C-C3C	3.30	1.47	1.38
87	F2	202	CLA	C4D-ND	-3.30	1.33	1.37
82	c1	202	PEB	CHB-C1C	3.30	1.48	1.40
82	O5	202	PEB	CHB-C1C	3.30	1.48	1.40
82	NQ	202	PEB	C1A-NA	-3.30	1.33	1.37
87	C6	515	CLA	C1D-ND	3.30	1.41	1.37
87	4N	602	CLA	C4D-ND	-3.30	1.33	1.37
82	WD	202	PEB	C2C-C3C	3.30	1.47	1.38
82	TQ	201	PEB	C2C-C3C	3.30	1.47	1.38
87	cL	513	CLA	C3B-C4B	3.30	1.50	1.42
82	rF	202	PEB	CHB-C1C	3.30	1.48	1.40
82	KA	202	PEB	OD-C4D	3.30	1.29	1.23
82	dO	202	PEB	CHB-C1C	3.30	1.48	1.40
82	nK	201	PEB	C2C-C3C	3.30	1.47	1.38
82	SP	203	PEB	C1A-NA	-3.30	1.33	1.37
82	u8	202	PEB	C1A-NA	-3.30	1.33	1.37
82	lM	202	PEB	CHB-C1C	3.30	1.48	1.40
82	EA	201	PEB	C2C-C3C	3.30	1.47	1.38
82	UM	202	PEB	CHB-C1C	3.30	1.48	1.40
82	bK	202	PEB	C2C-C3C	3.30	1.47	1.38
87	AN	823	CLA	C1D-ND	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	J4	1001	CYC	C1D-C2D	3.30	1.49	1.41
84	D4	1001	CYC	CHA-C4D	3.30	1.48	1.40
82	O7	202	PEB	CHA-C1B	3.30	1.48	1.40
87	6N	610	CLA	C4B-NB	3.30	1.41	1.37
82	eF	202	PEB	C2C-C3C	3.30	1.47	1.38
87	C6	516	CLA	C4D-ND	-3.30	1.33	1.37
82	IM	203	PEB	C2C-C3C	3.30	1.47	1.38
82	L4	1002	PEB	C2C-C3C	3.30	1.47	1.38
82	G7	202	PEB	C2C-C3C	3.30	1.47	1.38
82	OA	202	PEB	OD-C4D	3.30	1.29	1.23
82	YJ	203	PEB	CHB-C1C	3.30	1.48	1.40
82	Y7	304	PEB	CHB-C1C	3.30	1.48	1.40
82	J7	203	PEB	C1A-NA	-3.29	1.33	1.37
82	AK	201	PEB	C2C-C3C	3.29	1.47	1.38
87	A6	402	CLA	C4D-ND	-3.29	1.33	1.37
82	UK	202	PEB	OD-C4D	3.29	1.29	1.23
82	B7	202	PEB	C2C-C3C	3.29	1.47	1.38
82	NA	203	PEB	C2A-C1A	-3.29	1.49	1.52
87	J2	101	CLA	C4B-NB	3.29	1.41	1.37
82	DI	202	PEB	CHB-C1C	3.29	1.48	1.40
82	RI	203	PEB	CHB-C1C	3.29	1.48	1.40
82	BM	301	PEB	C2C-C3C	3.29	1.47	1.38
82	l4	202	PEB	C2C-C3C	3.29	1.47	1.38
82	SE	201	PEB	CHB-C1C	3.29	1.48	1.40
82	i4	201	PEB	C2C-C3C	3.29	1.47	1.38
82	fK	201	PEB	C2C-C3C	3.29	1.47	1.38
82	FM	202	PEB	CHB-C1C	3.29	1.48	1.40
82	NO	1002	PEB	CHB-C1C	3.29	1.48	1.40
87	42	602	CLA	C4D-ND	-3.29	1.33	1.37
82	b1	201	PEB	CHA-C1B	3.29	1.48	1.40
87	AN	837	CLA	C1D-ND	3.29	1.41	1.37
87	RN	202	CLA	C4B-NB	3.29	1.41	1.37
82	CD	202	PEB	C2C-C3C	3.29	1.47	1.38
82	LH	1003	PEB	C2C-C3C	3.29	1.47	1.38
82	CB	202	PEB	CHB-C1C	3.29	1.48	1.40
82	YQ	202	PEB	CHA-C1B	3.29	1.48	1.40
82	cK	202	PEB	CHA-C1B	3.29	1.48	1.40
82	F1	1002	PEB	C2A-C1A	-3.29	1.49	1.52
82	eJ	202	PEB	C2C-C3C	3.29	1.47	1.38
82	kJ	202	PEB	CHB-C1C	3.29	1.48	1.40
82	RJ	201	PEB	C2C-C3C	3.29	1.47	1.38
82	CP	201	PEB	CHA-C1B	3.29	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	IP	203	PEB	CHA-C1B	3.29	1.48	1.40
82	RD	203	PEB	C2C-C3C	3.29	1.47	1.38
82	lJ	202	PEB	C2C-C3C	3.29	1.47	1.38
87	A2	807	CLA	C1D-ND	3.29	1.41	1.37
87	B2	810	CLA	C1D-ND	3.29	1.41	1.37
82	B5	201	PEB	C2A-C1A	-3.29	1.49	1.52
82	vK	202	PEB	CHB-C1C	3.29	1.48	1.40
82	TP	202	PEB	C2C-C3C	3.29	1.47	1.38
82	iJ	201	PEB	C1C-NC	-3.29	1.32	1.37
82	l1	203	PEB	OD-C4D	3.29	1.29	1.23
82	OP	202	PEB	C2C-C3C	3.29	1.47	1.38
82	O1	201	PEB	C2C-C3C	3.29	1.47	1.38
82	QF	201	PEB	C1A-NA	-3.29	1.33	1.37
87	BN	819	CLA	C4B-NB	3.29	1.41	1.37
87	AN	832	CLA	C4D-ND	-3.29	1.33	1.37
87	A2	802	CLA	C4D-ND	-3.29	1.33	1.37
87	B6	610	CLA	C4D-ND	-3.29	1.33	1.37
84	ME	1001	CYC	CHA-C4D	3.29	1.48	1.40
82	RQ	203	PEB	C2C-C3C	3.29	1.47	1.38
82	V4	201	PEB	C2C-C3C	3.29	1.47	1.38
82	A4	304	PEB	C1A-NA	-3.29	1.33	1.37
82	f1	203	PEB	CHA-C1B	3.29	1.48	1.40
87	AN	812	CLA	C4B-NB	3.29	1.41	1.37
82	UF	201	PEB	C3B-C2B	3.29	1.43	1.36
82	SH	202	PEB	C2C-C3C	3.29	1.47	1.38
82	mK	202	PEB	CHB-C1C	3.29	1.48	1.40
82	ZI	401	PEB	C1C-NC	-3.29	1.32	1.37
82	jM	201	PEB	CHB-C1C	3.29	1.48	1.40
87	b6	614	CLA	C4D-ND	-3.29	1.33	1.37
87	BN	827	CLA	C4B-NB	3.29	1.41	1.37
82	TJ	202	PEB	C2C-C3C	3.29	1.47	1.38
82	aO	203	PEB	C2C-C3C	3.29	1.47	1.38
82	YG	201	PEB	CHA-C1B	3.29	1.48	1.40
82	S4	202	PEB	C2C-C3C	3.29	1.47	1.38
82	SJ	202	PEB	C1A-NA	-3.29	1.33	1.37
82	eE	202	PEB	C1A-NA	-3.29	1.33	1.37
82	R4	202	PEB	CHB-C1C	3.29	1.48	1.40
84	FH	1001	CYC	C1D-C2D	3.29	1.49	1.41
82	EP	203	PEB	C2C-C3C	3.29	1.47	1.38
82	eO	201	PEB	C2A-C1A	-3.29	1.49	1.52
82	JQ	202	PEB	C1A-NA	-3.29	1.33	1.37
82	L7	203	PEB	C2C-C3C	3.29	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	eM	201	PEB	C2C-C3C	3.29	1.47	1.38
87	BN	820	CLA	C4D-ND	-3.29	1.33	1.37
87	A2	832	CLA	C4D-ND	-3.29	1.33	1.37
82	F9	202	PEB	C1A-NA	-3.29	1.33	1.37
82	qK	201	PEB	C1A-NA	-3.29	1.33	1.37
82	PO	203	PEB	C2C-C3C	3.29	1.47	1.38
82	LP	202	PEB	C2C-C3C	3.29	1.47	1.38
82	B7	203	PEB	C2C-C3C	3.29	1.47	1.38
82	nF	201	PEB	C2C-C3C	3.29	1.47	1.38
82	JB	202	PEB	C2C-C3C	3.29	1.47	1.38
82	c1	201	PEB	CHB-C1C	3.29	1.48	1.40
82	tC	202	PEB	C4B-C3B	3.29	1.50	1.45
82	D9	201	PEB	C2C-C3C	3.29	1.47	1.38
82	rK	202	PEB	CHB-C1C	3.29	1.48	1.40
87	12	601	CLA	C4D-ND	-3.29	1.33	1.37
87	dL	404	CLA	C4D-ND	-3.29	1.33	1.37
84	JH	1001	CYC	C1D-C2D	3.29	1.49	1.41
82	YB	202	PEB	CHB-C1C	3.28	1.48	1.40
82	WG	202	PEB	CHB-C1C	3.28	1.48	1.40
82	e1	201	PEB	CHB-C1C	3.28	1.48	1.40
82	XD	203	PEB	C1A-NA	-3.28	1.33	1.37
82	ZE	202	PEB	C2C-C3C	3.28	1.47	1.38
82	ZG	202	PEB	C2C-C3C	3.28	1.47	1.38
82	WG	201	PEB	C2C-C3C	3.28	1.47	1.38
82	TJ	202	PEB	C2A-C1A	-3.28	1.49	1.52
82	JJ	201	PEB	CHB-C1C	3.28	1.48	1.40
82	IA	201	PEB	C2C-C3C	3.28	1.47	1.38
82	LA	203	PEB	C2C-C3C	3.28	1.47	1.38
82	TF	201	PEB	C2C-C3C	3.28	1.47	1.38
82	Z4	201	PEB	CHA-C1B	3.28	1.48	1.40
84	LO	1001	CYC	C1D-C2D	3.28	1.49	1.41
82	mF	202	PEB	CHB-C1C	3.28	1.48	1.40
87	A2	823	CLA	C1D-ND	3.28	1.41	1.37
87	8N	301	CLA	C4B-NB	3.28	1.41	1.37
82	qK	203	PEB	C2C-C3C	3.28	1.47	1.38
87	I2	102	CLA	C4D-ND	-3.28	1.33	1.37
87	C6	510	CLA	C4D-ND	-3.28	1.33	1.37
82	X9	201	PEB	C1A-NA	-3.28	1.33	1.37
82	PF	201	PEB	C2C-C3C	3.28	1.47	1.38
82	NJ	202	PEB	C2C-C3C	3.28	1.47	1.38
82	BP	201	PEB	C2C-C3C	3.28	1.47	1.38
82	yK	301	PEB	C2C-C3C	3.28	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	72	603	CLA	C4B-NB	3.28	1.41	1.37
82	CP	202	PEB	C2C-C3C	3.28	1.47	1.38
87	AN	833	CLA	C4D-ND	-3.28	1.33	1.37
82	uC	203	PEB	C1A-NA	-3.28	1.33	1.37
82	iH	202	PEB	C1A-NA	-3.28	1.33	1.37
82	cB	403	PEB	CHB-C1C	3.28	1.48	1.40
82	SI	202	PEB	C2C-C3C	3.28	1.47	1.38
82	HJ	202	PEB	C2C-C3C	3.28	1.47	1.38
82	KM	202	PEB	C2C-C3C	3.28	1.47	1.38
82	eK	202	PEB	C2C-C3C	3.28	1.47	1.38
82	EJ	203	PEB	CHB-C1C	3.28	1.48	1.40
82	aG	202	PEB	CHB-C1C	3.28	1.48	1.40
87	6N	603	CLA	C4B-NB	3.28	1.41	1.37
82	RM	201	PEB	C2A-C1A	-3.28	1.49	1.52
82	AD	301	PEB	C1A-NA	-3.28	1.33	1.37
87	BL	623	CLA	C4D-ND	-3.28	1.33	1.37
82	FB	201	PEB	C2C-C3C	3.28	1.47	1.38
87	B2	818	CLA	C4B-NB	3.28	1.41	1.37
82	Y9	203	PEB	CHB-C1C	3.28	1.48	1.40
82	MJ	203	PEB	C1A-NA	-3.28	1.33	1.37
82	WP	202	PEB	C2C-C3C	3.28	1.47	1.38
82	D5	201	PEB	CHA-C1B	3.28	1.48	1.40
82	RJ	202	PEB	C2A-C1A	-3.28	1.49	1.52
87	c6	608	CLA	C4D-ND	-3.28	1.33	1.37
82	CF	201	PEB	C2C-C3C	3.28	1.47	1.38
82	fE	203	PEB	C2C-C3C	3.28	1.47	1.38
83	M9	303	PUB	C3B-C2B	3.28	1.47	1.38
84	NH	1001	CYC	C1D-C2D	3.28	1.49	1.41
84	L1	1001	CYC	CHA-C4D	3.28	1.48	1.40
82	Z4	202	PEB	C1A-NA	-3.28	1.33	1.37
82	VA	201	PEB	CHA-C1B	3.28	1.48	1.40
82	YB	201	PEB	CHB-C1C	3.28	1.48	1.40
87	A2	829	CLA	C4D-ND	-3.28	1.33	1.37
82	lM	202	PEB	C2C-C3C	3.28	1.47	1.38
82	mM	201	PEB	CHB-C1C	3.28	1.48	1.40
84	NE	201	CYC	CHA-C4D	3.28	1.48	1.40
84	KG	202	CYC	CHA-C4D	3.28	1.48	1.40
82	AH	305	PEB	C1A-NA	-3.28	1.33	1.37
82	AJ	302	PEB	CHB-C1C	3.28	1.48	1.40
82	l1	202	PEB	C2C-C3C	3.28	1.47	1.38
82	E7	201	PEB	C2C-C3C	3.28	1.47	1.38
82	NP	202	PEB	C2C-C3C	3.28	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	A4	303	PUB	C3B-C2B	3.28	1.47	1.38
84	C4	1001	CYC	C1D-C2D	3.28	1.49	1.41
82	lK	202	PEB	CHB-C1C	3.28	1.48	1.40
82	QA	202	PEB	OD-C4D	3.28	1.29	1.23
82	S1	202	PEB	C2C-C3C	3.28	1.47	1.38
82	dH	203	PEB	C1A-NA	-3.28	1.33	1.37
82	sK	202	PEB	OD-C4D	3.28	1.29	1.23
84	FO	1001	CYC	C1D-C2D	3.28	1.49	1.41
83	xK	306	PUB	CHB-C4B	3.28	1.48	1.40
84	LO	1001	CYC	CHA-C4D	3.28	1.48	1.40
82	jG	201	PEB	C1A-NA	-3.28	1.33	1.37
87	dL	402	CLA	C1D-ND	3.28	1.41	1.37
82	M5	304	PEB	CHA-C1B	3.28	1.48	1.40
82	PD	203	PEB	CHB-C1C	3.28	1.48	1.40
82	y8	202	PEB	CHA-C1B	3.28	1.48	1.40
82	KB	302	PEB	C2C-C3C	3.28	1.47	1.38
82	FJ	202	PEB	C2C-C3C	3.28	1.47	1.38
82	PK	201	PEB	C2C-C3C	3.28	1.47	1.38
82	J7	203	PEB	C2C-C3C	3.28	1.47	1.38
82	TD	202	PEB	C1A-NA	-3.28	1.33	1.37
82	hF	202	PEB	C1A-NA	-3.28	1.33	1.37
82	UB	302	PEB	C2A-C1A	-3.28	1.49	1.52
82	K7	201	PEB	CHA-C1B	3.28	1.48	1.40
82	WE	202	PEB	CHB-C1C	3.28	1.48	1.40
82	SF	203	PEB	CHB-C1C	3.28	1.48	1.40
82	AG	304	PEB	CHB-C1C	3.28	1.48	1.40
82	xK	302	PEB	CHB-C1C	3.28	1.48	1.40
82	TB	202	PEB	C2C-C3C	3.28	1.47	1.38
82	IM	202	PEB	C2C-C3C	3.28	1.47	1.38
84	E4	1001	CYC	C3D-C2D	3.28	1.47	1.38
82	R1	202	PEB	C1A-NA	-3.28	1.33	1.37
87	b6	618	CLA	C4D-ND	-3.28	1.33	1.37
82	NP	201	PEB	C2C-C3C	3.28	1.47	1.38
82	BQ	202	PEB	C2C-C3C	3.28	1.47	1.38
82	DQ	203	PEB	CHB-C1C	3.27	1.48	1.40
82	LH	1003	PEB	C1A-NA	-3.27	1.33	1.37
82	YM	203	PEB	C1A-NA	-3.27	1.33	1.37
82	P9	201	PEB	C1A-NA	-3.27	1.33	1.37
82	KE	201	PEB	C2C-C3C	3.27	1.47	1.38
82	hH	201	PEB	C2C-C3C	3.27	1.47	1.38
82	DQ	203	PEB	OD-C4D	3.27	1.29	1.23
82	hG	201	PEB	CHA-C1B	3.27	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VD	201	PEB	CHB-C1C	3.27	1.48	1.40
82	SE	202	PEB	CHA-C1B	3.27	1.48	1.40
83	Z9	302	PUB	C3B-C2B	3.27	1.47	1.38
82	WF	202	PEB	CHB-C1C	3.27	1.48	1.40
82	hM	203	PEB	CHB-C1C	3.27	1.48	1.40
82	iO	201	PEB	C2C-C3C	3.27	1.47	1.38
82	DF	202	PEB	C1A-NA	-3.27	1.33	1.37
82	T9	201	PEB	C1A-NA	-3.27	1.33	1.37
82	ZI	401	PEB	C4B-C3B	3.27	1.50	1.45
82	CM	201	PEB	C2C-C3C	3.27	1.47	1.38
82	gE	201	PEB	C2C-C3C	3.27	1.47	1.38
87	4N	601	CLA	C4B-NB	3.27	1.41	1.37
82	m4	201	PEB	CHB-C1C	3.27	1.48	1.40
82	VO	202	PEB	CHA-C1B	3.27	1.48	1.40
82	Z4	202	PEB	C2C-C3C	3.27	1.47	1.38
87	a6	607	CLA	C4D-ND	-3.27	1.33	1.37
87	62	309	CLA	C3B-C4B	3.27	1.50	1.42
82	dJ	202	PEB	CHA-C1B	3.27	1.48	1.40
84	I4	1001	CYC	C1D-C2D	3.27	1.49	1.41
82	KJ	202	PEB	C1A-NA	-3.27	1.33	1.37
82	L7	203	PEB	C1A-NA	-3.27	1.33	1.37
87	A2	813	CLA	C1D-ND	3.27	1.41	1.37
82	LQ	203	PEB	CHB-C1C	3.27	1.48	1.40
82	C9	201	PEB	C1A-NA	-3.27	1.33	1.37
82	I9	201	PEB	C1A-NA	-3.27	1.33	1.37
82	eF	203	PEB	C1A-NA	-3.27	1.33	1.37
82	AD	303	PEB	CHB-C1C	3.27	1.48	1.40
87	AL	404	CLA	C1D-ND	3.27	1.41	1.37
87	BL	620	CLA	C1D-ND	3.27	1.41	1.37
82	UH	203	PEB	C2C-C3C	3.27	1.47	1.38
82	P7	201	PEB	C2C-C3C	3.27	1.47	1.38
82	R7	203	PEB	C2C-C3C	3.27	1.47	1.38
82	WP	201	PEB	CHB-C1C	3.27	1.48	1.40
82	yK	301	PEB	CHA-C1B	3.27	1.48	1.40
87	b6	609	CLA	C1D-ND	3.27	1.41	1.37
87	5N	611	CLA	C4B-NB	3.27	1.41	1.37
82	BB	202	PEB	CHB-C1C	3.27	1.48	1.40
82	aJ	202	PEB	CHB-C1C	3.27	1.48	1.40
82	CD	201	PEB	CHA-C1B	3.27	1.48	1.40
82	hO	201	PEB	C2C-C3C	3.27	1.47	1.38
87	c6	609	CLA	C4D-ND	-3.27	1.33	1.37
82	TO	203	PEB	C1A-NA	-3.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EP	201	PEB	C2C-C3C	3.27	1.47	1.38
82	KD	202	PEB	CHB-C1C	3.27	1.48	1.40
82	RQ	202	PEB	C2C-C3C	3.27	1.47	1.38
82	fG	203	PEB	CHA-C1B	3.27	1.48	1.40
82	hM	201	PEB	CHA-C1B	3.27	1.48	1.40
82	aJ	203	PEB	C2C-C3C	3.27	1.47	1.38
82	J4	1002	PEB	C2C-C3C	3.27	1.47	1.38
87	6N	601	CLA	C4B-NB	3.27	1.41	1.37
84	L4	1001	CYC	C1D-C2D	3.27	1.49	1.41
82	D4	1002	PEB	C1A-NA	-3.27	1.33	1.37
82	EK	201	PEB	C2C-C3C	3.27	1.47	1.38
82	HP	202	PEB	C2C-C3C	3.27	1.47	1.38
82	lE	201	PEB	C2C-C3C	3.27	1.47	1.38
82	qF	203	PEB	C2C-C3C	3.27	1.47	1.38
82	mJ	202	PEB	C2C-C3C	3.27	1.47	1.38
82	SA	202	PEB	C2C-C3C	3.27	1.47	1.38
82	ZO	202	PEB	C2C-C3C	3.27	1.47	1.38
84	M4	1001	CYC	C3D-C2D	3.27	1.47	1.38
87	ON	201	CLA	C4D-ND	-3.27	1.33	1.37
87	B2	821	CLA	C4D-ND	-3.27	1.33	1.37
82	AE	304	PEB	CHB-C1C	3.27	1.48	1.40
82	FI	202	PEB	CHB-C1C	3.27	1.48	1.40
82	EJ	203	PEB	CHA-C1B	3.27	1.48	1.40
82	BQ	201	PEB	CHA-C1B	3.27	1.48	1.40
84	M1	201	CYC	C1D-C2D	3.27	1.49	1.41
82	WJ	202	PEB	C2C-C3C	3.27	1.47	1.38
82	Y4	201	PEB	C1A-NA	-3.27	1.33	1.37
82	eJ	202	PEB	CHB-C1C	3.27	1.48	1.40
82	FD	202	PEB	OD-C4D	3.27	1.29	1.23
82	QK	202	PEB	C2C-C3C	3.27	1.47	1.38
82	PP	202	PEB	C2C-C3C	3.27	1.47	1.38
84	EO	1001	CYC	C3D-C2D	3.27	1.47	1.38
82	FQ	202	PEB	C1A-NA	-3.27	1.33	1.37
82	V4	202	PEB	CHA-C1B	3.27	1.48	1.40
87	1N	606	CLA	C4D-ND	-3.27	1.33	1.37
82	PE	202	PEB	C2A-C1A	-3.27	1.49	1.52
82	iJ	202	PEB	C2A-C1A	-3.27	1.49	1.52
87	AN	816	CLA	C4B-NB	3.26	1.41	1.37
82	NH	1002	PEB	C2C-C3C	3.26	1.47	1.38
82	fF	201	PEB	C2C-C3C	3.26	1.47	1.38
82	DA	201	PEB	C1A-NA	-3.26	1.33	1.37
84	73	1002	CYC	C1D-C2D	3.26	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Z5	304	PEB	CHA-C1B	3.26	1.48	1.40
82	l4	201	PEB	C2C-C3C	3.26	1.47	1.38
82	CK	201	PEB	C2C-C3C	3.26	1.47	1.38
82	SP	203	PEB	C1C-NC	-3.26	1.32	1.37
82	HI	203	PEB	CHB-C1C	3.26	1.48	1.40
82	V4	202	PEB	CHB-C1C	3.26	1.48	1.40
87	A2	850	CLA	C3B-C4B	3.26	1.50	1.42
82	gK	202	PEB	C2C-C3C	3.26	1.47	1.38
87	2N	309	CLA	C1D-ND	3.26	1.41	1.37
82	G9	201	PEB	C1A-NA	-3.26	1.33	1.37
82	V4	201	PEB	CHB-C1C	3.26	1.48	1.40
82	gF	201	PEB	C2C-C3C	3.26	1.47	1.38
82	KJ	202	PEB	CHB-C1C	3.26	1.48	1.40
82	yF	301	PEB	C2C-C3C	3.26	1.47	1.38
82	A9	201	PEB	CHA-C1B	3.26	1.48	1.40
82	yF	301	PEB	CHA-C1B	3.26	1.48	1.40
82	XQ	203	PEB	C1A-NA	-3.26	1.33	1.37
82	N9	201	PEB	C1A-NA	-3.26	1.33	1.37
82	xF	302	PEB	CHB-C1C	3.26	1.48	1.40
83	M9	303	PUB	CHB-C4B	3.26	1.48	1.40
87	BN	807	CLA	C4D-ND	-3.26	1.33	1.37
82	JH	1002	PEB	C2C-C3C	3.26	1.47	1.38
82	aJ	204	PEB	C2A-C1A	-3.26	1.49	1.52
82	yK	301	PEB	C2A-C1A	-3.26	1.49	1.52
82	ZI	401	PEB	C1C-C2C	3.26	1.50	1.42
82	WG	201	PEB	CHB-C1C	3.26	1.48	1.40
82	cK	201	PEB	C2C-C3C	3.26	1.47	1.38
84	DE	1001	CYC	C1D-C2D	3.26	1.49	1.41
82	E9	201	PEB	CHA-C1B	3.26	1.48	1.40
82	V9	201	PEB	CHA-C1B	3.26	1.48	1.40
82	jO	202	PEB	CHB-C1C	3.26	1.48	1.40
87	bL	620	CLA	C1D-ND	3.26	1.41	1.37
82	wK	301	PEB	C2C-C3C	3.26	1.47	1.38
82	SB	202	PEB	CHB-C1C	3.26	1.48	1.40
82	RE	201	PEB	CHB-C1C	3.26	1.48	1.40
82	uF	203	PEB	C1A-NA	-3.26	1.33	1.37
87	CL	512	CLA	C4D-ND	-3.26	1.33	1.37
82	gF	202	PEB	CHA-C1B	3.26	1.48	1.40
82	RK	202	PEB	C2C-C3C	3.26	1.47	1.38
82	UM	202	PEB	C2C-C3C	3.26	1.47	1.38
87	AN	850	CLA	C3B-C4B	3.26	1.50	1.42
82	L1	1002	PEB	C2C-C3C	3.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GM	203	PEB	CHA-C1B	3.26	1.48	1.40
82	dH	202	PEB	CHC-C4C	3.26	1.53	1.49
87	1N	610	CLA	C4D-ND	-3.26	1.33	1.37
82	AM	301	PEB	C1A-NA	-3.26	1.33	1.37
87	O2	201	CLA	C4B-NB	3.26	1.41	1.37
82	mG	201	PEB	C2C-C3C	3.26	1.47	1.38
87	82	302	CLA	C4C-C3C	3.26	1.50	1.45
82	HQ	201	PEB	CHB-C1C	3.26	1.48	1.40
87	A2	826	CLA	C4D-ND	-3.26	1.33	1.37
82	K9	201	PEB	C1A-NA	-3.26	1.33	1.37
82	BA	203	PEB	C2C-C3C	3.26	1.47	1.38
82	WB	402	PEB	CHB-C1C	3.26	1.48	1.40
82	GD	202	PEB	C1A-NA	-3.26	1.33	1.37
82	OF	201	PEB	C1A-NA	-3.26	1.33	1.37
82	UF	202	PEB	OD-C4D	3.26	1.29	1.23
82	TA	202	PEB	CHB-C4B	3.26	1.45	1.38
82	K9	201	PEB	CHA-C1B	3.26	1.48	1.40
82	BA	203	PEB	CHB-C1C	3.26	1.48	1.40
87	1N	611	CLA	C4D-ND	-3.26	1.33	1.37
82	J9	203	PEB	C1A-NA	-3.26	1.33	1.37
82	tC	201	PEB	C1A-NA	-3.26	1.33	1.37
82	MP	201	PEB	CHA-C1B	3.26	1.48	1.40
82	BA	202	PEB	C2C-C3C	3.26	1.47	1.38
83	xF	305	PUB	C3B-C2B	3.26	1.47	1.38
82	LI	202	PEB	CHB-C1C	3.26	1.48	1.40
87	AN	838	CLA	C1D-ND	3.26	1.41	1.37
87	AN	840	CLA	C1D-ND	3.26	1.41	1.37
82	MB	202	PEB	OD-C4D	3.26	1.29	1.23
82	P9	201	PEB	CHA-C1B	3.26	1.48	1.40
82	DK	203	PEB	CHB-C1C	3.26	1.48	1.40
82	eH	201	PEB	CHB-C1C	3.26	1.48	1.40
87	BL	619	CLA	C4D-ND	-3.26	1.33	1.37
87	B6	603	CLA	C4D-ND	-3.26	1.33	1.37
82	QE	202	PEB	C2C-C3C	3.26	1.47	1.38
82	hB	301	PEB	C2C-C3C	3.26	1.47	1.38
82	LM	202	PEB	C2A-C1A	-3.26	1.49	1.52
84	N1	1001	CYC	C1D-C2D	3.26	1.49	1.41
82	GP	202	PEB	C2C-C3C	3.26	1.47	1.38
87	bL	619	CLA	C4D-ND	-3.26	1.33	1.37
82	SD	201	PEB	CHB-C1C	3.26	1.48	1.40
82	S4	201	PEB	C2C-C3C	3.26	1.47	1.38
82	Z4	202	PEB	CHB-C1C	3.26	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	836	CLA	C4B-NB	3.26	1.41	1.37
87	62	311	CLA	C4B-NB	3.26	1.41	1.37
82	KM	201	PEB	C2C-C3C	3.26	1.47	1.38
82	mE	201	PEB	C2C-C3C	3.26	1.47	1.38
87	b6	610	CLA	C4D-ND	-3.26	1.33	1.37
82	WM	203	PEB	CHB-C1C	3.25	1.48	1.40
82	YG	201	PEB	C2C-C3C	3.25	1.47	1.38
82	S5	202	PEB	CHA-C1B	3.25	1.48	1.40
87	A2	836	CLA	C4B-NB	3.25	1.41	1.37
87	1N	610	CLA	C1D-ND	3.25	1.41	1.37
82	cK	202	PEB	C2C-C3C	3.25	1.47	1.38
82	SH	202	PEB	CHB-C1C	3.25	1.48	1.40
82	YE	201	PEB	C2C-C3C	3.25	1.47	1.38
82	RB	201	PEB	CHB-C1C	3.25	1.48	1.40
82	U5	203	PEB	CHB-C1C	3.25	1.48	1.40
87	C6	513	CLA	C1D-ND	3.25	1.41	1.37
82	VJ	201	PEB	C2C-C3C	3.25	1.47	1.38
82	D5	201	PEB	C2C-C3C	3.25	1.47	1.38
83	AJ	304	PUB	CHB-C4B	3.25	1.48	1.40
82	gF	202	PEB	C2C-C3C	3.25	1.47	1.38
87	AN	801	CLA	C4D-ND	-3.25	1.33	1.37
87	C6	514	CLA	C4D-ND	-3.25	1.33	1.37
82	H4	1002	PEB	CHA-C1B	3.25	1.48	1.40
82	N9	201	PEB	CHA-C1B	3.25	1.48	1.40
82	KB	302	PEB	C2A-C1A	-3.25	1.49	1.52
82	dB	201	PEB	C2A-C1A	-3.25	1.49	1.52
84	DH	1001	CYC	C3D-C2D	3.25	1.47	1.38
82	BD	202	PEB	C2C-C3C	3.25	1.47	1.38
87	62	304	CLA	C4B-NB	3.25	1.41	1.37
87	B6	610	CLA	C1D-ND	3.25	1.41	1.37
82	KP	201	PEB	CHB-C1C	3.25	1.48	1.40
82	xC	201	PEB	C1A-NA	-3.25	1.33	1.37
82	hK	202	PEB	C1A-NA	-3.25	1.33	1.37
82	EK	202	PEB	CHB-C1C	3.25	1.48	1.40
82	fE	203	PEB	CHA-C1B	3.25	1.48	1.40
82	KA	201	PEB	C1C-C2C	3.25	1.50	1.42
87	c6	612	CLA	C4D-ND	-3.25	1.33	1.37
82	BI	201	PEB	C4B-C3B	3.25	1.50	1.45
87	b6	607	CLA	C1D-ND	3.25	1.41	1.37
87	dL	401	CLA	C1D-ND	3.25	1.41	1.37
87	6N	606	CLA	C4B-NB	3.25	1.41	1.37
82	DJ	201	PEB	CHB-C1C	3.25	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	HG	1001	CYC	CHA-C4D	3.25	1.48	1.40
82	L9	203	PEB	C1A-NA	-3.25	1.33	1.37
82	KK	202	PEB	CHB-C1C	3.25	1.48	1.40
82	CM	201	PEB	CHB-C1C	3.25	1.48	1.40
82	O9	202	PEB	CHB-C1C	3.25	1.48	1.40
82	KQ	201	PEB	C2C-C3C	3.25	1.47	1.38
82	h4	201	PEB	C2C-C3C	3.25	1.47	1.38
87	BN	814	CLA	C4D-ND	-3.25	1.33	1.37
87	72	609	CLA	C4B-NB	3.25	1.41	1.37
87	B2	833	CLA	C1D-ND	3.25	1.41	1.37
82	R9	201	PEB	CHA-C1B	3.25	1.48	1.40
87	cL	506	CLA	C4D-ND	-3.25	1.33	1.37
83	wF	304	PUB	C3B-C2B	3.25	1.47	1.38
82	IM	202	PEB	C2A-C1A	-3.25	1.49	1.52
82	P1	202	PEB	C2A-C1A	-3.25	1.49	1.52
87	bL	608	CLA	C4D-ND	-3.25	1.33	1.37
82	Y4	201	PEB	CHB-C1C	3.25	1.48	1.40
82	dM	201	PEB	CHA-C1B	3.25	1.48	1.40
87	A2	817	CLA	C1D-ND	3.25	1.41	1.37
87	b6	610	CLA	C4B-NB	3.25	1.41	1.37
82	BI	203	PEB	C1A-NA	-3.25	1.33	1.37
87	82	303	CLA	C4D-ND	-3.25	1.33	1.37
87	A2	808	CLA	C4D-ND	-3.25	1.33	1.37
82	OE	201	PEB	C2C-C3C	3.25	1.47	1.38
82	UJ	203	PEB	C2C-C3C	3.25	1.47	1.38
84	KH	1001	CYC	C2C-C1C	-3.25	1.49	1.52
82	C9	201	PEB	CHA-C1B	3.25	1.48	1.40
82	w8	202	PEB	C1A-NA	-3.25	1.33	1.37
82	QG	203	PEB	C2C-C3C	3.25	1.47	1.38
82	L5	201	PEB	C2C-C3C	3.25	1.47	1.38
82	wF	301	PEB	C2C-C3C	3.25	1.47	1.38
83	AM	303	PUB	CHB-C4B	3.25	1.48	1.40
82	kH	202	PEB	C2A-C1A	-3.25	1.49	1.52
82	QM	202	PEB	C1A-NA	-3.25	1.33	1.37
87	BN	826	CLA	C4D-ND	-3.25	1.33	1.37
87	B6	606	CLA	C4D-ND	-3.25	1.33	1.37
87	B6	615	CLA	C4D-ND	-3.25	1.33	1.37
82	BB	201	PEB	C2C-C3C	3.25	1.47	1.38
82	UB	303	PEB	C2C-C3C	3.25	1.47	1.38
82	FD	203	PEB	CHA-C1B	3.25	1.48	1.40
82	G9	201	PEB	CHA-C1B	3.25	1.48	1.40
82	OI	203	PEB	C2C-C3C	3.25	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MK	202	PEB	C2C-C3C	3.25	1.47	1.38
82	TO	201	PEB	C2C-C3C	3.25	1.47	1.38
82	UP	203	PEB	CHB-C1C	3.25	1.48	1.40
84	MG	1001	CYC	CHA-C4D	3.25	1.48	1.40
87	6N	608	CLA	C3B-C4B	3.25	1.50	1.42
82	x8	201	PEB	C1A-NA	-3.25	1.33	1.37
82	CF	203	PEB	C2C-C3C	3.25	1.47	1.38
84	ME	1001	CYC	C3D-C2D	3.25	1.47	1.38
82	IB	201	PEB	CHB-C1C	3.25	1.48	1.40
82	B9	203	PEB	CHB-C1C	3.25	1.48	1.40
82	EK	202	PEB	CHA-C1B	3.25	1.48	1.40
82	aK	202	PEB	C2C-C3C	3.25	1.47	1.38
82	QB	201	PEB	CHB-C1C	3.25	1.48	1.40
82	E7	202	PEB	OD-C4D	3.25	1.29	1.23
82	W9	203	PEB	C1A-NA	-3.25	1.33	1.37
87	A2	816	CLA	C4D-ND	-3.25	1.33	1.37
87	AN	807	CLA	C1D-ND	3.25	1.41	1.37
87	B2	826	CLA	C1D-ND	3.25	1.41	1.37
87	1N	611	CLA	C4B-NB	3.25	1.41	1.37
82	MM	202	PEB	C2C-C3C	3.25	1.47	1.38
82	DI	201	PEB	CHB-C1C	3.25	1.48	1.40
82	PE	201	PEB	C2C-C3C	3.25	1.47	1.38
82	L1	1002	PEB	C2A-C1A	-3.24	1.49	1.52
82	PH	201	PEB	CHB-C1C	3.24	1.48	1.40
82	A9	201	PEB	C1A-NA	-3.24	1.33	1.37
82	SO	201	PEB	C2C-C3C	3.24	1.47	1.38
82	DP	202	PEB	C2C-C3C	3.24	1.47	1.38
82	fJ	203	PEB	CHA-C1B	3.24	1.48	1.40
82	P1	201	PEB	CHB-C1C	3.24	1.48	1.40
82	N9	202	PEB	C1A-NA	-3.24	1.33	1.37
82	l1	201	PEB	CHA-C1B	3.24	1.48	1.40
82	mJ	201	PEB	C2A-C1A	-3.24	1.49	1.52
82	jO	201	PEB	CHB-C1C	3.24	1.48	1.40
87	A2	812	CLA	C4B-NB	3.24	1.41	1.37
87	cL	512	CLA	C1D-ND	3.24	1.41	1.37
83	BM	302	PUB	C3B-C2B	3.24	1.47	1.38
82	tF	201	PEB	C2A-C1A	-3.24	1.49	1.52
82	XD	201	PEB	CHA-C1B	3.24	1.48	1.40
82	XQ	201	PEB	CHA-C1B	3.24	1.48	1.40
82	wC	202	PEB	C1A-NA	-3.24	1.33	1.37
82	DG	1002	PEB	C2C-C3C	3.24	1.47	1.38
82	BP	202	PEB	C2C-C3C	3.24	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	wF	301	PEB	CHB-C1C	3.24	1.48	1.40
82	DB	202	PEB	C2C-C3C	3.24	1.47	1.38
82	SG	201	PEB	CHB-C1C	3.24	1.48	1.40
82	YO	201	PEB	CHB-C1C	3.24	1.48	1.40
87	CL	503	CLA	C4D-ND	-3.24	1.33	1.37
87	CL	508	CLA	C4D-ND	-3.24	1.33	1.37
87	B6	611	CLA	C4D-ND	-3.24	1.33	1.37
82	MQ	202	PEB	C1A-NA	-3.24	1.33	1.37
82	WG	203	PEB	CHA-C1B	3.24	1.48	1.40
82	DD	201	PEB	C2A-C1A	-3.24	1.49	1.52
82	CQ	202	PEB	C2C-C3C	3.24	1.47	1.38
82	K7	202	PEB	OD-C4D	3.24	1.29	1.23
82	QB	204	PEB	C2C-C3C	3.24	1.47	1.38
82	CP	202	PEB	CHB-C1C	3.24	1.48	1.40
82	R1	201	PEB	CHB-C1C	3.24	1.48	1.40
87	7N	601	CLA	C4B-NB	3.24	1.41	1.37
82	LA	201	PEB	C2C-C3C	3.24	1.47	1.38
82	aG	201	PEB	C2A-C1A	-3.24	1.49	1.52
82	jK	201	PEB	C2A-C1A	-3.24	1.49	1.52
82	M9	304	PEB	C2A-C1A	-3.24	1.49	1.52
82	H7	203	PEB	C2C-C3C	3.24	1.47	1.38
82	fG	203	PEB	C2C-C3C	3.24	1.47	1.38
82	TD	203	PEB	C1A-NA	-3.24	1.33	1.37
82	CQ	201	PEB	CHA-C1B	3.24	1.48	1.40
82	VB	201	PEB	C2C-C3C	3.24	1.47	1.38
82	H9	203	PEB	C2C-C3C	3.24	1.47	1.38
82	YA	304	PEB	CHB-C1C	3.24	1.48	1.40
82	GQ	202	PEB	C1A-NA	-3.24	1.33	1.37
84	D1	1001	CYC	C1C-NC	-3.24	1.33	1.37
82	QJ	202	PEB	C2A-C1A	-3.24	1.49	1.52
82	X9	201	PEB	CHA-C1B	3.24	1.48	1.40
82	mK	201	PEB	C2C-C3C	3.24	1.47	1.38
82	VO	202	PEB	CHB-C1C	3.24	1.48	1.40
87	7N	603	CLA	C4B-NB	3.24	1.41	1.37
82	JO	1002	PEB	CHC-C4C	3.24	1.53	1.49
82	ND	204	PEB	C2C-C3C	3.24	1.47	1.38
82	lK	201	PEB	CHA-C1B	3.24	1.48	1.40
82	KQ	202	PEB	CHB-C1C	3.24	1.48	1.40
87	AN	819	CLA	C3B-C4B	3.24	1.50	1.42
82	L5	201	PEB	CHB-C1C	3.24	1.48	1.40
87	IN	102	CLA	C1D-ND	3.24	1.41	1.37
82	d4	201	PEB	C2C-C3C	3.24	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	D9	202	PEB	C2C-C3C	3.24	1.47	1.38
82	gG	201	PEB	C2C-C3C	3.24	1.47	1.38
82	DH	1002	PEB	C1A-NA	-3.24	1.33	1.37
82	RQ	201	PEB	C1A-NA	-3.24	1.33	1.37
82	Z9	304	PEB	C1A-NA	-3.24	1.33	1.37
82	I9	201	PEB	CHA-C1B	3.24	1.48	1.40
82	GK	203	PEB	OD-C4D	3.24	1.29	1.23
82	L1	1002	PEB	CHB-C1C	3.24	1.48	1.40
82	UF	201	PEB	C2C-C3C	3.24	1.47	1.38
87	b6	607	CLA	C4D-ND	-3.24	1.33	1.37
87	bL	616	CLA	C4D-ND	-3.24	1.33	1.37
82	AD	303	PEB	C1A-NA	-3.24	1.33	1.37
82	CJ	201	PEB	CHB-C1C	3.24	1.48	1.40
82	QF	202	PEB	C2C-C3C	3.24	1.47	1.38
82	fB	301	PEB	C2C-C3C	3.24	1.47	1.38
87	3N	309	CLA	C4D-ND	-3.24	1.33	1.37
82	AJ	301	PEB	CHB-C1C	3.24	1.48	1.40
82	BB	202	PEB	C2C-C3C	3.24	1.47	1.38
82	OA	201	PEB	CHA-C1B	3.24	1.48	1.40
82	EF	202	PEB	CHB-C1C	3.24	1.48	1.40
82	DM	201	PEB	CHB-C1C	3.24	1.48	1.40
82	eM	201	PEB	CHB-C1C	3.24	1.48	1.40
82	uF	201	PEB	C2C-C3C	3.24	1.47	1.38
87	aL	605	CLA	C4D-ND	-3.24	1.33	1.37
82	Q1	203	PEB	C2C-C3C	3.24	1.47	1.38
82	SM	202	PEB	CHA-C1B	3.24	1.48	1.40
82	B7	203	PEB	CHB-C1C	3.24	1.48	1.40
82	MB	202	PEB	CHB-C1C	3.24	1.48	1.40
82	MK	201	PEB	C2C-C3C	3.23	1.47	1.38
82	R7	201	PEB	C2C-C3C	3.23	1.47	1.38
82	GB	202	PEB	C2A-C1A	-3.23	1.49	1.52
82	UG	203	PEB	C2C-C3C	3.23	1.47	1.38
82	FP	202	PEB	C2C-C3C	3.23	1.47	1.38
82	YO	203	PEB	C2C-C3C	3.23	1.47	1.38
87	BN	833	CLA	C1D-ND	3.23	1.41	1.37
87	12	610	CLA	C1D-ND	3.23	1.41	1.37
87	42	611	CLA	C4B-NB	3.23	1.41	1.37
87	b6	613	CLA	C1D-ND	3.23	1.41	1.37
87	bL	615	CLA	C1D-ND	3.23	1.41	1.37
82	P9	202	PEB	C1A-NA	-3.23	1.33	1.37
87	B6	607	CLA	C4D-ND	-3.23	1.33	1.37
82	ZF	201	PEB	C2C-C3C	3.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	I4	1001	CYC	C3D-C2D	3.23	1.47	1.38
84	DO	1001	CYC	CHA-C4D	3.23	1.48	1.40
82	SE	201	PEB	C2C-C3C	3.23	1.47	1.38
82	S1	202	PEB	CHB-C1C	3.23	1.48	1.40
82	OJ	202	PEB	CHA-C1B	3.23	1.48	1.40
82	ZH	201	PEB	CHB-C1C	3.23	1.48	1.40
82	YA	301	PEB	CHA-C1B	3.23	1.48	1.40
92	J6	102	LMG	O8-C28	3.23	1.42	1.33
82	GM	201	PEB	C2A-C1A	-3.23	1.49	1.52
87	AN	851	CLA	C1D-ND	3.23	1.41	1.37
87	22	606	CLA	C4B-NB	3.23	1.41	1.37
87	32	309	CLA	C4D-ND	-3.23	1.33	1.37
82	AP	203	PEB	C2C-C3C	3.23	1.47	1.38
82	QG	202	PEB	C2C-C3C	3.23	1.47	1.38
87	d6	401	CLA	C4D-ND	-3.23	1.33	1.37
82	RI	201	PEB	CHB-C1C	3.23	1.48	1.40
87	8N	303	CLA	C4C-C3C	3.23	1.50	1.45
82	DE	1002	PEB	C2C-C3C	3.23	1.47	1.38
82	KP	202	PEB	C2C-C3C	3.23	1.47	1.38
83	Z9	302	PUB	CHB-C4B	3.23	1.48	1.40
82	UE	201	PEB	CHA-C1B	3.23	1.48	1.40
87	8N	307	CLA	C4D-ND	-3.23	1.33	1.37
82	DI	202	PEB	C2C-C3C	3.23	1.47	1.38
82	LQ	202	PEB	C2C-C3C	3.23	1.47	1.38
84	F1	1001	CYC	C1D-C2D	3.23	1.49	1.41
82	LD	202	PEB	C2C-C3C	3.23	1.47	1.38
82	jE	201	PEB	C2C-C3C	3.23	1.47	1.38
82	p8	201	PEB	C1A-NA	-3.23	1.33	1.37
82	a4	203	PEB	C2C-C3C	3.23	1.47	1.38
82	hE	203	PEB	C2C-C3C	3.23	1.47	1.38
87	AN	803	CLA	C4B-NB	3.23	1.41	1.37
87	A2	838	CLA	C1D-ND	3.23	1.41	1.37
82	U7	202	PEB	CHA-C1B	3.23	1.48	1.40
82	GI	202	PEB	CHB-C1C	3.23	1.48	1.40
82	Q9	203	PEB	C1A-NA	-3.23	1.33	1.37
82	aM	201	PEB	C1A-NA	-3.23	1.33	1.37
82	J5	202	PEB	CHA-C1B	3.23	1.48	1.40
82	HJ	201	PEB	C2A-C1A	-3.23	1.49	1.52
82	SP	202	PEB	C2A-C1A	-3.23	1.49	1.52
82	U4	201	PEB	C2A-C1A	-3.23	1.49	1.52
82	Z9	303	PEB	C2A-C1A	-3.23	1.49	1.52
82	WQ	202	PEB	C2C-C3C	3.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	aF	203	PEB	C2C-C3C	3.23	1.47	1.38
87	B6	609	CLA	C4D-ND	-3.23	1.33	1.37
82	JD	202	PEB	C2C-C3C	3.23	1.47	1.38
82	CK	203	PEB	C2C-C3C	3.23	1.47	1.38
82	NO	1002	PEB	C2C-C3C	3.23	1.47	1.38
87	7N	609	CLA	C4B-NB	3.23	1.41	1.37
82	BK	201	PEB	OD-C4D	3.23	1.29	1.23
82	tK	203	PEB	C2C-C3C	3.23	1.47	1.38
82	eH	201	PEB	C2A-C1A	-3.23	1.49	1.52
82	D4	1002	PEB	C2C-C3C	3.23	1.47	1.38
87	52	611	CLA	C4B-NB	3.23	1.41	1.37
82	JA	203	PEB	C2C-C3C	3.23	1.47	1.38
82	kG	201	PEB	C2C-C3C	3.23	1.47	1.38
82	ND	202	PEB	C2C-C3C	3.23	1.47	1.38
82	Q1	201	PEB	C2C-C3C	3.23	1.47	1.38
82	fB	301	PEB	C1A-NA	-3.23	1.33	1.37
82	TK	202	PEB	C2A-C1A	-3.23	1.49	1.52
87	82	306	CLA	C4B-NB	3.23	1.41	1.37
82	PA	201	PEB	C2C-C3C	3.23	1.47	1.38
87	A2	822	CLA	C4D-ND	-3.23	1.33	1.37
82	QE	201	PEB	CHB-C1C	3.23	1.48	1.40
87	I2	102	CLA	C1D-ND	3.23	1.41	1.37
82	PM	201	PEB	C2C-C3C	3.23	1.47	1.38
82	DO	1002	PEB	C2A-C1A	-3.23	1.49	1.52
82	BA	201	PEB	CHB-C1C	3.23	1.47	1.40
82	RH	201	PEB	CHB-C1C	3.23	1.47	1.40
82	EJ	202	PEB	CHB-C1C	3.23	1.47	1.40
82	H7	202	PEB	C2C-C3C	3.23	1.47	1.38
84	KH	1001	CYC	C3D-C2D	3.23	1.47	1.38
82	dO	201	PEB	C1A-NA	-3.23	1.33	1.37
82	XJ	202	PEB	C2C-C3C	3.23	1.47	1.38
82	EI	201	PEB	CHB-C1C	3.22	1.47	1.40
82	XI	201	PEB	CHB-C1C	3.22	1.47	1.40
82	WG	202	PEB	C1A-NA	-3.22	1.33	1.37
82	T9	202	PEB	C1A-NA	-3.22	1.33	1.37
82	UG	203	PEB	OD-C4D	3.22	1.29	1.23
82	T4	203	PEB	C2C-C3C	3.22	1.47	1.38
82	EP	201	PEB	CHB-C1C	3.22	1.47	1.40
87	B2	806	CLA	C1D-ND	3.22	1.41	1.37
87	A2	803	CLA	C4D-ND	-3.22	1.33	1.37
82	DB	202	PEB	CHB-C1C	3.22	1.47	1.40
82	KK	201	PEB	CHB-C1C	3.22	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ZK	201	PEB	C2C-C3C	3.22	1.47	1.38
82	UP	203	PEB	C2C-C3C	3.22	1.47	1.38
82	WE	201	PEB	CHB-C1C	3.22	1.47	1.40
82	RO	203	PEB	C2C-C3C	3.22	1.47	1.38
82	N1	1002	PEB	C2C-C3C	3.22	1.47	1.38
82	c1	202	PEB	C2C-C3C	3.22	1.47	1.38
82	m1	201	PEB	CHB-C1C	3.22	1.47	1.40
82	gJ	201	PEB	CHB-C1C	3.22	1.47	1.40
87	AN	803	CLA	C4D-ND	-3.22	1.33	1.37
87	B6	612	CLA	C4D-ND	-3.22	1.33	1.37
87	2N	307	CLA	C4B-NB	3.22	1.41	1.37
82	BI	201	PEB	CHA-C1B	3.22	1.48	1.40
82	MM	201	PEB	CHA-C1B	3.22	1.48	1.40
82	F9	203	PEB	CHB-C1C	3.22	1.47	1.40
82	DD	203	PEB	C2C-C3C	3.22	1.47	1.38
83	wK	304	PUB	C3B-C2B	3.22	1.47	1.38
87	12	610	CLA	C4D-ND	-3.22	1.33	1.37
87	A2	819	CLA	C3B-C4B	3.22	1.50	1.42
87	K2	101	CLA	C4B-NB	3.22	1.41	1.37
82	SG	201	PEB	C2C-C3C	3.22	1.47	1.38
83	Z5	303	PUB	C4B-C3B	3.22	1.50	1.42
82	VK	202	PEB	C1A-NA	-3.22	1.33	1.37
82	XQ	201	PEB	C1A-NA	-3.22	1.33	1.37
82	MA	202	PEB	CHA-C1B	3.22	1.48	1.40
87	AN	817	CLA	C4D-ND	-3.22	1.33	1.37
87	12	606	CLA	C4D-ND	-3.22	1.33	1.37
82	t8	202	PEB	C4B-C3B	3.22	1.50	1.45
84	J1	1001	CYC	C1D-C2D	3.22	1.49	1.41
82	kH	203	PEB	CHA-C1B	3.22	1.48	1.40
87	CL	514	CLA	C4D-ND	-3.22	1.33	1.37
87	AN	808	CLA	C4D-ND	-3.22	1.33	1.37
87	BN	818	CLA	C4D-ND	-3.22	1.33	1.37
87	B2	835	CLA	C4D-ND	-3.22	1.33	1.37
87	cL	512	CLA	C4D-ND	-3.22	1.33	1.37
82	mH	201	PEB	CHB-C1C	3.22	1.47	1.40
82	wK	301	PEB	CHB-C1C	3.22	1.47	1.40
82	bF	202	PEB	C1A-NA	-3.22	1.33	1.37
82	QH	201	PEB	C2C-C3C	3.22	1.47	1.38
87	b6	616	CLA	C4D-ND	-3.22	1.33	1.37
83	Z5	302	PUB	C4B-C3B	3.22	1.50	1.42
82	GB	201	PEB	C2C-C3C	3.22	1.47	1.38
82	WE	203	PEB	CHA-C1B	3.22	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	T9	201	PEB	CHA-C1B	3.22	1.48	1.40
82	UO	202	PEB	CHB-C1C	3.22	1.47	1.40
87	AN	816	CLA	C4D-ND	-3.22	1.33	1.37
82	AI	201	PEB	CHB-C1C	3.22	1.47	1.40
82	QK	201	PEB	C1A-NA	-3.22	1.33	1.37
82	U9	204	PEB	C1A-NA	-3.22	1.33	1.37
82	HA	202	PEB	C2C-C3C	3.22	1.47	1.38
82	LD	201	PEB	C2C-C3C	3.22	1.47	1.38
84	L1	1001	CYC	C1B-C2B	3.22	1.50	1.45
82	ZJ	201	PEB	C2C-C3C	3.22	1.47	1.38
84	KG	202	CYC	C3D-C2D	3.22	1.47	1.38
82	SH	202	PEB	OD-C4D	3.22	1.29	1.23
87	B2	807	CLA	C1D-ND	3.22	1.41	1.37
82	eG	202	PEB	C1A-NA	-3.22	1.33	1.37
82	RA	203	PEB	C2C-C3C	3.22	1.47	1.38
82	KF	203	PEB	CHB-C1C	3.22	1.47	1.40
82	SK	203	PEB	CHB-C1C	3.22	1.47	1.40
82	BB	203	PEB	CHB-C1C	3.22	1.47	1.40
87	A2	840	CLA	C1D-ND	3.22	1.41	1.37
87	BN	835	CLA	C4D-ND	-3.22	1.33	1.37
87	FN	201	CLA	C4D-ND	-3.22	1.33	1.37
87	B2	813	CLA	C4D-ND	-3.22	1.33	1.37
82	ND	202	PEB	C1A-NA	-3.22	1.33	1.37
82	IJ	201	PEB	C2A-C1A	-3.22	1.49	1.52
82	SF	202	PEB	CHB-C1C	3.22	1.47	1.40
82	Q5	201	PEB	CHB-C1C	3.22	1.47	1.40
82	QE	203	PEB	C2C-C3C	3.22	1.47	1.38
82	JP	202	PEB	CHB-C1C	3.22	1.47	1.40
82	AQ	303	PEB	CHB-C1C	3.22	1.47	1.40
82	hG	203	PEB	C2C-C3C	3.22	1.47	1.38
82	jG	201	PEB	C2C-C3C	3.22	1.47	1.38
82	G5	201	PEB	C2C-C3C	3.22	1.47	1.38
82	e1	202	PEB	C1A-NA	-3.22	1.33	1.37
87	b6	618	CLA	C1D-ND	3.22	1.41	1.37
87	B6	616	CLA	C4D-ND	-3.21	1.33	1.37
82	FO	1002	PEB	CHB-C1C	3.21	1.47	1.40
82	d4	201	PEB	CHB-C1C	3.21	1.47	1.40
83	xK	305	PUB	C3B-C2B	3.21	1.47	1.38
87	CL	506	CLA	C4D-ND	-3.21	1.33	1.37
82	AI	203	PEB	C1A-NA	-3.21	1.33	1.37
82	OK	201	PEB	C1A-NA	-3.21	1.33	1.37
82	h4	202	PEB	C1A-NA	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	OJ	201	PEB	CHB-C1C	3.21	1.47	1.40
82	U4	202	PEB	CHB-C1C	3.21	1.47	1.40
82	d1	201	PEB	CHA-C1B	3.21	1.47	1.40
82	gH	203	PEB	OD-C4D	3.21	1.29	1.23
82	HA	203	PEB	C2C-C3C	3.21	1.47	1.38
82	k1	202	PEB	C2C-C3C	3.21	1.47	1.38
82	E5	201	PEB	C2C-C3C	3.21	1.47	1.38
84	K1	1001	CYC	C3D-C2D	3.21	1.47	1.38
82	AP	201	PEB	CHB-C1C	3.21	1.47	1.40
82	U1	203	PEB	CHB-C1C	3.21	1.47	1.40
82	K5	201	PEB	C2C-C3C	3.21	1.47	1.38
82	FA	201	PEB	C1A-NA	-3.21	1.33	1.37
82	JJ	202	PEB	CHB-C1C	3.21	1.47	1.40
82	W5	203	PEB	CHB-C1C	3.21	1.47	1.40
87	AN	813	CLA	C1D-ND	3.21	1.41	1.37
82	C5	201	PEB	C2C-C3C	3.21	1.47	1.38
82	eJ	201	PEB	C2C-C3C	3.21	1.47	1.38
84	IG	1001	CYC	CHA-C4D	3.21	1.47	1.40
82	OP	203	PEB	CHA-C1B	3.21	1.47	1.40
82	J9	203	PEB	C2C-C3C	3.21	1.47	1.38
82	KE	201	PEB	C2A-C1A	-3.21	1.49	1.52
82	eJ	202	PEB	C2A-C1A	-3.21	1.49	1.52
82	V9	202	PEB	C1A-NA	-3.21	1.33	1.37
82	ED	202	PEB	CHB-C1C	3.21	1.47	1.40
82	DP	201	PEB	C2C-C3C	3.21	1.47	1.38
82	W7	202	PEB	OD-C4D	3.21	1.29	1.23
82	lM	201	PEB	CHA-C1B	3.21	1.47	1.40
82	QF	203	PEB	C2A-C1A	-3.21	1.49	1.52
82	P4	201	PEB	C2A-C1A	-3.21	1.49	1.52
87	C6	520	CLA	C4D-ND	-3.21	1.33	1.37
82	TO	203	PEB	C2C-C3C	3.21	1.47	1.38
82	cB	401	PEB	CHB-C1C	3.21	1.47	1.40
87	3N	313	CLA	C4B-NB	3.21	1.41	1.37
82	U5	201	PEB	CHA-C1B	3.21	1.47	1.40
82	lJ	203	PEB	CHA-C1B	3.21	1.47	1.40
87	BN	832	CLA	C4D-ND	-3.21	1.33	1.37
82	L7	201	PEB	C2C-C3C	3.21	1.47	1.38
82	DB	201	PEB	CHB-C1C	3.21	1.47	1.40
82	GB	201	PEB	CHB-C1C	3.21	1.47	1.40
82	T4	201	PEB	CHB-C1C	3.21	1.47	1.40
82	EJ	203	PEB	C1A-NA	-3.21	1.33	1.37
82	QJ	202	PEB	CHA-C1B	3.21	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	TD	201	PEB	C2C-C3C	3.21	1.47	1.38
82	MF	202	PEB	C2C-C3C	3.21	1.47	1.38
82	WK	202	PEB	CHB-C1C	3.21	1.47	1.40
87	bL	608	CLA	C4B-NB	3.21	1.41	1.37
87	B2	810	CLA	C4D-ND	-3.21	1.33	1.37
82	YF	203	PEB	OD-C4D	3.21	1.29	1.23
82	k4	201	PEB	C1A-NA	-3.21	1.33	1.37
82	RA	203	PEB	C2A-C1A	-3.21	1.49	1.52
82	TQ	202	PEB	C1A-NA	-3.21	1.33	1.37
82	X9	202	PEB	C1A-NA	-3.21	1.33	1.37
82	jH	202	PEB	C1A-NA	-3.21	1.33	1.37
82	TJ	202	PEB	CHB-C1C	3.21	1.47	1.40
87	82	306	CLA	C3B-C4B	3.21	1.50	1.42
82	VG	201	PEB	CHB-C1C	3.21	1.47	1.40
82	KI	202	PEB	CHB-C1C	3.21	1.47	1.40
82	hB	301	PEB	C1A-NA	-3.21	1.33	1.37
82	xC	202	PEB	C1A-NA	-3.21	1.33	1.37
82	CI	201	PEB	CHB-C1C	3.21	1.47	1.40
82	yF	301	PEB	CHB-C1C	3.21	1.47	1.40
82	aK	203	PEB	C2C-C3C	3.21	1.47	1.38
83	BJ	302	PUB	CHB-C4B	3.21	1.47	1.40
82	UG	201	PEB	CHA-C1B	3.21	1.47	1.40
82	A9	202	PEB	C1A-NA	-3.21	1.33	1.37
82	DO	1002	PEB	C2C-C3C	3.21	1.47	1.38
82	lK	203	PEB	OD-C4D	3.21	1.29	1.23
82	cH	201	PEB	CHB-C1C	3.21	1.47	1.40
87	82	307	CLA	C4D-ND	-3.21	1.33	1.37
82	WI	203	PEB	C2C-C3C	3.21	1.47	1.38
82	II	201	PEB	CHB-C1C	3.21	1.47	1.40
82	VI	201	PEB	CHB-C1C	3.21	1.47	1.40
82	RO	202	PEB	CHB-C1C	3.21	1.47	1.40
82	JD	202	PEB	C1A-NA	-3.21	1.33	1.37
82	Z4	201	PEB	C2C-C3C	3.21	1.47	1.38
87	1N	602	CLA	C1B-C2B	3.21	1.50	1.43
82	j4	201	PEB	CHB-C1C	3.21	1.47	1.40
82	EB	501	PEB	C2C-C3C	3.21	1.47	1.38
87	22	607	CLA	C4B-NB	3.21	1.41	1.37
82	QG	201	PEB	CHB-C1C	3.21	1.47	1.40
82	GA	202	PEB	C1A-NA	-3.21	1.33	1.37
87	cL	508	CLA	C4D-ND	-3.21	1.33	1.37
82	Q5	201	PEB	C2C-C3C	3.20	1.47	1.38
82	dO	201	PEB	C2C-C3C	3.20	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	K4	1001	CYC	C3D-C2D	3.20	1.47	1.38
87	CL	503	CLA	C1D-ND	3.20	1.41	1.37
87	12	611	CLA	C4B-NB	3.20	1.41	1.37
82	sK	201	PEB	CHB-C1C	3.20	1.47	1.40
82	A5	201	PEB	C2C-C3C	3.20	1.47	1.38
87	B2	804	CLA	CMC-C2C	-3.20	1.44	1.50
87	82	304	CLA	C4D-ND	-3.20	1.33	1.37
82	KM	201	PEB	C2A-C1A	-3.20	1.49	1.52
82	DA	202	PEB	CHA-C1B	3.20	1.47	1.40
82	QA	202	PEB	CHB-C1C	3.20	1.47	1.40
82	dB	202	PEB	C2C-C3C	3.20	1.47	1.38
82	kH	202	PEB	C2C-C3C	3.20	1.47	1.38
84	BE	1001	CYC	C1D-C2D	3.20	1.49	1.41
87	6N	613	CLA	C4B-NB	3.20	1.41	1.37
82	uK	202	PEB	C1A-NA	-3.20	1.33	1.37
82	TJ	201	PEB	C2C-C3C	3.20	1.47	1.38
82	I5	201	PEB	C2C-C3C	3.20	1.47	1.38
82	kK	203	PEB	C2C-C3C	3.20	1.47	1.38
82	BD	203	PEB	CHB-C1C	3.20	1.47	1.40
82	BQ	203	PEB	CHB-C1C	3.20	1.47	1.40
87	H6	102	CLA	C4D-ND	-3.20	1.33	1.37
82	QH	203	PEB	C2C-C3C	3.20	1.47	1.38
84	M1	201	CYC	C3D-C2D	3.20	1.47	1.38
87	2N	311	CLA	C4B-NB	3.20	1.41	1.37
87	BL	601	CLA	C4D-ND	-3.20	1.33	1.37
87	B2	832	CLA	C4D-ND	-3.20	1.33	1.37
82	RJ	201	PEB	CHB-C1C	3.20	1.47	1.40
82	hF	202	PEB	CHB-C1C	3.20	1.47	1.40
82	AJ	301	PEB	CHA-C1B	3.20	1.47	1.40
87	BN	827	CLA	C4D-ND	-3.20	1.33	1.37
82	TO	201	PEB	CHB-C1C	3.20	1.47	1.40
82	KG	201	PEB	C2C-C3C	3.20	1.47	1.38
82	f1	203	PEB	C1A-NA	-3.20	1.33	1.37
82	kF	203	PEB	C1A-NA	-3.20	1.33	1.37
82	YP	502	PEB	CHB-C1C	3.20	1.47	1.40
82	p8	202	PEB	CHB-C1C	3.20	1.47	1.40
103	8N	310	ZEX	C34-C33	-3.20	1.31	1.35
82	FQ	202	PEB	OD-C4D	3.20	1.29	1.23
87	B2	827	CLA	C4D-ND	-3.20	1.33	1.37
82	OJ	201	PEB	C2C-C3C	3.20	1.47	1.38
82	TI	202	PEB	CHB-C1C	3.20	1.47	1.40
82	PQ	203	PEB	CHB-C1C	3.20	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	i1	201	PEB	CHB-C1C	3.20	1.47	1.40
87	A2	817	CLA	C4D-ND	-3.20	1.33	1.37
82	VD	201	PEB	C2C-C3C	3.20	1.47	1.38
84	BG	1001	CYC	CHA-C4D	3.20	1.47	1.40
82	FD	203	PEB	C2A-C1A	-3.20	1.49	1.52
82	GF	201	PEB	C2A-C1A	-3.20	1.49	1.52
82	VQ	201	PEB	C2C-C3C	3.20	1.47	1.38
82	V5	201	PEB	C2C-C3C	3.20	1.47	1.38
82	Q9	202	PEB	C2C-C3C	3.20	1.47	1.38
84	HE	1001	CYC	C1D-C2D	3.20	1.49	1.41
82	x8	202	PEB	C1A-NA	-3.20	1.33	1.37
84	LH	1001	CYC	C3D-C2D	3.20	1.47	1.38
82	UI	201	PEB	C2A-C1A	-3.20	1.49	1.52
82	DQ	201	PEB	C2A-C1A	-3.20	1.49	1.52
82	MK	201	PEB	CHB-C1C	3.20	1.47	1.40
87	bL	613	CLA	C4D-ND	-3.20	1.33	1.37
82	pC	201	PEB	C1A-NA	-3.20	1.33	1.37
82	h1	201	PEB	OD-C4D	3.20	1.29	1.23
87	22	609	CLA	C1D-ND	3.20	1.41	1.37
82	UH	203	PEB	CHA-C1B	3.20	1.47	1.40
87	BN	810	CLA	C4D-ND	-3.20	1.33	1.37
82	O5	202	PEB	C2A-C1A	-3.20	1.49	1.52
82	NJ	201	PEB	CHC-C4C	3.20	1.53	1.49
82	D1	1002	PEB	C1A-NA	-3.20	1.33	1.37
82	dQ	401	PEB	CHB-C1C	3.20	1.47	1.40
87	A2	816	CLA	C4B-NB	3.20	1.41	1.37
82	S5	201	PEB	C1C-NC	-3.20	1.32	1.37
87	12	611	CLA	C4D-ND	-3.20	1.33	1.37
87	c6	605	CLA	C4D-ND	-3.20	1.33	1.37
82	OA	202	PEB	CHB-C1C	3.20	1.47	1.40
82	CK	203	PEB	C1A-NA	-3.20	1.33	1.37
82	uC	202	PEB	C1A-NA	-3.20	1.33	1.37
82	fE	203	PEB	C1A-NA	-3.20	1.33	1.37
82	O7	201	PEB	CHA-C1B	3.20	1.47	1.40
82	XB	201	PEB	C2C-C3C	3.20	1.47	1.38
82	YP	502	PEB	C2A-C1A	-3.20	1.49	1.52
82	E9	202	PEB	C1A-NA	-3.20	1.33	1.37
82	I9	202	PEB	C1A-NA	-3.20	1.33	1.37
82	R4	203	PEB	C2C-C3C	3.20	1.47	1.38
82	VJ	201	PEB	CHB-C1C	3.20	1.47	1.40
87	A2	803	CLA	C4B-NB	3.20	1.41	1.37
83	M5	302	PUB	C4B-C3B	3.20	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	P5	201	PEB	C2C-C3C	3.20	1.47	1.38
82	AD	301	PEB	CHB-C1C	3.20	1.47	1.40
82	hM	203	PEB	C1A-NA	-3.20	1.33	1.37
82	N5	201	PEB	C2C-C3C	3.20	1.47	1.38
82	M7	201	PEB	CHA-C1B	3.20	1.47	1.40
87	BL	609	CLA	C4D-ND	-3.19	1.33	1.37
87	1N	607	CLA	C4D-ND	-3.19	1.33	1.37
82	F4	1002	PEB	CHB-C1C	3.19	1.47	1.40
82	RA	201	PEB	C2C-C3C	3.19	1.47	1.38
82	UK	201	PEB	C2C-C3C	3.19	1.47	1.38
82	DD	202	PEB	CHB-C1C	3.19	1.47	1.40
82	B7	201	PEB	CHB-C1C	3.19	1.47	1.40
82	QK	202	PEB	OD-C4D	3.19	1.29	1.23
82	T5	201	PEB	C2C-C3C	3.19	1.47	1.38
84	N1	1001	CYC	C3D-C2D	3.19	1.47	1.38
82	VH	202	PEB	C1A-NA	-3.19	1.33	1.37
82	hJ	201	PEB	C1A-NA	-3.19	1.33	1.37
82	VB	202	PEB	CHB-C1C	3.19	1.47	1.40
87	72	605	CLA	C4B-NB	3.19	1.41	1.37
82	SA	201	PEB	CHB-C1C	3.19	1.47	1.40
82	UP	203	PEB	CHA-C1B	3.19	1.47	1.40
82	TJ	201	PEB	C2A-C1A	-3.19	1.49	1.52
87	4N	601	CLA	C4D-ND	-3.19	1.33	1.37
82	GP	201	PEB	C2C-C3C	3.19	1.47	1.38
82	Z5	305	PEB	C2C-C3C	3.19	1.47	1.38
82	PM	201	PEB	CHB-C1C	3.19	1.47	1.40
87	2N	309	CLA	C4D-ND	-3.19	1.33	1.37
87	A2	825	CLA	CMC-C2C	-3.19	1.44	1.50
87	B6	609	CLA	C4B-NB	3.19	1.41	1.37
82	wK	302	PEB	CHB-C1C	3.19	1.47	1.40
82	mK	201	PEB	C1A-NA	-3.19	1.33	1.37
87	B6	604	CLA	C4D-ND	-3.19	1.33	1.37
87	BN	826	CLA	C1D-ND	3.19	1.41	1.37
87	A2	803	CLA	C1D-ND	3.19	1.41	1.37
87	R2	201	CLA	C4B-NB	3.19	1.41	1.37
82	R9	202	PEB	C1A-NA	-3.19	1.33	1.37
82	tF	202	PEB	C1A-NA	-3.19	1.33	1.37
87	CL	507	CLA	C4D-ND	-3.19	1.33	1.37
87	HL	101	CLA	C4D-ND	-3.19	1.33	1.37
82	J5	201	PEB	CHB-C1C	3.19	1.47	1.40
82	JJ	202	PEB	C2C-C3C	3.19	1.47	1.38
82	R5	201	PEB	C2C-C3C	3.19	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4N	611	CLA	C4B-NB	3.19	1.41	1.37
82	EB	501	PEB	CHB-C1C	3.19	1.47	1.40
82	IQ	202	PEB	CHB-C1C	3.19	1.47	1.40
84	BE	1001	CYC	CHA-C4D	3.19	1.47	1.40
82	JJ	201	PEB	C2C-C3C	3.19	1.47	1.38
82	FM	201	PEB	CHC-C4C	3.19	1.53	1.49
82	K9	202	PEB	C1A-NA	-3.19	1.33	1.37
82	DD	202	PEB	C2A-C1A	-3.19	1.49	1.52
87	12	604	CLA	C4D-ND	-3.19	1.33	1.37
82	HI	201	PEB	C2C-C3C	3.19	1.47	1.38
82	B5	202	PEB	C2C-C3C	3.19	1.47	1.38
82	X5	201	PEB	C2C-C3C	3.19	1.47	1.38
84	NE	201	CYC	C3D-C2D	3.19	1.47	1.38
82	UH	203	PEB	CHB-C1C	3.19	1.47	1.40
82	AH	302	PEB	C1A-NA	-3.19	1.33	1.37
82	S1	202	PEB	OD-C4D	3.19	1.29	1.23
82	GB	203	PEB	C2C-C3C	3.19	1.47	1.38
82	NA	202	PEB	CHB-C1C	3.19	1.47	1.40
84	IE	1001	CYC	CHA-C4D	3.19	1.47	1.40
82	lK	202	PEB	C1A-NA	-3.19	1.33	1.37
82	MM	203	PEB	C2C-C3C	3.19	1.47	1.38
82	U5	203	PEB	C2C-C3C	3.19	1.47	1.38
83	M5	303	PUB	C4B-C3B	3.19	1.50	1.42
87	B2	826	CLA	C4D-ND	-3.19	1.33	1.37
87	cL	510	CLA	C4D-ND	-3.19	1.33	1.37
82	QJ	204	PEB	C2C-C3C	3.19	1.47	1.38
82	wF	301	PEB	CHA-C1B	3.19	1.47	1.40
82	EA	202	PEB	OD-C4D	3.19	1.29	1.23
82	DQ	203	PEB	C1A-NA	-3.19	1.33	1.37
82	TQ	203	PEB	C1A-NA	-3.19	1.33	1.37
83	AG	303	PUB	OD-C4D	3.19	1.29	1.23
82	PH	202	PEB	C2C-C3C	3.19	1.47	1.38
82	S5	203	PEB	CHB-C1C	3.19	1.47	1.40
84	DG	1001	CYC	C1D-C2D	3.19	1.49	1.41
82	QB	201	PEB	C2C-C3C	3.19	1.47	1.38
82	XJ	201	PEB	C2C-C3C	3.19	1.47	1.38
82	wF	302	PEB	CHB-C1C	3.18	1.47	1.40
84	q3	1001	CYC	C1D-C2D	3.18	1.49	1.41
82	WA	202	PEB	C2C-C3C	3.18	1.47	1.38
82	NI	201	PEB	CHB-C1C	3.18	1.47	1.40
82	oK	202	PEB	C1A-NA	-3.18	1.33	1.37
82	WH	201	PEB	C2C-C3C	3.18	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VQ	202	PEB	OD-C4D	3.18	1.29	1.23
87	12	607	CLA	C4D-ND	-3.18	1.33	1.37
87	B6	613	CLA	C4D-ND	-3.18	1.33	1.37
82	NB	203	PEB	C2C-C3C	3.18	1.47	1.38
82	KK	203	PEB	CHB-C1C	3.18	1.47	1.40
87	d6	403	CLA	C4B-NB	3.18	1.41	1.37
87	7N	604	CLA	C4B-NB	3.18	1.41	1.37
82	MF	201	PEB	C2C-C3C	3.18	1.47	1.38
82	tK	201	PEB	C2A-C1A	-3.18	1.49	1.52
82	A1	302	PEB	C1A-NA	-3.18	1.33	1.37
82	mF	201	PEB	C1A-NA	-3.18	1.33	1.37
82	S7	201	PEB	CHB-C1C	3.18	1.47	1.40
82	EF	201	PEB	C2C-C3C	3.18	1.47	1.38
82	P1	202	PEB	C2C-C3C	3.18	1.47	1.38
82	D7	202	PEB	CHA-C1B	3.18	1.47	1.40
82	cJ	201	PEB	CHB-C1C	3.18	1.47	1.40
87	3N	303	CLA	C1D-C2D	3.18	1.51	1.45
82	CJ	201	PEB	C2C-C3C	3.18	1.47	1.38
82	HI	202	PEB	OD-C4D	3.18	1.29	1.23
82	s8	203	PEB	OD-C4D	3.18	1.29	1.23
84	MG	1001	CYC	C3D-C2D	3.18	1.47	1.38
82	U1	203	PEB	CHA-C1B	3.18	1.47	1.40
82	NI	203	PEB	C1A-NA	-3.18	1.33	1.37
82	RP	202	PEB	C2C-C3C	3.18	1.47	1.38
87	2N	306	CLA	C4B-NB	3.18	1.41	1.37
84	FH	1001	CYC	C3D-C2D	3.18	1.47	1.38
82	GE	1002	PEB	CHB-C1C	3.18	1.47	1.40
82	M5	304	PEB	C1A-NA	-3.18	1.33	1.37
82	HD	202	PEB	C2C-C3C	3.18	1.47	1.38
87	22	608	CLA	C4D-ND	-3.18	1.33	1.37
82	UM	201	PEB	CHA-C1B	3.18	1.47	1.40
87	72	607	CLA	C4B-NB	3.18	1.41	1.37
82	YK	203	PEB	OD-C4D	3.18	1.29	1.23
82	FJ	201	PEB	CHB-C1C	3.18	1.47	1.40
82	mO	203	PEB	C1A-NA	-3.18	1.33	1.37
82	UA	202	PEB	CHA-C1B	3.18	1.47	1.40
82	a4	201	PEB	CHB-C1C	3.18	1.47	1.40
82	VD	202	PEB	OD-C4D	3.18	1.29	1.23
82	UE	203	PEB	OD-C4D	3.18	1.29	1.23
84	BG	1001	CYC	C1D-C2D	3.18	1.49	1.41
87	B2	809	CLA	C4D-ND	-3.18	1.33	1.37
87	2N	312	CLA	C4B-NB	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	7N	607	CLA	C4B-NB	3.18	1.41	1.37
82	IM	201	PEB	CHA-C1B	3.18	1.47	1.40
82	N4	1002	PEB	C2C-C3C	3.18	1.47	1.38
82	A1	305	PEB	C1A-NA	-3.18	1.33	1.37
82	CB	201	PEB	C2A-C1A	-3.18	1.49	1.52
84	F1	1001	CYC	C2C-C1C	-3.18	1.49	1.52
87	A2	811	CLA	C4D-ND	-3.18	1.33	1.37
87	c6	613	CLA	C4D-ND	-3.18	1.33	1.37
82	PA	202	PEB	CHA-C1B	3.18	1.47	1.40
82	WA	202	PEB	C1A-NA	-3.18	1.33	1.37
82	MM	203	PEB	C1A-NA	-3.18	1.33	1.37
87	AN	826	CLA	C4D-ND	-3.18	1.33	1.37
82	W4	201	PEB	CHA-C1B	3.18	1.47	1.40
82	RG	201	PEB	CHB-C1C	3.18	1.47	1.40
82	hK	202	PEB	CHB-C1C	3.18	1.47	1.40
82	jK	202	PEB	CHB-C1C	3.18	1.47	1.40
82	VI	203	PEB	C1A-NA	-3.18	1.33	1.37
87	AN	822	CLA	C4D-ND	-3.18	1.33	1.37
82	JI	202	PEB	CHB-C1C	3.18	1.47	1.40
82	YB	202	PEB	C2C-C3C	3.18	1.47	1.38
82	aF	202	PEB	C2C-C3C	3.18	1.47	1.38
87	CL	518	CLA	C4B-NB	3.18	1.41	1.37
82	WG	202	PEB	C2A-C1A	-3.18	1.49	1.52
82	m4	203	PEB	C1A-NA	-3.18	1.33	1.37
82	hM	201	PEB	C1A-NA	-3.18	1.33	1.37
87	d6	406	CLA	C4D-ND	-3.18	1.33	1.37
87	BN	807	CLA	C1D-ND	3.17	1.41	1.37
82	KF	201	PEB	CHB-C1C	3.17	1.47	1.40
82	Q7	202	PEB	CHB-C1C	3.17	1.47	1.40
87	A6	403	CLA	C4D-ND	-3.17	1.33	1.37
82	oF	203	PEB	C1A-NA	-3.17	1.33	1.37
82	BJ	301	PEB	C2C-C3C	3.17	1.47	1.38
82	DD	203	PEB	OD-C4D	3.17	1.29	1.23
87	DL	404	CLA	C1D-ND	3.17	1.41	1.37
87	bL	615	CLA	C4B-NB	3.17	1.41	1.37
87	A2	801	CLA	C4D-ND	-3.17	1.33	1.37
82	GB	203	PEB	CHB-C1C	3.17	1.47	1.40
82	hJ	201	PEB	CHA-C1B	3.17	1.47	1.40
87	22	610	CLA	C4B-NB	3.17	1.41	1.37
82	jE	201	PEB	C2A-C1A	-3.17	1.49	1.52
87	AN	802	CLA	C4D-ND	-3.17	1.33	1.37
87	AN	813	CLA	C4D-ND	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	52	604	CLA	C4D-ND	-3.17	1.33	1.37
82	PI	201	PEB	CHB-C1C	3.17	1.47	1.40
82	Z5	305	PEB	CHB-C1C	3.17	1.47	1.40
82	KF	203	PEB	C2C-C3C	3.17	1.47	1.38
82	H4	1002	PEB	C2C-C3C	3.17	1.47	1.38
82	T4	201	PEB	C2C-C3C	3.17	1.47	1.38
87	c6	610	CLA	C4D-ND	-3.17	1.33	1.37
87	AN	803	CLA	C1D-ND	3.17	1.41	1.37
87	A2	831	CLA	C1D-ND	3.17	1.41	1.37
82	TQ	201	PEB	OD-C4D	3.17	1.29	1.23
82	ZO	202	PEB	CHB-C1C	3.17	1.47	1.40
82	CB	201	PEB	C2C-C3C	3.17	1.47	1.38
82	OD	202	PEB	C2A-C1A	-3.17	1.49	1.52
87	8N	301	CLA	C3B-C4B	3.17	1.50	1.42
82	FD	202	PEB	C2C-C3C	3.17	1.47	1.38
84	IO	1001	CYC	C3D-C2D	3.17	1.47	1.38
82	W1	202	PEB	CHB-C1C	3.17	1.47	1.40
82	yK	301	PEB	CHB-C1C	3.17	1.47	1.40
87	dL	402	CLA	C4D-ND	-3.17	1.33	1.37
92	j6	101	LMG	O8-C28	3.17	1.42	1.33
87	bL	622	CLA	C4B-NB	3.17	1.41	1.37
82	fG	203	PEB	C1A-NA	-3.17	1.33	1.37
84	F3	1001	CYC	C1D-C2D	3.17	1.49	1.41
82	OB	201	PEB	C2C-C3C	3.17	1.47	1.38
82	HQ	202	PEB	C2C-C3C	3.17	1.47	1.38
84	I1	1001	CYC	C3D-C2D	3.17	1.47	1.38
82	BI	202	PEB	OD-C4D	3.17	1.29	1.23
84	M3	1001	CYC	C1B-C2B	3.17	1.50	1.45
84	f3	1001	CYC	C1B-C2B	3.17	1.50	1.45
82	Y1	201	PEB	C2A-C1A	-3.17	1.49	1.52
87	bL	617	CLA	CMB-C2B	-3.17	1.44	1.50
82	GB	202	PEB	CHB-C1C	3.17	1.47	1.40
87	52	611	CLA	C4D-ND	-3.17	1.33	1.37
82	XA	203	PEB	C2C-C3C	3.17	1.47	1.38
82	CJ	202	PEB	C2C-C3C	3.17	1.47	1.38
82	F9	202	PEB	C2C-C3C	3.17	1.47	1.38
82	ZE	202	PEB	CHB-C1C	3.17	1.47	1.40
82	JH	1002	PEB	CHB-C1C	3.17	1.47	1.40
82	dD	401	PEB	CHB-C1C	3.17	1.47	1.40
82	i1	202	PEB	C1A-NA	-3.17	1.33	1.37
87	62	307	CLA	C4B-NB	3.17	1.41	1.37
82	V1	203	PEB	C2A-C1A	-3.17	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	CG	1001	CYC	C2C-C1C	-3.17	1.49	1.52
84	I3	1001	CYC	C1D-C2D	3.17	1.49	1.41
82	RA	201	PEB	CHB-C1C	3.17	1.47	1.40
87	AN	811	CLA	C4D-ND	-3.17	1.33	1.37
82	GJ	201	PEB	C2C-C3C	3.17	1.47	1.38
84	h3	1001	CYC	C1B-C2B	3.17	1.50	1.45
82	SK	202	PEB	CHB-C1C	3.17	1.47	1.40
82	QK	203	PEB	C2A-C1A	-3.17	1.49	1.52
82	J1	1002	PEB	C1A-NA	-3.17	1.33	1.37
82	C9	202	PEB	C1A-NA	-3.17	1.33	1.37
84	q3	1001	CYC	C1B-C2B	3.17	1.50	1.45
87	AN	825	CLA	CMC-C2C	-3.17	1.44	1.50
87	BN	811	CLA	C4D-ND	-3.17	1.33	1.37
87	C6	513	CLA	C4D-ND	-3.17	1.33	1.37
87	c6	607	CLA	C4D-ND	-3.17	1.33	1.37
82	ND	203	PEB	OD-C4D	3.17	1.29	1.23
82	cH	202	PEB	C2C-C3C	3.17	1.47	1.38
82	hO	201	PEB	C2A-C1A	-3.17	1.49	1.52
82	QE	203	PEB	CHB-C1C	3.17	1.47	1.40
82	QP	202	PEB	CHB-C1C	3.17	1.47	1.40
87	BN	817	CLA	C4B-NB	3.17	1.41	1.37
87	BN	805	CLA	CMC-C2C	-3.17	1.44	1.50
82	dH	201	PEB	CHA-C1B	3.17	1.47	1.40
84	w3	1001	CYC	C1D-C2D	3.17	1.49	1.41
82	IB	203	PEB	CHB-C1C	3.17	1.47	1.40
82	Q4	201	PEB	C2C-C3C	3.17	1.47	1.38
87	c6	614	CLA	C4D-ND	-3.17	1.33	1.37
82	ZO	201	PEB	C2C-C3C	3.17	1.47	1.38
82	RG	202	PEB	C2A-C1A	-3.17	1.49	1.52
84	DH	1001	CYC	C1C-NC	-3.17	1.33	1.37
87	D6	405	CLA	C4D-ND	-3.17	1.33	1.37
82	gK	201	PEB	C2C-C3C	3.17	1.47	1.38
82	M5	305	PEB	CHB-C1C	3.17	1.47	1.40
82	HB	202	PEB	C2A-C1A	-3.17	1.49	1.52
82	eB	201	PEB	C2A-C1A	-3.17	1.49	1.52
87	A2	813	CLA	C4D-ND	-3.16	1.33	1.37
87	12	601	CLA	C4B-NB	3.16	1.41	1.37
87	bL	622	CLA	C1D-ND	3.16	1.41	1.37
82	J9	203	PEB	CHB-C1C	3.16	1.47	1.40
82	NQ	202	PEB	C2C-C3C	3.16	1.47	1.38
82	B5	202	PEB	CHA-C1B	3.16	1.47	1.40
82	SH	201	PEB	C2C-C3C	3.16	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	lJ	203	PEB	C2C-C3C	3.16	1.47	1.38
82	qC	202	PEB	C1A-NA	-3.16	1.33	1.37
82	FQ	203	PEB	C2A-C1A	-3.16	1.49	1.52
82	mO	201	PEB	C2A-C1A	-3.16	1.49	1.52
84	Q3	1001	CYC	C1D-C2D	3.16	1.49	1.41
82	B9	203	PEB	C1A-NA	-3.16	1.33	1.37
82	G9	202	PEB	C1A-NA	-3.16	1.33	1.37
82	UB	301	PEB	CHB-C1C	3.16	1.47	1.40
87	42	601	CLA	C4D-ND	-3.16	1.33	1.37
82	eH	203	PEB	CHA-C1B	3.16	1.47	1.40
95	C6	503	DGD	O2G-C1B	3.16	1.43	1.34
87	72	601	CLA	C4B-NB	3.16	1.41	1.37
87	1N	609	CLA	C4B-NB	3.16	1.41	1.37
82	VO	201	PEB	CHB-C1C	3.16	1.47	1.40
82	uC	201	PEB	C1C-C2C	3.16	1.50	1.42
83	AG	302	PUB	C3B-C2B	3.16	1.47	1.38
82	T1	202	PEB	C1A-NA	-3.16	1.33	1.37
82	Z5	304	PEB	C1A-NA	-3.16	1.33	1.37
82	oK	203	PEB	C1A-NA	-3.16	1.33	1.37
82	PP	201	PEB	CHB-C1C	3.16	1.47	1.40
87	bL	614	CLA	C4D-ND	-3.16	1.33	1.37
87	nL	101	CLA	C1D-ND	3.16	1.41	1.37
82	SB	203	PEB	CHB-C1C	3.16	1.47	1.40
82	GP	202	PEB	CHB-C1C	3.16	1.47	1.40
82	DQ	203	PEB	C2C-C3C	3.16	1.47	1.38
84	U3	1001	CYC	C1D-C2D	3.16	1.49	1.41
82	sF	202	PEB	C1A-NA	-3.16	1.33	1.37
87	62	301	CLA	C4B-NB	3.16	1.41	1.37
87	7N	605	CLA	C4B-NB	3.16	1.41	1.37
82	GG	1002	PEB	CHB-C1C	3.16	1.47	1.40
82	R7	201	PEB	CHB-C1C	3.16	1.47	1.40
82	sF	202	PEB	OD-C4D	3.16	1.29	1.23
103	8N	310	ZEX	C14-C13	-3.16	1.31	1.35
82	Y9	202	PEB	C2C-C3C	3.16	1.47	1.38
84	F1	1001	CYC	C3D-C2D	3.16	1.47	1.38
91	aL	610	PHO	CBD-CGD	-3.16	1.48	1.52
84	73	1001	CYC	C1D-C2D	3.16	1.49	1.41
87	BL	609	CLA	C4B-NB	3.16	1.41	1.37
87	7N	610	CLA	C4B-NB	3.16	1.41	1.37
82	NB	201	PEB	C2C-C3C	3.16	1.47	1.38
82	F5	201	PEB	C2A-C1A	-3.16	1.49	1.52
82	eH	202	PEB	C1A-NA	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	Z9	305	PUB	OD-C4D	3.16	1.29	1.23
82	LJ	202	PEB	C2C-C3C	3.16	1.47	1.38
82	SK	203	PEB	C2C-C3C	3.16	1.47	1.38
82	V1	203	PEB	C1A-NA	-3.16	1.33	1.37
82	eB	202	PEB	C2C-C3C	3.16	1.47	1.38
82	W7	202	PEB	C2C-C3C	3.16	1.47	1.38
87	CL	510	CLA	C1D-ND	3.16	1.41	1.37
87	R2	201	CLA	C4D-ND	-3.16	1.33	1.37
87	c6	616	CLA	C4D-ND	-3.16	1.33	1.37
82	LH	1003	PEB	CHB-C1C	3.16	1.47	1.40
82	iK	202	PEB	CHB-C1C	3.16	1.47	1.40
84	u3	1001	CYC	C1B-C2B	3.16	1.50	1.45
82	h4	201	PEB	C2A-C1A	-3.16	1.49	1.52
82	YJ	203	PEB	CHA-C1B	3.16	1.47	1.40
84	o3	1001	CYC	C1B-C2B	3.16	1.50	1.45
82	AP	201	PEB	C2C-C3C	3.16	1.47	1.38
87	32	313	CLA	C4D-ND	-3.16	1.33	1.37
82	tK	202	PEB	C1A-NA	-3.16	1.33	1.37
82	SJ	203	PEB	CHA-C1B	3.16	1.47	1.40
82	RB	202	PEB	C2C-C3C	3.16	1.47	1.38
84	NH	1001	CYC	C3D-C2D	3.16	1.47	1.38
82	kF	203	PEB	C2C-C3C	3.16	1.47	1.38
82	j1	202	PEB	C1A-NA	-3.16	1.33	1.37
82	u8	201	PEB	OD-C4D	3.16	1.29	1.23
87	HL	102	CLA	C4D-ND	-3.16	1.33	1.37
83	yK	303	PUB	CHB-C4B	3.16	1.47	1.40
82	b1	203	PEB	CHA-C1B	3.16	1.47	1.40
87	4N	609	CLA	C4B-NB	3.16	1.41	1.37
103	82	310	ZEX	C34-C33	-3.16	1.31	1.35
82	BB	203	PEB	C2C-C3C	3.16	1.47	1.38
82	uC	202	PEB	C2C-C3C	3.16	1.47	1.38
82	oK	203	PEB	OD-C4D	3.16	1.29	1.23
82	mJ	201	PEB	C2C-C3C	3.16	1.47	1.38
84	KO	1001	CYC	C3D-C2D	3.16	1.47	1.38
82	EQ	202	PEB	CHB-C1C	3.16	1.47	1.40
82	UJ	202	PEB	C2C-C3C	3.16	1.47	1.38
82	bO	201	PEB	C2C-C3C	3.16	1.47	1.38
82	ZG	202	PEB	CHB-C1C	3.15	1.47	1.40
82	Q4	201	PEB	CHA-C1B	3.15	1.47	1.40
84	O3	1001	CYC	C1D-C2D	3.15	1.49	1.41
82	ZJ	202	PEB	C2C-C3C	3.15	1.47	1.38
82	b4	201	PEB	C2C-C3C	3.15	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	805	CLA	C4D-ND	-3.15	1.33	1.37
82	LQ	201	PEB	C2C-C3C	3.15	1.47	1.38
84	D3	1001	CYC	C1D-C2D	3.15	1.49	1.41
87	2N	304	CLA	C4D-ND	-3.15	1.33	1.37
82	c4	202	PEB	C2C-C3C	3.15	1.47	1.38
82	UE	203	PEB	CHB-C1C	3.15	1.47	1.40
82	YJ	201	PEB	CHA-C1B	3.15	1.47	1.40
87	K2	101	CLA	C4D-ND	-3.15	1.33	1.37
82	HB	203	PEB	C2C-C3C	3.15	1.47	1.38
82	UK	202	PEB	C2C-C3C	3.15	1.47	1.38
84	V3	1001	CYC	C3D-C2D	3.15	1.47	1.38
82	XB	202	PEB	C2C-C3C	3.15	1.47	1.38
82	KK	203	PEB	C2C-C3C	3.15	1.47	1.38
82	S5	201	PEB	C2A-C1A	-3.15	1.49	1.52
87	82	307	CLA	C4B-NB	3.15	1.41	1.37
87	1N	604	CLA	C4D-ND	-3.15	1.33	1.37
87	12	602	CLA	C1B-C2B	3.15	1.50	1.43
82	aF	201	PEB	C2C-C3C	3.15	1.47	1.38
84	Q3	1001	CYC	C1B-C2B	3.15	1.50	1.45
82	bO	202	PEB	C1A-NA	-3.15	1.33	1.37
87	c6	604	CLA	C4B-NB	3.15	1.41	1.37
87	cL	515	CLA	C4B-NB	3.15	1.41	1.37
87	AN	806	CLA	C4D-ND	-3.15	1.33	1.37
82	iJ	201	PEB	C2A-C1A	-3.15	1.49	1.52
84	S3	1001	CYC	C1B-C2B	3.15	1.50	1.45
82	UI	202	PEB	CHB-C1C	3.15	1.47	1.40
82	N7	202	PEB	CHB-C1C	3.15	1.47	1.40
87	32	302	CLA	C1D-C2D	3.15	1.51	1.45
87	BL	609	CLA	C1D-ND	3.15	1.41	1.37
87	8N	305	CLA	C4D-ND	-3.15	1.33	1.37
82	WP	202	PEB	CHB-C1C	3.15	1.47	1.40
82	w8	202	PEB	C4B-C3B	3.15	1.50	1.45
87	CL	515	CLA	C4B-NB	3.15	1.41	1.37
87	cL	510	CLA	C4B-NB	3.15	1.41	1.37
82	bP	501	PEB	C2C-C3C	3.15	1.47	1.38
82	M9	305	PEB	C1A-NA	-3.15	1.33	1.37
87	BL	605	CLA	C4D-ND	-3.15	1.33	1.37
87	AN	835	CLA	C4D-ND	-3.15	1.33	1.37
82	bP	501	PEB	C2A-C1A	-3.15	1.49	1.52
82	QH	201	PEB	CHA-C1B	3.15	1.47	1.40
82	W7	202	PEB	C1A-NA	-3.15	1.33	1.37
84	k3	1001	CYC	C1D-C2D	3.15	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	805	CLA	C4D-ND	-3.15	1.33	1.37
87	2N	308	CLA	C4D-ND	-3.15	1.33	1.37
84	L1	1001	CYC	C3D-C2D	3.15	1.47	1.38
87	3N	305	CLA	O1D-CGD	3.15	1.29	1.21
82	MA	201	PEB	CHA-C1B	3.15	1.47	1.40
82	jM	203	PEB	CHA-C1B	3.15	1.47	1.40
82	DJ	202	PEB	C2A-C1A	-3.15	1.49	1.52
87	R2	204	CLA	C4D-ND	-3.15	1.33	1.37
82	DF	201	PEB	C2C-C3C	3.15	1.47	1.38
82	OH	202	PEB	CHA-C1B	3.15	1.47	1.40
82	OK	203	PEB	OD-C4D	3.15	1.29	1.23
87	LN	204	CLA	C1D-ND	3.15	1.41	1.37
87	62	303	CLA	C4B-NB	3.15	1.41	1.37
84	j3	1001	CYC	C1D-C2D	3.15	1.49	1.41
82	YK	203	PEB	C2C-C3C	3.15	1.47	1.38
87	A2	830	CLA	C4D-ND	-3.15	1.33	1.37
82	pC	202	PEB	CHB-C1C	3.15	1.47	1.40
82	hK	201	PEB	C2A-C1A	-3.15	1.49	1.52
82	WD	201	PEB	C2C-C3C	3.15	1.47	1.38
87	b6	612	CLA	C4D-ND	-3.15	1.33	1.37
82	WP	201	PEB	C2C-C3C	3.15	1.47	1.38
82	VE	201	PEB	CHB-C1C	3.15	1.47	1.40
82	QE	203	PEB	OD-C4D	3.15	1.29	1.23
82	GK	201	PEB	C2A-C1A	-3.15	1.49	1.52
83	KA	203	PUB	CHB-C4B	3.15	1.47	1.40
84	j3	1001	CYC	C1B-C2B	3.15	1.50	1.45
87	AN	830	CLA	C4D-ND	-3.15	1.33	1.37
82	GF	203	PEB	OD-C4D	3.15	1.29	1.23
82	HK	202	PEB	CHB-C1C	3.15	1.47	1.40
87	A2	849	CLA	C4D-ND	-3.15	1.33	1.37
82	RK	202	PEB	CHB-C1C	3.15	1.47	1.40
82	jE	201	PEB	C1A-NA	-3.15	1.33	1.37
82	fO	201	PEB	C2C-C3C	3.15	1.47	1.38
82	D7	201	PEB	C2A-C1A	-3.14	1.49	1.52
82	YP	502	PEB	C2C-C3C	3.14	1.47	1.38
82	VD	201	PEB	CHA-C1B	3.14	1.47	1.40
82	O1	202	PEB	CHA-C1B	3.14	1.47	1.40
87	BN	830	CLA	C4D-ND	-3.14	1.33	1.37
84	F3	1001	CYC	C1B-C2B	3.14	1.50	1.45
84	w3	1001	CYC	C1B-C2B	3.14	1.50	1.45
82	H5	203	PEB	C2C-C3C	3.14	1.47	1.38
82	ZJ	201	PEB	C1C-NC	-3.14	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	J4	1001	CYC	C2C-C1C	-3.14	1.49	1.52
87	32	308	CLA	C1D-ND	3.14	1.41	1.37
82	sC	203	PEB	OD-C4D	3.14	1.29	1.23
84	B3	1001	CYC	C1D-C2D	3.14	1.49	1.41
84	h3	1001	CYC	C1D-C2D	3.14	1.49	1.41
82	IJ	202	PEB	C2C-C3C	3.14	1.47	1.38
82	fJ	203	PEB	C2C-C3C	3.14	1.47	1.38
87	42	608	CLA	C4B-NB	3.14	1.41	1.37
82	WQ	201	PEB	C1A-NA	-3.14	1.33	1.37
82	XP	201	PEB	C2C-C3C	3.14	1.47	1.38
82	HA	201	PEB	C2A-C1A	-3.14	1.49	1.52
82	MM	201	PEB	C2A-C1A	-3.14	1.49	1.52
82	yF	301	PEB	C2A-C1A	-3.14	1.49	1.52
84	FE	1001	CYC	C2C-C1C	-3.14	1.49	1.52
82	ZM	201	PEB	CHB-C1C	3.14	1.47	1.40
84	H3	1001	CYC	C1D-C2D	3.14	1.49	1.41
87	B2	830	CLA	C4D-ND	-3.14	1.33	1.37
87	22	611	CLA	C4B-NB	3.14	1.41	1.37
82	X7	203	PEB	C2C-C3C	3.14	1.47	1.38
82	Y7	301	PEB	CHB-C1C	3.14	1.47	1.40
84	x3	1001	CYC	C3D-C2D	3.14	1.47	1.38
82	GB	201	PEB	C2A-C1A	-3.14	1.49	1.52
82	WM	203	PEB	C2A-C1A	-3.14	1.49	1.52
82	aJ	204	PEB	CHA-C1B	3.14	1.47	1.40
82	GJ	201	PEB	CHB-C1C	3.14	1.47	1.40
82	DQ	202	PEB	CHB-C1C	3.14	1.47	1.40
82	Z1	201	PEB	CHB-C1C	3.14	1.47	1.40
82	iH	201	PEB	CHB-C1C	3.14	1.47	1.40
82	jM	202	PEB	C1C-C2C	3.14	1.50	1.42
87	b6	615	CLA	C4D-ND	-3.14	1.33	1.37
87	BL	603	CLA	CMD-C2D	-3.14	1.44	1.50
82	O7	202	PEB	CHB-C1C	3.14	1.47	1.40
82	bE	201	PEB	CHB-C1C	3.14	1.47	1.40
82	bG	201	PEB	CHB-C1C	3.14	1.47	1.40
82	RD	201	PEB	C1A-NA	-3.14	1.33	1.37
82	gF	202	PEB	C1A-NA	-3.14	1.33	1.37
87	BL	602	CLA	C1D-ND	3.14	1.41	1.37
87	5N	605	CLA	C4B-NB	3.14	1.41	1.37
87	C6	518	CLA	C4D-ND	-3.14	1.33	1.37
87	c6	604	CLA	C4D-ND	-3.14	1.33	1.37
82	O4	201	PEB	C2C-C3C	3.14	1.47	1.38
82	D7	201	PEB	C1A-NA	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	808	CLA	C1D-ND	3.14	1.41	1.37
87	22	612	CLA	C4B-NB	3.14	1.41	1.37
82	UD	201	PEB	OD-C4D	3.14	1.29	1.23
87	B2	817	CLA	C4D-ND	-3.14	1.33	1.37
84	u3	1001	CYC	C1D-C2D	3.14	1.49	1.41
82	AM	302	PEB	C1A-NA	-3.14	1.33	1.37
87	3N	312	CLA	C4B-NB	3.14	1.41	1.37
82	S9	201	PEB	C2C-C3C	3.14	1.47	1.38
84	M3	1001	CYC	C1D-C2D	3.14	1.49	1.41
82	YH	202	PEB	C2A-C1A	-3.14	1.49	1.52
84	73	1001	CYC	C1B-C2B	3.14	1.50	1.45
84	S3	1001	CYC	C1D-C2D	3.14	1.49	1.41
87	bL	604	CLA	C4B-NB	3.14	1.41	1.37
82	RD	202	PEB	OD-C4D	3.14	1.29	1.23
103	82	310	ZEX	C14-C13	-3.14	1.31	1.35
84	H1	1001	CYC	C1D-C2D	3.14	1.49	1.41
82	MD	202	PEB	C1A-NA	-3.14	1.33	1.37
82	q8	202	PEB	C1A-NA	-3.14	1.33	1.37
87	RN	201	CLA	C4B-NB	3.14	1.41	1.37
87	4N	608	CLA	C4D-ND	-3.14	1.33	1.37
82	VA	203	PEB	C2C-C3C	3.14	1.47	1.38
82	OQ	202	PEB	C2A-C1A	-3.14	1.49	1.52
84	d3	1001	CYC	C1D-C2D	3.14	1.49	1.41
84	U3	1001	CYC	C1B-C2B	3.14	1.50	1.45
87	AN	841	CLA	C4B-NB	3.14	1.41	1.37
87	32	312	CLA	C4B-NB	3.14	1.41	1.37
82	WH	202	PEB	CHB-C1C	3.14	1.47	1.40
82	vC	202	PEB	CHB-C1C	3.14	1.47	1.40
82	QO	201	PEB	C2C-C3C	3.14	1.47	1.38
82	TH	201	PEB	C2C-C3C	3.14	1.47	1.38
82	HB	202	PEB	CHB-C1C	3.14	1.47	1.40
82	NB	201	PEB	CHB-C1C	3.14	1.47	1.40
82	XJ	202	PEB	CHB-C1C	3.14	1.47	1.40
84	n3	1001	CYC	C1D-C2D	3.14	1.49	1.41
87	B2	816	CLA	C3B-C4B	3.14	1.50	1.42
87	C6	511	CLA	C4D-ND	-3.14	1.33	1.37
82	UH	201	PEB	C2C-C3C	3.14	1.47	1.38
82	AB	501	PEB	CHB-C1C	3.14	1.47	1.40
82	QO	201	PEB	CHA-C1B	3.14	1.47	1.40
82	GB	202	PEB	C2C-C3C	3.14	1.47	1.38
82	KA	202	PEB	C1A-NA	-3.14	1.33	1.37
82	t8	201	PEB	C1A-NA	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kE	201	PEB	C2A-C1A	-3.13	1.49	1.52
82	sF	203	PEB	C2A-C1A	-3.13	1.49	1.52
87	CL	508	CLA	CMB-C2B	-3.13	1.44	1.50
82	UF	202	PEB	C2C-C3C	3.13	1.47	1.38
84	HH	1001	CYC	C1D-C2D	3.13	1.49	1.41
84	LH	1002	CYC	C1B-C2B	3.13	1.50	1.45
87	JN	101	CLA	C4D-ND	-3.13	1.33	1.37
87	J2	101	CLA	C4D-ND	-3.13	1.33	1.37
82	TH	202	PEB	C2C-C3C	3.13	1.47	1.38
84	f3	1001	CYC	C1D-C2D	3.13	1.49	1.41
87	A2	851	CLA	C1D-ND	3.13	1.41	1.37
82	F5	201	PEB	CHA-C1B	3.13	1.47	1.40
82	AK	201	PEB	C2A-C1A	-3.13	1.49	1.52
84	63	901	CYC	C1D-C2D	3.13	1.49	1.41
82	SH	203	PEB	C1A-NA	-3.13	1.33	1.37
87	A2	806	CLA	C4D-ND	-3.13	1.33	1.37
82	ID	202	PEB	CHB-C1C	3.13	1.47	1.40
82	fM	203	PEB	CHA-C1B	3.13	1.47	1.40
82	AD	303	PEB	OD-C4D	3.13	1.29	1.23
87	8N	304	CLA	C4D-ND	-3.13	1.33	1.37
82	RB	201	PEB	C2A-C1A	-3.13	1.49	1.52
82	lF	203	PEB	OD-C4D	3.13	1.29	1.23
87	B2	834	CLA	C1D-ND	3.13	1.41	1.37
82	IB	201	PEB	C2C-C3C	3.13	1.47	1.38
82	LB	201	PEB	C2C-C3C	3.13	1.47	1.38
82	f4	201	PEB	C2C-C3C	3.13	1.47	1.38
84	I3	1001	CYC	C1B-C2B	3.13	1.50	1.45
87	RN	204	CLA	C4D-ND	-3.13	1.33	1.37
87	5N	604	CLA	C4D-ND	-3.13	1.33	1.37
82	M5	305	PEB	C2C-C3C	3.13	1.47	1.38
82	SF	201	PEB	CHA-C1B	3.13	1.47	1.40
82	dB	201	PEB	C2C-C3C	3.13	1.47	1.38
82	KK	203	PEB	OD-C4D	3.13	1.29	1.23
87	2N	301	CLA	CAB-C3B	-3.13	1.44	1.50
82	J1	1002	PEB	CHB-C1C	3.13	1.47	1.40
82	TI	201	PEB	CHB-C1C	3.13	1.47	1.40
87	AN	831	CLA	C1D-ND	3.13	1.41	1.37
87	A2	841	CLA	C4B-NB	3.13	1.41	1.37
87	32	304	CLA	O1D-CGD	3.13	1.29	1.21
82	W5	202	PEB	C2A-C1A	-3.13	1.49	1.52
82	Q7	202	PEB	OD-C4D	3.13	1.29	1.23
82	kK	203	PEB	C1A-NA	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hE	201	PEB	C2C-C3C	3.13	1.47	1.38
82	hG	201	PEB	C2C-C3C	3.13	1.47	1.38
82	NI	202	PEB	CHB-C1C	3.13	1.47	1.40
82	iF	202	PEB	CHB-C1C	3.13	1.47	1.40
87	BL	620	CLA	C4D-ND	-3.13	1.33	1.37
87	B6	608	CLA	C4D-ND	-3.13	1.33	1.37
87	B6	607	CLA	C4B-NB	3.13	1.41	1.37
82	YM	203	PEB	C2C-C3C	3.13	1.47	1.38
82	FQ	202	PEB	C2C-C3C	3.13	1.47	1.38
82	WQ	201	PEB	C2C-C3C	3.13	1.47	1.38
82	cO	202	PEB	C2C-C3C	3.13	1.47	1.38
96	G2	201	HEM	CAB-C3B	3.13	1.56	1.47
82	II	202	PEB	CHB-C1C	3.13	1.47	1.40
84	o3	1001	CYC	C1D-C2D	3.13	1.49	1.41
82	KB	304	PEB	C2C-C3C	3.13	1.47	1.38
82	SF	203	PEB	C2C-C3C	3.13	1.47	1.38
82	KK	201	PEB	C2A-C1A	-3.13	1.49	1.52
87	RN	201	CLA	C4D-ND	-3.13	1.33	1.37
82	LM	201	PEB	CHB-C1C	3.13	1.47	1.40
87	12	609	CLA	C4B-NB	3.13	1.41	1.37
84	p3	1001	CYC	C1B-C2B	3.13	1.50	1.45
82	WM	202	PEB	C1C-C2C	3.13	1.50	1.42
82	AI	203	PEB	OD-C4D	3.13	1.29	1.23
87	CL	518	CLA	C4D-ND	-3.13	1.33	1.37
87	A6	404	CLA	C4D-ND	-3.13	1.33	1.37
84	D3	1001	CYC	C1B-C2B	3.13	1.50	1.45
84	d3	1001	CYC	C1B-C2B	3.13	1.50	1.45
82	XK	203	PEB	C2A-C1A	-3.13	1.49	1.52
87	42	609	CLA	C4B-NB	3.13	1.41	1.37
87	c6	612	CLA	C4B-NB	3.13	1.41	1.37
82	DB	201	PEB	C2C-C3C	3.13	1.47	1.38
82	u8	202	PEB	C2C-C3C	3.13	1.47	1.38
84	O3	1001	CYC	C1B-C2B	3.12	1.50	1.45
82	EM	202	PEB	C2A-C1A	-3.12	1.49	1.52
84	K1	1001	CYC	C2C-C1C	-3.12	1.49	1.52
82	XJ	201	PEB	C1C-NC	-3.12	1.32	1.37
82	OE	203	PEB	CHA-C1B	3.12	1.47	1.40
82	aK	201	PEB	C2C-C3C	3.12	1.47	1.38
82	gB	203	PEB	CHB-C1C	3.12	1.47	1.40
82	wC	202	PEB	C4B-C3B	3.12	1.50	1.45
82	T1	202	PEB	C2C-C3C	3.12	1.47	1.38
87	22	609	CLA	C4D-ND	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	e3	1001	CYC	C1B-C2B	3.12	1.50	1.45
82	YM	201	PEB	C2A-C1A	-3.12	1.49	1.52
82	RI	203	PEB	C1A-NA	-3.12	1.33	1.37
82	MF	201	PEB	CHB-C1C	3.12	1.47	1.40
87	22	605	CLA	CAB-C3B	-3.12	1.44	1.50
82	XD	202	PEB	C1A-NA	-3.12	1.33	1.37
82	Y9	203	PEB	C1A-NA	-3.12	1.33	1.37
82	NK	202	PEB	C1C-NC	-3.12	1.32	1.37
82	TE	201	PEB	CHB-C1C	3.12	1.47	1.40
87	AN	806	CLA	C4B-NB	3.12	1.41	1.37
82	T1	201	PEB	C2C-C3C	3.12	1.47	1.38
82	J4	1002	PEB	CHC-C4C	3.12	1.53	1.49
82	u8	201	PEB	C1C-C2C	3.12	1.50	1.42
87	7N	608	CLA	C4B-NB	3.12	1.41	1.37
83	K7	203	PUB	CHB-C4B	3.12	1.47	1.40
84	JH	1003	CYC	C3D-C2D	3.12	1.47	1.38
82	W9	202	PEB	C4B-C3B	3.12	1.50	1.45
82	UJ	203	PEB	C1A-NA	-3.12	1.33	1.37
82	F5	202	PEB	CHB-C1C	3.12	1.47	1.40
82	W9	201	PEB	CHB-C1C	3.12	1.47	1.40
84	L3	1001	CYC	C1D-C2D	3.12	1.49	1.41
83	yF	303	PUB	CHB-C4B	3.12	1.47	1.40
83	BJ	302	PUB	C3B-C2B	3.12	1.47	1.38
82	NE	202	PEB	C2A-C1A	-3.12	1.49	1.52
82	TM	201	PEB	CHB-C1C	3.12	1.47	1.40
84	k3	1001	CYC	C1B-C2B	3.12	1.50	1.45
82	RH	201	PEB	C1A-NA	-3.12	1.33	1.37
87	AN	849	CLA	C4D-ND	-3.12	1.33	1.37
87	cL	505	CLA	C4D-ND	-3.12	1.33	1.37
87	3N	313	CLA	C4D-ND	-3.12	1.33	1.37
87	6N	604	CLA	C4D-ND	-3.12	1.33	1.37
87	BN	811	CLA	CMB-C2B	-3.12	1.44	1.50
82	aM	204	PEB	C2C-C3C	3.12	1.47	1.38
87	82	303	CLA	C4B-NB	3.12	1.41	1.37
87	D6	403	CLA	C1D-ND	3.12	1.41	1.37
82	jF	202	PEB	CHB-C1C	3.12	1.47	1.40
82	O9	201	PEB	C4B-C3B	3.12	1.50	1.45
82	RQ	202	PEB	OD-C4D	3.12	1.29	1.23
87	5N	610	CLA	C4D-ND	-3.12	1.33	1.37
82	U9	201	PEB	C2A-C1A	-3.12	1.49	1.52
87	B2	804	CLA	C4B-NB	3.12	1.41	1.37
87	5N	601	CLA	C4D-ND	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	lG	201	PEB	C1A-NA	-3.12	1.33	1.37
82	bK	202	PEB	C1A-NA	-3.12	1.33	1.37
87	L2	204	CLA	C1D-ND	3.12	1.41	1.37
82	XF	203	PEB	C2A-C1A	-3.12	1.49	1.52
82	H5	201	PEB	C4D-ND	3.12	1.39	1.35
84	A3	1001	CYC	C1B-C2B	3.12	1.50	1.45
82	OG	203	PEB	CHA-C1B	3.12	1.47	1.40
82	JM	201	PEB	C2A-C1A	-3.12	1.49	1.52
82	jJ	203	PEB	C2C-C3C	3.12	1.47	1.38
87	bL	606	CLA	C1D-ND	3.12	1.41	1.37
82	UQ	201	PEB	OD-C4D	3.12	1.29	1.23
82	KI	203	PEB	CHB-C1C	3.12	1.47	1.40
82	iJ	201	PEB	CHB-C1C	3.12	1.47	1.40
82	hO	202	PEB	C1A-NA	-3.12	1.33	1.37
82	VP	201	PEB	C2A-C1A	-3.11	1.49	1.52
82	XA	203	PEB	CHB-C1C	3.11	1.47	1.40
82	v8	202	PEB	CHB-C1C	3.11	1.47	1.40
82	H7	202	PEB	CHA-C1B	3.11	1.47	1.40
82	O9	202	PEB	CHA-C1B	3.11	1.47	1.40
87	AN	835	CLA	C1D-ND	3.11	1.41	1.37
87	B2	816	CLA	C4B-NB	3.11	1.41	1.37
83	AE	302	PUB	C3B-C2B	3.11	1.47	1.38
87	BN	805	CLA	C3B-C4B	3.11	1.50	1.42
82	UI	201	PEB	C2C-C3C	3.11	1.47	1.38
84	H1	1001	CYC	C3D-C2D	3.11	1.47	1.38
82	X7	203	PEB	CHB-C1C	3.11	1.47	1.40
82	EM	201	PEB	CHA-C1B	3.11	1.47	1.40
87	BN	817	CLA	C3B-C4B	3.11	1.50	1.42
87	B2	828	CLA	C4D-ND	-3.11	1.33	1.37
82	NQ	203	PEB	OD-C4D	3.11	1.29	1.23
87	1N	601	CLA	C4B-NB	3.11	1.41	1.37
82	SB	201	PEB	CHB-C1C	3.11	1.47	1.40
87	B2	810	CLA	CMB-C2B	-3.11	1.44	1.50
82	P7	202	PEB	CHA-C1B	3.11	1.47	1.40
82	YB	201	PEB	C2C-C3C	3.11	1.47	1.38
82	VP	202	PEB	C2C-C3C	3.11	1.47	1.38
87	2N	306	CLA	C4D-ND	-3.11	1.33	1.37
87	cL	507	CLA	C4B-NB	3.11	1.41	1.37
82	N4	1002	PEB	C2A-C1A	-3.11	1.49	1.52
87	AN	823	CLA	C4D-ND	-3.11	1.33	1.37
87	8N	306	CLA	C4B-NB	3.11	1.41	1.37
82	HQ	203	PEB	C1A-NA	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	eO	201	PEB	CHB-C1C	3.11	1.47	1.40
87	42	603	CLA	C4D-ND	-3.11	1.33	1.37
87	5N	611	CLA	C4D-ND	-3.11	1.33	1.37
82	R7	203	PEB	C2A-C1A	-3.11	1.49	1.52
82	KP	201	PEB	C2C-C3C	3.11	1.47	1.38
82	eK	203	PEB	C2C-C3C	3.11	1.47	1.38
84	LH	1002	CYC	C3D-C2D	3.11	1.47	1.38
87	22	605	CLA	C4B-NB	3.11	1.41	1.37
87	B2	828	CLA	C4B-NB	3.11	1.41	1.37
84	l3	1001	CYC	C1B-C2B	3.11	1.50	1.45
84	HG	1001	CYC	C1D-C2D	3.11	1.49	1.41
82	mF	201	PEB	C2C-C3C	3.11	1.47	1.38
82	QB	204	PEB	CHB-C1C	3.11	1.47	1.40
82	OE	201	PEB	CHB-C1C	3.11	1.47	1.40
84	H3	1001	CYC	C1B-C2B	3.11	1.50	1.45
82	GP	202	PEB	C2A-C1A	-3.11	1.49	1.52
82	HO	1002	PEB	C2C-C3C	3.11	1.47	1.38
82	jF	201	PEB	C2C-C3C	3.11	1.47	1.38
82	sF	203	PEB	C2C-C3C	3.11	1.47	1.38
82	lM	201	PEB	C2C-C3C	3.11	1.47	1.38
82	s8	202	PEB	C1A-NA	-3.11	1.33	1.37
87	72	608	CLA	C4B-NB	3.11	1.41	1.37
87	2N	310	CLA	C4B-NB	3.11	1.41	1.37
82	mG	202	PEB	C2C-C3C	3.11	1.47	1.38
87	a6	608	CLA	C4D-ND	-3.11	1.33	1.37
84	DH	1003	CYC	C1D-C2D	3.11	1.49	1.41
82	XI	202	PEB	CHB-C1C	3.11	1.47	1.40
87	A2	835	CLA	C1D-ND	3.11	1.41	1.37
87	cL	514	CLA	C4D-ND	-3.11	1.33	1.37
87	32	313	CLA	C4B-NB	3.11	1.41	1.37
82	B9	201	PEB	C1A-NA	-3.11	1.33	1.37
87	42	606	CLA	C4D-ND	-3.11	1.33	1.37
87	52	601	CLA	C4D-ND	-3.11	1.33	1.37
84	B3	1001	CYC	C1B-C2B	3.11	1.50	1.45
82	DF	202	PEB	CHA-C1B	3.11	1.47	1.40
82	UA	202	PEB	OD-C4D	3.11	1.29	1.23
82	LQ	202	PEB	C2A-C1A	-3.11	1.49	1.52
82	iM	201	PEB	CHB-C1C	3.11	1.47	1.40
82	WJ	201	PEB	C2C-C3C	3.11	1.47	1.38
82	PP	201	PEB	C2C-C3C	3.11	1.47	1.38
82	dE	202	PEB	C2C-C3C	3.11	1.47	1.38
82	M9	302	PEB	C2C-C3C	3.11	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WD	201	PEB	C1A-NA	-3.11	1.33	1.37
82	IB	202	PEB	CHB-C1C	3.11	1.47	1.40
82	BK	202	PEB	CHB-C1C	3.11	1.47	1.40
82	FO	1002	PEB	C2C-C3C	3.11	1.47	1.38
82	U5	201	PEB	C2C-C3C	3.11	1.47	1.38
82	eF	203	PEB	C2C-C3C	3.11	1.47	1.38
87	ON	203	CLA	CHC-C1C	3.11	1.44	1.38
82	gG	202	PEB	CHB-C1C	3.11	1.47	1.40
82	WI	202	PEB	C1A-NA	-3.11	1.33	1.37
96	GN	201	HEM	CAB-C3B	3.10	1.55	1.47
82	iF	202	PEB	C2C-C3C	3.10	1.47	1.38
87	82	305	CLA	C4B-NB	3.10	1.41	1.37
82	SH	201	PEB	C2A-C1A	-3.10	1.49	1.52
82	IK	201	PEB	C2C-C3C	3.10	1.47	1.38
84	NO	1001	CYC	C3D-C2D	3.10	1.47	1.38
87	22	605	CLA	MG-NB	-3.10	1.99	2.05
82	wF	302	PEB	C1A-NA	-3.10	1.33	1.37
82	j1	201	PEB	CHA-C1B	3.10	1.47	1.40
87	A2	806	CLA	C4B-NB	3.10	1.41	1.37
87	c6	613	CLA	C4B-NB	3.10	1.41	1.37
82	XD	201	PEB	C2C-C3C	3.10	1.47	1.38
82	cB	401	PEB	C2C-C3C	3.10	1.47	1.38
84	G3	1001	CYC	C1B-C2B	3.10	1.50	1.45
84	N3	1001	CYC	C1B-C2B	3.10	1.50	1.45
83	AE	303	PUB	OD-C4D	3.10	1.29	1.23
82	O5	201	PEB	C1C-NC	-3.10	1.32	1.37
87	BN	828	CLA	C4B-NB	3.10	1.41	1.37
87	C6	518	CLA	C4B-NB	3.10	1.41	1.37
82	J9	202	PEB	C2C-C3C	3.10	1.47	1.38
82	RI	202	PEB	CHB-C1C	3.10	1.47	1.40
82	RB	201	PEB	C2C-C3C	3.10	1.47	1.38
87	62	308	CLA	C4B-NB	3.10	1.41	1.37
87	8N	303	CLA	C4B-NB	3.10	1.41	1.37
82	VB	202	PEB	C2C-C3C	3.10	1.47	1.38
87	B2	804	CLA	C3B-C4B	3.10	1.50	1.42
82	AK	202	PEB	OD-C4D	3.10	1.29	1.23
82	VB	201	PEB	CHB-C1C	3.10	1.47	1.40
82	Y5	203	PEB	CHB-C1C	3.10	1.47	1.40
82	sF	201	PEB	CHB-C1C	3.10	1.47	1.40
82	OJ	202	PEB	C2C-C3C	3.10	1.47	1.38
82	TH	202	PEB	C1A-NA	-3.10	1.33	1.37
82	AQ	301	PEB	CHB-C1C	3.10	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jH	201	PEB	CHB-C1C	3.10	1.47	1.40
82	SK	201	PEB	CHA-C1B	3.10	1.47	1.40
82	dG	202	PEB	C2C-C3C	3.10	1.47	1.38
84	HH	1001	CYC	C3D-C2D	3.10	1.47	1.38
82	GJ	202	PEB	C1A-NA	-3.10	1.33	1.37
82	gK	202	PEB	C1A-NA	-3.10	1.33	1.37
82	ZG	203	PEB	C2A-C1A	-3.10	1.49	1.52
82	XJ	201	PEB	C2A-C1A	-3.10	1.49	1.52
82	DB	203	PEB	C2C-C3C	3.10	1.47	1.38
87	3N	304	CLA	C4D-ND	-3.10	1.33	1.37
84	BG	1002	CYC	CHA-C4D	3.10	1.47	1.40
82	JH	1002	PEB	C1A-NA	-3.10	1.33	1.37
82	wC	201	PEB	C1A-NA	-3.10	1.33	1.37
82	kK	202	PEB	OD-C4D	3.10	1.29	1.23
82	O4	201	PEB	CHB-C1C	3.10	1.47	1.40
87	C6	509	CLA	C4D-ND	-3.10	1.33	1.37
87	DL	403	CLA	C1D-ND	3.10	1.41	1.37
82	CQ	201	PEB	C2A-C1A	-3.10	1.49	1.52
82	S1	201	PEB	C2C-C3C	3.10	1.47	1.38
82	UD	202	PEB	CHB-C1C	3.10	1.47	1.40
82	UQ	202	PEB	CHB-C1C	3.10	1.47	1.40
87	72	604	CLA	C4B-NB	3.10	1.41	1.37
82	YI	202	PEB	C2C-C3C	3.10	1.47	1.38
82	XJ	202	PEB	C2A-C1A	-3.10	1.49	1.52
84	FH	1001	CYC	C2C-C1C	-3.10	1.49	1.52
82	PD	201	PEB	C2C-C3C	3.10	1.47	1.38
82	B5	203	PEB	C2C-C3C	3.10	1.47	1.38
84	n3	1001	CYC	C1B-C2B	3.10	1.50	1.45
87	42	608	CLA	C4D-ND	-3.10	1.33	1.37
82	WO	201	PEB	CHA-C1B	3.10	1.47	1.40
82	OG	201	PEB	CHB-C1C	3.10	1.47	1.40
82	BI	203	PEB	C2C-C3C	3.10	1.47	1.38
87	52	601	CLA	C4B-NB	3.10	1.41	1.37
84	K3	1001	CYC	C1B-C2B	3.10	1.50	1.45
84	g3	1001	CYC	C1B-C2B	3.10	1.50	1.45
84	m3	1001	CYC	C1B-C2B	3.10	1.50	1.45
84	t3	1001	CYC	C1B-C2B	3.10	1.50	1.45
84	v3	1001	CYC	C1B-C2B	3.10	1.50	1.45
87	cL	517	CLA	C4D-ND	-3.10	1.33	1.37
82	VH	202	PEB	C2A-C1A	-3.10	1.49	1.52
82	SA	202	PEB	C1A-NA	-3.10	1.33	1.37
82	sK	201	PEB	C1A-NA	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NM	201	PEB	C2C-C3C	3.10	1.47	1.38
82	dO	201	PEB	CHB-C1C	3.10	1.47	1.40
84	T3	1001	CYC	C1B-C2B	3.10	1.50	1.45
82	DI	202	PEB	C1A-NA	-3.10	1.33	1.37
82	SQ	201	PEB	C2A-C1A	-3.10	1.49	1.52
87	4N	603	CLA	C4D-ND	-3.10	1.33	1.37
82	QG	203	PEB	CHB-C1C	3.10	1.47	1.40
82	ZI	401	PEB	C1A-NA	-3.09	1.33	1.37
87	BN	834	CLA	C1D-ND	3.09	1.41	1.37
84	c3	1001	CYC	C1B-C2B	3.09	1.50	1.45
82	EI	202	PEB	CHB-C1C	3.09	1.47	1.40
82	jF	202	PEB	C2A-C1A	-3.09	1.49	1.52
82	KJ	201	PEB	C2C-C3C	3.09	1.47	1.38
82	S9	202	PEB	C2C-C3C	3.09	1.47	1.38
82	R1	201	PEB	C1A-NA	-3.09	1.33	1.37
82	aO	201	PEB	CHB-C1C	3.09	1.47	1.40
83	AJ	303	PUB	CHB-C4B	3.09	1.47	1.40
87	3N	301	CLA	C1D-ND	3.09	1.41	1.37
87	3N	301	CLA	C4D-ND	-3.09	1.33	1.37
87	4N	611	CLA	C4D-ND	-3.09	1.33	1.37
82	DK	201	PEB	C2C-C3C	3.09	1.47	1.38
84	GE	1001	CYC	C3D-C2D	3.09	1.47	1.38
82	SB	201	PEB	C2A-C1A	-3.09	1.49	1.52
87	72	610	CLA	C4B-NB	3.09	1.41	1.37
87	O2	203	CLA	CHC-C1C	3.09	1.44	1.38
87	62	305	CLA	C4D-ND	-3.09	1.33	1.37
87	A2	824	CLA	C4D-ND	-3.09	1.33	1.37
82	aE	201	PEB	C2A-C1A	-3.09	1.49	1.52
82	OO	201	PEB	C2C-C3C	3.09	1.47	1.38
82	uF	203	PEB	OD-C4D	3.09	1.29	1.23
82	IK	203	PEB	CHB-C1C	3.09	1.47	1.40
82	S7	202	PEB	C1A-NA	-3.09	1.33	1.37
82	kF	202	PEB	C1A-NA	-3.09	1.33	1.37
82	iK	201	PEB	C1A-NA	-3.09	1.33	1.37
82	wK	302	PEB	C1A-NA	-3.09	1.33	1.37
82	V7	203	PEB	C2C-C3C	3.09	1.47	1.38
87	8N	302	CLA	C4B-NB	3.09	1.41	1.37
82	CI	202	PEB	CHB-C1C	3.09	1.47	1.40
87	CL	505	CLA	C4B-NB	3.09	1.41	1.37
87	B6	615	CLA	C4B-NB	3.09	1.41	1.37
82	e4	201	PEB	CHB-C1C	3.09	1.47	1.40
82	OF	203	PEB	CHB-C1C	3.09	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4N	606	CLA	C4D-ND	-3.09	1.33	1.37
87	A2	830	CLA	C1D-ND	3.09	1.41	1.37
87	4N	608	CLA	C4B-NB	3.09	1.41	1.37
87	6N	602	CLA	C4B-NB	3.09	1.41	1.37
82	KG	201	PEB	C2A-C1A	-3.09	1.49	1.52
82	b4	201	PEB	C2A-C1A	-3.09	1.49	1.52
82	iK	202	PEB	C2C-C3C	3.09	1.47	1.38
84	L3	1001	CYC	C1B-C2B	3.09	1.50	1.45
82	oF	203	PEB	OD-C4D	3.09	1.29	1.23
82	kK	202	PEB	C1A-NA	-3.09	1.33	1.37
82	VI	202	PEB	CHB-C1C	3.09	1.47	1.40
87	3N	309	CLA	C4B-NB	3.09	1.41	1.37
82	K7	202	PEB	C1A-NA	-3.09	1.33	1.37
82	q8	203	PEB	C1A-NA	-3.09	1.33	1.37
82	w8	201	PEB	C1A-NA	-3.09	1.33	1.37
82	PI	202	PEB	CHB-C1C	3.09	1.47	1.40
82	HO	1002	PEB	C2A-C1A	-3.09	1.49	1.52
82	AQ	303	PEB	OD-C4D	3.09	1.29	1.23
87	c6	615	CLA	C4D-ND	-3.09	1.33	1.37
87	AN	849	CLA	C3B-C4B	3.09	1.50	1.42
82	KF	203	PEB	OD-C4D	3.09	1.29	1.23
82	uF	201	PEB	CHC-C4C	3.09	1.53	1.49
87	AN	805	CLA	C4B-NB	3.09	1.41	1.37
82	YH	201	PEB	C2A-C1A	-3.09	1.49	1.52
82	LI	201	PEB	C2A-C1A	-3.09	1.49	1.52
82	NM	202	PEB	C2A-C1A	-3.09	1.49	1.52
82	H7	201	PEB	C2A-C1A	-3.09	1.49	1.52
82	fH	202	PEB	OD-C4D	3.09	1.29	1.23
87	bL	622	CLA	C4D-ND	-3.09	1.33	1.37
82	NI	203	PEB	OD-C4D	3.09	1.29	1.23
82	XF	201	PEB	C2C-C3C	3.09	1.47	1.38
82	X7	202	PEB	CHB-C1C	3.09	1.47	1.40
84	E1	1001	CYC	C3D-C2D	3.09	1.47	1.38
82	gE	202	PEB	CHB-C1C	3.09	1.47	1.40
82	kF	202	PEB	OD-C4D	3.09	1.29	1.23
82	dB	202	PEB	CHB-C1C	3.08	1.47	1.40
82	HB	202	PEB	C2C-C3C	3.08	1.47	1.38
82	RQ	203	PEB	CHA-C1B	3.08	1.47	1.40
82	q8	201	PEB	C1A-NA	-3.08	1.33	1.37
82	YJ	202	PEB	C2C-C3C	3.08	1.47	1.38
82	jJ	203	PEB	CHA-C1B	3.08	1.47	1.40
82	AF	202	PEB	OD-C4D	3.08	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	cL	506	CLA	C4B-NB	3.08	1.41	1.37
82	U1	201	PEB	C2C-C3C	3.08	1.47	1.38
82	qK	201	PEB	C2C-C3C	3.08	1.47	1.38
87	52	605	CLA	C4B-NB	3.08	1.41	1.37
82	a1	202	PEB	C1A-NA	-3.08	1.33	1.37
82	TI	203	PEB	CHB-C1C	3.08	1.47	1.40
82	lF	203	PEB	C2C-C3C	3.08	1.47	1.38
82	IB	203	PEB	C2C-C3C	3.08	1.47	1.38
87	52	610	CLA	C4D-ND	-3.08	1.33	1.37
82	SK	203	PEB	OD-C4D	3.08	1.29	1.23
82	lM	203	PEB	C1A-NA	-3.08	1.33	1.37
82	WE	202	PEB	C2A-C1A	-3.08	1.49	1.52
82	JQ	202	PEB	CHA-C1B	3.08	1.47	1.40
87	cL	507	CLA	C4D-ND	-3.08	1.33	1.37
87	bL	615	CLA	C4D-ND	-3.08	1.33	1.37
82	XM	202	PEB	C2A-C1A	-3.08	1.49	1.52
87	2N	301	CLA	MG-NB	-3.08	1.99	2.05
82	V1	202	PEB	C2C-C3C	3.08	1.47	1.38
87	BN	829	CLA	C4D-ND	-3.08	1.33	1.37
82	IF	203	PEB	CHB-C1C	3.08	1.47	1.40
82	g1	202	PEB	OD-C4D	3.08	1.29	1.23
82	fG	202	PEB	OD-C4D	3.08	1.29	1.23
82	YI	201	PEB	C2A-C1A	-3.08	1.49	1.52
82	H5	202	PEB	CHA-C1B	3.08	1.47	1.40
82	HD	203	PEB	C1A-NA	-3.08	1.33	1.37
87	AN	824	CLA	C4D-ND	-3.08	1.33	1.37
82	QG	203	PEB	OD-C4D	3.08	1.29	1.23
82	LQ	201	PEB	CHA-C1B	3.08	1.47	1.40
82	IF	201	PEB	C2C-C3C	3.08	1.47	1.38
82	Z9	301	PEB	C2C-C3C	3.08	1.47	1.38
87	bL	604	CLA	C4D-ND	-3.08	1.33	1.37
82	YA	301	PEB	CHB-C1C	3.08	1.47	1.40
82	LH	1003	PEB	CHA-C1B	3.08	1.47	1.40
82	L9	202	PEB	C2C-C3C	3.08	1.47	1.38
82	OK	203	PEB	CHB-C1C	3.08	1.47	1.40
82	F9	202	PEB	CHA-C1B	3.08	1.47	1.40
82	BJ	301	PEB	C2A-C1A	-3.08	1.49	1.52
87	42	611	CLA	C4D-ND	-3.08	1.33	1.37
87	52	609	CLA	C4D-ND	-3.08	1.33	1.37
87	L2	206	CLA	C4D-ND	-3.08	1.33	1.37
82	pF	202	PEB	C4B-C3B	3.08	1.50	1.45
87	BL	606	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	811	CLA	C4D-ND	-3.08	1.33	1.37
87	6N	607	CLA	C4B-NB	3.08	1.41	1.37
82	IB	201	PEB	C2A-C1A	-3.08	1.49	1.52
82	C7	201	PEB	C2A-C1A	-3.08	1.49	1.52
82	sK	203	PEB	C2A-C1A	-3.08	1.49	1.52
82	F4	1002	PEB	C2C-C3C	3.08	1.47	1.38
82	QF	201	PEB	C2C-C3C	3.07	1.47	1.38
82	HQ	203	PEB	OD-C4D	3.07	1.29	1.23
87	AN	830	CLA	C1D-ND	3.07	1.41	1.37
82	SB	201	PEB	C2C-C3C	3.07	1.47	1.38
82	Q1	201	PEB	CHA-C1B	3.07	1.47	1.40
87	BN	828	CLA	C4D-ND	-3.07	1.33	1.37
87	A2	835	CLA	C4D-ND	-3.07	1.33	1.37
82	DK	202	PEB	CHA-C1B	3.07	1.47	1.40
87	AN	805	CLA	C1D-ND	3.07	1.41	1.37
87	62	306	CLA	C4B-NB	3.07	1.41	1.37
82	TD	201	PEB	OD-C4D	3.07	1.29	1.23
87	nL	101	CLA	CMC-C2C	-3.07	1.44	1.50
82	T7	202	PEB	CHB-C1C	3.07	1.47	1.40
82	jM	203	PEB	C2C-C3C	3.07	1.47	1.38
82	ZM	201	PEB	C2A-C1A	-3.07	1.49	1.52
82	HA	202	PEB	CHA-C1B	3.07	1.47	1.40
84	FG	1001	CYC	C3D-C2D	3.07	1.47	1.38
87	3N	308	CLA	C1C-NC	-3.07	1.33	1.37
87	52	607	CLA	C4B-NB	3.07	1.41	1.37
91	aL	610	PHO	C3A-C2A	-3.07	1.51	1.54
82	M5	304	PEB	C2C-C3C	3.07	1.47	1.38
84	J3	1001	CYC	C1B-C2B	3.07	1.50	1.45
82	lF	202	PEB	C1A-NA	-3.07	1.33	1.37
83	Z5	302	PUB	C4B-NB	-3.07	1.32	1.37
82	RM	201	PEB	C2C-C3C	3.07	1.47	1.38
82	RD	203	PEB	CHA-C1B	3.07	1.47	1.40
87	B6	605	CLA	C4D-ND	-3.07	1.33	1.37
87	C6	519	CLA	C4D-ND	-3.07	1.33	1.37
82	lO	201	PEB	CHB-C1C	3.07	1.47	1.40
82	sK	203	PEB	C2C-C3C	3.07	1.47	1.38
87	dL	402	CLA	C3B-C4B	3.07	1.49	1.42
82	R4	203	PEB	C1A-NA	-3.07	1.33	1.37
87	b6	607	CLA	C4B-NB	3.07	1.41	1.37
87	32	305	CLA	C4D-ND	-3.07	1.33	1.37
82	GA	201	PEB	C2C-C3C	3.07	1.47	1.38
87	LN	204	CLA	C3C-C2C	3.07	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	P3	1001	CYC	C1B-C2B	3.07	1.50	1.45
84	N4	1001	CYC	C3D-C2D	3.07	1.47	1.38
82	l4	201	PEB	CHB-C1C	3.07	1.47	1.40
82	lK	203	PEB	C2C-C3C	3.07	1.47	1.38
82	GI	203	PEB	CHB-C1C	3.07	1.47	1.40
84	J1	1001	CYC	CHA-C4D	3.07	1.47	1.40
87	2N	301	CLA	C4B-NB	3.07	1.41	1.37
82	d1	202	PEB	CHC-C4C	3.07	1.53	1.49
84	D1	1003	CYC	C1D-C2D	3.07	1.48	1.41
82	OQ	201	PEB	OD-C4D	3.07	1.29	1.23
82	NF	202	PEB	C1C-NC	-3.07	1.32	1.37
82	AI	202	PEB	CHB-C1C	3.07	1.47	1.40
82	JD	202	PEB	OD-C4D	3.07	1.29	1.23
82	IP	202	PEB	C1A-NA	-3.07	1.33	1.37
82	dJ	201	PEB	CHA-C1B	3.07	1.47	1.40
84	C3	1001	CYC	C1B-C2B	3.07	1.50	1.45
82	bB	201	PEB	C2C-C3C	3.07	1.47	1.38
82	HF	202	PEB	CHB-C1C	3.07	1.47	1.40
82	ZG	201	PEB	CHB-C1C	3.07	1.47	1.40
82	LI	201	PEB	C2C-C3C	3.07	1.47	1.38
82	UG	203	PEB	CHB-C1C	3.07	1.47	1.40
82	HD	203	PEB	OD-C4D	3.07	1.29	1.23
87	32	303	CLA	C4D-ND	-3.07	1.33	1.37
84	R3	1001	CYC	C1B-C2B	3.07	1.50	1.45
82	uC	201	PEB	OD-C4D	3.07	1.29	1.23
82	TB	201	PEB	C4A-NA	-3.07	1.30	1.37
82	JA	201	PEB	CHB-C1C	3.07	1.47	1.40
82	J7	201	PEB	CHB-C1C	3.07	1.47	1.40
87	BL	602	CLA	CMC-C2C	-3.07	1.44	1.50
87	8N	307	CLA	C4B-NB	3.07	1.41	1.37
82	aM	204	PEB	C2A-C1A	-3.07	1.49	1.52
82	QH	201	PEB	C1A-NA	-3.06	1.33	1.37
82	KF	201	PEB	C2A-C1A	-3.06	1.49	1.52
82	RJ	201	PEB	C2A-C1A	-3.06	1.49	1.52
82	MA	202	PEB	C1A-NA	-3.06	1.33	1.37
82	aH	202	PEB	C1A-NA	-3.06	1.33	1.37
87	5N	603	CLA	C4B-NB	3.06	1.41	1.37
82	JB	201	PEB	C4A-NA	-3.06	1.30	1.37
84	E3	1001	CYC	C1B-C2B	3.06	1.50	1.45
82	JF	202	PEB	C2A-C1A	-3.06	1.49	1.52
82	PG	202	PEB	C2A-C1A	-3.06	1.49	1.52
82	KM	203	PEB	CHA-C1B	3.06	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VQ	201	PEB	CHA-C1B	3.06	1.47	1.40
82	XA	202	PEB	CHB-C1C	3.06	1.47	1.40
82	F5	201	PEB	CHB-C1C	3.06	1.47	1.40
87	6N	605	CLA	C4B-NB	3.06	1.41	1.37
82	jH	201	PEB	CHA-C1B	3.06	1.47	1.40
82	JF	201	PEB	C2C-C3C	3.06	1.47	1.38
82	Z5	304	PEB	C2C-C3C	3.06	1.47	1.38
82	Z9	304	PEB	CHB-C1C	3.06	1.47	1.40
82	VJ	201	PEB	C2A-C1A	-3.06	1.49	1.52
87	BN	805	CLA	C4B-NB	3.06	1.41	1.37
87	B2	836	CLA	C1D-ND	3.06	1.41	1.37
82	Q7	202	PEB	C2C-C3C	3.06	1.47	1.38
82	XB	202	PEB	CHB-C1C	3.06	1.47	1.40
82	IF	201	PEB	C4A-NA	-3.06	1.30	1.37
87	L2	204	CLA	C3C-C2C	3.06	1.43	1.36
87	c6	609	CLA	C4B-NB	3.06	1.41	1.37
87	8N	304	CLA	C4B-NB	3.06	1.41	1.37
82	RO	203	PEB	C1A-NA	-3.06	1.33	1.37
82	qC	203	PEB	C1A-NA	-3.06	1.33	1.37
82	QK	201	PEB	C2C-C3C	3.06	1.47	1.38
87	5N	607	CLA	C4B-NB	3.06	1.41	1.37
82	IK	201	PEB	C4A-NA	-3.06	1.30	1.37
82	WI	203	PEB	CHB-C1C	3.06	1.47	1.40
82	bP	502	PEB	C2C-C3C	3.06	1.47	1.38
87	B2	829	CLA	C4D-ND	-3.06	1.33	1.37
87	b6	606	CLA	C4D-ND	-3.06	1.33	1.37
82	uF	202	PEB	C1A-NA	-3.06	1.33	1.37
87	BL	620	CLA	CMB-C2B	-3.06	1.44	1.50
87	B6	609	CLA	C3B-C4B	3.06	1.49	1.42
82	IB	202	PEB	CHA-C1B	3.06	1.47	1.40
87	5N	606	CLA	C4D-ND	-3.06	1.33	1.37
82	j1	203	PEB	C2C-C3C	3.06	1.47	1.38
87	32	307	CLA	C1C-NC	-3.06	1.33	1.37
82	f1	202	PEB	OD-C4D	3.06	1.29	1.23
87	cL	516	CLA	C4D-ND	-3.06	1.33	1.37
87	3N	306	CLA	C4D-ND	-3.06	1.33	1.37
82	BF	201	PEB	C2C-C3C	3.06	1.47	1.38
82	M9	305	PEB	CHB-C1C	3.06	1.47	1.40
82	eF	201	PEB	C2C-C3C	3.06	1.47	1.38
87	A2	850	CLA	C4B-NB	3.06	1.41	1.37
87	1N	604	CLA	C4B-NB	3.06	1.41	1.37
87	AN	836	CLA	C4D-ND	-3.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CB	201	PEB	CHB-C1C	3.06	1.47	1.40
82	J5	203	PEB	CHB-C1C	3.06	1.47	1.40
87	32	311	CLA	C4D-ND	-3.06	1.33	1.37
82	hM	201	PEB	C2C-C3C	3.06	1.47	1.38
82	B9	201	PEB	C4B-C3B	3.06	1.50	1.45
82	EQ	202	PEB	C2C-C3C	3.06	1.47	1.38
87	52	603	CLA	C4B-NB	3.06	1.41	1.37
82	lJ	202	PEB	CHB-C1C	3.05	1.47	1.40
82	gB	201	PEB	C1A-NA	-3.05	1.33	1.37
82	uK	201	PEB	C1A-NA	-3.05	1.33	1.37
82	fE	202	PEB	OD-C4D	3.05	1.29	1.23
82	HM	202	PEB	C2A-C1A	-3.05	1.49	1.52
82	qC	201	PEB	C1A-NA	-3.05	1.33	1.37
82	HI	203	PEB	C2C-C3C	3.05	1.47	1.38
82	d1	203	PEB	OD-C4D	3.05	1.29	1.23
82	WI	202	PEB	C2C-C3C	3.05	1.47	1.38
87	b6	611	CLA	C4B-NB	3.05	1.41	1.37
82	UK	202	PEB	CHA-C1B	3.05	1.47	1.40
82	sF	203	PEB	CHA-C1B	3.05	1.47	1.40
82	YI	202	PEB	C2A-C1A	-3.05	1.49	1.52
82	JM	202	PEB	C2A-C1A	-3.05	1.49	1.52
82	LM	201	PEB	C2A-C1A	-3.05	1.49	1.52
82	oK	203	PEB	C2A-C1A	-3.05	1.49	1.52
87	H6	103	CLA	C4B-NB	3.05	1.41	1.37
82	H5	202	PEB	C2C-C3C	3.05	1.47	1.38
87	bL	620	CLA	C4D-ND	-3.05	1.33	1.37
82	ID	202	PEB	C2C-C3C	3.05	1.47	1.38
82	j1	201	PEB	CHB-C1C	3.05	1.47	1.40
82	MF	203	PEB	C2C-C3C	3.05	1.47	1.38
82	XQ	201	PEB	C2C-C3C	3.05	1.47	1.38
82	TA	202	PEB	CHB-C1C	3.05	1.47	1.40
82	jH	203	PEB	C2C-C3C	3.05	1.47	1.38
82	XQ	202	PEB	C1A-NA	-3.05	1.33	1.37
87	LN	206	CLA	C4D-ND	-3.05	1.33	1.37
84	FE	1002	CYC	C3D-C2D	3.05	1.47	1.38
82	BF	202	PEB	CHB-C1C	3.05	1.47	1.40
82	lO	201	PEB	CHA-C1B	3.05	1.47	1.40
82	CA	201	PEB	C2A-C1A	-3.05	1.49	1.52
82	a4	202	PEB	C2A-C1A	-3.05	1.49	1.52
82	AB	501	PEB	C2C-C3C	3.05	1.47	1.38
82	YI	201	PEB	C2C-C3C	3.05	1.47	1.38
87	12	610	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	3N	311	CLA	C4D-ND	-3.05	1.33	1.37
82	M9	302	PEB	CHA-C1B	3.05	1.47	1.40
82	SF	202	PEB	C2C-C3C	3.05	1.47	1.38
82	mE	202	PEB	C2C-C3C	3.05	1.47	1.38
82	cK	202	PEB	OD-C4D	3.05	1.29	1.23
82	lK	201	PEB	OD-C4D	3.05	1.29	1.23
82	RD	201	PEB	CHA-C1B	3.05	1.47	1.40
82	YM	201	PEB	CHA-C1B	3.05	1.47	1.40
87	c6	606	CLA	C4D-ND	-3.05	1.33	1.37
87	BN	816	CLA	C4B-NB	3.05	1.41	1.37
82	UP	201	PEB	CHB-C1C	3.05	1.47	1.40
82	WO	201	PEB	C2C-C3C	3.05	1.47	1.38
82	r8	202	PEB	C1A-NA	-3.05	1.33	1.37
82	PB	201	PEB	CHB-C1C	3.05	1.47	1.40
82	dH	201	PEB	C2C-C3C	3.05	1.47	1.38
87	BN	812	CLA	C4D-ND	-3.05	1.33	1.37
87	A2	814	CLA	C4D-ND	-3.05	1.33	1.37
82	dK	201	PEB	C2A-C1A	-3.05	1.49	1.52
82	Y1	202	PEB	C2C-C3C	3.05	1.47	1.38
82	Q5	202	PEB	C2C-C3C	3.05	1.47	1.38
84	i3	1001	CYC	C1B-C2B	3.05	1.50	1.45
82	KF	203	PEB	CHA-C1B	3.05	1.47	1.40
87	CL	515	CLA	C4D-ND	-3.05	1.33	1.37
82	jK	201	PEB	C2C-C3C	3.05	1.47	1.38
82	NB	203	PEB	CHB-C1C	3.05	1.47	1.40
82	BP	202	PEB	C2A-C1A	-3.05	1.49	1.52
87	22	603	CLA	C4D-ND	-3.04	1.33	1.37
87	22	606	CLA	C4D-ND	-3.04	1.33	1.37
87	A2	823	CLA	C4D-ND	-3.04	1.33	1.37
82	SK	202	PEB	C2C-C3C	3.04	1.47	1.38
82	G7	201	PEB	C2C-C3C	3.04	1.47	1.38
87	A2	805	CLA	C4B-NB	3.04	1.41	1.37
82	BK	201	PEB	C2C-C3C	3.04	1.47	1.38
82	KP	202	PEB	CHB-C1C	3.04	1.47	1.40
82	tK	203	PEB	CHC-C4C	3.04	1.53	1.49
82	W5	201	PEB	C2C-C3C	3.04	1.47	1.38
84	BG	1001	CYC	C3D-C2D	3.04	1.47	1.38
87	A2	829	CLA	C1D-ND	3.04	1.41	1.37
82	uK	202	PEB	OD-C4D	3.04	1.29	1.23
87	12	605	CLA	C4B-NB	3.04	1.41	1.37
82	lE	201	PEB	C1A-NA	-3.04	1.33	1.37
82	hH	201	PEB	CHA-C1B	3.04	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GF	201	PEB	C4B-NB	-3.04	1.32	1.38
82	WK	203	PEB	OD-C4D	3.04	1.29	1.23
87	52	606	CLA	C4D-ND	-3.04	1.33	1.37
84	GG	1001	CYC	C3D-C2D	3.04	1.47	1.38
84	C4	1001	CYC	C3D-C2D	3.04	1.47	1.38
82	l4	201	PEB	CHA-C1B	3.04	1.47	1.40
84	JH	1001	CYC	CHA-C4D	3.04	1.47	1.40
82	hG	203	PEB	OD-C4D	3.04	1.29	1.23
82	OO	201	PEB	CHB-C1C	3.04	1.47	1.40
87	32	309	CLA	C4B-NB	3.04	1.41	1.37
82	QA	202	PEB	C2C-C3C	3.04	1.47	1.38
82	ZG	203	PEB	OD-C4D	3.04	1.29	1.23
87	CL	507	CLA	C1D-ND	3.04	1.41	1.37
82	sF	201	PEB	C1A-NA	-3.04	1.33	1.37
82	TG	201	PEB	CHB-C1C	3.04	1.47	1.40
87	2N	309	CLA	C4C-C3C	3.04	1.50	1.45
87	F2	201	CLA	C3B-C4B	3.04	1.49	1.42
82	ZB	201	PEB	C2A-C1A	-3.04	1.49	1.52
96	f6	101	HEM	C3B-C4B	3.04	1.50	1.44
82	gH	202	PEB	OD-C4D	3.04	1.29	1.23
82	VF	202	PEB	CHB-C1C	3.04	1.47	1.40
87	M2	101	CLA	C4D-ND	-3.04	1.33	1.37
82	SF	203	PEB	OD-C4D	3.04	1.29	1.23
82	NO	1002	PEB	C2A-C1A	-3.04	1.49	1.52
82	aJ	201	PEB	C1A-NA	-3.04	1.33	1.37
87	B2	809	CLA	C4B-NB	3.04	1.41	1.37
82	CP	203	PEB	OD-C4D	3.04	1.29	1.23
82	CF	202	PEB	C1A-NA	-3.04	1.33	1.37
82	JD	202	PEB	CHA-C1B	3.04	1.47	1.40
82	S1	201	PEB	C2A-C1A	-3.03	1.49	1.52
82	L5	203	PEB	C2A-C1A	-3.03	1.49	1.52
87	52	610	CLA	C4B-NB	3.03	1.41	1.37
87	C6	514	CLA	C4B-NB	3.03	1.41	1.37
87	c6	615	CLA	C4B-NB	3.03	1.41	1.37
87	5N	610	CLA	C4B-NB	3.03	1.41	1.37
82	qF	201	PEB	C2C-C3C	3.03	1.46	1.38
82	QH	202	PEB	C2C-C3C	3.03	1.46	1.38
84	CO	1001	CYC	C3D-C2D	3.03	1.46	1.38
87	LN	202	CLA	C4B-NB	3.03	1.41	1.37
87	K2	106	CLA	C1D-ND	3.03	1.41	1.37
82	PG	201	PEB	CHB-C1C	3.03	1.47	1.40
87	82	302	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SM	203	PEB	C2C-C3C	3.03	1.46	1.38
82	e4	201	PEB	C2A-C1A	-3.03	1.49	1.52
82	QB	203	PEB	C2C-C3C	3.03	1.46	1.38
82	WF	203	PEB	OD-C4D	3.03	1.29	1.23
87	AN	814	CLA	C4D-ND	-3.03	1.33	1.37
82	hE	203	PEB	OD-C4D	3.03	1.29	1.23
82	sC	202	PEB	C1A-NA	-3.03	1.33	1.37
82	iF	201	PEB	C1A-NA	-3.03	1.33	1.37
82	sK	202	PEB	C1A-NA	-3.03	1.33	1.37
82	PB	201	PEB	C2A-C1A	-3.03	1.49	1.52
82	e1	201	PEB	C2A-C1A	-3.03	1.49	1.52
82	JK	201	PEB	C2C-C3C	3.03	1.46	1.38
82	OF	203	PEB	OD-C4D	3.03	1.29	1.23
82	WI	202	PEB	OD-C4D	3.03	1.29	1.23
82	fM	203	PEB	C2C-C3C	3.03	1.46	1.38
87	AN	829	CLA	C1D-ND	3.03	1.41	1.37
87	c6	614	CLA	C4B-NB	3.03	1.41	1.37
82	jE	202	PEB	OD-C4D	3.03	1.29	1.23
82	pF	202	PEB	C2A-C1A	-3.03	1.49	1.52
87	5N	609	CLA	C4D-ND	-3.03	1.33	1.37
82	SP	203	PEB	C1C-C2C	3.03	1.50	1.42
82	NA	203	PEB	C1C-NC	-3.03	1.32	1.37
82	N7	203	PEB	C1C-NC	-3.03	1.32	1.37
82	U5	202	PEB	C2C-C3C	3.03	1.46	1.38
87	D6	403	CLA	C4B-NB	3.03	1.41	1.37
87	2N	304	CLA	C4B-NB	3.03	1.41	1.37
82	18	203	PEB	OD-C4D	3.03	1.29	1.23
87	AN	850	CLA	C4B-NB	3.03	1.41	1.37
87	B2	834	CLA	C4B-NB	3.03	1.41	1.37
87	A2	849	CLA	C3B-C4B	3.03	1.49	1.42
82	WH	202	PEB	OD-C4D	3.03	1.29	1.23
82	RF	201	PEB	C2C-C3C	3.03	1.46	1.38
82	d1	201	PEB	C2C-C3C	3.03	1.46	1.38
84	BE	1001	CYC	C3D-C2D	3.03	1.46	1.38
87	BL	621	CLA	C1D-ND	3.03	1.41	1.37
87	72	607	CLA	C4D-ND	-3.03	1.33	1.37
82	NA	203	PEB	C2C-C3C	3.03	1.46	1.38
82	YH	202	PEB	C2C-C3C	3.03	1.46	1.38
82	EQ	201	PEB	C2C-C3C	3.03	1.46	1.38
83	M5	302	PUB	C4B-NB	-3.03	1.32	1.37
82	D5	203	PEB	CHB-C1C	3.03	1.47	1.40
82	OD	201	PEB	OD-C4D	3.03	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gH	203	PEB	C1A-NA	-3.03	1.33	1.37
82	W9	201	PEB	C4B-C3B	3.03	1.50	1.45
87	b6	612	CLA	C4B-NB	3.03	1.41	1.37
82	ZE	203	PEB	OD-C4D	3.03	1.29	1.23
87	FN	203	CLA	C3B-C4B	3.03	1.49	1.42
82	CA	201	PEB	C2C-C3C	3.03	1.46	1.38
87	RN	203	CLA	C4B-NB	3.03	1.41	1.37
82	aJ	204	PEB	C2C-C3C	3.03	1.46	1.38
82	M7	202	PEB	C1A-NA	-3.03	1.33	1.37
82	IQ	202	PEB	C2C-C3C	3.03	1.46	1.38
82	IB	202	PEB	C2A-C1A	-3.02	1.49	1.52
82	YO	203	PEB	C1A-NA	-3.02	1.33	1.37
82	PA	203	PEB	CHB-C1C	3.02	1.47	1.40
84	BE	1002	CYC	CHA-C4D	3.02	1.47	1.40
82	NM	201	PEB	CHC-C4C	3.02	1.53	1.49
82	fH	203	PEB	C1A-NA	-3.02	1.33	1.37
82	O1	201	PEB	CHA-C1B	3.02	1.47	1.40
82	WD	201	PEB	CHB-C1C	3.02	1.47	1.40
87	AN	818	CLA	C4D-ND	-3.02	1.33	1.37
82	UI	202	PEB	C2A-C1A	-3.02	1.49	1.52
87	AN	814	CLA	C4B-NB	3.02	1.41	1.37
82	O5	202	PEB	C2C-C3C	3.02	1.46	1.38
84	EH	1001	CYC	C3D-C2D	3.02	1.46	1.38
82	XM	201	PEB	CHC-C4C	3.02	1.53	1.49
82	EI	202	PEB	CHA-C1B	3.02	1.47	1.40
82	RD	203	PEB	OD-C4D	3.02	1.29	1.23
84	BG	1002	CYC	C3D-C2D	3.02	1.46	1.38
84	DE	1001	CYC	CHB-C4A	3.02	1.47	1.40
82	ZE	201	PEB	CHA-C1B	3.02	1.47	1.40
82	P7	203	PEB	CHB-C1C	3.02	1.47	1.40
87	72	610	CLA	C4D-ND	-3.02	1.33	1.37
82	SB	203	PEB	C2A-C1A	-3.02	1.49	1.52
82	IP	202	PEB	OD-C4D	3.02	1.29	1.23
87	cL	514	CLA	C4B-NB	3.02	1.41	1.37
82	ZG	201	PEB	CHA-C1B	3.02	1.47	1.40
82	IB	202	PEB	C2C-C3C	3.02	1.46	1.38
82	UO	201	PEB	CHA-C1B	3.02	1.47	1.40
87	32	308	CLA	C4D-ND	-3.02	1.33	1.37
87	bL	605	CLA	C4D-ND	-3.02	1.33	1.37
87	6N	602	CLA	C4D-ND	-3.02	1.33	1.37
82	EI	201	PEB	C1C-NC	-3.02	1.32	1.37
82	ED	201	PEB	CHB-C1C	3.02	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	F4	1001	CYC	C3D-C2D	3.02	1.46	1.38
82	jK	202	PEB	C2A-C1A	-3.02	1.49	1.52
82	L1	1002	PEB	CHA-C1B	3.02	1.47	1.40
87	A2	836	CLA	C4D-ND	-3.02	1.33	1.37
87	R2	203	CLA	C4B-NB	3.02	1.41	1.37
87	C6	513	CLA	C4B-NB	3.02	1.41	1.37
82	XI	201	PEB	C1C-NC	-3.02	1.32	1.37
82	aB	202	PEB	C2C-C3C	3.02	1.46	1.38
87	MN	101	CLA	C4D-ND	-3.02	1.33	1.37
87	B2	827	CLA	CMD-C2D	-3.02	1.44	1.50
82	sC	201	PEB	OD-C4D	3.02	1.29	1.23
82	jO	201	PEB	CHA-C1B	3.02	1.47	1.40
82	N7	203	PEB	C2C-C3C	3.02	1.46	1.38
82	DI	201	PEB	C1C-C2C	3.02	1.49	1.42
87	22	604	CLA	C4B-NB	3.02	1.41	1.37
82	WA	201	PEB	C2A-C1A	-3.02	1.49	1.52
82	DE	1002	PEB	C2A-C1A	-3.02	1.49	1.52
87	62	303	CLA	C4D-ND	-3.02	1.33	1.37
87	A2	824	CLA	C4B-NB	3.02	1.41	1.37
82	PQ	201	PEB	C2C-C3C	3.01	1.46	1.38
82	IJ	202	PEB	CHB-C1C	3.01	1.47	1.40
84	DG	1001	CYC	CHB-C4A	3.01	1.47	1.40
82	LI	201	PEB	C1C-NC	-3.01	1.32	1.37
82	rC	202	PEB	C4B-C3B	3.01	1.50	1.45
82	sK	203	PEB	CHA-C1B	3.01	1.47	1.40
82	JP	202	PEB	C2C-C3C	3.01	1.46	1.38
84	BE	1002	CYC	C3D-C2D	3.01	1.46	1.38
82	TH	201	PEB	CHB-C1C	3.01	1.47	1.40
82	L5	201	PEB	CHA-C1B	3.01	1.47	1.40
82	ZM	202	PEB	C2A-C1A	-3.01	1.49	1.52
82	MJ	202	PEB	C2C-C3C	3.01	1.46	1.38
82	VQ	203	PEB	CHA-C1B	3.01	1.47	1.40
82	J7	202	PEB	CHA-C1B	3.01	1.47	1.40
82	MB	201	PEB	C2C-C3C	3.01	1.46	1.38
87	AN	806	CLA	C3B-C4B	3.01	1.49	1.42
87	1N	610	CLA	C4B-NB	3.01	1.41	1.37
82	MJ	203	PEB	C2C-C3C	3.01	1.46	1.38
82	U7	202	PEB	OD-C4D	3.01	1.29	1.23
82	DA	202	PEB	C2C-C3C	3.01	1.46	1.38
87	62	302	CLA	C4D-ND	-3.01	1.33	1.37
87	22	609	CLA	C4C-C3C	3.01	1.50	1.45
82	J7	202	PEB	C2C-C3C	3.01	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	KK	203	PEB	CHA-C1B	3.01	1.47	1.40
87	2N	311	CLA	C3B-C4B	3.01	1.49	1.42
82	dH	203	PEB	OD-C4D	3.01	1.29	1.23
82	r8	201	PEB	OD-C4D	3.01	1.29	1.23
82	hJ	201	PEB	C2C-C3C	3.01	1.46	1.38
87	7N	607	CLA	C4D-ND	-3.01	1.33	1.37
87	BN	836	CLA	C1D-ND	3.01	1.41	1.37
87	2N	305	CLA	C4B-NB	3.01	1.41	1.37
82	MK	202	PEB	OD-C4D	3.01	1.29	1.23
82	f4	201	PEB	CHA-C1B	3.01	1.47	1.40
82	W4	201	PEB	C2C-C3C	3.01	1.46	1.38
82	SF	203	PEB	C2A-C1A	-3.01	1.49	1.52
82	QG	202	PEB	C2A-C1A	-3.01	1.49	1.52
82	S5	203	PEB	C2C-C3C	3.01	1.46	1.38
83	yF	302	PUB	C3B-C2B	3.01	1.46	1.38
87	A2	851	CLA	C4D-ND	-3.01	1.33	1.37
82	SK	203	PEB	C2A-C1A	-3.01	1.49	1.52
87	22	603	CLA	C4B-NB	3.01	1.41	1.37
87	c6	606	CLA	C4B-NB	3.01	1.41	1.37
87	22	611	CLA	C3B-C4B	3.01	1.49	1.42
82	S4	201	PEB	CHB-C1C	3.01	1.47	1.40
87	22	601	CLA	C4B-NB	3.01	1.41	1.37
82	y8	202	PEB	CHC-C4C	3.01	1.53	1.49
82	CQ	202	PEB	C2A-C1A	-3.01	1.49	1.52
82	SH	203	PEB	C2C-C3C	3.01	1.46	1.38
82	WI	201	PEB	C4B-C3B	3.01	1.50	1.45
82	L5	202	PEB	C2C-C3C	3.01	1.46	1.38
82	Y5	202	PEB	C2C-C3C	3.01	1.46	1.38
82	lJ	201	PEB	CHA-C1B	3.01	1.47	1.40
82	YF	203	PEB	C2C-C3C	3.01	1.46	1.38
82	bB	201	PEB	CHB-C1C	3.01	1.47	1.40
82	UP	202	PEB	C1C-C2C	3.01	1.49	1.42
82	kE	201	PEB	C1C-C2C	3.01	1.49	1.42
87	AN	810	CLA	C4D-ND	-3.01	1.33	1.37
82	1C	203	PEB	OD-C4D	3.01	1.29	1.23
82	EM	201	PEB	C2C-C3C	3.01	1.46	1.38
82	M5	304	PEB	CHB-C1C	3.01	1.47	1.40
82	QI	201	PEB	C2C-C3C	3.00	1.46	1.38
87	6N	613	CLA	C4D-ND	-3.00	1.33	1.37
87	B2	815	CLA	C4B-NB	3.00	1.41	1.37
82	YF	202	PEB	OD-C4D	3.00	1.29	1.23
82	KK	201	PEB	CHA-C1B	3.00	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EQ	201	PEB	CHB-C1C	3.00	1.47	1.40
82	eH	201	PEB	OD-C4D	3.00	1.29	1.23
82	iK	203	PEB	OD-C4D	3.00	1.29	1.23
82	WQ	201	PEB	CHB-C1C	3.00	1.47	1.40
82	UF	202	PEB	CHA-C1B	3.00	1.47	1.40
82	LI	202	PEB	C2C-C3C	3.00	1.46	1.38
82	TJ	201	PEB	C1C-NC	-3.00	1.32	1.37
82	N7	201	PEB	C2C-C3C	3.00	1.46	1.38
82	TA	203	PEB	CHB-C1C	3.00	1.47	1.40
82	O5	203	PEB	C2C-C3C	3.00	1.46	1.38
82	xC	202	PEB	CHB-C1C	3.00	1.47	1.40
82	PJ	202	PEB	C2A-C1A	-3.00	1.49	1.52
82	1C	202	PEB	C4B-C3B	3.00	1.50	1.45
82	C7	201	PEB	C2C-C3C	3.00	1.46	1.38
84	73	1001	CYC	C3D-C2D	3.00	1.46	1.38
87	AN	827	CLA	C4B-NB	3.00	1.41	1.37
87	cL	508	CLA	C4B-NB	3.00	1.41	1.37
87	2N	302	CLA	C4B-NB	3.00	1.41	1.37
87	A2	806	CLA	C3B-C4B	3.00	1.49	1.42
82	HB	201	PEB	C2C-C3C	3.00	1.46	1.38
82	eH	203	PEB	C2C-C3C	3.00	1.46	1.38
87	32	310	CLA	C4B-NB	3.00	1.41	1.37
87	1N	605	CLA	C4B-NB	3.00	1.41	1.37
82	XI	202	PEB	CHA-C1B	3.00	1.47	1.40
82	I7	202	PEB	CHA-C1B	3.00	1.47	1.40
87	A2	821	CLA	C4D-ND	-3.00	1.33	1.37
87	A2	852	CLA	CHD-C4C	3.00	1.46	1.39
87	82	301	CLA	C4B-NB	3.00	1.41	1.37
82	sC	202	PEB	OD-C4D	3.00	1.29	1.23
82	II	202	PEB	CHA-C1B	3.00	1.47	1.40
82	Y5	202	PEB	CHA-C1B	3.00	1.47	1.40
82	XK	203	PEB	C1C-NC	-3.00	1.32	1.37
87	AN	851	CLA	C4D-ND	-3.00	1.33	1.37
82	ZE	201	PEB	CHB-C1C	3.00	1.47	1.40
82	VP	202	PEB	C2A-C1A	-3.00	1.49	1.52
82	L5	202	PEB	CHA-C1B	3.00	1.47	1.40
82	iK	201	PEB	C2C-C3C	3.00	1.46	1.38
82	YI	201	PEB	C1C-NC	-3.00	1.32	1.37
87	BL	602	CLA	CMB-C2B	-3.00	1.44	1.50
87	A2	805	CLA	C1D-ND	3.00	1.41	1.37
87	b6	617	CLA	C4B-NB	3.00	1.41	1.37
82	pK	202	PEB	C2A-C1A	-3.00	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	yC	202	PEB	CHC-C4C	3.00	1.53	1.49
82	Z9	301	PEB	CHA-C1B	3.00	1.47	1.40
87	A2	819	CLA	C1D-ND	3.00	1.41	1.37
82	HB	201	PEB	CHB-C1C	3.00	1.47	1.40
84	q3	1001	CYC	C3D-C2D	3.00	1.46	1.38
82	j4	201	PEB	CHA-C1B	3.00	1.47	1.40
87	AN	818	CLA	C4B-NB	3.00	1.41	1.37
82	rC	201	PEB	OD-C4D	3.00	1.29	1.23
82	NI	202	PEB	CHA-C1B	3.00	1.47	1.40
82	rC	202	PEB	OD-C4D	3.00	1.29	1.23
82	kJ	202	PEB	C2A-C1A	-3.00	1.49	1.52
82	XK	201	PEB	C2C-C3C	3.00	1.46	1.38
84	w3	1001	CYC	C3D-C2D	3.00	1.46	1.38
82	VK	202	PEB	CHB-C1C	3.00	1.47	1.40
82	R4	201	PEB	CHB-C1C	3.00	1.47	1.40
87	82	304	CLA	C4B-NB	2.99	1.41	1.37
82	F5	202	PEB	C2A-C1A	-2.99	1.49	1.52
82	eB	202	PEB	C2A-C1A	-2.99	1.49	1.52
82	nK	201	PEB	C2A-C1A	-2.99	1.49	1.52
87	6N	601	CLA	C4D-ND	-2.99	1.33	1.37
82	v8	202	PEB	OD-C4D	2.99	1.29	1.23
87	3N	310	CLA	C4B-NB	2.99	1.41	1.37
82	gF	203	PEB	C2C-C3C	2.99	1.46	1.38
82	kH	202	PEB	C1A-NA	-2.99	1.33	1.37
87	A2	818	CLA	C4D-ND	-2.99	1.33	1.37
87	cL	509	CLA	C4D-ND	-2.99	1.33	1.37
82	LK	201	PEB	C2C-C3C	2.99	1.46	1.38
82	AK	201	PEB	CHB-C1C	2.99	1.47	1.40
82	II	201	PEB	C1C-NC	-2.99	1.32	1.37
87	CL	510	CLA	CMB-C2B	-2.99	1.44	1.50
82	UP	201	PEB	CHA-C1B	2.99	1.47	1.40
82	UJ	201	PEB	C2A-C1A	-2.99	1.49	1.52
82	JI	202	PEB	OD-C4D	2.99	1.29	1.23
87	5N	603	CLA	C4D-ND	-2.99	1.33	1.37
82	Q1	202	PEB	C2C-C3C	2.99	1.46	1.38
82	aK	201	PEB	CHA-C1B	2.99	1.47	1.40
82	MK	203	PEB	C2C-C3C	2.99	1.46	1.38
82	x8	202	PEB	CHB-C1C	2.99	1.47	1.40
87	52	603	CLA	C4D-ND	-2.99	1.33	1.37
87	FN	205	CLA	C3B-C4B	2.99	1.49	1.42
82	fK	202	PEB	OD-C4D	2.99	1.29	1.23
82	bO	201	PEB	C2A-C1A	-2.99	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	T7	203	PEB	CHB-C1C	2.99	1.47	1.40
82	iG	201	PEB	OD-C4D	2.99	1.29	1.23
82	CI	202	PEB	CHA-C1B	2.99	1.47	1.40
82	CI	201	PEB	C1C-NC	-2.99	1.32	1.37
87	12	605	CLA	C4D-ND	-2.99	1.33	1.37
87	32	302	CLA	C4D-ND	-2.99	1.33	1.37
87	bL	607	CLA	C4D-ND	-2.99	1.33	1.37
87	8N	303	CLA	C1D-ND	2.99	1.41	1.37
82	HJ	201	PEB	C1C-NC	-2.99	1.32	1.37
82	RF	202	PEB	CHB-C1C	2.99	1.47	1.40
82	L5	203	PEB	CHB-C1C	2.99	1.47	1.40
82	KI	203	PEB	CHA-C1B	2.99	1.47	1.40
82	D5	202	PEB	CHA-C1B	2.99	1.47	1.40
84	M3	1001	CYC	C3D-C2D	2.99	1.46	1.38
87	BN	827	CLA	CMD-C2D	-2.99	1.44	1.50
84	Q3	1001	CYC	C3D-C2D	2.99	1.46	1.38
82	W1	202	PEB	OD-C4D	2.99	1.29	1.23
82	T1	201	PEB	CHB-C1C	2.99	1.47	1.40
87	aL	606	CLA	C4D-ND	-2.99	1.33	1.37
82	GI	203	PEB	CHA-C1B	2.99	1.47	1.40
82	S7	202	PEB	CHA-C1B	2.99	1.47	1.40
82	KI	202	PEB	C1C-NC	-2.99	1.32	1.37
87	CL	506	CLA	C4B-NB	2.99	1.41	1.37
87	KN	102	CLA	C1D-ND	2.99	1.41	1.37
87	cL	515	CLA	C3B-C4B	2.99	1.49	1.42
82	XQ	201	PEB	OD-C4D	2.99	1.29	1.23
84	k3	1001	CYC	C3D-C2D	2.99	1.46	1.38
84	o3	1001	CYC	C3D-C2D	2.99	1.46	1.38
87	AN	824	CLA	C4B-NB	2.99	1.41	1.37
82	D7	202	PEB	C2C-C3C	2.99	1.46	1.38
82	vC	202	PEB	OD-C4D	2.99	1.29	1.23
82	RI	201	PEB	C1C-NC	-2.99	1.32	1.37
87	CL	505	CLA	C4D-ND	-2.99	1.33	1.37
87	1N	606	CLA	C4B-NB	2.99	1.41	1.37
82	AF	201	PEB	CHB-C1C	2.98	1.47	1.40
87	2N	305	CLA	C3B-C4B	2.98	1.49	1.42
82	MD	201	PEB	C2A-C1A	-2.98	1.49	1.52
87	D6	405	CLA	C4B-NB	2.98	1.41	1.37
87	AL	404	CLA	C4D-ND	-2.98	1.33	1.37
87	7N	610	CLA	C4D-ND	-2.98	1.33	1.37
82	U4	201	PEB	CHA-C1B	2.98	1.47	1.40
82	q8	202	PEB	C2C-C3C	2.98	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	22	604	CLA	C3B-C4B	2.98	1.49	1.42
82	H5	201	PEB	C2C-C3C	2.98	1.46	1.38
82	RI	202	PEB	CHA-C1B	2.98	1.47	1.40
82	CM	203	PEB	CHA-C1B	2.98	1.47	1.40
87	3N	303	CLA	C4D-ND	-2.98	1.33	1.37
87	KN	105	CLA	C1D-ND	2.98	1.41	1.37
84	n3	1001	CYC	C3D-C2D	2.98	1.46	1.38
82	WK	201	PEB	CHA-C1B	2.98	1.47	1.40
82	QH	203	PEB	OD-C4D	2.98	1.29	1.23
82	JP	201	PEB	C2A-C1A	-2.98	1.49	1.52
82	QM	202	PEB	C2C-C3C	2.98	1.46	1.38
87	cL	510	CLA	CMB-C2B	-2.98	1.44	1.50
87	CL	513	CLA	C3B-C4B	2.98	1.49	1.42
84	FO	1001	CYC	C3D-C2D	2.98	1.46	1.38
82	WE	202	PEB	OD-C4D	2.98	1.29	1.23
82	NB	202	PEB	C2A-C1A	-2.98	1.49	1.52
82	ED	202	PEB	C2C-C3C	2.98	1.46	1.38
84	h3	1001	CYC	C3D-C2D	2.98	1.46	1.38
87	DL	406	CLA	C4D-ND	-2.98	1.33	1.37
87	bL	621	CLA	C4D-ND	-2.98	1.33	1.37
87	AN	852	CLA	CHD-C4C	2.98	1.46	1.39
82	YO	201	PEB	C2A-C1A	-2.98	1.49	1.52
82	JA	202	PEB	C2C-C3C	2.98	1.46	1.38
87	BN	810	CLA	C4B-NB	2.98	1.41	1.37
87	2N	309	CLA	C3B-C4B	2.98	1.49	1.42
82	WI	202	PEB	CHB-C1C	2.98	1.47	1.40
87	82	308	CLA	C1D-ND	2.98	1.41	1.37
82	r8	202	PEB	C4B-C3B	2.98	1.50	1.45
82	RK	201	PEB	C2C-C3C	2.98	1.46	1.38
82	MF	202	PEB	OD-C4D	2.98	1.29	1.23
84	F3	1001	CYC	C3D-C2D	2.98	1.46	1.38
82	LF	201	PEB	C2C-C3C	2.98	1.46	1.38
82	HD	202	PEB	C2A-C1A	-2.98	1.49	1.52
82	ZE	203	PEB	C2A-C1A	-2.98	1.49	1.52
82	AA	201	PEB	C4B-C3B	2.98	1.50	1.45
82	eK	201	PEB	C2C-C3C	2.98	1.46	1.38
87	cL	517	CLA	C3B-C4B	2.98	1.49	1.42
82	VI	202	PEB	CHA-C1B	2.98	1.47	1.40
82	ZJ	201	PEB	CHB-C1C	2.98	1.47	1.40
84	I3	1001	CYC	C3D-C2D	2.98	1.46	1.38
82	HM	201	PEB	C1C-NC	-2.98	1.32	1.37
87	7N	605	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B6	610	CLA	C4B-NB	2.98	1.41	1.37
82	h1	201	PEB	C1A-NA	-2.98	1.33	1.37
82	AI	202	PEB	CHA-C1B	2.98	1.47	1.40
82	fO	201	PEB	CHA-C1B	2.98	1.47	1.40
82	NQ	204	PEB	CHC-C4C	2.98	1.53	1.49
87	4N	609	CLA	C4D-ND	-2.97	1.33	1.37
84	u3	1001	CYC	C3D-C2D	2.97	1.46	1.38
87	5N	601	CLA	C4B-NB	2.97	1.41	1.37
82	YJ	202	PEB	CHB-C1C	2.97	1.47	1.40
87	b6	608	CLA	C4D-ND	-2.97	1.33	1.37
82	OH	201	PEB	CHA-C1B	2.97	1.47	1.40
82	VQ	203	PEB	C2C-C3C	2.97	1.46	1.38
87	B2	830	CLA	C4B-NB	2.97	1.41	1.37
82	MM	202	PEB	CHB-C1C	2.97	1.47	1.40
82	CD	201	PEB	C2A-C1A	-2.97	1.49	1.52
82	YJ	203	PEB	C2C-C3C	2.97	1.46	1.38
84	U3	1001	CYC	C3D-C2D	2.97	1.46	1.38
82	VB	202	PEB	OD-C4D	2.97	1.29	1.23
87	BN	823	CLA	C1D-ND	2.97	1.41	1.37
87	d6	406	CLA	C4B-NB	2.97	1.41	1.37
82	tC	201	PEB	OD-C4D	2.97	1.29	1.23
82	FI	201	PEB	C2C-C3C	2.97	1.46	1.38
82	iH	202	PEB	C2A-C1A	-2.97	1.49	1.52
82	qC	202	PEB	C2C-C3C	2.97	1.46	1.38
84	L3	1001	CYC	C3D-C2D	2.97	1.46	1.38
82	Q1	201	PEB	C1A-NA	-2.97	1.33	1.37
82	GK	201	PEB	C4B-NB	-2.97	1.32	1.38
82	WB	402	PEB	C2A-C1A	-2.97	1.49	1.52
82	XJ	201	PEB	CHB-C1C	2.97	1.47	1.40
84	H3	1001	CYC	C3D-C2D	2.97	1.46	1.38
84	S3	1001	CYC	C3D-C2D	2.97	1.46	1.38
87	cL	511	CLA	C1D-ND	2.97	1.41	1.37
82	PI	202	PEB	CHA-C1B	2.97	1.47	1.40
82	TQ	203	PEB	OD-C4D	2.97	1.29	1.23
82	aK	201	PEB	OD-C4D	2.97	1.29	1.23
82	V1	202	PEB	C1A-NA	-2.97	1.33	1.37
87	62	301	CLA	C4D-ND	-2.97	1.33	1.37
82	AP	202	PEB	OD-C4D	2.97	1.29	1.23
82	s8	202	PEB	OD-C4D	2.97	1.29	1.23
87	AN	836	CLA	C3B-C4B	2.97	1.49	1.42
82	IA	202	PEB	CHA-C1B	2.97	1.47	1.40
82	Z5	304	PEB	CHB-C1C	2.97	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	306	CLA	C4B-NB	2.97	1.41	1.37
87	bL	608	CLA	C3B-C4B	2.97	1.49	1.42
82	NA	201	PEB	C2C-C3C	2.97	1.46	1.38
82	RQ	201	PEB	CHA-C1B	2.97	1.47	1.40
82	uF	201	PEB	OD-C4D	2.97	1.29	1.23
87	3N	310	CLA	C4D-ND	-2.97	1.33	1.37
82	J7	203	PEB	CHB-C1C	2.97	1.47	1.40
82	WG	202	PEB	OD-C4D	2.97	1.29	1.23
87	B6	604	CLA	C4B-NB	2.97	1.41	1.37
84	j3	1001	CYC	C3D-C2D	2.97	1.46	1.38
82	aF	201	PEB	C4B-C3B	2.97	1.50	1.45
87	B2	817	CLA	C4B-NB	2.97	1.41	1.37
82	MA	201	PEB	C2C-C3C	2.97	1.46	1.38
82	dM	201	PEB	C2C-C3C	2.97	1.46	1.38
87	A2	835	CLA	C3B-C4B	2.97	1.49	1.42
87	F2	205	CLA	C3B-C4B	2.97	1.49	1.42
87	cL	512	CLA	CMB-C2B	-2.97	1.44	1.50
87	B2	805	CLA	C3B-C4B	2.96	1.49	1.42
82	k1	202	PEB	OD-C4D	2.96	1.29	1.23
87	72	606	CLA	C4B-NB	2.96	1.41	1.37
82	LB	201	PEB	CHB-C1C	2.96	1.47	1.40
82	FM	201	PEB	CHB-C1C	2.96	1.47	1.40
82	SO	201	PEB	CHB-C1C	2.96	1.47	1.40
82	UI	202	PEB	C2C-C3C	2.96	1.46	1.38
82	s8	201	PEB	OD-C4D	2.96	1.29	1.23
82	eF	201	PEB	OD-C4D	2.96	1.29	1.23
87	72	605	CLA	C4D-ND	-2.96	1.33	1.37
82	w8	203	PEB	C1A-NA	-2.96	1.33	1.37
82	eO	203	PEB	C1A-NA	-2.96	1.33	1.37
87	22	609	CLA	C3B-C4B	2.96	1.49	1.42
82	AI	203	PEB	C1D-ND	2.96	1.50	1.45
82	WF	201	PEB	CHA-C1B	2.96	1.47	1.40
82	r8	202	PEB	OD-C4D	2.96	1.29	1.23
87	BN	830	CLA	C4B-NB	2.96	1.41	1.37
82	Y5	201	PEB	CHB-C1C	2.96	1.47	1.40
83	yK	302	PUB	C3B-C2B	2.96	1.46	1.38
82	TD	203	PEB	OD-C4D	2.96	1.29	1.23
82	j1	203	PEB	OD-C4D	2.96	1.29	1.23
82	z8	201	PEB	OD-C4D	2.96	1.29	1.23
82	h1	202	PEB	CHA-C1B	2.96	1.47	1.40
82	KF	201	PEB	CHA-C1B	2.96	1.47	1.40
82	F7	202	PEB	CHA-C1B	2.96	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B5	203	PEB	CHB-C1C	2.96	1.47	1.40
82	pK	202	PEB	C4B-C3B	2.96	1.50	1.45
82	iE	201	PEB	OD-C4D	2.96	1.29	1.23
87	AL	403	CLA	CMD-C2D	-2.96	1.44	1.50
82	HI	202	PEB	C1A-NA	-2.96	1.33	1.37
82	pC	202	PEB	C2A-C1A	-2.96	1.49	1.52
82	JQ	202	PEB	OD-C4D	2.96	1.29	1.23
82	VD	203	PEB	CHA-C1B	2.96	1.47	1.40
82	U5	202	PEB	CHA-C1B	2.96	1.47	1.40
87	A2	827	CLA	C4B-NB	2.96	1.41	1.37
87	7N	602	CLA	C3B-C4B	2.96	1.49	1.42
84	D3	1001	CYC	C3D-C2D	2.96	1.46	1.38
82	lF	201	PEB	OD-C4D	2.96	1.29	1.23
82	aH	201	PEB	OD-C4D	2.96	1.29	1.23
82	AF	201	PEB	C2A-C1A	-2.96	1.49	1.52
82	jG	201	PEB	C2A-C1A	-2.96	1.49	1.52
82	JA	203	PEB	CHB-C1C	2.96	1.47	1.40
82	JK	202	PEB	CHB-C1C	2.96	1.47	1.40
82	LK	202	PEB	C1C-NC	-2.96	1.32	1.37
82	Z1	203	PEB	OD-C4D	2.96	1.29	1.23
87	LN	204	CLA	C4B-NB	2.96	1.41	1.37
82	OI	202	PEB	OD-C4D	2.96	1.29	1.23
82	HQ	202	PEB	C2A-C1A	-2.96	1.49	1.52
87	12	606	CLA	C4B-NB	2.96	1.41	1.37
82	ED	201	PEB	C2C-C3C	2.96	1.46	1.38
82	F5	203	PEB	C2C-C3C	2.96	1.46	1.38
82	D7	203	PEB	CHB-C1C	2.96	1.47	1.40
87	62	307	CLA	C4D-ND	-2.96	1.33	1.37
82	W7	201	PEB	C2C-C3C	2.96	1.46	1.38
82	eE	203	PEB	C2A-C1A	-2.96	1.49	1.52
87	BN	829	CLA	C4B-NB	2.96	1.41	1.37
87	A2	818	CLA	C4B-NB	2.96	1.41	1.37
82	VI	201	PEB	C1C-NC	-2.95	1.32	1.37
87	72	609	CLA	C4D-ND	-2.95	1.33	1.37
87	1N	605	CLA	C4D-ND	-2.95	1.33	1.37
82	GM	203	PEB	C2C-C3C	2.95	1.46	1.38
82	PE	201	PEB	CHB-C1C	2.95	1.47	1.40
87	BN	806	CLA	C3B-C4B	2.95	1.49	1.42
82	JJ	201	PEB	CHC-C4C	2.95	1.53	1.49
82	KD	202	PEB	C1A-NA	-2.95	1.33	1.37
87	B2	824	CLA	C4D-ND	-2.95	1.33	1.37
87	6N	603	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	d3	1001	CYC	C3D-C2D	2.95	1.46	1.38
87	L2	202	CLA	C4B-NB	2.95	1.41	1.37
82	LD	201	PEB	CHA-C1B	2.95	1.47	1.40
87	A2	814	CLA	C4B-NB	2.95	1.41	1.37
87	c6	616	CLA	C4B-NB	2.95	1.41	1.37
87	A2	827	CLA	C3B-C4B	2.95	1.49	1.42
82	LA	202	PEB	CHA-C1B	2.95	1.47	1.40
87	AN	817	CLA	C4B-NB	2.95	1.41	1.37
87	M2	101	CLA	C4B-NB	2.95	1.41	1.37
82	kG	201	PEB	C2A-C1A	-2.95	1.49	1.52
82	JA	202	PEB	CHA-C1B	2.95	1.47	1.40
87	AN	821	CLA	C4D-ND	-2.95	1.33	1.37
82	b1	203	PEB	C2C-C3C	2.95	1.46	1.38
82	KQ	202	PEB	C1A-NA	-2.95	1.33	1.37
82	jG	202	PEB	OD-C4D	2.95	1.29	1.23
87	BL	602	CLA	C4B-NB	2.95	1.41	1.37
87	42	607	CLA	C4B-NB	2.95	1.41	1.37
87	2N	309	CLA	C4B-NB	2.95	1.41	1.37
82	CD	201	PEB	CHB-C1C	2.95	1.47	1.40
82	TI	203	PEB	CHA-C1B	2.95	1.47	1.40
87	A2	841	CLA	CMB-C2B	-2.95	1.44	1.50
87	8N	305	CLA	C4B-NB	2.95	1.41	1.37
87	8N	308	CLA	C1D-ND	2.95	1.41	1.37
82	GA	202	PEB	OD-C4D	2.95	1.29	1.23
84	f3	1001	CYC	C3D-C2D	2.95	1.46	1.38
82	gK	202	PEB	OD-C4D	2.95	1.29	1.23
82	RO	201	PEB	CHB-C1C	2.95	1.47	1.40
82	eJ	201	PEB	CHB-C1C	2.95	1.47	1.40
82	aF	201	PEB	CHA-C1B	2.95	1.47	1.40
82	sK	203	PEB	OD-C4D	2.95	1.29	1.23
82	F5	202	PEB	C2C-C3C	2.95	1.46	1.38
87	AN	841	CLA	CMB-C2B	-2.95	1.44	1.50
87	AN	835	CLA	C3B-C4B	2.95	1.49	1.42
87	72	602	CLA	C3B-C4B	2.95	1.49	1.42
82	Z1	202	PEB	CHA-C1B	2.95	1.47	1.40
82	F5	203	PEB	CHB-C1C	2.95	1.47	1.40
87	FN	203	CLA	C4B-NB	2.95	1.41	1.37
82	QJ	202	PEB	C2C-C3C	2.94	1.46	1.38
82	Y1	202	PEB	OD-C4D	2.94	1.29	1.23
87	62	304	CLA	C4D-ND	-2.94	1.33	1.37
82	D5	201	PEB	C1C-NC	-2.94	1.32	1.37
87	12	604	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VA	203	PEB	OD-C4D	2.94	1.29	1.23
82	qF	202	PEB	OD-C4D	2.94	1.29	1.23
87	AN	811	CLA	CMB-C2B	-2.94	1.44	1.50
87	AN	827	CLA	C3B-C4B	2.94	1.49	1.42
87	cL	507	CLA	C3B-C4B	2.94	1.49	1.42
87	A2	812	CLA	C4D-ND	-2.94	1.33	1.37
82	zC	201	PEB	OD-C4D	2.94	1.29	1.23
82	iF	203	PEB	OD-C4D	2.94	1.29	1.23
87	4N	611	CLA	C3B-C4B	2.94	1.49	1.42
82	OJ	203	PEB	CHA-C1B	2.94	1.47	1.40
82	O1	203	PEB	C2C-C3C	2.94	1.46	1.38
82	NI	201	PEB	C1C-NC	-2.94	1.32	1.37
82	dF	201	PEB	C2A-C1A	-2.94	1.49	1.52
87	62	313	CLA	C1B-C2B	2.94	1.50	1.43
82	a1	202	PEB	OD-C4D	2.94	1.29	1.23
82	hO	201	PEB	CHA-C1B	2.94	1.47	1.40
87	MN	101	CLA	C4B-NB	2.94	1.41	1.37
82	XQ	203	PEB	OD-C4D	2.94	1.29	1.23
82	XK	203	PEB	CHB-C1C	2.94	1.47	1.40
82	AH	302	PEB	OD-C4D	2.94	1.29	1.23
82	IJ	203	PEB	C1C-C2C	2.94	1.49	1.42
87	BL	622	CLA	C4D-ND	-2.94	1.33	1.37
82	kH	203	PEB	C2C-C3C	2.94	1.46	1.38
82	DG	1002	PEB	C2A-C1A	-2.94	1.49	1.52
82	Q1	203	PEB	OD-C4D	2.94	1.29	1.23
87	4N	607	CLA	C4B-NB	2.94	1.41	1.37
82	YK	202	PEB	OD-C4D	2.94	1.29	1.23
82	iF	201	PEB	C2C-C3C	2.94	1.46	1.38
82	aK	201	PEB	C4B-C3B	2.94	1.50	1.45
87	BN	811	CLA	C4B-NB	2.94	1.41	1.37
87	52	604	CLA	C4B-NB	2.94	1.41	1.37
82	UM	203	PEB	OD-C4D	2.94	1.29	1.23
82	F9	201	PEB	C2A-C1A	-2.94	1.49	1.52
82	eM	201	PEB	C2A-C1A	-2.94	1.49	1.52
87	A2	836	CLA	C3B-C4B	2.94	1.49	1.42
84	O3	1001	CYC	C3D-C2D	2.94	1.46	1.38
82	YA	301	PEB	C1C-NC	-2.94	1.32	1.37
87	CL	509	CLA	C1D-ND	2.94	1.41	1.37
87	B2	820	CLA	C3B-C4B	2.94	1.49	1.42
82	XF	203	PEB	C1C-NC	-2.94	1.32	1.37
82	m4	201	PEB	C2A-C1A	-2.94	1.49	1.52
82	WH	201	PEB	CHA-C1B	2.94	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	819	CLA	C4B-NB	2.94	1.41	1.37
82	G7	202	PEB	OD-C4D	2.94	1.29	1.23
87	B6	606	CLA	C4B-NB	2.94	1.41	1.37
87	bL	613	CLA	C4B-NB	2.94	1.41	1.37
82	AI	201	PEB	C1C-NC	-2.94	1.32	1.37
82	M9	304	PEB	OD-C4D	2.94	1.29	1.23
82	kG	201	PEB	C1C-C2C	2.94	1.49	1.42
87	72	604	CLA	C4D-ND	-2.94	1.33	1.37
82	DA	201	PEB	C2A-C1A	-2.94	1.49	1.52
82	CD	202	PEB	C2A-C1A	-2.94	1.49	1.52
82	Z5	304	PEB	C2A-C1A	-2.94	1.49	1.52
82	UJ	201	PEB	CHA-C1B	2.94	1.47	1.40
82	VA	201	PEB	C2C-C3C	2.93	1.46	1.38
87	22	609	CLA	C4B-NB	2.93	1.41	1.37
87	82	305	CLA	C3B-C4B	2.93	1.49	1.42
96	FL	102	HEM	C1C-C2C	-2.93	1.39	1.45
82	A7	201	PEB	C4B-C3B	2.93	1.50	1.45
82	pC	201	PEB	OD-C4D	2.93	1.29	1.23
87	BL	609	CLA	C3B-C4B	2.93	1.49	1.42
82	HB	203	PEB	C2A-C1A	-2.93	1.49	1.52
82	ZH	203	PEB	OD-C4D	2.93	1.29	1.23
82	Z9	303	PEB	OD-C4D	2.93	1.29	1.23
82	W1	201	PEB	CHA-C1B	2.93	1.47	1.40
87	BN	834	CLA	C4B-NB	2.93	1.41	1.37
84	B3	1001	CYC	C3D-C2D	2.93	1.46	1.38
87	6N	610	CLA	C4D-ND	-2.93	1.33	1.37
82	SA	202	PEB	CHA-C1B	2.93	1.47	1.40
87	A2	828	CLA	C3B-C4B	2.93	1.49	1.42
82	M7	202	PEB	OD-C4D	2.93	1.29	1.23
82	jE	201	PEB	OD-C4D	2.93	1.29	1.23
82	cF	201	PEB	OD-C4D	2.93	1.29	1.23
82	fF	202	PEB	OD-C4D	2.93	1.29	1.23
82	PI	201	PEB	C1C-NC	-2.93	1.32	1.37
82	JP	201	PEB	C4B-C3B	2.93	1.50	1.45
82	UM	201	PEB	C2C-C3C	2.93	1.46	1.38
87	4N	610	CLA	C4D-ND	-2.93	1.33	1.37
82	gF	202	PEB	OD-C4D	2.93	1.29	1.23
82	GI	202	PEB	C1C-NC	-2.93	1.32	1.37
87	B6	613	CLA	C4B-NB	2.93	1.41	1.37
82	uF	201	PEB	C1A-NA	-2.93	1.33	1.37
82	VD	203	PEB	C2C-C3C	2.93	1.46	1.38
82	W5	203	PEB	C2C-C3C	2.93	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	825	CLA	C4D-ND	-2.93	1.33	1.37
82	h4	201	PEB	CHA-C1B	2.93	1.47	1.40
87	22	605	CLA	CMB-C2B	-2.93	1.44	1.50
82	BB	201	PEB	C2A-C1A	-2.93	1.49	1.52
82	hF	201	PEB	C2A-C1A	-2.93	1.49	1.52
82	eK	201	PEB	OD-C4D	2.93	1.29	1.23
87	2N	302	CLA	C4D-ND	-2.93	1.33	1.37
82	M7	201	PEB	C2C-C3C	2.93	1.46	1.38
84	DG	1001	CYC	C3D-C2D	2.93	1.46	1.38
82	aO	202	PEB	C2A-C1A	-2.93	1.49	1.52
87	bL	618	CLA	CMD-C2D	-2.93	1.44	1.50
82	TQ	201	PEB	C1A-NA	-2.93	1.33	1.37
87	12	603	CLA	C4B-NB	2.93	1.41	1.37
87	K2	103	CLA	C1D-ND	2.93	1.41	1.37
82	OH	201	PEB	OD-C4D	2.93	1.29	1.23
87	5N	605	CLA	C4D-ND	-2.93	1.33	1.37
87	b6	605	CLA	C1B-C2B	2.93	1.50	1.43
82	XF	203	PEB	CHB-C1C	2.93	1.47	1.40
82	18	202	PEB	C4B-C3B	2.93	1.50	1.45
82	k1	202	PEB	C1A-NA	-2.93	1.33	1.37
82	rC	202	PEB	C1A-NA	-2.93	1.33	1.37
82	J5	203	PEB	C2C-C3C	2.93	1.46	1.38
87	AN	828	CLA	C3B-C4B	2.93	1.49	1.42
82	OA	201	PEB	C4A-NA	-2.93	1.31	1.37
82	WK	201	PEB	C2C-C3C	2.93	1.46	1.38
87	BL	608	CLA	C4B-NB	2.93	1.41	1.37
87	BL	623	CLA	C4B-NB	2.93	1.41	1.37
87	A2	849	CLA	C4B-NB	2.93	1.41	1.37
87	L2	204	CLA	C4B-NB	2.93	1.41	1.37
83	KA	203	PUB	OA-C1A	2.93	1.29	1.23
87	42	609	CLA	C4D-ND	-2.93	1.33	1.37
87	A2	838	CLA	C4B-NB	2.93	1.41	1.37
87	K6	101	CLA	C4B-NB	2.93	1.41	1.37
87	62	311	CLA	C4D-ND	-2.93	1.33	1.37
82	SI	201	PEB	C2C-C3C	2.93	1.46	1.38
82	S5	202	PEB	C2C-C3C	2.93	1.46	1.38
82	JF	202	PEB	CHB-C1C	2.93	1.47	1.40
82	W5	202	PEB	CHA-C1B	2.93	1.47	1.40
82	GI	201	PEB	C1A-NA	-2.93	1.33	1.37
87	A2	819	CLA	CMC-C2C	-2.92	1.44	1.50
87	22	611	CLA	C4D-ND	-2.92	1.33	1.37
82	zF	501	PEB	C1A-NA	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gK	203	PEB	C2C-C3C	2.92	1.46	1.38
82	RQ	203	PEB	OD-C4D	2.92	1.29	1.23
82	TI	202	PEB	C1C-NC	-2.92	1.32	1.37
87	2N	301	CLA	CMB-C2B	-2.92	1.44	1.50
87	C6	515	CLA	C4B-NB	2.92	1.41	1.37
82	LF	202	PEB	C1C-NC	-2.92	1.32	1.37
87	8N	306	CLA	C3B-C4B	2.92	1.49	1.42
82	ZH	201	PEB	OD-C4D	2.92	1.29	1.23
82	wC	203	PEB	C1A-NA	-2.92	1.33	1.37
84	y3	1001	CYC	C1B-C2B	2.92	1.50	1.45
87	CL	513	CLA	C4D-ND	-2.92	1.33	1.37
82	Y7	301	PEB	C1C-NC	-2.92	1.32	1.37
83	Z9	302	PUB	OA-C1A	2.92	1.29	1.23
82	FA	202	PEB	CHA-C1B	2.92	1.47	1.40
82	S7	202	PEB	CHB-C1C	2.92	1.47	1.40
87	32	310	CLA	C4D-ND	-2.92	1.33	1.37
82	WQ	201	PEB	OD-C4D	2.92	1.29	1.23
82	rF	202	PEB	OD-C4D	2.92	1.29	1.23
87	HL	102	CLA	C4B-NB	2.92	1.41	1.37
82	MQ	201	PEB	C2A-C1A	-2.92	1.49	1.52
82	c1	202	PEB	C2A-C1A	-2.92	1.49	1.52
82	O7	201	PEB	C4A-NA	-2.92	1.31	1.37
82	LJ	201	PEB	CHB-C1C	2.92	1.47	1.40
82	IP	202	PEB	CHB-C1C	2.92	1.47	1.40
82	cK	201	PEB	OD-C4D	2.92	1.29	1.23
87	4N	602	CLA	C3B-C4B	2.92	1.49	1.42
82	O1	201	PEB	OD-C4D	2.92	1.29	1.23
82	SA	202	PEB	CHB-C1C	2.92	1.47	1.40
82	F5	203	PEB	C2A-C1A	-2.92	1.49	1.52
82	A1	301	PEB	C1A-NA	-2.92	1.33	1.37
82	CJ	203	PEB	CHA-C1B	2.92	1.47	1.40
87	A2	811	CLA	CMB-C2B	-2.92	1.44	1.50
82	EK	202	PEB	OD-C4D	2.92	1.29	1.23
82	c1	201	PEB	OD-C4D	2.92	1.29	1.23
82	hF	202	PEB	OD-C4D	2.92	1.29	1.23
87	82	302	CLA	C1D-ND	2.92	1.41	1.37
87	BN	821	CLA	C3B-C4B	2.92	1.49	1.42
87	3N	305	CLA	C4D-ND	-2.92	1.33	1.37
82	F7	202	PEB	C2C-C3C	2.92	1.46	1.38
87	BN	801	CLA	C4B-NB	2.92	1.41	1.37
82	qC	203	PEB	OD-C4D	2.92	1.29	1.23
82	e4	202	PEB	C2C-C3C	2.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	22	607	CLA	C4D-ND	-2.92	1.33	1.37
82	XD	203	PEB	OD-C4D	2.92	1.29	1.23
87	1N	603	CLA	C4B-NB	2.92	1.41	1.37
82	QG	201	PEB	CHA-C1B	2.92	1.47	1.40
82	IJ	201	PEB	CHA-C1B	2.92	1.47	1.40
82	VF	202	PEB	C2A-C1A	-2.92	1.49	1.52
82	eG	203	PEB	C2A-C1A	-2.92	1.49	1.52
82	PQ	201	PEB	OD-C4D	2.92	1.29	1.23
82	F9	202	PEB	OD-C4D	2.92	1.29	1.23
87	CL	518	CLA	C3B-C4B	2.92	1.49	1.42
83	xK	301	PUB	C3B-C2B	2.92	1.46	1.38
84	y3	1001	CYC	C4C-NC	-2.92	1.31	1.37
82	SE	201	PEB	C2A-C1A	-2.92	1.49	1.52
82	VK	202	PEB	C2A-C1A	-2.92	1.49	1.52
82	W7	201	PEB	C2A-C1A	-2.92	1.49	1.52
82	XI	202	PEB	OD-C4D	2.92	1.29	1.23
82	wC	202	PEB	CHC-C4C	2.92	1.53	1.49
82	MJ	201	PEB	CHA-C1B	2.92	1.47	1.40
82	t8	201	PEB	OD-C4D	2.92	1.29	1.23
83	K7	203	PUB	OA-C1A	2.92	1.29	1.23
82	DA	203	PEB	CHB-C1C	2.92	1.47	1.40
87	62	309	CLA	CMB-C2B	-2.92	1.44	1.50
82	RD	203	PEB	CHC-C4C	2.92	1.53	1.49
82	RQ	203	PEB	CHC-C4C	2.92	1.53	1.49
82	NI	202	PEB	OD-C4D	2.92	1.29	1.23
87	c6	610	CLA	C4B-NB	2.92	1.41	1.37
82	OK	201	PEB	C2C-C3C	2.92	1.46	1.38
82	ZG	201	PEB	C2A-C1A	-2.91	1.49	1.52
82	S9	201	PEB	C2A-C1A	-2.91	1.49	1.52
96	E6	101	HEM	C3B-C4B	2.91	1.50	1.44
82	GJ	203	PEB	CHA-C1B	2.91	1.47	1.40
82	jG	201	PEB	OD-C4D	2.91	1.29	1.23
87	62	311	CLA	C3B-C4B	2.91	1.49	1.42
84	V3	1001	CYC	C4D-ND	-2.91	1.32	1.37
82	GK	202	PEB	C3B-C2B	2.91	1.42	1.36
82	JB	201	PEB	C2C-C3C	2.91	1.46	1.38
87	6N	612	CLA	C1B-C2B	2.91	1.50	1.43
82	HB	201	PEB	C2A-C1A	-2.91	1.49	1.52
82	a4	203	PEB	C2A-C1A	-2.91	1.49	1.52
82	QE	201	PEB	CHA-C1B	2.91	1.47	1.40
87	BN	820	CLA	C4B-NB	2.91	1.41	1.37
87	c6	605	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	W3	1001	CYC	C1B-C2B	2.91	1.50	1.45
87	12	603	CLA	C4D-ND	-2.91	1.33	1.37
82	SB	203	PEB	C2C-C3C	2.91	1.46	1.38
87	6N	610	CLA	C3B-C4B	2.91	1.49	1.42
82	PD	203	PEB	OD-C4D	2.91	1.29	1.23
84	L4	1001	CYC	C4B-NB	-2.91	1.31	1.38
82	JK	202	PEB	C2A-C1A	-2.91	1.49	1.52
82	rF	201	PEB	C2A-C1A	-2.91	1.49	1.52
82	gH	202	PEB	C2A-C1A	-2.91	1.49	1.52
82	WI	202	PEB	C1D-ND	2.91	1.50	1.45
87	6N	602	CLA	C3B-C4B	2.91	1.49	1.42
82	gH	201	PEB	OD-C4D	2.91	1.29	1.23
82	cH	201	PEB	OD-C4D	2.91	1.29	1.23
87	AN	849	CLA	C4B-NB	2.91	1.41	1.37
87	BN	812	CLA	C4B-NB	2.91	1.41	1.37
87	cL	505	CLA	C4B-NB	2.91	1.41	1.37
87	22	601	CLA	C4D-ND	-2.91	1.33	1.37
87	7N	604	CLA	C4D-ND	-2.91	1.33	1.37
82	aO	203	PEB	C2A-C1A	-2.91	1.49	1.52
82	b1	203	PEB	OD-C4D	2.91	1.29	1.23
87	AN	813	CLA	C4B-NB	2.91	1.41	1.37
87	AN	835	CLA	C4B-NB	2.91	1.41	1.37
82	ND	204	PEB	CHC-C4C	2.91	1.53	1.49
82	BQ	201	PEB	C2C-C3C	2.91	1.46	1.38
87	6N	608	CLA	CMB-C2B	-2.91	1.44	1.50
87	BN	822	CLA	C4B-NB	2.91	1.41	1.37
82	CB	201	PEB	OD-C4D	2.91	1.29	1.23
84	J1	1001	CYC	C3D-C2D	2.91	1.46	1.38
82	g1	201	PEB	OD-C4D	2.91	1.29	1.23
82	kH	202	PEB	OD-C4D	2.91	1.29	1.23
87	A2	813	CLA	C4B-NB	2.91	1.41	1.37
82	L9	202	PEB	C4B-C3B	2.91	1.50	1.45
82	OJ	202	PEB	OD-C4D	2.91	1.29	1.23
82	p8	201	PEB	OD-C4D	2.91	1.29	1.23
87	c6	608	CLA	C4B-NB	2.91	1.41	1.37
82	LQ	203	PEB	OD-C4D	2.91	1.29	1.23
82	O9	202	PEB	OD-C4D	2.91	1.29	1.23
82	dJ	201	PEB	C2C-C3C	2.91	1.46	1.38
82	BM	301	PEB	C1C-C2C	2.91	1.49	1.42
82	JQ	203	PEB	CHA-C1B	2.91	1.47	1.40
82	L7	202	PEB	CHA-C1B	2.91	1.47	1.40
82	YM	203	PEB	OD-C4D	2.91	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	xK	302	PEB	OD-C4D	2.91	1.29	1.23
82	e4	203	PEB	C1A-NA	-2.91	1.33	1.37
87	cL	515	CLA	C4D-ND	-2.91	1.33	1.37
82	iO	203	PEB	OD-C4D	2.91	1.29	1.23
87	BN	818	CLA	C4B-NB	2.91	1.41	1.37
87	52	602	CLA	C4B-NB	2.91	1.41	1.37
84	W3	1001	CYC	C4C-NC	-2.91	1.31	1.37
87	AN	812	CLA	C4D-ND	-2.91	1.33	1.37
82	L9	202	PEB	OD-C4D	2.91	1.29	1.23
82	xF	303	PEB	OD-C4D	2.91	1.29	1.23
87	42	602	CLA	C3B-C4B	2.91	1.49	1.42
82	Z9	301	PEB	CHB-C1C	2.91	1.47	1.40
87	B6	603	CLA	C4B-NB	2.91	1.41	1.37
82	PI	202	PEB	OD-C4D	2.91	1.29	1.23
82	iO	202	PEB	C2C-C3C	2.91	1.46	1.38
82	SD	201	PEB	C2A-C1A	-2.91	1.49	1.52
82	Y7	301	PEB	C1A-NA	-2.91	1.33	1.37
82	W1	203	PEB	C2C-C3C	2.91	1.46	1.38
82	eF	201	PEB	CHA-C1B	2.91	1.47	1.40
82	e1	201	PEB	OD-C4D	2.91	1.29	1.23
87	L2	203	CLA	C4B-NB	2.91	1.41	1.37
82	NG	201	PEB	C2A-C1A	-2.90	1.49	1.52
82	nF	202	PEB	CHC-C4C	2.90	1.53	1.49
87	bL	621	CLA	C4B-NB	2.90	1.41	1.37
82	CK	203	PEB	OD-C4D	2.90	1.29	1.23
82	dE	201	PEB	OD-C4D	2.90	1.29	1.23
82	eH	203	PEB	OD-C4D	2.90	1.29	1.23
87	A2	810	CLA	C4D-ND	-2.90	1.33	1.37
87	BL	622	CLA	C4B-NB	2.90	1.41	1.37
87	A2	819	CLA	C4B-NB	2.90	1.41	1.37
87	B2	822	CLA	C1D-ND	2.90	1.41	1.37
87	6N	606	CLA	C4D-ND	-2.90	1.33	1.37
82	LB	201	PEB	C2A-C1A	-2.90	1.49	1.52
82	XM	201	PEB	C2A-C1A	-2.90	1.49	1.52
82	rK	201	PEB	C2A-C1A	-2.90	1.49	1.52
87	42	603	CLA	C3B-C4B	2.90	1.49	1.42
84	LO	1001	CYC	C3D-C2D	2.90	1.46	1.38
84	L4	1001	CYC	C3D-C2D	2.90	1.46	1.38
82	dK	201	PEB	OD-C4D	2.90	1.29	1.23
82	IJ	201	PEB	C2C-C3C	2.90	1.46	1.38
82	nF	201	PEB	C2A-C1A	-2.90	1.49	1.52
82	BA	203	PEB	OD-C4D	2.90	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	819	CLA	C1D-ND	2.90	1.41	1.37
82	OH	203	PEB	C2C-C3C	2.90	1.46	1.38
82	V7	201	PEB	C2C-C3C	2.90	1.46	1.38
82	U9	202	PEB	C2C-C3C	2.90	1.46	1.38
82	wF	302	PEB	OD-C4D	2.90	1.29	1.23
82	S5	203	PEB	C2A-C1A	-2.90	1.49	1.52
82	MA	202	PEB	OD-C4D	2.90	1.29	1.23
82	qC	202	PEB	OD-C4D	2.90	1.29	1.23
82	M9	302	PEB	CHB-C1C	2.90	1.47	1.40
82	WA	201	PEB	C2C-C3C	2.90	1.46	1.38
82	UJ	201	PEB	C2C-C3C	2.90	1.46	1.38
87	AN	841	CLA	C1D-ND	2.90	1.41	1.37
87	5N	604	CLA	C4B-NB	2.90	1.41	1.37
82	i4	202	PEB	C2C-C3C	2.90	1.46	1.38
82	TD	201	PEB	C1A-NA	-2.90	1.33	1.37
82	GI	203	PEB	OD-C4D	2.90	1.29	1.23
82	aK	203	PEB	OD-C4D	2.90	1.29	1.23
87	AN	825	CLA	C3B-C4B	2.90	1.49	1.42
87	B2	829	CLA	C4B-NB	2.90	1.41	1.37
82	B7	203	PEB	OD-C4D	2.90	1.29	1.23
82	TB	202	PEB	CHA-C1B	2.90	1.47	1.40
87	2N	307	CLA	C4D-ND	-2.90	1.33	1.37
82	XD	201	PEB	OD-C4D	2.90	1.29	1.23
82	AO	305	PEB	OD-C4D	2.90	1.29	1.23
82	QE	202	PEB	C2A-C1A	-2.90	1.49	1.52
82	GE	1002	PEB	C2C-C3C	2.90	1.46	1.38
87	A2	817	CLA	C4B-NB	2.90	1.41	1.37
87	7N	601	CLA	C4D-ND	-2.90	1.33	1.37
84	x3	1001	CYC	C4D-ND	-2.90	1.33	1.37
82	Q9	202	PEB	OD-C4D	2.90	1.29	1.23
82	eJ	201	PEB	C2A-C1A	-2.90	1.49	1.52
87	7N	609	CLA	C4D-ND	-2.90	1.33	1.37
82	GP	203	PEB	OD-C4D	2.90	1.29	1.23
82	R9	202	PEB	OD-C4D	2.90	1.29	1.23
82	HA	202	PEB	OD-C4D	2.90	1.29	1.23
82	PD	201	PEB	OD-C4D	2.90	1.29	1.23
82	l1	201	PEB	C2C-C3C	2.90	1.46	1.38
82	tK	202	PEB	CHC-C4C	2.90	1.53	1.49
82	DI	201	PEB	C2A-C1A	-2.90	1.49	1.52
82	fB	301	PEB	C2A-C1A	-2.90	1.49	1.52
82	KJ	202	PEB	C2C-C3C	2.90	1.46	1.38
82	FF	202	PEB	CHB-C1C	2.90	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MP	202	PEB	OD-C4D	2.90	1.29	1.23
82	aM	203	PEB	C1C-C2C	2.90	1.49	1.42
87	BN	821	CLA	C4B-NB	2.90	1.41	1.37
87	B2	827	CLA	C1D-ND	2.90	1.41	1.37
87	62	308	CLA	C4D-ND	-2.90	1.33	1.37
82	qF	202	PEB	C2C-C3C	2.90	1.46	1.38
82	l1	201	PEB	OD-C4D	2.90	1.29	1.23
82	Q5	203	PEB	CHB-C1C	2.90	1.47	1.40
87	62	306	CLA	C4D-ND	-2.89	1.33	1.37
87	bL	617	CLA	CMC-C2C	-2.89	1.44	1.50
82	OM	203	PEB	C2A-C1A	-2.89	1.49	1.52
87	b6	611	CLA	C3B-C4B	2.89	1.49	1.42
82	RI	202	PEB	OD-C4D	2.89	1.29	1.23
82	GQ	202	PEB	OD-C4D	2.89	1.29	1.23
82	TB	201	PEB	C2C-C3C	2.89	1.46	1.38
82	lF	203	PEB	C1A-NA	-2.89	1.33	1.37
82	UA	201	PEB	C2C-C3C	2.89	1.46	1.38
87	BN	827	CLA	C1D-ND	2.89	1.41	1.37
87	B6	614	CLA	C4B-NB	2.89	1.41	1.37
83	xK	305	PUB	OA-C1A	2.89	1.29	1.23
82	xK	304	PEB	C1A-NA	-2.89	1.33	1.37
87	BL	621	CLA	CMB-C2B	-2.89	1.44	1.50
82	Y9	202	PEB	OD-C4D	2.89	1.29	1.23
82	LD	202	PEB	C2A-C1A	-2.89	1.49	1.52
87	LN	203	CLA	C4B-NB	2.89	1.41	1.37
87	B2	811	CLA	C4B-NB	2.89	1.41	1.37
82	VI	202	PEB	OD-C4D	2.89	1.29	1.23
82	HA	201	PEB	OD-C4D	2.89	1.29	1.23
82	q8	202	PEB	OD-C4D	2.89	1.29	1.23
82	eO	202	PEB	C2C-C3C	2.89	1.46	1.38
82	FQ	201	PEB	C2C-C3C	2.89	1.46	1.38
87	22	601	CLA	C1B-C2B	2.89	1.50	1.43
82	OH	202	PEB	OD-C4D	2.89	1.29	1.23
82	KI	203	PEB	OD-C4D	2.89	1.29	1.23
82	NI	203	PEB	C2C-C3C	2.89	1.46	1.38
82	ID	202	PEB	C2A-C1A	-2.89	1.49	1.52
87	C6	519	CLA	C4B-NB	2.89	1.41	1.37
87	1N	603	CLA	C3B-C4B	2.89	1.49	1.42
87	32	304	CLA	C4D-ND	-2.89	1.33	1.37
83	M9	303	PUB	OA-C1A	2.89	1.29	1.23
82	WF	201	PEB	OD-C4D	2.89	1.29	1.23
87	1N	609	CLA	C4D-ND	-2.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	YB	201	PEB	OD-C4D	2.89	1.29	1.23
82	jM	201	PEB	OD-C4D	2.89	1.29	1.23
82	CQ	201	PEB	CHB-C1C	2.89	1.47	1.40
87	BL	620	CLA	C4B-NB	2.89	1.41	1.37
87	AN	838	CLA	C4B-NB	2.89	1.41	1.37
87	A2	825	CLA	C3B-C4B	2.89	1.49	1.42
82	JD	203	PEB	CHA-C1B	2.89	1.47	1.40
82	MF	202	PEB	C2A-C1A	-2.89	1.49	1.52
82	W1	201	PEB	OD-C4D	2.89	1.29	1.23
84	p3	1001	CYC	C4B-NB	-2.89	1.31	1.38
87	42	610	CLA	C4D-ND	-2.89	1.33	1.37
87	3N	307	CLA	C4B-NB	2.89	1.41	1.37
82	JP	202	PEB	C2A-C1A	-2.89	1.49	1.52
87	b6	616	CLA	C4B-NB	2.89	1.41	1.37
82	fM	202	PEB	OD-C4D	2.89	1.29	1.23
83	AG	302	PUB	OD-C4D	2.89	1.29	1.23
82	Y5	201	PEB	C1C-NC	-2.89	1.33	1.37
87	6N	605	CLA	C4D-ND	-2.89	1.33	1.37
82	II	202	PEB	OD-C4D	2.89	1.29	1.23
82	TP	202	PEB	OD-C4D	2.89	1.29	1.23
87	BN	816	CLA	C3B-C4B	2.89	1.49	1.42
82	cF	201	PEB	CHA-C1B	2.89	1.47	1.40
96	G2	201	HEM	FE-NB	2.89	2.03	1.94
82	PB	201	PEB	C2C-C3C	2.89	1.46	1.38
87	bL	617	CLA	C4B-NB	2.89	1.41	1.37
87	B2	823	CLA	C3B-C4B	2.89	1.49	1.42
87	6N	611	CLA	C3B-C4B	2.88	1.49	1.42
82	WK	201	PEB	OD-C4D	2.88	1.29	1.23
83	AD	302	PUB	OA-C1A	2.88	1.29	1.23
87	BN	832	CLA	C4B-NB	2.88	1.41	1.37
87	42	611	CLA	C3B-C4B	2.88	1.49	1.42
82	RB	201	PEB	OD-C4D	2.88	1.29	1.23
82	k4	201	PEB	OD-C4D	2.88	1.29	1.23
82	hO	202	PEB	OD-C4D	2.88	1.29	1.23
83	xF	306	PUB	OA-C1A	2.88	1.29	1.23
82	NJ	201	PEB	C2C-C3C	2.88	1.46	1.38
82	QP	202	PEB	C2C-C3C	2.88	1.46	1.38
87	AN	819	CLA	CMC-C2C	-2.88	1.44	1.50
87	12	603	CLA	C3B-C4B	2.88	1.49	1.42
82	DB	203	PEB	CHB-C1C	2.88	1.47	1.40
87	7N	606	CLA	C4B-NB	2.88	1.41	1.37
82	NK	202	PEB	C2A-C1A	-2.88	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	c4	203	PEB	OD-C4D	2.88	1.29	1.23
82	GF	202	PEB	C3B-C2B	2.88	1.42	1.36
82	eE	203	PEB	C1C-C2C	2.88	1.49	1.42
87	12	610	CLA	C3B-C4B	2.88	1.49	1.42
87	C6	512	CLA	C4B-NB	2.88	1.41	1.37
82	GK	202	PEB	CMB-C2B	-2.88	1.44	1.50
82	eK	201	PEB	CHA-C1B	2.88	1.47	1.40
82	GD	202	PEB	OD-C4D	2.88	1.29	1.23
82	O4	202	PEB	OD-C4D	2.88	1.29	1.23
82	OM	203	PEB	C2C-C3C	2.88	1.46	1.38
82	U5	201	PEB	C4D-ND	2.88	1.39	1.35
82	EI	202	PEB	OD-C4D	2.88	1.29	1.23
87	B2	825	CLA	C4B-NB	2.88	1.41	1.37
82	mK	201	PEB	OD-C4D	2.88	1.29	1.23
82	HI	201	PEB	C2A-C1A	-2.88	1.49	1.52
82	EJ	201	PEB	CHA-C1B	2.88	1.47	1.40
87	52	605	CLA	C4D-ND	-2.88	1.33	1.37
83	xF	301	PUB	C3B-C2B	2.88	1.46	1.38
82	MQ	202	PEB	OD-C4D	2.88	1.29	1.23
82	U9	201	PEB	OD-C4D	2.88	1.29	1.23
87	B2	815	CLA	C3B-C4B	2.88	1.49	1.42
82	O1	203	PEB	CHA-C1B	2.88	1.47	1.40
82	EP	202	PEB	OD-C4D	2.88	1.29	1.23
82	a1	201	PEB	OD-C4D	2.88	1.29	1.23
82	kH	203	PEB	OD-C4D	2.88	1.29	1.23
82	SM	201	PEB	C2A-C1A	-2.88	1.49	1.52
82	NI	203	PEB	C1D-ND	2.88	1.50	1.45
82	YH	202	PEB	OD-C4D	2.88	1.29	1.23
82	D9	202	PEB	OD-C4D	2.88	1.29	1.23
82	JB	202	PEB	CHA-C1B	2.88	1.47	1.40
87	6N	607	CLA	C4D-ND	-2.88	1.33	1.37
87	A2	835	CLA	C4B-NB	2.88	1.41	1.37
87	BN	823	CLA	MG-NB	-2.88	2.00	2.05
82	ZB	203	PEB	OD-C4D	2.88	1.29	1.23
82	rK	202	PEB	OD-C4D	2.88	1.29	1.23
82	tK	203	PEB	OD-C4D	2.88	1.29	1.23
82	OI	203	PEB	C2A-C1A	-2.88	1.49	1.52
82	TI	203	PEB	OD-C4D	2.88	1.29	1.23
82	GG	1002	PEB	C2C-C3C	2.88	1.46	1.38
84	i3	1001	CYC	C4B-NB	-2.88	1.31	1.38
82	E9	202	PEB	OD-C4D	2.88	1.29	1.23
87	12	608	CLA	C4B-NB	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	C6	509	CLA	C4B-NB	2.88	1.41	1.37
87	2N	302	CLA	C1B-C2B	2.88	1.50	1.43
82	eG	202	PEB	C2C-C3C	2.88	1.46	1.38
82	qK	202	PEB	C2C-C3C	2.88	1.46	1.38
82	SJ	203	PEB	C2C-C3C	2.88	1.46	1.38
82	QK	203	PEB	OD-C4D	2.88	1.29	1.23
87	BL	621	CLA	CMD-C2D	-2.88	1.44	1.50
82	SG	201	PEB	C2A-C1A	-2.88	1.49	1.52
87	c6	611	CLA	C4B-NB	2.88	1.41	1.37
82	W9	202	PEB	OD-C4D	2.87	1.29	1.23
82	kE	201	PEB	OD-C4D	2.87	1.29	1.23
82	WI	201	PEB	C2A-C1A	-2.87	1.49	1.52
82	IM	201	PEB	C2C-C3C	2.87	1.46	1.38
82	OJ	202	PEB	C1C-C2C	2.87	1.49	1.42
82	AA	201	PEB	OD-C4D	2.87	1.29	1.23
82	A7	201	PEB	OD-C4D	2.87	1.29	1.23
82	jJ	202	PEB	OD-C4D	2.87	1.29	1.23
82	cK	201	PEB	CHA-C1B	2.87	1.47	1.40
82	hK	201	PEB	C1A-NA	-2.87	1.33	1.37
87	DL	404	CLA	C3B-C4B	2.87	1.49	1.42
87	52	607	CLA	C4D-ND	-2.87	1.33	1.37
87	62	303	CLA	C3B-C4B	2.87	1.49	1.42
82	YD	201	PEB	OD-C4D	2.87	1.29	1.23
82	eH	202	PEB	OD-C4D	2.87	1.29	1.23
83	AQ	302	PUB	OA-C1A	2.87	1.29	1.23
82	QF	201	PEB	CHB-C1C	2.87	1.47	1.40
87	B2	810	CLA	C4B-NB	2.87	1.41	1.37
82	YQ	201	PEB	OD-C4D	2.87	1.29	1.23
82	aF	201	PEB	OD-C4D	2.87	1.29	1.23
87	BN	828	CLA	C3B-C4B	2.87	1.49	1.42
84	T3	1001	CYC	C4B-NB	-2.87	1.31	1.38
87	1N	610	CLA	C3B-C4B	2.87	1.49	1.42
87	BL	603	CLA	CMC-C2C	-2.87	1.44	1.50
82	p8	202	PEB	C2A-C1A	-2.87	1.49	1.52
82	CI	202	PEB	OD-C4D	2.87	1.29	1.23
87	ON	203	CLA	C4B-NB	2.87	1.41	1.37
87	L2	202	CLA	C4D-ND	-2.87	1.33	1.37
87	4N	604	CLA	C4D-CHA	2.87	1.48	1.38
82	DM	201	PEB	C2A-C1A	-2.87	1.49	1.52
82	Q5	203	PEB	OD-C4D	2.87	1.29	1.23
87	RN	204	CLA	C4B-NB	2.87	1.41	1.37
82	H7	202	PEB	OD-C4D	2.87	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	JQ	203	PEB	C2C-C3C	2.87	1.46	1.38
84	DE	1001	CYC	C3D-C2D	2.87	1.46	1.38
82	DB	202	PEB	C2A-C1A	-2.87	1.49	1.52
87	1N	603	CLA	C4D-ND	-2.87	1.33	1.37
82	OO	202	PEB	OD-C4D	2.87	1.29	1.23
82	g4	202	PEB	C2C-C3C	2.87	1.46	1.38
87	62	312	CLA	C3B-C4B	2.87	1.49	1.42
87	3N	305	CLA	C3B-C4B	2.87	1.49	1.42
82	V9	202	PEB	OD-C4D	2.87	1.29	1.23
82	zK	501	PEB	C1A-NA	-2.87	1.33	1.37
87	B2	819	CLA	C4B-NB	2.87	1.41	1.37
82	UJ	203	PEB	OD-C4D	2.87	1.29	1.23
82	IP	202	PEB	C1C-NC	-2.87	1.33	1.37
82	J5	202	PEB	C2C-C3C	2.87	1.46	1.38
82	QM	204	PEB	OD-C4D	2.87	1.29	1.23
82	fH	201	PEB	OD-C4D	2.87	1.29	1.23
82	WP	201	PEB	C2A-C1A	-2.87	1.49	1.52
82	cE	201	PEB	C2A-C1A	-2.87	1.49	1.52
84	V3	1001	CYC	C4D-C3D	2.87	1.49	1.42
87	b6	609	CLA	C4B-NB	2.87	1.41	1.37
82	GF	201	PEB	C4A-NA	-2.87	1.31	1.37
82	PK	202	PEB	OD-C4D	2.87	1.29	1.23
84	v3	1001	CYC	C4B-NB	-2.87	1.31	1.38
82	TF	202	PEB	CHB-C1C	2.87	1.47	1.40
87	72	609	CLA	C3B-C4B	2.87	1.49	1.42
87	BL	621	CLA	C4D-ND	-2.87	1.33	1.37
82	XB	202	PEB	C2A-C1A	-2.87	1.49	1.52
82	TA	203	PEB	C2C-C3C	2.87	1.46	1.38
87	6N	605	CLA	C3B-C4B	2.86	1.49	1.42
82	P7	203	PEB	C2A-C1A	-2.86	1.49	1.52
82	U4	201	PEB	C2C-C3C	2.86	1.46	1.38
82	BA	201	PEB	OD-C4D	2.86	1.29	1.23
82	GM	202	PEB	OD-C4D	2.86	1.29	1.23
82	B9	202	PEB	OD-C4D	2.86	1.29	1.23
82	LK	202	PEB	C1C-C2C	2.86	1.49	1.42
87	2N	311	CLA	C4D-ND	-2.86	1.33	1.37
82	YA	301	PEB	C1A-NA	-2.86	1.33	1.37
82	lE	201	PEB	C2A-C1A	-2.86	1.49	1.52
82	FD	201	PEB	C2C-C3C	2.86	1.46	1.38
84	J3	1001	CYC	C4B-NB	-2.86	1.31	1.38
96	GN	201	HEM	FE-NB	2.86	2.03	1.94
82	FD	201	PEB	OD-C4D	2.86	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q5	203	PEB	C2C-C3C	2.86	1.46	1.38
82	UG	202	PEB	C2A-C1A	-2.86	1.49	1.52
82	aM	203	PEB	OD-C4D	2.86	1.29	1.23
82	W5	201	PEB	CHB-C1C	2.86	1.47	1.40
82	OE	202	PEB	OD-C4D	2.86	1.29	1.23
82	OG	202	PEB	OD-C4D	2.86	1.29	1.23
82	hK	202	PEB	OD-C4D	2.86	1.29	1.23
82	xK	304	PEB	OD-C4D	2.86	1.29	1.23
87	72	601	CLA	C4D-ND	-2.86	1.33	1.37
82	JA	202	PEB	C1A-NA	-2.86	1.33	1.37
84	JH	1001	CYC	C2C-C1C	-2.86	1.49	1.52
82	I9	202	PEB	OD-C4D	2.86	1.29	1.23
84	J1	1001	CYC	OB-C4B	2.86	1.29	1.23
98	B2	837	PQN	C10-C1	2.86	1.53	1.48
82	FK	202	PEB	CHB-C1C	2.86	1.47	1.40
82	X9	202	PEB	OD-C4D	2.86	1.29	1.23
82	I5	201	PEB	CHB-C1C	2.86	1.47	1.40
87	b6	618	CLA	C4B-NB	2.86	1.41	1.37
82	ZE	201	PEB	C2A-C1A	-2.86	1.49	1.52
83	Z5	303	PUB	OA-C1A	2.86	1.29	1.23
82	U7	201	PEB	C2C-C3C	2.86	1.46	1.38
82	CK	202	PEB	C1A-NA	-2.86	1.33	1.37
82	HB	203	PEB	CHB-C1C	2.86	1.47	1.40
82	DI	202	PEB	OD-C4D	2.86	1.29	1.23
82	DJ	202	PEB	OD-C4D	2.86	1.29	1.23
82	xC	201	PEB	OD-C4D	2.86	1.29	1.23
82	aF	203	PEB	OD-C4D	2.86	1.29	1.23
87	BN	824	CLA	C3B-C4B	2.86	1.49	1.42
84	P3	1001	CYC	C4B-NB	-2.86	1.31	1.38
82	TF	202	PEB	C1C-NC	-2.86	1.33	1.37
87	32	304	CLA	C3B-C4B	2.86	1.49	1.42
82	FI	202	PEB	OD-C4D	2.86	1.29	1.23
82	xF	304	PEB	OD-C4D	2.86	1.29	1.23
84	K3	1001	CYC	C4B-NB	-2.86	1.31	1.38
82	ND	203	PEB	C1A-NA	-2.86	1.33	1.37
82	FA	202	PEB	C2C-C3C	2.86	1.46	1.38
87	5N	602	CLA	C4B-NB	2.86	1.41	1.37
82	TJ	201	PEB	CHB-C1C	2.86	1.47	1.40
82	gG	201	PEB	OD-C4D	2.86	1.29	1.23
82	OJ	203	PEB	C2C-C3C	2.86	1.46	1.38
82	T7	203	PEB	C2C-C3C	2.86	1.46	1.38
82	eF	201	PEB	C2A-C1A	-2.86	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	82	306	CLA	C3C-C2C	2.86	1.42	1.36
84	C3	1001	CYC	C4B-NB	-2.86	1.31	1.38
82	QF	203	PEB	OD-C4D	2.86	1.29	1.23
82	PM	202	PEB	OD-C4D	2.86	1.29	1.23
82	B9	202	PEB	C2C-C3C	2.86	1.46	1.38
82	T1	201	PEB	OD-C4D	2.86	1.29	1.23
82	lJ	201	PEB	C2C-C3C	2.86	1.46	1.38
87	42	604	CLA	C4D-CHA	2.86	1.48	1.38
82	QI	201	PEB	OD-C4D	2.86	1.29	1.23
82	pK	202	PEB	OD-C4D	2.86	1.29	1.23
87	BL	606	CLA	C4B-NB	2.86	1.41	1.37
87	42	605	CLA	C4B-NB	2.86	1.41	1.37
87	ON	201	CLA	C3B-C4B	2.85	1.49	1.42
82	AH	305	PEB	OD-C4D	2.85	1.29	1.23
82	IM	203	PEB	OD-C4D	2.85	1.29	1.23
82	GJ	203	PEB	C2A-C1A	-2.85	1.49	1.52
82	W9	201	PEB	C2A-C1A	-2.85	1.49	1.52
87	R2	204	CLA	C4B-NB	2.85	1.41	1.37
82	Y4	203	PEB	C1A-NA	-2.85	1.33	1.37
82	kH	203	PEB	C1A-NA	-2.85	1.33	1.37
82	HI	203	PEB	OD-C4D	2.85	1.29	1.23
82	sF	203	PEB	OD-C4D	2.85	1.29	1.23
82	DE	1002	PEB	C4B-C3B	2.85	1.50	1.45
82	ZO	201	PEB	C4A-NA	-2.85	1.31	1.37
82	eE	203	PEB	OD-C4D	2.85	1.29	1.23
82	nF	202	PEB	OD-C4D	2.85	1.29	1.23
82	dO	202	PEB	OD-C4D	2.85	1.29	1.23
82	PQ	203	PEB	OD-C4D	2.85	1.29	1.23
82	Z1	201	PEB	OD-C4D	2.85	1.29	1.23
82	wC	204	PEB	OD-C4D	2.85	1.29	1.23
87	F2	201	CLA	C4B-NB	2.85	1.41	1.37
87	A2	849	CLA	CMD-C2D	-2.85	1.44	1.50
84	x3	1001	CYC	C4D-C3D	2.85	1.49	1.42
82	ED	201	PEB	C1C-NC	-2.85	1.33	1.37
87	B2	821	CLA	C4B-NB	2.85	1.41	1.37
82	LG	1002	PEB	C2A-C1A	-2.85	1.49	1.52
82	w8	202	PEB	CHC-C4C	2.85	1.53	1.49
82	1C	201	PEB	OD-C4D	2.85	1.29	1.23
82	eE	202	PEB	C2C-C3C	2.85	1.46	1.38
82	A4	301	PEB	OD-C4D	2.85	1.29	1.23
82	b4	202	PEB	OD-C4D	2.85	1.29	1.23
82	O5	201	PEB	OD-C4D	2.85	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B7	201	PEB	OD-C4D	2.85	1.29	1.23
82	A9	202	PEB	OD-C4D	2.85	1.29	1.23
82	N9	202	PEB	OD-C4D	2.85	1.29	1.23
82	eB	201	PEB	OD-C4D	2.85	1.29	1.23
82	aH	202	PEB	OD-C4D	2.85	1.29	1.23
82	V1	202	PEB	C2A-C1A	-2.85	1.49	1.52
84	t3	1001	CYC	C4B-NB	-2.85	1.31	1.38
82	CM	203	PEB	C2C-C3C	2.85	1.46	1.38
82	m4	202	PEB	C2C-C3C	2.85	1.46	1.38
87	B6	608	CLA	C4B-NB	2.85	1.41	1.37
82	ZH	202	PEB	CHA-C1B	2.85	1.47	1.40
82	R7	203	PEB	CHB-C1C	2.85	1.47	1.40
82	TA	202	PEB	C1A-NA	-2.85	1.33	1.37
82	BB	203	PEB	C2A-C1A	-2.85	1.49	1.52
82	eK	202	PEB	C2A-C1A	-2.85	1.49	1.52
87	B2	828	CLA	C3B-C4B	2.85	1.49	1.42
82	FP	202	PEB	OD-C4D	2.85	1.29	1.23
82	P9	202	PEB	OD-C4D	2.85	1.29	1.23
87	A2	809	CLA	C4D-ND	-2.85	1.33	1.37
82	IP	202	PEB	C2C-C3C	2.85	1.46	1.38
82	u8	203	PEB	OD-C4D	2.85	1.29	1.23
82	G9	202	PEB	OD-C4D	2.85	1.29	1.23
83	AE	302	PUB	OD-C4D	2.85	1.29	1.23
82	MJ	201	PEB	C2C-C3C	2.85	1.46	1.38
82	EP	201	PEB	C2A-C1A	-2.85	1.49	1.52
82	VQ	203	PEB	C2A-C1A	-2.85	1.49	1.52
82	bF	201	PEB	OD-C4D	2.85	1.29	1.23
82	C5	201	PEB	C1C-NC	-2.85	1.33	1.37
87	1N	607	CLA	C3B-C4B	2.85	1.49	1.42
82	t8	202	PEB	OD-C4D	2.85	1.29	1.23
82	OF	201	PEB	C2C-C3C	2.85	1.46	1.38
82	M5	304	PEB	C2A-C1A	-2.85	1.49	1.52
82	cH	202	PEB	C2A-C1A	-2.85	1.49	1.52
98	B2	837	PQN	C2-C1	2.85	1.54	1.48
82	WF	201	PEB	C2C-C3C	2.85	1.46	1.38
82	vF	201	PEB	OD-C4D	2.85	1.29	1.23
82	dG	204	PEB	OD-C4D	2.85	1.29	1.23
87	A2	831	CLA	C4B-NB	2.85	1.41	1.37
82	RA	203	PEB	CHB-C1C	2.85	1.47	1.40
82	QK	201	PEB	CHB-C1C	2.85	1.47	1.40
82	cO	203	PEB	OD-C4D	2.85	1.29	1.23
83	QM	201	PUB	OD-C4D	2.85	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	62	306	CLA	C3B-C4B	2.85	1.49	1.42
82	mO	202	PEB	C2C-C3C	2.85	1.46	1.38
82	B9	202	PEB	CHC-C4C	2.84	1.53	1.49
82	PF	202	PEB	OD-C4D	2.84	1.29	1.23
82	K9	202	PEB	OD-C4D	2.84	1.29	1.23
87	AN	832	CLA	MG-NB	-2.84	2.00	2.05
82	TK	202	PEB	C1C-NC	-2.84	1.33	1.37
82	lG	201	PEB	OD-C4D	2.84	1.29	1.23
82	HJ	201	PEB	CHB-C1C	2.84	1.47	1.40
82	O1	202	PEB	OD-C4D	2.84	1.29	1.23
84	G3	1001	CYC	C4B-NB	-2.84	1.32	1.38
82	mM	202	PEB	OD-C4D	2.84	1.29	1.23
82	nK	202	PEB	CHC-C4C	2.84	1.53	1.49
87	AN	840	CLA	C4B-NB	2.84	1.41	1.37
82	LF	202	PEB	C1C-C2C	2.84	1.49	1.42
84	e3	1001	CYC	C4B-NB	-2.84	1.32	1.38
87	O2	201	CLA	C3B-C4B	2.84	1.49	1.42
84	V3	1001	CYC	C4B-NB	-2.84	1.32	1.38
87	8N	308	CLA	C4B-NB	2.84	1.41	1.37
87	4N	603	CLA	C3B-C4B	2.84	1.49	1.42
82	j4	203	PEB	C2A-C1A	-2.84	1.49	1.52
82	UP	202	PEB	OD-C4D	2.84	1.29	1.23
82	hG	201	PEB	OD-C4D	2.84	1.29	1.23
87	bL	607	CLA	CMB-C2B	-2.84	1.44	1.50
82	K5	201	PEB	CHB-C1C	2.84	1.47	1.40
82	LD	203	PEB	OD-C4D	2.84	1.29	1.23
82	AI	202	PEB	OD-C4D	2.84	1.29	1.23
82	A1	305	PEB	OD-C4D	2.84	1.29	1.23
82	rF	201	PEB	OD-C4D	2.84	1.29	1.23
82	OH	203	PEB	CHA-C1B	2.84	1.47	1.40
87	BN	805	CLA	C1D-ND	2.84	1.41	1.37
87	I2	102	CLA	C4B-NB	2.84	1.41	1.37
82	x8	201	PEB	OD-C4D	2.84	1.29	1.23
98	BN	837	PQN	C10-C1	2.84	1.53	1.48
82	QB	204	PEB	C2A-C1A	-2.84	1.49	1.52
82	UJ	202	PEB	CHB-C1C	2.84	1.47	1.40
87	42	606	CLA	C4B-NB	2.84	1.41	1.37
87	C6	520	CLA	C4B-NB	2.84	1.41	1.37
82	xF	302	PEB	OD-C4D	2.84	1.29	1.23
82	gJ	202	PEB	OD-C4D	2.84	1.29	1.23
87	6N	604	CLA	C3B-C4B	2.84	1.49	1.42
82	dK	201	PEB	C1A-NA	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UD	202	PEB	OD-C4D	2.84	1.29	1.23
82	D7	203	PEB	OD-C4D	2.84	1.29	1.23
84	NH	1001	CYC	OB-C4B	2.84	1.29	1.23
87	A2	841	CLA	C1D-ND	2.84	1.41	1.37
82	x8	202	PEB	C4B-C3B	2.84	1.50	1.45
87	52	608	CLA	C3B-C4B	2.84	1.49	1.42
87	7N	609	CLA	C3B-C4B	2.84	1.49	1.42
82	c4	201	PEB	OD-C4D	2.84	1.29	1.23
82	z8	202	PEB	OD-C4D	2.84	1.29	1.23
82	II	203	PEB	C1A-NA	-2.84	1.33	1.37
87	6N	603	CLA	C3B-C4B	2.84	1.49	1.42
82	TK	202	PEB	CHB-C1C	2.84	1.47	1.40
82	D9	203	PEB	OD-C4D	2.84	1.29	1.23
82	dG	201	PEB	OD-C4D	2.84	1.29	1.23
87	12	607	CLA	C3B-C4B	2.84	1.49	1.42
82	OP	203	PEB	CHB-C1C	2.84	1.47	1.40
87	IN	102	CLA	C4B-NB	2.84	1.41	1.37
87	a6	607	CLA	C4B-NB	2.84	1.41	1.37
82	WH	201	PEB	OD-C4D	2.84	1.29	1.23
82	NM	202	PEB	OD-C4D	2.84	1.29	1.23
82	MD	202	PEB	OD-C4D	2.84	1.29	1.23
82	A1	302	PEB	OD-C4D	2.84	1.29	1.23
82	S9	202	PEB	OD-C4D	2.84	1.29	1.23
82	j4	203	PEB	C2C-C3C	2.84	1.46	1.38
82	hF	201	PEB	C1A-NA	-2.84	1.33	1.37
87	A6	402	CLA	C4B-NB	2.84	1.41	1.37
87	42	610	CLA	C3B-C4B	2.84	1.49	1.42
82	AQ	304	PEB	OD-C4D	2.84	1.29	1.23
82	f4	202	PEB	OD-C4D	2.84	1.29	1.23
82	w8	204	PEB	OD-C4D	2.84	1.29	1.23
82	gM	202	PEB	OD-C4D	2.84	1.29	1.23
82	eG	203	PEB	C1C-C2C	2.84	1.49	1.42
87	32	311	CLA	C3B-C4B	2.84	1.49	1.42
87	62	304	CLA	C3B-C4B	2.84	1.49	1.42
82	XB	201	PEB	C2A-C1A	-2.84	1.49	1.52
82	Y4	201	PEB	C2A-C1A	-2.84	1.49	1.52
87	1N	608	CLA	C4B-NB	2.84	1.41	1.37
82	TH	201	PEB	OD-C4D	2.84	1.29	1.23
82	jJ	201	PEB	OD-C4D	2.84	1.29	1.23
83	BM	302	PUB	OD-C4D	2.84	1.29	1.23
82	A5	201	PEB	CHB-C1C	2.84	1.47	1.40
82	G5	201	PEB	CHB-C1C	2.84	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	831	CLA	C4B-NB	2.84	1.41	1.37
87	8N	301	CLA	C3C-C2C	2.84	1.42	1.36
82	W4	201	PEB	CHB-C1C	2.84	1.47	1.40
87	C6	511	CLA	C4B-NB	2.83	1.41	1.37
87	bL	605	CLA	C4B-NB	2.83	1.41	1.37
82	FQ	201	PEB	OD-C4D	2.83	1.29	1.23
82	U9	203	PEB	OD-C4D	2.83	1.29	1.23
82	dF	201	PEB	OD-C4D	2.83	1.29	1.23
84	g3	1001	CYC	C4B-NB	-2.83	1.32	1.38
87	72	608	CLA	C3B-C4B	2.83	1.49	1.42
82	H9	202	PEB	C2C-C3C	2.83	1.46	1.38
82	PP	202	PEB	C2A-C1A	-2.83	1.49	1.52
82	F7	203	PEB	OD-C4D	2.83	1.29	1.23
82	H9	203	PEB	OD-C4D	2.83	1.29	1.23
84	c3	1001	CYC	C4B-NB	-2.83	1.32	1.38
82	UO	201	PEB	C2C-C3C	2.83	1.46	1.38
82	D5	203	PEB	OD-C4D	2.83	1.29	1.23
82	xC	202	PEB	OD-C4D	2.83	1.29	1.23
82	WJ	203	PEB	CHA-C1B	2.83	1.47	1.40
87	BL	604	CLA	C4B-NB	2.83	1.41	1.37
84	E3	1001	CYC	C4B-NB	-2.83	1.32	1.38
82	LI	202	PEB	C2A-C1A	-2.83	1.49	1.52
87	12	609	CLA	C4D-ND	-2.83	1.33	1.37
82	NK	202	PEB	CHB-C1C	2.83	1.47	1.40
84	l3	1001	CYC	C4B-NB	-2.83	1.32	1.38
87	c6	614	CLA	C3B-C4B	2.83	1.49	1.42
82	BD	202	PEB	OD-C4D	2.83	1.29	1.23
83	M5	303	PUB	OA-C1A	2.83	1.29	1.23
82	BQ	202	PEB	OD-C4D	2.83	1.29	1.23
82	kG	201	PEB	OD-C4D	2.83	1.29	1.23
82	FI	202	PEB	C2A-C1A	-2.83	1.49	1.52
82	RJ	201	PEB	CHC-C4C	2.83	1.53	1.49
82	tF	202	PEB	CHC-C4C	2.83	1.53	1.49
87	A2	833	CLA	C4B-NB	2.83	1.41	1.37
82	L5	202	PEB	OD-C4D	2.83	1.29	1.23
82	W5	203	PEB	OD-C4D	2.83	1.29	1.23
82	bK	201	PEB	OD-C4D	2.83	1.29	1.23
84	DO	1001	CYC	C3D-C2D	2.83	1.46	1.38
87	AN	849	CLA	CMD-C2D	-2.83	1.44	1.50
87	B2	822	CLA	MG-NB	-2.83	2.00	2.05
82	C9	202	PEB	OD-C4D	2.83	1.29	1.23
82	cM	202	PEB	OD-C4D	2.83	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kM	201	PEB	OD-C4D	2.83	1.29	1.23
82	Z9	301	PEB	OD-C4D	2.83	1.29	1.23
82	JD	203	PEB	C2C-C3C	2.83	1.46	1.38
84	73	1002	CYC	C3D-C2D	2.83	1.46	1.38
87	6N	607	CLA	C3B-C4B	2.83	1.49	1.42
87	7N	608	CLA	C3B-C4B	2.83	1.49	1.42
87	bL	620	CLA	C4B-NB	2.83	1.41	1.37
82	LA	202	PEB	C2C-C3C	2.83	1.46	1.38
82	MM	201	PEB	C2C-C3C	2.83	1.46	1.38
82	M9	305	PEB	OD-C4D	2.83	1.29	1.23
83	xF	305	PUB	OA-C1A	2.83	1.29	1.23
82	X5	201	PEB	CHB-C1C	2.83	1.47	1.40
87	B6	607	CLA	C3B-C4B	2.83	1.49	1.42
82	WD	201	PEB	OD-C4D	2.83	1.29	1.23
82	YD	202	PEB	OD-C4D	2.83	1.29	1.23
82	AG	304	PEB	OD-C4D	2.83	1.29	1.23
82	mE	202	PEB	OD-C4D	2.83	1.29	1.23
82	mG	202	PEB	OD-C4D	2.83	1.29	1.23
82	cH	202	PEB	OD-C4D	2.83	1.29	1.23
82	vK	201	PEB	OD-C4D	2.83	1.29	1.23
87	DL	406	CLA	C4B-NB	2.83	1.41	1.37
87	B2	820	CLA	C4B-NB	2.83	1.41	1.37
82	gO	202	PEB	C2C-C3C	2.83	1.46	1.38
82	q8	202	PEB	C2A-C1A	-2.83	1.49	1.52
82	T5	201	PEB	CHB-C1C	2.83	1.47	1.40
82	O9	201	PEB	OD-C4D	2.83	1.29	1.23
82	J5	201	PEB	C1C-NC	-2.83	1.33	1.37
82	BD	201	PEB	C2C-C3C	2.83	1.46	1.38
82	eK	201	PEB	C2A-C1A	-2.83	1.49	1.52
82	c1	202	PEB	OD-C4D	2.83	1.29	1.23
83	Z5	302	PUB	OA-C1A	2.83	1.29	1.23
87	62	308	CLA	C3B-C4B	2.83	1.49	1.42
82	zC	202	PEB	OD-C4D	2.83	1.29	1.23
87	R2	202	CLA	C4D-ND	-2.83	1.33	1.37
87	bL	616	CLA	C4B-NB	2.83	1.41	1.37
82	TH	201	PEB	C2A-C1A	-2.83	1.49	1.52
82	oF	203	PEB	C2A-C1A	-2.83	1.49	1.52
82	cB	402	PEB	OD-C4D	2.83	1.29	1.23
82	wC	202	PEB	OD-C4D	2.83	1.29	1.23
82	tK	201	PEB	OD-C4D	2.83	1.29	1.23
87	BL	606	CLA	C1B-C2B	2.83	1.49	1.43
82	HB	201	PEB	C1C-NC	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gE	201	PEB	OD-C4D	2.83	1.29	1.23
82	gO	201	PEB	OD-C4D	2.83	1.29	1.23
82	SG	203	PEB	C2C-C3C	2.83	1.46	1.38
87	82	308	CLA	C4B-NB	2.83	1.41	1.37
87	A2	832	CLA	C1D-ND	2.83	1.41	1.37
82	jH	203	PEB	OD-C4D	2.83	1.29	1.23
83	xK	306	PUB	OA-C1A	2.83	1.29	1.23
87	AN	802	CLA	C3B-C4B	2.83	1.49	1.42
82	IA	201	PEB	OD-C4D	2.83	1.29	1.23
84	A3	1001	CYC	C4B-NB	-2.83	1.32	1.38
82	w8	202	PEB	OD-C4D	2.83	1.29	1.23
82	fO	201	PEB	OD-C4D	2.83	1.29	1.23
82	xC	202	PEB	C4B-C3B	2.83	1.50	1.45
84	JH	1001	CYC	C3D-C2D	2.82	1.46	1.38
82	EF	202	PEB	OD-C4D	2.82	1.29	1.23
84	N1	1001	CYC	OB-C4B	2.82	1.29	1.23
84	R3	1001	CYC	C4B-NB	-2.82	1.32	1.38
84	LO	1001	CYC	C1B-NB	-2.82	1.33	1.37
82	T9	202	PEB	OD-C4D	2.82	1.29	1.23
82	dG	203	PEB	OD-C4D	2.82	1.29	1.23
83	QJ	201	PUB	OD-C4D	2.82	1.29	1.23
84	D1	1001	CYC	OB-C4B	2.82	1.29	1.23
82	aH	201	PEB	C1A-NA	-2.82	1.33	1.37
82	QM	203	PEB	C2A-C1A	-2.82	1.49	1.52
87	cL	513	CLA	C4D-ND	-2.82	1.33	1.37
82	R5	201	PEB	CHB-C1C	2.82	1.47	1.40
82	R1	201	PEB	OD-C4D	2.82	1.29	1.23
87	AN	811	CLA	C4B-NB	2.82	1.41	1.37
87	dL	401	CLA	C4B-NB	2.82	1.41	1.37
82	sK	203	PEB	C4B-C3B	2.82	1.50	1.45
87	5N	607	CLA	C4D-ND	-2.82	1.33	1.37
84	y3	1001	CYC	C4B-NB	-2.82	1.32	1.38
87	A2	801	CLA	C3B-C4B	2.82	1.49	1.42
82	xK	303	PEB	OD-C4D	2.82	1.29	1.23
82	M9	302	PEB	OD-C4D	2.82	1.29	1.23
87	B2	827	CLA	MG-NB	-2.82	2.00	2.05
82	kO	202	PEB	C2C-C3C	2.82	1.46	1.38
87	AN	832	CLA	C1D-ND	2.82	1.41	1.37
82	NM	201	PEB	CHB-C1C	2.82	1.47	1.40
87	82	303	CLA	C3B-C4B	2.82	1.49	1.42
82	AH	301	PEB	C1A-NA	-2.82	1.33	1.37
82	lK	203	PEB	C1A-NA	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NK	202	PEB	OD-C4D	2.82	1.29	1.23
82	B9	201	PEB	OD-C4D	2.82	1.29	1.23
82	HM	201	PEB	CHB-C1C	2.82	1.47	1.40
87	c6	609	CLA	C3B-C4B	2.82	1.49	1.42
87	b6	605	CLA	C4D-ND	-2.82	1.33	1.37
82	tK	203	PEB	C1A-NA	-2.82	1.33	1.37
82	BI	203	PEB	OD-C4D	2.82	1.29	1.23
82	B9	202	PEB	CHA-C1B	2.82	1.47	1.40
87	B6	613	CLA	C3B-C4B	2.82	1.49	1.42
87	BN	806	CLA	C1D-ND	2.82	1.41	1.37
87	I2	103	CLA	C4B-NB	2.82	1.41	1.37
82	RO	202	PEB	C2C-C3C	2.82	1.46	1.38
82	g1	202	PEB	C2A-C1A	-2.82	1.49	1.52
82	Q5	202	PEB	C2A-C1A	-2.82	1.49	1.52
82	ZK	202	PEB	OD-C4D	2.82	1.28	1.23
82	h4	202	PEB	OD-C4D	2.82	1.28	1.23
87	4N	610	CLA	C3B-C4B	2.82	1.49	1.42
82	SJ	203	PEB	C2A-C1A	-2.82	1.49	1.52
82	U9	204	PEB	C4B-C3B	2.82	1.50	1.45
87	BL	619	CLA	C4B-NB	2.82	1.41	1.37
82	OF	201	PEB	CHA-C1B	2.82	1.47	1.40
83	M5	302	PUB	CHB-C4B	2.82	1.47	1.40
82	VP	201	PEB	C1C-NC	-2.82	1.33	1.37
87	4N	605	CLA	C4B-NB	2.82	1.41	1.37
82	V4	202	PEB	C2A-C1A	-2.82	1.49	1.52
82	eM	202	PEB	C2A-C1A	-2.82	1.49	1.52
82	QF	203	PEB	C4A-NA	-2.82	1.31	1.37
84	LO	1001	CYC	C4B-NB	-2.82	1.32	1.38
82	JP	201	PEB	OD-C4D	2.82	1.28	1.23
82	uK	201	PEB	OD-C4D	2.82	1.28	1.23
87	62	305	CLA	C3B-C4B	2.82	1.49	1.42
84	W3	1001	CYC	C4B-NB	-2.82	1.32	1.38
82	mE	203	PEB	OD-C4D	2.82	1.28	1.23
82	mG	201	PEB	OD-C4D	2.82	1.28	1.23
87	22	612	CLA	C3B-C4B	2.82	1.49	1.42
82	AO	304	PEB	OD-C4D	2.82	1.28	1.23
82	L9	203	PEB	OD-C4D	2.82	1.28	1.23
82	Z9	304	PEB	OD-C4D	2.82	1.28	1.23
87	72	603	CLA	C4D-ND	-2.82	1.33	1.37
84	N3	1001	CYC	C4B-NB	-2.82	1.32	1.38
82	l1	201	PEB	C1A-NA	-2.82	1.34	1.37
82	W9	203	PEB	OD-C4D	2.82	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	sK	201	PEB	OD-C4D	2.82	1.28	1.23
82	cM	201	PEB	OD-C4D	2.82	1.28	1.23
87	BL	601	CLA	C4B-NB	2.82	1.41	1.37
87	B2	832	CLA	C4B-NB	2.82	1.41	1.37
87	LN	202	CLA	C4D-ND	-2.82	1.33	1.37
87	7N	603	CLA	C4D-ND	-2.82	1.33	1.37
87	6N	609	CLA	C3B-C4B	2.82	1.49	1.42
82	SD	202	PEB	OD-C4D	2.82	1.28	1.23
82	q8	203	PEB	OD-C4D	2.82	1.28	1.23
84	F1	1001	CYC	C1B-C2B	2.82	1.50	1.45
82	E5	201	PEB	CHB-C1C	2.82	1.47	1.40
87	BL	623	CLA	C3B-C4B	2.82	1.49	1.42
87	L2	206	CLA	C4B-NB	2.82	1.41	1.37
82	FH	1002	PEB	OD-C4D	2.82	1.28	1.23
82	mJ	202	PEB	OD-C4D	2.82	1.28	1.23
84	m3	1001	CYC	C4B-NB	-2.82	1.32	1.38
84	J1	1001	CYC	C2C-C1C	-2.81	1.49	1.52
82	jH	201	PEB	OD-C4D	2.81	1.28	1.23
87	AN	809	CLA	C4D-ND	-2.81	1.33	1.37
87	A2	811	CLA	C4B-NB	2.81	1.41	1.37
87	B2	814	CLA	C4B-NB	2.81	1.41	1.37
82	cF	203	PEB	C2C-C3C	2.81	1.46	1.38
82	kE	202	PEB	OD-C4D	2.81	1.28	1.23
82	R4	202	PEB	C2C-C3C	2.81	1.46	1.38
82	VB	201	PEB	C2A-C1A	-2.81	1.49	1.52
82	NM	201	PEB	C2A-C1A	-2.81	1.49	1.52
82	P5	201	PEB	CHB-C1C	2.81	1.47	1.40
82	O7	201	PEB	CHB-C1C	2.81	1.47	1.40
82	JA	203	PEB	OD-C4D	2.81	1.28	1.23
82	XP	202	PEB	OD-C4D	2.81	1.28	1.23
87	AN	833	CLA	C4B-NB	2.81	1.41	1.37
82	j1	201	PEB	OD-C4D	2.81	1.28	1.23
82	V5	201	PEB	CHB-C1C	2.81	1.47	1.40
87	B6	605	CLA	C4B-NB	2.81	1.41	1.37
87	3N	301	CLA	C4B-NB	2.81	1.41	1.37
82	fJ	202	PEB	OD-C4D	2.81	1.28	1.23
82	A5	201	PEB	C1C-NC	-2.81	1.33	1.37
98	BN	837	PQN	C2-C1	2.81	1.54	1.48
87	K2	101	CLA	C3B-C4B	2.81	1.49	1.42
87	7N	601	CLA	C3B-C4B	2.81	1.49	1.42
82	B9	203	PEB	OD-C4D	2.81	1.28	1.23
82	H9	201	PEB	OD-C4D	2.81	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hE	201	PEB	OD-C4D	2.81	1.28	1.23
87	b6	607	CLA	C3B-C4B	2.81	1.49	1.42
83	Z5	302	PUB	CHB-C4B	2.81	1.47	1.40
82	UE	202	PEB	C2A-C1A	-2.81	1.49	1.52
82	H7	201	PEB	OD-C4D	2.81	1.28	1.23
84	JH	1001	CYC	OB-C4B	2.81	1.28	1.23
87	BN	801	CLA	C3B-C4B	2.81	1.49	1.42
82	V5	201	PEB	C1C-NC	-2.81	1.33	1.37
82	VJ	202	PEB	OD-C4D	2.81	1.28	1.23
87	BL	608	CLA	CMC-C2C	-2.81	1.44	1.50
82	IM	201	PEB	C2A-C1A	-2.81	1.49	1.52
82	C5	201	PEB	CHB-C1C	2.81	1.47	1.40
82	HP	202	PEB	OD-C4D	2.81	1.28	1.23
87	c6	613	CLA	C3B-C4B	2.81	1.49	1.42
82	I5	201	PEB	C1C-NC	-2.81	1.33	1.37
82	Q9	203	PEB	OD-C4D	2.81	1.28	1.23
87	R2	203	CLA	C3B-C4B	2.81	1.49	1.42
87	5N	608	CLA	C3B-C4B	2.81	1.49	1.42
82	SH	203	PEB	C2A-C1A	-2.81	1.49	1.52
82	JI	202	PEB	C2A-C1A	-2.81	1.49	1.52
82	pC	201	PEB	C2A-C1A	-2.81	1.49	1.52
82	FA	202	PEB	C1A-NA	-2.81	1.34	1.37
82	GM	203	PEB	OD-C4D	2.81	1.28	1.23
82	eE	201	PEB	OD-C4D	2.81	1.28	1.23
82	kG	202	PEB	OD-C4D	2.81	1.28	1.23
82	wK	302	PEB	OD-C4D	2.81	1.28	1.23
82	S9	201	PEB	CHB-C1C	2.81	1.47	1.40
82	SB	202	PEB	C2C-C3C	2.81	1.46	1.38
82	KI	201	PEB	OD-C4D	2.81	1.28	1.23
82	SJ	202	PEB	OD-C4D	2.81	1.28	1.23
82	i1	202	PEB	C2A-C1A	-2.81	1.49	1.52
82	H4	1002	PEB	C2A-C1A	-2.81	1.49	1.52
82	lG	201	PEB	C2A-C1A	-2.81	1.49	1.52
82	WQ	202	PEB	OD-C4D	2.81	1.28	1.23
82	cB	401	PEB	OD-C4D	2.81	1.28	1.23
82	N5	201	PEB	CHB-C1C	2.81	1.46	1.40
82	DA	203	PEB	OD-C4D	2.81	1.28	1.23
82	OA	202	PEB	C2C-C3C	2.81	1.46	1.38
82	lG	202	PEB	C2A-C1A	-2.81	1.49	1.52
87	B2	832	CLA	C3B-C4B	2.81	1.49	1.42
82	BQ	203	PEB	CHA-C1B	2.81	1.47	1.40
82	gO	203	PEB	OD-C4D	2.81	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L2	206	CLA	C3B-C4B	2.81	1.49	1.42
82	YJ	201	PEB	C2C-C3C	2.81	1.46	1.38
87	62	310	CLA	C3B-C4B	2.81	1.49	1.42
87	KN	102	CLA	C4B-NB	2.81	1.41	1.37
82	i4	203	PEB	OD-C4D	2.81	1.28	1.23
83	xK	301	PUB	OD-C4D	2.81	1.28	1.23
82	QE	201	PEB	C2A-C1A	-2.81	1.49	1.52
82	DG	1002	PEB	C4B-C3B	2.81	1.50	1.45
87	bL	619	CLA	C4B-NB	2.81	1.41	1.37
82	RE	202	PEB	OD-C4D	2.81	1.28	1.23
82	m4	203	PEB	OD-C4D	2.81	1.28	1.23
82	JM	202	PEB	OD-C4D	2.80	1.28	1.23
82	yF	301	PEB	OD-C4D	2.80	1.28	1.23
87	AN	801	CLA	C4B-NB	2.80	1.41	1.37
87	B2	805	CLA	C1D-ND	2.80	1.41	1.37
87	BN	832	CLA	C3B-C4B	2.80	1.49	1.42
87	72	601	CLA	C3B-C4B	2.80	1.49	1.42
87	3N	301	CLA	C3B-C4B	2.80	1.49	1.42
82	TO	202	PEB	C2C-C3C	2.80	1.46	1.38
82	AI	203	PEB	CHB-C1C	2.80	1.46	1.40
87	B2	804	CLA	C1D-ND	2.80	1.41	1.37
82	AO	301	PEB	OD-C4D	2.80	1.28	1.23
82	F1	1002	PEB	OD-C4D	2.80	1.28	1.23
82	uC	203	PEB	OD-C4D	2.80	1.28	1.23
82	E5	201	PEB	C1C-NC	-2.80	1.33	1.37
87	RN	203	CLA	C3B-C4B	2.80	1.49	1.42
82	AD	304	PEB	OD-C4D	2.80	1.28	1.23
82	EM	203	PEB	OD-C4D	2.80	1.28	1.23
82	mG	203	PEB	OD-C4D	2.80	1.28	1.23
82	lF	202	PEB	CHC-C4C	2.80	1.53	1.49
82	FA	201	PEB	OD-C4D	2.80	1.28	1.23
82	iM	202	PEB	OD-C4D	2.80	1.28	1.23
87	2N	308	CLA	C3B-C4B	2.80	1.49	1.42
87	AN	802	CLA	C4B-NB	2.80	1.41	1.37
87	32	305	CLA	C4B-NB	2.80	1.41	1.37
82	NF	202	PEB	CHB-C1C	2.80	1.46	1.40
82	F7	202	PEB	C1C-C2C	2.80	1.49	1.42
82	M5	301	PEB	CHB-C1C	2.80	1.46	1.40
82	VM	201	PEB	C2A-C1A	-2.80	1.49	1.52
87	3N	311	CLA	C3B-C4B	2.80	1.49	1.42
82	CQ	201	PEB	OD-C4D	2.80	1.28	1.23
82	gM	201	PEB	OD-C4D	2.80	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	xK	305	PUB	OD-C4D	2.80	1.28	1.23
87	A2	840	CLA	C4B-NB	2.80	1.41	1.37
87	b6	615	CLA	C4B-NB	2.80	1.41	1.37
87	4N	603	CLA	C4B-NB	2.80	1.41	1.37
82	GF	202	PEB	CMB-C2B	-2.80	1.44	1.50
82	LI	202	PEB	OD-C4D	2.80	1.28	1.23
82	U5	202	PEB	OD-C4D	2.80	1.28	1.23
82	lE	201	PEB	OD-C4D	2.80	1.28	1.23
82	cO	201	PEB	OD-C4D	2.80	1.28	1.23
87	a6	608	CLA	C4B-NB	2.80	1.41	1.37
82	mO	202	PEB	C2A-C1A	-2.80	1.49	1.52
82	Q9	201	PEB	OD-C4D	2.80	1.28	1.23
82	mE	201	PEB	OD-C4D	2.80	1.28	1.23
87	A2	832	CLA	MG-NB	-2.80	2.00	2.05
82	ZF	202	PEB	OD-C4D	2.80	1.28	1.23
82	OP	203	PEB	OD-C4D	2.80	1.28	1.23
82	18	201	PEB	OD-C4D	2.80	1.28	1.23
87	A2	828	CLA	CMD-C2D	-2.80	1.44	1.50
82	U7	201	PEB	C4A-NA	-2.80	1.31	1.37
87	C6	510	CLA	C4B-NB	2.80	1.41	1.37
82	ED	202	PEB	OD-C4D	2.80	1.28	1.23
82	JP	202	PEB	OD-C4D	2.80	1.28	1.23
82	J7	203	PEB	OD-C4D	2.80	1.28	1.23
82	yC	203	PEB	OD-C4D	2.80	1.28	1.23
82	dH	201	PEB	OD-C4D	2.80	1.28	1.23
87	52	610	CLA	C3B-C4B	2.80	1.49	1.42
82	D9	201	PEB	C2A-C1A	-2.80	1.49	1.52
82	KI	201	PEB	C2C-C3C	2.80	1.46	1.38
87	D6	402	CLA	C4B-NB	2.80	1.41	1.37
82	G5	201	PEB	C1C-NC	-2.80	1.33	1.37
82	OK	201	PEB	CHA-C1B	2.80	1.47	1.40
87	B2	825	CLA	C3B-C4B	2.80	1.49	1.42
87	8N	304	CLA	C3B-C4B	2.80	1.49	1.42
82	OF	202	PEB	CHB-C1C	2.80	1.46	1.40
82	QD	201	PEB	OD-C4D	2.80	1.28	1.23
82	HM	202	PEB	OD-C4D	2.80	1.28	1.23
82	f1	201	PEB	OD-C4D	2.80	1.28	1.23
82	qC	202	PEB	C2A-C1A	-2.80	1.49	1.52
87	CL	514	CLA	C4B-NB	2.80	1.41	1.37
87	4N	606	CLA	C4B-NB	2.80	1.41	1.37
87	3N	312	CLA	C3B-C4B	2.80	1.49	1.42
82	Z5	301	PEB	CHB-C1C	2.80	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BI	202	PEB	C1D-ND	2.80	1.49	1.45
82	RD	201	PEB	OD-C4D	2.80	1.28	1.23
82	FM	202	PEB	OD-C4D	2.80	1.28	1.23
87	22	608	CLA	C3B-C4B	2.80	1.49	1.42
87	3N	312	CLA	C4D-ND	-2.80	1.33	1.37
82	YF	201	PEB	OD-C4D	2.80	1.28	1.23
82	Q5	201	PEB	C2A-C1A	-2.80	1.49	1.52
82	RO	201	PEB	C1C-NC	-2.80	1.33	1.37
82	T5	201	PEB	C1C-NC	-2.80	1.33	1.37
82	SM	203	PEB	OD-C4D	2.80	1.28	1.23
84	HE	1001	CYC	C3D-C2D	2.80	1.46	1.38
82	T4	202	PEB	C2C-C3C	2.80	1.46	1.38
82	U1	202	PEB	OD-C4D	2.80	1.28	1.23
84	FH	1001	CYC	C1B-C2B	2.80	1.50	1.45
82	CJ	203	PEB	C2C-C3C	2.80	1.46	1.38
82	EJ	201	PEB	C2C-C3C	2.80	1.46	1.38
87	AN	803	CLA	C3B-C4B	2.80	1.49	1.42
82	Q4	201	PEB	CHB-C1C	2.80	1.46	1.40
83	A4	302	PUB	OD-C4D	2.80	1.28	1.23
82	DD	202	PEB	C2C-C3C	2.79	1.46	1.38
82	d1	202	PEB	C2A-C1A	-2.79	1.49	1.52
82	T1	202	PEB	OD-C4D	2.79	1.28	1.23
82	FM	201	PEB	C1C-NC	-2.79	1.33	1.37
82	R5	201	PEB	C1C-NC	-2.79	1.33	1.37
82	T1	201	PEB	C4B-C3B	2.79	1.50	1.45
87	32	308	CLA	C3B-C4B	2.79	1.49	1.42
82	XB	201	PEB	OD-C4D	2.79	1.28	1.23
82	RH	201	PEB	OD-C4D	2.79	1.28	1.23
87	A2	825	CLA	C4B-NB	2.79	1.41	1.37
87	K2	103	CLA	C4B-NB	2.79	1.41	1.37
87	72	608	CLA	C4D-ND	-2.79	1.33	1.37
87	bL	622	CLA	C3B-C4B	2.79	1.49	1.42
82	T7	202	PEB	C1A-NA	-2.79	1.34	1.37
87	BN	827	CLA	MG-NB	-2.79	2.00	2.05
82	DF	203	PEB	OD-C4D	2.79	1.28	1.23
82	nK	202	PEB	OD-C4D	2.79	1.28	1.23
87	3N	307	CLA	C3B-C4B	2.79	1.49	1.42
82	d4	202	PEB	OD-C4D	2.79	1.28	1.23
82	V7	201	PEB	OD-C4D	2.79	1.28	1.23
87	22	602	CLA	C3B-C4B	2.79	1.49	1.42
87	5N	604	CLA	C3B-C4B	2.79	1.49	1.42
87	7N	608	CLA	C4D-ND	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	a1	201	PEB	C1A-NA	-2.79	1.34	1.37
82	dF	201	PEB	C1A-NA	-2.79	1.34	1.37
87	32	306	CLA	C3B-C4B	2.79	1.49	1.42
82	aM	201	PEB	OD-C4D	2.79	1.28	1.23
82	HE	1002	PEB	C2A-C1A	-2.79	1.49	1.52
82	fE	201	PEB	C2A-C1A	-2.79	1.49	1.52
83	ND	201	PUB	C4B-C3B	2.79	1.49	1.42
82	F9	201	PEB	CHB-C1C	2.79	1.46	1.40
87	c6	604	CLA	C3B-C4B	2.79	1.49	1.42
82	JF	202	PEB	OD-C4D	2.79	1.28	1.23
83	xF	305	PUB	OD-C4D	2.79	1.28	1.23
82	N7	203	PEB	CHB-C1C	2.79	1.46	1.40
87	AN	831	CLA	C4B-NB	2.79	1.41	1.37
87	A2	818	CLA	C3B-C4B	2.79	1.49	1.42
87	bL	618	CLA	MG-NB	-2.79	2.00	2.05
82	IK	203	PEB	CHA-C1B	2.79	1.47	1.40
82	g4	203	PEB	OD-C4D	2.79	1.28	1.23
82	nK	201	PEB	OD-C4D	2.79	1.28	1.23
83	AE	303	PUB	OA-C1A	2.79	1.28	1.23
82	GJ	203	PEB	C2C-C3C	2.79	1.46	1.38
82	HI	203	PEB	C2A-C1A	-2.79	1.49	1.52
84	D1	1003	CYC	C2C-C1C	-2.79	1.49	1.52
87	bL	604	CLA	C3B-C4B	2.79	1.49	1.42
84	JH	1003	CYC	C4D-C3D	2.79	1.49	1.42
84	D4	1001	CYC	C3D-C2D	2.79	1.46	1.38
87	CL	509	CLA	C4B-NB	2.79	1.41	1.37
82	CD	202	PEB	OD-C4D	2.79	1.28	1.23
82	JI	201	PEB	OD-C4D	2.79	1.28	1.23
82	bH	202	PEB	OD-C4D	2.79	1.28	1.23
82	TF	202	PEB	OD-C4D	2.79	1.28	1.23
82	OM	202	PEB	OD-C4D	2.79	1.28	1.23
82	YQ	202	PEB	OD-C4D	2.79	1.28	1.23
87	12	604	CLA	C3B-C4B	2.79	1.49	1.42
82	OG	203	PEB	C2C-C3C	2.79	1.46	1.38
82	XP	202	PEB	C2A-C1A	-2.79	1.49	1.52
82	R7	203	PEB	C1C-NC	-2.79	1.33	1.37
82	OA	201	PEB	CHB-C1C	2.79	1.46	1.40
82	AB	501	PEB	OD-C4D	2.79	1.28	1.23
82	OI	203	PEB	OD-C4D	2.79	1.28	1.23
82	WH	203	PEB	C2C-C3C	2.79	1.46	1.38
87	B6	603	CLA	C3B-C4B	2.79	1.49	1.42
82	JD	203	PEB	OD-C4D	2.79	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PQ	202	PEB	OD-C4D	2.79	1.28	1.23
82	jF	202	PEB	OD-C4D	2.79	1.28	1.23
82	vF	202	PEB	OD-C4D	2.79	1.28	1.23
82	fO	202	PEB	OD-C4D	2.79	1.28	1.23
82	OP	202	PEB	C2A-C1A	-2.79	1.49	1.52
82	X5	201	PEB	C1C-NC	-2.79	1.33	1.37
82	dF	202	PEB	OD-C4D	2.79	1.28	1.23
82	eK	202	PEB	OD-C4D	2.79	1.28	1.23
82	YO	202	PEB	C2C-C3C	2.79	1.46	1.38
87	BL	619	CLA	C3B-C4B	2.79	1.49	1.42
82	RK	202	PEB	OD-C4D	2.79	1.28	1.23
82	x8	202	PEB	OD-C4D	2.79	1.28	1.23
82	U9	202	PEB	OD-C4D	2.79	1.28	1.23
84	C1	1001	CYC	OB-C4B	2.79	1.28	1.23
87	AN	818	CLA	C3B-C4B	2.79	1.49	1.42
87	O2	203	CLA	C4B-NB	2.79	1.41	1.37
83	yK	303	PUB	C3B-C2B	2.79	1.46	1.38
82	RM	202	PEB	OD-C4D	2.79	1.28	1.23
82	V7	203	PEB	OD-C4D	2.79	1.28	1.23
82	K5	201	PEB	C1C-NC	-2.79	1.33	1.37
82	O7	202	PEB	C2C-C3C	2.79	1.46	1.38
82	YK	201	PEB	OD-C4D	2.79	1.28	1.23
82	D5	201	PEB	OD-C4D	2.79	1.28	1.23
82	IJ	202	PEB	C4A-NA	-2.79	1.31	1.37
87	cL	516	CLA	C4B-NB	2.79	1.41	1.37
82	HG	1002	PEB	C4B-C3B	2.78	1.50	1.45
82	DQ	202	PEB	C2C-C3C	2.78	1.46	1.38
82	R7	202	PEB	C2C-C3C	2.78	1.46	1.38
82	eG	201	PEB	OD-C4D	2.78	1.28	1.23
87	52	608	CLA	C4D-ND	-2.78	1.33	1.37
82	WG	203	PEB	C2C-C3C	2.78	1.46	1.38
87	CL	512	CLA	C4B-NB	2.78	1.41	1.37
87	2N	303	CLA	C3B-C4B	2.78	1.49	1.42
84	x3	1001	CYC	C4B-NB	-2.78	1.32	1.38
82	FA	203	PEB	OD-C4D	2.78	1.28	1.23
82	A4	305	PEB	OD-C4D	2.78	1.28	1.23
82	G9	201	PEB	OD-C4D	2.78	1.28	1.23
82	gJ	201	PEB	OD-C4D	2.78	1.28	1.23
82	D5	203	PEB	C2C-C3C	2.78	1.46	1.38
87	A2	816	CLA	C3B-C4B	2.78	1.49	1.42
82	Y4	202	PEB	C2A-C1A	-2.78	1.49	1.52
82	vK	202	PEB	OD-C4D	2.78	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	LN	206	CLA	C4B-NB	2.78	1.41	1.37
87	BN	830	CLA	C3B-C4B	2.78	1.49	1.42
87	1N	601	CLA	C3B-C4B	2.78	1.49	1.42
82	QJ	204	PEB	OD-C4D	2.78	1.28	1.23
82	fE	203	PEB	OD-C4D	2.78	1.28	1.23
82	dG	202	PEB	OD-C4D	2.78	1.28	1.23
82	y8	202	PEB	C2C-C3C	2.78	1.46	1.38
82	BD	203	PEB	CHA-C1B	2.78	1.46	1.40
82	UF	201	PEB	C4A-NA	-2.78	1.31	1.37
82	Z4	201	PEB	C4A-NA	-2.78	1.31	1.37
87	82	307	CLA	C3B-C4B	2.78	1.49	1.42
87	5N	603	CLA	C3B-C4B	2.78	1.49	1.42
87	5N	610	CLA	C3B-C4B	2.78	1.49	1.42
82	J5	202	PEB	OD-C4D	2.78	1.28	1.23
82	Y4	202	PEB	C2C-C3C	2.78	1.46	1.38
82	a4	202	PEB	C2C-C3C	2.78	1.46	1.38
82	WD	202	PEB	C2A-C1A	-2.78	1.49	1.52
82	mG	201	PEB	C2A-C1A	-2.78	1.49	1.52
82	i1	201	PEB	OD-C4D	2.78	1.28	1.23
82	mF	201	PEB	OD-C4D	2.78	1.28	1.23
82	jO	202	PEB	OD-C4D	2.78	1.28	1.23
87	A2	829	CLA	C3B-C4B	2.78	1.49	1.42
87	2N	312	CLA	C3B-C4B	2.78	1.49	1.42
82	WO	201	PEB	CHB-C1C	2.78	1.46	1.40
82	dK	202	PEB	OD-C4D	2.78	1.28	1.23
82	NJ	201	PEB	C1C-NC	-2.78	1.33	1.37
82	YB	202	PEB	C2A-C1A	-2.78	1.49	1.52
82	HA	203	PEB	OD-C4D	2.78	1.28	1.23
82	VK	201	PEB	OD-C4D	2.78	1.28	1.23
82	Z1	202	PEB	OD-C4D	2.78	1.28	1.23
82	fM	201	PEB	OD-C4D	2.78	1.28	1.23
82	L7	203	PEB	OD-C4D	2.78	1.28	1.23
87	bL	613	CLA	C3B-C4B	2.78	1.49	1.42
82	BJ	301	PEB	C1C-C2C	2.78	1.49	1.42
87	BN	806	CLA	C4B-NB	2.78	1.41	1.37
87	32	312	CLA	C3B-C4B	2.78	1.49	1.42
82	OK	202	PEB	CHB-C1C	2.78	1.46	1.40
82	KM	203	PEB	C2C-C3C	2.78	1.46	1.38
87	B2	806	CLA	C4B-NB	2.78	1.41	1.37
87	H6	102	CLA	C4B-NB	2.78	1.41	1.37
82	D9	201	PEB	OD-C4D	2.78	1.28	1.23
83	AO	302	PUB	OD-C4D	2.78	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	312	CLA	C4D-ND	-2.78	1.33	1.37
83	AQ	302	PUB	OD-C4D	2.78	1.28	1.23
87	BN	820	CLA	C3B-C4B	2.78	1.49	1.42
82	D9	201	PEB	CHB-C1C	2.78	1.46	1.40
82	VA	201	PEB	OD-C4D	2.78	1.28	1.23
82	YP	503	PEB	OD-C4D	2.78	1.28	1.23
82	UQ	202	PEB	OD-C4D	2.78	1.28	1.23
96	GN	201	HEM	FE-NC	2.78	2.04	1.95
82	qF	202	PEB	C4B-C3B	2.78	1.50	1.45
82	O5	201	PEB	C2A-C1A	-2.78	1.49	1.52
82	eG	202	PEB	OD-C4D	2.78	1.28	1.23
87	CL	507	CLA	C4B-NB	2.78	1.41	1.37
87	C6	517	CLA	C4B-NB	2.78	1.41	1.37
87	c6	607	CLA	C4B-NB	2.78	1.41	1.37
87	62	307	CLA	C3B-C4B	2.78	1.49	1.42
82	QB	203	PEB	OD-C4D	2.78	1.28	1.23
82	F7	201	PEB	OD-C4D	2.78	1.28	1.23
87	b6	610	CLA	C3B-C4B	2.78	1.49	1.42
82	SI	202	PEB	C2A-C1A	-2.78	1.49	1.52
82	AE	304	PEB	OD-C4D	2.78	1.28	1.23
82	fG	203	PEB	OD-C4D	2.78	1.28	1.23
83	AM	303	PUB	OA-C1A	2.78	1.28	1.23
82	jM	202	PEB	OD-C4D	2.78	1.28	1.23
82	O5	203	PEB	CHB-C1C	2.78	1.46	1.40
82	kM	202	PEB	C2A-C1A	-2.78	1.49	1.52
82	PG	202	PEB	OD-C4D	2.78	1.28	1.23
82	PM	201	PEB	C1C-NC	-2.78	1.33	1.37
82	N5	201	PEB	C1C-NC	-2.78	1.33	1.37
87	A6	404	CLA	C4B-NB	2.78	1.41	1.37
82	LD	202	PEB	OD-C4D	2.78	1.28	1.23
82	ZH	202	PEB	OD-C4D	2.78	1.28	1.23
82	O9	203	PEB	OD-C4D	2.78	1.28	1.23
82	U1	202	PEB	CHC-C4C	2.78	1.53	1.49
82	NJ	201	PEB	CHB-C1C	2.77	1.46	1.40
82	SQ	201	PEB	C1C-NC	-2.77	1.33	1.37
87	a6	608	CLA	C3B-C4B	2.77	1.49	1.42
82	j4	202	PEB	OD-C4D	2.77	1.28	1.23
87	2N	307	CLA	C3B-C4B	2.77	1.49	1.42
82	IF	203	PEB	CHA-C1B	2.77	1.46	1.40
82	U1	202	PEB	CHA-C1B	2.77	1.46	1.40
82	V9	201	PEB	OD-C4D	2.77	1.28	1.23
82	iM	201	PEB	OD-C4D	2.77	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	AM	304	PUB	OD-C4D	2.77	1.28	1.23
87	c6	612	CLA	C3B-C4B	2.77	1.49	1.42
82	GK	202	PEB	C2C-C3C	2.77	1.46	1.38
87	cL	512	CLA	C4B-NB	2.77	1.41	1.37
82	NQ	202	PEB	OD-C4D	2.77	1.28	1.23
82	WE	203	PEB	C2C-C3C	2.77	1.46	1.38
82	WQ	202	PEB	C2A-C1A	-2.77	1.49	1.52
82	m4	202	PEB	C2A-C1A	-2.77	1.49	1.52
87	5N	608	CLA	C4D-ND	-2.77	1.33	1.37
87	LN	206	CLA	C3B-C4B	2.77	1.49	1.42
82	QK	203	PEB	C4A-NA	-2.77	1.31	1.37
82	AE	301	PEB	OD-C4D	2.77	1.28	1.23
82	I7	201	PEB	C2A-C1A	-2.77	1.49	1.52
82	GK	201	PEB	C4A-NA	-2.77	1.31	1.37
82	NF	202	PEB	OD-C4D	2.77	1.28	1.23
82	PP	202	PEB	OD-C4D	2.77	1.28	1.23
82	lF	202	PEB	OD-C4D	2.77	1.28	1.23
87	1N	604	CLA	C3B-C4B	2.77	1.49	1.42
82	NP	202	PEB	OD-C4D	2.77	1.28	1.23
82	H5	203	PEB	OD-C4D	2.77	1.28	1.23
82	Q5	201	PEB	OD-C4D	2.77	1.28	1.23
82	y8	202	PEB	OD-C4D	2.77	1.28	1.23
82	jO	201	PEB	OD-C4D	2.77	1.28	1.23
87	BN	815	CLA	C4B-NB	2.77	1.41	1.37
84	JO	1001	CYC	C1B-NB	-2.77	1.33	1.37
82	PE	202	PEB	OD-C4D	2.77	1.28	1.23
87	62	313	CLA	C3B-C4B	2.77	1.49	1.42
82	JK	202	PEB	OD-C4D	2.77	1.28	1.23
82	F9	203	PEB	OD-C4D	2.77	1.28	1.23
82	AJ	302	PEB	OD-C4D	2.77	1.28	1.23
82	iH	201	PEB	OD-C4D	2.77	1.28	1.23
82	dH	202	PEB	OD-C4D	2.77	1.28	1.23
96	FL	102	HEM	FE-ND	-2.77	1.86	1.94
87	IN	103	CLA	C4B-NB	2.77	1.41	1.37
87	32	308	CLA	C4B-NB	2.77	1.41	1.37
84	x3	1001	CYC	C1B-C2B	2.77	1.50	1.45
83	AH	304	PUB	OD-C4D	2.77	1.28	1.23
83	wK	304	PUB	OD-C4D	2.77	1.28	1.23
87	DL	406	CLA	C3B-C4B	2.77	1.49	1.42
87	6N	612	CLA	C3B-C4B	2.77	1.49	1.42
87	B6	616	CLA	CMB-C2B	-2.77	1.44	1.50
82	M7	201	PEB	C2A-C1A	-2.77	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	CL	504	CLA	MG-NB	-2.77	2.00	2.05
82	WI	203	PEB	OD-C4D	2.77	1.28	1.23
82	yC	202	PEB	OD-C4D	2.77	1.28	1.23
82	aE	202	PEB	OD-C4D	2.77	1.28	1.23
82	lK	202	PEB	OD-C4D	2.77	1.28	1.23
87	72	605	CLA	C3B-C4B	2.77	1.49	1.42
82	l1	203	PEB	C4B-C3B	2.77	1.50	1.45
82	MK	201	PEB	OD-C4D	2.77	1.28	1.23
87	12	601	CLA	C3B-C4B	2.77	1.49	1.42
87	AN	825	CLA	C4B-NB	2.77	1.41	1.37
87	52	605	CLA	C3B-C4B	2.77	1.49	1.42
87	5N	606	CLA	C3B-C4B	2.77	1.49	1.42
82	g4	201	PEB	OD-C4D	2.77	1.28	1.23
82	mO	203	PEB	OD-C4D	2.77	1.28	1.23
84	DH	1001	CYC	OB-C4B	2.77	1.28	1.23
87	52	604	CLA	C3B-C4B	2.77	1.49	1.42
87	A2	803	CLA	C3B-C4B	2.77	1.49	1.42
82	tC	202	PEB	OD-C4D	2.77	1.28	1.23
82	pF	202	PEB	OD-C4D	2.77	1.28	1.23
87	12	602	CLA	C4D-ND	-2.77	1.33	1.37
82	bH	201	PEB	OD-C4D	2.77	1.28	1.23
84	L1	1001	CYC	C4B-NB	-2.77	1.32	1.38
87	62	302	CLA	C3B-C4B	2.77	1.49	1.42
82	ZK	201	PEB	OD-C4D	2.77	1.28	1.23
87	BN	822	CLA	C3B-C4B	2.77	1.49	1.42
87	8N	307	CLA	C3B-C4B	2.77	1.49	1.42
82	HB	202	PEB	OD-C4D	2.77	1.28	1.23
82	fJ	201	PEB	OD-C4D	2.77	1.28	1.23
82	Y9	202	PEB	C2A-C1A	-2.77	1.49	1.52
82	RA	202	PEB	C2C-C3C	2.77	1.46	1.38
87	A2	810	CLA	C1D-ND	2.77	1.41	1.37
87	B6	616	CLA	C4B-NB	2.77	1.41	1.37
87	BL	606	CLA	C3B-C4B	2.77	1.49	1.42
82	XM	202	PEB	OD-C4D	2.77	1.28	1.23
95	c6	601	DGD	O6D-C5D	-2.77	1.37	1.44
87	52	606	CLA	C3B-C4B	2.76	1.49	1.42
87	c6	606	CLA	C3B-C4B	2.76	1.49	1.42
82	X7	203	PEB	C1C-NC	-2.76	1.33	1.37
82	WD	202	PEB	OD-C4D	2.76	1.28	1.23
82	UH	202	PEB	OD-C4D	2.76	1.28	1.23
82	bF	202	PEB	OD-C4D	2.76	1.28	1.23
87	22	607	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6N	606	CLA	C3B-C4B	2.76	1.49	1.42
87	B2	821	CLA	C3B-C4B	2.76	1.49	1.42
87	J2	101	CLA	C3B-C4B	2.76	1.49	1.42
87	BN	833	CLA	C4B-NB	2.76	1.41	1.37
96	G2	201	HEM	FE-NC	2.76	2.04	1.95
82	eG	203	PEB	OD-C4D	2.76	1.28	1.23
82	mK	202	PEB	C2A-C1A	-2.76	1.49	1.52
82	LB	201	PEB	OD-C4D	2.76	1.28	1.23
82	ZM	201	PEB	OD-C4D	2.76	1.28	1.23
82	L7	202	PEB	C2C-C3C	2.76	1.46	1.38
82	C9	201	PEB	OD-C4D	2.76	1.28	1.23
87	BL	621	CLA	C4B-NB	2.76	1.41	1.37
84	LG	1001	CYC	C1B-NB	-2.76	1.33	1.37
82	UB	303	PEB	C2A-C1A	-2.76	1.49	1.52
82	V1	201	PEB	C2A-C1A	-2.76	1.49	1.52
82	lO	201	PEB	C2A-C1A	-2.76	1.49	1.52
82	JQ	203	PEB	OD-C4D	2.76	1.28	1.23
82	L5	201	PEB	OD-C4D	2.76	1.28	1.23
82	gB	203	PEB	OD-C4D	2.76	1.28	1.23
82	B5	201	PEB	C1C-NC	-2.76	1.33	1.37
82	ZB	202	PEB	OD-C4D	2.76	1.28	1.23
82	DP	202	PEB	OD-C4D	2.76	1.28	1.23
87	AN	810	CLA	C1D-ND	2.76	1.41	1.37
87	5N	605	CLA	C3B-C4B	2.76	1.49	1.42
82	RQ	201	PEB	OD-C4D	2.76	1.28	1.23
82	f4	201	PEB	OD-C4D	2.76	1.28	1.23
82	bK	202	PEB	OD-C4D	2.76	1.28	1.23
82	OI	202	PEB	C4B-NB	-2.76	1.32	1.38
87	AN	829	CLA	C3B-C4B	2.76	1.49	1.42
82	B5	202	PEB	C2A-C1A	-2.76	1.49	1.52
82	GJ	202	PEB	OD-C4D	2.76	1.28	1.23
82	b1	201	PEB	OD-C4D	2.76	1.28	1.23
82	P9	201	PEB	OD-C4D	2.76	1.28	1.23
87	AN	824	CLA	C3B-C4B	2.76	1.49	1.42
82	AF	201	PEB	OD-C4D	2.76	1.28	1.23
82	Y9	203	PEB	OD-C4D	2.76	1.28	1.23
82	QO	201	PEB	CHB-C1C	2.76	1.46	1.40
82	YM	201	PEB	C2C-C3C	2.76	1.46	1.38
87	AN	816	CLA	C3B-C4B	2.76	1.49	1.42
87	72	603	CLA	C3B-C4B	2.76	1.49	1.42
82	e1	202	PEB	OD-C4D	2.76	1.28	1.23
82	g4	202	PEB	OD-C4D	2.76	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S9	203	PEB	OD-C4D	2.76	1.28	1.23
82	eM	202	PEB	OD-C4D	2.76	1.28	1.23
82	lM	203	PEB	OD-C4D	2.76	1.28	1.23
82	gO	202	PEB	OD-C4D	2.76	1.28	1.23
83	wF	304	PUB	OD-C4D	2.76	1.28	1.23
87	A2	801	CLA	C4B-NB	2.76	1.41	1.37
82	VA	202	PEB	OD-C4D	2.76	1.28	1.23
82	DF	201	PEB	OD-C4D	2.76	1.28	1.23
82	DM	202	PEB	C2A-C1A	-2.76	1.49	1.52
82	LP	202	PEB	C2A-C1A	-2.76	1.49	1.52
82	kJ	201	PEB	C2A-C1A	-2.76	1.49	1.52
82	KF	201	PEB	C2C-C3C	2.76	1.46	1.38
87	52	603	CLA	C3B-C4B	2.76	1.49	1.42
87	A2	808	CLA	C4B-NB	2.76	1.41	1.37
82	kJ	202	PEB	OD-C4D	2.76	1.28	1.23
87	B2	806	CLA	C1B-C2B	2.76	1.49	1.43
82	XA	203	PEB	C4A-NA	-2.76	1.31	1.37
82	NA	203	PEB	CHB-C1C	2.76	1.46	1.40
87	AN	828	CLA	CMD-C2D	-2.76	1.45	1.50
82	U1	203	PEB	OD-C4D	2.76	1.28	1.23
82	R9	201	PEB	OD-C4D	2.76	1.28	1.23
82	yK	301	PEB	OD-C4D	2.76	1.28	1.23
87	B2	824	CLA	C3B-C4B	2.76	1.49	1.42
82	JQ	201	PEB	C2A-C1A	-2.76	1.49	1.52
82	l4	201	PEB	C2A-C1A	-2.76	1.49	1.52
82	zC	202	PEB	C4B-C3B	2.76	1.50	1.45
82	KI	201	PEB	C1D-ND	2.76	1.49	1.45
82	A9	201	PEB	OD-C4D	2.76	1.28	1.23
82	dE	204	PEB	OD-C4D	2.76	1.28	1.23
82	KI	201	PEB	C1A-NA	-2.76	1.34	1.37
82	YP	503	PEB	C2A-C1A	-2.76	1.49	1.52
82	h1	202	PEB	CHC-C4C	2.76	1.53	1.49
82	QB	204	PEB	OD-C4D	2.76	1.28	1.23
82	QE	202	PEB	OD-C4D	2.76	1.28	1.23
82	XM	201	PEB	OD-C4D	2.76	1.28	1.23
82	UK	201	PEB	CHB-C4B	2.76	1.44	1.38
82	ZH	201	PEB	C2C-C3C	2.76	1.46	1.38
82	A4	304	PEB	OD-C4D	2.75	1.28	1.23
82	I7	201	PEB	OD-C4D	2.75	1.28	1.23
82	EQ	202	PEB	OD-C4D	2.75	1.28	1.23
82	lJ	203	PEB	OD-C4D	2.75	1.28	1.23
83	A1	304	PUB	OD-C4D	2.75	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	TP	201	PEB	C4B-C3B	2.75	1.50	1.45
82	FA	202	PEB	C1C-C2C	2.75	1.49	1.42
87	a6	609	CLA	C4B-NB	2.75	1.41	1.37
82	dH	202	PEB	C2A-C1A	-2.75	1.49	1.52
82	RJ	202	PEB	OD-C4D	2.75	1.28	1.23
82	T9	201	PEB	OD-C4D	2.75	1.28	1.23
82	yC	202	PEB	C2C-C3C	2.75	1.46	1.38
87	RN	202	CLA	C4D-ND	-2.75	1.33	1.37
82	Y5	203	PEB	OD-C4D	2.75	1.28	1.23
82	nF	201	PEB	OD-C4D	2.75	1.28	1.23
83	Z9	305	PUB	OA-C1A	2.75	1.28	1.23
87	1N	608	CLA	C3B-C4B	2.75	1.49	1.42
82	XF	203	PEB	OD-C4D	2.75	1.28	1.23
82	y8	203	PEB	OD-C4D	2.75	1.28	1.23
82	QA	201	PEB	C4A-NA	-2.75	1.31	1.37
87	12	608	CLA	C3B-C4B	2.75	1.49	1.42
82	jJ	201	PEB	C2A-C1A	-2.75	1.49	1.52
82	QE	201	PEB	C2C-C3C	2.75	1.46	1.38
82	Z1	201	PEB	C2C-C3C	2.75	1.46	1.38
82	L4	1002	PEB	OD-C4D	2.75	1.28	1.23
87	72	602	CLA	C4B-NB	2.75	1.41	1.37
87	5N	606	CLA	C4B-NB	2.75	1.41	1.37
87	32	310	CLA	C3B-C4B	2.75	1.49	1.42
82	BK	202	PEB	OD-C4D	2.75	1.28	1.23
82	IQ	201	PEB	OD-C4D	2.75	1.28	1.23
83	M5	302	PUB	OA-C1A	2.75	1.28	1.23
82	1C	201	PEB	C4B-C3B	2.75	1.50	1.45
82	lK	202	PEB	CHC-C4C	2.75	1.53	1.49
87	3N	306	CLA	C4B-NB	2.75	1.41	1.37
82	SD	201	PEB	OD-C4D	2.75	1.28	1.23
82	TM	201	PEB	OD-C4D	2.75	1.28	1.23
82	K9	201	PEB	OD-C4D	2.75	1.28	1.23
82	N9	201	PEB	OD-C4D	2.75	1.28	1.23
82	kK	201	PEB	OD-C4D	2.75	1.28	1.23
82	eO	201	PEB	OD-C4D	2.75	1.28	1.23
82	iH	201	PEB	C2A-C1A	-2.75	1.49	1.52
87	B2	829	CLA	C3B-C4B	2.75	1.49	1.42
82	TM	201	PEB	C1C-NC	-2.75	1.33	1.37
82	P5	201	PEB	C1C-NC	-2.75	1.33	1.37
84	LG	1001	CYC	C4B-NB	-2.75	1.32	1.38
82	WM	202	PEB	OD-C4D	2.75	1.28	1.23
82	kF	201	PEB	OD-C4D	2.75	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	805	CLA	C3B-C4B	2.75	1.49	1.42
87	BN	807	CLA	C4B-NB	2.75	1.41	1.37
82	XD	202	PEB	OD-C4D	2.75	1.28	1.23
82	sF	201	PEB	OD-C4D	2.75	1.28	1.23
82	kJ	201	PEB	OD-C4D	2.75	1.28	1.23
82	jK	202	PEB	OD-C4D	2.75	1.28	1.23
82	kO	201	PEB	OD-C4D	2.75	1.28	1.23
82	PA	203	PEB	C2A-C1A	-2.75	1.49	1.52
82	Q5	201	PEB	C1C-NC	-2.75	1.33	1.37
87	A2	802	CLA	C4B-NB	2.75	1.41	1.37
84	HG	1001	CYC	C3D-C2D	2.75	1.46	1.38
82	E9	201	PEB	OD-C4D	2.75	1.28	1.23
82	LE	1002	PEB	C2A-C1A	-2.75	1.49	1.52
82	HF	202	PEB	C2A-C1A	-2.75	1.49	1.52
82	UG	201	PEB	C2A-C1A	-2.75	1.49	1.52
82	EM	201	PEB	C2A-C1A	-2.75	1.49	1.52
82	fJ	201	PEB	C2A-C1A	-2.75	1.49	1.52
82	ID	201	PEB	OD-C4D	2.75	1.28	1.23
82	MP	201	PEB	OD-C4D	2.75	1.28	1.23
82	qC	201	PEB	OD-C4D	2.75	1.28	1.23
82	cO	202	PEB	OD-C4D	2.75	1.28	1.23
82	U5	201	PEB	C4B-C3B	2.75	1.50	1.45
82	UJ	202	PEB	C4A-NA	-2.75	1.31	1.37
87	42	607	CLA	C3B-C4B	2.75	1.49	1.42
82	tF	201	PEB	OD-C4D	2.75	1.28	1.23
82	kM	202	PEB	OD-C4D	2.75	1.28	1.23
82	PG	201	PEB	C1C-NC	-2.75	1.33	1.37
82	HE	1002	PEB	C4B-C3B	2.75	1.50	1.45
82	UH	202	PEB	CHA-C1B	2.75	1.46	1.40
87	CL	514	CLA	C3B-C4B	2.75	1.49	1.42
87	CL	508	CLA	C4B-NB	2.75	1.41	1.37
87	d6	401	CLA	C4B-NB	2.75	1.41	1.37
82	lE	203	PEB	OD-C4D	2.75	1.28	1.23
82	eF	202	PEB	OD-C4D	2.75	1.28	1.23
82	cJ	202	PEB	OD-C4D	2.75	1.28	1.23
82	gK	201	PEB	OD-C4D	2.75	1.28	1.23
82	bO	202	PEB	OD-C4D	2.75	1.28	1.23
87	82	308	CLA	CMD-C2D	-2.75	1.45	1.50
87	7N	603	CLA	C3B-C4B	2.75	1.49	1.42
82	VD	203	PEB	CHC-C4C	2.75	1.53	1.49
87	1N	602	CLA	C4D-ND	-2.74	1.33	1.37
87	BN	807	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WI	201	PEB	OD-C4D	2.74	1.28	1.23
87	bL	606	CLA	CMB-C2B	-2.74	1.45	1.50
82	TB	201	PEB	CHB-C1C	2.74	1.46	1.40
82	dE	203	PEB	OD-C4D	2.74	1.28	1.23
82	KA	201	PEB	OD-C4D	2.74	1.28	1.23
82	SQ	202	PEB	OD-C4D	2.74	1.28	1.23
82	hJ	203	PEB	OD-C4D	2.74	1.28	1.23
87	A2	832	CLA	C4B-NB	2.74	1.41	1.37
82	GF	202	PEB	C2C-C3C	2.74	1.46	1.38
87	A2	851	CLA	C3B-C4B	2.74	1.49	1.42
82	JB	201	PEB	CHB-C1C	2.74	1.46	1.40
82	NI	203	PEB	CHA-C1B	2.74	1.46	1.40
87	3N	310	CLA	C3B-C4B	2.74	1.49	1.42
84	E1	1001	CYC	C4C-NC	-2.74	1.31	1.37
87	B2	818	CLA	CMB-C2B	-2.74	1.45	1.50
82	JM	201	PEB	OD-C4D	2.74	1.28	1.23
82	TO	203	PEB	OD-C4D	2.74	1.28	1.23
83	AJ	303	PUB	OA-C1A	2.74	1.28	1.23
82	I9	201	PEB	OD-C4D	2.74	1.28	1.23
82	jF	201	PEB	OD-C4D	2.74	1.28	1.23
87	AN	831	CLA	MG-NB	-2.74	2.00	2.05
87	B2	834	CLA	C3B-C4B	2.74	1.49	1.42
82	K7	201	PEB	OD-C4D	2.74	1.28	1.23
87	82	301	CLA	CMD-C2D	-2.74	1.45	1.50
82	LP	202	PEB	OD-C4D	2.74	1.28	1.23
82	X7	202	PEB	CHA-C1B	2.74	1.46	1.40
82	w8	201	PEB	C4B-C3B	2.74	1.50	1.45
82	cF	201	PEB	CHC-C4C	2.74	1.53	1.49
82	MF	201	PEB	OD-C4D	2.74	1.28	1.23
87	A2	828	CLA	C4D-ND	-2.74	1.33	1.37
87	AN	851	CLA	C4B-NB	2.74	1.41	1.37
82	UF	201	PEB	CHB-C4B	2.74	1.44	1.38
87	AN	828	CLA	C4D-ND	-2.74	1.33	1.37
82	ZM	201	PEB	C1C-NC	-2.74	1.33	1.37
82	RM	201	PEB	OD-C4D	2.74	1.28	1.23
96	VL	201	HEM	FE-ND	-2.74	1.86	1.94
82	PH	202	PEB	OD-C4D	2.74	1.28	1.23
82	b1	202	PEB	OD-C4D	2.74	1.28	1.23
82	i4	202	PEB	OD-C4D	2.74	1.28	1.23
82	fM	203	PEB	OD-C4D	2.74	1.28	1.23
82	VO	202	PEB	C2A-C1A	-2.74	1.49	1.52
82	TQ	202	PEB	C2A-C1A	-2.74	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WM	203	PEB	C2C-C3C	2.74	1.46	1.38
87	ON	202	CLA	C3B-C4B	2.74	1.49	1.42
82	RG	201	PEB	OD-C4D	2.74	1.28	1.23
82	CQ	202	PEB	OD-C4D	2.74	1.28	1.23
87	72	604	CLA	C3B-C4B	2.74	1.49	1.42
82	sK	203	PEB	CHC-C4C	2.74	1.53	1.49
82	LA	203	PEB	OD-C4D	2.74	1.28	1.23
82	jK	201	PEB	OD-C4D	2.74	1.28	1.23
82	kK	202	PEB	C4B-C3B	2.74	1.50	1.45
87	2N	310	CLA	C3B-C4B	2.74	1.49	1.42
82	TE	201	PEB	OD-C4D	2.74	1.28	1.23
82	iG	202	PEB	OD-C4D	2.74	1.28	1.23
82	PJ	201	PEB	C2A-C1A	-2.74	1.49	1.52
84	LH	1002	CYC	C4B-NB	-2.74	1.32	1.38
87	DL	403	CLA	C4B-NB	2.74	1.41	1.37
82	RF	202	PEB	OD-C4D	2.74	1.28	1.23
82	WF	202	PEB	OD-C4D	2.74	1.28	1.23
83	AD	302	PUB	OD-C4D	2.74	1.28	1.23
83	AM	304	PUB	OA-C1A	2.74	1.28	1.23
82	TB	201	PEB	OD-C4D	2.74	1.28	1.23
82	RE	201	PEB	OD-C4D	2.74	1.28	1.23
82	U4	202	PEB	OD-C4D	2.74	1.28	1.23
87	52	606	CLA	C4B-NB	2.74	1.41	1.37
82	NQ	203	PEB	C1A-NA	-2.74	1.34	1.37
82	J7	202	PEB	C1A-NA	-2.74	1.34	1.37
82	TH	202	PEB	OD-C4D	2.74	1.28	1.23
84	CH	1001	CYC	OB-C4B	2.74	1.28	1.23
87	BN	825	CLA	C3B-C4B	2.74	1.49	1.42
87	3N	313	CLA	C3B-C4B	2.74	1.49	1.42
82	EQ	201	PEB	C1C-NC	-2.73	1.33	1.37
82	PD	202	PEB	OD-C4D	2.73	1.28	1.23
87	bL	617	CLA	C1D-ND	2.73	1.41	1.37
87	MN	101	CLA	C3B-C4B	2.73	1.49	1.42
87	M2	101	CLA	C3B-C4B	2.73	1.49	1.42
84	E1	1001	CYC	C1B-NB	-2.73	1.33	1.37
82	iE	202	PEB	OD-C4D	2.73	1.28	1.23
82	aG	202	PEB	OD-C4D	2.73	1.28	1.23
82	mM	201	PEB	OD-C4D	2.73	1.28	1.23
83	QM	201	PUB	OA-C1A	2.73	1.28	1.23
82	18	201	PEB	C4B-C3B	2.73	1.50	1.45
87	JN	101	CLA	C3B-C4B	2.73	1.49	1.42
82	CD	201	PEB	OD-C4D	2.73	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CM	202	PEB	OD-C4D	2.73	1.28	1.23
82	YJ	202	PEB	C4A-NA	-2.73	1.31	1.37
82	IA	201	PEB	C2A-C1A	-2.73	1.49	1.52
82	HG	1002	PEB	C2A-C1A	-2.73	1.49	1.52
82	TM	201	PEB	C2A-C1A	-2.73	1.49	1.52
82	iM	201	PEB	C2A-C1A	-2.73	1.49	1.52
87	AN	851	CLA	C3B-C4B	2.73	1.49	1.42
87	B2	819	CLA	C3B-C4B	2.73	1.49	1.42
87	7N	604	CLA	C3B-C4B	2.73	1.49	1.42
82	eJ	201	PEB	C1C-NC	-2.73	1.33	1.37
82	VM	202	PEB	OD-C4D	2.73	1.28	1.23
83	AH	304	PUB	OA-C1A	2.73	1.28	1.23
87	bL	620	CLA	C3B-C4B	2.73	1.49	1.42
87	7N	605	CLA	C3B-C4B	2.73	1.49	1.42
82	WJ	203	PEB	C4A-NA	-2.73	1.31	1.37
82	XP	201	PEB	OD-C4D	2.73	1.28	1.23
82	P7	203	PEB	OD-C4D	2.73	1.28	1.23
82	uF	202	PEB	OD-C4D	2.73	1.28	1.23
82	hM	202	PEB	OD-C4D	2.73	1.28	1.23
82	P1	202	PEB	OD-C4D	2.73	1.28	1.23
82	J5	201	PEB	OD-C4D	2.73	1.28	1.23
87	AN	849	CLA	CMC-C2C	-2.73	1.45	1.50
87	BN	819	CLA	CMB-C2B	-2.73	1.45	1.50
82	SB	203	PEB	OD-C4D	2.73	1.28	1.23
82	dB	202	PEB	OD-C4D	2.73	1.28	1.23
84	W3	1001	CYC	C4D-C3D	2.73	1.49	1.42
87	BN	829	CLA	C3B-C4B	2.73	1.49	1.42
82	xF	304	PEB	C4B-C3B	2.73	1.50	1.45
82	IQ	201	PEB	C1C-NC	-2.73	1.33	1.37
83	QJ	201	PUB	C4B-NB	-2.73	1.33	1.37
84	EH	1001	CYC	C1B-NB	-2.73	1.33	1.37
82	EJ	203	PEB	OD-C4D	2.73	1.28	1.23
82	HB	201	PEB	CHC-C4C	2.73	1.53	1.49
82	SE	202	PEB	C2C-C3C	2.73	1.46	1.38
87	BN	834	CLA	MG-NB	-2.73	2.00	2.05
87	42	609	CLA	C3B-C4B	2.73	1.49	1.42
87	8N	305	CLA	C3B-C4B	2.73	1.49	1.42
82	QG	202	PEB	OD-C4D	2.73	1.28	1.23
82	lO	201	PEB	OD-C4D	2.73	1.28	1.23
82	TD	201	PEB	C1D-ND	2.73	1.49	1.45
82	YA	301	PEB	C2A-C1A	-2.73	1.49	1.52
84	M1	201	CYC	C4D-C3D	2.73	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	824	CLA	C3B-C4B	2.73	1.49	1.42
87	7N	610	CLA	C3B-C4B	2.73	1.49	1.42
82	fF	201	PEB	OD-C4D	2.73	1.28	1.23
82	mF	202	PEB	OD-C4D	2.73	1.28	1.23
82	IK	201	PEB	C3B-C2B	2.73	1.42	1.36
84	63	901	CYC	C3D-C2D	2.73	1.46	1.38
82	VH	201	PEB	C2A-C1A	-2.73	1.49	1.52
82	D5	201	PEB	CHB-C1C	2.73	1.46	1.40
82	LA	202	PEB	OD-C4D	2.73	1.28	1.23
82	UH	203	PEB	OD-C4D	2.73	1.28	1.23
82	Y1	201	PEB	OD-C4D	2.73	1.28	1.23
87	KN	105	CLA	C3B-C4B	2.73	1.49	1.42
82	SP	201	PEB	C1C-NC	-2.73	1.33	1.37
82	R4	202	PEB	OD-C4D	2.73	1.28	1.23
83	A1	304	PUB	OA-C1A	2.73	1.28	1.23
82	VA	202	PEB	C2C-C3C	2.73	1.46	1.38
82	TM	202	PEB	OD-C4D	2.73	1.28	1.23
82	eE	202	PEB	OD-C4D	2.73	1.28	1.23
87	AN	805	CLA	C3B-C4B	2.73	1.49	1.42
87	4N	609	CLA	C3B-C4B	2.73	1.49	1.42
87	32	313	CLA	C3B-C4B	2.73	1.49	1.42
82	UE	201	PEB	C2A-C1A	-2.73	1.49	1.52
82	W5	201	PEB	C2A-C1A	-2.73	1.49	1.52
87	8N	302	CLA	CMD-C2D	-2.73	1.45	1.50
82	F7	202	PEB	C1A-NA	-2.73	1.34	1.37
82	cE	202	PEB	OD-C4D	2.73	1.28	1.23
83	xF	306	PUB	OD-C4D	2.73	1.28	1.23
82	D7	201	PEB	OD-C4D	2.73	1.28	1.23
82	W5	202	PEB	C4B-C3B	2.73	1.50	1.45
87	BN	819	CLA	MG-NB	-2.72	2.00	2.05
87	B2	818	CLA	MG-NB	-2.72	2.00	2.05
96	vL	201	HEM	FE-ND	-2.72	1.86	1.94
87	A2	851	CLA	C4B-NB	2.72	1.41	1.37
82	YE	202	PEB	OD-C4D	2.72	1.28	1.23
82	PG	201	PEB	OD-C4D	2.72	1.28	1.23
82	aJ	203	PEB	OD-C4D	2.72	1.28	1.23
82	LD	201	PEB	OD-C4D	2.72	1.28	1.23
82	UO	202	PEB	OD-C4D	2.72	1.28	1.23
82	L7	202	PEB	C2A-C1A	-2.72	1.49	1.52
82	PB	201	PEB	OD-C4D	2.72	1.28	1.23
82	SI	202	PEB	OD-C4D	2.72	1.28	1.23
82	hK	201	PEB	OD-C4D	2.72	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BQ	203	PEB	C2C-C3C	2.72	1.46	1.38
87	AN	810	CLA	C4B-NB	2.72	1.41	1.37
87	B2	805	CLA	C4B-NB	2.72	1.41	1.37
82	VE	201	PEB	OD-C4D	2.72	1.28	1.23
87	d6	406	CLA	C3B-C4B	2.72	1.49	1.42
87	6N	601	CLA	C3B-C4B	2.72	1.49	1.42
82	BP	201	PEB	C2A-C1A	-2.72	1.49	1.52
87	AN	840	CLA	C3B-C4B	2.72	1.49	1.42
87	72	610	CLA	C3B-C4B	2.72	1.49	1.42
82	J9	202	PEB	OD-C4D	2.72	1.28	1.23
82	rK	201	PEB	OD-C4D	2.72	1.28	1.23
87	BN	834	CLA	C3B-C4B	2.72	1.49	1.42
82	dF	202	PEB	C1C-NC	-2.72	1.33	1.37
82	PJ	202	PEB	OD-C4D	2.72	1.28	1.23
82	sF	203	PEB	C4B-C3B	2.72	1.50	1.45
82	VQ	203	PEB	CHC-C4C	2.72	1.53	1.49
82	OK	201	PEB	C2A-C1A	-2.72	1.49	1.52
82	cG	201	PEB	C2A-C1A	-2.72	1.49	1.52
87	BL	622	CLA	C3B-C4B	2.72	1.49	1.42
87	K2	106	CLA	C3B-C4B	2.72	1.49	1.42
82	IM	201	PEB	OD-C4D	2.72	1.28	1.23
87	A2	849	CLA	CMC-C2C	-2.72	1.45	1.50
82	WK	202	PEB	C2A-C1A	-2.72	1.49	1.52
82	OP	203	PEB	C2A-C1A	-2.72	1.49	1.52
82	RG	202	PEB	OD-C4D	2.72	1.28	1.23
82	XJ	201	PEB	OD-C4D	2.72	1.28	1.23
82	HI	202	PEB	CHB-C1C	2.72	1.46	1.40
87	BN	826	CLA	C3B-C4B	2.72	1.49	1.42
87	O2	203	CLA	C3B-C4B	2.72	1.49	1.42
84	V3	1001	CYC	C1B-C2B	2.72	1.50	1.45
82	d1	201	PEB	OD-C4D	2.72	1.28	1.23
82	H7	203	PEB	OD-C4D	2.72	1.28	1.23
82	w8	203	PEB	OD-C4D	2.72	1.28	1.23
82	J9	201	PEB	OD-C4D	2.72	1.28	1.23
95	C6	502	DGD	O6D-C5D	-2.72	1.37	1.44
87	4N	607	CLA	C3B-C4B	2.72	1.49	1.42
82	EF	202	PEB	C2A-C1A	-2.72	1.49	1.52
82	DK	203	PEB	OD-C4D	2.72	1.28	1.23
82	W5	201	PEB	OD-C4D	2.72	1.28	1.23
82	MD	201	PEB	C1C-C2C	2.72	1.49	1.42
82	SD	201	PEB	C1C-NC	-2.72	1.33	1.37
87	CL	505	CLA	C3B-C4B	2.72	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AM	302	PEB	OD-C4D	2.72	1.28	1.23
82	QQ	201	PEB	OD-C4D	2.72	1.28	1.23
82	HD	201	PEB	CHA-C1B	2.72	1.46	1.40
83	xF	306	PUB	C4B-NB	-2.72	1.33	1.37
82	VM	201	PEB	CHC-C4C	2.72	1.53	1.49
82	YG	202	PEB	OD-C4D	2.72	1.28	1.23
82	JJ	202	PEB	OD-C4D	2.72	1.28	1.23
82	PO	201	PEB	OD-C4D	2.72	1.28	1.23
82	i1	202	PEB	OD-C4D	2.72	1.28	1.23
87	H6	102	CLA	C3B-C4B	2.72	1.49	1.42
87	A2	831	CLA	C1B-NB	-2.72	1.34	1.37
87	ON	203	CLA	C3B-C4B	2.72	1.49	1.42
87	82	304	CLA	C3B-C4B	2.72	1.49	1.42
84	L4	1001	CYC	C1B-NB	-2.72	1.33	1.37
82	BF	202	PEB	C2A-C1A	-2.72	1.49	1.52
82	SJ	203	PEB	OD-C4D	2.72	1.28	1.23
82	TK	202	PEB	OD-C4D	2.72	1.28	1.23
82	aB	201	PEB	OD-C4D	2.72	1.28	1.23
82	dE	202	PEB	OD-C4D	2.72	1.28	1.23
82	iO	202	PEB	OD-C4D	2.72	1.28	1.23
83	QJ	201	PUB	OA-C1A	2.72	1.28	1.23
83	AO	302	PUB	OA-C1A	2.72	1.28	1.23
83	A4	302	PUB	OA-C1A	2.72	1.28	1.23
82	JA	203	PEB	C4B-C3B	2.72	1.50	1.45
82	HJ	202	PEB	OD-C4D	2.72	1.28	1.23
82	LJ	202	PEB	OD-C4D	2.72	1.28	1.23
82	RP	202	PEB	OD-C4D	2.72	1.28	1.23
82	JQ	201	PEB	OD-C4D	2.72	1.28	1.23
87	B2	836	CLA	C4B-NB	2.72	1.41	1.37
82	kM	201	PEB	CHC-C4C	2.72	1.53	1.49
82	KK	201	PEB	C2C-C3C	2.72	1.46	1.38
87	62	310	CLA	C4D-ND	-2.72	1.34	1.37
82	BB	201	PEB	OD-C4D	2.72	1.28	1.23
82	QB	203	PEB	C2A-C1A	-2.72	1.49	1.52
82	VI	203	PEB	CHB-C1C	2.72	1.46	1.40
87	C6	518	CLA	C3B-C4B	2.72	1.49	1.42
82	ND	202	PEB	OD-C4D	2.72	1.28	1.23
82	XQ	202	PEB	OD-C4D	2.72	1.28	1.23
82	II	203	PEB	C4B-NB	-2.72	1.32	1.38
87	B2	830	CLA	C3B-C4B	2.72	1.49	1.42
82	DM	202	PEB	OD-C4D	2.72	1.28	1.23
87	BN	813	CLA	C4B-NB	2.72	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	812	CLA	C4B-NB	2.72	1.41	1.37
82	WF	202	PEB	C2A-C1A	-2.72	1.49	1.52
84	J4	1001	CYC	C1B-NB	-2.72	1.33	1.37
82	AD	301	PEB	OD-C4D	2.71	1.28	1.23
83	AH	303	PUB	OD-C4D	2.71	1.28	1.23
87	aL	606	CLA	C4B-NB	2.71	1.41	1.37
82	cK	203	PEB	C2C-C3C	2.71	1.46	1.38
87	A2	838	CLA	C3B-C4B	2.71	1.49	1.42
87	bL	615	CLA	C3B-C4B	2.71	1.49	1.42
82	JI	201	PEB	C4B-C3B	2.71	1.50	1.45
82	TP	201	PEB	OD-C4D	2.71	1.28	1.23
82	H5	202	PEB	OD-C4D	2.71	1.28	1.23
83	A4	303	PUB	OD-C4D	2.71	1.28	1.23
87	KN	103	CLA	C4B-NB	2.71	1.41	1.37
87	b6	614	CLA	C4B-NB	2.71	1.41	1.37
87	A2	831	CLA	MG-NB	-2.71	2.00	2.05
82	HF	202	PEB	OD-C4D	2.71	1.28	1.23
87	8N	308	CLA	CMD-C2D	-2.71	1.45	1.50
82	DK	203	PEB	C2A-C1A	-2.71	1.49	1.52
82	PM	202	PEB	C2A-C1A	-2.71	1.49	1.52
87	12	609	CLA	C3B-C4B	2.71	1.49	1.42
87	6N	612	CLA	C4D-ND	-2.71	1.34	1.37
82	KQ	201	PEB	OD-C4D	2.71	1.28	1.23
82	V7	202	PEB	OD-C4D	2.71	1.28	1.23
82	mK	202	PEB	OD-C4D	2.71	1.28	1.23
87	cL	514	CLA	C3B-C4B	2.71	1.49	1.42
82	QG	201	PEB	C2C-C3C	2.71	1.46	1.38
82	UK	201	PEB	C4A-NA	-2.71	1.31	1.37
82	KP	202	PEB	C4A-NA	-2.71	1.31	1.37
87	A2	822	CLA	C4B-NB	2.71	1.41	1.37
82	RH	202	PEB	OD-C4D	2.71	1.28	1.23
82	UH	201	PEB	OD-C4D	2.71	1.28	1.23
82	QM	202	PEB	OD-C4D	2.71	1.28	1.23
87	A2	821	CLA	C4B-NB	2.71	1.41	1.37
87	b6	604	CLA	C4B-NB	2.71	1.41	1.37
87	cL	506	CLA	C3B-C4B	2.71	1.49	1.42
82	QK	201	PEB	OD-C4D	2.71	1.28	1.23
82	LO	1002	PEB	OD-C4D	2.71	1.28	1.23
82	LQ	202	PEB	OD-C4D	2.71	1.28	1.23
83	yF	303	PUB	C3B-C2B	2.71	1.46	1.38
82	YP	501	PEB	OD-C4D	2.71	1.28	1.23
87	62	313	CLA	C4D-ND	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	832	CLA	C4B-NB	2.71	1.41	1.37
87	B2	831	CLA	C4B-NB	2.71	1.41	1.37
82	lH	202	PEB	C4B-C3B	2.71	1.50	1.45
82	LM	201	PEB	OD-C4D	2.71	1.28	1.23
82	fH	203	PEB	OD-C4D	2.71	1.28	1.23
82	eM	201	PEB	OD-C4D	2.71	1.28	1.23
87	52	601	CLA	C3B-C4B	2.71	1.49	1.42
82	JD	201	PEB	C2A-C1A	-2.71	1.49	1.52
82	p8	201	PEB	C2A-C1A	-2.71	1.49	1.52
82	bP	502	PEB	C2A-C1A	-2.71	1.49	1.52
82	CF	203	PEB	OD-C4D	2.71	1.28	1.23
82	AM	301	PEB	OD-C4D	2.71	1.28	1.23
82	qK	202	PEB	OD-C4D	2.71	1.28	1.23
84	LE	1001	CYC	C4B-NB	-2.71	1.32	1.38
82	OE	203	PEB	C2C-C3C	2.71	1.46	1.38
82	BI	201	PEB	OD-C4D	2.71	1.28	1.23
82	L7	202	PEB	OD-C4D	2.71	1.28	1.23
84	DH	1003	CYC	OB-C4B	2.71	1.28	1.23
87	22	610	CLA	C3B-C4B	2.71	1.49	1.42
82	JB	201	PEB	OD-C4D	2.71	1.28	1.23
82	j4	201	PEB	OD-C4D	2.71	1.28	1.23
82	J9	203	PEB	OD-C4D	2.71	1.28	1.23
82	BK	202	PEB	C2A-C1A	-2.71	1.49	1.52
82	mF	202	PEB	C2A-C1A	-2.71	1.49	1.52
82	qK	202	PEB	C4B-C3B	2.71	1.50	1.45
87	AN	821	CLA	C3B-C4B	2.71	1.49	1.42
82	VE	202	PEB	OD-C4D	2.71	1.28	1.23
82	KF	201	PEB	OD-C4D	2.71	1.28	1.23
82	CJ	202	PEB	OD-C4D	2.71	1.28	1.23
82	VP	202	PEB	OD-C4D	2.71	1.28	1.23
82	Y4	201	PEB	OD-C4D	2.71	1.28	1.23
87	B2	834	CLA	MG-NB	-2.71	2.00	2.05
82	QJ	203	PEB	C2A-C1A	-2.71	1.49	1.52
82	UM	201	PEB	C2A-C1A	-2.71	1.49	1.52
87	AN	813	CLA	C3B-C4B	2.71	1.49	1.42
87	aL	605	CLA	C4B-NB	2.71	1.41	1.37
87	AN	838	CLA	C3B-C4B	2.71	1.49	1.42
87	12	605	CLA	C3B-C4B	2.71	1.49	1.42
87	C6	511	CLA	C3B-C4B	2.71	1.49	1.42
82	DI	201	PEB	OD-C4D	2.71	1.28	1.23
82	R1	202	PEB	OD-C4D	2.71	1.28	1.23
82	gB	202	PEB	OD-C4D	2.71	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	42	603	CLA	C4B-NB	2.71	1.41	1.37
82	QI	201	PEB	C2A-C1A	-2.71	1.49	1.52
82	DK	202	PEB	C2C-C3C	2.71	1.46	1.38
82	fG	201	PEB	OD-C4D	2.71	1.28	1.23
82	J5	201	PEB	C4A-NA	-2.71	1.31	1.37
82	aO	202	PEB	C2C-C3C	2.71	1.46	1.38
82	SO	202	PEB	OD-C4D	2.71	1.28	1.23
82	V1	202	PEB	OD-C4D	2.71	1.28	1.23
82	WJ	202	PEB	C2A-C1A	-2.70	1.49	1.52
82	mE	201	PEB	C2A-C1A	-2.70	1.49	1.52
82	X7	203	PEB	C4A-NA	-2.70	1.31	1.37
82	gG	202	PEB	OD-C4D	2.70	1.28	1.23
82	iO	201	PEB	OD-C4D	2.70	1.28	1.23
87	A6	403	CLA	C3B-C4B	2.70	1.49	1.42
87	32	303	CLA	C4B-NB	2.70	1.41	1.37
82	RJ	201	PEB	C1C-NC	-2.70	1.33	1.37
82	iM	201	PEB	C1C-NC	-2.70	1.33	1.37
87	7N	607	CLA	C3B-C4B	2.70	1.49	1.42
82	tK	202	PEB	C1C-C2C	2.70	1.49	1.42
82	DP	201	PEB	C2A-C1A	-2.70	1.49	1.52
82	eF	201	PEB	CHC-C4C	2.70	1.53	1.49
87	1N	605	CLA	C3B-C4B	2.70	1.49	1.42
82	HB	203	PEB	OD-C4D	2.70	1.28	1.23
82	hM	201	PEB	OD-C4D	2.70	1.28	1.23
84	BG	1002	CYC	OB-C4B	2.70	1.28	1.23
87	c6	616	CLA	C3B-C4B	2.70	1.49	1.42
82	RD	201	PEB	C4B-C3B	2.70	1.50	1.45
82	F5	201	PEB	OD-C4D	2.70	1.28	1.23
87	4N	605	CLA	C4D-ND	-2.70	1.34	1.37
82	V7	202	PEB	CHA-C1B	2.70	1.46	1.40
82	MK	202	PEB	C2A-C1A	-2.70	1.49	1.52
82	KM	202	PEB	OD-C4D	2.70	1.28	1.23
82	bP	502	PEB	OD-C4D	2.70	1.28	1.23
87	BL	603	CLA	MG-NB	-2.70	2.00	2.05
87	A2	823	CLA	C4B-NB	2.70	1.41	1.37
82	UA	201	PEB	C4A-NA	-2.70	1.31	1.37
82	OF	201	PEB	C2A-C1A	-2.70	1.49	1.52
82	PE	201	PEB	OD-C4D	2.70	1.28	1.23
82	oF	201	PEB	OD-C4D	2.70	1.28	1.23
87	CL	515	CLA	C3B-C4B	2.70	1.49	1.42
87	O2	202	CLA	C3B-C4B	2.70	1.49	1.42
82	b1	202	PEB	C1C-C2C	2.70	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	KK	201	PEB	OD-C4D	2.70	1.28	1.23
82	EM	201	PEB	OD-C4D	2.70	1.28	1.23
82	cG	201	PEB	OD-C4D	2.70	1.28	1.23
82	iH	202	PEB	OD-C4D	2.70	1.28	1.23
82	m1	202	PEB	C1C-C2C	2.70	1.49	1.42
87	AN	822	CLA	C4B-NB	2.70	1.41	1.37
82	X7	201	PEB	C1C-C2C	2.70	1.49	1.42
82	XM	201	PEB	C1C-NC	-2.70	1.33	1.37
82	YB	202	PEB	OD-C4D	2.70	1.28	1.23
82	kF	203	PEB	C1C-C2C	2.70	1.49	1.42
84	ME	1001	CYC	C4C-NC	-2.70	1.31	1.37
82	TE	201	PEB	C1C-NC	-2.70	1.33	1.37
82	IB	203	PEB	OD-C4D	2.70	1.28	1.23
82	NK	201	PEB	OD-C4D	2.70	1.28	1.23
82	m4	202	PEB	OD-C4D	2.70	1.28	1.23
82	v8	201	PEB	OD-C4D	2.70	1.28	1.23
82	XA	202	PEB	CHA-C1B	2.70	1.46	1.40
82	VF	201	PEB	OD-C4D	2.70	1.28	1.23
82	X9	201	PEB	OD-C4D	2.70	1.28	1.23
84	HH	1001	CYC	OB-C4B	2.70	1.28	1.23
87	B2	826	CLA	C3B-C4B	2.70	1.49	1.42
87	7N	606	CLA	C3B-C4B	2.70	1.49	1.42
82	eB	202	PEB	OD-C4D	2.70	1.28	1.23
83	AO	303	PUB	OA-C1A	2.70	1.28	1.23
82	UI	201	PEB	C1C-NC	-2.70	1.33	1.37
82	OK	202	PEB	OD-C4D	2.70	1.28	1.23
82	DM	201	PEB	OD-C4D	2.70	1.28	1.23
82	OM	203	PEB	OD-C4D	2.70	1.28	1.23
82	RJ	201	PEB	OD-C4D	2.70	1.28	1.23
87	BN	836	CLA	C4B-NB	2.70	1.41	1.37
82	V7	203	PEB	C4B-C3B	2.70	1.50	1.45
82	aB	202	PEB	OD-C4D	2.70	1.28	1.23
87	A2	840	CLA	C3B-C4B	2.70	1.49	1.42
83	YA	302	PUB	OD-C4D	2.70	1.28	1.23
84	M1	201	CYC	OB-C4B	2.70	1.28	1.23
87	F2	202	CLA	C1B-C2B	2.70	1.49	1.43
84	y3	1001	CYC	C4D-C3D	2.70	1.49	1.42
82	OI	202	PEB	C1A-NA	-2.70	1.34	1.37
82	PJ	201	PEB	OD-C4D	2.70	1.28	1.23
82	BP	201	PEB	OD-C4D	2.70	1.28	1.23
82	HI	202	PEB	C4B-NB	-2.70	1.32	1.38
87	AN	808	CLA	C4B-NB	2.70	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	807	CLA	C4B-NB	2.70	1.41	1.37
87	B6	611	CLA	C4B-NB	2.70	1.41	1.37
87	b6	618	CLA	C3B-C4B	2.70	1.49	1.42
87	bL	606	CLA	CMD-C2D	-2.70	1.45	1.50
82	DP	201	PEB	OD-C4D	2.70	1.28	1.23
83	AE	302	PUB	OA-C1A	2.70	1.28	1.23
82	LM	201	PEB	CHC-C4C	2.70	1.53	1.49
82	KQ	201	PEB	C2A-C1A	-2.69	1.49	1.52
87	cL	511	CLA	C4B-NB	2.69	1.41	1.37
82	ZM	202	PEB	OD-C4D	2.69	1.28	1.23
82	cE	201	PEB	OD-C4D	2.69	1.28	1.23
87	A2	821	CLA	C3B-C4B	2.69	1.49	1.42
87	A2	810	CLA	C4B-NB	2.69	1.41	1.37
87	FN	201	CLA	C3B-C4B	2.69	1.49	1.42
87	C6	520	CLA	C3B-C4B	2.69	1.49	1.42
82	AP	203	PEB	C2A-C1A	-2.69	1.49	1.52
82	T7	203	PEB	C4A-NA	-2.69	1.31	1.37
82	kK	203	PEB	C1C-C2C	2.69	1.49	1.42
82	MM	203	PEB	OD-C4D	2.69	1.28	1.23
82	S1	201	PEB	OD-C4D	2.69	1.28	1.23
82	e4	201	PEB	OD-C4D	2.69	1.28	1.23
82	HI	201	PEB	C4B-C3B	2.69	1.50	1.45
82	KP	201	PEB	C2A-C1A	-2.69	1.49	1.52
84	JH	1003	CYC	OB-C4B	2.69	1.28	1.23
87	BN	808	CLA	C4B-NB	2.69	1.41	1.37
82	XA	202	PEB	C2C-C3C	2.69	1.46	1.38
82	VP	201	PEB	OD-C4D	2.69	1.28	1.23
82	LQ	201	PEB	OD-C4D	2.69	1.28	1.23
84	EH	1001	CYC	C4C-NC	-2.69	1.31	1.37
82	U5	202	PEB	C4B-C3B	2.69	1.50	1.45
84	I1	1001	CYC	C4B-NB	-2.69	1.32	1.38
87	A2	826	CLA	C3B-C4B	2.69	1.49	1.42
87	5N	602	CLA	C3B-C4B	2.69	1.49	1.42
82	aG	201	PEB	C1C-C2C	2.69	1.49	1.42
82	TG	201	PEB	OD-C4D	2.69	1.28	1.23
82	QJ	202	PEB	OD-C4D	2.69	1.28	1.23
82	U9	204	PEB	OD-C4D	2.69	1.28	1.23
82	VM	202	PEB	C2A-C1A	-2.69	1.49	1.52
87	KN	102	CLA	C3B-C4B	2.69	1.49	1.42
82	z8	201	PEB	C1C-NC	-2.69	1.33	1.37
82	EJ	202	PEB	C4A-NA	-2.69	1.31	1.37
82	R7	203	PEB	OD-C4D	2.69	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mO	202	PEB	OD-C4D	2.69	1.28	1.23
87	K2	103	CLA	C3B-C4B	2.69	1.49	1.42
82	EF	201	PEB	CHB-C1C	2.69	1.46	1.40
87	A2	837	CLA	C4B-NB	2.69	1.41	1.37
87	B2	807	CLA	C4B-NB	2.69	1.41	1.37
82	AF	202	PEB	C4B-C3B	2.69	1.50	1.45
82	J1	1002	PEB	OD-C4D	2.69	1.28	1.23
82	mO	201	PEB	OD-C4D	2.69	1.28	1.23
83	AJ	304	PUB	OA-C1A	2.69	1.28	1.23
82	YO	202	PEB	C2A-C1A	-2.69	1.49	1.52
82	IB	201	PEB	OD-C4D	2.69	1.28	1.23
82	q8	201	PEB	OD-C4D	2.69	1.28	1.23
82	cG	202	PEB	OD-C4D	2.69	1.28	1.23
82	HF	201	PEB	C2C-C3C	2.69	1.46	1.38
82	PE	201	PEB	C1C-NC	-2.69	1.33	1.37
82	AI	203	PEB	C2C-C3C	2.69	1.46	1.38
82	MQ	201	PEB	C1C-C2C	2.69	1.49	1.42
87	B2	808	CLA	C3B-C4B	2.69	1.49	1.42
82	YH	201	PEB	OD-C4D	2.69	1.28	1.23
82	YI	202	PEB	OD-C4D	2.69	1.28	1.23
82	eO	203	PEB	OD-C4D	2.69	1.28	1.23
83	xF	301	PUB	OD-C4D	2.69	1.28	1.23
82	MA	201	PEB	C2A-C1A	-2.69	1.49	1.52
82	cK	201	PEB	CHC-C4C	2.69	1.53	1.49
87	7N	602	CLA	C4B-NB	2.69	1.41	1.37
87	F2	202	CLA	C3B-C4B	2.69	1.49	1.42
82	AH	301	PEB	OD-C4D	2.69	1.28	1.23
82	WJ	202	PEB	OD-C4D	2.69	1.28	1.23
82	RO	202	PEB	OD-C4D	2.69	1.28	1.23
82	PP	201	PEB	OD-C4D	2.69	1.28	1.23
83	YA	302	PUB	OA-C1A	2.69	1.28	1.23
83	AJ	304	PUB	OD-C4D	2.69	1.28	1.23
82	Q7	201	PEB	C4A-NA	-2.69	1.31	1.37
87	72	606	CLA	C3B-C4B	2.69	1.49	1.42
82	SJ	201	PEB	OD-C4D	2.69	1.28	1.23
87	CL	504	CLA	C4B-NB	2.69	1.41	1.37
83	NQ	201	PUB	C4B-C3B	2.69	1.49	1.42
82	NF	201	PEB	OD-C4D	2.69	1.28	1.23
87	52	602	CLA	C3B-C4B	2.69	1.49	1.42
82	SA	201	PEB	C2C-C3C	2.69	1.46	1.38
87	b6	606	CLA	C4B-NB	2.69	1.41	1.37
82	c4	202	PEB	OD-C4D	2.69	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	dL	403	PHO	C3A-C2A	-2.69	1.52	1.54
87	AN	841	CLA	C3B-C4B	2.69	1.49	1.42
82	cJ	201	PEB	OD-C4D	2.69	1.28	1.23
87	A2	841	CLA	C3B-C4B	2.69	1.49	1.42
82	GB	201	PEB	OD-C4D	2.69	1.28	1.23
82	e4	203	PEB	OD-C4D	2.69	1.28	1.23
82	X7	202	PEB	C1A-NA	-2.69	1.34	1.37
82	YO	203	PEB	OD-C4D	2.69	1.28	1.23
82	zK	501	PEB	OD-C4D	2.69	1.28	1.23
82	YE	201	PEB	CHB-C1C	2.69	1.46	1.40
82	AQ	301	PEB	OD-C4D	2.69	1.28	1.23
82	V5	202	PEB	OD-C4D	2.69	1.28	1.23
82	wC	201	PEB	OD-C4D	2.69	1.28	1.23
82	iJ	201	PEB	OD-C4D	2.69	1.28	1.23
87	A6	402	CLA	C3B-C4B	2.69	1.49	1.42
82	VJ	201	PEB	C1C-NC	-2.69	1.33	1.37
87	A2	820	CLA	MG-NB	-2.69	2.00	2.05
84	HO	1001	CYC	C3D-C2D	2.69	1.46	1.38
87	F2	202	CLA	C4B-NB	2.69	1.41	1.37
82	V7	203	PEB	C2A-C1A	-2.68	1.49	1.52
82	aM	202	PEB	C2A-C1A	-2.68	1.49	1.52
87	B2	813	CLA	C3B-C4B	2.68	1.49	1.42
82	DB	201	PEB	OD-C4D	2.68	1.28	1.23
82	SQ	201	PEB	OD-C4D	2.68	1.28	1.23
82	XF	202	PEB	C2C-C3C	2.68	1.46	1.38
82	S7	201	PEB	C2C-C3C	2.68	1.46	1.38
82	tF	202	PEB	C1C-C2C	2.68	1.49	1.42
87	HL	102	CLA	C3B-C4B	2.68	1.49	1.42
87	C6	510	CLA	C3B-C4B	2.68	1.49	1.42
82	TH	201	PEB	C4B-C3B	2.68	1.50	1.45
82	TJ	202	PEB	OD-C4D	2.68	1.28	1.23
82	LP	201	PEB	OD-C4D	2.68	1.28	1.23
82	UP	201	PEB	OD-C4D	2.68	1.28	1.23
82	wK	303	PEB	OD-C4D	2.68	1.28	1.23
87	B2	833	CLA	C4B-NB	2.68	1.41	1.37
82	FK	202	PEB	C1C-NC	-2.68	1.33	1.37
82	GB	203	PEB	OD-C4D	2.68	1.28	1.23
82	K5	202	PEB	OD-C4D	2.68	1.28	1.23
82	gB	201	PEB	OD-C4D	2.68	1.28	1.23
83	NQ	201	PUB	OA-C1A	2.68	1.28	1.23
82	VA	203	PEB	C4B-C3B	2.68	1.50	1.45
82	BI	203	PEB	C2A-C1A	-2.68	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	X7	202	PEB	C2C-C3C	2.68	1.46	1.38
87	L2	202	CLA	C3B-C4B	2.68	1.49	1.42
87	b6	613	CLA	C4B-NB	2.68	1.41	1.37
87	BN	815	CLA	C1B-C2B	2.68	1.49	1.43
82	BB	203	PEB	OD-C4D	2.68	1.28	1.23
82	OF	202	PEB	OD-C4D	2.68	1.28	1.23
82	QF	201	PEB	OD-C4D	2.68	1.28	1.23
82	TF	201	PEB	OD-C4D	2.68	1.28	1.23
82	HQ	201	PEB	OD-C4D	2.68	1.28	1.23
82	SM	202	PEB	OD-C4D	2.68	1.28	1.23
82	f1	203	PEB	OD-C4D	2.68	1.28	1.23
82	B5	201	PEB	OD-C4D	2.68	1.28	1.23
82	dJ	201	PEB	OD-C4D	2.68	1.28	1.23
87	D6	403	CLA	C3B-C4B	2.68	1.49	1.42
87	5N	601	CLA	C3B-C4B	2.68	1.49	1.42
82	kK	203	PEB	OD-C4D	2.68	1.28	1.23
83	Z9	305	PUB	C1C-C2C	2.68	1.50	1.45
87	BN	823	CLA	C4B-NB	2.68	1.41	1.37
87	b6	612	CLA	C3B-C4B	2.68	1.49	1.42
82	RA	203	PEB	OD-C4D	2.68	1.28	1.23
82	WH	203	PEB	OD-C4D	2.68	1.28	1.23
82	BQ	201	PEB	OD-C4D	2.68	1.28	1.23
82	hH	201	PEB	OD-C4D	2.68	1.28	1.23
83	A4	303	PUB	OA-C1A	2.68	1.28	1.23
82	SI	201	PEB	C2A-C1A	-2.68	1.49	1.52
82	EK	202	PEB	C2A-C1A	-2.68	1.49	1.52
82	GM	203	PEB	C2A-C1A	-2.68	1.49	1.52
82	DP	202	PEB	C2A-C1A	-2.68	1.49	1.52
87	b6	615	CLA	C3B-C4B	2.68	1.49	1.42
87	1N	609	CLA	C3B-C4B	2.68	1.49	1.42
82	VB	201	PEB	OD-C4D	2.68	1.28	1.23
96	V6	201	HEM	FE-ND	-2.68	1.86	1.94
82	YG	201	PEB	CHB-C1C	2.68	1.46	1.40
82	L5	203	PEB	C2C-C3C	2.68	1.46	1.38
82	XA	201	PEB	C1C-C2C	2.68	1.49	1.42
82	YG	201	PEB	OD-C4D	2.68	1.28	1.23
87	AN	826	CLA	C3B-C4B	2.68	1.49	1.42
82	DF	202	PEB	C2C-C3C	2.68	1.46	1.38
87	AN	823	CLA	C4B-NB	2.68	1.41	1.37
82	DB	201	PEB	C4A-NA	-2.68	1.31	1.37
87	BN	827	CLA	MG-ND	-2.68	2.00	2.05
82	RB	202	PEB	OD-C4D	2.68	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HD	201	PEB	OD-C4D	2.68	1.28	1.23
82	l1	202	PEB	OD-C4D	2.68	1.28	1.23
87	A2	813	CLA	C3B-C4B	2.68	1.49	1.42
87	d6	403	CLA	C3B-C4B	2.68	1.49	1.42
82	CK	202	PEB	OD-C4D	2.68	1.28	1.23
82	r8	202	PEB	C2A-C1A	-2.68	1.49	1.52
87	A2	817	CLA	C3B-C4B	2.68	1.49	1.42
87	b6	612	CLA	CMB-C2B	-2.68	1.45	1.50
87	1N	611	CLA	C3B-C4B	2.68	1.49	1.42
82	HF	201	PEB	C4A-NA	-2.68	1.31	1.37
82	DA	202	PEB	OD-C4D	2.68	1.28	1.23
82	OM	201	PEB	OD-C4D	2.68	1.28	1.23
83	xK	306	PUB	OD-C4D	2.68	1.28	1.23
82	TQ	201	PEB	C1D-ND	2.68	1.49	1.45
82	KB	304	PEB	OD-C4D	2.68	1.28	1.23
82	bP	501	PEB	OD-C4D	2.68	1.28	1.23
82	MJ	202	PEB	CHB-C1C	2.68	1.46	1.40
82	V7	202	PEB	C2C-C3C	2.68	1.46	1.38
84	JO	1001	CYC	C4B-NB	-2.68	1.32	1.38
82	SP	203	PEB	C2A-C1A	-2.68	1.49	1.52
87	nL	101	CLA	C4B-NB	2.68	1.41	1.37
82	lG	202	PEB	OD-C4D	2.68	1.28	1.23
82	Y5	203	PEB	C2C-C3C	2.68	1.46	1.38
87	b6	616	CLA	C3B-C4B	2.68	1.49	1.42
82	hM	202	PEB	C4B-C3B	2.68	1.50	1.45
87	B6	614	CLA	C3B-C4B	2.68	1.49	1.42
87	AN	821	CLA	C4B-NB	2.68	1.41	1.37
87	6N	609	CLA	C4D-ND	-2.68	1.34	1.37
82	TK	201	PEB	OD-C4D	2.68	1.28	1.23
82	iK	202	PEB	OD-C4D	2.68	1.28	1.23
87	32	305	CLA	C3B-C4B	2.68	1.49	1.42
87	A2	826	CLA	C4B-NB	2.68	1.41	1.37
82	PK	202	PEB	C1C-NC	-2.67	1.33	1.37
82	zC	201	PEB	C1C-NC	-2.67	1.33	1.37
82	PA	203	PEB	OD-C4D	2.67	1.28	1.23
82	cB	403	PEB	C2A-C1A	-2.67	1.49	1.52
87	B2	814	CLA	C1B-C2B	2.67	1.49	1.43
87	B2	827	CLA	MG-ND	-2.67	2.00	2.05
82	MM	201	PEB	OD-C4D	2.67	1.28	1.23
83	A1	303	PUB	OA-C1A	2.67	1.28	1.23
87	LN	202	CLA	C3B-C4B	2.67	1.49	1.42
87	B2	825	CLA	C1D-ND	2.67	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	c6	607	CLA	C3B-C4B	2.67	1.49	1.42
82	DA	201	PEB	OD-C4D	2.67	1.28	1.23
84	H1	1001	CYC	OB-C4B	2.67	1.28	1.23
82	XF	202	PEB	C4A-NA	-2.67	1.31	1.37
82	JH	1002	PEB	OD-C4D	2.67	1.28	1.23
84	BE	1002	CYC	OB-C4B	2.67	1.28	1.23
82	eF	202	PEB	CHB-C1C	2.67	1.46	1.40
87	c6	610	CLA	C3B-C4B	2.67	1.49	1.42
84	o3	1001	CYC	C4B-NB	-2.67	1.32	1.38
82	BP	202	PEB	OD-C4D	2.67	1.28	1.23
82	S4	202	PEB	OD-C4D	2.67	1.28	1.23
82	iJ	202	PEB	OD-C4D	2.67	1.28	1.23
82	aM	204	PEB	OD-C4D	2.67	1.28	1.23
87	72	606	CLA	C1B-C2B	2.67	1.49	1.43
87	C6	516	CLA	C4B-NB	2.67	1.41	1.37
82	FJ	202	PEB	OD-C4D	2.67	1.28	1.23
82	R7	201	PEB	OD-C4D	2.67	1.28	1.23
83	A1	303	PUB	OD-C4D	2.67	1.28	1.23
82	XA	203	PEB	C1C-NC	-2.67	1.33	1.37
82	PM	201	PEB	OD-C4D	2.67	1.28	1.23
82	D1	1002	PEB	OD-C4D	2.67	1.28	1.23
82	vC	201	PEB	OD-C4D	2.67	1.28	1.23
87	8N	303	CLA	C3B-C4B	2.67	1.49	1.42
87	A6	403	CLA	C4B-NB	2.67	1.41	1.37
82	VA	203	PEB	C2A-C1A	-2.67	1.49	1.52
82	JI	201	PEB	C2A-C1A	-2.67	1.49	1.52
87	A2	810	CLA	C3B-C4B	2.67	1.49	1.42
82	HK	201	PEB	C2C-C3C	2.67	1.46	1.38
87	bL	614	CLA	MG-NB	-2.67	2.00	2.05
82	fE	201	PEB	OD-C4D	2.67	1.28	1.23
82	ZH	203	PEB	C1B-C2B	2.67	1.51	1.45
87	BL	601	CLA	C3B-C4B	2.67	1.49	1.42
82	WP	202	PEB	C4A-NA	-2.67	1.31	1.37
82	fG	201	PEB	C2A-C1A	-2.67	1.49	1.52
84	DH	1003	CYC	C2C-C1C	-2.67	1.49	1.52
82	RA	203	PEB	C1C-NC	-2.67	1.33	1.37
87	32	309	CLA	C3B-C4B	2.67	1.49	1.42
87	bL	621	CLA	C3B-C4B	2.67	1.49	1.42
87	A2	839	CLA	C4B-NB	2.67	1.41	1.37
91	D6	404	PHO	CBD-CGD	-2.67	1.48	1.52
82	LM	202	PEB	OD-C4D	2.67	1.28	1.23
87	62	309	CLA	C3D-C4D	2.67	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HQ	201	PEB	C2C-C3C	2.67	1.46	1.38
82	VG	202	PEB	OD-C4D	2.67	1.28	1.23
82	MM	202	PEB	C4A-NA	-2.67	1.31	1.37
82	HI	202	PEB	C1D-ND	2.67	1.49	1.45
82	JD	201	PEB	OD-C4D	2.67	1.28	1.23
82	ZF	201	PEB	OD-C4D	2.67	1.28	1.23
82	J7	201	PEB	OD-C4D	2.67	1.28	1.23
82	hE	202	PEB	OD-C4D	2.67	1.28	1.23
82	NB	201	PEB	OD-C4D	2.67	1.28	1.23
87	AN	810	CLA	C3B-C4B	2.67	1.49	1.42
82	FK	201	PEB	C4B-C3B	2.67	1.50	1.45
83	Z9	305	PUB	C1C-NC	-2.67	1.32	1.38
82	UH	202	PEB	CHC-C4C	2.67	1.53	1.49
87	42	606	CLA	C3B-C4B	2.67	1.49	1.42
82	t8	202	PEB	C2A-C1A	-2.67	1.49	1.52
82	mM	202	PEB	C2A-C1A	-2.67	1.49	1.52
87	aL	606	CLA	CAA-C2A	-2.67	1.49	1.54
82	FF	201	PEB	C4B-C3B	2.67	1.50	1.45
82	WK	202	PEB	OD-C4D	2.67	1.28	1.23
82	rK	202	PEB	CHC-C4C	2.67	1.53	1.49
82	BD	203	PEB	C2C-C3C	2.66	1.46	1.38
87	B6	616	CLA	CMC-C2C	-2.66	1.45	1.50
82	Q1	201	PEB	OD-C4D	2.66	1.28	1.23
82	W1	203	PEB	OD-C4D	2.66	1.28	1.23
84	BG	1002	CYC	C4A-C3A	2.66	1.51	1.45
82	KB	304	PEB	C2A-C1A	-2.66	1.49	1.52
82	RA	201	PEB	OD-C4D	2.66	1.28	1.23
83	AH	303	PUB	OA-C1A	2.66	1.28	1.23
87	A2	849	CLA	MG-NB	-2.66	2.00	2.05
82	DD	201	PEB	C2C-C3C	2.66	1.46	1.38
82	OD	202	PEB	OD-C4D	2.66	1.28	1.23
82	E5	202	PEB	OD-C4D	2.66	1.28	1.23
82	oK	201	PEB	OD-C4D	2.66	1.28	1.23
82	EA	202	PEB	C1D-ND	2.66	1.49	1.45
87	FN	201	CLA	C1B-C2B	2.66	1.49	1.43
82	PF	202	PEB	C1C-NC	-2.66	1.33	1.37
82	cM	202	PEB	C2A-C1A	-2.66	1.49	1.52
82	hJ	201	PEB	OD-C4D	2.66	1.28	1.23
82	fK	201	PEB	OD-C4D	2.66	1.28	1.23
82	GI	201	PEB	OD-C4D	2.66	1.28	1.23
82	QP	201	PEB	OD-C4D	2.66	1.28	1.23
82	gF	201	PEB	OD-C4D	2.66	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	302	CLA	C3B-C4B	2.66	1.49	1.42
87	FN	201	CLA	C4B-NB	2.66	1.41	1.37
82	KJ	203	PEB	C2C-C3C	2.66	1.45	1.38
87	AN	823	CLA	C3B-C4B	2.66	1.49	1.42
82	XP	202	PEB	C4A-NA	-2.66	1.31	1.37
82	QG	201	PEB	OD-C4D	2.66	1.28	1.23
83	Y7	302	PUB	OD-C4D	2.66	1.28	1.23
87	BN	809	CLA	C3B-C4B	2.66	1.49	1.42
82	O5	201	PEB	CHB-C1C	2.66	1.46	1.40
87	42	605	CLA	C4D-ND	-2.66	1.34	1.37
82	LK	202	PEB	OD-C4D	2.66	1.28	1.23
82	UG	201	PEB	C2C-C3C	2.66	1.45	1.38
87	CL	512	CLA	C1B-C2B	2.66	1.49	1.43
91	DL	405	PHO	CBD-CGD	-2.66	1.48	1.52
82	GI	202	PEB	OD-C4D	2.66	1.28	1.23
87	AN	839	CLA	C4B-NB	2.66	1.41	1.37
87	A2	820	CLA	C4B-NB	2.66	1.41	1.37
87	12	611	CLA	C3B-C4B	2.66	1.49	1.42
82	SM	202	PEB	C1C-C2C	2.66	1.49	1.42
82	CF	202	PEB	OD-C4D	2.66	1.28	1.23
83	yK	303	PUB	OD-C4D	2.66	1.28	1.23
82	QK	203	PEB	CHA-C1B	2.66	1.46	1.40
82	W1	201	PEB	CHC-C4C	2.66	1.53	1.49
87	AL	405	CLA	C4B-NB	2.66	1.41	1.37
87	B2	835	CLA	C4B-NB	2.66	1.41	1.37
87	K2	104	CLA	C4B-NB	2.66	1.41	1.37
82	XA	202	PEB	C2A-C1A	-2.66	1.49	1.52
82	UE	201	PEB	OD-C4D	2.66	1.28	1.23
82	T5	202	PEB	OD-C4D	2.66	1.28	1.23
82	B5	202	PEB	C4B-C3B	2.66	1.49	1.45
82	jO	201	PEB	CHA-C4A	-2.66	1.31	1.36
82	ZB	201	PEB	OD-C4D	2.66	1.28	1.23
82	EP	201	PEB	OD-C4D	2.66	1.28	1.23
82	dD	401	PEB	OD-C4D	2.66	1.28	1.23
83	xK	306	PUB	C4B-NB	-2.66	1.33	1.37
87	22	606	CLA	C3B-C4B	2.66	1.49	1.42
87	72	607	CLA	C3B-C4B	2.66	1.49	1.42
87	4N	606	CLA	C3B-C4B	2.66	1.49	1.42
82	BM	301	PEB	OD-C4D	2.66	1.28	1.23
82	X5	202	PEB	OD-C4D	2.66	1.28	1.23
82	dQ	401	PEB	OD-C4D	2.66	1.28	1.23
91	a6	613	PHO	CBD-CGD	-2.66	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AL	404	CLA	MG-NB	-2.66	2.00	2.05
82	bB	201	PEB	OD-C4D	2.66	1.28	1.23
82	F9	201	PEB	C4A-NA	-2.66	1.31	1.37
82	N1	1002	PEB	OD-C4D	2.66	1.28	1.23
82	l4	201	PEB	OD-C4D	2.66	1.28	1.23
87	B2	822	CLA	C3B-C4B	2.66	1.49	1.42
82	ID	201	PEB	C1C-NC	-2.66	1.33	1.37
82	zF	501	PEB	OD-C4D	2.66	1.28	1.23
87	82	308	CLA	C3B-C4B	2.66	1.49	1.42
82	RO	203	PEB	C4B-C3B	2.66	1.49	1.45
82	I5	202	PEB	OD-C4D	2.66	1.28	1.23
84	F1	1001	CYC	OB-C4B	2.66	1.28	1.23
87	2N	310	CLA	C1B-C2B	2.66	1.49	1.43
82	WH	201	PEB	CHC-C4C	2.65	1.53	1.49
87	7N	606	CLA	C4D-ND	-2.65	1.34	1.37
82	AG	301	PEB	OD-C4D	2.65	1.28	1.23
87	BN	814	CLA	C3B-C4B	2.65	1.49	1.42
82	T1	201	PEB	C2A-C1A	-2.65	1.49	1.52
82	j4	201	PEB	C2A-C1A	-2.65	1.49	1.52
82	jO	201	PEB	C2A-C1A	-2.65	1.49	1.52
82	j4	201	PEB	CHA-C4A	-2.65	1.31	1.36
82	DH	1002	PEB	OD-C4D	2.65	1.28	1.23
87	AN	807	CLA	C4B-NB	2.65	1.41	1.37
82	VA	202	PEB	CHA-C1B	2.65	1.46	1.40
87	5N	609	CLA	C3B-C4B	2.65	1.49	1.42
82	BB	202	PEB	OD-C4D	2.65	1.28	1.23
82	TJ	201	PEB	OD-C4D	2.65	1.28	1.23
82	cB	403	PEB	OD-C4D	2.65	1.28	1.23
82	mO	203	PEB	C4B-C3B	2.65	1.49	1.45
87	B2	822	CLA	CMD-C2D	-2.65	1.45	1.50
87	K6	101	CLA	CMB-C2B	-2.65	1.45	1.50
82	VI	203	PEB	C4B-NB	-2.65	1.32	1.38
82	fM	201	PEB	C2A-C1A	-2.65	1.49	1.52
87	3N	306	CLA	C3B-C4B	2.65	1.49	1.42
82	NA	202	PEB	CHA-C1B	2.65	1.46	1.40
82	AK	201	PEB	OD-C4D	2.65	1.28	1.23
82	kO	202	PEB	OD-C4D	2.65	1.28	1.23
87	BN	823	CLA	CMD-C2D	-2.65	1.45	1.50
96	fL	102	HEM	FE-ND	-2.65	1.86	1.94
82	YM	201	PEB	OD-C4D	2.65	1.28	1.23
82	PO	203	PEB	OD-C4D	2.65	1.28	1.23
87	6N	608	CLA	C3D-C4D	2.65	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	52	611	CLA	C3B-C4B	2.65	1.49	1.42
87	82	302	CLA	C3B-C4B	2.65	1.49	1.42
84	k3	1001	CYC	C4B-NB	-2.65	1.32	1.38
82	jJ	203	PEB	C2A-C1A	-2.65	1.49	1.52
82	fJ	203	PEB	OD-C4D	2.65	1.28	1.23
82	mJ	201	PEB	OD-C4D	2.65	1.28	1.23
82	HD	201	PEB	C2C-C3C	2.65	1.45	1.38
82	WK	201	PEB	C4A-NA	-2.65	1.31	1.37
82	RQ	201	PEB	C4B-C3B	2.65	1.49	1.45
82	VG	201	PEB	OD-C4D	2.65	1.28	1.23
82	SH	201	PEB	OD-C4D	2.65	1.28	1.23
82	C5	202	PEB	OD-C4D	2.65	1.28	1.23
83	AO	303	PUB	OD-C4D	2.65	1.28	1.23
87	A2	812	CLA	C3B-C4B	2.65	1.49	1.42
82	HM	201	PEB	C2A-C1A	-2.65	1.49	1.52
82	lJ	201	PEB	C2A-C1A	-2.65	1.49	1.52
82	NJ	202	PEB	OD-C4D	2.65	1.28	1.23
82	18	202	PEB	OD-C4D	2.65	1.28	1.23
87	3N	304	CLA	C4B-NB	2.65	1.41	1.37
82	UE	201	PEB	C2C-C3C	2.65	1.45	1.38
82	SH	203	PEB	OD-C4D	2.65	1.28	1.23
87	AN	849	CLA	MG-NB	-2.65	2.00	2.05
82	w8	201	PEB	OD-C4D	2.65	1.28	1.23
82	Q7	201	PEB	C2C-C3C	2.65	1.45	1.38
87	A2	823	CLA	C3B-C4B	2.65	1.49	1.42
87	4N	605	CLA	C3B-C4B	2.65	1.49	1.42
82	ZJ	202	PEB	OD-C4D	2.65	1.28	1.23
82	VM	201	PEB	OD-C4D	2.65	1.28	1.23
82	h1	202	PEB	OD-C4D	2.65	1.28	1.23
84	K1	1001	CYC	OB-C4B	2.65	1.28	1.23
87	c6	615	CLA	C3B-C4B	2.65	1.49	1.42
84	LE	1001	CYC	C1B-NB	-2.65	1.33	1.37
82	BD	201	PEB	OD-C4D	2.65	1.28	1.23
82	LA	202	PEB	C2A-C1A	-2.65	1.49	1.52
84	H4	1001	CYC	C3D-C2D	2.65	1.45	1.38
87	cL	506	CLA	CMB-C2B	-2.65	1.45	1.50
82	R4	203	PEB	C4B-C3B	2.65	1.49	1.45
82	uC	202	PEB	C4B-C3B	2.65	1.49	1.45
82	H9	202	PEB	OD-C4D	2.65	1.28	1.23
82	wF	303	PEB	OD-C4D	2.65	1.28	1.23
87	1N	611	CLA	C1B-C2B	2.65	1.49	1.43
87	AN	852	CLA	CHD-C1D	2.65	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BL	620	CLA	CMD-C2D	-2.65	1.45	1.50
87	A2	830	CLA	C3B-C4B	2.65	1.49	1.42
82	fH	203	PEB	CHC-C4C	2.65	1.53	1.49
82	V1	201	PEB	OD-C4D	2.65	1.28	1.23
87	7N	601	CLA	C1B-C2B	2.65	1.49	1.43
82	u8	202	PEB	C4B-C3B	2.65	1.49	1.45
87	3N	309	CLA	C3B-C4B	2.65	1.49	1.42
82	RP	201	PEB	OD-C4D	2.65	1.28	1.23
87	4N	611	CLA	C1B-C2B	2.65	1.49	1.43
84	h3	1001	CYC	C4B-NB	-2.65	1.32	1.38
82	1C	202	PEB	OD-C4D	2.65	1.28	1.23
82	hF	201	PEB	OD-C4D	2.65	1.28	1.23
82	TD	202	PEB	C2A-C1A	-2.65	1.49	1.52
82	DF	203	PEB	C2A-C1A	-2.65	1.49	1.52
87	c6	608	CLA	C3B-C4B	2.65	1.49	1.42
87	bL	607	CLA	C4B-NB	2.65	1.41	1.37
87	5N	611	CLA	C3B-C4B	2.65	1.49	1.42
82	W5	201	PEB	CHA-C1B	2.65	1.46	1.40
82	wF	301	PEB	OD-C4D	2.65	1.28	1.23
82	JM	201	PEB	C1C-NC	-2.65	1.33	1.37
82	xF	304	PEB	C1A-NA	-2.64	1.34	1.37
87	8N	301	CLA	MG-NB	-2.64	2.00	2.05
84	Q3	1001	CYC	C4B-NB	-2.64	1.32	1.38
87	42	605	CLA	C3B-C4B	2.64	1.49	1.42
82	rF	202	PEB	CHC-C4C	2.64	1.52	1.49
82	1C	202	PEB	C2A-C1A	-2.64	1.49	1.52
87	BN	833	CLA	MG-NB	-2.64	2.00	2.05
82	JA	201	PEB	OD-C4D	2.64	1.28	1.23
82	DO	1002	PEB	OD-C4D	2.64	1.28	1.23
87	72	601	CLA	C1B-C2B	2.64	1.49	1.43
82	x8	201	PEB	C1C-NC	-2.64	1.33	1.37
82	lF	201	PEB	C4B-C3B	2.64	1.49	1.45
87	C6	519	CLA	C3B-C4B	2.64	1.49	1.42
82	QG	201	PEB	C2A-C1A	-2.64	1.49	1.52
82	W7	202	PEB	C2A-C1A	-2.64	1.49	1.52
82	AJ	301	PEB	OD-C4D	2.64	1.28	1.23
87	BN	812	CLA	C3B-C4B	2.64	1.48	1.42
82	BK	201	PEB	C4D-ND	2.64	1.38	1.35
82	DJ	201	PEB	OD-C4D	2.64	1.28	1.23
82	a4	202	PEB	OD-C4D	2.64	1.28	1.23
84	I3	1001	CYC	C4B-NB	-2.64	1.32	1.38
82	fB	301	PEB	OD-C4D	2.64	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	hB	301	PEB	OD-C4D	2.64	1.28	1.23
82	aF	202	PEB	C2A-C1A	-2.64	1.49	1.52
87	8N	308	CLA	C3B-C4B	2.64	1.48	1.42
82	BF	202	PEB	OD-C4D	2.64	1.28	1.23
82	EM	202	PEB	OD-C4D	2.64	1.28	1.23
84	NE	201	CYC	OB-C4B	2.64	1.28	1.23
82	QA	201	PEB	C2C-C3C	2.64	1.45	1.38
82	XK	202	PEB	C2C-C3C	2.64	1.45	1.38
82	VJ	201	PEB	OD-C4D	2.64	1.28	1.23
82	T4	203	PEB	OD-C4D	2.64	1.28	1.23
87	BN	835	CLA	C4B-NB	2.64	1.41	1.37
82	lK	203	PEB	C2A-C1A	-2.64	1.49	1.52
82	a4	203	PEB	OD-C4D	2.64	1.28	1.23
87	B2	813	CLA	C1B-C2B	2.64	1.49	1.43
82	YA	303	PEB	C1C-C2C	2.64	1.49	1.42
87	L2	204	CLA	C3B-C4B	2.64	1.48	1.42
87	C6	515	CLA	C3B-C4B	2.64	1.48	1.42
82	hB	301	PEB	C2A-C1A	-2.64	1.49	1.52
82	rC	202	PEB	C2A-C1A	-2.64	1.49	1.52
87	CL	510	CLA	CMC-C2C	-2.64	1.45	1.50
87	52	609	CLA	C3B-C4B	2.64	1.48	1.42
87	3N	303	CLA	C3B-C4B	2.64	1.48	1.42
87	A2	841	CLA	MG-NB	-2.64	2.00	2.05
87	cL	511	CLA	C3B-C4B	2.64	1.48	1.42
87	22	610	CLA	C1B-C2B	2.64	1.49	1.43
84	J4	1001	CYC	C4B-NB	-2.64	1.32	1.38
82	lH	201	PEB	OD-C4D	2.64	1.28	1.23
82	jH	202	PEB	C2A-C1A	-2.64	1.49	1.52
82	HF	201	PEB	CHA-C1B	2.64	1.46	1.40
87	AN	830	CLA	C3B-C4B	2.64	1.48	1.42
87	A2	852	CLA	CHD-C1D	2.64	1.43	1.38
82	XB	202	PEB	OD-C4D	2.64	1.28	1.23
82	DK	201	PEB	OD-C4D	2.64	1.28	1.23
82	OQ	202	PEB	OD-C4D	2.64	1.28	1.23
84	JO	1001	CYC	C3D-C2D	2.64	1.45	1.38
87	cL	505	CLA	C3B-C4B	2.64	1.48	1.42
82	mH	201	PEB	OD-C4D	2.64	1.28	1.23
82	eJ	202	PEB	OD-C4D	2.64	1.28	1.23
83	AG	302	PUB	OA-C1A	2.64	1.28	1.23
84	J4	1001	CYC	C3D-C2D	2.64	1.45	1.38
82	y8	203	PEB	C4B-C3B	2.64	1.49	1.45
82	cH	202	PEB	C1B-C2B	2.64	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AQ	303	PEB	C2A-C1A	-2.64	1.49	1.52
82	rK	202	PEB	C2A-C1A	-2.64	1.49	1.52
82	FP	201	PEB	OD-C4D	2.64	1.28	1.23
83	AG	303	PUB	OA-C1A	2.64	1.28	1.23
82	S7	201	PEB	C4A-NA	-2.64	1.31	1.37
87	b6	608	CLA	C3B-C4B	2.64	1.48	1.42
82	aE	201	PEB	C1C-C2C	2.64	1.49	1.42
87	B6	612	CLA	C3B-C4B	2.64	1.48	1.42
87	c6	605	CLA	C3B-C4B	2.64	1.48	1.42
87	aL	605	CLA	C3B-C4B	2.64	1.48	1.42
87	cL	509	CLA	C3B-C4B	2.64	1.48	1.42
82	R5	202	PEB	OD-C4D	2.64	1.28	1.23
82	N7	202	PEB	OD-C4D	2.64	1.28	1.23
87	AN	805	CLA	CMD-C2D	-2.64	1.45	1.50
82	L9	201	PEB	OD-C4D	2.64	1.28	1.23
82	aO	203	PEB	OD-C4D	2.64	1.28	1.23
87	B6	612	CLA	C4B-NB	2.64	1.41	1.37
82	MJ	202	PEB	C4A-NA	-2.64	1.31	1.37
82	XJ	202	PEB	OD-C4D	2.64	1.28	1.23
82	KI	201	PEB	CHA-C1B	2.64	1.46	1.40
82	Y7	301	PEB	C2A-C1A	-2.64	1.49	1.52
87	B2	822	CLA	C4B-NB	2.64	1.41	1.37
82	18	201	PEB	C1C-C2C	2.64	1.49	1.42
82	1C	201	PEB	C1C-C2C	2.64	1.49	1.42
82	KD	201	PEB	OD-C4D	2.64	1.28	1.23
82	JJ	201	PEB	OD-C4D	2.64	1.28	1.23
82	FJ	201	PEB	C1C-NC	-2.63	1.33	1.37
82	a4	201	PEB	C1C-NC	-2.63	1.33	1.37
82	T5	201	PEB	OD-C4D	2.63	1.28	1.23
87	42	611	CLA	C1B-C2B	2.63	1.49	1.43
87	8N	305	CLA	C1B-C2B	2.63	1.49	1.43
82	TG	201	PEB	C1C-NC	-2.63	1.33	1.37
84	u3	1001	CYC	C4B-NB	-2.63	1.32	1.38
82	YO	201	PEB	OD-C4D	2.63	1.28	1.23
82	V1	203	PEB	OD-C4D	2.63	1.28	1.23
82	kF	203	PEB	OD-C4D	2.63	1.28	1.23
82	eK	201	PEB	CHC-C4C	2.63	1.52	1.49
82	J7	203	PEB	C4B-C3B	2.63	1.49	1.45
87	B6	604	CLA	C3B-C4B	2.63	1.48	1.42
82	XK	203	PEB	OD-C4D	2.63	1.28	1.23
82	U5	203	PEB	OD-C4D	2.63	1.28	1.23
87	CL	510	CLA	MG-NB	-2.63	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	d3	1001	CYC	C4D-C3D	2.63	1.49	1.42
87	7N	606	CLA	C1B-C2B	2.63	1.49	1.43
87	c6	611	CLA	C3B-C4B	2.63	1.48	1.42
82	JM	201	PEB	CHC-C4C	2.63	1.52	1.49
84	L3	1001	CYC	C4B-NB	-2.63	1.32	1.38
82	NP	201	PEB	OD-C4D	2.63	1.28	1.23
82	lG	203	PEB	OD-C4D	2.63	1.28	1.23
87	82	306	CLA	MG-NB	-2.63	2.00	2.05
82	bK	202	PEB	C2A-C1A	-2.63	1.49	1.52
87	BN	819	CLA	C3B-C4B	2.63	1.48	1.42
82	EK	201	PEB	CHB-C1C	2.63	1.46	1.40
87	dL	404	CLA	C4B-NB	2.63	1.41	1.37
84	D3	1001	CYC	C4B-NB	-2.63	1.32	1.38
82	WE	203	PEB	OD-C4D	2.63	1.28	1.23
82	WG	203	PEB	OD-C4D	2.63	1.28	1.23
82	mH	202	PEB	OD-C4D	2.63	1.28	1.23
82	R4	201	PEB	C1C-NC	-2.63	1.33	1.37
87	c6	616	CLA	C1B-C2B	2.63	1.49	1.43
82	NM	201	PEB	OD-C4D	2.63	1.28	1.23
82	U1	201	PEB	OD-C4D	2.63	1.28	1.23
82	F4	1002	PEB	OD-C4D	2.63	1.28	1.23
82	M9	301	PEB	OD-C4D	2.63	1.28	1.23
82	s8	202	PEB	CHC-C4C	2.63	1.52	1.49
82	D7	202	PEB	OD-C4D	2.63	1.28	1.23
82	hG	202	PEB	OD-C4D	2.63	1.28	1.23
87	72	606	CLA	C4D-ND	-2.63	1.34	1.37
82	Z1	203	PEB	C1B-C2B	2.63	1.51	1.45
82	IP	201	PEB	OD-C4D	2.63	1.28	1.23
83	KA	203	PUB	OD-C4D	2.63	1.28	1.23
84	M3	1001	CYC	C4B-NB	-2.63	1.32	1.38
87	BN	814	CLA	C1B-C2B	2.63	1.49	1.43
82	kF	202	PEB	C4B-C3B	2.63	1.49	1.45
82	WF	201	PEB	C4A-NA	-2.63	1.31	1.37
82	VH	202	PEB	OD-C4D	2.63	1.28	1.23
82	G5	202	PEB	OD-C4D	2.63	1.28	1.23
87	BN	801	CLA	C1D-ND	2.63	1.41	1.37
87	2N	306	CLA	C3B-C4B	2.63	1.48	1.42
87	AN	841	CLA	MG-NB	-2.63	2.00	2.05
87	8N	303	CLA	C1B-C2B	2.63	1.49	1.43
82	OH	203	PEB	OD-C4D	2.63	1.28	1.23
87	AN	814	CLA	C3B-C4B	2.63	1.48	1.42
84	LH	1001	CYC	C1B-NB	-2.63	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	F3	1001	CYC	C4B-NB	-2.63	1.32	1.38
82	vC	201	PEB	C1C-C2C	2.63	1.49	1.42
87	22	612	CLA	C1B-C2B	2.63	1.49	1.43
84	H3	1001	CYC	C4B-NB	-2.63	1.32	1.38
82	UM	201	PEB	OD-C4D	2.63	1.28	1.23
82	DJ	201	PEB	C1C-NC	-2.63	1.33	1.37
84	B3	1001	CYC	C4B-NB	-2.63	1.32	1.38
82	CI	201	PEB	OD-C4D	2.63	1.28	1.23
82	GP	202	PEB	OD-C4D	2.63	1.28	1.23
82	SA	201	PEB	C4A-NA	-2.63	1.31	1.37
82	bH	202	PEB	C1C-C2C	2.63	1.49	1.42
82	i4	201	PEB	C2A-C1A	-2.63	1.49	1.52
82	gM	202	PEB	C2A-C1A	-2.63	1.49	1.52
87	B2	811	CLA	C3B-C4B	2.63	1.48	1.42
82	SB	201	PEB	OD-C4D	2.63	1.28	1.23
82	j4	203	PEB	OD-C4D	2.63	1.28	1.23
82	F7	202	PEB	OD-C4D	2.63	1.28	1.23
82	eO	202	PEB	OD-C4D	2.63	1.28	1.23
82	dK	202	PEB	C1C-NC	-2.63	1.33	1.37
87	D6	405	CLA	C3B-C4B	2.63	1.48	1.42
82	NH	1002	PEB	OD-C4D	2.63	1.28	1.23
82	SM	201	PEB	OD-C4D	2.63	1.28	1.23
82	HP	201	PEB	OD-C4D	2.63	1.28	1.23
84	K4	1001	CYC	OB-C4B	2.63	1.28	1.23
87	B2	833	CLA	C3B-C4B	2.63	1.48	1.42
82	TK	202	PEB	CHC-C4C	2.63	1.52	1.49
82	UP	202	PEB	C4B-C3B	2.63	1.49	1.45
82	FA	202	PEB	OD-C4D	2.63	1.28	1.23
82	EB	501	PEB	OD-C4D	2.63	1.28	1.23
82	PF	201	PEB	OD-C4D	2.63	1.28	1.23
82	CM	203	PEB	OD-C4D	2.63	1.28	1.23
87	6N	611	CLA	C4D-ND	-2.63	1.34	1.37
87	AN	817	CLA	C3B-C4B	2.63	1.48	1.42
84	S3	1001	CYC	C4D-C3D	2.63	1.49	1.42
82	SB	202	PEB	OD-C4D	2.63	1.28	1.23
82	P5	202	PEB	OD-C4D	2.63	1.28	1.23
87	62	301	CLA	C3B-C4B	2.63	1.48	1.42
84	D3	1001	CYC	C4D-C3D	2.63	1.49	1.42
82	mM	201	PEB	C1C-NC	-2.63	1.33	1.37
82	UB	303	PEB	OD-C4D	2.63	1.28	1.23
82	CM	203	PEB	C2A-C1A	-2.63	1.49	1.52
82	z8	202	PEB	C4B-C3B	2.63	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	II	201	PEB	OD-C4D	2.62	1.28	1.23
82	RO	203	PEB	OD-C4D	2.62	1.28	1.23
82	i4	201	PEB	OD-C4D	2.62	1.28	1.23
84	j3	1001	CYC	C4B-NB	-2.62	1.32	1.38
87	b6	616	CLA	C1B-C2B	2.62	1.49	1.43
87	AN	812	CLA	C3B-C4B	2.62	1.48	1.42
87	bL	616	CLA	C3B-C4B	2.62	1.48	1.42
87	AN	837	CLA	C4B-NB	2.62	1.41	1.37
82	m4	201	PEB	OD-C4D	2.62	1.28	1.23
82	gK	201	PEB	C2A-C1A	-2.62	1.49	1.52
87	62	301	CLA	C1B-C2B	2.62	1.49	1.43
87	2N	312	CLA	C1B-C2B	2.62	1.49	1.43
82	tC	202	PEB	C2A-C1A	-2.62	1.49	1.52
82	FF	202	PEB	C1C-NC	-2.62	1.33	1.37
82	O5	203	PEB	OD-C4D	2.62	1.28	1.23
96	v6	201	HEM	FE-ND	-2.62	1.86	1.94
87	AN	820	CLA	MG-NB	-2.62	2.00	2.05
82	NB	203	PEB	C1C-NC	-2.62	1.33	1.37
82	bO	201	PEB	OD-C4D	2.62	1.28	1.23
82	ZO	201	PEB	CHB-C1C	2.62	1.46	1.40
87	6N	613	CLA	C3B-C4B	2.62	1.48	1.42
82	Y9	201	PEB	OD-C4D	2.62	1.28	1.23
82	uC	202	PEB	OD-C4D	2.62	1.28	1.23
82	eK	202	PEB	CHB-C1C	2.62	1.46	1.40
87	dL	404	CLA	C3B-C4B	2.62	1.48	1.42
82	YE	201	PEB	OD-C4D	2.62	1.28	1.23
82	YI	201	PEB	OD-C4D	2.62	1.28	1.23
82	Q1	202	PEB	OD-C4D	2.62	1.28	1.23
82	wC	203	PEB	OD-C4D	2.62	1.28	1.23
87	5N	603	CLA	C1B-C2B	2.62	1.49	1.43
87	7N	609	CLA	C1B-C2B	2.62	1.49	1.43
87	BN	824	CLA	CMD-C2D	-2.62	1.45	1.50
82	PJ	201	PEB	C1C-NC	-2.62	1.33	1.37
87	R2	204	CLA	C3B-C4B	2.62	1.48	1.42
84	U3	1001	CYC	C4B-NB	-2.62	1.32	1.38
87	B2	815	CLA	C1B-C2B	2.62	1.49	1.43
82	XK	202	PEB	C4A-NA	-2.62	1.31	1.37
87	K2	104	CLA	C1B-C2B	2.62	1.49	1.43
82	HQ	201	PEB	CHA-C1B	2.62	1.46	1.40
82	18	202	PEB	C2A-C1A	-2.62	1.49	1.52
87	A2	829	CLA	C4B-NB	2.62	1.41	1.37
82	D4	1002	PEB	OD-C4D	2.62	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	N5	202	PEB	OD-C4D	2.62	1.28	1.23
82	S5	203	PEB	OD-C4D	2.62	1.28	1.23
87	52	603	CLA	C1B-C2B	2.62	1.49	1.43
87	2N	307	CLA	C1B-C2B	2.62	1.49	1.43
84	d3	1001	CYC	C4B-NB	-2.62	1.32	1.38
87	LN	204	CLA	C3B-C4B	2.62	1.48	1.42
87	cL	516	CLA	C3B-C4B	2.62	1.48	1.42
82	BM	301	PEB	C2A-C1A	-2.62	1.49	1.52
82	GM	201	PEB	OD-C4D	2.62	1.28	1.23
82	S9	201	PEB	C4A-NA	-2.62	1.31	1.37
82	m1	201	PEB	OD-C4D	2.62	1.28	1.23
82	DQ	201	PEB	C2C-C3C	2.62	1.45	1.38
82	YJ	203	PEB	OD-C4D	2.62	1.28	1.23
82	FO	1002	PEB	OD-C4D	2.62	1.28	1.23
82	BD	202	PEB	C2A-C1A	-2.62	1.49	1.52
87	1N	606	CLA	C3B-C4B	2.62	1.48	1.42
82	P4	202	PEB	C2C-C3C	2.62	1.45	1.38
82	v8	201	PEB	C1C-C2C	2.62	1.49	1.42
82	aJ	202	PEB	OD-C4D	2.62	1.28	1.23
82	lM	201	PEB	OD-C4D	2.62	1.28	1.23
87	6N	610	CLA	C1B-C2B	2.62	1.49	1.43
87	A2	814	CLA	C3B-C4B	2.62	1.48	1.42
82	GB	202	PEB	OD-C4D	2.62	1.28	1.23
82	UG	201	PEB	OD-C4D	2.62	1.28	1.23
82	RI	201	PEB	OD-C4D	2.62	1.28	1.23
82	P4	201	PEB	OD-C4D	2.62	1.28	1.23
84	LO	1001	CYC	OB-C4B	2.62	1.28	1.23
82	oK	202	PEB	C1C-C2C	2.62	1.49	1.42
84	O3	1001	CYC	C4B-NB	-2.62	1.32	1.38
82	kO	202	PEB	C2A-C1A	-2.62	1.49	1.52
82	IQ	202	PEB	C4B-C3B	2.62	1.49	1.45
82	QH	202	PEB	OD-C4D	2.61	1.28	1.23
82	IJ	203	PEB	OD-C4D	2.61	1.28	1.23
82	T4	202	PEB	OD-C4D	2.61	1.28	1.23
82	WJ	203	PEB	C2C-C3C	2.61	1.45	1.38
84	n3	1001	CYC	C4B-NB	-2.61	1.32	1.38
87	H6	103	CLA	C3B-C4B	2.61	1.48	1.42
82	HK	202	PEB	C2A-C1A	-2.61	1.49	1.52
87	LN	204	CLA	C1B-C2B	2.61	1.49	1.43
82	OP	203	PEB	C2C-C3C	2.61	1.45	1.38
82	LA	201	PEB	OD-C4D	2.61	1.28	1.23
82	NA	202	PEB	OD-C4D	2.61	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B5	203	PEB	OD-C4D	2.61	1.28	1.23
82	aE	201	PEB	OD-C4D	2.61	1.28	1.23
87	R2	201	CLA	C3B-C4B	2.61	1.48	1.42
87	BL	605	CLA	C4B-NB	2.61	1.41	1.37
82	NI	201	PEB	OD-C4D	2.61	1.28	1.23
82	S5	202	PEB	OD-C4D	2.61	1.28	1.23
82	TA	203	PEB	C4A-NA	-2.61	1.31	1.37
87	72	609	CLA	C1B-C2B	2.61	1.49	1.43
82	Y5	202	PEB	C2A-C1A	-2.61	1.49	1.52
87	b6	609	CLA	C3B-C4B	2.61	1.48	1.42
82	QD	201	PEB	C1C-C2C	2.61	1.49	1.42
82	qC	201	PEB	C1C-C2C	2.61	1.49	1.42
82	QH	201	PEB	OD-C4D	2.61	1.28	1.23
82	PI	201	PEB	OD-C4D	2.61	1.28	1.23
82	NJ	201	PEB	OD-C4D	2.61	1.28	1.23
82	u8	202	PEB	OD-C4D	2.61	1.28	1.23
87	AN	831	CLA	C1B-NB	-2.61	1.34	1.37
82	N7	201	PEB	OD-C4D	2.61	1.28	1.23
82	Z4	201	PEB	CHB-C1C	2.61	1.46	1.40
82	wC	201	PEB	C4B-C3B	2.61	1.49	1.45
82	f1	203	PEB	CHC-C4C	2.61	1.52	1.49
82	EQ	202	PEB	C2A-C1A	-2.61	1.49	1.52
82	iK	202	PEB	C2A-C1A	-2.61	1.49	1.52
82	iO	201	PEB	C2A-C1A	-2.61	1.49	1.52
84	LG	1001	CYC	C4C-NC	-2.61	1.31	1.37
82	Y4	203	PEB	OD-C4D	2.61	1.28	1.23
82	dM	202	PEB	OD-C4D	2.61	1.28	1.23
87	AL	403	CLA	C3B-C4B	2.61	1.48	1.42
82	U9	201	PEB	C4B-C3B	2.61	1.49	1.45
82	DB	202	PEB	OD-C4D	2.61	1.28	1.23
84	D1	1003	CYC	OB-C4B	2.61	1.28	1.23
82	q8	201	PEB	C1C-C2C	2.61	1.49	1.42
84	S3	1001	CYC	C4B-NB	-2.61	1.32	1.38
82	BF	201	PEB	C1D-ND	2.61	1.49	1.45
82	N7	202	PEB	CHA-C1B	2.61	1.46	1.40
82	LI	201	PEB	C4A-NA	-2.61	1.31	1.37
82	IP	203	PEB	C2A-C1A	-2.61	1.49	1.52
87	B6	611	CLA	C3B-C4B	2.61	1.48	1.42
82	A5	202	PEB	OD-C4D	2.61	1.28	1.23
87	HL	101	CLA	MG-NB	-2.61	2.00	2.05
82	ZF	202	PEB	C1C-C2C	2.61	1.49	1.42
82	mH	202	PEB	C1C-C2C	2.61	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	313	CLA	C1B-C2B	2.61	1.49	1.43
87	52	604	CLA	C1B-C2B	2.61	1.49	1.43
82	P4	202	PEB	OD-C4D	2.61	1.28	1.23
83	Y7	302	PUB	OA-C1A	2.61	1.28	1.23
87	12	606	CLA	C3B-C4B	2.61	1.48	1.42
87	C6	514	CLA	C3B-C4B	2.61	1.48	1.42
87	bL	614	CLA	C4B-NB	2.61	1.41	1.37
84	L3	1001	CYC	C4D-C3D	2.61	1.49	1.42
82	A5	201	PEB	OD-C4D	2.61	1.28	1.23
82	N7	203	PEB	OD-C4D	2.61	1.28	1.23
87	62	312	CLA	C4D-ND	-2.61	1.34	1.37
82	fJ	202	PEB	C1C-NC	-2.61	1.33	1.37
84	I1	1001	CYC	C1B-NB	-2.61	1.33	1.37
84	BE	1002	CYC	C4A-C3A	2.61	1.51	1.45
82	QE	201	PEB	OD-C4D	2.61	1.28	1.23
87	RN	204	CLA	C3B-C4B	2.61	1.48	1.42
87	AN	834	CLA	MG-NB	-2.61	2.00	2.05
87	22	607	CLA	C1B-C2B	2.61	1.49	1.43
82	U9	202	PEB	C4B-C3B	2.61	1.49	1.45
87	L2	204	CLA	C1B-C2B	2.61	1.49	1.43
83	K7	203	PUB	OD-C4D	2.61	1.28	1.23
84	n3	1001	CYC	C4D-C3D	2.61	1.49	1.42
82	TM	201	PEB	CHC-C4C	2.61	1.52	1.49
87	12	611	CLA	C1B-C2B	2.61	1.49	1.43
82	L7	201	PEB	OD-C4D	2.61	1.28	1.23
82	qK	201	PEB	OD-C4D	2.61	1.28	1.23
82	wK	301	PEB	OD-C4D	2.61	1.28	1.23
82	F5	203	PEB	C4A-NA	-2.61	1.31	1.37
82	QJ	203	PEB	OD-C4D	2.61	1.28	1.23
84	FH	1001	CYC	OB-C4B	2.61	1.28	1.23
87	A2	815	CLA	C3B-C4B	2.61	1.48	1.42
82	sF	203	PEB	CHC-C4C	2.61	1.52	1.49
82	AP	201	PEB	C4A-NA	-2.61	1.31	1.37
82	eA	301	PEB	OD-C4D	2.61	1.28	1.23
82	VH	201	PEB	OD-C4D	2.61	1.28	1.23
82	K5	201	PEB	OD-C4D	2.61	1.28	1.23
82	R5	201	PEB	OD-C4D	2.61	1.28	1.23
87	A6	404	CLA	C3B-C4B	2.61	1.48	1.42
82	WB	401	PEB	OD-C4D	2.61	1.28	1.23
82	VI	201	PEB	OD-C4D	2.61	1.28	1.23
82	L5	203	PEB	OD-C4D	2.61	1.28	1.23
82	lM	202	PEB	OD-C4D	2.61	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HP	201	PEB	C2A-C1A	-2.61	1.49	1.52
84	MG	1001	CYC	C4C-NC	-2.61	1.31	1.37
82	r8	202	PEB	C1C-C2C	2.61	1.49	1.42
87	RN	201	CLA	C3B-C4B	2.61	1.48	1.42
87	82	301	CLA	C3B-C4B	2.61	1.48	1.42
87	CL	511	CLA	MG-NB	-2.60	2.00	2.05
82	KI	202	PEB	OD-C4D	2.60	1.28	1.23
87	82	304	CLA	C1B-C2B	2.60	1.49	1.43
82	FD	203	PEB	C4A-NA	-2.60	1.31	1.37
87	AL	403	CLA	C4B-NB	2.60	1.41	1.37
82	YA	303	PEB	OD-C4D	2.60	1.28	1.23
82	ZE	201	PEB	OD-C4D	2.60	1.28	1.23
82	A1	301	PEB	OD-C4D	2.60	1.28	1.23
82	E7	202	PEB	C1D-ND	2.60	1.49	1.45
82	KD	201	PEB	C2A-C1A	-2.60	1.49	1.52
82	AK	202	PEB	C4B-C3B	2.60	1.49	1.45
82	d1	202	PEB	OD-C4D	2.60	1.28	1.23
82	N5	201	PEB	OD-C4D	2.60	1.28	1.23
82	gK	203	PEB	OD-C4D	2.60	1.28	1.23
87	22	605	CLA	C1B-NB	-2.60	1.34	1.37
87	AN	819	CLA	CHC-C1C	2.60	1.43	1.38
87	82	303	CLA	CMD-C2D	-2.60	1.45	1.50
84	B3	1001	CYC	C4D-C3D	2.60	1.49	1.42
84	H3	1001	CYC	C4D-C3D	2.60	1.49	1.42
82	MF	203	PEB	OD-C4D	2.60	1.28	1.23
82	P5	201	PEB	OD-C4D	2.60	1.28	1.23
82	hO	201	PEB	OD-C4D	2.60	1.28	1.23
84	f3	1001	CYC	C4D-C3D	2.60	1.49	1.42
87	bL	617	CLA	MG-NB	-2.60	2.00	2.05
82	F7	203	PEB	C2A-C1A	-2.60	1.49	1.52
87	cL	508	CLA	CMB-C2B	-2.60	1.45	1.50
87	KN	103	CLA	C1B-C2B	2.60	1.49	1.43
82	xK	304	PEB	C4B-C3B	2.60	1.49	1.45
87	1N	605	CLA	C1B-C2B	2.60	1.49	1.43
84	w3	1001	CYC	C4B-NB	-2.60	1.32	1.38
82	Q5	201	PEB	C4A-NA	-2.60	1.31	1.37
87	22	603	CLA	C1B-C2B	2.60	1.49	1.43
82	EI	201	PEB	OD-C4D	2.60	1.28	1.23
87	BN	823	CLA	C3B-C4B	2.60	1.48	1.42
82	TI	202	PEB	OD-C4D	2.60	1.28	1.23
82	XI	201	PEB	OD-C4D	2.60	1.28	1.23
82	b4	201	PEB	OD-C4D	2.60	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	ND	201	PUB	OA-C1A	2.60	1.28	1.23
84	KH	1001	CYC	OB-C4B	2.60	1.28	1.23
87	AN	815	CLA	C3B-C4B	2.60	1.48	1.42
82	O5	203	PEB	C1C-NC	-2.60	1.33	1.37
82	KE	201	PEB	OD-C4D	2.60	1.28	1.23
87	82	302	CLA	C1B-C2B	2.60	1.49	1.43
82	YA	301	PEB	OD-C4D	2.60	1.28	1.23
82	iF	202	PEB	OD-C4D	2.60	1.28	1.23
82	Q9	201	PEB	C2A-C1A	-2.60	1.49	1.52
87	a6	609	CLA	C3B-C4B	2.60	1.48	1.42
87	A2	805	CLA	CMD-C2D	-2.60	1.45	1.50
84	j3	1001	CYC	C4D-C3D	2.60	1.49	1.42
84	k3	1001	CYC	C4D-C3D	2.60	1.49	1.42
82	eJ	201	PEB	OD-C4D	2.60	1.28	1.23
82	XQ	202	PEB	C4B-C3B	2.60	1.49	1.45
84	f3	1001	CYC	C4B-NB	-2.60	1.32	1.38
82	l1	203	PEB	C1C-C2C	2.60	1.49	1.42
82	DG	1002	PEB	OD-C4D	2.60	1.28	1.23
82	S9	201	PEB	OD-C4D	2.60	1.28	1.23
87	B2	833	CLA	MG-NB	-2.60	2.00	2.05
82	PP	201	PEB	C2A-C1A	-2.60	1.49	1.52
82	BK	201	PEB	C1D-ND	2.60	1.49	1.45
82	m4	203	PEB	C4B-C3B	2.60	1.49	1.45
87	2N	304	CLA	C3B-C4B	2.60	1.48	1.42
82	HI	202	PEB	CHA-C1B	2.60	1.46	1.40
82	Y7	304	PEB	OD-C4D	2.60	1.28	1.23
82	TA	203	PEB	C1C-NC	-2.60	1.33	1.37
82	D5	201	PEB	C4A-NA	-2.60	1.31	1.37
87	6N	609	CLA	C1B-C2B	2.60	1.49	1.43
87	7N	605	CLA	C1B-C2B	2.60	1.49	1.43
82	XA	202	PEB	C1A-NA	-2.60	1.34	1.37
82	RA	201	PEB	C4A-NA	-2.60	1.31	1.37
82	R7	201	PEB	C4A-NA	-2.60	1.31	1.37
84	73	1001	CYC	C4B-NB	-2.60	1.32	1.38
84	73	1002	CYC	C1B-C2B	2.60	1.49	1.45
82	pK	201	PEB	OD-C4D	2.60	1.28	1.23
84	o3	1001	CYC	C4D-C3D	2.60	1.48	1.42
82	ZG	201	PEB	OD-C4D	2.60	1.28	1.23
87	L2	206	CLA	MG-NB	-2.60	2.00	2.05
82	RI	203	PEB	C4B-NB	-2.60	1.33	1.38
82	SP	203	PEB	C4B-C3B	2.60	1.49	1.45
82	VP	201	PEB	C4B-C3B	2.60	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	q3	1001	CYC	C4B-NB	-2.60	1.32	1.38
82	GD	201	PEB	OD-C4D	2.60	1.28	1.23
82	CJ	203	PEB	OD-C4D	2.60	1.28	1.23
87	5N	605	CLA	C1B-C2B	2.60	1.49	1.43
87	42	604	CLA	C3B-C4B	2.60	1.48	1.42
82	MF	202	PEB	C4B-C3B	2.60	1.49	1.45
82	YO	202	PEB	OD-C4D	2.59	1.28	1.23
87	a6	607	CLA	C3B-C4B	2.59	1.48	1.42
82	UM	203	PEB	C1C-C2C	2.59	1.48	1.42
84	L4	1001	CYC	OB-C4B	2.59	1.28	1.23
82	PO	202	PEB	C2A-C1A	-2.59	1.49	1.52
84	KG	202	CYC	OB-C4B	2.59	1.28	1.23
82	JI	201	PEB	C1C-NC	-2.59	1.33	1.37
96	fL	102	HEM	C1C-C2C	-2.59	1.40	1.45
87	AL	405	CLA	MG-NB	-2.59	2.00	2.05
82	aG	201	PEB	OD-C4D	2.59	1.28	1.23
87	12	604	CLA	C1B-C2B	2.59	1.49	1.43
87	62	302	CLA	C1B-C2B	2.59	1.49	1.43
82	dF	202	PEB	C1C-C2C	2.59	1.48	1.42
87	BN	814	CLA	C4B-NB	2.59	1.41	1.37
82	BI	201	PEB	C2A-C1A	-2.59	1.49	1.52
82	PB	201	PEB	C4A-NA	-2.59	1.31	1.37
82	II	203	PEB	OD-C4D	2.59	1.28	1.23
82	TO	202	PEB	OD-C4D	2.59	1.28	1.23
82	a4	201	PEB	OD-C4D	2.59	1.28	1.23
84	Q3	1001	CYC	C4D-C3D	2.59	1.48	1.42
82	Q1	201	PEB	C4B-C3B	2.59	1.49	1.45
82	N7	202	PEB	C1A-NA	-2.59	1.34	1.37
82	rF	201	PEB	C1A-NA	-2.59	1.34	1.37
87	5N	604	CLA	C1B-C2B	2.59	1.49	1.43
82	HK	201	PEB	C4A-NA	-2.59	1.31	1.37
87	B2	818	CLA	C3B-C4B	2.59	1.48	1.42
87	b6	604	CLA	C3B-C4B	2.59	1.48	1.42
82	FQ	203	PEB	C4A-NA	-2.59	1.31	1.37
82	AI	203	PEB	CHA-C1B	2.59	1.46	1.40
82	NF	202	PEB	C2A-C1A	-2.59	1.49	1.52
87	B2	823	CLA	CMD-C2D	-2.59	1.45	1.50
83	Z5	302	PUB	OD-C4D	2.59	1.28	1.23
82	X5	201	PEB	OD-C4D	2.59	1.28	1.23
82	aB	202	PEB	C2A-C1A	-2.59	1.49	1.52
82	mM	201	PEB	C2A-C1A	-2.59	1.49	1.52
82	IF	201	PEB	C3B-C2B	2.59	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Y7	301	PEB	CHC-C4C	2.59	1.52	1.49
87	AN	820	CLA	C4B-NB	2.59	1.41	1.37
87	72	608	CLA	C1B-C2B	2.59	1.49	1.43
82	ZK	202	PEB	C1C-C2C	2.59	1.48	1.42
87	B6	605	CLA	C3B-C4B	2.59	1.48	1.42
82	mH	201	PEB	C2A-C1A	-2.59	1.49	1.52
82	J5	203	PEB	OD-C4D	2.59	1.28	1.23
82	UI	202	PEB	OD-C4D	2.59	1.28	1.23
82	UP	203	PEB	OD-C4D	2.59	1.28	1.23
82	aO	202	PEB	OD-C4D	2.59	1.28	1.23
82	T7	203	PEB	C1C-NC	-2.59	1.33	1.37
87	BN	801	CLA	CMD-C2D	-2.59	1.45	1.50
82	IQ	202	PEB	C2A-C1A	-2.59	1.49	1.52
84	JH	1003	CYC	C2C-C1C	-2.59	1.49	1.52
82	DK	202	PEB	OD-C4D	2.59	1.28	1.23
82	G5	201	PEB	OD-C4D	2.59	1.28	1.23
82	KA	201	PEB	CHC-C4C	2.59	1.52	1.49
83	M9	303	PUB	CHA-C1B	2.59	1.52	1.49
87	12	605	CLA	C1B-C2B	2.59	1.49	1.43
84	M3	1001	CYC	C4D-C3D	2.59	1.48	1.42
82	GQ	201	PEB	OD-C4D	2.59	1.28	1.23
87	72	605	CLA	C1B-C2B	2.59	1.49	1.43
82	SJ	201	PEB	C2A-C1A	-2.59	1.49	1.52
87	6N	613	CLA	C1B-C2B	2.59	1.49	1.43
82	hJ	203	PEB	C1C-C2C	2.59	1.48	1.42
84	U3	1001	CYC	C4D-C3D	2.59	1.48	1.42
87	CL	503	CLA	C4B-NB	2.59	1.41	1.37
84	KG	202	CYC	C4C-NC	-2.59	1.31	1.37
82	NA	201	PEB	OD-C4D	2.59	1.28	1.23
82	EK	201	PEB	OD-C4D	2.59	1.28	1.23
83	xK	301	PUB	OA-C1A	2.59	1.28	1.23
87	RN	202	CLA	C3B-C4B	2.59	1.48	1.42
82	a1	202	PEB	C2A-C1A	-2.59	1.49	1.52
82	aO	201	PEB	C1C-NC	-2.59	1.33	1.37
82	QB	201	PEB	OD-C4D	2.59	1.28	1.23
82	RO	201	PEB	OD-C4D	2.59	1.28	1.23
82	M5	301	PEB	OD-C4D	2.59	1.28	1.23
82	gE	202	PEB	OD-C4D	2.59	1.28	1.23
82	EJ	202	PEB	OD-C4D	2.59	1.28	1.23
82	SP	203	PEB	OD-C4D	2.59	1.28	1.23
82	m1	202	PEB	OD-C4D	2.59	1.28	1.23
82	UO	201	PEB	C4A-NA	-2.59	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	oF	202	PEB	C1C-C2C	2.59	1.48	1.42
82	hE	201	PEB	C2A-C1A	-2.58	1.49	1.52
82	eF	202	PEB	C2A-C1A	-2.58	1.49	1.52
82	hG	201	PEB	C2A-C1A	-2.58	1.49	1.52
87	52	609	CLA	C1B-C2B	2.58	1.49	1.43
84	73	1001	CYC	C4D-C3D	2.58	1.48	1.42
82	ID	202	PEB	C4B-C3B	2.58	1.49	1.45
87	B2	813	CLA	C4B-NB	2.58	1.41	1.37
87	B2	804	CLA	CHC-C1C	2.58	1.43	1.38
87	62	311	CLA	C1B-C2B	2.58	1.49	1.43
87	c6	615	CLA	C1B-C2B	2.58	1.49	1.43
87	bL	621	CLA	C1B-C2B	2.58	1.49	1.43
82	aK	202	PEB	C2A-C1A	-2.58	1.49	1.52
87	bL	605	CLA	C3B-C4B	2.58	1.48	1.42
87	c6	612	CLA	C1B-C2B	2.58	1.49	1.43
87	A2	830	CLA	C4B-NB	2.58	1.41	1.37
82	GJ	203	PEB	OD-C4D	2.58	1.28	1.23
87	KN	103	CLA	C3B-C4B	2.58	1.48	1.42
82	Y4	201	PEB	C1C-NC	-2.58	1.33	1.37
82	UD	201	PEB	C2A-C1A	-2.58	1.49	1.52
82	aJ	201	PEB	C2A-C1A	-2.58	1.49	1.52
87	AN	830	CLA	C4B-NB	2.58	1.41	1.37
82	YB	201	PEB	C4A-NA	-2.58	1.31	1.37
82	KJ	201	PEB	C4A-NA	-2.58	1.31	1.37
87	K2	104	CLA	C3B-C4B	2.58	1.48	1.42
82	KM	203	PEB	OD-C4D	2.58	1.28	1.23
103	82	310	ZEX	C10-C9	-2.58	1.32	1.35
82	xC	201	PEB	C1C-NC	-2.58	1.33	1.37
87	FN	203	CLA	MG-NB	-2.58	2.00	2.05
82	JK	201	PEB	OD-C4D	2.58	1.28	1.23
82	PO	202	PEB	OD-C4D	2.58	1.28	1.23
82	cK	203	PEB	OD-C4D	2.58	1.28	1.23
83	xF	301	PUB	OA-C1A	2.58	1.28	1.23
84	u3	1001	CYC	C4D-C3D	2.58	1.48	1.42
82	EJ	201	PEB	C2A-C1A	-2.58	1.49	1.52
87	BN	805	CLA	CMD-C2D	-2.58	1.45	1.50
82	EJ	201	PEB	OD-C4D	2.58	1.28	1.23
82	Z5	301	PEB	OD-C4D	2.58	1.28	1.23
83	yF	303	PUB	OD-C4D	2.58	1.28	1.23
84	BG	1001	CYC	C4B-NB	-2.58	1.32	1.38
87	b6	614	CLA	C3B-C4B	2.58	1.48	1.42
84	O3	1001	CYC	C4D-C3D	2.58	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	607	CLA	CMD-C2D	-2.58	1.45	1.50
82	JK	202	PEB	C1C-NC	-2.58	1.33	1.37
87	A2	822	CLA	MG-NB	-2.58	2.00	2.05
87	A2	830	CLA	MG-NB	-2.58	2.00	2.05
87	DL	403	CLA	C3B-C4B	2.58	1.48	1.42
87	8N	302	CLA	C3B-C4B	2.58	1.48	1.42
84	q3	1001	CYC	C4D-C3D	2.58	1.48	1.42
82	kG	202	PEB	C4A-NA	-2.58	1.31	1.37
87	aL	605	CLA	CMD-C2D	-2.58	1.45	1.50
82	JB	202	PEB	C2A-C1A	-2.58	1.49	1.52
82	WI	203	PEB	C2A-C1A	-2.58	1.49	1.52
82	YP	502	PEB	OD-C4D	2.58	1.28	1.23
87	C6	511	CLA	C1B-C2B	2.58	1.49	1.43
87	1N	601	CLA	C1B-C2B	2.58	1.49	1.43
87	4N	601	CLA	C1B-C2B	2.58	1.49	1.43
82	QF	203	PEB	CHA-C1B	2.58	1.46	1.40
82	E5	201	PEB	OD-C4D	2.58	1.28	1.23
87	A2	834	CLA	MG-NB	-2.58	2.00	2.05
87	CL	504	CLA	C3B-C4B	2.58	1.48	1.42
82	OG	202	PEB	C2A-C1A	-2.58	1.49	1.52
82	ZE	203	PEB	C4A-NA	-2.58	1.31	1.37
87	62	310	CLA	C1B-C2B	2.58	1.49	1.43
82	OE	203	PEB	OD-C4D	2.58	1.28	1.23
82	e4	202	PEB	OD-C4D	2.58	1.28	1.23
82	pF	201	PEB	OD-C4D	2.58	1.28	1.23
82	HI	201	PEB	C1C-NC	-2.58	1.33	1.37
87	BN	833	CLA	C3B-C4B	2.58	1.48	1.42
82	ZE	201	PEB	C2C-C3C	2.58	1.45	1.38
84	F3	1001	CYC	C4D-C3D	2.58	1.48	1.42
82	bB	201	PEB	C2A-C1A	-2.58	1.49	1.52
82	CK	201	PEB	OD-C4D	2.58	1.28	1.23
82	NO	1002	PEB	OD-C4D	2.58	1.28	1.23
82	RE	201	PEB	C1C-NC	-2.58	1.33	1.37
87	6N	607	CLA	C1B-C2B	2.58	1.49	1.43
82	DB	203	PEB	OD-C4D	2.58	1.28	1.23
82	qF	201	PEB	OD-C4D	2.58	1.28	1.23
82	lJ	201	PEB	OD-C4D	2.58	1.28	1.23
87	6N	602	CLA	C1B-C2B	2.58	1.49	1.43
82	dK	202	PEB	C1C-C2C	2.58	1.48	1.42
87	cL	509	CLA	C4B-NB	2.58	1.41	1.37
87	7N	608	CLA	C1B-C2B	2.57	1.49	1.43
82	D5	202	PEB	OD-C4D	2.57	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	KO	1001	CYC	OB-C4B	2.57	1.28	1.23
87	BN	834	CLA	CMD-C2D	-2.57	1.45	1.50
82	Z5	305	PEB	CHA-C1B	2.57	1.46	1.40
82	V4	201	PEB	C1C-NC	-2.57	1.33	1.37
87	B2	817	CLA	C3B-C4B	2.57	1.48	1.42
87	AN	826	CLA	C4B-NB	2.57	1.40	1.37
82	HK	202	PEB	OD-C4D	2.57	1.28	1.23
87	BL	608	CLA	C3B-C4B	2.57	1.48	1.42
82	KM	201	PEB	OD-C4D	2.57	1.28	1.23
82	W5	201	PEB	C4A-NA	-2.57	1.31	1.37
82	bF	202	PEB	C2A-C1A	-2.57	1.49	1.52
82	rF	202	PEB	C2A-C1A	-2.57	1.49	1.52
87	B6	615	CLA	C3B-C4B	2.57	1.48	1.42
87	1N	604	CLA	C1B-C2B	2.57	1.49	1.43
82	MJ	201	PEB	C4A-NA	-2.57	1.31	1.37
87	2N	304	CLA	C1B-C2B	2.57	1.49	1.43
87	A2	822	CLA	C1B-C2B	2.57	1.49	1.43
87	AN	829	CLA	C4B-NB	2.57	1.40	1.37
82	AI	201	PEB	OD-C4D	2.57	1.28	1.23
83	yF	303	PUB	OA-C1A	2.57	1.28	1.23
84	j3	1001	CYC	OB-C4B	2.57	1.28	1.23
82	MP	203	PEB	C2A-C1A	-2.57	1.49	1.52
82	gF	201	PEB	C2A-C1A	-2.57	1.49	1.52
87	52	607	CLA	C1B-C2B	2.57	1.49	1.43
87	62	303	CLA	C1B-C2B	2.57	1.49	1.43
82	IB	202	PEB	OD-C4D	2.57	1.28	1.23
82	F5	202	PEB	OD-C4D	2.57	1.28	1.23
87	BN	805	CLA	CHC-C1C	2.57	1.43	1.38
87	42	601	CLA	C1B-C2B	2.57	1.49	1.43
82	yC	203	PEB	C4B-C3B	2.57	1.49	1.45
87	aL	606	CLA	C3B-C4B	2.57	1.48	1.42
82	KA	201	PEB	C2A-C1A	-2.57	1.49	1.52
82	iH	202	PEB	C1B-C2B	2.57	1.51	1.45
84	LH	1001	CYC	C4C-NC	-2.57	1.31	1.37
82	H9	201	PEB	C4B-C3B	2.57	1.49	1.45
87	AN	809	CLA	C3B-C4B	2.57	1.48	1.42
87	C6	517	CLA	C3B-C4B	2.57	1.48	1.42
82	TJ	201	PEB	CHC-C4C	2.57	1.52	1.49
82	TQ	202	PEB	CHC-C4C	2.57	1.52	1.49
87	B2	804	CLA	MG-NB	-2.57	2.00	2.05
87	BN	818	CLA	C3B-C4B	2.57	1.48	1.42
82	FA	202	PEB	C4B-C3B	2.57	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	NE	201	CYC	C4C-NC	-2.57	1.31	1.37
87	8N	302	CLA	CMC-C2C	-2.57	1.45	1.50
82	AK	202	PEB	C2A-C1A	-2.57	1.49	1.52
82	QM	203	PEB	OD-C4D	2.57	1.28	1.23
82	I5	201	PEB	OD-C4D	2.57	1.28	1.23
84	CG	1001	CYC	C1B-C2B	2.57	1.49	1.45
82	C5	201	PEB	C4A-NA	-2.57	1.31	1.37
82	QH	201	PEB	C4B-C3B	2.57	1.49	1.45
87	BN	816	CLA	C4D-ND	-2.57	1.34	1.37
82	HM	201	PEB	CHC-C4C	2.57	1.52	1.49
87	BN	816	CLA	C1B-C2B	2.57	1.49	1.43
87	6N	601	CLA	C1B-C2B	2.57	1.49	1.43
84	I3	1001	CYC	C4D-C3D	2.57	1.48	1.42
87	AN	849	CLA	C1B-NB	-2.57	1.34	1.37
87	d6	401	CLA	C3B-C4B	2.57	1.48	1.42
84	h3	1001	CYC	C4D-C3D	2.57	1.48	1.42
82	gJ	202	PEB	C2A-C1A	-2.57	1.49	1.52
82	YA	304	PEB	OD-C4D	2.57	1.28	1.23
82	aM	202	PEB	OD-C4D	2.57	1.28	1.23
82	lO	202	PEB	OD-C4D	2.57	1.28	1.23
87	B2	834	CLA	CMD-C2D	-2.57	1.45	1.50
87	cL	514	CLA	CMD-C2D	-2.57	1.45	1.50
87	AN	808	CLA	C3B-C4B	2.57	1.48	1.42
84	W3	1001	CYC	OB-C4B	2.57	1.28	1.23
87	IN	102	CLA	C3B-C4B	2.57	1.48	1.42
82	YD	201	PEB	C2A-C1A	-2.57	1.49	1.52
82	ZK	202	PEB	C2A-C1A	-2.57	1.49	1.52
82	IF	203	PEB	C4A-NA	-2.57	1.32	1.37
87	HL	101	CLA	C3B-C4B	2.57	1.48	1.42
82	WP	201	PEB	OD-C4D	2.57	1.28	1.23
87	32	312	CLA	C1B-C2B	2.57	1.49	1.43
87	82	308	CLA	C3C-C2C	2.57	1.42	1.36
82	VK	202	PEB	OD-C4D	2.57	1.28	1.23
83	yK	303	PUB	OA-C1A	2.57	1.28	1.23
82	JA	201	PEB	C2A-C1A	-2.57	1.49	1.52
82	i4	202	PEB	C2A-C1A	-2.57	1.49	1.52
87	4N	606	CLA	C1B-C2B	2.57	1.49	1.43
87	R2	202	CLA	C3B-C4B	2.57	1.48	1.42
83	AJ	303	PUB	C3C-C4C	2.57	1.52	1.43
82	MK	203	PEB	OD-C4D	2.57	1.28	1.23
83	ND	201	PUB	OD-C4D	2.57	1.28	1.23
82	sC	202	PEB	CHC-C4C	2.57	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PO	202	PEB	C2C-C3C	2.57	1.45	1.38
87	B6	608	CLA	C3B-C4B	2.57	1.48	1.42
82	YO	201	PEB	C1C-NC	-2.57	1.33	1.37
103	8N	310	ZEX	C10-C9	-2.57	1.32	1.35
87	3N	312	CLA	C1B-C2B	2.57	1.49	1.43
82	EF	201	PEB	OD-C4D	2.57	1.28	1.23
82	ZI	401	PEB	OD-C4D	2.57	1.28	1.23
82	UM	202	PEB	OD-C4D	2.57	1.28	1.23
87	B6	610	CLA	C3B-C4B	2.57	1.48	1.42
82	rC	202	PEB	C1C-C2C	2.57	1.48	1.42
82	RA	202	PEB	OD-C4D	2.56	1.28	1.23
82	OI	201	PEB	OD-C4D	2.56	1.28	1.23
82	ZG	201	PEB	C2C-C3C	2.56	1.45	1.38
82	cB	402	PEB	C2A-C1A	-2.56	1.49	1.52
87	BN	835	CLA	MG-NB	-2.56	2.00	2.05
87	A2	808	CLA	C3B-C4B	2.56	1.48	1.42
87	A2	809	CLA	C3B-C4B	2.56	1.48	1.42
82	NG	201	PEB	OD-C4D	2.56	1.28	1.23
82	QQ	202	PEB	OD-C4D	2.56	1.28	1.23
87	3N	313	CLA	C1B-C2B	2.56	1.49	1.43
82	R4	203	PEB	OD-C4D	2.56	1.28	1.23
83	NQ	201	PUB	OD-C4D	2.56	1.28	1.23
87	B2	808	CLA	C4B-NB	2.56	1.40	1.37
87	B2	826	CLA	CMD-C2D	-2.56	1.45	1.50
82	uC	203	PEB	C2A-C1A	-2.56	1.49	1.52
87	AN	830	CLA	MG-NB	-2.56	2.00	2.05
87	6N	606	CLA	C1B-C2B	2.56	1.49	1.43
82	g4	203	PEB	C4B-C3B	2.56	1.49	1.45
87	AN	815	CLA	C4B-NB	2.56	1.40	1.37
83	xK	306	PUB	C4B-C3B	2.56	1.48	1.42
87	4N	604	CLA	C3B-C4B	2.56	1.48	1.42
82	N4	1002	PEB	OD-C4D	2.56	1.28	1.23
82	VD	203	PEB	C2A-C1A	-2.56	1.49	1.52
82	VE	201	PEB	C2A-C1A	-2.56	1.49	1.52
82	MJ	203	PEB	C2A-C1A	-2.56	1.49	1.52
82	FP	202	PEB	C2A-C1A	-2.56	1.49	1.52
87	C6	509	CLA	C3B-C4B	2.56	1.48	1.42
87	BN	826	CLA	CMB-C2B	-2.56	1.45	1.50
84	w3	1001	CYC	C4D-C3D	2.56	1.48	1.42
94	aL	601	PL9	C6-C5	2.56	1.48	1.35
82	XD	202	PEB	C4B-C3B	2.56	1.49	1.45
83	BJ	302	PUB	OD-C4D	2.56	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	805	CLA	MG-NB	-2.56	2.00	2.05
87	CL	504	CLA	CMB-C2B	-2.56	1.45	1.50
87	CL	506	CLA	CMB-C2B	-2.56	1.45	1.50
87	62	308	CLA	C1B-C2B	2.56	1.49	1.43
83	wK	304	PUB	OA-C1A	2.56	1.28	1.23
87	LN	206	CLA	MG-NB	-2.56	2.00	2.05
87	F2	201	CLA	MG-NB	-2.56	2.00	2.05
82	BB	203	PEB	C4A-NA	-2.56	1.32	1.37
87	B2	804	CLA	CMD-C2D	-2.56	1.45	1.50
87	cL	516	CLA	C1B-C2B	2.56	1.49	1.43
82	KD	202	PEB	OD-C4D	2.56	1.28	1.23
82	M5	305	PEB	OD-C4D	2.56	1.28	1.23
87	52	605	CLA	C1B-C2B	2.56	1.49	1.43
82	PK	201	PEB	OD-C4D	2.56	1.28	1.23
82	V5	201	PEB	OD-C4D	2.56	1.28	1.23
87	C6	520	CLA	C1B-C2B	2.56	1.49	1.43
87	5N	609	CLA	C1B-C2B	2.56	1.49	1.43
87	bL	614	CLA	C3B-C4B	2.56	1.48	1.42
82	XF	201	PEB	OD-C4D	2.56	1.28	1.23
82	NA	202	PEB	C2C-C3C	2.56	1.45	1.38
82	DB	203	PEB	C4A-NA	-2.56	1.32	1.37
82	ZJ	201	PEB	OD-C4D	2.56	1.28	1.23
82	C5	201	PEB	OD-C4D	2.56	1.28	1.23
87	cL	512	CLA	MG-NB	-2.56	2.00	2.05
87	2N	301	CLA	MG-ND	-2.56	2.00	2.05
87	I2	102	CLA	C3B-C4B	2.56	1.48	1.42
87	AL	404	CLA	C4B-NB	2.56	1.40	1.37
87	c6	606	CLA	C1B-C2B	2.56	1.49	1.43
82	MK	202	PEB	C4B-C3B	2.56	1.49	1.45
82	MJ	203	PEB	OD-C4D	2.56	1.28	1.23
82	L5	201	PEB	C4A-NA	-2.56	1.32	1.37
87	BN	807	CLA	C3B-C4B	2.56	1.48	1.42
82	gF	201	PEB	CHB-C1C	2.56	1.46	1.40
87	62	312	CLA	C1B-C2B	2.56	1.49	1.43
82	HK	201	PEB	CHA-C1B	2.56	1.46	1.40
87	A2	849	CLA	C1B-NB	-2.56	1.34	1.37
82	LI	201	PEB	OD-C4D	2.56	1.28	1.23
83	wF	304	PUB	OA-C1A	2.56	1.28	1.23
87	AN	805	CLA	MG-NB	-2.56	2.00	2.05
82	i1	201	PEB	C2A-C1A	-2.56	1.49	1.52
82	w8	203	PEB	C2A-C1A	-2.56	1.49	1.52
87	7N	610	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	cJ	201	PEB	C1C-NC	-2.56	1.33	1.37
82	JA	202	PEB	C1C-C2C	2.56	1.48	1.42
82	dJ	202	PEB	OD-C4D	2.56	1.28	1.23
87	2N	309	CLA	MG-NB	-2.56	2.00	2.05
82	O7	201	PEB	C2C-C3C	2.56	1.45	1.38
82	Y7	303	PEB	C1C-C2C	2.56	1.48	1.42
82	VD	201	PEB	OD-C4D	2.56	1.28	1.23
82	UH	201	PEB	C2A-C1A	-2.56	1.49	1.52
82	gO	203	PEB	C2A-C1A	-2.56	1.49	1.52
87	BN	815	CLA	C4D-ND	-2.56	1.34	1.37
82	hB	301	PEB	C4B-C3B	2.56	1.49	1.45
82	R7	202	PEB	OD-C4D	2.56	1.28	1.23
82	U4	201	PEB	C4A-NA	-2.56	1.32	1.37
87	BN	811	CLA	MG-NB	-2.56	2.00	2.05
82	VD	203	PEB	OD-C4D	2.56	1.28	1.23
82	T4	201	PEB	OD-C4D	2.56	1.28	1.23
82	VE	202	PEB	C2A-C1A	-2.56	1.49	1.52
82	cB	401	PEB	C2A-C1A	-2.56	1.49	1.52
82	VF	202	PEB	OD-C4D	2.56	1.28	1.23
82	MJ	201	PEB	OD-C4D	2.56	1.28	1.23
82	O1	203	PEB	OD-C4D	2.56	1.28	1.23
82	Z5	305	PEB	OD-C4D	2.56	1.28	1.23
87	BN	826	CLA	CMD-C2D	-2.56	1.45	1.50
87	B2	823	CLA	C4B-NB	2.55	1.40	1.37
82	Y9	201	PEB	C2A-C1A	-2.55	1.49	1.52
82	PA	202	PEB	C1A-NA	-2.55	1.34	1.37
87	BN	826	CLA	C4B-NB	2.55	1.40	1.37
87	AN	817	CLA	MG-NB	-2.55	2.00	2.05
87	A2	819	CLA	CHC-C1C	2.55	1.43	1.38
87	AN	832	CLA	CMD-C2D	-2.55	1.45	1.50
87	BL	605	CLA	C3B-C4B	2.55	1.48	1.42
82	YA	301	PEB	CHC-C4C	2.55	1.52	1.49
82	X7	202	PEB	C2A-C1A	-2.55	1.49	1.52
84	HO	1001	CYC	C1B-C2B	2.55	1.49	1.45
87	52	608	CLA	CMD-C2D	-2.55	1.45	1.50
82	OA	201	PEB	C2C-C3C	2.55	1.45	1.38
87	22	609	CLA	MG-NB	-2.55	2.00	2.05
82	aK	202	PEB	OD-C4D	2.55	1.28	1.23
87	BN	805	CLA	MG-NB	-2.55	2.00	2.05
82	KJ	203	PEB	CHA-C1B	2.55	1.46	1.40
82	M5	305	PEB	CHA-C1B	2.55	1.46	1.40
82	DE	1002	PEB	OD-C4D	2.55	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NE	202	PEB	OD-C4D	2.55	1.28	1.23
82	R4	201	PEB	OD-C4D	2.55	1.28	1.23
82	QQ	201	PEB	C1C-C2C	2.55	1.48	1.42
87	K6	101	CLA	C3B-C4B	2.55	1.48	1.42
87	42	606	CLA	C1B-C2B	2.55	1.49	1.43
84	d3	1001	CYC	OB-C4B	2.55	1.28	1.23
87	BN	809	CLA	C4B-NB	2.55	1.40	1.37
87	BL	621	CLA	MG-NB	-2.55	2.00	2.05
87	AN	822	CLA	MG-NB	-2.55	2.00	2.05
82	NB	201	PEB	C4A-NA	-2.55	1.32	1.37
82	aJ	203	PEB	C1C-C2C	2.55	1.48	1.42
84	LH	1001	CYC	C4B-NB	-2.55	1.32	1.38
82	TF	202	PEB	CHC-C4C	2.55	1.52	1.49
82	hH	201	PEB	CHC-C4C	2.55	1.52	1.49
87	B2	807	CLA	C3B-C4B	2.55	1.48	1.42
82	BI	202	PEB	C1A-NA	-2.55	1.34	1.37
82	dM	201	PEB	OD-C4D	2.55	1.28	1.23
87	cL	514	CLA	C1B-C2B	2.55	1.49	1.43
82	B5	203	PEB	C1C-NC	-2.55	1.33	1.37
84	N4	1001	CYC	C1B-NB	-2.55	1.33	1.37
87	8N	308	CLA	C3C-C2C	2.55	1.42	1.36
82	WI	202	PEB	C4D-ND	2.55	1.38	1.35
82	IM	202	PEB	OD-C4D	2.55	1.28	1.23
82	Y5	201	PEB	OD-C4D	2.55	1.28	1.23
82	IJ	201	PEB	OD-C4D	2.55	1.28	1.23
87	A2	815	CLA	C4B-NB	2.55	1.40	1.37
82	X7	202	PEB	OD-C4D	2.55	1.28	1.23
82	aJ	201	PEB	OD-C4D	2.55	1.28	1.23
87	BN	836	CLA	C1B-C2B	2.55	1.49	1.43
87	42	608	CLA	CMB-C2B	-2.55	1.45	1.50
82	h4	201	PEB	OD-C4D	2.55	1.28	1.23
84	LE	1001	CYC	C4C-NC	-2.55	1.32	1.37
82	UO	201	PEB	CHA-C4A	-2.55	1.31	1.36
82	UP	202	PEB	C2A-C1A	-2.55	1.49	1.52
82	VO	201	PEB	C1C-NC	-2.55	1.33	1.37
87	2N	301	CLA	C1B-NB	-2.55	1.34	1.37
82	K7	201	PEB	CHC-C4C	2.55	1.52	1.49
82	BF	201	PEB	C4D-ND	2.55	1.38	1.35
87	5N	607	CLA	C1B-C2B	2.55	1.49	1.43
82	XA	202	PEB	OD-C4D	2.55	1.28	1.23
84	H3	1001	CYC	OB-C4B	2.55	1.28	1.23
82	HA	203	PEB	C2A-C1A	-2.55	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	m4	203	PEB	C2A-C1A	-2.55	1.49	1.52
82	WH	203	PEB	C1C-C2C	2.55	1.48	1.42
82	PA	202	PEB	OD-C4D	2.55	1.28	1.23
82	SE	202	PEB	OD-C4D	2.55	1.28	1.23
84	h3	1001	CYC	OB-C4B	2.55	1.28	1.23
87	8N	304	CLA	CMD-C2D	-2.55	1.45	1.50
82	jK	201	PEB	C1A-NA	-2.55	1.34	1.37
83	yF	302	PUB	OA-C1A	2.55	1.28	1.23
82	GI	201	PEB	C4A-NA	-2.55	1.32	1.37
82	VI	203	PEB	C4A-NA	-2.55	1.32	1.37
82	MF	201	PEB	C2A-C1A	-2.55	1.49	1.52
87	AN	822	CLA	C1B-C2B	2.55	1.49	1.43
82	WM	203	PEB	OD-C4D	2.55	1.28	1.23
82	ZK	202	PEB	C4B-C3B	2.55	1.49	1.45
87	L2	202	CLA	C1B-C2B	2.55	1.49	1.43
87	B2	814	CLA	C4D-ND	-2.55	1.34	1.37
82	KG	201	PEB	OD-C4D	2.54	1.28	1.23
87	b6	617	CLA	CMC-C2C	-2.54	1.45	1.50
82	J7	201	PEB	C2A-C1A	-2.54	1.49	1.52
82	F9	201	PEB	OD-C4D	2.54	1.28	1.23
82	IP	201	PEB	C4A-NA	-2.54	1.32	1.37
87	BL	606	CLA	CMC-C2C	-2.54	1.45	1.50
87	62	307	CLA	C1B-C2B	2.54	1.49	1.43
82	H1	1002	PEB	OD-C4D	2.54	1.28	1.23
87	B2	815	CLA	C4D-ND	-2.54	1.34	1.37
82	uF	201	PEB	C1D-ND	2.54	1.49	1.45
87	B2	826	CLA	C4B-NB	2.54	1.40	1.37
87	22	606	CLA	C1B-C2B	2.54	1.49	1.43
87	JN	101	CLA	MG-NB	-2.54	2.00	2.05
82	B7	201	PEB	C2A-C1A	-2.54	1.49	1.52
82	z8	201	PEB	C1C-C2C	2.54	1.48	1.42
87	6N	605	CLA	C1B-C2B	2.54	1.49	1.43
82	Y9	202	PEB	C4B-C3B	2.54	1.49	1.45
82	CF	201	PEB	C2A-C1A	-2.54	1.49	1.52
82	UQ	202	PEB	C2A-C1A	-2.54	1.49	1.52
87	C6	518	CLA	C1B-C2B	2.54	1.49	1.43
82	P7	202	PEB	C2C-C3C	2.54	1.45	1.38
84	EE	1001	CYC	C4C-NC	-2.54	1.32	1.37
84	HG	1001	CYC	C4C-NC	-2.54	1.32	1.37
82	Y7	301	PEB	OD-C4D	2.54	1.28	1.23
84	w3	1001	CYC	OB-C4B	2.54	1.28	1.23
82	BA	202	PEB	OD-C4D	2.54	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NB	202	PEB	OD-C4D	2.54	1.28	1.23
82	B7	202	PEB	OD-C4D	2.54	1.28	1.23
82	P7	202	PEB	OD-C4D	2.54	1.28	1.23
82	F7	203	PEB	C1C-C2C	2.54	1.48	1.42
87	A2	817	CLA	MG-NB	-2.54	2.00	2.05
82	OG	203	PEB	OD-C4D	2.54	1.28	1.23
82	Y7	303	PEB	OD-C4D	2.54	1.28	1.23
87	B2	825	CLA	CMD-C2D	-2.54	1.45	1.50
84	HH	1001	CYC	C4C-NC	-2.54	1.32	1.37
82	DF	202	PEB	OD-C4D	2.54	1.28	1.23
82	TO	201	PEB	OD-C4D	2.54	1.28	1.23
82	hM	203	PEB	OD-C4D	2.54	1.28	1.23
82	OE	201	PEB	C1C-NC	-2.54	1.33	1.37
82	dJ	202	PEB	C1C-C2C	2.54	1.48	1.42
87	bL	622	CLA	CMD-C2D	-2.54	1.45	1.50
82	FQ	203	PEB	OD-C4D	2.54	1.28	1.23
84	S3	1001	CYC	OB-C4B	2.54	1.28	1.23
87	BN	808	CLA	C3B-C4B	2.54	1.48	1.42
87	B6	610	CLA	CMB-C2B	-2.54	1.45	1.50
87	C6	513	CLA	C3B-C4B	2.54	1.48	1.42
82	YJ	201	PEB	OD-C4D	2.54	1.28	1.23
82	VQ	203	PEB	OD-C4D	2.54	1.28	1.23
82	GF	201	PEB	CHA-C1B	2.54	1.46	1.40
82	ZB	202	PEB	C2A-C1A	-2.54	1.49	1.52
82	U1	201	PEB	C2A-C1A	-2.54	1.49	1.52
82	fE	202	PEB	C2A-C1A	-2.54	1.49	1.52
82	Z5	301	PEB	C1C-NC	-2.54	1.33	1.37
82	SG	203	PEB	OD-C4D	2.54	1.28	1.23
83	M5	302	PUB	OD-C4D	2.54	1.28	1.23
87	LN	202	CLA	C1B-C2B	2.54	1.49	1.43
87	72	610	CLA	C1B-C2B	2.54	1.49	1.43
87	22	603	CLA	C3B-C4B	2.54	1.48	1.42
87	B2	826	CLA	CMB-C2B	-2.54	1.45	1.50
82	KP	201	PEB	OD-C4D	2.54	1.28	1.23
82	VQ	201	PEB	OD-C4D	2.54	1.28	1.23
82	OF	201	PEB	C4B-C3B	2.54	1.49	1.45
82	D7	201	PEB	C4B-C3B	2.54	1.49	1.45
87	cL	510	CLA	C3B-C4B	2.54	1.48	1.42
87	A2	832	CLA	CMD-C2D	-2.54	1.45	1.50
82	T7	202	PEB	C4B-NB	-2.54	1.33	1.38
82	SO	201	PEB	OD-C4D	2.54	1.28	1.23
82	aO	201	PEB	OD-C4D	2.54	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BL	605	CLA	CMD-C2D	-2.54	1.45	1.50
82	GK	203	PEB	C4B-C3B	2.54	1.49	1.45
82	TA	201	PEB	C4A-NA	-2.54	1.32	1.37
82	FJ	202	PEB	C4A-NA	-2.54	1.32	1.37
82	OG	203	PEB	C2A-C1A	-2.54	1.49	1.52
82	zC	201	PEB	C1C-C2C	2.54	1.48	1.42
82	lH	202	PEB	C1C-C2C	2.54	1.48	1.42
87	4N	608	CLA	CMB-C2B	-2.54	1.45	1.50
82	ZG	203	PEB	C4A-NA	-2.54	1.32	1.37
82	lJ	202	PEB	C4A-NA	-2.54	1.32	1.37
82	KQ	202	PEB	OD-C4D	2.54	1.28	1.23
87	BL	609	CLA	CMB-C2B	-2.54	1.45	1.50
87	12	601	CLA	C1B-C2B	2.54	1.49	1.43
87	12	609	CLA	C1B-C2B	2.54	1.49	1.43
82	fK	202	PEB	C2A-C1A	-2.54	1.49	1.52
82	EQ	201	PEB	OD-C4D	2.54	1.28	1.23
82	NQ	204	PEB	OD-C4D	2.53	1.28	1.23
82	B5	202	PEB	OD-C4D	2.53	1.28	1.23
84	I3	1001	CYC	OB-C4B	2.53	1.28	1.23
87	AN	826	CLA	MG-NB	-2.53	2.00	2.05
87	KN	102	CLA	MG-NB	-2.53	2.00	2.05
87	22	605	CLA	MG-ND	-2.53	2.00	2.05
87	A2	826	CLA	MG-NB	-2.53	2.00	2.05
84	Q3	1001	CYC	OB-C4B	2.53	1.28	1.23
96	V6	201	HEM	C1C-C2C	-2.53	1.40	1.45
87	dL	402	CLA	CMD-C2D	-2.53	1.45	1.50
82	qC	203	PEB	C4B-C3B	2.53	1.49	1.45
82	XF	202	PEB	OD-C4D	2.53	1.28	1.23
82	SG	201	PEB	OD-C4D	2.53	1.28	1.23
82	Y7	304	PEB	C1C-NC	-2.53	1.33	1.37
82	CK	201	PEB	C2A-C1A	-2.53	1.49	1.52
82	dJ	202	PEB	C2A-C1A	-2.53	1.49	1.52
87	L2	203	CLA	CMB-C2B	-2.53	1.45	1.50
82	P5	201	PEB	C4A-NA	-2.53	1.32	1.37
82	aB	201	PEB	C4A-NA	-2.53	1.32	1.37
87	c6	605	CLA	C1B-C2B	2.53	1.49	1.43
82	XK	202	PEB	OD-C4D	2.53	1.28	1.23
82	M5	304	PEB	C1C-NC	-2.53	1.33	1.37
82	GF	203	PEB	C4B-C3B	2.53	1.49	1.45
82	LA	202	PEB	C1A-NA	-2.53	1.34	1.37
82	NA	202	PEB	C1A-NA	-2.53	1.34	1.37
82	gK	201	PEB	CHB-C1C	2.53	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	W3	1001	CYC	C4D-ND	-2.53	1.33	1.37
87	82	301	CLA	CMC-C2C	-2.53	1.45	1.50
87	R2	203	CLA	C1B-C2B	2.53	1.49	1.43
87	c6	608	CLA	C1B-C2B	2.53	1.49	1.43
82	DD	201	PEB	OD-C4D	2.53	1.28	1.23
82	hJ	202	PEB	OD-C4D	2.53	1.28	1.23
82	jJ	203	PEB	OD-C4D	2.53	1.28	1.23
84	O3	1001	CYC	OB-C4B	2.53	1.28	1.23
82	WI	202	PEB	C4B-NB	-2.53	1.33	1.38
87	RN	203	CLA	C1B-C2B	2.53	1.49	1.43
87	62	306	CLA	C1B-C2B	2.53	1.49	1.43
82	G5	201	PEB	C4A-NA	-2.53	1.32	1.37
82	M5	305	PEB	C4A-NA	-2.53	1.32	1.37
82	lK	201	PEB	C4B-C3B	2.53	1.49	1.45
84	y3	1001	CYC	C4D-ND	-2.53	1.33	1.37
87	A2	823	CLA	MG-NB	-2.53	2.00	2.05
82	DQ	201	PEB	OD-C4D	2.53	1.28	1.23
82	QO	201	PEB	C4A-NA	-2.53	1.32	1.37
82	DB	203	PEB	C1C-NC	-2.53	1.33	1.37
87	B6	607	CLA	C1B-C2B	2.53	1.49	1.43
87	bL	617	CLA	CMD-C2D	-2.53	1.45	1.50
82	cF	203	PEB	OD-C4D	2.53	1.28	1.23
87	BL	602	CLA	C3B-C4B	2.53	1.48	1.42
82	i1	202	PEB	C1B-C2B	2.53	1.51	1.45
82	GK	201	PEB	CHA-C1B	2.53	1.46	1.40
82	Y5	201	PEB	C2A-C1A	-2.53	1.49	1.52
87	A2	818	CLA	C1B-C2B	2.53	1.49	1.43
87	42	608	CLA	MG-NB	-2.53	2.00	2.05
87	bL	607	CLA	MG-NB	-2.53	2.00	2.05
87	BL	604	CLA	C3B-C4B	2.53	1.48	1.42
82	YM	203	PEB	C1C-C2C	2.53	1.48	1.42
84	BG	1002	CYC	C4C-NC	-2.53	1.32	1.37
87	B2	810	CLA	MG-NB	-2.53	2.00	2.05
82	kF	201	PEB	C1B-C2B	2.53	1.51	1.45
84	y3	1001	CYC	OB-C4B	2.53	1.28	1.23
87	B2	836	CLA	C1B-C2B	2.53	1.49	1.43
87	8N	302	CLA	C1B-C2B	2.53	1.49	1.43
82	qK	202	PEB	C1C-C2C	2.53	1.48	1.42
82	L5	201	PEB	C1C-NC	-2.53	1.33	1.37
82	gJ	201	PEB	C1C-NC	-2.53	1.33	1.37
87	B2	835	CLA	MG-NB	-2.53	2.00	2.05
87	K2	103	CLA	MG-NB	-2.53	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	12	603	CLA	C1B-C2B	2.53	1.49	1.43
87	A2	831	CLA	MG-ND	-2.53	2.00	2.05
87	BN	802	CLA	C1B-C2B	2.53	1.49	1.43
82	NJ	202	PEB	C4A-NA	-2.53	1.32	1.37
82	BI	202	PEB	C2C-C3C	2.53	1.45	1.38
82	DA	201	PEB	C4B-C3B	2.53	1.49	1.45
84	BE	1002	CYC	C4C-NC	-2.53	1.32	1.37
82	QB	201	PEB	C2A-C1A	-2.53	1.49	1.52
82	CF	201	PEB	OD-C4D	2.53	1.28	1.23
87	62	304	CLA	C1B-C2B	2.53	1.49	1.43
87	H6	103	CLA	C1B-C2B	2.53	1.49	1.43
87	L2	203	CLA	MG-NB	-2.53	2.00	2.05
82	CP	201	PEB	C1C-NC	-2.53	1.33	1.37
87	nL	101	CLA	C1B-C2B	2.53	1.49	1.43
84	73	1002	CYC	OB-C4B	2.53	1.28	1.23
87	A2	814	CLA	C1B-C2B	2.53	1.49	1.43
82	L9	201	PEB	C1C-NC	-2.53	1.33	1.37
82	TP	202	PEB	C2A-C1A	-2.53	1.49	1.52
82	kK	201	PEB	C1B-C2B	2.52	1.51	1.45
82	QD	202	PEB	OD-C4D	2.52	1.28	1.23
84	GO	1001	CYC	OB-C4B	2.52	1.28	1.23
84	o3	1001	CYC	OB-C4B	2.52	1.28	1.23
82	I5	201	PEB	C4A-NA	-2.52	1.32	1.37
84	L4	1001	CYC	C4C-NC	-2.52	1.32	1.37
87	1N	603	CLA	C1B-C2B	2.52	1.49	1.43
82	i4	203	PEB	C4B-C3B	2.52	1.49	1.45
82	Z5	304	PEB	OD-C4D	2.52	1.28	1.23
82	V7	201	PEB	C4A-NA	-2.52	1.32	1.37
82	XJ	201	PEB	CHC-C4C	2.52	1.52	1.49
87	B2	809	CLA	C3B-C4B	2.52	1.48	1.42
87	J2	101	CLA	C1B-C2B	2.52	1.49	1.43
82	MD	201	PEB	OD-C4D	2.52	1.28	1.23
82	kK	203	PEB	C4A-NA	-2.52	1.32	1.37
82	DQ	203	PEB	CHA-C1B	2.52	1.46	1.40
82	FA	203	PEB	C1C-C2C	2.52	1.48	1.42
82	Q9	202	PEB	C1C-C2C	2.52	1.48	1.42
82	WE	201	PEB	C4A-NA	-2.52	1.32	1.37
87	CL	506	CLA	CAC-C3C	-2.52	1.44	1.51
82	Y4	202	PEB	OD-C4D	2.52	1.28	1.23
84	B3	1001	CYC	OB-C4B	2.52	1.28	1.23
82	VM	201	PEB	C1C-NC	-2.52	1.33	1.37
82	GP	201	PEB	C1C-NC	-2.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	N7	202	PEB	C2C-C3C	2.52	1.45	1.38
84	E4	1001	CYC	C4C-NC	-2.52	1.32	1.37
82	YQ	201	PEB	C2A-C1A	-2.52	1.49	1.52
82	hJ	202	PEB	C2A-C1A	-2.52	1.49	1.52
82	K5	201	PEB	C4A-NA	-2.52	1.32	1.37
82	N5	201	PEB	C4A-NA	-2.52	1.32	1.37
84	f3	1001	CYC	OB-C4B	2.52	1.28	1.23
82	S5	201	PEB	C4A-NA	-2.52	1.32	1.37
82	Z5	304	PEB	C1C-NC	-2.52	1.33	1.37
82	JA	202	PEB	OD-C4D	2.52	1.28	1.23
82	RF	201	PEB	OD-C4D	2.52	1.28	1.23
82	XK	201	PEB	OD-C4D	2.52	1.28	1.23
87	AN	827	CLA	CMD-C2D	-2.52	1.45	1.50
82	ED	202	PEB	C2A-C1A	-2.52	1.49	1.52
82	XK	202	PEB	C2A-C1A	-2.52	1.49	1.52
82	X9	202	PEB	C4B-C3B	2.52	1.49	1.45
82	OJ	203	PEB	OD-C4D	2.52	1.28	1.23
82	A5	201	PEB	C4A-NA	-2.52	1.32	1.37
82	E5	201	PEB	C4A-NA	-2.52	1.32	1.37
82	WJ	203	PEB	OD-C4D	2.52	1.28	1.23
84	NO	1001	CYC	OB-C4B	2.52	1.28	1.23
84	N4	1001	CYC	OB-C4B	2.52	1.28	1.23
82	WE	201	PEB	C1C-NC	-2.52	1.33	1.37
82	WG	201	PEB	C1C-NC	-2.52	1.33	1.37
87	LN	203	CLA	CMB-C2B	-2.52	1.45	1.50
87	A2	829	CLA	CMC-C2C	-2.52	1.45	1.50
87	6N	609	CLA	CMD-C2D	-2.52	1.45	1.50
82	h1	201	PEB	C1C-C2C	2.52	1.48	1.42
87	A2	839	CLA	C3B-C4B	2.52	1.48	1.42
87	BL	603	CLA	MG-ND	-2.52	2.00	2.05
82	jH	203	PEB	C4B-C3B	2.52	1.49	1.45
82	GI	201	PEB	CHA-C1B	2.52	1.46	1.40
82	MK	203	PEB	C1C-C2C	2.52	1.48	1.42
87	BL	604	CLA	C1B-C2B	2.52	1.49	1.43
87	AN	831	CLA	MG-ND	-2.52	2.00	2.05
87	J2	101	CLA	MG-NB	-2.52	2.00	2.05
82	ZJ	201	PEB	C4A-NA	-2.52	1.32	1.37
82	V9	202	PEB	C4B-C3B	2.52	1.49	1.45
82	ZG	202	PEB	C1C-NC	-2.52	1.33	1.37
87	5N	608	CLA	CMD-C2D	-2.52	1.45	1.50
82	J9	203	PEB	C2A-C1A	-2.52	1.49	1.52
87	FN	205	CLA	C4D-ND	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	837	CLA	C3B-C4B	2.52	1.48	1.42
82	vC	202	PEB	C1C-NC	-2.52	1.33	1.37
82	HB	201	PEB	OD-C4D	2.52	1.28	1.23
84	k3	1001	CYC	OB-C4B	2.52	1.28	1.23
82	OG	201	PEB	C1C-NC	-2.52	1.33	1.37
82	F9	202	PEB	C4B-C3B	2.52	1.49	1.45
87	AN	837	CLA	C3B-C4B	2.52	1.48	1.42
82	HD	202	PEB	C1B-C2B	2.52	1.51	1.45
82	HQ	202	PEB	C1B-C2B	2.52	1.51	1.45
82	EP	203	PEB	OD-C4D	2.52	1.28	1.23
82	VG	201	PEB	C2A-C1A	-2.52	1.49	1.52
82	N9	202	PEB	C4B-C3B	2.52	1.49	1.45
87	A2	801	CLA	C1B-C2B	2.52	1.49	1.43
82	ND	204	PEB	OD-C4D	2.52	1.28	1.23
84	M3	1001	CYC	OB-C4B	2.52	1.28	1.23
87	3N	303	CLA	C1B-C2B	2.52	1.49	1.43
87	HL	101	CLA	C4B-NB	2.52	1.40	1.37
82	YA	304	PEB	C1C-NC	-2.52	1.33	1.37
82	OJ	201	PEB	OD-C4D	2.52	1.28	1.23
87	42	607	CLA	CMC-C2C	-2.52	1.45	1.50
82	dE	201	PEB	C1C-C2C	2.52	1.48	1.42
82	qF	202	PEB	C1C-C2C	2.52	1.48	1.42
82	X5	201	PEB	C4A-NA	-2.52	1.32	1.37
84	D3	1001	CYC	OB-C4B	2.52	1.28	1.23
84	F3	1001	CYC	OB-C4B	2.52	1.28	1.23
82	SH	201	PEB	C4A-NA	-2.52	1.32	1.37
82	IK	203	PEB	C4A-NA	-2.52	1.32	1.37
82	O5	201	PEB	C4A-NA	-2.52	1.32	1.37
84	CO	1001	CYC	C4C-NC	-2.52	1.32	1.37
82	FA	203	PEB	C2A-C1A	-2.52	1.49	1.52
82	QM	202	PEB	C2A-C1A	-2.52	1.49	1.52
82	kH	201	PEB	C4B-C3B	2.52	1.49	1.45
87	BN	824	CLA	C4B-NB	2.52	1.40	1.37
82	JP	201	PEB	C1C-NC	-2.51	1.33	1.37
82	c1	202	PEB	C1B-C2B	2.51	1.51	1.45
82	dB	202	PEB	C2A-C1A	-2.51	1.49	1.52
87	D6	402	CLA	C3B-C4B	2.51	1.48	1.42
82	kE	202	PEB	C4A-NA	-2.51	1.32	1.37
87	A2	838	CLA	MG-NB	-2.51	2.00	2.05
82	DM	201	PEB	C1C-NC	-2.51	1.33	1.37
84	DE	1001	CYC	C1B-NB	-2.51	1.33	1.37
82	S1	201	PEB	C4A-NA	-2.51	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	NH	1001	CYC	C1B-C2B	2.51	1.49	1.45
82	KJ	202	PEB	OD-C4D	2.51	1.28	1.23
84	L1	1001	CYC	OB-C4B	2.51	1.28	1.23
84	u3	1001	CYC	OB-C4B	2.51	1.28	1.23
87	32	302	CLA	C1B-C2B	2.51	1.49	1.43
87	4N	608	CLA	MG-NB	-2.51	2.00	2.05
82	U5	201	PEB	C2A-C1A	-2.51	1.49	1.52
82	W9	201	PEB	C4A-NA	-2.51	1.32	1.37
82	UB	302	PEB	C1D-ND	2.51	1.49	1.45
82	KJ	203	PEB	OD-C4D	2.51	1.28	1.23
87	A2	811	CLA	MG-NB	-2.51	2.00	2.05
82	WG	201	PEB	C4A-NA	-2.51	1.32	1.37
82	PA	202	PEB	C2C-C3C	2.51	1.45	1.38
84	N4	1001	CYC	C4B-NB	-2.51	1.32	1.38
82	S4	202	PEB	C1D-ND	2.51	1.49	1.45
82	HA	202	PEB	C1C-C2C	2.51	1.48	1.42
87	A2	827	CLA	MG-NB	-2.51	2.00	2.05
87	IN	103	CLA	C1B-C2B	2.51	1.49	1.43
82	GB	201	PEB	C4A-NA	-2.51	1.32	1.37
82	MB	201	PEB	C4A-NA	-2.51	1.32	1.37
82	UQ	201	PEB	C2A-C1A	-2.51	1.49	1.52
82	S4	201	PEB	OD-C4D	2.51	1.28	1.23
82	t8	201	PEB	C1C-C2C	2.51	1.48	1.42
82	T5	201	PEB	C4A-NA	-2.51	1.32	1.37
84	I1	1001	CYC	C4C-NC	-2.51	1.32	1.37
82	P7	202	PEB	C1A-NA	-2.51	1.34	1.37
82	JF	201	PEB	OD-C4D	2.51	1.28	1.23
87	82	301	CLA	C1B-C2B	2.51	1.49	1.43
82	sK	203	PEB	C4B-NB	-2.51	1.33	1.38
87	CL	503	CLA	CMD-C2D	-2.51	1.45	1.50
87	A2	827	CLA	CMD-C2D	-2.51	1.45	1.50
84	n3	1001	CYC	OB-C4B	2.51	1.28	1.23
84	HE	1001	CYC	C1B-NB	-2.51	1.33	1.37
87	bL	606	CLA	MG-NB	-2.51	2.00	2.05
82	T9	202	PEB	C4B-C3B	2.51	1.49	1.45
82	UE	202	PEB	OD-C4D	2.51	1.28	1.23
82	R5	201	PEB	C4A-NA	-2.51	1.32	1.37
87	C6	509	CLA	C1B-C2B	2.51	1.49	1.43
82	eA	301	PEB	C2A-C1A	-2.51	1.49	1.52
82	HJ	201	PEB	OD-C4D	2.51	1.28	1.23
84	q3	1001	CYC	OB-C4B	2.51	1.28	1.23
87	c6	609	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	N4	1001	CYC	C1B-C2B	2.51	1.49	1.45
87	CL	503	CLA	C3B-C4B	2.51	1.48	1.42
87	AN	839	CLA	C3B-C4B	2.51	1.48	1.42
84	J1	1001	CYC	C4A-C3A	2.51	1.51	1.45
82	V4	201	PEB	OD-C4D	2.51	1.28	1.23
82	T7	203	PEB	OD-C4D	2.51	1.28	1.23
84	73	1001	CYC	OB-C4B	2.51	1.28	1.23
82	U4	201	PEB	CHA-C4A	-2.51	1.31	1.36
87	B2	816	CLA	MG-NB	-2.51	2.00	2.05
87	b6	617	CLA	C3B-C4B	2.51	1.48	1.42
87	2N	306	CLA	C1B-C2B	2.51	1.49	1.43
82	KJ	203	PEB	C4A-NA	-2.51	1.32	1.37
82	HM	201	PEB	OD-C4D	2.51	1.28	1.23
84	U3	1001	CYC	OB-C4B	2.51	1.28	1.23
87	CL	503	CLA	MG-NB	-2.51	2.00	2.05
82	hO	201	PEB	CHA-C4A	-2.51	1.31	1.36
82	VG	202	PEB	C2A-C1A	-2.51	1.49	1.52
83	xF	306	PUB	C4B-C3B	2.51	1.48	1.42
87	AN	818	CLA	C1B-C2B	2.51	1.49	1.43
96	FL	102	HEM	C4B-NB	-2.51	1.33	1.38
87	3N	310	CLA	C1B-C2B	2.51	1.49	1.43
87	6N	603	CLA	C1B-C2B	2.51	1.49	1.43
82	WJ	201	PEB	C4A-NA	-2.51	1.32	1.37
84	IG	1001	CYC	C4B-NB	-2.51	1.32	1.38
82	KB	301	PEB	OD-C4D	2.51	1.28	1.23
82	P1	201	PEB	OD-C4D	2.51	1.28	1.23
87	B6	608	CLA	C1B-C2B	2.51	1.49	1.43
87	c6	610	CLA	C1B-C2B	2.51	1.49	1.43
87	7N	603	CLA	C1B-C2B	2.51	1.49	1.43
82	L5	202	PEB	C4B-C3B	2.51	1.49	1.45
82	P1	201	PEB	C1C-NC	-2.51	1.33	1.37
82	AD	303	PEB	C2A-C1A	-2.51	1.49	1.52
82	dO	201	PEB	C2A-C1A	-2.51	1.49	1.52
82	hH	201	PEB	C4A-NA	-2.51	1.32	1.37
82	tC	201	PEB	C1C-C2C	2.51	1.48	1.42
82	B5	201	PEB	C4A-NA	-2.51	1.32	1.37
87	32	310	CLA	C1B-C2B	2.51	1.49	1.43
82	XA	203	PEB	C2A-C1A	-2.51	1.49	1.52
82	J9	202	PEB	C2A-C1A	-2.51	1.49	1.52
82	R9	202	PEB	C4B-C3B	2.51	1.49	1.45
87	bL	607	CLA	CMC-C2C	-2.51	1.45	1.50
84	BE	1001	CYC	C4B-NB	-2.50	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	806	CLA	C3B-C4B	2.50	1.48	1.42
82	j4	203	PEB	C4B-C3B	2.50	1.49	1.45
82	J4	1002	PEB	OD-C4D	2.50	1.28	1.23
82	gF	203	PEB	OD-C4D	2.50	1.28	1.23
82	GK	202	PEB	OA-C1A	2.50	1.28	1.23
82	JH	1002	PEB	C1C-NC	-2.50	1.33	1.37
87	AN	814	CLA	C1B-C2B	2.50	1.49	1.43
82	f1	201	PEB	C4B-C3B	2.50	1.49	1.45
82	SB	202	PEB	C4A-NA	-2.50	1.32	1.37
82	PH	201	PEB	OD-C4D	2.50	1.28	1.23
87	b6	617	CLA	C1B-C2B	2.50	1.49	1.43
87	dL	402	CLA	C1B-C2B	2.50	1.49	1.43
87	BN	836	CLA	C3B-C4B	2.50	1.48	1.42
82	XD	201	PEB	C1C-C2C	2.50	1.48	1.42
82	TI	201	PEB	C4B-NB	-2.50	1.33	1.38
82	XD	202	PEB	C2A-C1A	-2.50	1.49	1.52
82	CM	201	PEB	C4A-NA	-2.50	1.32	1.37
82	SP	202	PEB	OD-C4D	2.50	1.28	1.23
82	t8	202	PEB	C1C-NC	-2.50	1.33	1.37
87	AN	811	CLA	MG-NB	-2.50	2.00	2.05
87	A2	821	CLA	CMB-C2B	-2.50	1.45	1.50
83	yK	302	PUB	OA-C1A	2.50	1.28	1.23
82	TB	202	PEB	C2A-C1A	-2.50	1.49	1.52
82	WB	401	PEB	C2A-C1A	-2.50	1.49	1.52
82	U5	203	PEB	C2A-C1A	-2.50	1.49	1.52
82	lF	203	PEB	C2A-C1A	-2.50	1.49	1.52
82	H7	202	PEB	C1C-C2C	2.50	1.48	1.42
87	I2	103	CLA	C1B-C2B	2.50	1.49	1.43
87	6N	611	CLA	C1B-C2B	2.50	1.49	1.43
84	IG	1001	CYC	OB-C4B	2.50	1.28	1.23
82	PD	201	PEB	C1C-C2C	2.50	1.48	1.42
82	18	202	PEB	C1C-C2C	2.50	1.48	1.42
87	AN	823	CLA	CMB-C2B	-2.50	1.45	1.50
87	4N	607	CLA	CMC-C2C	-2.50	1.45	1.50
82	tC	202	PEB	C1C-NC	-2.50	1.33	1.37
82	dO	201	PEB	OD-C4D	2.50	1.28	1.23
87	12	608	CLA	C4D-ND	-2.50	1.34	1.37
82	vC	201	PEB	C2A-C1A	-2.50	1.49	1.52
82	ZF	202	PEB	C4B-C3B	2.50	1.49	1.45
82	eK	201	PEB	C4B-C3B	2.50	1.49	1.45
87	A2	820	CLA	C3B-C4B	2.50	1.48	1.42
87	AN	839	CLA	MG-NB	-2.50	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gB	203	PEB	CHC-C4C	2.50	1.52	1.49
82	UG	202	PEB	OD-C4D	2.50	1.28	1.23
84	EH	1001	CYC	C4B-NB	-2.50	1.32	1.38
87	AN	805	CLA	C1B-C2B	2.50	1.49	1.43
87	4N	610	CLA	C1B-C2B	2.50	1.49	1.43
82	VO	201	PEB	OD-C4D	2.50	1.28	1.23
87	C6	516	CLA	MG-NB	-2.50	2.00	2.05
82	X7	203	PEB	C2A-C1A	-2.50	1.49	1.52
82	L9	203	PEB	C2A-C1A	-2.50	1.49	1.52
82	kO	202	PEB	C4B-C3B	2.50	1.49	1.45
82	O9	202	PEB	C2C-C3C	2.50	1.45	1.38
82	O5	202	PEB	OD-C4D	2.50	1.28	1.23
82	gH	203	PEB	C1C-C2C	2.50	1.48	1.42
82	DA	203	PEB	C1C-NC	-2.50	1.33	1.37
87	BN	829	CLA	C1B-C2B	2.50	1.49	1.43
87	42	610	CLA	C1B-C2B	2.50	1.49	1.43
82	T7	201	PEB	C4A-NA	-2.50	1.32	1.37
87	6N	604	CLA	C1B-C2B	2.50	1.49	1.43
87	C6	512	CLA	C3B-C4B	2.50	1.48	1.42
82	V5	201	PEB	C4A-NA	-2.50	1.32	1.37
82	J7	202	PEB	C1C-C2C	2.50	1.48	1.42
87	AN	802	CLA	C1B-C2B	2.50	1.49	1.43
82	E9	202	PEB	C4B-C3B	2.50	1.49	1.45
82	fH	201	PEB	C4B-C3B	2.50	1.49	1.45
94	DL	401	PL9	O1-C4	2.50	1.28	1.23
87	b6	609	CLA	MG-NB	-2.50	2.00	2.05
87	CL	507	CLA	C3B-C4B	2.50	1.48	1.42
87	JN	101	CLA	C1B-C2B	2.50	1.49	1.43
94	a6	601	PL9	C6-C5	2.50	1.48	1.35
82	ED	201	PEB	OD-C4D	2.50	1.28	1.23
84	H4	1001	CYC	OB-C4B	2.50	1.28	1.23
87	A2	802	CLA	C3B-C4B	2.50	1.48	1.42
87	B2	801	CLA	C1B-C2B	2.50	1.49	1.43
82	TH	201	PEB	C1C-NC	-2.50	1.33	1.37
91	A6	407	PHO	CBD-CGD	-2.50	1.49	1.52
82	ND	202	PEB	C2A-C1A	-2.50	1.49	1.52
82	UJ	201	PEB	OD-C4D	2.50	1.28	1.23
87	AN	823	CLA	MG-NB	-2.50	2.00	2.05
82	DD	203	PEB	CHA-C1B	2.50	1.46	1.40
103	8N	310	ZEX	C22-C23	-2.50	1.49	1.53
87	AN	851	CLA	CMD-C2D	-2.50	1.45	1.50
87	IN	103	CLA	C3B-C4B	2.50	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	dL	409	CLA	C3B-C4B	2.50	1.48	1.42
82	VG	202	PEB	C1C-C2C	2.50	1.48	1.42
87	AN	827	CLA	C1D-ND	2.50	1.40	1.37
94	DL	401	PL9	C6-C5	2.50	1.48	1.35
82	bF	201	PEB	C2A-C1A	-2.50	1.49	1.52
82	qK	203	PEB	C2A-C1A	-2.50	1.49	1.52
82	dM	203	PEB	C1C-C2C	2.50	1.48	1.42
87	B6	615	CLA	C1B-C2B	2.50	1.49	1.43
82	Z5	305	PEB	C4A-NA	-2.49	1.32	1.37
87	CL	510	CLA	C3B-C4B	2.49	1.48	1.42
82	M5	301	PEB	C1C-NC	-2.49	1.33	1.37
84	M4	1001	CYC	OB-C4B	2.49	1.28	1.23
87	c6	614	CLA	C1B-C2B	2.49	1.49	1.43
87	1N	609	CLA	C1B-C2B	2.49	1.49	1.43
82	Q5	203	PEB	C2A-C1A	-2.49	1.49	1.52
87	BN	826	CLA	MG-NB	-2.49	2.00	2.05
82	C7	201	PEB	OD-C4D	2.49	1.28	1.23
82	cF	203	PEB	C1B-C2B	2.49	1.51	1.45
87	cL	512	CLA	C3B-C4B	2.49	1.48	1.42
82	aB	202	PEB	C4A-NA	-2.49	1.32	1.37
82	UQ	201	PEB	C1C-NC	-2.49	1.33	1.37
82	FQ	203	PEB	C4B-C3B	2.49	1.49	1.45
82	HF	201	PEB	C2A-C1A	-2.49	1.49	1.52
82	LF	202	PEB	OD-C4D	2.49	1.28	1.23
82	JJ	201	PEB	C1C-NC	-2.49	1.33	1.37
82	F9	201	PEB	C1C-NC	-2.49	1.33	1.37
87	BN	810	CLA	C3B-C4B	2.49	1.48	1.42
87	B6	606	CLA	C3B-C4B	2.49	1.48	1.42
82	hK	202	PEB	C4B-C3B	2.49	1.49	1.45
87	12	607	CLA	C1B-C2B	2.49	1.49	1.43
82	Y1	201	PEB	C1C-C2C	2.49	1.48	1.42
82	gH	202	PEB	C1C-C2C	2.49	1.48	1.42
87	32	308	CLA	C1B-C2B	2.49	1.49	1.43
82	W4	201	PEB	C4A-NA	-2.49	1.32	1.37
82	jF	201	PEB	C1A-NA	-2.49	1.34	1.37
87	A2	815	CLA	MG-NB	-2.49	2.00	2.05
83	Z9	302	PUB	CHA-C1B	2.49	1.52	1.49
82	s8	201	PEB	C1B-C2B	2.49	1.51	1.45
82	QP	201	PEB	C4A-NA	-2.49	1.32	1.37
82	C9	202	PEB	C4B-C3B	2.49	1.49	1.45
82	JO	1002	PEB	OD-C4D	2.49	1.28	1.23
82	JO	1002	PEB	C1C-NC	-2.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q4	201	PEB	C4A-NA	-2.49	1.32	1.37
82	F5	201	PEB	C4A-NA	-2.49	1.32	1.37
82	OP	201	PEB	C2A-C1A	-2.49	1.49	1.52
87	32	306	CLA	MG-NB	-2.49	2.00	2.05
82	S9	201	PEB	C1C-NC	-2.49	1.33	1.37
82	SE	201	PEB	OD-C4D	2.49	1.28	1.23
87	cL	513	CLA	CMB-C2B	-2.49	1.45	1.50
87	b6	606	CLA	C3B-C4B	2.49	1.48	1.42
82	HF	201	PEB	C4B-NB	-2.49	1.33	1.38
82	HK	201	PEB	OD-C4D	2.49	1.28	1.23
91	dL	403	PHO	CBD-CGD	-2.49	1.49	1.52
82	MJ	203	PEB	C1C-C2C	2.49	1.48	1.42
82	Z9	301	PEB	C4A-NA	-2.49	1.32	1.37
82	AQ	304	PEB	C1C-NC	-2.49	1.33	1.37
82	jK	202	PEB	C1C-NC	-2.49	1.33	1.37
82	tK	203	PEB	C1D-ND	2.49	1.49	1.45
82	WO	201	PEB	C4A-NA	-2.49	1.32	1.37
82	FD	203	PEB	OD-C4D	2.49	1.28	1.23
82	TQ	202	PEB	OD-C4D	2.49	1.28	1.23
87	LN	203	CLA	MG-NB	-2.49	2.00	2.05
82	P4	202	PEB	C2A-C1A	-2.49	1.49	1.52
82	OP	202	PEB	OD-C4D	2.49	1.28	1.23
84	J4	1001	CYC	OB-C4B	2.49	1.28	1.23
87	AN	827	CLA	MG-NB	-2.49	2.00	2.05
87	3N	301	CLA	C1B-C2B	2.49	1.49	1.43
84	63	901	CYC	C1B-C2B	2.49	1.49	1.45
82	MF	203	PEB	C1C-C2C	2.49	1.48	1.42
82	EB	501	PEB	C2A-C1A	-2.49	1.49	1.52
82	aE	202	PEB	C2A-C1A	-2.49	1.49	1.52
82	gO	201	PEB	C2A-C1A	-2.49	1.49	1.52
84	NO	1001	CYC	C4B-NB	-2.49	1.32	1.38
82	LK	201	PEB	C4B-C3B	2.49	1.49	1.45
87	cL	506	CLA	MG-NB	-2.49	2.00	2.05
87	A2	851	CLA	CMD-C2D	-2.49	1.45	1.50
82	GI	201	PEB	C4B-NB	-2.49	1.33	1.38
82	k1	201	PEB	OD-C4D	2.49	1.28	1.23
82	GI	201	PEB	CHB-C1C	2.49	1.46	1.40
82	SK	201	PEB	C2A-C1A	-2.49	1.49	1.52
82	AQ	304	PEB	C2A-C1A	-2.49	1.49	1.52
87	1N	607	CLA	C1B-C2B	2.49	1.49	1.43
82	WB	402	PEB	OD-C4D	2.49	1.28	1.23
87	AN	801	CLA	C3B-C4B	2.49	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	cL	511	CLA	C1B-C2B	2.49	1.49	1.43
82	kK	202	PEB	C1C-C2C	2.49	1.48	1.42
94	DL	401	PL9	C2-C1	-2.49	1.38	1.44
87	c6	611	CLA	MG-NB	-2.49	2.00	2.05
82	sF	203	PEB	C4B-NB	-2.49	1.33	1.38
82	v8	202	PEB	C4B-C3B	2.49	1.49	1.45
82	JB	202	PEB	OD-C4D	2.48	1.28	1.23
82	RK	201	PEB	OD-C4D	2.48	1.28	1.23
84	G4	1001	CYC	OB-C4B	2.48	1.28	1.23
82	vC	201	PEB	C1C-NC	-2.48	1.33	1.37
87	AN	820	CLA	C3B-C4B	2.48	1.48	1.42
87	AN	825	CLA	CHC-C1C	2.48	1.43	1.38
82	HO	1002	PEB	OD-C4D	2.48	1.28	1.23
87	bL	614	CLA	CMB-C2B	-2.48	1.45	1.50
87	B2	830	CLA	C1B-C2B	2.48	1.49	1.43
82	YH	201	PEB	C1C-C2C	2.48	1.48	1.42
82	eM	201	PEB	CHC-C4C	2.48	1.52	1.49
82	l4	202	PEB	OD-C4D	2.48	1.28	1.23
84	L3	1001	CYC	OB-C4B	2.48	1.28	1.23
82	1C	202	PEB	C1C-C2C	2.48	1.48	1.42
82	dH	203	PEB	C1C-C2C	2.48	1.48	1.42
82	M5	304	PEB	OD-C4D	2.48	1.28	1.23
82	F7	202	PEB	C4B-C3B	2.48	1.49	1.45
87	A2	808	CLA	C1B-C2B	2.48	1.49	1.43
82	d4	201	PEB	OD-C4D	2.48	1.28	1.23
82	Q7	201	PEB	C2A-C1A	-2.48	1.49	1.52
82	AD	301	PEB	C1C-C2C	2.48	1.48	1.42
87	BN	807	CLA	MG-NB	-2.48	2.00	2.05
87	42	609	CLA	MG-NB	-2.48	2.00	2.05
82	MQ	201	PEB	OD-C4D	2.48	1.28	1.23
87	A2	833	CLA	C3B-C4B	2.48	1.48	1.42
87	B2	836	CLA	C3B-C4B	2.48	1.48	1.42
82	qK	201	PEB	C1C-C2C	2.48	1.48	1.42
83	Z5	302	PUB	C4C-NC	2.48	1.39	1.35
87	72	604	CLA	C1B-C2B	2.48	1.49	1.43
82	TD	203	PEB	C1C-C2C	2.48	1.48	1.42
87	3N	310	CLA	MG-NB	-2.48	2.00	2.05
87	dL	409	CLA	C4B-NB	2.48	1.40	1.37
82	TO	202	PEB	C2A-C1A	-2.48	1.49	1.52
82	T4	202	PEB	C2A-C1A	-2.48	1.49	1.52
82	XD	202	PEB	CHC-C4C	2.48	1.52	1.49
87	BL	602	CLA	MG-NB	-2.48	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HI	201	PEB	OD-C4D	2.48	1.28	1.23
84	EG	1001	CYC	OB-C4B	2.48	1.28	1.23
84	FG	1001	CYC	OB-C4B	2.48	1.28	1.23
84	63	901	CYC	OB-C4B	2.48	1.28	1.23
82	k1	201	PEB	C4B-C3B	2.48	1.49	1.45
82	fB	301	PEB	C4B-C3B	2.48	1.49	1.45
82	GJ	203	PEB	C4A-NA	-2.48	1.32	1.37
87	B2	820	CLA	C1B-C2B	2.48	1.49	1.43
87	AN	833	CLA	C3B-C4B	2.48	1.48	1.42
87	B2	828	CLA	MG-NB	-2.48	2.00	2.05
82	CD	201	PEB	C4A-NA	-2.48	1.32	1.37
82	q8	203	PEB	C4B-C3B	2.48	1.49	1.45
87	b6	613	CLA	C3B-C4B	2.48	1.48	1.42
82	QK	203	PEB	C4B-C3B	2.48	1.49	1.45
82	J9	202	PEB	C4B-C3B	2.48	1.49	1.45
82	BB	201	PEB	C4A-NA	-2.48	1.32	1.37
82	LI	202	PEB	C4A-NA	-2.48	1.32	1.37
82	CP	203	PEB	C1C-C2C	2.48	1.48	1.42
94	d6	408	PL9	C6-C5	2.48	1.48	1.35
82	UE	202	PEB	C4A-NA	-2.48	1.32	1.37
82	LJ	202	PEB	C4A-NA	-2.48	1.32	1.37
87	AN	821	CLA	CMB-C2B	-2.48	1.45	1.50
87	A2	825	CLA	CHC-C1C	2.48	1.43	1.38
82	dG	201	PEB	C1C-C2C	2.48	1.48	1.42
82	SF	201	PEB	C2C-C3C	2.48	1.45	1.38
82	UD	201	PEB	C1C-NC	-2.48	1.33	1.37
87	B2	806	CLA	MG-NB	-2.48	2.00	2.05
82	rK	201	PEB	C1A-NA	-2.48	1.34	1.37
82	NA	203	PEB	OD-C4D	2.48	1.28	1.23
82	MM	202	PEB	OD-C4D	2.48	1.28	1.23
82	Z4	202	PEB	OD-C4D	2.48	1.28	1.23
82	18	202	PEB	CHC-C4C	2.48	1.52	1.49
82	MQ	201	PEB	C4A-NA	-2.48	1.32	1.37
82	NM	201	PEB	C1C-NC	-2.48	1.33	1.37
82	R7	202	PEB	CHA-C1B	2.48	1.46	1.40
96	v6	201	HEM	C1C-C2C	-2.48	1.40	1.45
82	bE	201	PEB	C4A-NA	-2.48	1.32	1.37
84	CH	1001	CYC	C2C-C1C	-2.48	1.49	1.52
82	JF	202	PEB	C1C-NC	-2.48	1.33	1.37
82	HH	1002	PEB	OD-C4D	2.48	1.28	1.23
82	FP	201	PEB	C4B-C3B	2.48	1.49	1.45
82	R1	201	PEB	C4B-C3B	2.48	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	CG	1001	CYC	C4C-NC	-2.48	1.32	1.37
83	BJ	302	PUB	OA-C1A	2.48	1.28	1.23
82	IQ	201	PEB	C4A-NA	-2.48	1.32	1.37
87	L2	204	CLA	CMD-C2D	-2.48	1.45	1.50
87	CL	509	CLA	C1B-C2B	2.48	1.49	1.43
82	P9	202	PEB	C4B-C3B	2.48	1.49	1.45
87	dL	401	CLA	C3B-C4B	2.48	1.48	1.42
82	RD	201	PEB	C2A-C1A	-2.48	1.49	1.52
87	32	305	CLA	C1B-C2B	2.48	1.49	1.43
82	EP	201	PEB	C4A-NA	-2.48	1.32	1.37
87	A2	823	CLA	CMD-C2D	-2.48	1.45	1.50
87	cL	508	CLA	C3B-C4B	2.48	1.48	1.42
87	AN	819	CLA	MG-NB	-2.48	2.00	2.05
82	VA	201	PEB	C4A-NA	-2.48	1.32	1.37
82	EP	203	PEB	C1C-NC	-2.48	1.33	1.37
82	II	203	PEB	CHB-C1C	2.48	1.46	1.40
82	HA	202	PEB	C1A-NA	-2.48	1.34	1.37
82	F5	203	PEB	OD-C4D	2.47	1.28	1.23
82	AB	501	PEB	C2A-C1A	-2.47	1.49	1.52
82	MK	201	PEB	C2A-C1A	-2.47	1.49	1.52
82	uK	201	PEB	C1D-ND	2.47	1.49	1.45
82	RG	201	PEB	C1C-NC	-2.47	1.33	1.37
87	C6	512	CLA	C1B-C2B	2.47	1.49	1.43
82	kH	201	PEB	OD-C4D	2.47	1.28	1.23
83	M5	302	PUB	C4C-NC	2.47	1.39	1.35
87	bL	616	CLA	MG-NB	-2.47	2.00	2.05
82	PF	202	PEB	C2A-C1A	-2.47	1.49	1.52
82	I9	202	PEB	C4B-C3B	2.47	1.49	1.45
87	O2	203	CLA	C1C-C2C	2.47	1.49	1.44
87	I2	103	CLA	C3B-C4B	2.47	1.48	1.42
87	62	310	CLA	CMD-C2D	-2.47	1.45	1.50
87	A2	823	CLA	CMB-C2B	-2.47	1.45	1.50
82	ZJ	202	PEB	C4A-NA	-2.47	1.32	1.37
82	O1	203	PEB	C1C-C2C	2.47	1.48	1.42
82	Y5	202	PEB	OD-C4D	2.47	1.28	1.23
82	UM	203	PEB	C2A-C1A	-2.47	1.49	1.52
87	BL	603	CLA	C1B-C2B	2.47	1.49	1.43
87	C6	513	CLA	C1B-C2B	2.47	1.49	1.43
87	BN	817	CLA	MG-NB	-2.47	2.00	2.05
87	4N	609	CLA	MG-NB	-2.47	2.00	2.05
82	gB	203	PEB	C1C-NC	-2.47	1.33	1.37
87	BN	830	CLA	C1B-C2B	2.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	62	305	CLA	C1B-C2B	2.47	1.49	1.43
82	TA	202	PEB	C4B-NB	-2.47	1.33	1.38
82	OH	203	PEB	C1C-C2C	2.47	1.48	1.42
84	R3	1001	CYC	C4D-C3D	2.47	1.48	1.42
82	LK	201	PEB	OD-C4D	2.47	1.28	1.23
87	B2	831	CLA	C1B-C2B	2.47	1.49	1.43
82	IM	202	PEB	C4A-NA	-2.47	1.32	1.37
83	Y7	302	PUB	C4B-NB	-2.47	1.33	1.37
82	qF	201	PEB	C1C-C2C	2.47	1.48	1.42
87	B2	826	CLA	MG-NB	-2.47	2.00	2.05
82	MP	203	PEB	C1C-NC	-2.47	1.33	1.37
84	K3	1001	CYC	C4D-C3D	2.47	1.48	1.42
87	bL	622	CLA	CMB-C2B	-2.47	1.45	1.50
84	NO	1001	CYC	C1B-C2B	2.47	1.49	1.45
82	OK	201	PEB	C4B-C3B	2.47	1.49	1.45
82	QB	201	PEB	C1C-NC	-2.47	1.33	1.37
82	ZO	202	PEB	OD-C4D	2.47	1.28	1.23
82	fF	202	PEB	C4B-C3B	2.47	1.49	1.45
87	CL	512	CLA	MG-NB	-2.47	2.00	2.05
87	A2	833	CLA	MG-NB	-2.47	2.00	2.05
84	EO	1001	CYC	OB-C4B	2.47	1.28	1.23
83	NQ	201	PUB	C4C-NC	2.47	1.39	1.35
82	SB	201	PEB	C4A-NA	-2.47	1.32	1.37
82	wC	201	PEB	C1C-C2C	2.47	1.48	1.42
82	CD	201	PEB	C1C-NC	-2.47	1.33	1.37
94	dL	406	PL9	C6-C5	2.47	1.48	1.35
87	bL	617	CLA	C3B-C4B	2.47	1.48	1.42
82	mJ	201	PEB	C4A-NA	-2.47	1.32	1.37
84	N1	1001	CYC	C1B-C2B	2.47	1.49	1.45
82	W5	202	PEB	OD-C4D	2.47	1.28	1.23
84	HG	1001	CYC	C1B-NB	-2.47	1.33	1.37
87	cL	517	CLA	C1B-C2B	2.47	1.49	1.43
84	m3	1001	CYC	C4D-C3D	2.47	1.48	1.42
87	dL	409	CLA	MG-NB	-2.47	2.00	2.05
84	NO	1001	CYC	C1B-NB	-2.47	1.33	1.37
82	TP	201	PEB	C1C-C2C	2.47	1.48	1.42
84	C4	1001	CYC	C4C-NC	-2.47	1.32	1.37
87	b6	612	CLA	MG-NB	-2.47	2.00	2.05
82	OI	202	PEB	CHB-C1C	2.47	1.46	1.40
82	UP	203	PEB	C1C-NC	-2.47	1.33	1.37
87	72	603	CLA	C1B-C2B	2.47	1.49	1.43
87	bL	618	CLA	MG-ND	-2.47	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MM	203	PEB	C1C-C2C	2.47	1.48	1.42
82	PQ	201	PEB	C1C-C2C	2.47	1.48	1.42
82	T4	203	PEB	C4B-C3B	2.47	1.49	1.45
82	G9	202	PEB	C4B-C3B	2.47	1.49	1.45
84	HE	1001	CYC	C4C-NC	-2.47	1.32	1.37
82	j1	203	PEB	C1C-C2C	2.47	1.48	1.42
82	J7	202	PEB	OD-C4D	2.46	1.28	1.23
82	ZG	201	PEB	C4A-NA	-2.46	1.32	1.37
87	AN	817	CLA	C1B-C2B	2.46	1.49	1.43
87	2N	301	CLA	C1D-ND	2.46	1.40	1.37
82	TB	202	PEB	C1C-NC	-2.46	1.33	1.37
87	BN	802	CLA	CMD-C2D	-2.46	1.45	1.50
84	E4	1001	CYC	OB-C4B	2.46	1.28	1.23
84	J3	1001	CYC	C4D-C3D	2.46	1.48	1.42
82	OH	201	PEB	C4B-C3B	2.46	1.49	1.45
82	QB	201	PEB	CHC-C4C	2.46	1.52	1.49
87	A2	807	CLA	C1B-C2B	2.46	1.49	1.43
82	PO	201	PEB	C1C-NC	-2.46	1.33	1.37
84	H4	1001	CYC	C1B-C2B	2.46	1.49	1.45
82	H5	201	PEB	C4B-C3B	2.46	1.49	1.45
82	B9	203	PEB	C2A-C1A	-2.46	1.49	1.52
84	FE	1001	CYC	C4C-NC	-2.46	1.32	1.37
82	vC	202	PEB	C4B-C3B	2.46	1.49	1.45
87	ON	203	CLA	C1C-C2C	2.46	1.49	1.44
87	AN	823	CLA	CMD-C2D	-2.46	1.45	1.50
82	ZB	203	PEB	C4A-NA	-2.46	1.32	1.37
82	TP	201	PEB	C2A-C1A	-2.46	1.49	1.52
82	J5	203	PEB	C2A-C1A	-2.46	1.49	1.52
82	NK	202	PEB	CHC-C4C	2.46	1.52	1.49
82	kJ	201	PEB	CHC-C4C	2.46	1.52	1.49
82	cO	202	PEB	CHC-C4C	2.46	1.52	1.49
87	F2	205	CLA	C4D-ND	-2.46	1.34	1.37
82	jH	203	PEB	C1C-C2C	2.46	1.48	1.42
82	YJ	202	PEB	OD-C4D	2.46	1.28	1.23
84	FE	1001	CYC	OB-C4B	2.46	1.28	1.23
87	BN	835	CLA	CMB-C2B	-2.46	1.45	1.50
82	bE	201	PEB	C1C-NC	-2.46	1.33	1.37
87	H6	102	CLA	C1B-C2B	2.46	1.49	1.43
82	EJ	203	PEB	C2A-C1A	-2.46	1.49	1.52
82	MP	202	PEB	C2A-C1A	-2.46	1.49	1.52
82	cH	201	PEB	C2A-C1A	-2.46	1.49	1.52
82	dE	203	PEB	C1C-C2C	2.46	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	O1	201	PEB	C4B-C3B	2.46	1.49	1.45
87	AL	403	CLA	MG-NB	-2.46	2.00	2.05
87	AN	838	CLA	MG-NB	-2.46	2.00	2.05
82	iG	202	PEB	C1C-C2C	2.46	1.48	1.42
87	b6	609	CLA	CMB-C2B	-2.46	1.45	1.50
82	ZH	203	PEB	C4A-NA	-2.46	1.32	1.37
82	U4	201	PEB	CHB-C1C	2.46	1.46	1.40
82	lF	202	PEB	C4B-C3B	2.46	1.49	1.45
82	oK	201	PEB	C4B-C3B	2.46	1.49	1.45
82	gO	203	PEB	C4B-C3B	2.46	1.49	1.45
87	C6	514	CLA	CMB-C2B	-2.46	1.45	1.50
87	bL	618	CLA	CMC-C2C	-2.46	1.45	1.50
82	NB	203	PEB	OD-C4D	2.46	1.28	1.23
87	BN	828	CLA	MG-NB	-2.46	2.00	2.05
87	32	310	CLA	MG-NB	-2.46	2.00	2.05
87	C6	517	CLA	MG-NB	-2.46	2.00	2.05
103	82	310	ZEX	C22-C23	-2.46	1.49	1.53
84	IG	1001	CYC	C4C-NC	-2.46	1.32	1.37
82	dG	203	PEB	C1C-C2C	2.46	1.48	1.42
87	A2	840	CLA	MG-NB	-2.46	2.00	2.05
87	62	309	CLA	C1B-C2B	2.46	1.49	1.43
87	B2	835	CLA	CMB-C2B	-2.46	1.45	1.50
84	g3	1001	CYC	C4D-C3D	2.46	1.48	1.42
82	TB	202	PEB	OD-C4D	2.46	1.28	1.23
82	FF	202	PEB	OD-C4D	2.46	1.28	1.23
82	DA	203	PEB	C2A-C1A	-2.46	1.49	1.52
82	K7	201	PEB	C2A-C1A	-2.46	1.49	1.52
87	b6	604	CLA	C1B-C2B	2.46	1.49	1.43
82	bP	501	PEB	C4A-NA	-2.46	1.32	1.37
87	7N	604	CLA	C1B-C2B	2.46	1.49	1.43
87	BN	813	CLA	C3B-C4B	2.46	1.48	1.42
87	b6	613	CLA	MG-NB	-2.46	2.00	2.05
82	c1	201	PEB	C2A-C1A	-2.46	1.49	1.52
82	LA	201	PEB	C1C-C2C	2.46	1.48	1.42
87	8N	301	CLA	CHC-C1C	2.46	1.43	1.38
82	dM	203	PEB	OD-C4D	2.46	1.28	1.23
84	c3	1001	CYC	C4D-C3D	2.46	1.48	1.42
82	j1	202	PEB	C4B-C3B	2.46	1.49	1.45
82	BA	202	PEB	CHC-C4C	2.46	1.52	1.49
83	AQ	302	PUB	C4B-C3B	2.46	1.48	1.42
84	HO	1001	CYC	OB-C4B	2.46	1.28	1.23
82	gK	202	PEB	C2A-C1A	-2.46	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AL	404	CLA	C3B-C4B	2.46	1.48	1.42
87	CL	508	CLA	C3B-C4B	2.46	1.48	1.42
87	c6	604	CLA	C1B-C2B	2.46	1.49	1.43
82	rC	202	PEB	C1C-NC	-2.46	1.33	1.37
84	A3	1001	CYC	C4D-C3D	2.46	1.48	1.42
87	AN	815	CLA	MG-NB	-2.46	2.00	2.05
87	c6	611	CLA	CMB-C2B	-2.46	1.45	1.50
95	c6	601	DGD	O2G-C2G	-2.46	1.40	1.46
84	e3	1001	CYC	C4D-C3D	2.46	1.48	1.42
82	UK	201	PEB	CMB-C2B	-2.46	1.45	1.50
82	dM	201	PEB	C2A-C1A	-2.46	1.49	1.52
84	DG	1001	CYC	C1B-NB	-2.46	1.33	1.37
87	B2	829	CLA	C1B-C2B	2.46	1.49	1.43
82	YM	202	PEB	OD-C4D	2.46	1.28	1.23
82	qF	202	PEB	C4A-NA	-2.46	1.32	1.37
82	g1	202	PEB	C1C-C2C	2.46	1.48	1.42
87	A2	805	CLA	C1B-C2B	2.46	1.49	1.43
87	AN	837	CLA	MG-NB	-2.46	2.00	2.05
87	A2	837	CLA	MG-NB	-2.46	2.00	2.05
87	B2	823	CLA	MG-NB	-2.46	2.00	2.05
82	SK	201	PEB	C2C-C3C	2.46	1.45	1.38
82	CP	202	PEB	OD-C4D	2.46	1.28	1.23
82	tC	202	PEB	C1C-C2C	2.45	1.48	1.42
82	O7	202	PEB	C2A-C1A	-2.45	1.49	1.52
87	BN	831	CLA	C1B-C2B	2.45	1.49	1.43
87	AN	832	CLA	CMB-C2B	-2.45	1.45	1.50
82	CA	201	PEB	OD-C4D	2.45	1.28	1.23
82	K9	202	PEB	C4B-C3B	2.45	1.49	1.45
82	cF	201	PEB	C4B-C3B	2.45	1.49	1.45
82	kF	203	PEB	C4A-NA	-2.45	1.32	1.37
84	MO	1001	CYC	OB-C4B	2.45	1.28	1.23
87	3N	306	CLA	C1B-C2B	2.45	1.49	1.43
82	JB	202	PEB	C1C-NC	-2.45	1.33	1.37
82	QA	201	PEB	C2A-C1A	-2.45	1.49	1.52
82	WF	201	PEB	C2A-C1A	-2.45	1.49	1.52
82	ZM	202	PEB	C4A-NA	-2.45	1.32	1.37
82	w8	201	PEB	C1C-C2C	2.45	1.48	1.42
82	SI	201	PEB	C1C-NC	-2.45	1.33	1.37
82	OK	202	PEB	C4A-NA	-2.45	1.32	1.37
87	cL	507	CLA	C1B-C2B	2.45	1.49	1.43
82	t8	202	PEB	C1C-C2C	2.45	1.48	1.42
82	K7	201	PEB	C4A-NA	-2.45	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	M9	302	PEB	C4A-NA	-2.45	1.32	1.37
82	MD	201	PEB	C1C-NC	-2.45	1.33	1.37
87	AN	840	CLA	MG-NB	-2.45	2.00	2.05
87	d6	406	CLA	C1B-C2B	2.45	1.49	1.43
82	WA	202	PEB	C2A-C1A	-2.45	1.49	1.52
82	Z5	305	PEB	C2A-C1A	-2.45	1.49	1.52
82	aF	202	PEB	OD-C4D	2.45	1.28	1.23
87	bL	604	CLA	C1B-C2B	2.45	1.49	1.43
82	sC	201	PEB	C1B-C2B	2.45	1.51	1.45
82	IP	203	PEB	C1C-NC	-2.45	1.33	1.37
82	v8	202	PEB	C1C-NC	-2.45	1.33	1.37
87	A2	852	CLA	C3B-C4B	2.45	1.48	1.42
84	DG	1001	CYC	C4C-NC	-2.45	1.32	1.37
87	AN	833	CLA	MG-NB	-2.45	2.00	2.05
82	OE	203	PEB	C2A-C1A	-2.45	1.49	1.52
82	iO	202	PEB	C2A-C1A	-2.45	1.49	1.52
87	A2	807	CLA	C3B-C4B	2.45	1.48	1.42
82	UJ	203	PEB	C1C-C2C	2.45	1.48	1.42
82	F5	203	PEB	C1C-NC	-2.45	1.33	1.37
83	wF	304	PUB	C4B-NB	-2.45	1.33	1.37
84	BG	1001	CYC	C1B-NB	-2.45	1.33	1.37
87	22	605	CLA	C1D-ND	2.45	1.40	1.37
82	QJ	204	PEB	C1C-C2C	2.45	1.48	1.42
82	TD	201	PEB	C4B-C3B	2.45	1.49	1.45
82	hE	201	PEB	C4B-C3B	2.45	1.49	1.45
82	jG	201	PEB	C1C-C2C	2.45	1.48	1.42
84	EO	1001	CYC	C4C-NC	-2.45	1.32	1.37
82	DD	203	PEB	C2A-C1A	-2.45	1.49	1.52
82	lF	203	PEB	C4B-NB	-2.45	1.33	1.38
87	A2	839	CLA	MG-NB	-2.45	2.00	2.05
87	BN	810	CLA	C1B-C2B	2.45	1.49	1.43
87	32	304	CLA	C1B-C2B	2.45	1.49	1.43
82	bG	201	PEB	OD-C4D	2.45	1.28	1.23
87	cL	515	CLA	C1D-C2D	2.45	1.50	1.45
82	aH	202	PEB	CHC-C4C	2.45	1.52	1.49
82	SF	201	PEB	C4A-NA	-2.45	1.32	1.37
87	D6	403	CLA	C1B-C2B	2.45	1.49	1.43
87	BL	621	CLA	C1B-NB	-2.45	1.34	1.37
82	k4	201	PEB	C2A-C1A	-2.45	1.49	1.52
82	gB	201	PEB	C2A-C1A	-2.45	1.49	1.52
82	W1	203	PEB	C1C-C2C	2.45	1.48	1.42
84	N3	1001	CYC	C4D-C3D	2.45	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	823	CLA	CMB-C2B	-2.45	1.45	1.50
84	DH	1003	CYC	C1B-C2B	2.45	1.49	1.45
82	d1	203	PEB	C1C-C2C	2.45	1.48	1.42
82	BD	203	PEB	C4A-NA	-2.45	1.32	1.37
82	SO	201	PEB	C4A-NA	-2.45	1.32	1.37
82	Z1	203	PEB	C4A-NA	-2.45	1.32	1.37
95	C6	502	DGD	O2G-C2G	-2.45	1.40	1.46
82	QP	203	PEB	OD-C4D	2.45	1.28	1.23
87	CL	507	CLA	CMD-C2D	-2.45	1.45	1.50
82	TQ	201	PEB	C4B-C3B	2.45	1.49	1.45
87	5N	610	CLA	C1B-C2B	2.45	1.49	1.43
82	dK	202	PEB	C4A-NA	-2.45	1.32	1.37
82	DP	201	PEB	C1C-NC	-2.45	1.33	1.37
82	B7	202	PEB	C1C-C2C	2.45	1.48	1.42
82	SK	202	PEB	C4A-NA	-2.45	1.32	1.37
82	XQ	201	PEB	C1C-C2C	2.45	1.48	1.42
87	A2	826	CLA	CMD-C2D	-2.45	1.45	1.50
87	BN	821	CLA	C1B-C2B	2.45	1.49	1.43
87	C6	519	CLA	C1B-C2B	2.45	1.49	1.43
87	A2	807	CLA	MG-NB	-2.45	2.00	2.05
84	T3	1001	CYC	C4D-C3D	2.45	1.48	1.42
82	m1	201	PEB	C2A-C1A	-2.45	1.49	1.52
82	JB	201	PEB	C1C-NC	-2.45	1.33	1.37
82	e4	201	PEB	C1C-NC	-2.45	1.33	1.37
82	D7	203	PEB	C1C-NC	-2.45	1.33	1.37
87	AN	852	CLA	C1B-C2B	2.45	1.49	1.43
82	H4	1002	PEB	OD-C4D	2.45	1.28	1.23
87	BL	603	CLA	C3B-C4B	2.45	1.48	1.42
87	AN	825	CLA	MG-NB	-2.45	2.00	2.05
82	cK	203	PEB	C1B-C2B	2.45	1.51	1.45
82	VO	202	PEB	OD-C4D	2.45	1.28	1.23
82	V4	202	PEB	OD-C4D	2.45	1.28	1.23
84	P3	1001	CYC	C4D-C3D	2.45	1.48	1.42
84	p3	1001	CYC	C4D-C3D	2.45	1.48	1.42
82	H5	201	PEB	C4A-NA	-2.45	1.32	1.37
82	bG	201	PEB	C4A-NA	-2.45	1.32	1.37
87	82	306	CLA	CHC-C1C	2.45	1.43	1.38
82	RB	202	PEB	C2A-C1A	-2.45	1.49	1.52
82	BQ	202	PEB	C2A-C1A	-2.45	1.49	1.52
82	qF	203	PEB	C2A-C1A	-2.45	1.49	1.52
82	vF	202	PEB	C1C-C2C	2.45	1.48	1.42
82	E7	201	PEB	OD-C4D	2.45	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	3N	307	CLA	MG-NB	-2.45	2.00	2.05
82	HJ	201	PEB	C4A-NA	-2.45	1.32	1.37
85	B6	621	BCR	C30-C25	-2.45	1.50	1.53
82	SO	202	PEB	C1D-ND	2.45	1.49	1.45
82	TD	202	PEB	CHC-C4C	2.45	1.52	1.49
87	AN	826	CLA	CMD-C2D	-2.45	1.45	1.50
87	bL	616	CLA	CMB-C2B	-2.45	1.45	1.50
82	FJ	201	PEB	C4A-NA	-2.45	1.32	1.37
87	4N	603	CLA	MG-NB	-2.45	2.00	2.05
82	ZG	202	PEB	OD-C4D	2.45	1.28	1.23
82	X7	203	PEB	OD-C4D	2.45	1.28	1.23
82	GP	203	PEB	C1C-C2C	2.44	1.48	1.42
84	E3	1001	CYC	C4D-C3D	2.44	1.48	1.42
82	FP	201	PEB	C2A-C1A	-2.44	1.49	1.52
82	u8	203	PEB	C2A-C1A	-2.44	1.49	1.52
82	jM	203	PEB	C2A-C1A	-2.44	1.49	1.52
87	BL	620	CLA	MG-NB	-2.44	2.00	2.05
87	bL	619	CLA	C1B-C2B	2.44	1.49	1.43
87	AN	807	CLA	C3B-C4B	2.44	1.48	1.42
82	CB	201	PEB	C1C-NC	-2.44	1.33	1.37
82	jH	202	PEB	C4B-C3B	2.44	1.49	1.45
87	A2	817	CLA	C1B-C2B	2.44	1.49	1.43
82	A9	202	PEB	C4B-C3B	2.44	1.49	1.45
82	eF	201	PEB	C4B-C3B	2.44	1.49	1.45
82	GJ	202	PEB	C2A-C1A	-2.44	1.49	1.52
83	BM	302	PUB	OA-C1A	2.44	1.28	1.23
82	V7	203	PEB	C1C-C2C	2.44	1.48	1.42
84	GG	1001	CYC	C1B-NB	-2.44	1.33	1.37
87	DL	403	CLA	MG-NB	-2.44	2.00	2.05
87	AN	829	CLA	CMC-C2C	-2.44	1.45	1.50
87	BL	608	CLA	C1B-C2B	2.44	1.49	1.43
82	BF	202	PEB	CHC-C4C	2.44	1.52	1.49
87	1N	602	CLA	C3B-C4B	2.44	1.48	1.42
87	bL	613	CLA	C1B-NB	-2.44	1.34	1.37
87	1N	608	CLA	C4D-ND	-2.44	1.34	1.37
87	bL	606	CLA	CMC-C2C	-2.44	1.45	1.50
84	C1	1001	CYC	C2C-C1C	-2.44	1.49	1.52
87	BN	801	CLA	MG-NB	-2.44	2.00	2.05
87	BL	609	CLA	CMD-C2D	-2.44	1.45	1.50
82	KB	301	PEB	C1C-NC	-2.44	1.33	1.37
82	YF	201	PEB	CHC-C4C	2.44	1.52	1.49
84	l3	1001	CYC	C4D-C3D	2.44	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	LO	1001	CYC	C4C-NC	-2.44	1.32	1.37
87	BL	622	CLA	C1B-C2B	2.44	1.49	1.43
87	CL	515	CLA	C1B-C2B	2.44	1.49	1.43
82	j1	203	PEB	C4B-C3B	2.44	1.49	1.45
82	ID	202	PEB	OD-C4D	2.44	1.28	1.23
84	LH	1002	CYC	OB-C4B	2.44	1.28	1.23
82	ID	201	PEB	C4A-NA	-2.44	1.32	1.37
84	FE	1001	CYC	C1B-C2B	2.44	1.49	1.45
82	TA	203	PEB	OD-C4D	2.44	1.28	1.23
87	MN	101	CLA	MG-NB	-2.44	2.00	2.05
87	C6	510	CLA	MG-NB	-2.44	2.00	2.05
87	42	602	CLA	O1D-CGD	2.44	1.27	1.21
82	MD	201	PEB	C4A-NA	-2.44	1.32	1.37
82	BQ	203	PEB	OD-C4D	2.44	1.28	1.23
82	LJ	201	PEB	OD-C4D	2.44	1.28	1.23
84	JO	1001	CYC	OB-C4B	2.44	1.28	1.23
82	wC	203	PEB	C2A-C1A	-2.44	1.49	1.52
87	b6	618	CLA	C1B-C2B	2.44	1.49	1.43
82	RK	202	PEB	C4A-NA	-2.44	1.32	1.37
87	AN	850	CLA	C1B-C2B	2.44	1.49	1.43
87	D6	405	CLA	C1B-C2B	2.44	1.49	1.43
82	GF	201	PEB	C4B-C3B	2.44	1.49	1.45
82	SM	203	PEB	C2A-C1A	-2.44	1.49	1.52
82	uF	202	PEB	C1B-C2B	2.44	1.51	1.45
87	AN	812	CLA	C1B-C2B	2.44	1.49	1.43
87	BN	822	CLA	C1B-C2B	2.44	1.49	1.43
87	R2	202	CLA	C1B-C2B	2.44	1.49	1.43
87	8N	304	CLA	C1B-C2B	2.44	1.49	1.43
82	tK	202	PEB	OD-C4D	2.44	1.28	1.23
82	QB	202	PEB	C4A-NA	-2.44	1.32	1.37
82	YP	501	PEB	C4A-NA	-2.44	1.32	1.37
87	B2	801	CLA	CMD-C2D	-2.44	1.45	1.50
82	ZE	202	PEB	C1C-NC	-2.44	1.33	1.37
82	QJ	204	PEB	C1C-NC	-2.44	1.33	1.37
82	KF	202	PEB	C4A-NA	-2.44	1.32	1.37
82	M5	301	PEB	C4A-NA	-2.44	1.32	1.37
82	UP	203	PEB	C2A-C1A	-2.44	1.49	1.52
82	cF	203	PEB	C2A-C1A	-2.44	1.49	1.52
87	AL	403	CLA	CMC-C2C	-2.44	1.45	1.50
82	HP	201	PEB	C4B-C3B	2.44	1.49	1.45
82	W9	202	PEB	C1C-C2C	2.44	1.48	1.42
82	J4	1002	PEB	C1C-NC	-2.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	KM	202	PEB	C1C-C2C	2.44	1.48	1.42
82	U9	204	PEB	C1C-C2C	2.44	1.48	1.42
82	vK	202	PEB	C1C-C2C	2.44	1.48	1.42
82	S5	201	PEB	OD-C4D	2.44	1.28	1.23
87	4N	609	CLA	C1B-C2B	2.44	1.49	1.43
87	AN	805	CLA	CMB-C2B	-2.44	1.45	1.50
84	v3	1001	CYC	C4D-C3D	2.43	1.48	1.42
87	AN	807	CLA	MG-NB	-2.43	2.01	2.05
87	6N	608	CLA	C1B-C2B	2.43	1.49	1.43
82	PH	201	PEB	C1C-NC	-2.43	1.33	1.37
82	A7	202	PEB	C1C-C2C	2.43	1.48	1.42
82	OE	202	PEB	C2A-C1A	-2.43	1.49	1.52
82	RP	201	PEB	C2A-C1A	-2.43	1.49	1.52
87	CL	508	CLA	CMC-C2C	-2.43	1.45	1.50
82	RP	201	PEB	C4B-C3B	2.43	1.49	1.45
82	OF	202	PEB	C4A-NA	-2.43	1.32	1.37
82	NJ	201	PEB	C4A-NA	-2.43	1.32	1.37
82	HB	203	PEB	C1C-NC	-2.43	1.33	1.37
82	O7	201	PEB	C4B-NB	-2.43	1.33	1.38
82	KA	201	PEB	C4A-NA	-2.43	1.32	1.37
82	CB	201	PEB	C4A-NA	-2.43	1.32	1.37
82	FF	202	PEB	C4A-NA	-2.43	1.32	1.37
82	CM	201	PEB	OD-C4D	2.43	1.28	1.23
82	FQ	203	PEB	CHC-C4C	2.43	1.52	1.49
82	QB	201	PEB	C4A-NA	-2.43	1.32	1.37
82	SB	203	PEB	C4A-NA	-2.43	1.32	1.37
87	A2	819	CLA	MG-NB	-2.43	2.01	2.05
82	vK	202	PEB	C4B-C3B	2.43	1.49	1.45
82	eF	202	PEB	C1C-NC	-2.43	1.33	1.37
83	wK	304	PUB	C4B-NB	-2.43	1.33	1.37
87	BL	603	CLA	C4B-NB	2.43	1.40	1.37
82	GB	203	PEB	C4A-NA	-2.43	1.32	1.37
87	CL	505	CLA	C1B-C2B	2.43	1.49	1.43
82	ZE	202	PEB	OD-C4D	2.43	1.28	1.23
82	VJ	202	PEB	C1C-C2C	2.43	1.48	1.42
84	BE	1001	CYC	C1B-NB	-2.43	1.33	1.37
82	CF	203	PEB	C2A-C1A	-2.43	1.49	1.52
82	xC	202	PEB	C2A-C1A	-2.43	1.49	1.52
82	CI	201	PEB	C4A-NA	-2.43	1.32	1.37
84	H1	1001	CYC	C4C-NC	-2.43	1.32	1.37
87	A2	821	CLA	C1B-NB	-2.43	1.34	1.37
87	AN	832	CLA	MG-ND	-2.43	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	M2	101	CLA	MG-NB	-2.43	2.01	2.05
82	LB	201	PEB	C1C-NC	-2.43	1.33	1.37
84	EE	1001	CYC	OB-C4B	2.43	1.28	1.23
82	cM	201	PEB	C1C-NC	-2.43	1.33	1.37
82	WM	201	PEB	C4A-NA	-2.43	1.32	1.37
94	D6	408	PL9	C6-C5	2.43	1.48	1.35
82	eK	202	PEB	C1C-NC	-2.43	1.33	1.37
87	5N	601	CLA	C1B-C2B	2.43	1.49	1.43
87	B6	611	CLA	MG-NB	-2.43	2.01	2.05
82	VI	201	PEB	C4A-NA	-2.43	1.32	1.37
87	AN	852	CLA	C4D-ND	-2.43	1.34	1.37
87	ON	201	CLA	C1B-C2B	2.43	1.49	1.43
87	42	605	CLA	C1B-C2B	2.43	1.49	1.43
82	RA	202	PEB	CHA-C1B	2.43	1.46	1.40
82	x8	202	PEB	C2A-C1A	-2.43	1.49	1.52
82	Y1	202	PEB	C1B-C2B	2.43	1.51	1.45
82	BQ	203	PEB	C4A-NA	-2.43	1.32	1.37
87	C6	516	CLA	C1B-C2B	2.43	1.49	1.43
87	A2	818	CLA	CMD-C2D	-2.43	1.45	1.50
82	YE	201	PEB	C1C-NC	-2.43	1.33	1.37
82	CQ	201	PEB	C1C-NC	-2.43	1.33	1.37
82	eH	201	PEB	C1C-NC	-2.43	1.33	1.37
82	pC	202	PEB	C1C-C2C	2.43	1.48	1.42
82	gE	201	PEB	C2A-C1A	-2.43	1.49	1.52
82	II	201	PEB	C4A-NA	-2.43	1.32	1.37
84	IE	1001	CYC	C4C-NC	-2.43	1.32	1.37
87	AN	808	CLA	C1B-C2B	2.43	1.49	1.43
82	Q1	201	PEB	C1C-C2C	2.43	1.48	1.42
87	AN	852	CLA	C3B-C4B	2.43	1.48	1.42
82	FI	201	PEB	C4B-C3B	2.43	1.49	1.45
87	CL	511	CLA	CMB-C2B	-2.43	1.45	1.50
87	AN	807	CLA	C1B-C2B	2.43	1.49	1.43
82	Z5	301	PEB	C4A-NA	-2.43	1.32	1.37
87	4N	602	CLA	O1D-CGD	2.43	1.27	1.21
87	B2	812	CLA	C3B-C4B	2.43	1.48	1.42
82	HK	201	PEB	C4B-NB	-2.43	1.33	1.38
82	TD	202	PEB	OD-C4D	2.43	1.28	1.23
87	BN	808	CLA	C1B-C2B	2.43	1.49	1.43
82	VI	203	PEB	CHA-C1B	2.43	1.46	1.40
82	v8	201	PEB	C1C-NC	-2.43	1.33	1.37
87	LN	204	CLA	MG-NB	-2.43	2.01	2.05
87	B2	831	CLA	MG-NB	-2.43	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ED	201	PEB	C1C-C2C	2.43	1.48	1.42
87	RN	201	CLA	C1B-C2B	2.43	1.49	1.43
82	D7	203	PEB	C2A-C1A	-2.43	1.49	1.52
82	lK	202	PEB	C4B-C3B	2.43	1.49	1.45
84	EG	1001	CYC	C4C-NC	-2.43	1.32	1.37
82	W5	201	PEB	C1C-NC	-2.43	1.33	1.37
87	AL	405	CLA	CMD-C2D	-2.43	1.45	1.50
82	UM	202	PEB	C4A-NA	-2.43	1.32	1.37
87	BN	809	CLA	MG-NB	-2.43	2.01	2.05
82	TB	201	PEB	C1C-NC	-2.43	1.33	1.37
82	PA	201	PEB	OD-C4D	2.43	1.28	1.23
82	jM	203	PEB	OD-C4D	2.43	1.28	1.23
82	VP	201	PEB	C4A-NA	-2.43	1.32	1.37
82	V4	202	PEB	C2C-C3C	2.43	1.45	1.38
87	B2	822	CLA	CMB-C2B	-2.43	1.45	1.50
82	NO	1002	PEB	C1C-NC	-2.43	1.33	1.37
82	N4	1002	PEB	C1C-NC	-2.43	1.33	1.37
82	OP	201	PEB	OD-C4D	2.43	1.28	1.23
82	fH	203	PEB	C4B-C3B	2.42	1.49	1.45
82	AQ	301	PEB	C1C-C2C	2.42	1.48	1.42
82	gK	203	PEB	CHC-C4C	2.42	1.52	1.49
82	pC	201	PEB	C1C-NC	-2.42	1.33	1.37
82	LF	201	PEB	OD-C4D	2.42	1.28	1.23
82	FK	202	PEB	OD-C4D	2.42	1.28	1.23
83	Y7	302	PUB	C4C-NC	2.42	1.39	1.35
82	YQ	201	PEB	C1C-C2C	2.42	1.48	1.42
82	BA	202	PEB	C1C-C2C	2.42	1.48	1.42
84	i3	1001	CYC	C4D-C3D	2.42	1.48	1.42
87	AN	832	CLA	C1B-C2B	2.42	1.49	1.43
82	LF	201	PEB	C4B-C3B	2.42	1.49	1.45
87	BN	825	CLA	CMD-C2D	-2.42	1.45	1.50
87	bL	608	CLA	CMD-C2D	-2.42	1.45	1.50
82	WI	203	PEB	C1C-NC	-2.42	1.33	1.37
82	eM	201	PEB	C1C-NC	-2.42	1.33	1.37
82	HD	201	PEB	C2A-C1A	-2.42	1.49	1.52
87	AN	838	CLA	CMB-C2B	-2.42	1.45	1.50
82	UF	201	PEB	OD-C4D	2.42	1.28	1.23
96	VL	201	HEM	C1D-ND	-2.42	1.33	1.38
87	42	609	CLA	C1B-C2B	2.42	1.49	1.43
82	M5	305	PEB	C2A-C1A	-2.42	1.49	1.52
87	K2	101	CLA	C1B-C2B	2.42	1.49	1.43
87	52	601	CLA	MG-NB	-2.42	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	808	CLA	MG-NB	-2.42	2.01	2.05
82	DP	201	PEB	C4A-NA	-2.42	1.32	1.37
82	mG	203	PEB	C1C-C2C	2.42	1.48	1.42
87	1N	610	CLA	C1B-C2B	2.42	1.49	1.43
87	bL	606	CLA	CHC-C4B	-2.42	1.34	1.39
84	IO	1001	CYC	OB-C4B	2.42	1.28	1.23
82	ZE	201	PEB	C4A-NA	-2.42	1.32	1.37
84	GE	1001	CYC	C4C-NC	-2.42	1.32	1.37
87	CL	507	CLA	C1B-C2B	2.42	1.49	1.43
87	B2	812	CLA	C1B-C2B	2.42	1.49	1.43
82	hE	202	PEB	C2A-C1A	-2.42	1.49	1.52
82	hG	201	PEB	C4B-C3B	2.42	1.49	1.45
82	J1	1002	PEB	C1C-NC	-2.42	1.33	1.37
82	QQ	202	PEB	C1C-C2C	2.42	1.48	1.42
82	KI	202	PEB	C4A-NA	-2.42	1.32	1.37
82	MP	201	PEB	C4A-NA	-2.42	1.32	1.37
82	W9	202	PEB	CHC-C4C	2.42	1.52	1.49
82	Q9	202	PEB	C4B-C3B	2.42	1.49	1.45
82	BA	202	PEB	C2A-C1A	-2.42	1.49	1.52
82	j4	202	PEB	C2A-C1A	-2.42	1.49	1.52
82	jO	202	PEB	C2A-C1A	-2.42	1.49	1.52
87	4N	605	CLA	C1B-C2B	2.42	1.49	1.43
87	BN	824	CLA	MG-NB	-2.42	2.01	2.05
87	AN	818	CLA	CMD-C2D	-2.42	1.45	1.50
87	A2	812	CLA	CMB-C2B	-2.42	1.45	1.50
87	A6	403	CLA	C1B-C2B	2.42	1.49	1.43
83	yK	302	PUB	OD-C4D	2.42	1.28	1.23
82	iO	203	PEB	C4B-C3B	2.42	1.49	1.45
82	MM	203	PEB	C2A-C1A	-2.42	1.49	1.52
87	DL	404	CLA	CMD-C2D	-2.42	1.45	1.50
82	WI	201	PEB	C1C-C2C	2.42	1.48	1.42
82	WJ	202	PEB	C4A-NA	-2.42	1.32	1.37
82	L7	201	PEB	C1C-C2C	2.42	1.48	1.42
82	mJ	201	PEB	C1C-NC	-2.42	1.33	1.37
87	B2	807	CLA	C1B-C2B	2.42	1.48	1.43
82	GF	202	PEB	OA-C1A	2.42	1.28	1.23
82	sC	201	PEB	C2A-C1A	-2.42	1.49	1.52
84	G3	1001	CYC	C4D-C3D	2.42	1.48	1.42
84	t3	1001	CYC	C4D-C3D	2.42	1.48	1.42
82	WI	201	PEB	C1C-NC	-2.42	1.33	1.37
87	52	601	CLA	C1B-C2B	2.42	1.48	1.43
87	72	606	CLA	MG-NB	-2.42	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	R1	202	PEB	C4B-C3B	2.42	1.49	1.45
82	XJ	201	PEB	C4A-NA	-2.42	1.32	1.37
87	cL	509	CLA	CMD-C2D	-2.42	1.45	1.50
82	VD	203	PEB	C4B-NB	-2.42	1.33	1.38
82	tF	201	PEB	C1C-C2C	2.42	1.48	1.42
82	FA	202	PEB	C2A-C1A	-2.42	1.49	1.52
82	E7	201	PEB	C2A-C1A	-2.42	1.49	1.52
82	PE	201	PEB	C4A-NA	-2.42	1.32	1.37
82	PG	201	PEB	C4A-NA	-2.42	1.32	1.37
82	qK	202	PEB	C4A-NA	-2.42	1.32	1.37
84	HG	1001	CYC	C4B-NB	-2.42	1.32	1.38
87	AN	829	CLA	C1B-C2B	2.42	1.48	1.43
87	R2	201	CLA	C1B-C2B	2.42	1.48	1.43
84	JH	1001	CYC	C4A-C3A	2.42	1.51	1.45
82	oF	201	PEB	CHC-C4C	2.42	1.52	1.49
87	bL	619	CLA	C3B-C4B	2.42	1.48	1.42
82	FD	203	PEB	C4B-C3B	2.42	1.49	1.45
87	RN	202	CLA	C1B-C2B	2.42	1.48	1.43
82	YI	202	PEB	C4A-NA	-2.42	1.32	1.37
84	HE	1001	CYC	C4B-NB	-2.42	1.32	1.38
82	LP	201	PEB	C1C-NC	-2.42	1.33	1.37
82	HQ	201	PEB	C2A-C1A	-2.42	1.49	1.52
82	D5	201	PEB	C2A-C1A	-2.42	1.49	1.52
87	5N	601	CLA	MG-NB	-2.42	2.01	2.05
84	73	1002	CYC	C4B-NB	-2.42	1.32	1.38
84	IG	1001	CYC	C1B-NB	-2.41	1.33	1.37
82	B9	201	PEB	C1C-C2C	2.41	1.48	1.42
87	BN	822	CLA	MG-NB	-2.41	2.01	2.05
87	B6	606	CLA	MG-NB	-2.41	2.01	2.05
82	cK	201	PEB	C4B-C3B	2.41	1.49	1.45
87	62	309	CLA	C3A-C4A	2.41	1.59	1.51
82	hJ	201	PEB	C2A-C1A	-2.41	1.49	1.52
84	C3	1001	CYC	C4D-C3D	2.41	1.48	1.42
82	TO	203	PEB	C4B-C3B	2.41	1.49	1.45
83	yF	302	PUB	OD-C4D	2.41	1.28	1.23
87	B2	825	CLA	MG-NB	-2.41	2.01	2.05
87	d6	401	CLA	MG-NB	-2.41	2.01	2.05
82	A1	302	PEB	C1C-C2C	2.41	1.48	1.42
82	S4	201	PEB	C4A-NA	-2.41	1.32	1.37
84	BG	1001	CYC	C4C-NC	-2.41	1.32	1.37
82	DQ	203	PEB	C2A-C1A	-2.41	1.49	1.52
82	AD	301	PEB	C1C-NC	-2.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	LN	204	CLA	CMD-C2D	-2.41	1.45	1.50
82	RH	201	PEB	C4B-C3B	2.41	1.49	1.45
87	22	610	CLA	MG-NB	-2.41	2.01	2.05
87	3N	305	CLA	C1B-C2B	2.41	1.48	1.43
82	NF	202	PEB	CHC-C4C	2.41	1.52	1.49
82	QH	201	PEB	C1C-C2C	2.41	1.48	1.42
82	YP	502	PEB	C4A-NA	-2.41	1.32	1.37
87	H6	103	CLA	MG-NB	-2.41	2.01	2.05
84	FE	1002	CYC	OB-C4B	2.41	1.28	1.23
84	IE	1001	CYC	OB-C4B	2.41	1.28	1.23
84	GG	1001	CYC	OB-C4B	2.41	1.28	1.23
87	O2	203	CLA	C1B-C2B	2.41	1.48	1.43
87	a6	608	CLA	MG-NB	-2.41	2.01	2.05
82	BI	202	PEB	CHA-C1B	2.41	1.46	1.40
82	GQ	201	PEB	C1C-NC	-2.41	1.33	1.37
82	GI	202	PEB	C4A-NA	-2.41	1.32	1.37
87	BN	806	CLA	MG-NB	-2.41	2.01	2.05
87	A2	832	CLA	CMB-C2B	-2.41	1.45	1.50
82	TQ	203	PEB	C1C-C2C	2.41	1.48	1.42
87	BN	832	CLA	MG-NB	-2.41	2.01	2.05
87	7N	606	CLA	MG-NB	-2.41	2.01	2.05
87	82	303	CLA	C1B-C2B	2.41	1.48	1.43
87	C6	515	CLA	C1B-C2B	2.41	1.48	1.43
87	b6	606	CLA	C1B-C2B	2.41	1.48	1.43
82	TF	202	PEB	C4A-NA	-2.41	1.32	1.37
82	RI	201	PEB	C4A-NA	-2.41	1.32	1.37
82	aG	201	PEB	C4A-NA	-2.41	1.32	1.37
87	A2	829	CLA	CMD-C2D	-2.41	1.45	1.50
82	QD	202	PEB	C1C-C2C	2.41	1.48	1.42
87	12	610	CLA	C1B-C2B	2.41	1.48	1.43
87	A2	827	CLA	C1D-ND	2.41	1.40	1.37
82	Q9	202	PEB	C2A-C1A	-2.41	1.49	1.52
87	aL	605	CLA	C1B-C2B	2.41	1.48	1.43
82	p8	201	PEB	C1C-NC	-2.41	1.33	1.37
82	TK	202	PEB	C4A-NA	-2.41	1.32	1.37
84	DE	1001	CYC	C4C-NC	-2.41	1.32	1.37
82	OB	201	PEB	OD-C4D	2.41	1.28	1.23
84	CG	1001	CYC	OB-C4B	2.41	1.28	1.23
87	CL	518	CLA	C1B-C2B	2.41	1.48	1.43
87	B6	605	CLA	C1B-C2B	2.41	1.48	1.43
87	82	307	CLA	C1B-C2B	2.41	1.48	1.43
82	uF	201	PEB	C1C-C2C	2.41	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	3N	311	CLA	C1B-C2B	2.41	1.48	1.43
82	SI	201	PEB	OD-C4D	2.41	1.28	1.23
87	A2	832	CLA	MG-ND	-2.41	2.01	2.05
87	2N	310	CLA	MG-NB	-2.41	2.01	2.05
82	aF	203	PEB	C1B-C2B	2.41	1.51	1.45
84	H1	1001	CYC	C4B-NB	-2.41	1.32	1.38
82	KB	302	PEB	C4A-NA	-2.41	1.32	1.37
82	HD	202	PEB	C4A-NA	-2.41	1.32	1.37
87	BN	815	CLA	C3B-C4B	2.41	1.48	1.42
84	DH	1003	CYC	C4D-C3D	2.41	1.48	1.42
87	52	610	CLA	C1B-C2B	2.41	1.48	1.43
82	AI	201	PEB	C4A-NA	-2.41	1.32	1.37
82	JP	202	PEB	C4A-NA	-2.41	1.32	1.37
82	OP	202	PEB	C4A-NA	-2.41	1.32	1.37
82	PP	201	PEB	C4A-NA	-2.41	1.32	1.37
84	CG	1001	CYC	C1B-NB	-2.41	1.33	1.37
82	RI	203	PEB	C2C-C3C	2.41	1.45	1.38
84	J1	1001	CYC	C1B-C2B	2.41	1.49	1.45
87	a6	609	CLA	MG-NB	-2.41	2.01	2.05
82	AP	201	PEB	OD-C4D	2.41	1.28	1.23
82	ND	202	PEB	CHC-C4C	2.41	1.52	1.49
84	EO	1001	CYC	C1B-NB	-2.41	1.33	1.37
87	A2	805	CLA	CMB-C2B	-2.41	1.45	1.50
82	UD	202	PEB	C2A-C1A	-2.41	1.49	1.52
82	CF	201	PEB	C1C-C2C	2.41	1.48	1.42
82	YG	201	PEB	C4A-NA	-2.41	1.32	1.37
82	R4	201	PEB	C4A-NA	-2.41	1.32	1.37
83	YA	302	PUB	C4B-NB	-2.41	1.33	1.37
82	TJ	201	PEB	C4A-NA	-2.41	1.32	1.37
87	22	611	CLA	C1B-C2B	2.41	1.48	1.43
82	J5	202	PEB	C2A-C1A	-2.41	1.49	1.52
82	fH	203	PEB	C2A-C1A	-2.41	1.49	1.52
82	KI	201	PEB	C4B-C3B	2.41	1.49	1.45
87	AL	405	CLA	C3B-C4B	2.41	1.48	1.42
87	bL	618	CLA	C3B-C4B	2.41	1.48	1.42
82	RF	202	PEB	C4A-NA	-2.41	1.32	1.37
82	O7	202	PEB	C4A-NA	-2.41	1.32	1.37
82	KK	202	PEB	OD-C4D	2.41	1.28	1.23
82	h4	201	PEB	CHA-C4A	-2.41	1.32	1.36
87	AN	803	CLA	C1B-C2B	2.41	1.48	1.43
82	T4	201	PEB	C1C-NC	-2.40	1.33	1.37
82	jF	202	PEB	C1C-NC	-2.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	O9	201	PEB	C1C-C2C	2.40	1.48	1.42
87	AN	849	CLA	MG-ND	-2.40	2.01	2.05
87	32	310	CLA	MG-ND	-2.40	2.01	2.05
82	HD	202	PEB	OD-C4D	2.40	1.28	1.23
82	UO	201	PEB	CHB-C1C	2.40	1.46	1.40
83	ND	201	PUB	C4C-NC	2.40	1.39	1.35
82	YQ	202	PEB	C1C-C2C	2.40	1.48	1.42
82	H7	203	PEB	C2A-C1A	-2.40	1.49	1.52
87	A2	825	CLA	MG-NB	-2.40	2.01	2.05
82	UB	301	PEB	CHC-C4C	2.40	1.52	1.49
82	tF	202	PEB	OD-C4D	2.40	1.28	1.23
82	fK	202	PEB	C4A-NA	-2.40	1.32	1.37
82	V9	201	PEB	C1C-NC	-2.40	1.33	1.37
82	tC	201	PEB	C1C-NC	-2.40	1.33	1.37
82	Y4	203	PEB	C4B-C3B	2.40	1.49	1.45
87	8N	307	CLA	C1B-C2B	2.40	1.48	1.43
87	AN	821	CLA	MG-NB	-2.40	2.01	2.05
87	I2	103	CLA	MG-NB	-2.40	2.01	2.05
82	kM	201	PEB	C2A-C1A	-2.40	1.49	1.52
82	kH	201	PEB	C1C-C2C	2.40	1.48	1.42
87	7N	605	CLA	CMD-C2D	-2.40	1.45	1.50
82	MQ	202	PEB	C1C-C2C	2.40	1.48	1.42
82	hG	201	PEB	C1C-C2C	2.40	1.48	1.42
82	EI	201	PEB	C4A-NA	-2.40	1.32	1.37
82	U1	202	PEB	C4A-NA	-2.40	1.32	1.37
87	B2	814	CLA	C3B-C4B	2.40	1.48	1.42
82	JQ	203	PEB	C1C-C2C	2.40	1.48	1.42
87	HL	101	CLA	C1B-NB	-2.40	1.34	1.37
82	F4	1002	PEB	C1C-NC	-2.40	1.33	1.37
82	R9	201	PEB	C1C-NC	-2.40	1.33	1.37
82	AQ	304	PEB	C1C-C2C	2.40	1.48	1.42
87	B2	807	CLA	MG-NB	-2.40	2.01	2.05
82	YD	202	PEB	C4B-C3B	2.40	1.49	1.45
82	BJ	301	PEB	C4A-NA	-2.40	1.32	1.37
82	RQ	201	PEB	C1C-C2C	2.40	1.48	1.42
84	EG	1001	CYC	C1B-NB	-2.40	1.33	1.37
87	A2	852	CLA	C1B-C2B	2.40	1.48	1.43
87	d6	401	CLA	C1B-C2B	2.40	1.48	1.43
87	AN	821	CLA	C1B-NB	-2.40	1.34	1.37
87	A2	827	CLA	CHC-C1C	2.40	1.43	1.38
84	63	901	CYC	C4C-NC	-2.40	1.32	1.37
82	EA	201	PEB	OD-C4D	2.40	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VE	202	PEB	C1C-C2C	2.40	1.48	1.42
83	QM	201	PUB	C4B-C3B	2.40	1.48	1.42
82	V7	201	PEB	C2A-C1A	-2.40	1.49	1.52
87	AN	850	CLA	CMD-C2D	-2.40	1.45	1.50
87	42	603	CLA	MG-NB	-2.40	2.01	2.05
87	B2	832	CLA	MG-NB	-2.40	2.01	2.05
84	CH	1001	CYC	C1B-C2B	2.40	1.49	1.45
87	B2	809	CLA	C1B-C2B	2.40	1.48	1.43
87	CL	511	CLA	CMD-C2D	-2.40	1.45	1.50
87	6N	608	CLA	C3A-C4A	2.40	1.59	1.51
82	mE	203	PEB	C4B-C3B	2.40	1.49	1.45
82	mH	202	PEB	C4B-C3B	2.40	1.49	1.45
82	H7	202	PEB	C1A-NA	-2.40	1.34	1.37
82	hE	201	PEB	C1C-C2C	2.40	1.48	1.42
82	UP	201	PEB	C4A-NA	-2.40	1.32	1.37
82	BD	203	PEB	OD-C4D	2.40	1.28	1.23
82	BJ	301	PEB	OD-C4D	2.40	1.28	1.23
87	L2	204	CLA	MG-NB	-2.40	2.01	2.05
82	wC	203	PEB	C4B-C3B	2.40	1.49	1.45
87	AN	836	CLA	C1B-C2B	2.40	1.48	1.43
87	B2	811	CLA	C1B-C2B	2.40	1.48	1.43
87	B6	614	CLA	C1B-C2B	2.40	1.48	1.43
87	D6	402	CLA	C1B-C2B	2.40	1.48	1.43
82	j4	201	PEB	C4A-NA	-2.40	1.32	1.37
82	jO	201	PEB	C4A-NA	-2.40	1.32	1.37
87	12	602	CLA	C3B-C4B	2.40	1.48	1.42
82	MP	202	PEB	C1C-C2C	2.40	1.48	1.42
87	B6	606	CLA	C1B-C2B	2.40	1.48	1.43
87	c6	607	CLA	C1B-C2B	2.40	1.48	1.43
87	4N	604	CLA	C1B-C2B	2.40	1.48	1.43
82	UG	202	PEB	C4A-NA	-2.40	1.32	1.37
84	K4	1001	CYC	C4C-NC	-2.40	1.32	1.37
82	BI	201	PEB	C1C-C2C	2.40	1.48	1.42
87	bL	606	CLA	C4B-NB	2.40	1.40	1.37
87	22	603	CLA	MG-NB	-2.40	2.01	2.05
87	A2	821	CLA	MG-NB	-2.40	2.01	2.05
82	W1	203	PEB	C2A-C1A	-2.40	1.49	1.52
82	aG	202	PEB	C2A-C1A	-2.40	1.49	1.52
83	Z9	305	PUB	C3B-C2B	2.40	1.45	1.38
84	KG	202	CYC	C1B-C2B	2.40	1.49	1.45
82	VA	203	PEB	C1C-C2C	2.40	1.48	1.42
82	ZB	203	PEB	C1C-NC	-2.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	bG	201	PEB	C1C-NC	-2.40	1.33	1.37
87	B6	604	CLA	C1B-C2B	2.40	1.48	1.43
82	DD	202	PEB	C4A-NA	-2.40	1.32	1.37
82	FK	202	PEB	C4A-NA	-2.40	1.32	1.37
87	5N	606	CLA	C1B-C2B	2.40	1.48	1.43
82	lJ	202	PEB	OD-C4D	2.40	1.28	1.23
87	a6	607	CLA	MG-NB	-2.40	2.01	2.05
82	gB	203	PEB	C4A-NA	-2.40	1.32	1.37
87	22	601	CLA	C3B-C4B	2.40	1.48	1.42
94	A6	410	PL9	C6-C5	2.40	1.47	1.35
87	BN	831	CLA	MG-NB	-2.40	2.01	2.05
87	cL	511	CLA	CMD-C2D	-2.40	1.45	1.50
82	YD	201	PEB	C1C-C2C	2.40	1.48	1.42
82	OQ	201	PEB	C1C-C2C	2.40	1.48	1.42
87	A2	803	CLA	C1B-C2B	2.40	1.48	1.43
82	WA	202	PEB	C1D-ND	2.40	1.49	1.45
82	dB	201	PEB	OD-C4D	2.40	1.28	1.23
82	WM	203	PEB	C4A-NA	-2.40	1.32	1.37
82	iE	201	PEB	C1C-C2C	2.40	1.48	1.42
87	8N	306	CLA	CMD-C2D	-2.40	1.45	1.50
87	DL	404	CLA	C1B-C2B	2.40	1.48	1.43
87	ON	202	CLA	C1B-C2B	2.40	1.48	1.43
82	AP	203	PEB	C1C-NC	-2.40	1.33	1.37
82	v8	201	PEB	C2A-C1A	-2.40	1.49	1.52
82	HP	201	PEB	C1C-C2C	2.40	1.48	1.42
82	RB	201	PEB	C4A-NA	-2.40	1.32	1.37
82	PI	201	PEB	C4A-NA	-2.40	1.32	1.37
87	a6	609	CLA	C1B-C2B	2.40	1.48	1.43
82	BP	201	PEB	C4B-C3B	2.40	1.49	1.45
87	L2	203	CLA	C1B-C2B	2.40	1.48	1.43
82	PP	201	PEB	C1C-NC	-2.40	1.33	1.37
87	B2	811	CLA	MG-NB	-2.40	2.01	2.05
87	nL	101	CLA	C3B-C4B	2.39	1.48	1.42
87	O2	202	CLA	C1B-C2B	2.39	1.48	1.43
87	FN	201	CLA	CMD-C2D	-2.39	1.45	1.50
82	r8	202	PEB	C1C-NC	-2.39	1.33	1.37
82	kF	202	PEB	C1C-C2C	2.39	1.48	1.42
82	YB	202	PEB	C4A-NA	-2.39	1.32	1.37
82	F5	202	PEB	C4A-NA	-2.39	1.32	1.37
87	B6	616	CLA	CMD-C2D	-2.39	1.45	1.50
82	aH	202	PEB	C2A-C1A	-2.39	1.50	1.52
87	B2	831	CLA	C3B-C4B	2.39	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VK	201	PEB	C1A-NA	-2.39	1.34	1.37
82	vK	201	PEB	C4B-C3B	2.39	1.49	1.45
82	c4	202	PEB	CHC-C4C	2.39	1.52	1.49
82	E7	201	PEB	C1C-C2C	2.39	1.48	1.42
82	p8	202	PEB	C1C-C2C	2.39	1.48	1.42
87	B2	805	CLA	MG-NB	-2.39	2.01	2.05
87	B6	603	CLA	C1B-C2B	2.39	1.48	1.43
82	HI	201	PEB	C4A-NA	-2.39	1.32	1.37
84	I4	1001	CYC	C4C-NC	-2.39	1.32	1.37
85	b6	601	BCR	C30-C25	-2.39	1.50	1.53
82	B7	202	PEB	C2A-C1A	-2.39	1.50	1.52
82	O9	203	PEB	C2A-C1A	-2.39	1.50	1.52
82	RP	201	PEB	C1C-NC	-2.39	1.33	1.37
82	DQ	202	PEB	C4A-NA	-2.39	1.32	1.37
87	O2	201	CLA	C1B-C2B	2.39	1.48	1.43
82	GQ	201	PEB	C4B-C3B	2.39	1.49	1.45
82	fM	202	PEB	C1C-C2C	2.39	1.48	1.42
82	UJ	202	PEB	C1C-NC	-2.39	1.33	1.37
82	N9	201	PEB	C1C-NC	-2.39	1.33	1.37
87	aL	605	CLA	MG-NB	-2.39	2.01	2.05
82	H9	201	PEB	C1C-C2C	2.39	1.48	1.42
82	X9	202	PEB	C2A-C1A	-2.39	1.50	1.52
87	BL	622	CLA	CMD-C2D	-2.39	1.45	1.50
87	DL	404	CLA	CMC-C2C	-2.39	1.45	1.50
82	QJ	203	PEB	C4A-NA	-2.39	1.32	1.37
82	AD	304	PEB	C1C-NC	-2.39	1.33	1.37
82	YG	201	PEB	C1C-NC	-2.39	1.33	1.37
87	DL	406	CLA	C1B-C2B	2.39	1.48	1.43
87	A2	813	CLA	C1B-C2B	2.39	1.48	1.43
82	CJ	201	PEB	OD-C4D	2.39	1.28	1.23
87	82	305	CLA	CMD-C2D	-2.39	1.45	1.50
82	TP	201	PEB	C1C-NC	-2.39	1.33	1.37
83	AD	302	PUB	C4B-C3B	2.39	1.48	1.42
87	K2	106	CLA	C4D-ND	-2.39	1.34	1.37
87	LN	203	CLA	C1B-C2B	2.39	1.48	1.43
82	RG	201	PEB	C4A-NA	-2.39	1.32	1.37
82	YJ	201	PEB	C4A-NA	-2.39	1.32	1.37
82	FK	201	PEB	OD-C4D	2.39	1.28	1.23
82	mG	203	PEB	C4B-C3B	2.39	1.49	1.45
87	CL	514	CLA	C1B-C2B	2.39	1.48	1.43
87	AN	812	CLA	CMB-C2B	-2.39	1.45	1.50
82	VO	202	PEB	C2C-C3C	2.39	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GE	1002	PEB	C4A-NA	-2.39	1.32	1.37
82	NI	201	PEB	C4A-NA	-2.39	1.32	1.37
82	NM	202	PEB	C4A-NA	-2.39	1.32	1.37
82	RA	202	PEB	C2A-C1A	-2.39	1.50	1.52
82	CP	201	PEB	C2A-C1A	-2.39	1.50	1.52
87	12	611	CLA	MG-NB	-2.39	2.01	2.05
82	UF	201	PEB	CMB-C2B	-2.39	1.45	1.50
87	B2	824	CLA	CMD-C2D	-2.39	1.45	1.50
87	4N	605	CLA	CMD-C2D	-2.39	1.45	1.50
82	oK	201	PEB	CHC-C4C	2.39	1.52	1.49
84	C4	1001	CYC	OB-C4B	2.39	1.28	1.23
84	EE	1001	CYC	C1B-NB	-2.39	1.33	1.37
87	b6	608	CLA	MG-NB	-2.39	2.01	2.05
87	F2	202	CLA	CMD-C2D	-2.39	1.45	1.50
82	e1	201	PEB	C1C-NC	-2.39	1.33	1.37
82	I9	201	PEB	C1C-NC	-2.39	1.33	1.37
84	DO	1001	CYC	C4B-NB	-2.39	1.32	1.38
84	E1	1001	CYC	C4B-NB	-2.39	1.32	1.38
87	dL	401	CLA	MG-NB	-2.39	2.01	2.05
82	RO	202	PEB	C4A-NA	-2.39	1.32	1.37
84	M1	201	CYC	C2C-C1C	-2.39	1.50	1.52
87	BL	605	CLA	CMB-C2B	-2.39	1.45	1.50
82	nF	201	PEB	C1C-C2C	2.39	1.48	1.42
82	J9	201	PEB	C4A-NA	-2.39	1.32	1.37
87	B2	836	CLA	MG-NB	-2.39	2.01	2.05
82	GK	201	PEB	C4B-C3B	2.39	1.49	1.45
82	VE	202	PEB	C4A-NA	-2.39	1.32	1.37
82	gF	202	PEB	C2A-C1A	-2.39	1.50	1.52
82	iF	202	PEB	C2A-C1A	-2.39	1.50	1.52
87	42	607	CLA	C1B-C2B	2.39	1.48	1.43
87	1N	611	CLA	MG-NB	-2.39	2.01	2.05
82	mM	202	PEB	C1C-C2C	2.39	1.48	1.42
87	AN	803	CLA	MG-NB	-2.39	2.01	2.05
82	RH	202	PEB	C4B-C3B	2.39	1.49	1.45
84	D1	1003	CYC	C4D-C3D	2.39	1.48	1.42
87	b6	613	CLA	C1B-C2B	2.39	1.48	1.43
82	eO	201	PEB	C1C-NC	-2.39	1.33	1.37
87	BL	623	CLA	CMC-C2C	-2.39	1.45	1.50
82	CP	201	PEB	OD-C4D	2.39	1.28	1.23
82	UJ	201	PEB	C4A-NA	-2.39	1.32	1.37
82	FQ	201	PEB	C4A-NA	-2.39	1.32	1.37
87	52	611	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A6	402	CLA	C1B-C2B	2.39	1.48	1.43
82	w8	203	PEB	C4B-C3B	2.39	1.49	1.45
82	PD	202	PEB	C1B-C2B	2.39	1.51	1.45
82	Y5	201	PEB	C4A-NA	-2.39	1.32	1.37
82	VA	201	PEB	C2A-C1A	-2.39	1.50	1.52
82	fF	202	PEB	C2A-C1A	-2.39	1.50	1.52
82	SK	201	PEB	OD-C4D	2.39	1.28	1.23
82	MJ	202	PEB	C1C-NC	-2.39	1.33	1.37
87	BN	813	CLA	MG-NB	-2.38	2.01	2.05
87	2N	304	CLA	MG-NB	-2.38	2.01	2.05
87	52	606	CLA	C1B-C2B	2.38	1.48	1.43
82	OA	202	PEB	C4A-NA	-2.38	1.32	1.37
82	JI	201	PEB	C4A-NA	-2.38	1.32	1.37
82	R7	203	PEB	C1C-C2C	2.38	1.48	1.42
82	hM	203	PEB	C1C-C2C	2.38	1.48	1.42
87	b6	608	CLA	C4B-NB	2.38	1.40	1.37
82	s8	201	PEB	C2A-C1A	-2.38	1.50	1.52
87	A2	818	CLA	MG-NB	-2.38	2.01	2.05
87	3N	301	CLA	MG-NB	-2.38	2.01	2.05
82	QF	203	PEB	C4B-C3B	2.38	1.49	1.45
82	T1	201	PEB	C1C-NC	-2.38	1.33	1.37
82	IF	201	PEB	CHB-C4B	2.38	1.43	1.38
82	CD	202	PEB	C1C-C2C	2.38	1.48	1.42
82	h1	202	PEB	C4A-NA	-2.38	1.32	1.37
82	PQ	202	PEB	C1B-C2B	2.38	1.51	1.45
82	iE	202	PEB	C1C-C2C	2.38	1.48	1.42
82	GJ	201	PEB	C4A-NA	-2.38	1.32	1.37
82	IQ	202	PEB	OD-C4D	2.38	1.28	1.23
82	p8	202	PEB	OD-C4D	2.38	1.28	1.23
87	AN	813	CLA	C1B-C2B	2.38	1.48	1.43
87	A6	402	CLA	CMD-C2D	-2.38	1.45	1.50
82	SP	201	PEB	C2A-C1A	-2.38	1.50	1.52
82	V4	202	PEB	C4A-NA	-2.38	1.32	1.37
82	j4	202	PEB	C1D-ND	2.38	1.49	1.45
82	rF	202	PEB	C1C-NC	-2.38	1.33	1.37
82	HD	202	PEB	CHC-C4C	2.38	1.52	1.49
87	cL	510	CLA	CMC-C2C	-2.38	1.45	1.50
82	RJ	201	PEB	C4A-NA	-2.38	1.32	1.37
82	OF	203	PEB	C1C-NC	-2.38	1.33	1.37
87	B2	821	CLA	C1B-C2B	2.38	1.48	1.43
87	2N	311	CLA	C1B-C2B	2.38	1.48	1.43
87	42	606	CLA	MG-NB	-2.38	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ZH	202	PEB	C4A-NA	-2.38	1.32	1.37
87	KN	105	CLA	C4D-ND	-2.38	1.34	1.37
82	TD	201	PEB	C2A-C1A	-2.38	1.50	1.52
82	BK	202	PEB	CHC-C4C	2.38	1.52	1.49
82	K9	201	PEB	C1C-NC	-2.38	1.33	1.37
87	BN	836	CLA	MG-NB	-2.38	2.01	2.05
82	KB	301	PEB	C4A-NA	-2.38	1.32	1.37
82	UM	203	PEB	C4B-C3B	2.38	1.49	1.45
82	J7	202	PEB	C4B-C3B	2.38	1.49	1.45
82	xF	302	PEB	C4B-C3B	2.38	1.49	1.45
87	A2	812	CLA	C1B-C2B	2.38	1.48	1.43
82	OJ	203	PEB	C4A-NA	-2.38	1.32	1.37
82	MM	201	PEB	C4A-NA	-2.38	1.32	1.37
82	OF	202	PEB	C1C-NC	-2.38	1.33	1.37
82	P4	201	PEB	C1C-NC	-2.38	1.33	1.37
82	QB	202	PEB	OD-C4D	2.38	1.28	1.23
82	SK	202	PEB	OD-C4D	2.38	1.28	1.23
84	CO	1001	CYC	OB-C4B	2.38	1.28	1.23
82	R7	202	PEB	C1A-NA	-2.38	1.34	1.37
82	iH	201	PEB	CHC-C4C	2.38	1.52	1.49
87	AN	824	CLA	C1B-C2B	2.38	1.48	1.43
87	BL	602	CLA	CMD-C2D	-2.38	1.45	1.50
87	IN	103	CLA	MG-NB	-2.38	2.01	2.05
87	B2	821	CLA	MG-NB	-2.38	2.01	2.05
82	IB	202	PEB	C4A-NA	-2.38	1.32	1.37
95	C6	504	DGD	O2G-C2G	-2.38	1.40	1.46
82	NP	201	PEB	C4B-C3B	2.38	1.49	1.45
87	72	607	CLA	CMB-C2B	-2.38	1.45	1.50
87	1N	606	CLA	C1B-C2B	2.38	1.48	1.43
82	gE	201	PEB	C1C-C2C	2.38	1.48	1.42
84	I4	1001	CYC	OB-C4B	2.38	1.28	1.23
87	52	607	CLA	C3B-C4B	2.38	1.48	1.42
87	C6	516	CLA	C3B-C4B	2.38	1.48	1.42
87	BN	834	CLA	CMB-C2B	-2.38	1.45	1.50
87	AN	816	CLA	C1B-C2B	2.38	1.48	1.43
87	52	602	CLA	C1B-C2B	2.38	1.48	1.43
82	hK	201	PEB	C1C-C2C	2.38	1.48	1.42
83	QJ	201	PUB	C4B-C3B	2.38	1.48	1.42
84	IE	1001	CYC	C4B-NB	-2.38	1.32	1.38
82	DI	202	PEB	C2A-C1A	-2.38	1.50	1.52
87	B2	822	CLA	MG-ND	-2.38	2.01	2.05
82	iJ	201	PEB	CHC-C4C	2.38	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NE	202	PEB	C4A-NA	-2.38	1.32	1.37
82	GJ	201	PEB	OD-C4D	2.38	1.28	1.23
87	32	311	CLA	C1B-C2B	2.38	1.48	1.43
82	RA	202	PEB	C1A-NA	-2.38	1.34	1.37
82	ID	202	PEB	C4A-NA	-2.38	1.32	1.37
82	N7	202	PEB	C2A-C1A	-2.38	1.50	1.52
82	gB	202	PEB	C2A-C1A	-2.38	1.50	1.52
87	5N	607	CLA	C3B-C4B	2.38	1.48	1.42
82	VJ	201	PEB	C4A-NA	-2.38	1.32	1.37
82	u8	202	PEB	C1C-C2C	2.38	1.48	1.42
82	FB	201	PEB	OD-C4D	2.38	1.28	1.23
82	LH	1003	PEB	OD-C4D	2.38	1.28	1.23
82	II	203	PEB	C4B-C3B	2.38	1.49	1.45
82	YQ	202	PEB	C4B-C3B	2.38	1.49	1.45
82	lF	203	PEB	C4B-C3B	2.38	1.49	1.45
82	TH	201	PEB	C4A-NA	-2.38	1.32	1.37
87	H6	102	CLA	MG-NB	-2.38	2.01	2.05
87	cL	511	CLA	MG-NB	-2.38	2.01	2.05
82	TQ	201	PEB	CHC-C4C	2.38	1.52	1.49
87	RN	204	CLA	C1B-C2B	2.38	1.48	1.43
82	OM	202	PEB	C1C-C2C	2.38	1.48	1.42
82	f1	203	PEB	C1C-C2C	2.38	1.48	1.42
87	BN	813	CLA	C1B-C2B	2.38	1.48	1.43
87	42	604	CLA	C1B-C2B	2.38	1.48	1.43
87	A2	824	CLA	C1B-C2B	2.38	1.48	1.43
82	xF	303	PEB	C1C-C2C	2.38	1.48	1.42
87	b6	611	CLA	MG-NB	-2.38	2.01	2.05
87	CL	510	CLA	C4B-NB	2.38	1.40	1.37
82	OI	202	PEB	C1D-ND	2.38	1.49	1.45
82	CA	201	PEB	C4A-NA	-2.38	1.32	1.37
82	lM	203	PEB	C1C-C2C	2.38	1.48	1.42
87	ON	203	CLA	C1B-C2B	2.38	1.48	1.43
82	DK	203	PEB	C1C-NC	-2.38	1.33	1.37
87	1N	602	CLA	C4B-NB	2.38	1.40	1.37
87	42	605	CLA	CMD-C2D	-2.38	1.45	1.50
87	B6	610	CLA	CMC-C2C	-2.38	1.45	1.50
82	YO	203	PEB	C4B-C3B	2.38	1.49	1.45
87	AN	828	CLA	C1B-C2B	2.38	1.48	1.43
82	fJ	203	PEB	C1C-C2C	2.38	1.48	1.42
87	2N	307	CLA	MG-NB	-2.38	2.01	2.05
82	QK	203	PEB	C2C-C3C	2.38	1.45	1.38
87	B2	809	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	QG	202	PEB	C4A-NA	-2.38	1.32	1.37
82	dQ	401	PEB	C4A-NA	-2.38	1.32	1.37
87	B6	615	CLA	MG-NB	-2.37	2.01	2.05
87	BN	812	CLA	C1B-C2B	2.37	1.48	1.43
82	iK	201	PEB	CHC-C4C	2.37	1.52	1.49
82	qC	201	PEB	C4B-C3B	2.37	1.49	1.45
82	kE	201	PEB	C4B-C3B	2.37	1.49	1.45
82	kO	201	PEB	C4B-C3B	2.37	1.49	1.45
87	AN	818	CLA	MG-NB	-2.37	2.01	2.05
87	82	306	CLA	MG-ND	-2.37	2.01	2.05
82	XI	201	PEB	C4A-NA	-2.37	1.32	1.37
82	RM	201	PEB	C4A-NA	-2.37	1.32	1.37
82	AI	203	PEB	C4B-NB	-2.37	1.33	1.38
82	bE	201	PEB	OD-C4D	2.37	1.28	1.23
82	KA	202	PEB	C1D-ND	2.37	1.49	1.45
82	EQ	201	PEB	C1C-C2C	2.37	1.48	1.42
82	L9	202	PEB	C1C-C2C	2.37	1.48	1.42
84	H1	1001	CYC	C1B-C2B	2.37	1.49	1.45
87	BN	812	CLA	MG-NB	-2.37	2.01	2.05
82	RQ	201	PEB	C2A-C1A	-2.37	1.50	1.52
82	O1	201	PEB	C2A-C1A	-2.37	1.50	1.52
82	WK	203	PEB	C4B-C3B	2.37	1.49	1.45
82	S5	202	PEB	C4B-C3B	2.37	1.49	1.45
82	UI	201	PEB	C4A-NA	-2.37	1.32	1.37
82	NE	202	PEB	C1C-NC	-2.37	1.33	1.37
84	H4	1001	CYC	C1B-NB	-2.37	1.33	1.37
87	K2	106	CLA	C1B-C2B	2.37	1.48	1.43
82	fJ	202	PEB	C1C-C2C	2.37	1.48	1.42
82	P7	201	PEB	OD-C4D	2.37	1.28	1.23
96	E6	101	HEM	C1D-ND	-2.37	1.33	1.38
87	CL	507	CLA	MG-NB	-2.37	2.01	2.05
87	8N	301	CLA	MG-ND	-2.37	2.01	2.05
87	CL	509	CLA	C3B-C4B	2.37	1.48	1.42
82	WH	203	PEB	C4A-NA	-2.37	1.32	1.37
82	TI	202	PEB	C4A-NA	-2.37	1.32	1.37
87	AN	827	CLA	CHC-C1C	2.37	1.43	1.38
82	TI	201	PEB	OD-C4D	2.37	1.28	1.23
87	AN	851	CLA	MG-NB	-2.37	2.01	2.05
87	A2	828	CLA	C1B-C2B	2.37	1.48	1.43
82	YH	202	PEB	C1B-C2B	2.37	1.50	1.45
82	f1	203	PEB	C4B-C3B	2.37	1.49	1.45
82	XA	203	PEB	OD-C4D	2.37	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	LG	1002	PEB	OD-C4D	2.37	1.28	1.23
87	A2	836	CLA	C1B-C2B	2.37	1.48	1.43
87	bL	617	CLA	C1B-NB	-2.37	1.34	1.37
82	UB	303	PEB	C1C-C2C	2.37	1.48	1.42
84	D1	1003	CYC	C1B-C2B	2.37	1.49	1.45
87	72	605	CLA	CMD-C2D	-2.37	1.45	1.50
87	A2	829	CLA	C1B-C2B	2.37	1.48	1.43
84	F4	1001	CYC	C4B-NB	-2.37	1.33	1.38
82	BI	202	PEB	C4B-NB	-2.37	1.33	1.38
82	h1	201	PEB	CHC-C4C	2.37	1.52	1.49
82	l1	201	PEB	CHC-C4C	2.37	1.52	1.49
82	WP	201	PEB	C1C-NC	-2.37	1.33	1.37
82	m1	202	PEB	C4B-C3B	2.37	1.49	1.45
82	Y9	201	PEB	C1C-C2C	2.37	1.48	1.42
87	A2	849	CLA	MG-ND	-2.37	2.01	2.05
87	2N	305	CLA	MG-NB	-2.37	2.01	2.05
82	FA	203	PEB	C4B-C3B	2.37	1.49	1.45
87	A2	838	CLA	CMB-C2B	-2.37	1.45	1.50
82	DD	203	PEB	CHC-C4C	2.37	1.52	1.49
82	f1	203	PEB	C2A-C1A	-2.37	1.50	1.52
87	IN	102	CLA	MG-NB	-2.37	2.01	2.05
87	B2	812	CLA	MG-NB	-2.37	2.01	2.05
87	c6	605	CLA	MG-NB	-2.37	2.01	2.05
82	tK	201	PEB	C1C-C2C	2.37	1.48	1.42
87	42	602	CLA	MG-NB	-2.37	2.01	2.05
82	1C	202	PEB	CHC-C4C	2.37	1.52	1.49
87	BN	806	CLA	CHC-C1C	2.37	1.43	1.38
82	BP	201	PEB	C4A-NA	-2.37	1.32	1.37
82	B9	202	PEB	C4B-C3B	2.37	1.49	1.45
82	lH	201	PEB	C2A-C1A	-2.37	1.50	1.52
82	fJ	203	PEB	C2A-C1A	-2.37	1.50	1.52
87	22	604	CLA	MG-NB	-2.37	2.01	2.05
87	1N	608	CLA	C1B-C2B	2.37	1.48	1.43
82	L1	1002	PEB	OD-C4D	2.37	1.28	1.23
82	FM	201	PEB	C4A-NA	-2.37	1.32	1.37
82	aE	201	PEB	C4A-NA	-2.37	1.32	1.37
84	BE	1001	CYC	C4C-NC	-2.37	1.32	1.37
87	2N	302	CLA	C3B-C4B	2.37	1.48	1.42
82	gM	201	PEB	C1C-NC	-2.37	1.33	1.37
82	QB	204	PEB	CHC-C4C	2.37	1.52	1.49
82	F7	203	PEB	C4B-C3B	2.37	1.49	1.45
82	aJ	204	PEB	OD-C4D	2.37	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	CL	510	CLA	C1B-NB	-2.37	1.34	1.37
82	cG	202	PEB	C4A-NA	-2.37	1.32	1.37
82	fE	202	PEB	C1C-C2C	2.37	1.48	1.42
87	b6	618	CLA	MG-NB	-2.37	2.01	2.05
82	J7	203	PEB	C2A-C1A	-2.37	1.50	1.52
82	WP	202	PEB	OD-C4D	2.37	1.28	1.23
87	BN	809	CLA	CMC-C2C	-2.37	1.45	1.50
84	D4	1001	CYC	C4B-NB	-2.37	1.33	1.38
82	xF	304	PEB	C1C-C2C	2.37	1.48	1.42
82	fH	201	PEB	C1C-C2C	2.37	1.48	1.42
87	AN	828	CLA	MG-ND	-2.37	2.01	2.05
87	A2	850	CLA	MG-NB	-2.37	2.01	2.05
82	NP	201	PEB	C1C-NC	-2.37	1.33	1.37
82	ZI	401	PEB	CAA-C3A	-2.37	1.49	1.54
87	aL	606	CLA	MG-NB	-2.37	2.01	2.05
82	SF	201	PEB	C2A-C1A	-2.37	1.50	1.52
82	XF	202	PEB	C2A-C1A	-2.37	1.50	1.52
82	II	203	PEB	C2A-C1A	-2.37	1.50	1.52
87	BN	831	CLA	C3B-C4B	2.37	1.48	1.42
87	MN	101	CLA	C1B-C2B	2.37	1.48	1.43
82	GM	202	PEB	C1C-C2C	2.37	1.48	1.42
87	CL	508	CLA	MG-NB	-2.37	2.01	2.05
82	FK	201	PEB	C1C-C2C	2.37	1.48	1.42
82	jE	201	PEB	C1C-C2C	2.37	1.48	1.42
82	dM	201	PEB	C1C-C2C	2.37	1.48	1.42
82	H7	201	PEB	CHC-C4C	2.37	1.52	1.49
82	HQ	202	PEB	C4A-NA	-2.37	1.32	1.37
84	NE	201	CYC	C1B-NB	-2.37	1.33	1.37
87	12	606	CLA	C1B-C2B	2.37	1.48	1.43
87	A2	850	CLA	C1B-C2B	2.37	1.48	1.43
87	2N	308	CLA	C1B-C2B	2.37	1.48	1.43
82	xK	303	PEB	C1C-C2C	2.37	1.48	1.42
87	42	607	CLA	MG-NB	-2.37	2.01	2.05
82	l4	201	PEB	C4A-NA	-2.37	1.32	1.37
82	VE	201	PEB	C4B-C3B	2.37	1.49	1.45
82	W9	201	PEB	C1C-NC	-2.37	1.33	1.37
84	GE	1001	CYC	C1B-NB	-2.37	1.33	1.37
82	YI	201	PEB	C4A-NA	-2.37	1.32	1.37
82	h4	201	PEB	C4A-NA	-2.37	1.32	1.37
82	YI	201	PEB	C1C-C2C	2.37	1.48	1.42
82	EP	203	PEB	C2A-C1A	-2.36	1.50	1.52
87	D6	405	CLA	MG-NB	-2.36	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	d6	406	CLA	MG-NB	-2.36	2.01	2.05
82	RB	201	PEB	C1C-NC	-2.36	1.33	1.37
84	CO	1001	CYC	C1B-NB	-2.36	1.33	1.37
82	CQ	202	PEB	C1C-C2C	2.36	1.48	1.42
82	RO	201	PEB	C4A-NA	-2.36	1.32	1.37
87	CL	512	CLA	C3B-C4B	2.36	1.48	1.42
87	5N	611	CLA	C1B-C2B	2.36	1.48	1.43
87	A2	805	CLA	CMC-C2C	-2.36	1.45	1.50
87	BN	835	CLA	C3B-C4B	2.36	1.48	1.42
84	KO	1001	CYC	C4C-NC	-2.36	1.32	1.37
82	ZK	201	PEB	C2A-C1A	-2.36	1.50	1.52
96	vL	201	HEM	C1D-ND	-2.36	1.33	1.38
82	hG	201	PEB	CHC-C4C	2.36	1.52	1.49
82	KF	203	PEB	C4A-NA	-2.36	1.32	1.37
82	JD	203	PEB	C1C-C2C	2.36	1.48	1.42
87	4N	607	CLA	MG-NB	-2.36	2.01	2.05
82	IK	201	PEB	CHB-C4B	2.36	1.43	1.38
87	7N	607	CLA	CMB-C2B	-2.36	1.45	1.50
82	zC	202	PEB	C1C-NC	-2.36	1.33	1.37
82	nK	201	PEB	C1C-C2C	2.36	1.48	1.42
82	FD	203	PEB	CHC-C4C	2.36	1.52	1.49
87	F2	201	CLA	MG-ND	-2.36	2.01	2.05
87	K6	101	CLA	MG-NB	-2.36	2.01	2.05
82	b1	201	PEB	C1D-ND	2.36	1.49	1.45
82	b1	203	PEB	C2A-C1A	-2.36	1.50	1.52
87	BN	802	CLA	CMC-C2C	-2.36	1.45	1.50
82	lK	203	PEB	C4B-C3B	2.36	1.49	1.45
84	GE	1001	CYC	OB-C4B	2.36	1.28	1.23
82	iG	201	PEB	C1C-C2C	2.36	1.48	1.42
82	rK	201	PEB	C1C-C2C	2.36	1.48	1.42
82	UB	302	PEB	C1C-NC	-2.36	1.33	1.37
82	MQ	201	PEB	C1C-NC	-2.36	1.33	1.37
82	L7	202	PEB	C1A-NA	-2.36	1.34	1.37
87	FN	205	CLA	C1B-C2B	2.36	1.48	1.43
87	B2	814	CLA	CMD-C2D	-2.36	1.45	1.50
87	B2	834	CLA	CMB-C2B	-2.36	1.45	1.50
82	S9	202	PEB	C1C-C2C	2.36	1.48	1.42
87	A2	852	CLA	C4D-ND	-2.36	1.34	1.37
82	iM	201	PEB	CHC-C4C	2.36	1.52	1.49
82	X7	201	PEB	OD-C4D	2.36	1.28	1.23
82	NP	201	PEB	C2A-C1A	-2.36	1.50	1.52
82	k1	201	PEB	C1C-C2C	2.36	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	aL	606	CLA	C1B-C2B	2.36	1.48	1.43
82	VA	202	PEB	C1A-NA	-2.36	1.34	1.37
82	oK	203	PEB	C1C-C2C	2.36	1.48	1.42
84	M1	201	CYC	C1B-C2B	2.36	1.49	1.45
82	HP	201	PEB	C4A-NA	-2.36	1.32	1.37
87	bL	607	CLA	C1B-NB	-2.36	1.34	1.37
87	dL	404	CLA	C1B-C2B	2.36	1.48	1.43
82	HK	201	PEB	C2A-C1A	-2.36	1.50	1.52
82	UK	201	PEB	OD-C4D	2.36	1.28	1.23
87	A2	837	CLA	MG-ND	-2.36	2.01	2.05
87	A2	828	CLA	CMC-C2C	-2.36	1.45	1.50
87	5N	605	CLA	CMD-C2D	-2.36	1.45	1.50
87	4N	607	CLA	C1B-C2B	2.36	1.48	1.43
82	HG	1002	PEB	OD-C4D	2.36	1.28	1.23
82	MB	202	PEB	C1B-C2B	2.36	1.50	1.45
82	II	203	PEB	C4A-NA	-2.36	1.32	1.37
82	hE	201	PEB	CHC-C4C	2.36	1.52	1.49
82	VB	201	PEB	C1C-NC	-2.36	1.33	1.37
82	GD	201	PEB	C1C-NC	-2.36	1.33	1.37
82	XA	201	PEB	OD-C4D	2.36	1.28	1.23
82	OI	201	PEB	C2A-C1A	-2.36	1.50	1.52
82	NP	201	PEB	C4A-NA	-2.36	1.32	1.37
83	YA	302	PUB	C4C-NC	2.36	1.39	1.35
82	Z1	202	PEB	C4A-NA	-2.36	1.32	1.37
82	JF	202	PEB	CHC-C4C	2.36	1.52	1.49
87	A6	403	CLA	MG-NB	-2.36	2.01	2.05
87	c6	607	CLA	MG-NB	-2.36	2.01	2.05
87	BN	801	CLA	CHC-C1C	2.36	1.43	1.38
82	SM	202	PEB	C2A-C1A	-2.36	1.50	1.52
82	T9	201	PEB	C1C-NC	-2.36	1.33	1.37
82	JA	202	PEB	C4B-C3B	2.36	1.49	1.45
82	hF	202	PEB	C4B-C3B	2.36	1.49	1.45
87	KN	105	CLA	C1B-C2B	2.36	1.48	1.43
87	12	608	CLA	C1B-C2B	2.36	1.48	1.43
87	3N	307	CLA	C1B-C2B	2.36	1.48	1.43
82	cK	203	PEB	C1C-C2C	2.36	1.48	1.42
82	KF	202	PEB	OD-C4D	2.36	1.28	1.23
82	KJ	201	PEB	OD-C4D	2.36	1.28	1.23
82	q8	201	PEB	C4B-C3B	2.36	1.49	1.45
87	AN	829	CLA	CMD-C2D	-2.36	1.45	1.50
87	1N	608	CLA	MG-NB	-2.36	2.01	2.05
84	H4	1001	CYC	C4C-NC	-2.36	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gG	201	PEB	C2A-C1A	-2.36	1.50	1.52
82	V7	202	PEB	C1C-C2C	2.36	1.48	1.42
83	AM	303	PUB	C3C-C4C	2.36	1.51	1.43
87	BN	823	CLA	MG-ND	-2.36	2.01	2.05
82	JB	202	PEB	C4A-NA	-2.36	1.32	1.37
82	qF	203	PEB	C1D-ND	2.36	1.49	1.45
82	X9	201	PEB	C1C-NC	-2.36	1.33	1.37
82	V1	202	PEB	C4B-C3B	2.36	1.49	1.45
82	KK	203	PEB	C4A-NA	-2.36	1.32	1.37
82	O1	203	PEB	C4A-NA	-2.36	1.32	1.37
84	J1	1001	CYC	C4C-NC	-2.36	1.32	1.37
87	A2	830	CLA	CMD-C2D	-2.36	1.45	1.50
82	iM	202	PEB	C2A-C1A	-2.36	1.50	1.52
87	5N	608	CLA	C1B-C2B	2.36	1.48	1.43
82	IB	203	PEB	C4A-NA	-2.36	1.32	1.37
82	AA	202	PEB	C1C-C2C	2.36	1.48	1.42
82	AD	304	PEB	C1C-C2C	2.36	1.48	1.42
87	A2	849	CLA	C1D-ND	2.36	1.40	1.37
87	BN	811	CLA	CMD-C2D	-2.36	1.45	1.50
87	B2	814	CLA	CMC-C2C	-2.36	1.45	1.50
82	B5	203	PEB	C4A-NA	-2.36	1.32	1.37
87	52	608	CLA	MG-NB	-2.36	2.01	2.05
87	A6	402	CLA	MG-NB	-2.36	2.01	2.05
82	OP	201	PEB	C1C-NC	-2.36	1.33	1.37
82	Y9	201	PEB	C1C-NC	-2.36	1.33	1.37
82	j1	203	PEB	CHC-C4C	2.36	1.52	1.49
82	GD	201	PEB	C4B-C3B	2.35	1.49	1.45
84	LH	1002	CYC	CBA-CGA	2.35	1.56	1.50
87	A2	832	CLA	C1B-C2B	2.35	1.48	1.43
87	R2	204	CLA	C1B-C2B	2.35	1.48	1.43
82	f4	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	hG	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	UH	202	PEB	C4A-NA	-2.35	1.32	1.37
82	eB	202	PEB	C4A-NA	-2.35	1.32	1.37
87	3N	310	CLA	MG-ND	-2.35	2.01	2.05
82	KI	201	PEB	C4B-NB	-2.35	1.33	1.38
87	AN	834	CLA	CMB-C2B	-2.35	1.45	1.50
84	HH	1001	CYC	C4B-NB	-2.35	1.33	1.38
82	RI	203	PEB	CHA-C1B	2.35	1.45	1.40
82	JJ	201	PEB	C4A-NA	-2.35	1.32	1.37
82	LJ	201	PEB	C4A-NA	-2.35	1.32	1.37
87	B2	817	CLA	MG-NB	-2.35	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	801	CLA	CMC-C2C	-2.35	1.45	1.50
87	bL	605	CLA	C1B-C2B	2.35	1.48	1.43
82	bF	202	PEB	C1C-NC	-2.35	1.33	1.37
82	R7	202	PEB	C2A-C1A	-2.35	1.50	1.52
87	cL	508	CLA	CAC-C3C	-2.35	1.45	1.51
87	dL	401	CLA	C1B-C2B	2.35	1.48	1.43
87	5N	602	CLA	C1B-C2B	2.35	1.48	1.43
83	A4	302	PUB	C4B-C3B	2.35	1.48	1.42
82	P9	201	PEB	C1C-NC	-2.35	1.33	1.37
82	jH	202	PEB	C1D-ND	2.35	1.49	1.45
82	aK	203	PEB	C1B-C2B	2.35	1.50	1.45
87	12	608	CLA	MG-NB	-2.35	2.01	2.05
87	4N	606	CLA	MG-NB	-2.35	2.01	2.05
87	cL	512	CLA	CMC-C2C	-2.35	1.45	1.50
82	gG	201	PEB	C1C-C2C	2.35	1.48	1.42
82	JD	203	PEB	C1D-ND	2.35	1.49	1.45
82	JQ	203	PEB	C1D-ND	2.35	1.49	1.45
87	BN	815	CLA	CMD-C2D	-2.35	1.45	1.50
82	e1	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	lO	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	AP	203	PEB	OD-C4D	2.35	1.28	1.23
87	B2	808	CLA	C1B-NB	-2.35	1.34	1.37
87	2N	308	CLA	MG-NB	-2.35	2.01	2.05
84	KG	202	CYC	C1B-NB	-2.35	1.33	1.37
82	LE	1002	PEB	OD-C4D	2.35	1.28	1.23
82	tK	202	PEB	C4B-C3B	2.35	1.49	1.45
82	S9	201	PEB	CHC-C4C	2.35	1.52	1.49
82	eK	202	PEB	C4A-NA	-2.35	1.32	1.37
82	RP	202	PEB	C2A-C1A	-2.35	1.50	1.52
87	bL	619	CLA	MG-NB	-2.35	2.01	2.05
87	C6	514	CLA	C1B-C2B	2.35	1.48	1.43
84	NH	1001	CYC	C4C-NC	-2.35	1.32	1.37
84	D4	1001	CYC	C4C-NC	-2.35	1.32	1.37
87	B2	827	CLA	C3B-C4B	2.35	1.48	1.42
87	AN	817	CLA	CMD-C2D	-2.35	1.45	1.50
87	AL	403	CLA	MG-ND	-2.35	2.01	2.05
82	l4	202	PEB	C1D-ND	2.35	1.49	1.45
87	A6	404	CLA	C1B-C2B	2.35	1.48	1.43
87	B6	612	CLA	C1B-C2B	2.35	1.48	1.43
82	YM	201	PEB	C4A-NA	-2.35	1.32	1.37
82	VO	202	PEB	C4A-NA	-2.35	1.32	1.37
82	rK	202	PEB	C1C-NC	-2.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	615	CLA	CMD-C2D	-2.35	1.45	1.50
82	AH	302	PEB	C1C-C2C	2.35	1.48	1.42
82	c4	202	PEB	C1C-C2C	2.35	1.48	1.42
82	cO	202	PEB	C1C-C2C	2.35	1.48	1.42
82	lO	202	PEB	C1D-ND	2.35	1.49	1.45
87	BL	620	CLA	C1B-NB	-2.35	1.34	1.37
87	b6	610	CLA	C1B-C2B	2.35	1.48	1.43
87	bL	606	CLA	C1B-C2B	2.35	1.48	1.43
82	dD	401	PEB	C4A-NA	-2.35	1.32	1.37
87	BN	810	CLA	CMD-C2D	-2.35	1.45	1.50
82	cO	203	PEB	C4B-C3B	2.35	1.49	1.45
82	uF	202	PEB	C1D-ND	2.35	1.49	1.45
82	NA	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	QD	202	PEB	C2A-C1A	-2.35	1.50	1.52
87	A6	404	CLA	MG-NB	-2.35	2.01	2.05
82	JJ	202	PEB	C4A-NA	-2.35	1.32	1.37
82	OJ	201	PEB	C4A-NA	-2.35	1.32	1.37
84	LH	1002	CYC	C4A-C3A	2.35	1.50	1.45
87	BN	827	CLA	C1B-NB	-2.35	1.34	1.37
87	bL	618	CLA	C1B-NB	-2.35	1.34	1.37
82	zC	202	PEB	C1C-C2C	2.35	1.48	1.42
82	jM	203	PEB	C4B-C3B	2.35	1.49	1.45
87	12	610	CLA	MG-NB	-2.35	2.01	2.05
87	B2	824	CLA	MG-ND	-2.35	2.01	2.05
82	Z9	304	PEB	C1D-ND	2.35	1.49	1.45
82	WE	203	PEB	C4A-NA	-2.35	1.32	1.37
82	WG	203	PEB	C4A-NA	-2.35	1.32	1.37
82	PQ	202	PEB	C4A-NA	-2.35	1.32	1.37
82	WD	201	PEB	C1C-NC	-2.35	1.33	1.37
84	63	901	CYC	C4D-C3D	2.35	1.48	1.42
87	A2	828	CLA	MG-ND	-2.35	2.01	2.05
87	1N	604	CLA	MG-NB	-2.35	2.01	2.05
82	KG	201	PEB	C4A-NA	-2.35	1.32	1.37
87	C6	510	CLA	C1B-C2B	2.35	1.48	1.43
87	cL	505	CLA	C1B-C2B	2.35	1.48	1.43
82	LO	1002	PEB	C1C-NC	-2.35	1.33	1.37
82	G9	201	PEB	C1C-NC	-2.35	1.33	1.37
84	FO	1001	CYC	C4B-NB	-2.35	1.33	1.38
82	lM	201	PEB	C1C-C2C	2.35	1.48	1.42
87	BN	815	CLA	CMC-C2C	-2.35	1.45	1.50
82	dK	202	PEB	CHC-C4C	2.35	1.52	1.49
87	BN	809	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	dL	406	PL9	C2-C1	-2.35	1.38	1.44
82	eF	202	PEB	C4A-NA	-2.35	1.32	1.37
87	22	607	CLA	MG-NB	-2.35	2.01	2.05
82	J9	201	PEB	C1C-C2C	2.35	1.48	1.42
87	RN	201	CLA	CMB-C2B	-2.35	1.45	1.50
87	52	605	CLA	CMD-C2D	-2.35	1.45	1.50
82	IA	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	l1	203	PEB	C2A-C1A	-2.35	1.50	1.52
82	RA	202	PEB	C4B-C3B	2.35	1.49	1.45
84	DE	1001	CYC	OB-C4B	2.35	1.28	1.23
84	DG	1001	CYC	OB-C4B	2.35	1.28	1.23
82	YD	202	PEB	C1C-C2C	2.35	1.48	1.42
87	32	308	CLA	MG-NB	-2.35	2.01	2.05
87	A2	851	CLA	MG-NB	-2.35	2.01	2.05
87	AN	802	CLA	CMC-C2C	-2.35	1.45	1.50
87	dL	401	CLA	CMD-C2D	-2.35	1.45	1.50
82	tK	203	PEB	C1C-C2C	2.35	1.48	1.42
82	cF	203	PEB	C4A-NA	-2.35	1.32	1.37
84	NO	1001	CYC	C4C-NC	-2.35	1.32	1.37
82	OI	202	PEB	CHA-C1B	2.35	1.45	1.40
82	K7	202	PEB	C1D-ND	2.35	1.49	1.45
87	22	608	CLA	C1B-C2B	2.35	1.48	1.43
87	6N	602	CLA	CHC-C1C	2.35	1.43	1.38
82	BA	201	PEB	C2A-C1A	-2.35	1.50	1.52
82	CP	203	PEB	C2A-C1A	-2.35	1.50	1.52
82	G9	202	PEB	C2A-C1A	-2.35	1.50	1.52
82	bK	201	PEB	C2A-C1A	-2.35	1.50	1.52
82	jM	201	PEB	C2A-C1A	-2.35	1.50	1.52
82	HF	201	PEB	OD-C4D	2.35	1.28	1.23
87	22	608	CLA	MG-NB	-2.35	2.01	2.05
82	lK	203	PEB	C4B-NB	-2.35	1.33	1.38
84	E4	1001	CYC	C1B-NB	-2.35	1.33	1.37
87	HL	101	CLA	CMB-C2B	-2.35	1.45	1.50
87	2N	309	CLA	CMB-C2B	-2.35	1.45	1.50
82	LJ	202	PEB	C1C-C2C	2.35	1.48	1.42
82	x8	201	PEB	C1C-C2C	2.35	1.48	1.42
82	OB	201	PEB	C4A-NA	-2.35	1.32	1.37
82	VG	202	PEB	C4A-NA	-2.35	1.32	1.37
82	W1	203	PEB	C4A-NA	-2.35	1.32	1.37
87	AN	801	CLA	MG-NB	-2.35	2.01	2.05
87	BN	817	CLA	CMB-C2B	-2.35	1.45	1.50
82	A9	201	PEB	C1C-NC	-2.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	vC	201	PEB	C4B-C3B	2.34	1.49	1.45
82	R7	203	PEB	C4A-NA	-2.34	1.32	1.37
87	A2	838	CLA	C1B-C2B	2.34	1.48	1.43
87	F2	205	CLA	C1B-C2B	2.34	1.48	1.43
82	U7	201	PEB	C4B-NB	-2.34	1.33	1.38
82	oK	203	PEB	C1D-ND	2.34	1.49	1.45
82	Y5	203	PEB	C1C-NC	-2.34	1.33	1.37
82	HM	202	PEB	C4A-NA	-2.34	1.32	1.37
82	fK	202	PEB	C4B-C3B	2.34	1.49	1.45
87	BL	619	CLA	C1B-C2B	2.34	1.48	1.43
87	AN	805	CLA	CMC-C2C	-2.34	1.45	1.50
87	RN	202	CLA	CMB-C2B	-2.34	1.45	1.50
87	B2	824	CLA	CMC-C2C	-2.34	1.45	1.50
87	BN	827	CLA	C3B-C4B	2.34	1.48	1.42
82	TI	201	PEB	C1D-ND	2.34	1.49	1.45
82	AA	201	PEB	C4A-NA	-2.34	1.32	1.37
87	M2	101	CLA	C1B-C2B	2.34	1.48	1.43
82	HK	202	PEB	C1C-NC	-2.34	1.33	1.37
82	uF	201	PEB	C4B-C3B	2.34	1.49	1.45
87	RN	203	CLA	MG-NB	-2.34	2.01	2.05
82	gK	203	PEB	C4A-NA	-2.34	1.32	1.37
84	GG	1001	CYC	C4C-NC	-2.34	1.32	1.37
82	C9	201	PEB	C1C-NC	-2.34	1.33	1.37
87	BN	825	CLA	CMC-C2C	-2.34	1.45	1.50
87	c6	613	CLA	C1B-C2B	2.34	1.48	1.43
82	WI	202	PEB	C4A-NA	-2.34	1.32	1.37
85	C6	507	BCR	C30-C25	-2.34	1.50	1.53
82	YP	502	PEB	C1C-NC	-2.34	1.33	1.37
87	bL	618	CLA	C4B-NB	2.34	1.40	1.37
82	FI	201	PEB	OD-C4D	2.34	1.28	1.23
82	iO	203	PEB	C1C-C2C	2.34	1.48	1.42
87	2N	312	CLA	C3C-C2C	2.34	1.41	1.36
87	A2	841	CLA	CMD-C2D	-2.34	1.45	1.50
87	bL	605	CLA	CMD-C2D	-2.34	1.45	1.50
87	bL	620	CLA	CMD-C2D	-2.34	1.45	1.50
87	CL	509	CLA	MG-ND	-2.34	2.01	2.05
87	R2	203	CLA	MG-NB	-2.34	2.01	2.05
82	rF	201	PEB	C1C-C2C	2.34	1.48	1.42
82	NB	202	PEB	C4A-NA	-2.34	1.32	1.37
87	bL	618	CLA	C1D-ND	2.34	1.40	1.37
87	CL	511	CLA	MG-ND	-2.34	2.01	2.05
87	C6	509	CLA	MG-NB	-2.34	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UH	201	PEB	C1C-C2C	2.34	1.48	1.42
82	II	203	PEB	CHA-C1B	2.34	1.45	1.40
82	PD	203	PEB	C4A-NA	-2.34	1.32	1.37
82	pC	202	PEB	OD-C4D	2.34	1.28	1.23
82	VK	202	PEB	C1C-NC	-2.34	1.33	1.37
82	CP	202	PEB	C1C-NC	-2.34	1.33	1.37
82	a1	202	PEB	CHC-C4C	2.34	1.52	1.49
87	AN	811	CLA	CMD-C2D	-2.34	1.45	1.50
82	HB	202	PEB	C4A-NA	-2.34	1.32	1.37
87	A2	816	CLA	C1B-C2B	2.34	1.48	1.43
82	WJ	202	PEB	C1C-NC	-2.34	1.33	1.37
87	BN	808	CLA	MG-NB	-2.34	2.01	2.05
82	IB	201	PEB	C4A-NA	-2.34	1.32	1.37
82	CQ	201	PEB	C4A-NA	-2.34	1.32	1.37
87	MN	101	CLA	CMC-C2C	-2.34	1.45	1.50
82	VA	202	PEB	C1C-C2C	2.34	1.48	1.42
82	dE	203	PEB	C2A-C1A	-2.34	1.50	1.52
87	I2	102	CLA	MG-NB	-2.34	2.01	2.05
82	eE	201	PEB	C4A-NA	-2.34	1.32	1.37
87	52	608	CLA	C1B-C2B	2.34	1.48	1.43
87	B2	810	CLA	C1B-C2B	2.34	1.48	1.43
87	42	606	CLA	CMD-C2D	-2.34	1.45	1.50
87	A2	816	CLA	CMD-C2D	-2.34	1.45	1.50
87	4N	606	CLA	CMD-C2D	-2.34	1.45	1.50
82	v8	201	PEB	C4B-C3B	2.34	1.49	1.45
82	WM	201	PEB	OD-C4D	2.34	1.28	1.23
82	QF	203	PEB	C2C-C3C	2.34	1.45	1.38
82	dB	202	PEB	C1C-NC	-2.34	1.33	1.37
87	I2	102	CLA	C1B-C2B	2.34	1.48	1.43
82	CM	203	PEB	C4A-NA	-2.34	1.32	1.37
87	B2	805	CLA	CHC-C1C	2.34	1.43	1.38
82	VE	201	PEB	C1C-C2C	2.34	1.48	1.42
82	LD	201	PEB	C4B-C3B	2.34	1.49	1.45
87	IN	102	CLA	C1B-C2B	2.34	1.48	1.43
82	KA	202	PEB	C2A-C1A	-2.34	1.50	1.52
82	SA	202	PEB	C2A-C1A	-2.34	1.50	1.52
87	AN	850	CLA	MG-NB	-2.34	2.01	2.05
87	b6	614	CLA	MG-NB	-2.34	2.01	2.05
82	GF	203	PEB	C1C-NC	-2.34	1.33	1.37
84	FE	1001	CYC	C1B-NB	-2.34	1.33	1.37
87	A2	849	CLA	CHC-C1C	2.34	1.43	1.38
82	YK	203	PEB	CHC-C4C	2.34	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jH	203	PEB	CHC-C4C	2.34	1.52	1.49
82	wK	302	PEB	C4A-NA	-2.34	1.32	1.37
82	U9	203	PEB	C1C-C2C	2.34	1.48	1.42
87	A2	829	CLA	MG-NB	-2.34	2.01	2.05
87	4N	608	CLA	C3B-C4B	2.34	1.48	1.42
82	EJ	201	PEB	C4A-NA	-2.34	1.32	1.37
84	HO	1001	CYC	C4C-NC	-2.34	1.32	1.37
87	AN	830	CLA	CMD-C2D	-2.34	1.45	1.50
82	EA	201	PEB	CHC-C4C	2.34	1.52	1.49
82	XB	201	PEB	C4A-NA	-2.34	1.32	1.37
82	KK	202	PEB	C4A-NA	-2.34	1.32	1.37
87	82	306	CLA	CMD-C2D	-2.34	1.45	1.50
87	A2	831	CLA	CMC-C2C	-2.34	1.45	1.50
82	Q1	202	PEB	C1B-C2B	2.34	1.50	1.45
82	YF	203	PEB	C1C-C2C	2.34	1.48	1.42
82	W9	203	PEB	C1C-C2C	2.34	1.48	1.42
82	uC	202	PEB	C1C-C2C	2.34	1.48	1.42
82	AA	202	PEB	C1D-ND	2.34	1.49	1.45
82	RP	201	PEB	C4A-NA	-2.34	1.32	1.37
82	R4	202	PEB	C4A-NA	-2.34	1.32	1.37
87	DL	403	CLA	CMD-C2D	-2.34	1.45	1.50
87	A2	817	CLA	CMD-C2D	-2.34	1.45	1.50
87	FN	203	CLA	O2A-CGA	2.34	1.38	1.30
82	mE	203	PEB	C1C-C2C	2.34	1.48	1.42
82	cF	203	PEB	C1C-C2C	2.34	1.48	1.42
82	I7	202	PEB	C2A-C1A	-2.34	1.50	1.52
87	a6	608	CLA	C1B-C2B	2.34	1.48	1.43
87	A2	815	CLA	CMB-C2B	-2.34	1.45	1.50
87	B6	604	CLA	MG-NB	-2.34	2.01	2.05
87	1N	610	CLA	MG-NB	-2.34	2.01	2.05
87	3N	306	CLA	MG-NB	-2.34	2.01	2.05
87	B2	835	CLA	C3B-C4B	2.34	1.48	1.42
82	HQ	202	PEB	OD-C4D	2.34	1.28	1.23
87	BL	601	CLA	MG-NB	-2.34	2.01	2.05
82	kM	201	PEB	C1C-NC	-2.34	1.33	1.37
82	LD	201	PEB	C1C-C2C	2.34	1.48	1.42
82	LQ	201	PEB	C1C-C2C	2.34	1.48	1.42
87	b6	605	CLA	C3B-C4B	2.34	1.48	1.42
87	AN	826	CLA	C1B-C2B	2.34	1.48	1.43
82	RD	202	PEB	C2A-C1A	-2.34	1.50	1.52
82	MK	203	PEB	C2A-C1A	-2.34	1.50	1.52
82	cM	201	PEB	C2A-C1A	-2.34	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B2	816	CLA	CMB-C2B	-2.34	1.45	1.50
84	D1	1001	CYC	C1B-C2B	2.34	1.49	1.45
83	AO	302	PUB	C4B-C3B	2.34	1.48	1.42
87	1N	605	CLA	MG-NB	-2.34	2.01	2.05
82	NA	201	PEB	C1C-NC	-2.34	1.33	1.37
87	b6	607	CLA	C1B-C2B	2.34	1.48	1.43
82	T4	202	PEB	CHC-C4C	2.34	1.52	1.49
87	82	306	CLA	C1B-NB	-2.34	1.34	1.37
87	AN	841	CLA	CMD-C2D	-2.34	1.45	1.50
87	B2	808	CLA	C1B-C2B	2.33	1.48	1.43
82	BM	301	PEB	C4A-NA	-2.33	1.32	1.37
82	gH	201	PEB	C1C-C2C	2.33	1.48	1.42
87	A2	834	CLA	CMB-C2B	-2.33	1.45	1.50
87	C6	519	CLA	MG-NB	-2.33	2.01	2.05
87	22	612	CLA	C3C-C2C	2.33	1.41	1.36
84	HO	1001	CYC	C1B-NB	-2.33	1.33	1.37
87	cL	509	CLA	C1B-C2B	2.33	1.48	1.43
87	L2	204	CLA	MG-ND	-2.33	2.01	2.05
87	A2	819	CLA	CMD-C2D	-2.33	1.45	1.50
87	cL	512	CLA	C1B-NB	-2.33	1.34	1.37
82	UI	201	PEB	C4B-C3B	2.33	1.49	1.45
82	XK	201	PEB	C4B-C3B	2.33	1.49	1.45
87	B2	834	CLA	MG-ND	-2.33	2.01	2.05
82	RQ	202	PEB	C2A-C1A	-2.33	1.50	1.52
82	SJ	202	PEB	C1C-C2C	2.33	1.48	1.42
82	H9	201	PEB	C4A-NA	-2.33	1.32	1.37
87	42	608	CLA	C3B-C4B	2.33	1.48	1.42
87	BN	811	CLA	C1B-C2B	2.33	1.48	1.43
82	DF	203	PEB	C1C-NC	-2.33	1.33	1.37
82	RD	201	PEB	C1C-C2C	2.33	1.48	1.42
82	wC	203	PEB	C1C-C2C	2.33	1.48	1.42
82	hF	201	PEB	C1C-C2C	2.33	1.48	1.42
87	AN	837	CLA	MG-ND	-2.33	2.01	2.05
87	C6	511	CLA	MG-NB	-2.33	2.01	2.05
87	B2	827	CLA	C1B-NB	-2.33	1.34	1.37
82	gJ	202	PEB	C1C-C2C	2.33	1.48	1.42
94	dL	406	PL9	O1-C4	2.33	1.28	1.23
87	KN	103	CLA	MG-NB	-2.33	2.01	2.05
82	NG	201	PEB	C4A-NA	-2.33	1.32	1.37
82	iF	201	PEB	C4A-NA	-2.33	1.32	1.37
82	IP	202	PEB	C2A-C1A	-2.33	1.50	1.52
82	S5	203	PEB	C4A-NA	-2.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PB	201	PEB	C1C-NC	-2.33	1.33	1.37
82	c4	203	PEB	C4B-C3B	2.33	1.49	1.45
87	22	612	CLA	CHC-C1C	2.33	1.43	1.38
87	K2	104	CLA	MG-NB	-2.33	2.01	2.05
87	D6	402	CLA	MG-NB	-2.33	2.01	2.05
82	eM	202	PEB	C4A-NA	-2.33	1.32	1.37
82	OI	201	PEB	C1C-C2C	2.33	1.48	1.42
82	t8	201	PEB	C1C-NC	-2.33	1.33	1.37
82	QP	202	PEB	C2A-C1A	-2.33	1.50	1.52
82	I9	202	PEB	C2A-C1A	-2.33	1.50	1.52
87	a6	607	CLA	C1B-C2B	2.33	1.48	1.43
82	D9	201	PEB	C4B-C3B	2.33	1.49	1.45
82	SP	202	PEB	C4A-NA	-2.33	1.32	1.37
87	A2	816	CLA	MG-NB	-2.33	2.01	2.05
87	bL	617	CLA	MG-ND	-2.33	2.01	2.05
87	BN	809	CLA	CMB-C2B	-2.33	1.45	1.50
87	M2	101	CLA	CMC-C2C	-2.33	1.45	1.50
82	YF	202	PEB	C1C-C2C	2.33	1.48	1.42
87	BN	825	CLA	C1B-C2B	2.33	1.48	1.43
82	AP	202	PEB	C1C-C2C	2.33	1.48	1.42
82	dE	204	PEB	C1C-C2C	2.33	1.48	1.42
87	A2	802	CLA	C1B-C2B	2.33	1.48	1.43
82	v8	202	PEB	C2A-C1A	-2.33	1.50	1.52
82	LK	202	PEB	C4A-NA	-2.33	1.32	1.37
82	QF	202	PEB	C1C-C2C	2.33	1.48	1.42
82	pC	201	PEB	C1C-C2C	2.33	1.48	1.42
87	RN	204	CLA	MG-NB	-2.33	2.01	2.05
82	A9	202	PEB	C1C-C2C	2.33	1.48	1.42
82	xK	304	PEB	C1C-C2C	2.33	1.48	1.42
82	KM	203	PEB	C4A-NA	-2.33	1.32	1.37
82	T1	201	PEB	C4A-NA	-2.33	1.32	1.37
82	gF	203	PEB	C4A-NA	-2.33	1.32	1.37
87	5N	608	CLA	MG-NB	-2.33	2.01	2.05
82	M9	305	PEB	C1D-ND	2.33	1.49	1.45
82	cK	203	PEB	C4A-NA	-2.33	1.32	1.37
87	AN	807	CLA	CMD-C2D	-2.33	1.45	1.50
91	d6	404	PHO	CBD-CGD	-2.33	1.49	1.52
82	TA	202	PEB	C2C-C3C	2.33	1.45	1.38
82	EA	201	PEB	C1C-C2C	2.33	1.48	1.42
82	jM	203	PEB	C1C-C2C	2.33	1.48	1.42
87	AN	830	CLA	C1B-NB	-2.33	1.34	1.37
82	JP	201	PEB	C4A-NA	-2.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	CL	509	CLA	MG-NB	-2.33	2.01	2.05
87	B6	605	CLA	MG-NB	-2.33	2.01	2.05
87	c6	615	CLA	MG-NB	-2.33	2.01	2.05
82	OB	201	PEB	CHC-C4C	2.33	1.52	1.49
82	OD	201	PEB	C1C-C2C	2.33	1.48	1.42
82	gM	202	PEB	C1C-C2C	2.33	1.48	1.42
82	z8	202	PEB	C1C-NC	-2.33	1.33	1.37
87	62	303	CLA	CHC-C1C	2.33	1.43	1.38
87	b6	609	CLA	CMD-C2D	-2.33	1.45	1.50
87	32	307	CLA	O2A-CGA	2.33	1.38	1.30
87	A2	824	CLA	MG-NB	-2.33	2.01	2.05
87	c6	613	CLA	MG-NB	-2.33	2.01	2.05
82	RA	203	PEB	C1C-C2C	2.33	1.48	1.42
82	FF	201	PEB	C1C-C2C	2.33	1.48	1.42
82	w8	203	PEB	C1C-C2C	2.33	1.48	1.42
87	B2	822	CLA	C1B-NB	-2.33	1.34	1.37
82	SH	202	PEB	C2A-C1A	-2.33	1.50	1.52
82	HE	1002	PEB	OD-C4D	2.33	1.28	1.23
82	UB	301	PEB	C4A-NA	-2.33	1.32	1.37
82	PD	202	PEB	C4A-NA	-2.33	1.32	1.37
82	NG	201	PEB	C1C-NC	-2.33	1.33	1.37
82	jO	202	PEB	C1D-ND	2.33	1.49	1.45
87	c6	608	CLA	CMD-C2D	-2.33	1.45	1.50
87	AN	837	CLA	C1B-NB	-2.33	1.34	1.37
87	b6	606	CLA	MG-NB	-2.33	2.01	2.05
82	NB	203	PEB	O1B-CGB	2.33	1.29	1.22
82	NB	203	PEB	C4A-NA	-2.33	1.32	1.37
82	CJ	203	PEB	C4A-NA	-2.33	1.32	1.37
82	JA	203	PEB	C2A-C1A	-2.33	1.50	1.52
82	MF	203	PEB	C2A-C1A	-2.33	1.50	1.52
82	HI	202	PEB	C4B-C3B	2.33	1.49	1.45
87	3N	308	CLA	O2A-CGA	2.33	1.38	1.30
87	A2	802	CLA	MG-NB	-2.33	2.01	2.05
87	B6	611	CLA	C1B-C2B	2.33	1.48	1.43
82	FD	201	PEB	C4A-NA	-2.33	1.32	1.37
82	PK	202	PEB	C4A-NA	-2.33	1.32	1.37
82	sK	202	PEB	C1C-C2C	2.33	1.48	1.42
87	BN	834	CLA	CHC-C1C	2.33	1.43	1.38
84	JH	1001	CYC	C1B-C2B	2.33	1.49	1.45
87	A2	826	CLA	C1B-C2B	2.33	1.48	1.43
84	MG	1001	CYC	C4B-NB	-2.33	1.33	1.38
82	ZJ	201	PEB	CHC-C4C	2.33	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WM	202	PEB	C4A-NA	-2.33	1.32	1.37
82	fF	202	PEB	C4A-NA	-2.33	1.32	1.37
82	SH	203	PEB	C1C-C2C	2.33	1.48	1.42
82	VI	203	PEB	C2A-C1A	-2.33	1.50	1.52
82	Q1	203	PEB	C2A-C1A	-2.33	1.50	1.52
87	CL	503	CLA	C1B-NB	-2.33	1.34	1.37
82	WQ	202	PEB	C4A-NA	-2.33	1.32	1.37
82	ZK	202	PEB	CHC-C4C	2.33	1.52	1.49
82	xC	201	PEB	C1C-C2C	2.32	1.48	1.42
82	VJ	202	PEB	C4A-NA	-2.32	1.32	1.37
82	EQ	202	PEB	C4A-NA	-2.32	1.32	1.37
87	B2	809	CLA	CMB-C2B	-2.32	1.45	1.50
82	AO	305	PEB	C2A-C1A	-2.32	1.50	1.52
82	iO	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	gK	201	PEB	C1B-C2B	2.32	1.50	1.45
87	BN	815	CLA	MG-NB	-2.32	2.01	2.05
82	DJ	202	PEB	C4A-NA	-2.32	1.32	1.37
82	IQ	202	PEB	C4A-NA	-2.32	1.32	1.37
82	LE	1002	PEB	C1C-NC	-2.32	1.33	1.37
82	FO	1002	PEB	C1C-NC	-2.32	1.33	1.37
82	OP	203	PEB	C1C-NC	-2.32	1.33	1.37
87	FN	203	CLA	MG-ND	-2.32	2.01	2.05
87	B2	826	CLA	MG-ND	-2.32	2.01	2.05
87	cL	514	CLA	MG-NB	-2.32	2.01	2.05
82	PA	201	PEB	C4A-NA	-2.32	1.32	1.37
82	aJ	204	PEB	C4A-NA	-2.32	1.32	1.37
87	CL	512	CLA	CMD-C2D	-2.32	1.45	1.50
82	V1	202	PEB	C1C-C2C	2.32	1.48	1.42
82	ZK	201	PEB	C4B-C3B	2.32	1.49	1.45
82	GE	1002	PEB	C1C-NC	-2.32	1.33	1.37
82	GG	1002	PEB	C1C-NC	-2.32	1.33	1.37
82	S5	203	PEB	C1C-NC	-2.32	1.33	1.37
87	12	605	CLA	MG-NB	-2.32	2.01	2.05
82	TM	201	PEB	C4A-NA	-2.32	1.32	1.37
82	TO	202	PEB	CHC-C4C	2.32	1.52	1.49
82	HA	203	PEB	C1C-C2C	2.32	1.48	1.42
82	K9	202	PEB	C1C-C2C	2.32	1.48	1.42
82	OF	201	PEB	OD-C4D	2.32	1.28	1.23
87	A2	837	CLA	C1B-NB	-2.32	1.34	1.37
87	BN	818	CLA	MG-NB	-2.32	2.01	2.05
87	B6	613	CLA	MG-NB	-2.32	2.01	2.05
87	CL	510	CLA	CMD-C2D	-2.32	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	613	CLA	CMC-C2C	-2.32	1.45	1.50
82	LQ	202	PEB	C1B-C2B	2.32	1.50	1.45
82	WF	203	PEB	C4B-C3B	2.32	1.49	1.45
82	AA	201	PEB	C2A-C1A	-2.32	1.50	1.52
82	ZB	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	K9	202	PEB	C2A-C1A	-2.32	1.50	1.52
87	AN	838	CLA	C1B-C2B	2.32	1.48	1.43
87	b6	614	CLA	C1B-C2B	2.32	1.48	1.43
87	A2	850	CLA	CMD-C2D	-2.32	1.45	1.50
87	AN	824	CLA	MG-NB	-2.32	2.01	2.05
96	vL	201	HEM	C4B-NB	-2.32	1.34	1.38
87	BN	827	CLA	CMC-C2C	-2.32	1.45	1.50
82	W9	201	PEB	OD-C4D	2.32	1.28	1.23
87	AN	829	CLA	MG-NB	-2.32	2.01	2.05
87	BL	621	CLA	C3B-C4B	2.32	1.48	1.42
82	A4	305	PEB	C2A-C1A	-2.32	1.50	1.52
82	u8	202	PEB	C2A-C1A	-2.32	1.50	1.52
82	B9	201	PEB	C2A-C1A	-2.32	1.50	1.52
82	dE	204	PEB	C2A-C1A	-2.32	1.50	1.52
82	cK	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	MD	202	PEB	C1C-C2C	2.32	1.48	1.42
82	F1	1002	PEB	C4A-NA	-2.32	1.32	1.37
82	uC	203	PEB	C4B-C3B	2.32	1.49	1.45
87	LN	204	CLA	MG-ND	-2.32	2.01	2.05
82	VM	202	PEB	C1C-C2C	2.32	1.48	1.42
87	A2	826	CLA	C1B-NB	-2.32	1.34	1.37
82	EP	201	PEB	C1C-NC	-2.32	1.33	1.37
82	QP	202	PEB	C1C-NC	-2.32	1.33	1.37
84	N1	1001	CYC	C1B-NB	-2.32	1.33	1.37
87	BN	835	CLA	C1B-C2B	2.32	1.48	1.43
82	QB	202	PEB	C1C-C2C	2.32	1.48	1.42
82	SE	202	PEB	C1C-C2C	2.32	1.48	1.42
82	MA	201	PEB	C4A-NA	-2.32	1.32	1.37
87	bL	605	CLA	CMC-C2C	-2.32	1.45	1.50
82	cJ	201	PEB	C2A-C1A	-2.32	1.50	1.52
82	qK	203	PEB	C1D-ND	2.32	1.49	1.45
87	32	305	CLA	MG-NB	-2.32	2.01	2.05
82	AQ	301	PEB	C1C-NC	-2.32	1.33	1.37
87	AN	816	CLA	CMD-C2D	-2.32	1.45	1.50
87	bL	613	CLA	CMD-C2D	-2.32	1.45	1.50
82	DD	202	PEB	C1B-C2B	2.32	1.50	1.45
82	J5	203	PEB	C1C-NC	-2.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gH	201	PEB	C1C-NC	-2.32	1.33	1.37
84	L1	1001	CYC	C4C-NC	-2.32	1.32	1.37
82	OM	202	PEB	C4B-C3B	2.32	1.49	1.45
87	42	601	CLA	MG-NB	-2.32	2.01	2.05
82	mO	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	DJ	201	PEB	C4A-NA	-2.32	1.32	1.37
82	hO	201	PEB	C4A-NA	-2.32	1.32	1.37
87	CL	505	CLA	CMD-C2D	-2.32	1.45	1.50
82	OK	203	PEB	C1C-NC	-2.32	1.33	1.37
82	VQ	203	PEB	C4B-NB	-2.32	1.33	1.38
87	dL	409	CLA	C1B-C2B	2.32	1.48	1.43
82	U5	201	PEB	C1D-ND	2.32	1.49	1.45
87	BN	825	CLA	MG-ND	-2.32	2.01	2.05
82	u8	203	PEB	C4B-C3B	2.32	1.49	1.45
82	D9	202	PEB	C4B-C3B	2.32	1.49	1.45
82	UI	201	PEB	OD-C4D	2.32	1.28	1.23
82	LD	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	WH	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	IJ	203	PEB	C2A-C1A	-2.32	1.50	1.52
82	NA	203	PEB	C4A-NA	-2.32	1.32	1.37
82	W1	202	PEB	C1C-C2C	2.32	1.48	1.42
82	s8	202	PEB	C1C-C2C	2.32	1.48	1.42
87	bL	618	CLA	C1B-C2B	2.32	1.48	1.43
87	42	601	CLA	C3B-C4B	2.32	1.48	1.42
82	O4	202	PEB	C1C-C2C	2.32	1.48	1.42
82	JK	201	PEB	C4B-C3B	2.32	1.49	1.45
82	RA	201	PEB	C1C-NC	-2.32	1.33	1.37
83	Z5	303	PUB	C4B-NB	-2.32	1.33	1.37
87	DL	406	CLA	MG-NB	-2.32	2.01	2.05
82	YK	202	PEB	C1C-C2C	2.32	1.48	1.42
82	OE	201	PEB	C4A-NA	-2.32	1.32	1.37
82	sF	203	PEB	C4A-NA	-2.32	1.32	1.37
82	dM	202	PEB	C2A-C1A	-2.32	1.50	1.52
82	QH	202	PEB	C1B-C2B	2.32	1.50	1.45
87	4N	602	CLA	MG-NB	-2.32	2.01	2.05
84	E4	1001	CYC	C4B-NB	-2.32	1.33	1.38
87	A2	810	CLA	MG-NB	-2.32	2.01	2.05
87	2N	312	CLA	MG-NB	-2.32	2.01	2.05
87	A2	839	CLA	C1B-C2B	2.32	1.48	1.43
87	F2	201	CLA	C1B-C2B	2.32	1.48	1.43
82	gF	203	PEB	CHC-C4C	2.32	1.52	1.49
87	d6	403	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BL	609	CLA	MG-NB	-2.32	2.01	2.05
82	YE	201	PEB	C4A-NA	-2.32	1.32	1.37
82	UA	202	PEB	C4A-NA	-2.31	1.32	1.37
87	B6	614	CLA	MG-NB	-2.31	2.01	2.05
87	C6	515	CLA	MG-NB	-2.31	2.01	2.05
87	BN	808	CLA	CMD-C2D	-2.31	1.45	1.50
82	mH	201	PEB	C1B-C2B	2.31	1.50	1.45
82	TI	201	PEB	CHA-C1B	2.31	1.45	1.40
87	c6	613	CLA	CMD-C2D	-2.31	1.45	1.50
87	B2	814	CLA	MG-NB	-2.31	2.01	2.05
82	pC	202	PEB	C1C-NC	-2.31	1.33	1.37
84	K4	1001	CYC	C1B-NB	-2.31	1.33	1.37
87	AN	828	CLA	CMC-C2C	-2.31	1.45	1.50
87	A2	808	CLA	MG-NB	-2.31	2.01	2.05
82	R9	202	PEB	C1C-C2C	2.31	1.48	1.42
87	bL	608	CLA	C1B-C2B	2.31	1.48	1.43
87	b6	618	CLA	CMD-C2D	-2.31	1.45	1.50
82	BK	202	PEB	C1C-NC	-2.31	1.33	1.37
82	EP	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	KP	202	PEB	OD-C4D	2.31	1.28	1.23
82	WH	203	PEB	CHC-C4C	2.31	1.52	1.49
82	XQ	202	PEB	CHC-C4C	2.31	1.52	1.49
87	22	612	CLA	MG-NB	-2.31	2.01	2.05
87	B6	612	CLA	MG-NB	-2.31	2.01	2.05
87	3N	309	CLA	MG-NB	-2.31	2.01	2.05
82	ZF	202	PEB	C1C-NC	-2.31	1.33	1.37
82	sF	202	PEB	C1C-C2C	2.31	1.48	1.42
82	dG	204	PEB	C1C-C2C	2.31	1.48	1.42
82	C7	201	PEB	C4A-NA	-2.31	1.32	1.37
87	A2	801	CLA	CMC-C2C	-2.31	1.45	1.50
87	dL	409	CLA	CMD-C2D	-2.31	1.45	1.50
82	nK	202	PEB	C1C-C2C	2.31	1.48	1.42
82	P9	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	RI	203	PEB	C4A-NA	-2.31	1.32	1.37
82	FM	202	PEB	C4A-NA	-2.31	1.32	1.37
87	A2	807	CLA	CMD-C2D	-2.31	1.45	1.50
87	B2	806	CLA	CMD-C2D	-2.31	1.45	1.50
82	lK	203	PEB	C1D-ND	2.31	1.49	1.45
87	A2	852	CLA	CHC-C4B	-2.31	1.34	1.39
96	VL	201	HEM	C4B-NB	-2.31	1.34	1.38
82	JF	201	PEB	C1C-C2C	2.31	1.48	1.42
82	J5	203	PEB	C4A-NA	-2.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	832	CLA	CMD-C2D	-2.31	1.45	1.50
82	IQ	202	PEB	C1C-NC	-2.31	1.33	1.37
84	L1	1001	CYC	CBA-CGA	2.31	1.56	1.50
82	G9	202	PEB	C1C-C2C	2.31	1.48	1.42
82	JO	1002	PEB	C4A-NA	-2.31	1.32	1.37
82	XP	201	PEB	C4A-NA	-2.31	1.32	1.37
82	O4	201	PEB	C4A-NA	-2.31	1.32	1.37
82	e4	202	PEB	C4A-NA	-2.31	1.32	1.37
84	JH	1001	CYC	C4C-NC	-2.31	1.32	1.37
87	B2	808	CLA	CMC-C2C	-2.31	1.45	1.50
82	CK	203	PEB	C2A-C1A	-2.31	1.50	1.52
82	OO	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	l1	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	eH	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	hJ	203	PEB	C4B-C3B	2.31	1.49	1.45
87	BN	823	CLA	C1B-NB	-2.31	1.34	1.37
82	PQ	203	PEB	C4A-NA	-2.31	1.32	1.37
87	R2	202	CLA	CMB-C2B	-2.31	1.45	1.50
87	bL	621	CLA	CMC-C2C	-2.31	1.45	1.50
82	JD	201	PEB	C1D-ND	2.31	1.49	1.45
82	Q9	201	PEB	C1C-C2C	2.31	1.48	1.42
82	kH	203	PEB	CHC-C4C	2.31	1.52	1.49
87	AN	801	CLA	C1B-C2B	2.31	1.48	1.43
87	B2	827	CLA	CMC-C2C	-2.31	1.45	1.50
82	TB	202	PEB	C4A-NA	-2.31	1.32	1.37
82	UF	202	PEB	C4A-NA	-2.31	1.32	1.37
82	eB	201	PEB	C4A-NA	-2.31	1.32	1.37
87	BN	805	CLA	MG-ND	-2.31	2.01	2.05
87	22	609	CLA	CMB-C2B	-2.31	1.45	1.50
84	FE	1002	CYC	C4C-NC	-2.31	1.32	1.37
87	F2	201	CLA	O2A-CGA	2.31	1.38	1.30
82	D9	203	PEB	C1C-C2C	2.31	1.48	1.42
82	Q9	203	PEB	C1C-C2C	2.31	1.48	1.42
87	FN	203	CLA	C1B-C2B	2.31	1.48	1.43
87	BN	834	CLA	MG-ND	-2.31	2.01	2.05
87	aL	605	CLA	CMC-C2C	-2.31	1.45	1.50
82	I9	202	PEB	C1C-C2C	2.31	1.48	1.42
83	QM	201	PUB	C4B-NB	-2.31	1.33	1.37
87	B2	835	CLA	C1B-C2B	2.31	1.48	1.43
87	2N	312	CLA	CHC-C1C	2.31	1.43	1.38
87	12	604	CLA	MG-NB	-2.31	2.01	2.05
82	g1	201	PEB	C1C-C2C	2.31	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EM	202	PEB	C4A-NA	-2.31	1.32	1.37
87	AN	814	CLA	CMD-C2D	-2.31	1.45	1.50
87	IN	102	CLA	CMB-C2B	-2.31	1.45	1.50
82	LD	202	PEB	C1B-C2B	2.31	1.50	1.45
87	cL	513	CLA	C1B-C2B	2.31	1.48	1.43
87	A2	803	CLA	MG-NB	-2.31	2.01	2.05
87	c6	608	CLA	MG-NB	-2.31	2.01	2.05
87	3N	313	CLA	MG-NB	-2.31	2.01	2.05
82	TP	201	PEB	C4A-NA	-2.31	1.32	1.37
87	B6	609	CLA	C1B-C2B	2.31	1.48	1.43
82	E9	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	AI	203	PEB	C4D-ND	2.31	1.38	1.35
82	CK	201	PEB	C1C-C2C	2.31	1.48	1.42
82	VQ	203	PEB	C1C-C2C	2.31	1.48	1.42
82	JA	203	PEB	C1C-NC	-2.31	1.33	1.37
82	PD	203	PEB	C1C-NC	-2.31	1.33	1.37
82	TO	201	PEB	C1C-NC	-2.31	1.33	1.37
87	A2	815	CLA	CMD-C2D	-2.31	1.45	1.50
87	nL	101	CLA	CMD-C2D	-2.31	1.45	1.50
84	HH	1001	CYC	C1B-C2B	2.31	1.49	1.45
82	OE	202	PEB	C4A-NA	-2.31	1.32	1.37
82	TE	201	PEB	C4A-NA	-2.31	1.32	1.37
82	RH	201	PEB	C4A-NA	-2.31	1.32	1.37
82	bB	201	PEB	C4A-NA	-2.31	1.32	1.37
87	7N	602	CLA	CHC-C1C	2.31	1.43	1.38
87	AN	839	CLA	C1B-C2B	2.31	1.48	1.43
87	b6	611	CLA	CMD-C2D	-2.31	1.45	1.50
82	jF	202	PEB	C4A-NA	-2.31	1.32	1.37
82	gH	202	PEB	C1A-NA	-2.31	1.34	1.37
82	TM	202	PEB	C1C-C2C	2.31	1.48	1.42
82	EA	201	PEB	C2A-C1A	-2.31	1.50	1.52
82	l4	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	hM	202	PEB	C2A-C1A	-2.31	1.50	1.52
82	M7	201	PEB	C4A-NA	-2.31	1.32	1.37
82	fG	202	PEB	C1C-C2C	2.31	1.48	1.42
82	a1	202	PEB	C1B-C2B	2.31	1.50	1.45
87	BN	810	CLA	CMB-C2B	-2.31	1.45	1.50
87	A2	833	CLA	CMB-C2B	-2.31	1.45	1.50
82	VG	201	PEB	C1C-C2C	2.31	1.48	1.42
82	mJ	202	PEB	C1C-C2C	2.31	1.48	1.42
82	KP	202	PEB	C1C-NC	-2.31	1.33	1.37
87	62	307	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WD	202	PEB	C4A-NA	-2.31	1.32	1.37
82	GG	1002	PEB	C4A-NA	-2.31	1.32	1.37
82	fH	203	PEB	C1C-C2C	2.31	1.48	1.42
87	C6	514	CLA	MG-NB	-2.31	2.01	2.05
82	R1	202	PEB	CHC-C4C	2.31	1.52	1.49
87	32	306	CLA	C1B-C2B	2.31	1.48	1.43
82	UE	203	PEB	C1C-NC	-2.30	1.33	1.37
82	HP	201	PEB	C1C-NC	-2.30	1.33	1.37
87	R2	201	CLA	CMB-C2B	-2.30	1.45	1.50
82	SF	202	PEB	C4A-NA	-2.30	1.32	1.37
82	W5	202	PEB	C4A-NA	-2.30	1.32	1.37
82	LK	202	PEB	C4B-C3B	2.30	1.49	1.45
82	LQ	201	PEB	C4B-C3B	2.30	1.49	1.45
82	C5	202	PEB	C4A-NA	-2.30	1.32	1.37
82	jH	201	PEB	C4A-NA	-2.30	1.32	1.37
87	HL	102	CLA	MG-NB	-2.30	2.01	2.05
87	AN	810	CLA	MG-NB	-2.30	2.01	2.05
87	B6	610	CLA	MG-NB	-2.30	2.01	2.05
82	E9	202	PEB	C1C-C2C	2.30	1.48	1.42
87	B2	834	CLA	CHC-C1C	2.30	1.43	1.38
82	OG	201	PEB	C4A-NA	-2.30	1.32	1.37
87	AL	404	CLA	CMD-C2D	-2.30	1.45	1.50
82	S7	201	PEB	C4B-NB	-2.30	1.33	1.38
82	W7	202	PEB	C1D-ND	2.30	1.49	1.45
82	T9	202	PEB	C1C-C2C	2.30	1.48	1.42
82	j1	203	PEB	C2A-C1A	-2.30	1.50	1.52
87	B2	807	CLA	CMD-C2D	-2.30	1.45	1.50
82	KF	201	PEB	C4A-NA	-2.30	1.32	1.37
84	EH	1001	CYC	C1B-C2B	2.30	1.49	1.45
87	R2	204	CLA	MG-NB	-2.30	2.01	2.05
82	HH	1002	PEB	C1C-C2C	2.30	1.48	1.42
87	AN	830	CLA	C1B-C2B	2.30	1.48	1.43
82	EB	501	PEB	C4A-NA	-2.30	1.32	1.37
82	YP	503	PEB	C4A-NA	-2.30	1.32	1.37
82	aO	201	PEB	C4A-NA	-2.30	1.32	1.37
82	NB	201	PEB	C1C-NC	-2.30	1.34	1.37
82	E9	201	PEB	C1C-NC	-2.30	1.34	1.37
82	p8	201	PEB	C1C-C2C	2.30	1.48	1.42
82	TH	202	PEB	C1C-C2C	2.30	1.48	1.42
82	YK	203	PEB	C1C-C2C	2.30	1.48	1.42
87	c6	609	CLA	MG-NB	-2.30	2.01	2.05
84	DH	1001	CYC	C1B-C2B	2.30	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q7	202	PEB	C4A-NA	-2.30	1.32	1.37
87	72	602	CLA	CHC-C1C	2.30	1.43	1.38
84	LH	1002	CYC	C4D-C3D	2.30	1.48	1.42
82	OK	201	PEB	CHC-C4C	2.30	1.52	1.49
82	lK	203	PEB	CHC-C4C	2.30	1.52	1.49
82	iF	201	PEB	OD-C4D	2.30	1.28	1.23
87	B6	610	CLA	C1B-C2B	2.30	1.48	1.43
94	AL	413	PL9	C6-C5	2.30	1.47	1.35
82	GA	202	PEB	C4B-C3B	2.30	1.49	1.45
82	H7	203	PEB	C1C-C2C	2.30	1.48	1.42
82	OQ	202	PEB	C1D-ND	2.30	1.49	1.45
82	Q4	201	PEB	OD-C4D	2.30	1.28	1.23
82	L9	203	PEB	C4B-C3B	2.30	1.49	1.45
82	DJ	202	PEB	C1C-C2C	2.30	1.48	1.42
82	D5	203	PEB	C1C-NC	-2.30	1.34	1.37
82	YF	203	PEB	CHC-C4C	2.30	1.52	1.49
82	E7	201	PEB	CHC-C4C	2.30	1.52	1.49
82	ZB	201	PEB	C1C-C2C	2.30	1.48	1.42
87	BN	807	CLA	CMD-C2D	-2.30	1.45	1.50
82	SA	201	PEB	C4B-NB	-2.30	1.33	1.38
82	AI	203	PEB	C4A-NA	-2.30	1.32	1.37
82	lO	201	PEB	C4A-NA	-2.30	1.32	1.37
87	AN	849	CLA	CHC-C1C	2.30	1.43	1.38
87	AN	819	CLA	CMD-C2D	-2.30	1.45	1.50
87	B2	808	CLA	CMB-C2B	-2.30	1.45	1.50
87	B2	810	CLA	CMC-C2C	-2.30	1.45	1.50
87	A2	833	CLA	C1B-C2B	2.30	1.48	1.43
82	D9	202	PEB	C1D-ND	2.30	1.49	1.45
84	JH	1003	CYC	C1B-C2B	2.30	1.49	1.45
82	KA	202	PEB	C1C-C2C	2.30	1.48	1.42
87	bL	622	CLA	C1B-C2B	2.30	1.48	1.43
82	eG	201	PEB	C4A-NA	-2.30	1.32	1.37
82	XQ	202	PEB	C2A-C1A	-2.30	1.50	1.52
87	B2	832	CLA	C1B-C2B	2.30	1.48	1.43
82	g1	202	PEB	C4B-C3B	2.30	1.49	1.45
82	JI	202	PEB	C1C-NC	-2.30	1.34	1.37
82	zF	501	PEB	CHB-C1C	2.30	1.45	1.40
87	8N	308	CLA	MG-NB	-2.30	2.01	2.05
82	UI	201	PEB	C1C-C2C	2.30	1.48	1.42
87	AN	849	CLA	C1D-ND	2.30	1.40	1.37
82	A7	201	PEB	C4A-NA	-2.30	1.32	1.37
82	jJ	203	PEB	C4A-NA	-2.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AH	305	PEB	C1C-C2C	2.30	1.48	1.42
82	WH	202	PEB	C1C-C2C	2.30	1.48	1.42
82	AF	202	PEB	C2A-C1A	-2.30	1.50	1.52
82	f4	201	PEB	C2A-C1A	-2.30	1.50	1.52
82	TD	201	PEB	CHC-C4C	2.30	1.52	1.49
82	NG	201	PEB	CHC-C4C	2.30	1.52	1.49
87	AN	831	CLA	C3B-C4B	2.30	1.48	1.42
87	b6	608	CLA	CMD-C2D	-2.30	1.45	1.50
82	GP	202	PEB	C4A-NA	-2.30	1.32	1.37
82	R7	202	PEB	C4B-C3B	2.30	1.49	1.45
87	4N	601	CLA	C3B-C4B	2.30	1.48	1.42
87	b6	615	CLA	CMB-C2B	-2.30	1.45	1.50
82	UG	203	PEB	C4A-NA	-2.30	1.32	1.37
82	KM	201	PEB	C4A-NA	-2.30	1.32	1.37
82	W7	201	PEB	C4A-NA	-2.30	1.32	1.37
82	OO	202	PEB	C1C-C2C	2.30	1.48	1.42
82	N9	202	PEB	C1C-C2C	2.30	1.48	1.42
82	lK	201	PEB	CHC-C4C	2.30	1.52	1.49
82	OA	201	PEB	C4B-NB	-2.30	1.33	1.38
87	I2	102	CLA	CMB-C2B	-2.30	1.45	1.50
87	B6	606	CLA	CMB-C2B	-2.30	1.45	1.50
82	R1	201	PEB	C2A-C1A	-2.30	1.50	1.52
82	lH	202	PEB	C2A-C1A	-2.30	1.50	1.52
82	CJ	202	PEB	C1C-C2C	2.30	1.48	1.42
82	HB	201	PEB	C4A-NA	-2.30	1.32	1.37
82	QJ	202	PEB	C4A-NA	-2.30	1.32	1.37
87	AN	810	CLA	C1B-C2B	2.30	1.48	1.43
87	bL	620	CLA	C1B-C2B	2.30	1.48	1.43
87	2N	305	CLA	C1B-C2B	2.30	1.48	1.43
87	D6	403	CLA	MG-NB	-2.30	2.01	2.05
82	L9	201	PEB	C4B-C3B	2.30	1.49	1.45
82	QM	203	PEB	C4A-NA	-2.30	1.32	1.37
82	cF	201	PEB	C4A-NA	-2.30	1.32	1.37
82	BP	201	PEB	C1C-NC	-2.30	1.34	1.37
84	C4	1001	CYC	C1B-NB	-2.30	1.34	1.37
82	C9	202	PEB	C2A-C1A	-2.30	1.50	1.52
82	CB	202	PEB	C1B-C2B	2.30	1.50	1.45
82	C9	201	PEB	C1C-C2C	2.30	1.48	1.42
87	dL	401	CLA	CMB-C2B	-2.30	1.45	1.50
82	FJ	202	PEB	C1C-NC	-2.29	1.34	1.37
87	BN	820	CLA	MG-NB	-2.29	2.01	2.05
87	b6	617	CLA	MG-NB	-2.29	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	830	CLA	C1B-C2B	2.29	1.48	1.43
87	AN	839	CLA	CMD-C2D	-2.29	1.45	1.50
87	2N	308	CLA	CMD-C2D	-2.29	1.45	1.50
87	8N	301	CLA	CMD-C2D	-2.29	1.45	1.50
82	U5	201	PEB	C4A-NA	-2.29	1.32	1.37
84	IO	1001	CYC	C4C-NC	-2.29	1.32	1.37
82	C9	202	PEB	C1C-C2C	2.29	1.48	1.42
82	vC	202	PEB	C1C-C2C	2.29	1.48	1.42
82	H7	202	PEB	C2A-C1A	-2.29	1.50	1.52
82	R9	202	PEB	C2A-C1A	-2.29	1.50	1.52
82	T9	202	PEB	C2A-C1A	-2.29	1.50	1.52
82	QO	201	PEB	OD-C4D	2.29	1.27	1.23
82	WI	202	PEB	CHA-C1B	2.29	1.45	1.40
82	J4	1002	PEB	C4A-NA	-2.29	1.32	1.37
82	M9	304	PEB	C1C-C2C	2.29	1.48	1.42
87	BN	811	CLA	CMC-C2C	-2.29	1.45	1.50
84	BE	1001	CYC	OB-C4B	2.29	1.27	1.23
82	IJ	201	PEB	C4A-NA	-2.29	1.32	1.37
87	b6	611	CLA	C1B-C2B	2.29	1.48	1.43
82	RH	201	PEB	C2A-C1A	-2.29	1.50	1.52
82	ZE	202	PEB	C4A-NA	-2.29	1.32	1.37
84	MO	1001	CYC	C4C-NC	-2.29	1.32	1.37
84	LG	1001	CYC	C4D-ND	-2.29	1.34	1.37
87	12	602	CLA	C4B-NB	2.29	1.40	1.37
82	uK	201	PEB	C1B-C2B	2.29	1.50	1.45
87	b6	608	CLA	C1B-C2B	2.29	1.48	1.43
82	N7	203	PEB	C4A-NA	-2.29	1.32	1.37
82	fO	201	PEB	C4A-NA	-2.29	1.32	1.37
87	cL	515	CLA	C1B-C2B	2.29	1.48	1.43
87	AN	803	CLA	CMB-C2B	-2.29	1.45	1.50
87	B2	832	CLA	CMD-C2D	-2.29	1.45	1.50
87	D6	403	CLA	CMD-C2D	-2.29	1.45	1.50
82	VM	202	PEB	C4A-NA	-2.29	1.32	1.37
82	KK	202	PEB	C1B-C2B	2.29	1.50	1.45
82	PA	203	PEB	C1C-NC	-2.29	1.34	1.37
82	P7	203	PEB	C1C-NC	-2.29	1.34	1.37
82	lJ	203	PEB	C1C-NC	-2.29	1.34	1.37
84	DH	1001	CYC	C4D-C3D	2.29	1.48	1.42
87	B6	613	CLA	C1B-C2B	2.29	1.48	1.43
87	BN	809	CLA	C1B-NB	-2.29	1.35	1.37
82	WD	201	PEB	C1C-C2C	2.29	1.48	1.42
87	K2	106	CLA	CMD-C2D	-2.29	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	c6	611	CLA	C1B-C2B	2.29	1.48	1.43
82	E5	202	PEB	C4A-NA	-2.29	1.32	1.37
83	AH	304	PUB	C1C-C2C	2.29	1.49	1.45
82	L9	203	PEB	C1C-C2C	2.29	1.48	1.42
82	QH	203	PEB	C2A-C1A	-2.29	1.50	1.52
82	K7	202	PEB	C2A-C1A	-2.29	1.50	1.52
82	YJ	203	PEB	C4A-NA	-2.29	1.32	1.37
82	L5	203	PEB	C4A-NA	-2.29	1.32	1.37
82	gF	201	PEB	C4A-NA	-2.29	1.32	1.37
82	eO	201	PEB	C4A-NA	-2.29	1.32	1.37
82	ZM	201	PEB	CHC-C4C	2.29	1.52	1.49
87	B2	801	CLA	C3B-C4B	2.29	1.48	1.42
82	BF	202	PEB	C1C-NC	-2.29	1.34	1.37
82	R7	201	PEB	C1C-NC	-2.29	1.34	1.37
84	IE	1001	CYC	C1B-NB	-2.29	1.34	1.37
82	PK	202	PEB	C1C-C2C	2.29	1.48	1.42
87	AN	815	CLA	CMB-C2B	-2.29	1.45	1.50
87	BN	802	CLA	C3B-C4B	2.29	1.48	1.42
87	AN	808	CLA	MG-NB	-2.29	2.01	2.05
82	i4	203	PEB	C1C-C2C	2.29	1.48	1.42
82	z8	202	PEB	C1C-C2C	2.29	1.48	1.42
82	v8	202	PEB	C1C-C2C	2.29	1.48	1.42
87	AN	833	CLA	C1B-C2B	2.29	1.48	1.43
87	B2	831	CLA	CMB-C2B	-2.29	1.45	1.50
82	HA	201	PEB	CHC-C4C	2.29	1.52	1.49
82	RE	201	PEB	C4A-NA	-2.29	1.32	1.37
82	R1	201	PEB	C1C-NC	-2.29	1.34	1.37
84	C1	1001	CYC	C4A-C3A	2.29	1.50	1.45
87	K2	106	CLA	MG-NB	-2.29	2.01	2.05
82	zK	501	PEB	CHB-C1C	2.29	1.45	1.40
87	AN	841	CLA	C1B-NB	-2.29	1.35	1.37
82	cB	403	PEB	C4A-NA	-2.29	1.32	1.37
82	I9	201	PEB	C1C-C2C	2.29	1.48	1.42
87	B2	819	CLA	C1B-C2B	2.29	1.48	1.43
87	8N	307	CLA	MG-NB	-2.29	2.01	2.05
82	eK	201	PEB	CHA-C4A	-2.29	1.32	1.36
82	M5	301	PEB	C2A-C1A	-2.29	1.50	1.52
82	U7	202	PEB	C2A-C1A	-2.29	1.50	1.52
82	D9	202	PEB	C2A-C1A	-2.29	1.50	1.52
82	D9	203	PEB	C2A-C1A	-2.29	1.50	1.52
82	uF	203	PEB	C2A-C1A	-2.29	1.50	1.52
82	GI	201	PEB	C1D-ND	2.29	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	H5	201	PEB	C1D-ND	2.29	1.49	1.45
87	BL	620	CLA	C3B-C4B	2.29	1.48	1.42
87	dL	402	CLA	CMC-C2C	-2.29	1.45	1.50
82	SK	201	PEB	C4A-NA	-2.29	1.32	1.37
82	AM	302	PEB	C1C-C2C	2.29	1.48	1.42
84	L1	1001	CYC	C4A-C3A	2.29	1.50	1.45
87	AN	852	CLA	CHC-C4B	-2.29	1.34	1.39
82	vF	202	PEB	C1C-NC	-2.29	1.34	1.37
87	AN	826	CLA	C1B-NB	-2.29	1.35	1.37
87	8N	301	CLA	C1B-NB	-2.29	1.35	1.37
84	FG	1001	CYC	C4C-NC	-2.29	1.32	1.37
84	73	1002	CYC	C4C-NC	-2.29	1.32	1.37
82	RM	201	PEB	C1B-C2B	2.29	1.50	1.45
82	uC	201	PEB	C4B-C3B	2.29	1.49	1.45
87	BN	826	CLA	MG-ND	-2.29	2.01	2.05
87	82	307	CLA	MG-NB	-2.29	2.01	2.05
87	B2	819	CLA	MG-NB	-2.29	2.01	2.05
87	C6	518	CLA	MG-NB	-2.29	2.01	2.05
87	A2	831	CLA	CMD-C2D	-2.29	1.46	1.50
82	A4	304	PEB	C1C-C2C	2.29	1.48	1.42
82	cE	202	PEB	C4A-NA	-2.29	1.32	1.37
87	bL	622	CLA	MG-NB	-2.29	2.01	2.05
82	LA	203	PEB	C1C-C2C	2.29	1.48	1.42
82	dO	202	PEB	C1D-ND	2.29	1.49	1.45
87	AN	834	CLA	C4B-NB	2.29	1.40	1.37
82	ZK	202	PEB	C1C-NC	-2.29	1.34	1.37
82	L5	203	PEB	C1C-NC	-2.29	1.34	1.37
82	N4	1002	PEB	C4A-NA	-2.29	1.32	1.37
82	GP	203	PEB	C2A-C1A	-2.29	1.50	1.52
82	X9	202	PEB	C1C-C2C	2.29	1.48	1.42
87	A2	820	CLA	MG-ND	-2.29	2.01	2.05
87	B6	608	CLA	MG-NB	-2.29	2.01	2.05
87	HL	102	CLA	C1B-C2B	2.29	1.48	1.43
82	Z5	305	PEB	C1C-NC	-2.29	1.34	1.37
84	MG	1001	CYC	OB-C4B	2.29	1.27	1.23
82	TO	202	PEB	C1C-C2C	2.29	1.48	1.42
82	T4	202	PEB	C1C-C2C	2.29	1.48	1.42
87	BN	832	CLA	C1B-C2B	2.29	1.48	1.43
87	A2	841	CLA	C1B-NB	-2.29	1.35	1.37
87	82	308	CLA	MG-NB	-2.29	2.01	2.05
87	A2	840	CLA	CMB-C2B	-2.29	1.46	1.50
82	KK	201	PEB	C4A-NA	-2.29	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	FP	201	PEB	C1C-C2C	2.29	1.48	1.42
82	LG	1002	PEB	C1C-NC	-2.29	1.34	1.37
82	WK	201	PEB	C2A-C1A	-2.29	1.50	1.52
87	bL	608	CLA	CMB-C2B	-2.29	1.46	1.50
82	WK	202	PEB	C1B-C2B	2.29	1.50	1.45
82	XQ	202	PEB	C1C-C2C	2.28	1.48	1.42
82	J9	202	PEB	C1C-C2C	2.28	1.48	1.42
87	b6	615	CLA	C1B-C2B	2.28	1.48	1.43
87	CL	514	CLA	C1B-NB	-2.28	1.35	1.37
82	RK	202	PEB	C1C-NC	-2.28	1.34	1.37
82	V7	201	PEB	C1C-NC	-2.28	1.34	1.37
87	A2	807	CLA	CMC-C2C	-2.28	1.46	1.50
85	AN	848	BCR	C19-C18	2.28	1.50	1.45
82	Q5	202	PEB	C4B-C3B	2.28	1.49	1.45
82	j1	202	PEB	C1D-ND	2.28	1.49	1.45
82	CJ	201	PEB	C4A-NA	-2.28	1.32	1.37
82	XD	202	PEB	C1C-C2C	2.28	1.48	1.42
87	22	608	CLA	CMD-C2D	-2.28	1.46	1.50
82	AP	202	PEB	C2A-C1A	-2.28	1.50	1.52
82	OM	203	PEB	C4A-NA	-2.28	1.32	1.37
82	dF	202	PEB	C4A-NA	-2.28	1.32	1.37
82	K7	202	PEB	C1C-C2C	2.28	1.48	1.42
87	b6	606	CLA	CMB-C2B	-2.28	1.46	1.50
82	P9	202	PEB	C1C-C2C	2.28	1.48	1.42
82	YJ	202	PEB	C1C-NC	-2.28	1.34	1.37
84	C1	1001	CYC	C1B-C2B	2.28	1.49	1.45
87	6N	606	CLA	CMD-C2D	-2.28	1.46	1.50
82	FD	203	PEB	C2C-C3C	2.28	1.44	1.38
82	g4	201	PEB	C4A-NA	-2.28	1.32	1.37
82	DB	201	PEB	C1C-NC	-2.28	1.34	1.37
84	IE	1001	CYC	C4D-ND	-2.28	1.34	1.37
84	IG	1001	CYC	C4D-ND	-2.28	1.34	1.37
87	AN	833	CLA	CMB-C2B	-2.28	1.46	1.50
87	AN	852	CLA	C4B-NB	2.28	1.40	1.37
82	iJ	202	PEB	C1C-C2C	2.28	1.48	1.42
87	CL	513	CLA	C1B-C2B	2.28	1.48	1.43
87	A2	810	CLA	C1B-C2B	2.28	1.48	1.43
87	8N	306	CLA	C1B-C2B	2.28	1.48	1.43
87	c6	606	CLA	MG-NB	-2.28	2.01	2.05
87	c6	616	CLA	MG-NB	-2.28	2.01	2.05
87	2N	310	CLA	MG-ND	-2.28	2.01	2.05
82	RH	202	PEB	CHC-C4C	2.28	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	E7	201	PEB	C4B-C3B	2.28	1.49	1.45
82	u8	201	PEB	C4B-C3B	2.28	1.49	1.45
84	ME	1001	CYC	OB-C4B	2.28	1.27	1.23
82	PF	202	PEB	C1C-C2C	2.28	1.48	1.42
82	hJ	201	PEB	C1C-C2C	2.28	1.48	1.42
82	Y9	203	PEB	C2A-C1A	-2.28	1.50	1.52
82	dG	203	PEB	C2A-C1A	-2.28	1.50	1.52
82	mJ	202	PEB	C4A-NA	-2.28	1.32	1.37
82	RQ	203	PEB	C1C-C2C	2.28	1.48	1.42
82	V9	202	PEB	C1C-C2C	2.28	1.48	1.42
94	aL	601	PL9	C2-C1	-2.28	1.38	1.44
87	DL	403	CLA	CMB-C2B	-2.28	1.46	1.50
87	cL	505	CLA	CMD-C2D	-2.28	1.46	1.50
82	JQ	201	PEB	C1D-ND	2.28	1.49	1.45
87	1N	607	CLA	MG-NB	-2.28	2.01	2.05
82	OI	201	PEB	C1C-NC	-2.28	1.34	1.37
82	FF	201	PEB	OD-C4D	2.28	1.27	1.23
84	BG	1001	CYC	OB-C4B	2.28	1.27	1.23
87	A2	839	CLA	CMD-C2D	-2.28	1.46	1.50
82	gH	202	PEB	C4B-C3B	2.28	1.49	1.45
82	tK	203	PEB	C4B-C3B	2.28	1.49	1.45
82	uC	202	PEB	C2A-C1A	-2.28	1.50	1.52
84	DO	1001	CYC	C4C-NC	-2.28	1.32	1.37
82	m4	203	PEB	C1C-C2C	2.28	1.48	1.42
82	Y9	202	PEB	C1C-C2C	2.28	1.48	1.42
84	L1	1001	CYC	C4D-C3D	2.28	1.48	1.42
87	d6	403	CLA	MG-NB	-2.28	2.01	2.05
82	MP	203	PEB	OD-C4D	2.28	1.27	1.23
87	KN	103	CLA	CMD-C2D	-2.28	1.46	1.50
82	tF	202	PEB	C4B-C3B	2.28	1.49	1.45
84	BG	1001	CYC	C4D-C3D	2.28	1.48	1.42
87	6N	608	CLA	C4B-NB	2.28	1.40	1.37
82	U5	203	PEB	C1C-NC	-2.28	1.34	1.37
82	f1	201	PEB	C1C-C2C	2.28	1.48	1.42
82	jJ	202	PEB	C1C-C2C	2.28	1.48	1.42
82	AQ	304	PEB	C4B-C3B	2.28	1.49	1.45
87	AN	831	CLA	CMC-C2C	-2.28	1.46	1.50
82	U1	202	PEB	CHA-C4A	-2.28	1.32	1.36
82	CM	202	PEB	C1C-C2C	2.28	1.48	1.42
82	RA	203	PEB	C4A-NA	-2.28	1.32	1.37
87	CL	506	CLA	C3B-C4B	2.28	1.48	1.42
87	42	609	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	DG	1001	CYC	C4B-NB	-2.28	1.33	1.38
84	GG	1001	CYC	C4B-NB	-2.28	1.33	1.38
82	H1	1002	PEB	C1C-C2C	2.28	1.48	1.42
82	P4	202	PEB	C4A-NA	-2.28	1.32	1.37
82	P7	201	PEB	C4A-NA	-2.28	1.32	1.37
82	bH	201	PEB	C1D-ND	2.28	1.49	1.45
87	BL	604	CLA	MG-NB	-2.28	2.01	2.05
82	OA	202	PEB	C2A-C1A	-2.28	1.50	1.52
82	RO	203	PEB	C1C-C2C	2.28	1.48	1.42
82	eF	201	PEB	CHA-C4A	-2.28	1.32	1.36
87	A2	832	CLA	C1B-NB	-2.28	1.35	1.37
82	RP	201	PEB	C1C-C2C	2.28	1.48	1.42
82	fE	201	PEB	C1C-C2C	2.28	1.48	1.42
87	c6	610	CLA	MG-NB	-2.28	2.01	2.05
82	JM	201	PEB	C4A-NA	-2.28	1.32	1.37
82	VP	202	PEB	C4A-NA	-2.28	1.32	1.37
103	8N	310	ZEX	C31-C30	2.28	1.50	1.43
82	L4	1002	PEB	C1C-C2C	2.28	1.48	1.42
82	JJ	202	PEB	C1C-NC	-2.28	1.34	1.37
82	UB	303	PEB	C4A-NA	-2.28	1.32	1.37
82	HK	202	PEB	C4A-NA	-2.28	1.32	1.37
82	XM	202	PEB	C4A-NA	-2.28	1.32	1.37
82	AD	304	PEB	C2A-C1A	-2.28	1.50	1.52
82	OH	201	PEB	C2A-C1A	-2.28	1.50	1.52
82	A7	201	PEB	C2A-C1A	-2.28	1.50	1.52
82	WO	201	PEB	OD-C4D	2.28	1.27	1.23
87	B2	819	CLA	CMD-C2D	-2.28	1.46	1.50
82	DQ	201	PEB	C4B-C3B	2.28	1.49	1.45
82	fM	203	PEB	C1C-C2C	2.28	1.48	1.42
87	A2	851	CLA	C1B-C2B	2.28	1.48	1.43
82	WH	203	PEB	C4B-C3B	2.28	1.49	1.45
82	A1	305	PEB	C1C-C2C	2.28	1.48	1.42
82	X7	203	PEB	C1C-C2C	2.28	1.48	1.42
82	GP	201	PEB	C2A-C1A	-2.28	1.50	1.52
82	CK	202	PEB	CHB-C1C	2.28	1.45	1.40
96	f6	101	HEM	C1D-ND	-2.28	1.34	1.38
82	R1	201	PEB	C4A-NA	-2.28	1.32	1.37
82	iJ	201	PEB	C4A-NA	-2.28	1.32	1.37
84	FE	1001	CYC	C4D-C3D	2.28	1.48	1.42
82	sK	201	PEB	C1D-ND	2.28	1.49	1.45
82	JI	201	PEB	C1C-C2C	2.28	1.48	1.42
82	dJ	202	PEB	C4A-NA	-2.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	K2	104	CLA	CMD-C2D	-2.28	1.46	1.50
84	KO	1001	CYC	C1B-NB	-2.28	1.34	1.37
84	JH	1001	CYC	C4D-C3D	2.28	1.48	1.42
82	V5	202	PEB	C4A-NA	-2.27	1.32	1.37
82	XA	203	PEB	C4B-C3B	2.27	1.49	1.45
82	kG	201	PEB	C4B-C3B	2.27	1.49	1.45
82	GA	201	PEB	C4A-NA	-2.27	1.32	1.37
82	AE	304	PEB	C4A-NA	-2.27	1.32	1.37
82	U7	202	PEB	C4A-NA	-2.27	1.32	1.37
87	cL	505	CLA	MG-NB	-2.27	2.01	2.05
87	BN	821	CLA	C4D-ND	-2.27	1.34	1.37
87	3N	308	CLA	C4D-ND	-2.27	1.34	1.37
103	82	310	ZEX	C31-C30	2.27	1.50	1.43
82	LH	1003	PEB	C4A-NA	-2.27	1.32	1.37
87	AN	820	CLA	MG-ND	-2.27	2.01	2.05
87	7N	607	CLA	MG-NB	-2.27	2.01	2.05
82	fO	202	PEB	C2A-C1A	-2.27	1.50	1.52
82	iM	201	PEB	C1D-ND	2.27	1.49	1.45
82	SM	201	PEB	C1C-C2C	2.27	1.48	1.42
87	22	604	CLA	C1B-C2B	2.27	1.48	1.43
82	KB	304	PEB	C4A-NA	-2.27	1.32	1.37
87	KN	102	CLA	C1B-C2B	2.27	1.48	1.43
82	gF	201	PEB	C1C-NC	-2.27	1.34	1.37
82	I5	202	PEB	C4A-NA	-2.27	1.32	1.37
82	wF	302	PEB	C4A-NA	-2.27	1.32	1.37
87	AN	832	CLA	C3B-C4B	2.27	1.48	1.42
87	A2	831	CLA	C3B-C4B	2.27	1.48	1.42
82	lF	201	PEB	C1C-C2C	2.27	1.48	1.42
84	IO	1001	CYC	C1B-NB	-2.27	1.34	1.37
82	qF	203	PEB	C4B-C3B	2.27	1.49	1.45
82	DB	202	PEB	C4A-NA	-2.27	1.32	1.37
82	WB	402	PEB	C4A-NA	-2.27	1.32	1.37
82	RI	203	PEB	OD-C4D	2.27	1.27	1.23
87	K2	103	CLA	C1B-C2B	2.27	1.48	1.43
84	CG	1001	CYC	C4D-C3D	2.27	1.48	1.42
87	A2	840	CLA	MG-ND	-2.27	2.01	2.05
85	b6	603	BCR	C30-C25	-2.27	1.50	1.53
82	SH	203	PEB	C4B-C3B	2.27	1.49	1.45
87	22	610	CLA	MG-ND	-2.27	2.01	2.05
82	DI	201	PEB	C4A-NA	-2.27	1.32	1.37
87	B2	824	CLA	C1B-C2B	2.27	1.48	1.43
82	TO	203	PEB	C1C-C2C	2.27	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	T7	202	PEB	C2C-C3C	2.27	1.44	1.38
87	CL	513	CLA	CHC-C1C	2.27	1.43	1.38
82	CB	202	PEB	C1C-NC	-2.27	1.34	1.37
84	CO	1001	CYC	C4B-NB	-2.27	1.33	1.38
87	22	605	CLA	C4B-C3B	2.27	1.48	1.43
82	KE	201	PEB	C1C-C2C	2.27	1.48	1.42
82	HJ	202	PEB	C4A-NA	-2.27	1.32	1.37
82	SF	201	PEB	OD-C4D	2.27	1.27	1.23
87	dL	404	CLA	MG-NB	-2.27	2.01	2.05
87	AL	405	CLA	CMB-C2B	-2.27	1.46	1.50
82	aF	201	PEB	CHC-C4C	2.27	1.52	1.49
82	N7	201	PEB	C1C-NC	-2.27	1.34	1.37
87	AN	851	CLA	C1B-C2B	2.27	1.48	1.43
82	SQ	201	PEB	C1C-C2C	2.27	1.48	1.42
82	A9	201	PEB	C1C-C2C	2.27	1.48	1.42
82	sC	203	PEB	C4B-C3B	2.27	1.49	1.45
82	d4	202	PEB	C1D-ND	2.27	1.49	1.45
87	CL	514	CLA	MG-NB	-2.27	2.01	2.05
87	CL	512	CLA	CMB-C2B	-2.27	1.46	1.50
87	A2	811	CLA	CMD-C2D	-2.27	1.46	1.50
87	C6	517	CLA	C1B-C2B	2.27	1.48	1.43
82	aF	201	PEB	C1C-C2C	2.27	1.48	1.42
82	BB	203	PEB	C1C-NC	-2.27	1.34	1.37
82	LF	202	PEB	C4A-NA	-2.27	1.32	1.37
82	D5	203	PEB	C4A-NA	-2.27	1.32	1.37
82	eJ	201	PEB	C4A-NA	-2.27	1.32	1.37
82	gK	201	PEB	C4A-NA	-2.27	1.32	1.37
87	62	305	CLA	C1D-C2D	2.27	1.49	1.45
87	CL	504	CLA	C1B-NB	-2.27	1.35	1.37
82	DQ	202	PEB	C1B-C2B	2.27	1.50	1.45
82	qK	201	PEB	C1B-C2B	2.27	1.50	1.45
82	H5	202	PEB	C4B-C3B	2.27	1.49	1.45
82	rF	201	PEB	C4B-C3B	2.27	1.49	1.45
87	BL	604	CLA	CMC-C2C	-2.27	1.46	1.50
87	AN	808	CLA	CMD-C2D	-2.27	1.46	1.50
87	A2	814	CLA	CMD-C2D	-2.27	1.46	1.50
83	A1	304	PUB	C4B-C3B	2.27	1.48	1.42
82	DK	203	PEB	C4A-NA	-2.27	1.32	1.37
82	a4	201	PEB	C4A-NA	-2.27	1.32	1.37
82	D9	203	PEB	C4A-NA	-2.27	1.32	1.37
82	yF	301	PEB	C4A-NA	-2.27	1.32	1.37
82	KK	203	PEB	C1C-NC	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kH	201	PEB	C1C-NC	-2.27	1.34	1.37
82	XQ	203	PEB	C2A-C1A	-2.27	1.50	1.52
87	AN	816	CLA	MG-NB	-2.27	2.01	2.05
87	AN	840	CLA	MG-ND	-2.27	2.01	2.05
85	F6	101	BCR	C1-C6	-2.27	1.50	1.53
87	6N	608	CLA	CHC-C4B	-2.27	1.34	1.39
87	B2	828	CLA	C1B-C2B	2.27	1.48	1.43
87	bL	616	CLA	CMC-C2C	-2.27	1.46	1.50
82	TO	202	PEB	C4A-NA	-2.27	1.32	1.37
82	OK	202	PEB	C1C-NC	-2.27	1.34	1.37
82	WQ	201	PEB	C1C-NC	-2.27	1.34	1.37
87	KN	105	CLA	MG-NB	-2.27	2.01	2.05
87	32	313	CLA	MG-NB	-2.27	2.01	2.05
87	8N	302	CLA	MG-NB	-2.27	2.01	2.05
84	DO	1001	CYC	OB-C4B	2.27	1.27	1.23
82	mJ	202	PEB	C2A-C1A	-2.27	1.50	1.52
82	eO	202	PEB	C2A-C1A	-2.27	1.50	1.52
82	uC	201	PEB	C4A-NA	-2.27	1.32	1.37
87	A2	806	CLA	C1B-C2B	2.27	1.48	1.43
82	EA	201	PEB	C4B-C3B	2.27	1.49	1.45
82	RQ	203	PEB	C4B-C3B	2.27	1.49	1.45
82	nF	202	PEB	C1C-C2C	2.27	1.48	1.42
82	p8	202	PEB	C1C-NC	-2.27	1.34	1.37
82	QA	202	PEB	C4A-NA	-2.27	1.32	1.37
82	SG	201	PEB	C4A-NA	-2.27	1.32	1.37
82	LP	201	PEB	C4A-NA	-2.27	1.32	1.37
82	OG	201	PEB	OD-C4D	2.27	1.27	1.23
82	M7	201	PEB	OD-C4D	2.27	1.27	1.23
82	PM	202	PEB	C1C-C2C	2.27	1.48	1.42
82	U1	201	PEB	C1C-C2C	2.27	1.48	1.42
82	N9	201	PEB	C1C-C2C	2.27	1.48	1.42
82	ZF	202	PEB	CHC-C4C	2.27	1.52	1.49
87	AN	814	CLA	MG-NB	-2.27	2.01	2.05
82	sK	203	PEB	C4A-NA	-2.27	1.32	1.37
82	KF	202	PEB	C1B-C2B	2.27	1.50	1.45
82	kM	202	PEB	C1C-C2C	2.27	1.48	1.42
82	OM	202	PEB	C2A-C1A	-2.27	1.50	1.52
87	R2	203	CLA	CMD-C2D	-2.27	1.46	1.50
82	HQ	203	PEB	C1C-C2C	2.27	1.48	1.42
82	BB	202	PEB	C4A-NA	-2.27	1.32	1.37
87	b6	610	CLA	CMB-C2B	-2.27	1.46	1.50
87	bL	619	CLA	CMD-C2D	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	K5	202	PEB	C4A-NA	-2.27	1.32	1.37
87	32	309	CLA	MG-NB	-2.27	2.01	2.05
87	B2	806	CLA	CMB-C2B	-2.27	1.46	1.50
82	OD	202	PEB	C1C-C2C	2.27	1.48	1.42
82	OQ	202	PEB	C1C-C2C	2.27	1.48	1.42
82	lK	201	PEB	C1C-C2C	2.27	1.48	1.42
83	AH	304	PUB	C4B-C3B	2.27	1.48	1.42
82	PP	202	PEB	C4A-NA	-2.27	1.32	1.37
82	A5	202	PEB	C4A-NA	-2.27	1.32	1.37
87	cL	509	CLA	MG-NB	-2.27	2.01	2.05
82	DM	202	PEB	C1C-C2C	2.27	1.48	1.42
82	BP	202	PEB	C4A-NA	-2.27	1.32	1.37
87	B6	603	CLA	MG-NB	-2.27	2.01	2.05
87	4N	601	CLA	MG-NB	-2.27	2.01	2.05
87	AN	820	CLA	C1B-NB	-2.27	1.35	1.37
87	cL	510	CLA	C1B-C2B	2.27	1.48	1.43
82	XA	203	PEB	C1C-C2C	2.27	1.48	1.42
82	UM	201	PEB	C1C-C2C	2.27	1.48	1.42
82	hJ	201	PEB	C4B-C3B	2.27	1.49	1.45
82	YM	202	PEB	C4A-NA	-2.27	1.32	1.37
82	PD	201	PEB	C2A-C1A	-2.27	1.50	1.52
82	FI	201	PEB	C2A-C1A	-2.27	1.50	1.52
82	CM	202	PEB	C2A-C1A	-2.27	1.50	1.52
82	dJ	201	PEB	C2A-C1A	-2.27	1.50	1.52
82	mE	202	PEB	CHC-C4C	2.26	1.52	1.49
87	1N	611	CLA	CMC-C2C	-2.26	1.46	1.50
82	T5	202	PEB	C4A-NA	-2.26	1.32	1.37
87	A2	852	CLA	C4B-NB	2.26	1.40	1.37
87	KN	105	CLA	CMD-C2D	-2.26	1.46	1.50
82	BA	203	PEB	C1C-NC	-2.26	1.34	1.37
82	OF	201	PEB	CHC-C4C	2.26	1.52	1.49
87	AN	811	CLA	MG-ND	-2.26	2.01	2.05
87	cL	508	CLA	MG-NB	-2.26	2.01	2.05
87	AN	815	CLA	CMD-C2D	-2.26	1.46	1.50
87	B2	821	CLA	CMD-C2D	-2.26	1.46	1.50
82	S5	201	PEB	C4B-C3B	2.26	1.49	1.45
82	dD	401	PEB	C1C-NC	-2.26	1.34	1.37
82	dG	201	PEB	C1C-NC	-2.26	1.34	1.37
82	P5	202	PEB	C4A-NA	-2.26	1.32	1.37
87	82	305	CLA	C1B-C2B	2.26	1.48	1.43
82	JK	201	PEB	C1C-C2C	2.26	1.48	1.42
82	D9	202	PEB	C1C-C2C	2.26	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	840	CLA	CMB-C2B	-2.26	1.46	1.50
87	bL	615	CLA	CMB-C2B	-2.26	1.46	1.50
82	lF	203	PEB	CHC-C4C	2.26	1.52	1.49
82	TA	201	PEB	C1C-C2C	2.26	1.48	1.42
82	AO	304	PEB	C1C-C2C	2.26	1.48	1.42
82	k1	201	PEB	C1C-NC	-2.26	1.34	1.37
82	c1	202	PEB	C1C-NC	-2.26	1.34	1.37
87	B6	610	CLA	CMD-C2D	-2.26	1.46	1.50
87	c6	610	CLA	CMD-C2D	-2.26	1.46	1.50
87	CL	518	CLA	MG-NB	-2.26	2.01	2.05
87	A2	814	CLA	MG-NB	-2.26	2.01	2.05
82	R9	201	PEB	C1C-C2C	2.26	1.48	1.42
82	SF	202	PEB	OD-C4D	2.26	1.27	1.23
87	AN	815	CLA	CMC-C2C	-2.26	1.46	1.50
82	VK	202	PEB	C1C-C2C	2.26	1.48	1.42
82	QE	202	PEB	C4A-NA	-2.26	1.32	1.37
82	PG	202	PEB	C4A-NA	-2.26	1.32	1.37
82	nF	202	PEB	C4A-NA	-2.26	1.32	1.37
82	aO	202	PEB	C4A-NA	-2.26	1.32	1.37
84	N1	1001	CYC	C4C-NC	-2.26	1.32	1.37
87	A2	803	CLA	CMB-C2B	-2.26	1.46	1.50
82	AA	202	PEB	C1C-NC	-2.26	1.34	1.37
82	A7	202	PEB	C1C-NC	-2.26	1.34	1.37
87	BL	621	CLA	C1B-C2B	2.26	1.48	1.43
84	73	1002	CYC	C4A-C3A	2.26	1.50	1.45
84	E1	1001	CYC	C1B-C2B	2.26	1.49	1.45
87	B2	825	CLA	CHC-C1C	2.26	1.43	1.38
82	B5	202	PEB	CHC-C4C	2.26	1.52	1.49
82	W5	203	PEB	C4A-NA	-2.26	1.32	1.37
82	hJ	202	PEB	C4A-NA	-2.26	1.32	1.37
82	lF	203	PEB	C1D-ND	2.26	1.49	1.45
82	q8	203	PEB	C1C-C2C	2.26	1.48	1.42
87	52	602	CLA	MG-NB	-2.26	2.01	2.05
82	LQ	203	PEB	C2A-C1A	-2.26	1.50	1.52
82	q8	201	PEB	C2A-C1A	-2.26	1.50	1.52
82	DF	203	PEB	C4A-NA	-2.26	1.32	1.37
82	PJ	202	PEB	C4A-NA	-2.26	1.32	1.37
82	dB	201	PEB	C4A-NA	-2.26	1.32	1.37
87	BN	818	CLA	C1B-C2B	2.26	1.48	1.43
87	B2	810	CLA	CMD-C2D	-2.26	1.46	1.50
84	J1	1001	CYC	C4D-C3D	2.26	1.48	1.42
82	JA	201	PEB	C1C-NC	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	F7	202	PEB	C2A-C1A	-2.26	1.50	1.52
82	qC	201	PEB	C2A-C1A	-2.26	1.50	1.52
82	RJ	202	PEB	C4A-NA	-2.26	1.32	1.37
82	f1	201	PEB	C4A-NA	-2.26	1.32	1.37
82	O4	202	PEB	C1D-ND	2.26	1.49	1.45
87	HL	102	CLA	CMB-C2B	-2.26	1.46	1.50
82	eJ	201	PEB	CHC-C4C	2.26	1.52	1.49
82	K9	201	PEB	C1C-C2C	2.26	1.48	1.42
82	OH	203	PEB	C4A-NA	-2.26	1.32	1.37
82	UQ	201	PEB	C4B-C3B	2.26	1.49	1.45
82	lE	201	PEB	C4B-C3B	2.26	1.49	1.45
94	D6	408	PL9	C2-C1	-2.26	1.38	1.44
87	B2	805	CLA	CMD-C2D	-2.26	1.46	1.50
82	gF	201	PEB	C1B-C2B	2.26	1.50	1.45
84	L4	1001	CYC	C4A-C3A	2.26	1.50	1.45
82	AO	305	PEB	C1C-C2C	2.26	1.48	1.42
82	P9	201	PEB	C1C-C2C	2.26	1.48	1.42
82	iM	202	PEB	C1C-C2C	2.26	1.48	1.42
82	QB	204	PEB	C4A-NA	-2.26	1.32	1.37
82	DE	1002	PEB	C4A-NA	-2.26	1.32	1.37
82	O9	203	PEB	C4A-NA	-2.26	1.32	1.37
83	M5	303	PUB	C4B-NB	-2.26	1.34	1.37
84	NH	1001	CYC	C1B-NB	-2.26	1.34	1.37
87	RN	203	CLA	CMD-C2D	-2.26	1.46	1.50
82	gH	203	PEB	CHC-C4C	2.26	1.52	1.49
82	SP	202	PEB	C1C-C2C	2.26	1.48	1.42
82	XB	202	PEB	C4A-NA	-2.26	1.32	1.37
82	N5	202	PEB	C4A-NA	-2.26	1.32	1.37
82	UH	202	PEB	CHA-C4A	-2.26	1.32	1.36
82	QK	202	PEB	C1C-C2C	2.26	1.48	1.42
82	Z1	203	PEB	C1C-C2C	2.26	1.48	1.42
82	L7	203	PEB	C1C-C2C	2.26	1.48	1.42
82	N1	1002	PEB	C4B-C3B	2.26	1.49	1.45
82	OG	202	PEB	C4A-NA	-2.26	1.32	1.37
82	TI	201	PEB	C4A-NA	-2.26	1.32	1.37
82	c4	201	PEB	C4A-NA	-2.26	1.32	1.37
87	C6	520	CLA	MG-NB	-2.26	2.01	2.05
94	aL	601	PL9	O1-C4	2.26	1.28	1.23
87	42	603	CLA	CMD-C2D	-2.26	1.46	1.50
82	fG	203	PEB	CHC-C4C	2.26	1.52	1.49
82	aK	201	PEB	C1C-C2C	2.26	1.48	1.42
82	fO	202	PEB	C1C-C2C	2.26	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	j1	202	PEB	C2A-C1A	-2.26	1.50	1.52
82	eH	203	PEB	C2A-C1A	-2.26	1.50	1.52
82	OM	201	PEB	C4A-NA	-2.26	1.32	1.37
82	Q5	203	PEB	C4A-NA	-2.26	1.32	1.37
87	b6	610	CLA	MG-NB	-2.26	2.01	2.05
87	7N	602	CLA	C1B-C2B	2.26	1.48	1.43
87	AN	831	CLA	CMD-C2D	-2.26	1.46	1.50
87	BN	831	CLA	MG-ND	-2.26	2.01	2.05
82	iK	201	PEB	OD-C4D	2.26	1.27	1.23
82	N1	1002	PEB	C2A-C1A	-2.26	1.50	1.52
82	r8	201	PEB	C2A-C1A	-2.26	1.50	1.52
82	A9	202	PEB	C2A-C1A	-2.26	1.50	1.52
82	OM	203	PEB	C1C-C2C	2.26	1.48	1.42
82	EP	202	PEB	C1C-C2C	2.26	1.48	1.42
87	b6	604	CLA	MG-NB	-2.26	2.01	2.05
82	NM	201	PEB	C4A-NA	-2.26	1.32	1.37
82	ZM	201	PEB	C4A-NA	-2.26	1.32	1.37
87	K2	101	CLA	CMD-C2D	-2.26	1.46	1.50
87	8N	303	CLA	CMD-C2D	-2.26	1.46	1.50
82	HF	202	PEB	C1C-NC	-2.26	1.34	1.37
84	D4	1001	CYC	OB-C4B	2.26	1.27	1.23
82	A7	202	PEB	C1D-ND	2.26	1.49	1.45
82	HH	1002	PEB	C4A-NA	-2.26	1.32	1.37
82	aO	203	PEB	C4B-C3B	2.26	1.49	1.45
82	HI	201	PEB	C1C-C2C	2.26	1.48	1.42
82	d4	202	PEB	C2A-C1A	-2.25	1.50	1.52
87	82	302	CLA	CMD-C2D	-2.25	1.46	1.50
87	bL	620	CLA	CMB-C2B	-2.25	1.46	1.50
82	QP	201	PEB	C1B-C2B	2.25	1.50	1.45
82	SF	202	PEB	C1C-NC	-2.25	1.34	1.37
82	U9	204	PEB	C1C-NC	-2.25	1.34	1.37
84	M4	1001	CYC	C4C-NC	-2.25	1.32	1.37
87	BL	601	CLA	CMB-C2B	-2.25	1.46	1.50
82	FI	201	PEB	C1C-NC	-2.25	1.34	1.37
82	HF	202	PEB	C4A-NA	-2.25	1.32	1.37
82	T4	202	PEB	C4A-NA	-2.25	1.32	1.37
87	4N	609	CLA	CMD-C2D	-2.25	1.46	1.50
82	CD	201	PEB	C1B-C2B	2.25	1.50	1.45
87	bL	615	CLA	MG-NB	-2.25	2.01	2.05
82	SA	202	PEB	C4A-NA	-2.25	1.32	1.37
82	eJ	202	PEB	C4A-NA	-2.25	1.32	1.37
82	cM	201	PEB	C4A-NA	-2.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	613	CLA	CMB-C2B	-2.25	1.46	1.50
87	K2	106	CLA	CAC-C3C	-2.25	1.45	1.51
87	B2	804	CLA	MG-ND	-2.25	2.01	2.05
82	qC	202	PEB	C1C-C2C	2.25	1.48	1.42
82	g1	201	PEB	C4B-C3B	2.25	1.49	1.45
82	OO	201	PEB	C4A-NA	-2.25	1.32	1.37
82	qC	201	PEB	C4A-NA	-2.25	1.32	1.37
87	b6	613	CLA	CMC-C2C	-2.25	1.46	1.50
82	CP	202	PEB	C1B-C2B	2.25	1.50	1.45
84	N1	1001	CYC	C4A-C3A	2.25	1.50	1.45
82	YO	201	PEB	C1C-C2C	2.25	1.48	1.42
82	Y4	201	PEB	C1C-C2C	2.25	1.48	1.42
87	5N	607	CLA	MG-NB	-2.25	2.01	2.05
82	cK	201	PEB	C4A-NA	-2.25	1.32	1.37
82	H9	202	PEB	C2A-C1A	-2.25	1.50	1.52
87	BN	828	CLA	C1B-C2B	2.25	1.48	1.43
87	AN	816	CLA	CMB-C2B	-2.25	1.46	1.50
87	BN	806	CLA	CMD-C2D	-2.25	1.46	1.50
82	IM	201	PEB	C1C-C2C	2.25	1.48	1.42
82	D7	202	PEB	C1C-C2C	2.25	1.48	1.42
82	L9	201	PEB	C1C-C2C	2.25	1.48	1.42
82	mE	201	PEB	C1C-C2C	2.25	1.48	1.42
84	EE	1001	CYC	C4B-NB	-2.25	1.33	1.38
82	r8	201	PEB	C1C-NC	-2.25	1.34	1.37
82	G5	202	PEB	C4A-NA	-2.25	1.32	1.37
87	D6	403	CLA	CMC-C2C	-2.25	1.46	1.50
82	lF	201	PEB	CHC-C4C	2.25	1.52	1.49
82	oF	203	PEB	C1D-ND	2.25	1.49	1.45
87	B6	616	CLA	CHC-C1C	2.25	1.43	1.38
87	AN	812	CLA	MG-NB	-2.25	2.01	2.05
87	52	607	CLA	MG-NB	-2.25	2.01	2.05
87	82	301	CLA	MG-NB	-2.25	2.01	2.05
83	Z9	302	PUB	C3C-C4C	2.25	1.51	1.43
82	O5	202	PEB	C4A-NA	-2.25	1.32	1.37
82	P7	201	PEB	C1C-C2C	2.25	1.48	1.42
82	h4	202	PEB	C2A-C1A	-2.25	1.50	1.52
82	W9	202	PEB	C2A-C1A	-2.25	1.50	1.52
82	ED	202	PEB	C4A-NA	-2.25	1.32	1.37
82	X5	202	PEB	C4A-NA	-2.25	1.32	1.37
82	w8	204	PEB	C4A-NA	-2.25	1.32	1.37
82	TD	202	PEB	C1C-C2C	2.25	1.48	1.42
82	ED	202	PEB	C1C-NC	-2.25	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	UG	203	PEB	C1C-NC	-2.25	1.34	1.37
82	L1	1002	PEB	C1C-NC	-2.25	1.34	1.37
87	a6	607	CLA	CMD-C2D	-2.25	1.46	1.50
82	IJ	202	PEB	OD-C4D	2.25	1.27	1.23
84	NE	201	CYC	C4B-NB	-2.25	1.33	1.38
87	A2	811	CLA	MG-ND	-2.25	2.01	2.05
82	f4	201	PEB	C4A-NA	-2.25	1.32	1.37
82	zC	201	PEB	C4A-NA	-2.25	1.32	1.37
82	TQ	202	PEB	C1C-C2C	2.25	1.48	1.42
82	WF	202	PEB	C1B-C2B	2.25	1.50	1.45
82	YM	203	PEB	C2A-C1A	-2.25	1.50	1.52
82	TQ	201	PEB	C2A-C1A	-2.25	1.50	1.52
82	ND	204	PEB	C1C-C2C	2.25	1.48	1.42
87	b6	607	CLA	MG-NB	-2.25	2.01	2.05
87	bL	604	CLA	CMD-C2D	-2.25	1.46	1.50
87	1N	606	CLA	CMD-C2D	-2.25	1.46	1.50
82	HH	1002	PEB	C4B-C3B	2.25	1.49	1.45
82	OK	201	PEB	OD-C4D	2.25	1.27	1.23
82	IP	203	PEB	OD-C4D	2.25	1.27	1.23
87	A2	830	CLA	C1B-NB	-2.25	1.35	1.37
82	V4	201	PEB	C4A-NA	-2.25	1.32	1.37
87	72	602	CLA	MG-NB	-2.25	2.01	2.05
82	KJ	202	PEB	C1C-C2C	2.25	1.48	1.42
82	X9	201	PEB	C1C-C2C	2.25	1.48	1.42
82	eH	203	PEB	CHC-C4C	2.25	1.52	1.49
82	VB	202	PEB	C2A-C1A	-2.25	1.50	1.52
87	bL	606	CLA	C1B-NB	-2.25	1.35	1.37
87	C6	512	CLA	MG-NB	-2.25	2.01	2.05
82	HB	202	PEB	C1C-NC	-2.25	1.34	1.37
82	vF	201	PEB	C4B-C3B	2.25	1.49	1.45
87	KN	105	CLA	CAC-C3C	-2.25	1.45	1.51
82	DA	203	PEB	C1C-C2C	2.25	1.48	1.42
82	gJ	201	PEB	C1C-C2C	2.25	1.48	1.42
82	B7	202	PEB	CHC-C4C	2.25	1.52	1.49
84	NE	201	CYC	C1B-C2B	2.25	1.49	1.45
84	LH	1002	CYC	C4C-NC	-2.25	1.32	1.37
87	BL	619	CLA	MG-NB	-2.25	2.01	2.05
87	b6	607	CLA	CMB-C2B	-2.25	1.46	1.50
82	MB	202	PEB	C1C-C2C	2.25	1.48	1.42
82	KD	201	PEB	C1C-C2C	2.25	1.48	1.42
82	T1	201	PEB	C1C-C2C	2.25	1.48	1.42
84	LE	1001	CYC	C4D-ND	-2.25	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CJ	202	PEB	C2A-C1A	-2.25	1.50	1.52
82	V9	202	PEB	C2A-C1A	-2.25	1.50	1.52
82	iE	201	PEB	C2A-C1A	-2.25	1.50	1.52
82	LD	202	PEB	C4A-NA	-2.25	1.32	1.37
87	6N	604	CLA	C1D-C2D	2.25	1.49	1.45
85	A2	848	BCR	C19-C18	2.25	1.50	1.45
87	12	607	CLA	MG-NB	-2.25	2.01	2.05
82	uK	202	PEB	C1C-C2C	2.25	1.48	1.42
83	Y7	302	PUB	C4B-C3B	2.25	1.48	1.42
82	IF	201	PEB	O1C-CGC	2.25	1.29	1.22
82	KE	201	PEB	C4A-NA	-2.25	1.32	1.37
84	F1	1001	CYC	C4C-NC	-2.25	1.32	1.37
87	72	602	CLA	C1B-C2B	2.25	1.48	1.43
82	q8	201	PEB	C4A-NA	-2.25	1.32	1.37
82	XK	203	PEB	C1C-C2C	2.25	1.48	1.42
87	A2	822	CLA	C3B-C4B	2.25	1.48	1.42
82	OO	202	PEB	C1D-ND	2.25	1.49	1.45
84	BE	1001	CYC	C4D-C3D	2.25	1.48	1.42
87	BL	619	CLA	CMD-C2D	-2.25	1.46	1.50
87	AN	841	CLA	CMC-C2C	-2.25	1.46	1.50
82	M5	305	PEB	C1C-NC	-2.25	1.34	1.37
82	V9	201	PEB	C1C-C2C	2.25	1.48	1.42
82	HM	202	PEB	C1B-C2B	2.25	1.50	1.45
82	gG	201	PEB	C4A-NA	-2.25	1.32	1.37
82	AI	203	PEB	C2A-C1A	-2.25	1.50	1.52
82	A7	202	PEB	C2A-C1A	-2.25	1.50	1.52
82	vC	202	PEB	C2A-C1A	-2.25	1.50	1.52
87	BN	831	CLA	CMB-C2B	-2.25	1.46	1.50
87	BN	808	CLA	MG-ND	-2.25	2.01	2.05
82	TD	201	PEB	C1C-C2C	2.25	1.48	1.42
82	NQ	203	PEB	C1C-C2C	2.25	1.48	1.42
82	O9	203	PEB	C1C-C2C	2.25	1.48	1.42
82	sC	202	PEB	C1C-C2C	2.25	1.48	1.42
82	WD	202	PEB	C4B-C3B	2.25	1.49	1.45
82	cJ	202	PEB	C4B-C3B	2.25	1.49	1.45
84	JO	1001	CYC	C4A-C3A	2.25	1.50	1.45
82	S4	202	PEB	C4A-NA	-2.25	1.32	1.37
82	wC	204	PEB	C4A-NA	-2.25	1.32	1.37
87	ON	203	CLA	CMB-C2B	-2.25	1.46	1.50
87	12	610	CLA	CHC-C1C	2.25	1.43	1.38
87	nL	101	CLA	MG-NB	-2.25	2.01	2.05
84	FO	1001	CYC	OB-C4B	2.25	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kH	203	PEB	C1C-C2C	2.25	1.48	1.42
82	mO	203	PEB	C1C-C2C	2.25	1.48	1.42
82	EJ	203	PEB	C1C-NC	-2.25	1.34	1.37
85	C6	508	BCR	C30-C25	-2.25	1.50	1.53
82	rK	202	PEB	C4A-NA	-2.25	1.32	1.37
87	62	309	CLA	CHC-C4B	-2.25	1.34	1.39
82	RD	203	PEB	C4B-C3B	2.24	1.49	1.45
87	AN	851	CLA	CMC-C2C	-2.24	1.46	1.50
82	Z9	303	PEB	C1C-C2C	2.24	1.48	1.42
82	UK	202	PEB	C1C-NC	-2.24	1.34	1.37
82	YA	303	PEB	C4B-C3B	2.24	1.49	1.45
82	cE	201	PEB	C4B-C3B	2.24	1.49	1.45
82	iK	202	PEB	CHC-C4C	2.24	1.52	1.49
87	BN	814	CLA	MG-NB	-2.24	2.01	2.05
95	C6	503	DGD	O2G-C2G	-2.24	1.41	1.46
82	OP	201	PEB	C4A-NA	-2.24	1.32	1.37
87	bL	607	CLA	C1B-C2B	2.24	1.48	1.43
82	Y5	203	PEB	C1C-C2C	2.24	1.48	1.42
87	CL	510	CLA	MG-ND	-2.24	2.01	2.05
87	RN	202	CLA	MG-NB	-2.24	2.01	2.05
82	ZF	201	PEB	C4B-C3B	2.24	1.49	1.45
82	h1	201	PEB	C4B-C3B	2.24	1.49	1.45
82	O4	202	PEB	C2A-C1A	-2.24	1.50	1.52
82	g4	203	PEB	C2A-C1A	-2.24	1.50	1.52
82	ZH	203	PEB	C1C-C2C	2.24	1.48	1.42
82	OQ	201	PEB	C1D-ND	2.24	1.49	1.45
82	G9	201	PEB	C1C-C2C	2.24	1.48	1.42
87	A2	815	CLA	CMC-C2C	-2.24	1.46	1.50
82	OJ	202	PEB	C1C-NC	-2.24	1.34	1.37
82	VH	201	PEB	C1B-C2B	2.24	1.50	1.45
82	M9	305	PEB	C1B-C2B	2.24	1.50	1.45
87	42	602	CLA	C1B-C2B	2.24	1.48	1.43
87	62	309	CLA	C4D-CHA	2.24	1.46	1.38
82	FB	201	PEB	C4A-NA	-2.24	1.32	1.37
82	WQ	201	PEB	C1C-C2C	2.24	1.48	1.42
87	4N	603	CLA	CMD-C2D	-2.24	1.46	1.50
82	wF	301	PEB	C2A-C1A	-2.24	1.50	1.52
87	FN	201	CLA	C3C-C2C	2.24	1.41	1.36
87	A2	832	CLA	C3B-C4B	2.24	1.48	1.42
87	B2	817	CLA	C1B-C2B	2.24	1.48	1.43
82	PG	202	PEB	C1C-NC	-2.24	1.34	1.37
82	D7	202	PEB	C1D-ND	2.24	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SD	201	PEB	C1C-C2C	2.24	1.48	1.42
82	KG	201	PEB	C1C-C2C	2.24	1.48	1.42
82	HA	203	PEB	C4A-NA	-2.24	1.32	1.37
82	JK	202	PEB	CHC-C4C	2.24	1.52	1.49
82	lM	203	PEB	C1C-NC	-2.24	1.34	1.37
82	vK	202	PEB	C2A-C1A	-2.24	1.50	1.52
82	DA	202	PEB	C1C-C2C	2.24	1.48	1.42
82	TO	201	PEB	C4A-NA	-2.24	1.32	1.37
82	R5	202	PEB	C4A-NA	-2.24	1.32	1.37
82	gO	201	PEB	C4A-NA	-2.24	1.32	1.37
87	BL	623	CLA	MG-NB	-2.24	2.01	2.05
87	AN	840	CLA	CMD-C2D	-2.24	1.46	1.50
87	B6	612	CLA	CMD-C2D	-2.24	1.46	1.50
84	v3	1001	CYC	OB-C4B	2.24	1.27	1.23
82	GM	203	PEB	C1C-C2C	2.24	1.48	1.42
82	Z9	304	PEB	C1B-C2B	2.24	1.50	1.45
82	XJ	202	PEB	C4A-NA	-2.24	1.32	1.37
87	AN	838	CLA	CMC-C2C	-2.24	1.46	1.50
87	FN	201	CLA	MG-NB	-2.24	2.01	2.05
87	32	309	CLA	C1B-C2B	2.24	1.48	1.43
82	DD	201	PEB	C4B-C3B	2.24	1.49	1.45
82	VD	203	PEB	C1C-C2C	2.24	1.48	1.42
82	hH	201	PEB	C1C-C2C	2.24	1.48	1.42
87	B2	801	CLA	C4D-ND	-2.24	1.34	1.37
82	lG	203	PEB	C2A-C1A	-2.24	1.50	1.52
87	BL	623	CLA	CMB-C2B	-2.24	1.46	1.50
87	RN	204	CLA	CMB-C2B	-2.24	1.46	1.50
87	I2	102	CLA	CMD-C2D	-2.24	1.46	1.50
84	ME	1001	CYC	C4B-NB	-2.24	1.33	1.38
82	BI	201	PEB	C1B-C2B	2.24	1.50	1.45
82	lM	201	PEB	C4B-C3B	2.24	1.49	1.45
82	FP	201	PEB	C4A-NA	-2.24	1.32	1.37
82	e4	201	PEB	C4A-NA	-2.24	1.32	1.37
87	AL	403	CLA	C1B-C2B	2.24	1.48	1.43
87	12	611	CLA	CMC-C2C	-2.24	1.46	1.50
82	aF	202	PEB	C1B-C2B	2.24	1.50	1.45
87	BN	820	CLA	C1B-C2B	2.24	1.48	1.43
82	FI	201	PEB	C4A-NA	-2.24	1.32	1.37
82	HM	201	PEB	C4A-NA	-2.24	1.32	1.37
82	nK	201	PEB	C4B-C3B	2.24	1.49	1.45
83	A1	304	PUB	C1C-C2C	2.24	1.49	1.45
87	42	604	CLA	CMB-C2B	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	841	CLA	CMC-C2C	-2.24	1.46	1.50
82	T7	201	PEB	C1C-C2C	2.24	1.48	1.42
82	L4	1002	PEB	C1C-NC	-2.24	1.34	1.37
82	NQ	202	PEB	C2A-C1A	-2.24	1.50	1.52
82	A4	301	PEB	C2A-C1A	-2.24	1.50	1.52
82	K5	202	PEB	C2A-C1A	-2.24	1.50	1.52
82	Z5	301	PEB	C2A-C1A	-2.24	1.50	1.52
82	kO	201	PEB	C2A-C1A	-2.24	1.50	1.52
82	SG	203	PEB	C1C-C2C	2.24	1.48	1.42
87	BL	620	CLA	CHC-C4B	-2.24	1.34	1.39
87	B2	807	CLA	MG-ND	-2.24	2.01	2.05
87	2N	301	CLA	C4B-C3B	2.24	1.48	1.43
82	QE	201	PEB	C4A-NA	-2.24	1.32	1.37
82	hG	202	PEB	C4A-NA	-2.24	1.32	1.37
82	bK	201	PEB	C1C-C2C	2.24	1.48	1.42
87	bL	616	CLA	CMD-C2D	-2.24	1.46	1.50
87	b6	615	CLA	MG-NB	-2.24	2.01	2.05
82	aK	202	PEB	C1B-C2B	2.24	1.50	1.45
82	dM	201	PEB	C4B-C3B	2.24	1.49	1.45
82	mE	203	PEB	C2A-C1A	-2.24	1.50	1.52
82	cO	201	PEB	C2A-C1A	-2.24	1.50	1.52
82	EK	202	PEB	C4A-NA	-2.24	1.32	1.37
82	S7	202	PEB	C4A-NA	-2.24	1.32	1.37
87	AN	820	CLA	CMB-C2B	-2.24	1.46	1.50
87	C6	513	CLA	CMD-C2D	-2.24	1.46	1.50
87	c6	614	CLA	MG-NB	-2.24	2.01	2.05
83	M9	303	PUB	C3C-C4C	2.24	1.51	1.43
82	BA	203	PEB	C4A-NA	-2.24	1.32	1.37
82	JF	202	PEB	C4A-NA	-2.24	1.32	1.37
82	FH	1002	PEB	C4A-NA	-2.24	1.32	1.37
82	c4	202	PEB	C4A-NA	-2.24	1.32	1.37
87	A2	816	CLA	CMC-C2C	-2.24	1.46	1.50
87	A2	832	CLA	CMC-C2C	-2.24	1.46	1.50
87	CL	503	CLA	C1B-C2B	2.24	1.48	1.43
82	rF	202	PEB	C1B-C2B	2.24	1.50	1.45
87	B2	813	CLA	MG-NB	-2.24	2.01	2.05
82	jK	202	PEB	C4A-NA	-2.24	1.32	1.37
82	yK	301	PEB	C4A-NA	-2.24	1.32	1.37
82	PK	202	PEB	C2A-C1A	-2.24	1.50	1.52
87	cL	513	CLA	CMD-C2D	-2.24	1.46	1.50
82	bH	202	PEB	C4B-C3B	2.24	1.49	1.45
84	KG	202	CYC	C4B-NB	-2.24	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DD	201	PEB	C4A-NA	-2.24	1.32	1.37
82	WI	201	PEB	C4A-NA	-2.24	1.32	1.37
84	JO	1001	CYC	C4C-NC	-2.24	1.32	1.37
87	CL	506	CLA	CMC-C2C	-2.24	1.46	1.50
82	S4	201	PEB	C1B-C2B	2.24	1.50	1.45
84	C4	1001	CYC	C4B-NB	-2.24	1.33	1.38
82	ID	202	PEB	C1C-NC	-2.24	1.34	1.37
82	y8	202	PEB	C4B-C3B	2.24	1.49	1.45
82	s8	203	PEB	C4B-C3B	2.24	1.49	1.45
82	fM	203	PEB	C4B-C3B	2.24	1.49	1.45
87	B2	825	CLA	MG-ND	-2.24	2.01	2.05
82	u8	201	PEB	C4A-NA	-2.24	1.32	1.37
82	HD	203	PEB	C1C-C2C	2.24	1.48	1.42
82	q8	202	PEB	C1C-C2C	2.24	1.48	1.42
82	S1	202	PEB	C2A-C1A	-2.24	1.50	1.52
82	DQ	203	PEB	CHC-C4C	2.24	1.52	1.49
87	72	607	CLA	MG-NB	-2.24	2.01	2.05
87	B2	801	CLA	MG-NB	-2.24	2.01	2.05
82	UB	301	PEB	C1C-NC	-2.24	1.34	1.37
82	DQ	201	PEB	C4A-NA	-2.24	1.32	1.37
82	g4	201	PEB	C1C-C2C	2.24	1.48	1.42
82	lE	203	PEB	C1C-C2C	2.24	1.48	1.42
87	BN	802	CLA	C4D-ND	-2.24	1.34	1.37
82	wF	303	PEB	C1B-C2B	2.24	1.50	1.45
82	W4	201	PEB	OD-C4D	2.24	1.27	1.23
82	LQ	202	PEB	C4A-NA	-2.24	1.32	1.37
82	j1	201	PEB	C4A-NA	-2.24	1.32	1.37
87	bL	606	CLA	CHC-C1C	2.24	1.43	1.38
87	1N	610	CLA	CHC-C1C	2.24	1.43	1.38
87	8N	301	CLA	C3D-C4D	2.24	1.49	1.44
82	bF	201	PEB	C1C-C2C	2.23	1.48	1.42
82	eH	201	PEB	C1C-C2C	2.23	1.48	1.42
96	VL	201	HEM	C1C-C2C	-2.23	1.40	1.45
87	AN	806	CLA	C1B-C2B	2.23	1.48	1.43
82	iG	202	PEB	C2A-C1A	-2.23	1.50	1.52
82	qK	201	PEB	C2A-C1A	-2.23	1.50	1.52
82	g1	201	PEB	C1C-NC	-2.23	1.34	1.37
82	ZG	202	PEB	C4A-NA	-2.23	1.32	1.37
82	UH	201	PEB	C4A-NA	-2.23	1.32	1.37
82	IB	202	PEB	C1C-NC	-2.23	1.34	1.37
87	12	608	CLA	C1D-C2D	2.23	1.49	1.45
82	HO	1002	PEB	C1C-C2C	2.23	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	H4	1002	PEB	C1C-C2C	2.23	1.48	1.42
82	fB	301	PEB	C1C-C2C	2.23	1.48	1.42
82	AG	304	PEB	C4A-NA	-2.23	1.32	1.37
82	U1	201	PEB	C4A-NA	-2.23	1.32	1.37
82	fH	201	PEB	C4A-NA	-2.23	1.32	1.37
87	BL	604	CLA	CMD-C2D	-2.23	1.46	1.50
87	4N	603	CLA	C1B-C2B	2.23	1.48	1.43
82	S5	203	PEB	C1C-C2C	2.23	1.48	1.42
82	Q9	203	PEB	C4B-C3B	2.23	1.49	1.45
82	iK	203	PEB	C4B-C3B	2.23	1.49	1.45
87	bL	615	CLA	C1B-C2B	2.23	1.48	1.43
82	AQ	303	PEB	C1C-C2C	2.23	1.48	1.42
87	1N	608	CLA	C1D-C2D	2.23	1.49	1.45
82	FM	202	PEB	C1C-NC	-2.23	1.34	1.37
82	bK	202	PEB	C1C-NC	-2.23	1.34	1.37
82	u8	201	PEB	C1D-ND	2.23	1.49	1.45
82	TF	202	PEB	C4B-C3B	2.23	1.49	1.45
82	UA	201	PEB	C4B-NB	-2.23	1.33	1.38
82	AA	201	PEB	CHC-C4C	2.23	1.52	1.49
82	H1	1002	PEB	C4A-NA	-2.23	1.32	1.37
87	bL	620	CLA	MG-NB	-2.23	2.01	2.05
82	QP	203	PEB	C1C-NC	-2.23	1.34	1.37
82	EQ	202	PEB	C1C-NC	-2.23	1.34	1.37
87	AN	832	CLA	C1B-NB	-2.23	1.35	1.37
82	UE	203	PEB	C4A-NA	-2.23	1.32	1.37
82	m1	201	PEB	C4A-NA	-2.23	1.32	1.37
82	mO	203	PEB	C4A-NA	-2.23	1.32	1.37
82	IK	203	PEB	OD-C4D	2.23	1.27	1.23
84	F4	1001	CYC	OB-C4B	2.23	1.27	1.23
82	IK	203	PEB	C2C-C3C	2.23	1.44	1.38
82	NP	202	PEB	C2A-C1A	-2.23	1.50	1.52
82	S5	202	PEB	C2A-C1A	-2.23	1.50	1.52
82	O9	202	PEB	C2A-C1A	-2.23	1.50	1.52
82	iG	201	PEB	C2A-C1A	-2.23	1.50	1.52
82	VB	201	PEB	C4A-NA	-2.23	1.32	1.37
84	N4	1001	CYC	C4C-NC	-2.23	1.32	1.37
87	AN	835	CLA	CMB-C2B	-2.23	1.46	1.50
82	LI	201	PEB	C1C-C2C	2.23	1.48	1.42
87	C6	513	CLA	MG-NB	-2.23	2.01	2.05
87	42	605	CLA	C1B-NB	-2.23	1.35	1.37
82	OO	201	PEB	OD-C4D	2.23	1.27	1.23
82	cB	403	PEB	C1C-NC	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	YE	202	PEB	C4A-NA	-2.23	1.32	1.37
82	MF	201	PEB	C4A-NA	-2.23	1.32	1.37
87	BN	824	CLA	CMC-C2C	-2.23	1.46	1.50
87	A2	813	CLA	CMD-C2D	-2.23	1.46	1.50
83	YA	302	PUB	C4B-C3B	2.23	1.48	1.42
82	QG	201	PEB	C4B-C3B	2.23	1.49	1.45
82	B5	201	PEB	C4B-C3B	2.23	1.49	1.45
82	CF	202	PEB	CHB-C1C	2.23	1.45	1.40
96	FL	102	HEM	C1D-ND	-2.23	1.34	1.38
82	X7	201	PEB	C4A-NA	-2.23	1.32	1.37
82	bP	502	PEB	C4A-NA	-2.23	1.32	1.37
87	bL	607	CLA	C3B-C4B	2.23	1.48	1.42
82	qC	203	PEB	C1C-C2C	2.23	1.48	1.42
82	LH	1003	PEB	C1C-NC	-2.23	1.34	1.37
82	RH	201	PEB	C1C-NC	-2.23	1.34	1.37
82	i4	203	PEB	C2A-C1A	-2.23	1.50	1.52
87	B2	831	CLA	MG-ND	-2.23	2.01	2.05
82	WA	201	PEB	C4A-NA	-2.23	1.32	1.37
82	R4	203	PEB	C1C-C2C	2.23	1.48	1.42
87	AN	810	CLA	CMC-C2C	-2.23	1.46	1.50
87	82	303	CLA	CMC-C2C	-2.23	1.46	1.50
82	SK	202	PEB	C1C-NC	-2.23	1.34	1.37
82	KQ	202	PEB	C1C-NC	-2.23	1.34	1.37
82	B9	203	PEB	C1C-C2C	2.23	1.48	1.42
82	aE	202	PEB	C1C-C2C	2.23	1.48	1.42
82	EF	202	PEB	C4A-NA	-2.23	1.32	1.37
82	TG	201	PEB	C4A-NA	-2.23	1.32	1.37
82	L1	1002	PEB	C4A-NA	-2.23	1.32	1.37
82	iG	202	PEB	C4B-C3B	2.23	1.49	1.45
87	AN	823	CLA	C1B-C2B	2.23	1.48	1.43
87	A2	834	CLA	C1B-C2B	2.23	1.48	1.43
87	CL	506	CLA	MG-NB	-2.23	2.01	2.05
82	QM	203	PEB	C1C-C2C	2.23	1.48	1.42
82	eM	201	PEB	C4A-NA	-2.23	1.32	1.37
84	KH	1001	CYC	C4C-NC	-2.23	1.32	1.37
82	QO	201	PEB	CHA-C4A	-2.23	1.32	1.36
84	NH	1001	CYC	C4A-C3A	2.23	1.50	1.45
82	DA	202	PEB	C1A-NA	-2.23	1.34	1.37
82	NH	1002	PEB	C4B-C3B	2.23	1.49	1.45
82	a4	203	PEB	C4B-C3B	2.23	1.49	1.45
82	I7	201	PEB	C4B-C3B	2.23	1.49	1.45
82	kK	203	PEB	C4B-C3B	2.23	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Z9	301	PEB	C1D-ND	2.23	1.49	1.45
82	PE	202	PEB	C1C-NC	-2.23	1.34	1.37
82	gE	201	PEB	C4A-NA	-2.23	1.32	1.37
87	bL	619	CLA	CMC-C2C	-2.23	1.46	1.50
82	CA	201	PEB	CHC-C4C	2.23	1.52	1.49
82	XK	203	PEB	CHC-C4C	2.23	1.52	1.49
82	l1	203	PEB	CHC-C4C	2.23	1.52	1.49
92	mL	101	LMG	O1-C1	2.23	1.44	1.40
82	J7	201	PEB	C1C-NC	-2.23	1.34	1.37
87	AN	852	CLA	CMB-C2B	-2.23	1.46	1.50
82	ZB	201	PEB	C4A-NA	-2.23	1.32	1.37
82	NO	1002	PEB	C4A-NA	-2.23	1.32	1.37
82	H7	203	PEB	C4A-NA	-2.23	1.32	1.37
82	eO	202	PEB	C4A-NA	-2.23	1.32	1.37
82	bP	501	PEB	C1C-NC	-2.23	1.34	1.37
87	6N	603	CLA	MG-NB	-2.23	2.01	2.05
87	B6	605	CLA	CMB-C2B	-2.23	1.46	1.50
82	PF	202	PEB	C4A-NA	-2.23	1.32	1.37
82	eG	203	PEB	C4A-NA	-2.23	1.32	1.37
82	ND	203	PEB	C1C-C2C	2.23	1.48	1.42
82	e1	201	PEB	C1C-C2C	2.23	1.48	1.42
87	62	304	CLA	MG-NB	-2.23	2.01	2.05
87	dL	409	CLA	MG-ND	-2.23	2.01	2.05
87	F2	202	CLA	C3C-C2C	2.23	1.41	1.36
87	AN	816	CLA	CMC-C2C	-2.23	1.46	1.50
82	XA	201	PEB	C4A-NA	-2.23	1.32	1.37
82	m1	201	PEB	C1B-C2B	2.23	1.50	1.45
82	RM	202	PEB	C1C-C2C	2.23	1.48	1.42
83	AM	304	PUB	C4B-C3B	2.23	1.48	1.42
82	lH	202	PEB	CHC-C4C	2.23	1.52	1.49
82	fG	203	PEB	C4B-C3B	2.23	1.49	1.45
87	AN	850	CLA	MG-ND	-2.23	2.01	2.05
87	5N	602	CLA	MG-NB	-2.23	2.01	2.05
87	CL	509	CLA	CMB-C2B	-2.23	1.46	1.50
87	AN	836	CLA	CMB-C2B	-2.23	1.46	1.50
87	A2	808	CLA	CMD-C2D	-2.23	1.46	1.50
84	J4	1001	CYC	C4A-C3A	2.23	1.50	1.45
87	AN	822	CLA	C3B-C4B	2.23	1.48	1.42
82	MA	202	PEB	C2A-C1A	-2.23	1.50	1.52
82	D7	202	PEB	C1A-NA	-2.23	1.34	1.37
82	OJ	202	PEB	C4A-NA	-2.23	1.32	1.37
84	J1	1001	CYC	C1B-NB	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	EO	1001	CYC	C4B-NB	-2.23	1.33	1.38
82	OI	203	PEB	C1C-C2C	2.23	1.48	1.42
82	m1	201	PEB	C1C-C2C	2.23	1.48	1.42
87	A2	840	CLA	CMD-C2D	-2.23	1.46	1.50
82	gB	203	PEB	O1B-CGB	2.22	1.29	1.22
82	MJ	203	PEB	C1C-NC	-2.22	1.34	1.37
82	xF	302	PEB	C1C-C2C	2.22	1.48	1.42
87	IN	102	CLA	CMD-C2D	-2.22	1.46	1.50
87	8N	304	CLA	CMC-C2C	-2.22	1.46	1.50
84	FO	1001	CYC	C4C-NC	-2.22	1.32	1.37
87	7N	602	CLA	CHD-C1D	2.22	1.42	1.38
87	82	306	CLA	C3D-C4D	2.22	1.49	1.44
82	DD	201	PEB	C1C-C2C	2.22	1.48	1.42
82	gH	203	PEB	C4B-C3B	2.22	1.49	1.45
87	3N	309	CLA	C1B-C2B	2.22	1.48	1.43
82	jO	202	PEB	C1C-C2C	2.22	1.48	1.42
87	2N	309	CLA	CMD-C2D	-2.22	1.46	1.50
82	XM	201	PEB	C4A-NA	-2.22	1.32	1.37
82	b1	203	PEB	CHC-C4C	2.22	1.52	1.49
82	bF	201	PEB	C1C-NC	-2.22	1.34	1.37
87	BL	601	CLA	C1B-C2B	2.22	1.48	1.43
82	l1	201	PEB	C1C-C2C	2.22	1.48	1.42
82	k4	201	PEB	C1C-C2C	2.22	1.48	1.42
82	H5	203	PEB	C1C-C2C	2.22	1.48	1.42
82	HB	203	PEB	C4A-NA	-2.22	1.32	1.37
82	O5	203	PEB	C4A-NA	-2.22	1.32	1.37
82	MA	201	PEB	OD-C4D	2.22	1.27	1.23
82	OE	201	PEB	OD-C4D	2.22	1.27	1.23
82	dQ	401	PEB	C1C-NC	-2.22	1.34	1.37
82	CF	203	PEB	C1C-C2C	2.22	1.48	1.42
82	gB	201	PEB	C1C-C2C	2.22	1.48	1.42
87	32	304	CLA	CMD-C2D	-2.22	1.46	1.50
87	A2	851	CLA	CMC-C2C	-2.22	1.46	1.50
82	SJ	201	PEB	C4A-NA	-2.22	1.32	1.37
84	J4	1001	CYC	C4C-NC	-2.22	1.32	1.37
82	l1	202	PEB	C1C-C2C	2.22	1.48	1.42
82	H7	201	PEB	C1C-C2C	2.22	1.48	1.42
87	cL	512	CLA	MG-ND	-2.22	2.01	2.05
82	XF	203	PEB	C4B-C3B	2.22	1.49	1.45
82	g4	201	PEB	C2A-C1A	-2.22	1.50	1.52
82	rC	201	PEB	C2A-C1A	-2.22	1.50	1.52
87	82	308	CLA	CHC-C1C	2.22	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PA	201	PEB	C1C-C2C	2.22	1.48	1.42
82	RD	202	PEB	C1C-C2C	2.22	1.48	1.42
84	DE	1001	CYC	C4B-NB	-2.22	1.33	1.38
87	12	606	CLA	CMD-C2D	-2.22	1.46	1.50
87	b6	608	CLA	CMB-C2B	-2.22	1.46	1.50
84	K1	1001	CYC	C4C-NC	-2.22	1.32	1.37
82	T9	201	PEB	C1C-C2C	2.22	1.48	1.42
84	J3	1001	CYC	OB-C4B	2.22	1.27	1.23
87	4N	602	CLA	C1B-C2B	2.22	1.48	1.43
82	KQ	201	PEB	C1C-C2C	2.22	1.48	1.42
82	U5	203	PEB	C1C-C2C	2.22	1.48	1.42
82	x8	202	PEB	C1C-C2C	2.22	1.48	1.42
82	F9	202	PEB	C1C-C2C	2.22	1.48	1.42
82	SE	201	PEB	C4A-NA	-2.22	1.32	1.37
82	xF	302	PEB	C4A-NA	-2.22	1.32	1.37
82	mO	201	PEB	C4A-NA	-2.22	1.32	1.37
84	ME	1001	CYC	C1B-NB	-2.22	1.34	1.37
82	iK	203	PEB	C2A-C1A	-2.22	1.50	1.52
82	jJ	203	PEB	C4B-C3B	2.22	1.49	1.45
82	SP	201	PEB	OD-C4D	2.22	1.27	1.23
82	CM	202	PEB	C4B-C3B	2.22	1.49	1.45
87	BN	807	CLA	CMC-C2C	-2.22	1.46	1.50
87	AN	840	CLA	C1B-C2B	2.22	1.48	1.43
87	42	603	CLA	C1B-C2B	2.22	1.48	1.43
82	IK	201	PEB	O1C-CGC	2.22	1.29	1.22
82	WM	202	PEB	C2A-C1A	-2.22	1.50	1.52
84	T3	1001	CYC	OB-C4B	2.22	1.27	1.23
87	F2	205	CLA	CMB-C2B	-2.22	1.46	1.50
87	B6	615	CLA	CMC-C2C	-2.22	1.46	1.50
82	rF	202	PEB	C4A-NA	-2.22	1.32	1.37
82	lG	201	PEB	C4A-NA	-2.22	1.32	1.37
82	mM	202	PEB	C4A-NA	-2.22	1.32	1.37
82	nF	201	PEB	C4B-C3B	2.22	1.49	1.45
87	A2	823	CLA	C1B-C2B	2.22	1.48	1.43
82	H9	202	PEB	C1C-C2C	2.22	1.48	1.42
82	gO	203	PEB	C1C-C2C	2.22	1.48	1.42
82	XB	202	PEB	C1C-NC	-2.22	1.34	1.37
87	A2	852	CLA	CMB-C2B	-2.22	1.46	1.50
82	QE	201	PEB	C4B-C3B	2.22	1.49	1.45
87	BL	605	CLA	MG-NB	-2.22	2.01	2.05
87	cL	516	CLA	MG-NB	-2.22	2.01	2.05
82	cO	201	PEB	C4A-NA	-2.22	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	SE	201	PEB	C1C-NC	-2.22	1.34	1.37
82	jH	202	PEB	C1C-C2C	2.22	1.48	1.42
96	E6	101	HEM	FE-ND	-2.22	1.87	1.94
82	OD	201	PEB	C1D-ND	2.22	1.49	1.45
87	cL	517	CLA	CHC-C1C	2.22	1.43	1.38
82	BM	301	PEB	C1C-NC	-2.22	1.34	1.37
84	EG	1001	CYC	C4B-NB	-2.22	1.33	1.38
82	yC	202	PEB	C4B-C3B	2.22	1.49	1.45
82	U4	202	PEB	C2A-C1A	-2.22	1.50	1.52
82	eG	202	PEB	C2A-C1A	-2.22	1.50	1.52
82	Q9	202	PEB	C1D-ND	2.22	1.49	1.45
87	32	307	CLA	C4D-ND	-2.22	1.34	1.37
87	BL	605	CLA	C1B-C2B	2.22	1.48	1.43
82	AM	302	PEB	C1C-NC	-2.22	1.34	1.37
87	22	609	CLA	CMD-C2D	-2.22	1.46	1.50
87	5N	604	CLA	CMC-C2C	-2.22	1.46	1.50
82	nK	202	PEB	C4B-C3B	2.22	1.49	1.45
82	NK	201	PEB	C1A-NA	-2.22	1.34	1.37
87	3N	306	CLA	CMD-C2D	-2.22	1.46	1.50
82	Z4	202	PEB	C4A-NA	-2.22	1.32	1.37
82	oF	203	PEB	C1C-C2C	2.22	1.48	1.42
82	fG	202	PEB	C4A-NA	-2.22	1.32	1.37
87	BL	603	CLA	C1B-NB	-2.22	1.35	1.37
82	UD	202	PEB	C1C-C2C	2.22	1.48	1.42
82	sF	203	PEB	C1C-C2C	2.22	1.48	1.42
87	32	305	CLA	CMD-C2D	-2.22	1.46	1.50
87	A2	822	CLA	CMD-C2D	-2.22	1.46	1.50
82	VG	201	PEB	C4B-C3B	2.22	1.49	1.45
82	H1	1002	PEB	C4B-C3B	2.22	1.49	1.45
87	b6	616	CLA	MG-NB	-2.22	2.01	2.05
82	QB	202	PEB	C1C-NC	-2.22	1.34	1.37
82	VF	202	PEB	C1C-NC	-2.22	1.34	1.37
82	rC	201	PEB	C1C-NC	-2.22	1.34	1.37
87	BN	828	CLA	CHC-C1C	2.22	1.43	1.38
82	TH	201	PEB	C1C-C2C	2.22	1.48	1.42
87	BL	623	CLA	CMD-C2D	-2.22	1.46	1.50
82	MK	203	PEB	C4A-NA	-2.22	1.32	1.37
87	F2	202	CLA	MG-NB	-2.22	2.01	2.05
87	CL	513	CLA	CMC-C2C	-2.22	1.46	1.50
87	AN	832	CLA	CMC-C2C	-2.22	1.46	1.50
87	B2	820	CLA	CMB-C2B	-2.22	1.46	1.50
87	B2	823	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AL	404	CLA	C1B-C2B	2.22	1.48	1.43
87	A2	840	CLA	C1B-C2B	2.22	1.48	1.43
82	WP	201	PEB	C4A-NA	-2.22	1.32	1.37
82	y8	203	PEB	C4A-NA	-2.22	1.32	1.37
82	iF	201	PEB	CHC-C4C	2.22	1.52	1.49
82	AM	301	PEB	C1C-C2C	2.21	1.48	1.42
82	h4	202	PEB	C1C-C2C	2.21	1.48	1.42
82	fE	203	PEB	C4B-C3B	2.21	1.49	1.45
87	72	602	CLA	CHD-C1D	2.21	1.42	1.38
87	KN	102	CLA	CMB-C2B	-2.21	1.46	1.50
84	C3	1001	CYC	OB-C4B	2.21	1.27	1.23
84	p3	1001	CYC	OB-C4B	2.21	1.27	1.23
84	t3	1001	CYC	OB-C4B	2.21	1.27	1.23
82	PQ	203	PEB	C1C-C2C	2.21	1.48	1.42
87	DL	403	CLA	C1B-C2B	2.21	1.48	1.43
87	C6	517	CLA	CMD-C2D	-2.21	1.46	1.50
82	TI	203	PEB	C4A-NA	-2.21	1.32	1.37
82	yC	203	PEB	C4A-NA	-2.21	1.32	1.37
82	NQ	204	PEB	C1C-C2C	2.21	1.48	1.42
82	E9	201	PEB	C1C-C2C	2.21	1.48	1.42
82	jK	201	PEB	C4B-C3B	2.21	1.49	1.45
87	c6	604	CLA	MG-NB	-2.21	2.01	2.05
82	G7	201	PEB	C4A-NA	-2.21	1.32	1.37
82	eO	203	PEB	C1C-C2C	2.21	1.48	1.42
87	cL	508	CLA	C1B-NB	-2.21	1.35	1.37
82	G7	202	PEB	C4B-C3B	2.21	1.49	1.45
82	gK	202	PEB	C1C-NC	-2.21	1.34	1.37
82	yK	301	PEB	C1C-NC	-2.21	1.34	1.37
84	F4	1001	CYC	C1B-NB	-2.21	1.34	1.37
87	BN	807	CLA	CMB-C2B	-2.21	1.46	1.50
87	A2	825	CLA	CMD-C2D	-2.21	1.46	1.50
96	f6	101	HEM	FE-ND	-2.21	1.87	1.94
82	V7	202	PEB	C1A-NA	-2.21	1.34	1.37
82	TH	201	PEB	C1D-ND	2.21	1.49	1.45
82	sF	201	PEB	C1D-ND	2.21	1.49	1.45
82	iK	201	PEB	C1C-C2C	2.21	1.48	1.42
82	j4	202	PEB	C1C-NC	-2.21	1.34	1.37
82	JQ	203	PEB	C4B-C3B	2.21	1.49	1.45
82	HP	202	PEB	C2A-C1A	-2.21	1.50	1.52
82	W9	203	PEB	C2A-C1A	-2.21	1.50	1.52
87	b6	612	CLA	C1B-C2B	2.21	1.48	1.43
82	wK	303	PEB	C1B-C2B	2.21	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	820	CLA	CMB-C2B	-2.21	1.46	1.50
82	KI	201	PEB	C4A-NA	-2.21	1.32	1.37
82	AJ	302	PEB	C1C-NC	-2.21	1.34	1.37
82	oK	202	PEB	C1B-C2B	2.21	1.50	1.45
82	iF	202	PEB	CHC-C4C	2.21	1.52	1.49
82	hK	202	PEB	CHC-C4C	2.21	1.52	1.49
82	b1	201	PEB	C1C-C2C	2.21	1.48	1.42
84	D1	1001	CYC	C4D-C3D	2.21	1.48	1.42
87	32	308	CLA	MG-ND	-2.21	2.01	2.05
87	R2	202	CLA	MG-NB	-2.21	2.01	2.05
87	B2	808	CLA	CMD-C2D	-2.21	1.46	1.50
84	N4	1001	CYC	C4A-C3A	2.21	1.50	1.45
82	UE	203	PEB	C2A-C1A	-2.21	1.50	1.52
82	D5	202	PEB	C2A-C1A	-2.21	1.50	1.52
82	UE	202	PEB	C1C-C2C	2.21	1.48	1.42
82	mG	201	PEB	C1C-C2C	2.21	1.48	1.42
82	NF	201	PEB	C1A-NA	-2.21	1.34	1.37
87	CL	509	CLA	CMD-C2D	-2.21	1.46	1.50
87	CL	514	CLA	CMD-C2D	-2.21	1.46	1.50
87	A2	835	CLA	CMB-C2B	-2.21	1.46	1.50
82	GF	201	PEB	C2C-C3C	2.21	1.44	1.38
82	lJ	203	PEB	C4A-NA	-2.21	1.32	1.37
82	gO	202	PEB	C1C-C2C	2.21	1.48	1.42
84	63	901	CYC	C4B-NB	-2.21	1.33	1.38
82	IF	203	PEB	OD-C4D	2.21	1.27	1.23
84	G3	1001	CYC	OB-C4B	2.21	1.27	1.23
82	WB	402	PEB	C1C-NC	-2.21	1.34	1.37
82	VE	201	PEB	C1C-NC	-2.21	1.34	1.37
87	BN	820	CLA	CMD-C2D	-2.21	1.46	1.50
87	5N	606	CLA	CMD-C2D	-2.21	1.46	1.50
82	k4	201	PEB	C4B-C3B	2.21	1.49	1.45
92	ML	101	LMG	O1-C1	2.21	1.44	1.40
82	F5	202	PEB	C1C-C2C	2.21	1.48	1.42
87	AN	813	CLA	CMD-C2D	-2.21	1.46	1.50
87	52	606	CLA	CMD-C2D	-2.21	1.46	1.50
87	A2	814	CLA	CMB-C2B	-2.21	1.46	1.50
87	K2	103	CLA	CMD-C2D	-2.21	1.46	1.50
82	J9	201	PEB	C2A-C1A	-2.21	1.50	1.52
82	L9	201	PEB	C2A-C1A	-2.21	1.50	1.52
82	ED	201	PEB	C4A-NA	-2.21	1.32	1.37
82	aO	202	PEB	C4B-NB	-2.21	1.33	1.38
87	a6	609	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	2N	305	CLA	CMC-C2C	-2.21	1.46	1.50
84	P3	1001	CYC	OB-C4B	2.21	1.27	1.23
87	6N	601	CLA	CHC-C1C	2.21	1.43	1.38
87	BN	816	CLA	MG-NB	-2.21	2.01	2.05
87	B6	609	CLA	MG-NB	-2.21	2.01	2.05
87	7N	610	CLA	MG-NB	-2.21	2.01	2.05
87	6N	608	CLA	C4D-CHA	2.21	1.46	1.38
82	VG	201	PEB	C1C-NC	-2.21	1.34	1.37
82	xF	302	PEB	C1C-NC	-2.21	1.34	1.37
87	AN	814	CLA	CMB-C2B	-2.21	1.46	1.50
87	I2	103	CLA	CMC-C2C	-2.21	1.46	1.50
87	b6	611	CLA	CMB-C2B	-2.21	1.46	1.50
87	4N	604	CLA	CMB-C2B	-2.21	1.46	1.50
82	N4	1002	PEB	C1C-C2C	2.21	1.48	1.42
82	KP	201	PEB	C4A-NA	-2.21	1.32	1.37
84	i3	1001	CYC	OB-C4B	2.21	1.27	1.23
87	K2	103	CLA	MG-ND	-2.21	2.01	2.05
84	M4	1001	CYC	C1B-NB	-2.21	1.34	1.37
87	22	604	CLA	CMC-C2C	-2.21	1.46	1.50
87	A2	836	CLA	CMB-C2B	-2.21	1.46	1.50
82	VH	201	PEB	C1C-C2C	2.21	1.48	1.42
82	D5	202	PEB	C4B-C3B	2.21	1.49	1.45
82	iF	203	PEB	C4B-C3B	2.21	1.49	1.45
82	D4	1002	PEB	C4A-NA	-2.21	1.32	1.37
82	J5	202	PEB	C4A-NA	-2.21	1.32	1.37
82	iE	201	PEB	C4A-NA	-2.21	1.32	1.37
87	2N	305	CLA	CHC-C1C	2.21	1.43	1.38
87	52	604	CLA	MG-NB	-2.21	2.01	2.05
87	A2	812	CLA	MG-NB	-2.21	2.01	2.05
82	AK	202	PEB	C1C-NC	-2.21	1.34	1.37
82	Q7	202	PEB	C1C-NC	-2.21	1.34	1.37
82	CB	202	PEB	C4A-NA	-2.21	1.32	1.37
82	C7	201	PEB	C1B-C2B	2.21	1.50	1.45
87	A2	850	CLA	MG-ND	-2.21	2.01	2.05
87	B2	830	CLA	MG-NB	-2.21	2.01	2.05
82	A4	304	PEB	C2A-C1A	-2.21	1.50	1.52
82	FQ	202	PEB	C1C-C2C	2.21	1.48	1.42
87	AN	807	CLA	CMC-C2C	-2.21	1.46	1.50
87	AN	822	CLA	CMD-C2D	-2.21	1.46	1.50
87	B2	806	CLA	CMC-C2C	-2.21	1.46	1.50
82	IM	201	PEB	C4A-NA	-2.21	1.32	1.37
82	sF	202	PEB	C1B-C2B	2.21	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	rK	201	PEB	C4B-C3B	2.21	1.49	1.45
82	hM	201	PEB	C1C-C2C	2.21	1.48	1.42
87	FN	205	CLA	CMB-C2B	-2.21	1.46	1.50
87	82	306	CLA	CMB-C2B	-2.21	1.46	1.50
82	PO	201	PEB	C4A-NA	-2.21	1.32	1.37
82	GQ	201	PEB	C4A-NA	-2.21	1.32	1.37
82	LO	1002	PEB	C1C-C2C	2.21	1.48	1.42
87	C6	511	CLA	CMD-C2D	-2.21	1.46	1.50
82	QB	203	PEB	C4A-NA	-2.21	1.32	1.37
84	LO	1001	CYC	C4A-C3A	2.21	1.50	1.45
87	8N	308	CLA	CHC-C1C	2.21	1.43	1.38
87	BN	811	CLA	MG-ND	-2.21	2.01	2.05
87	72	603	CLA	MG-NB	-2.21	2.01	2.05
87	B6	607	CLA	MG-NB	-2.21	2.01	2.05
87	b6	605	CLA	MG-NB	-2.21	2.01	2.05
82	XJ	202	PEB	C1C-NC	-2.21	1.34	1.37
87	A6	404	CLA	CMD-C2D	-2.21	1.46	1.50
82	IJ	203	PEB	C4A-NA	-2.21	1.32	1.37
82	e4	203	PEB	C1C-C2C	2.21	1.48	1.42
87	AN	835	CLA	MG-NB	-2.21	2.01	2.05
87	7N	602	CLA	MG-NB	-2.21	2.01	2.05
87	CL	506	CLA	C1B-C2B	2.21	1.48	1.43
82	T7	202	PEB	OD-C4D	2.21	1.27	1.23
87	82	304	CLA	CMD-C2D	-2.21	1.46	1.50
87	A2	837	CLA	CMB-C2B	-2.21	1.46	1.50
84	MG	1001	CYC	C1B-NB	-2.21	1.34	1.37
82	D1	1002	PEB	C4A-NA	-2.21	1.32	1.37
82	N9	202	PEB	C2A-C1A	-2.21	1.50	1.52
82	iE	202	PEB	C2A-C1A	-2.21	1.50	1.52
82	fG	202	PEB	C2A-C1A	-2.21	1.50	1.52
82	nK	202	PEB	C2A-C1A	-2.21	1.50	1.52
87	K6	101	CLA	C1B-C2B	2.21	1.48	1.43
87	BL	605	CLA	CMC-C2C	-2.21	1.46	1.50
87	AN	817	CLA	CMC-C2C	-2.21	1.46	1.50
82	gG	202	PEB	C1C-NC	-2.21	1.34	1.37
87	22	606	CLA	MG-NB	-2.20	2.01	2.05
87	CL	503	CLA	CMB-C2B	-2.20	1.46	1.50
87	B2	829	CLA	CMD-C2D	-2.20	1.46	1.50
82	XF	201	PEB	C4B-C3B	2.20	1.49	1.45
82	PM	202	PEB	C4A-NA	-2.20	1.32	1.37
82	PO	202	PEB	C4A-NA	-2.20	1.32	1.37
82	O7	202	PEB	C1C-NC	-2.20	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	KA	203	PUB	C4B-NB	-2.20	1.34	1.37
87	A2	835	CLA	MG-NB	-2.20	2.01	2.05
82	SM	203	PEB	C1C-C2C	2.20	1.48	1.42
82	NF	202	PEB	C4A-NA	-2.20	1.32	1.37
82	RM	202	PEB	C4A-NA	-2.20	1.32	1.37
82	AD	304	PEB	C4B-C3B	2.20	1.49	1.45
87	AN	827	CLA	C1B-C2B	2.20	1.48	1.43
87	DL	404	CLA	CHC-C1C	2.20	1.43	1.38
82	NQ	202	PEB	CHC-C4C	2.20	1.52	1.49
87	A2	806	CLA	CMD-C2D	-2.20	1.46	1.50
82	UM	203	PEB	C4A-NA	-2.20	1.32	1.37
82	B7	203	PEB	C4A-NA	-2.20	1.32	1.37
87	22	602	CLA	C1B-C2B	2.20	1.48	1.43
82	BQ	203	PEB	C1C-C2C	2.20	1.48	1.42
82	dO	202	PEB	C1C-C2C	2.20	1.48	1.42
87	3N	305	CLA	CMB-C2B	-2.20	1.46	1.50
87	AN	830	CLA	MG-ND	-2.20	2.01	2.05
87	KN	102	CLA	MG-ND	-2.20	2.01	2.05
82	O9	201	PEB	C1C-NC	-2.20	1.34	1.37
82	dE	201	PEB	C1C-NC	-2.20	1.34	1.37
82	AO	301	PEB	C2A-C1A	-2.20	1.50	1.52
82	XP	201	PEB	C2A-C1A	-2.20	1.50	1.52
82	fO	201	PEB	C2A-C1A	-2.20	1.50	1.52
82	VE	201	PEB	C4A-NA	-2.20	1.32	1.37
82	VG	201	PEB	C4A-NA	-2.20	1.32	1.37
82	KI	203	PEB	C4A-NA	-2.20	1.32	1.37
82	lE	201	PEB	C4A-NA	-2.20	1.32	1.37
87	22	604	CLA	CHC-C1C	2.20	1.43	1.38
87	2N	311	CLA	CHC-C1C	2.20	1.43	1.38
82	dF	202	PEB	CHC-C4C	2.20	1.52	1.49
82	GK	201	PEB	C2C-C3C	2.20	1.44	1.38
82	FM	202	PEB	C1C-C2C	2.20	1.48	1.42
84	H1	1001	CYC	C4D-C3D	2.20	1.48	1.42
87	AN	806	CLA	CMD-C2D	-2.20	1.46	1.50
87	A2	810	CLA	CMC-C2C	-2.20	1.46	1.50
87	D6	403	CLA	CMB-C2B	-2.20	1.46	1.50
82	xF	303	PEB	C4B-C3B	2.20	1.49	1.45
82	PJ	201	PEB	C4A-NA	-2.20	1.32	1.37
84	GO	1001	CYC	C4C-NC	-2.20	1.32	1.37
84	G4	1001	CYC	C4C-NC	-2.20	1.32	1.37
82	TJ	202	PEB	C1C-NC	-2.20	1.34	1.37
87	bL	608	CLA	CHC-C1C	2.20	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	dL	409	CLA	CMB-C2B	-2.20	1.46	1.50
82	TP	202	PEB	C4A-NA	-2.20	1.32	1.37
82	lG	201	PEB	C4B-C3B	2.20	1.49	1.45
82	i1	201	PEB	CHC-C4C	2.20	1.52	1.49
82	c1	202	PEB	C1C-C2C	2.20	1.48	1.42
82	SJ	202	PEB	C1C-NC	-2.20	1.34	1.37
82	mH	201	PEB	C1C-NC	-2.20	1.34	1.37
87	BN	802	CLA	MG-NB	-2.20	2.01	2.05
82	OE	203	PEB	C4A-NA	-2.20	1.32	1.37
82	MJ	203	PEB	C4A-NA	-2.20	1.32	1.37
82	v8	201	PEB	C4A-NA	-2.20	1.32	1.37
87	b6	610	CLA	CHC-C1C	2.20	1.43	1.38
82	J7	203	PEB	C1C-NC	-2.20	1.34	1.37
84	LH	1002	CYC	C1B-NB	-2.20	1.34	1.37
87	BN	809	CLA	CMD-C2D	-2.20	1.46	1.50
87	A2	802	CLA	CMC-C2C	-2.20	1.46	1.50
87	C6	510	CLA	CMD-C2D	-2.20	1.46	1.50
82	gO	201	PEB	C1C-C2C	2.20	1.48	1.42
87	2N	303	CLA	C1B-C2B	2.20	1.48	1.43
87	CL	512	CLA	CMC-C2C	-2.20	1.46	1.50
87	AN	824	CLA	CMB-C2B	-2.20	1.46	1.50
87	4N	605	CLA	C1B-NB	-2.20	1.35	1.37
82	PM	201	PEB	C2A-C1A	-2.20	1.50	1.52
82	dO	202	PEB	C2A-C1A	-2.20	1.50	1.52
82	vF	202	PEB	C4B-C3B	2.20	1.49	1.45
82	Y9	203	PEB	C1C-C2C	2.20	1.48	1.42
87	BN	801	CLA	MG-ND	-2.20	2.01	2.05
87	AL	403	CLA	CHC-C1C	2.20	1.43	1.38
82	d4	202	PEB	C1C-C2C	2.20	1.48	1.42
82	s8	201	PEB	C1C-C2C	2.20	1.48	1.42
82	CP	201	PEB	C4A-NA	-2.20	1.32	1.37
82	NI	203	PEB	C4B-NB	-2.20	1.33	1.38
82	GB	203	PEB	C1C-NC	-2.20	1.34	1.37
82	Q5	203	PEB	C1C-NC	-2.20	1.34	1.37
87	CL	505	CLA	CMB-C2B	-2.20	1.46	1.50
87	cL	512	CLA	CMD-C2D	-2.20	1.46	1.50
82	O9	203	PEB	C1B-C2B	2.20	1.50	1.45
84	c3	1001	CYC	OB-C4B	2.20	1.27	1.23
82	aG	202	PEB	C4A-NA	-2.20	1.32	1.37
87	AN	841	CLA	MG-ND	-2.20	2.01	2.05
87	c6	612	CLA	MG-NB	-2.20	2.01	2.05
84	GE	1001	CYC	C4B-NB	-2.20	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	F1	1001	CYC	C4B-NB	-2.20	1.33	1.38
87	IN	103	CLA	CMB-C2B	-2.20	1.46	1.50
87	4N	601	CLA	CMB-C2B	-2.20	1.46	1.50
82	UH	201	PEB	CHC-C4C	2.20	1.52	1.49
82	VO	202	PEB	CHC-C4C	2.20	1.52	1.49
82	W1	203	PEB	CHC-C4C	2.20	1.52	1.49
82	ZI	401	PEB	C1B-C2B	2.20	1.50	1.45
82	iH	201	PEB	C1B-C2B	2.20	1.50	1.45
82	JH	1002	PEB	C1C-C2C	2.20	1.48	1.42
82	EQ	201	PEB	C4A-NA	-2.20	1.32	1.37
82	j4	202	PEB	C1C-C2C	2.20	1.48	1.42
82	lG	203	PEB	C1C-C2C	2.20	1.48	1.42
87	AN	818	CLA	CMB-C2B	-2.20	1.46	1.50
87	A2	838	CLA	CMC-C2C	-2.20	1.46	1.50
82	c1	201	PEB	C1C-NC	-2.20	1.34	1.37
84	JH	1001	CYC	C1B-NB	-2.20	1.34	1.37
82	T1	201	PEB	C1D-ND	2.20	1.49	1.45
82	DK	202	PEB	C4A-NA	-2.20	1.32	1.37
82	HQ	201	PEB	C4A-NA	-2.20	1.32	1.37
82	QQ	202	PEB	C2A-C1A	-2.20	1.50	1.52
82	D1	1002	PEB	C2A-C1A	-2.20	1.50	1.52
82	iF	203	PEB	C2A-C1A	-2.20	1.50	1.52
87	F2	201	CLA	CMD-C2D	-2.20	1.46	1.50
87	bL	622	CLA	CMC-C2C	-2.20	1.46	1.50
87	3N	305	CLA	CMD-C2D	-2.20	1.46	1.50
82	g1	202	PEB	C1A-NA	-2.20	1.34	1.37
87	4N	608	CLA	C1B-NB	-2.20	1.35	1.37
82	VA	201	PEB	C1C-NC	-2.20	1.34	1.37
82	FQ	203	PEB	C2C-C3C	2.20	1.44	1.38
82	YG	202	PEB	C4A-NA	-2.20	1.32	1.37
82	OH	202	PEB	C4B-C3B	2.20	1.49	1.45
82	wC	202	PEB	C1C-C2C	2.20	1.48	1.42
82	fG	201	PEB	C1C-C2C	2.20	1.48	1.42
82	DP	202	PEB	C1C-NC	-2.20	1.34	1.37
82	XP	201	PEB	C1C-NC	-2.20	1.34	1.37
82	gE	202	PEB	C1C-NC	-2.20	1.34	1.37
84	BE	1002	CYC	C4D-ND	-2.20	1.34	1.37
82	B7	201	PEB	C1C-C2C	2.20	1.48	1.42
87	2N	306	CLA	MG-NB	-2.20	2.01	2.05
82	xK	302	PEB	C1D-ND	2.20	1.49	1.45
87	c6	605	CLA	CMB-C2B	-2.20	1.46	1.50
82	dG	204	PEB	C2A-C1A	-2.20	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HP	202	PEB	C4A-NA	-2.20	1.32	1.37
82	F7	203	PEB	C4A-NA	-2.20	1.32	1.37
82	BD	203	PEB	C1C-C2C	2.20	1.48	1.42
82	RD	203	PEB	C1C-C2C	2.20	1.48	1.42
87	CL	507	CLA	MG-ND	-2.20	2.01	2.05
87	A2	819	CLA	MG-ND	-2.20	2.01	2.05
87	CL	509	CLA	CMC-C2C	-2.20	1.46	1.50
87	AN	836	CLA	CMD-C2D	-2.20	1.46	1.50
96	vL	201	HEM	C1C-C2C	-2.20	1.41	1.45
82	oF	201	PEB	C4B-C3B	2.20	1.49	1.45
82	GM	203	PEB	C4A-NA	-2.20	1.32	1.37
82	F9	201	PEB	CHC-C4C	2.20	1.52	1.49
82	TP	202	PEB	C1C-C2C	2.20	1.48	1.42
82	f4	202	PEB	C1C-C2C	2.20	1.48	1.42
87	A2	827	CLA	C1B-C2B	2.20	1.48	1.43
87	B2	810	CLA	MG-ND	-2.20	2.01	2.05
82	m1	201	PEB	C1C-NC	-2.20	1.34	1.37
82	aO	202	PEB	C1C-C2C	2.20	1.48	1.42
87	B2	820	CLA	C4D-ND	-2.20	1.34	1.37
82	DH	1002	PEB	C2A-C1A	-2.20	1.50	1.52
84	K3	1001	CYC	OB-C4B	2.20	1.27	1.23
87	ON	202	CLA	CMD-C2D	-2.20	1.46	1.50
82	bH	201	PEB	C1C-C2C	2.20	1.48	1.42
87	6N	611	CLA	CHC-C1C	2.20	1.43	1.38
82	T4	201	PEB	C4A-NA	-2.20	1.32	1.37
82	Q5	203	PEB	C1B-C2B	2.20	1.50	1.45
87	72	604	CLA	CMC-C2C	-2.20	1.46	1.50
87	AN	851	CLA	MG-ND	-2.20	2.01	2.05
82	B9	202	PEB	C1D-ND	2.20	1.49	1.45
82	BD	201	PEB	C1C-C2C	2.20	1.48	1.42
82	PE	201	PEB	C1C-C2C	2.20	1.48	1.42
82	UQ	202	PEB	C1C-C2C	2.20	1.48	1.42
82	aF	202	PEB	C4A-NA	-2.20	1.32	1.37
84	FH	1001	CYC	C4C-NC	-2.20	1.32	1.37
82	UE	202	PEB	C1C-NC	-2.20	1.34	1.37
82	d4	201	PEB	C2A-C1A	-2.20	1.50	1.52
82	L7	202	PEB	C1C-C2C	2.20	1.48	1.42
87	A2	851	CLA	MG-ND	-2.20	2.01	2.05
82	FO	1002	PEB	C4A-NA	-2.20	1.32	1.37
82	P4	201	PEB	C4A-NA	-2.20	1.32	1.37
84	K4	1001	CYC	C4B-NB	-2.19	1.33	1.38
87	b6	617	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	8N	305	CLA	CMD-C2D	-2.19	1.46	1.50
82	cO	203	PEB	C1C-C2C	2.19	1.48	1.42
87	A2	830	CLA	MG-ND	-2.19	2.01	2.05
82	SM	203	PEB	C4A-NA	-2.19	1.32	1.37
82	Y7	301	PEB	C4A-NA	-2.19	1.32	1.37
82	dM	202	PEB	C4A-NA	-2.19	1.32	1.37
82	PM	201	PEB	C4B-C3B	2.19	1.49	1.45
87	22	611	CLA	CHC-C1C	2.19	1.43	1.38
82	CM	203	PEB	C1C-C2C	2.19	1.48	1.42
82	DQ	201	PEB	C1C-C2C	2.19	1.48	1.42
87	BN	822	CLA	CMD-C2D	-2.19	1.46	1.50
87	A2	817	CLA	CMC-C2C	-2.19	1.46	1.50
87	c6	612	CLA	CMD-C2D	-2.19	1.46	1.50
82	jM	202	PEB	C2A-C1A	-2.19	1.50	1.52
84	g3	1001	CYC	OB-C4B	2.19	1.27	1.23
82	AD	303	PEB	C4A-NA	-2.19	1.32	1.37
82	AQ	303	PEB	C4A-NA	-2.19	1.32	1.37
82	xC	202	PEB	C1C-C2C	2.19	1.48	1.42
82	cJ	202	PEB	C1C-C2C	2.19	1.48	1.42
82	LK	201	PEB	C1A-NA	-2.19	1.34	1.37
87	A2	823	CLA	CMC-C2C	-2.19	1.46	1.50
87	5N	604	CLA	MG-NB	-2.19	2.01	2.05
82	II	202	PEB	C4A-NA	-2.19	1.32	1.37
82	MK	201	PEB	C4A-NA	-2.19	1.32	1.37
84	e3	1001	CYC	OB-C4B	2.19	1.27	1.23
87	bL	614	CLA	C1B-NB	-2.19	1.35	1.37
82	uF	203	PEB	C1C-C2C	2.19	1.48	1.42
87	BN	821	CLA	CMB-C2B	-2.19	1.46	1.50
87	BN	830	CLA	CMD-C2D	-2.19	1.46	1.50
87	7N	603	CLA	MG-NB	-2.19	2.01	2.05
87	42	602	CLA	CHC-C1C	2.19	1.43	1.38
82	TA	202	PEB	OD-C4D	2.19	1.27	1.23
82	T1	202	PEB	C1C-C2C	2.19	1.48	1.42
82	iF	201	PEB	C1C-C2C	2.19	1.48	1.42
82	cH	202	PEB	C1C-NC	-2.19	1.34	1.37
82	uC	201	PEB	C1D-ND	2.19	1.49	1.45
82	CQ	201	PEB	C1B-C2B	2.19	1.50	1.45
87	C6	515	CLA	CMD-C2D	-2.19	1.46	1.50
84	E4	1001	CYC	C1B-C2B	2.19	1.49	1.45
87	A2	815	CLA	C1B-C2B	2.19	1.48	1.43
87	AN	851	CLA	CMB-C2B	-2.19	1.46	1.50
87	O2	202	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	IA	201	PEB	C1D-ND	2.19	1.49	1.45
82	fG	203	PEB	C1C-C2C	2.19	1.48	1.42
82	H9	202	PEB	C4B-C3B	2.19	1.49	1.45
87	B6	611	CLA	CMD-C2D	-2.19	1.46	1.50
82	GK	203	PEB	C1C-NC	-2.19	1.34	1.37
82	WJ	201	PEB	C4B-NB	-2.19	1.33	1.38
82	VM	201	PEB	C4A-NA	-2.19	1.32	1.37
87	a6	608	CLA	CHC-C1C	2.19	1.43	1.38
82	aH	202	PEB	C1B-C2B	2.19	1.50	1.45
87	B6	611	CLA	CMB-C2B	-2.19	1.46	1.50
82	TA	201	PEB	C4B-C3B	2.19	1.49	1.45
82	m4	202	PEB	C4B-C3B	2.19	1.49	1.45
82	T7	201	PEB	C4B-C3B	2.19	1.49	1.45
82	xK	302	PEB	C4B-C3B	2.19	1.49	1.45
82	QE	202	PEB	C1C-C2C	2.19	1.48	1.42
82	a4	202	PEB	C4A-NA	-2.19	1.32	1.37
82	aE	202	PEB	C4A-NA	-2.19	1.32	1.37
82	dJ	201	PEB	C4A-NA	-2.19	1.32	1.37
87	DL	403	CLA	C1B-NB	-2.19	1.35	1.37
87	B2	828	CLA	CHC-C1C	2.19	1.43	1.38
87	B6	609	CLA	CMB-C2B	-2.19	1.46	1.50
87	C6	519	CLA	CMD-C2D	-2.19	1.46	1.50
84	LG	1001	CYC	OB-C4B	2.19	1.27	1.23
82	aH	201	PEB	C1C-C2C	2.19	1.48	1.42
84	CG	1001	CYC	C4A-C3A	2.19	1.50	1.45
87	BN	833	CLA	CMD-C2D	-2.19	1.46	1.50
82	AA	201	PEB	C1C-C2C	2.19	1.48	1.42
82	GG	1002	PEB	OD-C4D	2.19	1.27	1.23
82	a4	202	PEB	C4B-NB	-2.19	1.33	1.38
87	62	309	CLA	C4B-NB	2.19	1.40	1.37
82	DM	202	PEB	C4A-NA	-2.19	1.32	1.37
82	S5	202	PEB	C4A-NA	-2.19	1.32	1.37
82	hO	202	PEB	C1C-C2C	2.19	1.48	1.42
82	TQ	203	PEB	C1C-NC	-2.19	1.34	1.37
87	32	304	CLA	CMB-C2B	-2.19	1.46	1.50
87	A2	802	CLA	CMB-C2B	-2.19	1.46	1.50
82	W7	202	PEB	C4A-NA	-2.19	1.32	1.37
82	L9	201	PEB	C4A-NA	-2.19	1.32	1.37
82	GD	202	PEB	C1C-C2C	2.19	1.48	1.42
82	PD	203	PEB	C1C-C2C	2.19	1.48	1.42
87	12	601	CLA	MG-NB	-2.19	2.01	2.05
87	dL	404	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	RP	202	PEB	C4A-NA	-2.19	1.32	1.37
82	Y1	201	PEB	C4A-NA	-2.19	1.32	1.37
82	W9	201	PEB	C1C-C2C	2.19	1.48	1.42
82	fM	201	PEB	C1C-C2C	2.19	1.48	1.42
82	RF	202	PEB	CHC-C4C	2.19	1.52	1.49
87	7N	607	CLA	C1B-C2B	2.19	1.48	1.43
87	B2	807	CLA	CMB-C2B	-2.19	1.46	1.50
87	d6	401	CLA	CMB-C2B	-2.19	1.46	1.50
82	YA	304	PEB	C1D-ND	2.19	1.49	1.45
82	UG	201	PEB	C4A-NA	-2.19	1.32	1.37
82	NK	202	PEB	C4A-NA	-2.19	1.32	1.37
82	kJ	201	PEB	C1C-NC	-2.19	1.34	1.37
82	FQ	201	PEB	C1B-C2B	2.19	1.50	1.45
82	sK	203	PEB	C1C-C2C	2.19	1.48	1.42
87	ON	201	CLA	CHC-C1C	2.19	1.43	1.38
82	WA	201	PEB	C1C-C2C	2.19	1.48	1.42
83	AE	302	PUB	C4B-C3B	2.19	1.48	1.42
83	AG	302	PUB	C4B-C3B	2.19	1.48	1.42
82	uC	202	PEB	CHC-C4C	2.19	1.52	1.49
87	KN	102	CLA	CMD-C2D	-2.19	1.46	1.50
87	O2	201	CLA	CHC-C1C	2.19	1.43	1.38
87	dL	402	CLA	CHC-C1C	2.19	1.43	1.38
87	12	603	CLA	MG-NB	-2.19	2.01	2.05
82	DG	1002	PEB	C4A-NA	-2.19	1.32	1.37
82	EI	202	PEB	C4A-NA	-2.19	1.32	1.37
82	V1	201	PEB	C1B-C2B	2.19	1.50	1.45
87	52	604	CLA	CMC-C2C	-2.19	1.46	1.50
82	JK	202	PEB	C4A-NA	-2.19	1.32	1.37
82	TM	202	PEB	C4A-NA	-2.19	1.32	1.37
82	b1	203	PEB	C4A-NA	-2.19	1.32	1.37
87	A2	836	CLA	CMD-C2D	-2.19	1.46	1.50
87	aL	605	CLA	CMB-C2B	-2.19	1.46	1.50
87	B2	829	CLA	MG-NB	-2.19	2.01	2.05
87	8N	303	CLA	MG-NB	-2.19	2.01	2.05
82	E5	202	PEB	C1C-C2C	2.19	1.48	1.42
83	xK	305	PUB	C4B-C3B	2.19	1.48	1.42
82	dG	204	PEB	C1D-ND	2.19	1.49	1.45
82	Y5	202	PEB	C4A-NA	-2.19	1.32	1.37
82	aK	202	PEB	C4A-NA	-2.19	1.32	1.37
84	JH	1001	CYC	C4B-NB	-2.19	1.33	1.38
82	d4	202	PEB	C4A-NA	-2.19	1.32	1.37
82	TK	202	PEB	C4B-C3B	2.19	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	M9	302	PEB	C1D-ND	2.19	1.49	1.45
87	BN	829	CLA	CMC-C2C	-2.19	1.46	1.50
87	A6	404	CLA	CMB-C2B	-2.19	1.46	1.50
82	y8	203	PEB	C1C-C2C	2.19	1.48	1.42
82	B9	202	PEB	C4B-NB	-2.19	1.33	1.38
82	IA	201	PEB	C4A-NA	-2.19	1.32	1.37
82	H4	1002	PEB	C4A-NA	-2.19	1.32	1.37
82	Y4	202	PEB	C4A-NA	-2.19	1.32	1.37
82	P7	203	PEB	C4A-NA	-2.19	1.32	1.37
82	HO	1002	PEB	C1C-NC	-2.19	1.34	1.37
82	uC	203	PEB	C1C-C2C	2.19	1.48	1.42
82	mH	201	PEB	C1C-C2C	2.19	1.48	1.42
87	A2	816	CLA	CMB-C2B	-2.19	1.46	1.50
87	K2	103	CLA	CMB-C2B	-2.19	1.46	1.50
82	fJ	202	PEB	C4B-C3B	2.19	1.49	1.45
84	63	901	CYC	C1A-NA	-2.19	1.33	1.38
82	FM	201	PEB	OD-C4D	2.19	1.27	1.23
96	V6	201	HEM	C3C-C4C	-2.19	1.42	1.46
82	RF	202	PEB	C1C-NC	-2.19	1.34	1.37
87	B6	612	CLA	CHC-C1C	2.19	1.43	1.38
82	hG	203	PEB	C4B-C3B	2.19	1.49	1.45
96	v6	201	HEM	C1D-ND	-2.19	1.34	1.38
82	Y7	304	PEB	C4A-NA	-2.19	1.32	1.37
82	iM	201	PEB	C4A-NA	-2.19	1.32	1.37
82	tF	202	PEB	C1D-ND	2.19	1.49	1.45
82	XB	202	PEB	CHC-C4C	2.19	1.52	1.49
82	VF	201	PEB	C1A-NA	-2.18	1.34	1.37
82	KM	202	PEB	C4A-NA	-2.18	1.32	1.37
82	DO	1002	PEB	C4A-NA	-2.18	1.32	1.37
82	fJ	203	PEB	C4A-NA	-2.18	1.32	1.37
82	nK	202	PEB	C4A-NA	-2.18	1.32	1.37
82	QG	202	PEB	C1C-C2C	2.18	1.48	1.42
82	YK	202	PEB	C4B-C3B	2.18	1.49	1.45
87	A2	833	CLA	CMD-C2D	-2.18	1.46	1.50
82	JM	202	PEB	C4A-NA	-2.18	1.32	1.37
82	WD	201	PEB	C2A-C1A	-2.18	1.50	1.52
87	A2	825	CLA	C1B-C2B	2.18	1.48	1.43
87	A2	808	CLA	CMB-C2B	-2.18	1.46	1.50
87	B2	833	CLA	CMD-C2D	-2.18	1.46	1.50
82	tC	201	PEB	C4B-C3B	2.18	1.49	1.45
87	BL	623	CLA	C1B-NB	-2.18	1.35	1.37
82	hE	202	PEB	C1C-C2C	2.18	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	VD	201	PEB	C4A-NA	-2.18	1.32	1.37
82	L7	201	PEB	C4A-NA	-2.18	1.32	1.37
82	PQ	201	PEB	C1D-ND	2.18	1.49	1.45
82	VG	202	PEB	C1C-NC	-2.18	1.34	1.37
82	QP	201	PEB	C1C-NC	-2.18	1.34	1.37
87	32	313	CLA	CMC-C2C	-2.18	1.46	1.50
87	B2	833	CLA	CMB-C2B	-2.18	1.46	1.50
87	b6	608	CLA	CMC-C2C	-2.18	1.46	1.50
82	OJ	202	PEB	C4B-C3B	2.18	1.49	1.45
82	W1	203	PEB	C4B-C3B	2.18	1.49	1.45
82	xK	303	PEB	C4B-C3B	2.18	1.49	1.45
82	mG	201	PEB	C4A-NA	-2.18	1.32	1.37
82	ZH	202	PEB	CHC-C4C	2.18	1.52	1.49
82	UJ	203	PEB	C2A-C1A	-2.18	1.50	1.52
82	AD	303	PEB	C1C-NC	-2.18	1.34	1.37
82	FK	201	PEB	C1C-NC	-2.18	1.34	1.37
95	AL	416	DGD	O5D-C1E	2.18	1.43	1.40
87	8N	306	CLA	CHC-C1C	2.18	1.43	1.38
82	YA	301	PEB	C4A-NA	-2.18	1.32	1.37
82	WF	202	PEB	C4A-NA	-2.18	1.32	1.37
82	i4	201	PEB	C4A-NA	-2.18	1.32	1.37
82	Y7	303	PEB	C4A-NA	-2.18	1.32	1.37
82	iJ	202	PEB	C4A-NA	-2.18	1.32	1.37
82	qK	203	PEB	C4B-C3B	2.18	1.49	1.45
87	O2	201	CLA	MG-NB	-2.18	2.01	2.05
87	I2	103	CLA	CMD-C2D	-2.18	1.46	1.50
82	aJ	204	PEB	C1C-C2C	2.18	1.48	1.42
82	mG	202	PEB	CHC-C4C	2.18	1.52	1.49
82	H4	1002	PEB	C1C-NC	-2.18	1.34	1.37
87	B2	823	CLA	C1B-NB	-2.18	1.35	1.37
84	JO	1001	CYC	C1B-C2B	2.18	1.49	1.45
87	O2	203	CLA	CMB-C2B	-2.18	1.46	1.50
87	5N	603	CLA	CMB-C2B	-2.18	1.46	1.50
87	8N	308	CLA	CMB-C2B	-2.18	1.46	1.50
82	F1	1002	PEB	C1C-C2C	2.18	1.48	1.42
82	N5	202	PEB	C1C-C2C	2.18	1.48	1.42
87	AN	834	CLA	C1B-C2B	2.18	1.48	1.43
82	eE	202	PEB	C2A-C1A	-2.18	1.50	1.52
82	VJ	202	PEB	C1C-NC	-2.18	1.34	1.37
82	dG	203	PEB	C1C-NC	-2.18	1.34	1.37
84	BG	1002	CYC	C4D-ND	-2.18	1.34	1.37
87	8N	301	CLA	CMB-C2B	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jE	202	PEB	C1C-C2C	2.18	1.48	1.42
87	BL	603	CLA	C1D-ND	2.18	1.40	1.37
82	KJ	202	PEB	C4A-NA	-2.18	1.32	1.37
82	YO	202	PEB	C4A-NA	-2.18	1.32	1.37
82	MP	203	PEB	C4A-NA	-2.18	1.32	1.37
82	aK	201	PEB	C4A-NA	-2.18	1.32	1.37
82	u8	203	PEB	C1C-C2C	2.18	1.48	1.42
82	DF	201	PEB	C1C-NC	-2.18	1.34	1.37
82	A1	305	PEB	C1C-NC	-2.18	1.34	1.37
87	B2	830	CLA	CMD-C2D	-2.18	1.46	1.50
87	BN	824	CLA	C1B-C2B	2.18	1.48	1.43
87	A2	837	CLA	C1B-C2B	2.18	1.48	1.43
87	AN	822	CLA	MG-ND	-2.18	2.01	2.05
82	Q4	201	PEB	CHA-C4A	-2.18	1.32	1.36
82	H5	202	PEB	C4A-NA	-2.18	1.32	1.37
82	vC	201	PEB	C4A-NA	-2.18	1.32	1.37
82	kE	201	PEB	C4A-NA	-2.18	1.32	1.37
82	jE	201	PEB	C4B-C3B	2.18	1.49	1.45
82	h1	202	PEB	C1C-C2C	2.18	1.48	1.42
82	aG	202	PEB	C1C-C2C	2.18	1.48	1.42
82	SO	202	PEB	C2A-C1A	-2.18	1.50	1.52
82	18	203	PEB	C2A-C1A	-2.18	1.50	1.52
87	A2	824	CLA	CMB-C2B	-2.18	1.46	1.50
87	R2	204	CLA	CMB-C2B	-2.18	1.46	1.50
87	C6	513	CLA	CMB-C2B	-2.18	1.46	1.50
82	xF	302	PEB	CHC-C4C	2.18	1.52	1.49
87	72	604	CLA	MG-NB	-2.18	2.01	2.05
82	DK	201	PEB	C1C-NC	-2.18	1.34	1.37
84	A3	1001	CYC	OB-C4B	2.18	1.27	1.23
82	NI	203	PEB	C4A-NA	-2.18	1.32	1.37
82	LP	202	PEB	C4A-NA	-2.18	1.32	1.37
82	B9	202	PEB	C4A-NA	-2.18	1.32	1.37
82	SD	202	PEB	C1C-C2C	2.18	1.48	1.42
82	EJ	203	PEB	C1C-C2C	2.18	1.48	1.42
87	AN	837	CLA	C1B-C2B	2.18	1.48	1.43
87	c6	612	CLA	CMB-C2B	-2.18	1.46	1.50
82	PA	202	PEB	C4B-C3B	2.18	1.49	1.45
87	6N	605	CLA	MG-NB	-2.18	2.01	2.05
84	FE	1001	CYC	C4A-C3A	2.18	1.50	1.45
82	FD	202	PEB	C1C-C2C	2.18	1.48	1.42
82	T4	203	PEB	C1C-C2C	2.18	1.48	1.42
82	xK	302	PEB	C1C-C2C	2.18	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	kO	201	PEB	C1C-C2C	2.18	1.48	1.42
87	42	608	CLA	C1B-NB	-2.18	1.35	1.37
87	B6	607	CLA	CMB-C2B	-2.18	1.46	1.50
87	B6	607	CLA	CMD-C2D	-2.18	1.46	1.50
87	B6	615	CLA	CMD-C2D	-2.18	1.46	1.50
87	b6	616	CLA	CMB-C2B	-2.18	1.46	1.50
82	PE	202	PEB	C4A-NA	-2.18	1.32	1.37
87	AL	405	CLA	C1B-C2B	2.18	1.48	1.43
87	c6	607	CLA	CMD-C2D	-2.18	1.46	1.50
82	MF	202	PEB	C1C-C2C	2.18	1.48	1.42
82	PA	203	PEB	C4A-NA	-2.18	1.32	1.37
82	SM	201	PEB	C4A-NA	-2.18	1.32	1.37
82	DP	202	PEB	C4A-NA	-2.18	1.32	1.37
87	c6	613	CLA	CHC-C1C	2.18	1.43	1.38
87	7N	604	CLA	CMC-C2C	-2.18	1.46	1.50
82	WP	202	PEB	C1C-NC	-2.18	1.34	1.37
82	MA	202	PEB	C1C-C2C	2.18	1.48	1.42
82	PG	201	PEB	C1C-C2C	2.18	1.48	1.42
82	JP	201	PEB	C1C-C2C	2.18	1.48	1.42
82	JQ	201	PEB	C1C-C2C	2.18	1.48	1.42
87	62	306	CLA	MG-NB	-2.18	2.01	2.05
82	xF	302	PEB	C1D-ND	2.18	1.49	1.45
84	EO	1001	CYC	C1B-C2B	2.18	1.49	1.45
82	b1	202	PEB	C4B-C3B	2.18	1.49	1.45
82	t8	201	PEB	C4B-C3B	2.18	1.49	1.45
82	g4	203	PEB	C1C-C2C	2.18	1.48	1.42
82	E7	202	PEB	C1C-C2C	2.18	1.48	1.42
82	CJ	202	PEB	C1C-NC	-2.18	1.34	1.37
82	CP	203	PEB	C1C-NC	-2.18	1.34	1.37
82	iG	201	PEB	C1C-NC	-2.18	1.34	1.37
82	KB	302	PEB	CHC-C4C	2.18	1.52	1.49
82	QJ	204	PEB	C4A-NA	-2.18	1.32	1.37
82	HO	1002	PEB	C4A-NA	-2.18	1.32	1.37
96	V6	201	HEM	C1D-ND	-2.18	1.34	1.38
84	N3	1001	CYC	OB-C4B	2.18	1.27	1.23
87	BN	833	CLA	CHC-C1C	2.18	1.42	1.38
87	B6	603	CLA	CMD-C2D	-2.18	1.46	1.50
82	rK	202	PEB	C1B-C2B	2.18	1.50	1.45
82	DA	202	PEB	C4B-C3B	2.18	1.49	1.45
82	wC	204	PEB	C4B-C3B	2.18	1.49	1.45
82	nF	202	PEB	C4B-C3B	2.18	1.49	1.45
82	VI	202	PEB	C4A-NA	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GQ	201	PEB	C2A-C1A	-2.18	1.50	1.52
82	a1	201	PEB	C2A-C1A	-2.18	1.50	1.52
87	BL	621	CLA	CMC-C2C	-2.18	1.46	1.50
87	CL	514	CLA	CMC-C2C	-2.18	1.46	1.50
87	AN	808	CLA	CMB-C2B	-2.18	1.46	1.50
87	a6	608	CLA	CMD-C2D	-2.18	1.46	1.50
87	b6	610	CLA	CMD-C2D	-2.18	1.46	1.50
82	hM	202	PEB	C1C-C2C	2.18	1.48	1.42
87	B2	823	CLA	C1B-C2B	2.18	1.48	1.43
82	WQ	202	PEB	C1D-ND	2.18	1.49	1.45
82	A1	305	PEB	C4B-C3B	2.18	1.49	1.45
82	SB	201	PEB	C1C-NC	-2.18	1.34	1.37
82	bB	201	PEB	C1C-NC	-2.18	1.34	1.37
82	G5	202	PEB	C1C-C2C	2.18	1.48	1.42
84	R3	1001	CYC	OB-C4B	2.18	1.27	1.23
82	SI	201	PEB	C4A-NA	-2.18	1.32	1.37
82	I7	201	PEB	C4A-NA	-2.18	1.32	1.37
82	xK	302	PEB	C4A-NA	-2.18	1.32	1.37
82	HA	201	PEB	C1C-C2C	2.18	1.48	1.42
82	A7	201	PEB	C1C-C2C	2.18	1.48	1.42
82	G7	202	PEB	C1C-C2C	2.18	1.48	1.42
87	BN	832	CLA	CMB-C2B	-2.18	1.46	1.50
87	C6	509	CLA	CMD-C2D	-2.18	1.46	1.50
87	cL	506	CLA	CMD-C2D	-2.18	1.46	1.50
87	62	302	CLA	CHC-C1C	2.18	1.42	1.38
82	fE	203	PEB	CHC-C4C	2.18	1.52	1.49
82	XD	203	PEB	C2A-C1A	-2.18	1.50	1.52
82	KJ	202	PEB	C2A-C1A	-2.18	1.50	1.52
82	QG	201	PEB	C4A-NA	-2.18	1.32	1.37
82	DM	201	PEB	C4A-NA	-2.18	1.32	1.37
82	mM	201	PEB	C4A-NA	-2.18	1.32	1.37
82	AD	303	PEB	C1C-C2C	2.18	1.48	1.42
82	JM	202	PEB	C1C-C2C	2.18	1.48	1.42
82	A4	305	PEB	C1C-C2C	2.18	1.48	1.42
82	jO	201	PEB	C1C-C2C	2.18	1.48	1.42
96	fL	102	HEM	C1D-ND	-2.18	1.34	1.38
87	8N	303	CLA	CMB-C2B	-2.18	1.46	1.50
82	UE	201	PEB	C4A-NA	-2.18	1.32	1.37
82	RH	201	PEB	C1C-C2C	2.18	1.48	1.42
87	BL	619	CLA	CMC-C2C	-2.18	1.46	1.50
82	GF	203	PEB	C4A-NA	-2.18	1.32	1.37
82	MF	203	PEB	C4A-NA	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	18	201	PEB	C4A-NA	-2.18	1.32	1.37
82	eF	201	PEB	C4A-NA	-2.18	1.32	1.37
87	IN	103	CLA	CMC-C2C	-2.18	1.46	1.50
87	KN	105	CLA	CMB-C2B	-2.18	1.46	1.50
87	12	603	CLA	CMB-C2B	-2.18	1.46	1.50
87	B2	820	CLA	CMD-C2D	-2.18	1.46	1.50
87	3N	313	CLA	CMB-C2B	-2.18	1.46	1.50
82	SP	202	PEB	C1B-C2B	2.18	1.50	1.45
87	82	305	CLA	CHC-C1C	2.17	1.42	1.38
87	4N	603	CLA	CHC-C1C	2.17	1.42	1.38
82	pK	201	PEB	C1C-C2C	2.17	1.48	1.42
82	1C	201	PEB	C4A-NA	-2.17	1.32	1.37
82	U1	201	PEB	CHC-C4C	2.17	1.52	1.49
82	hF	202	PEB	CHC-C4C	2.17	1.52	1.49
82	W4	201	PEB	C1C-NC	-2.17	1.34	1.37
87	42	608	CLA	MG-ND	-2.17	2.01	2.05
87	72	610	CLA	MG-NB	-2.17	2.01	2.05
87	AN	801	CLA	CMB-C2B	-2.17	1.46	1.50
87	b6	615	CLA	CMC-C2C	-2.17	1.46	1.50
82	r8	201	PEB	C1D-ND	2.17	1.49	1.45
82	w8	202	PEB	C1C-C2C	2.17	1.48	1.42
82	bO	201	PEB	C4A-NA	-2.17	1.32	1.37
82	cO	202	PEB	C4A-NA	-2.17	1.32	1.37
87	K2	101	CLA	MG-NB	-2.17	2.01	2.05
87	O2	203	CLA	MG-NB	-2.17	2.01	2.05
82	GD	201	PEB	C2A-C1A	-2.17	1.50	1.52
82	WJ	202	PEB	C1C-C2C	2.17	1.48	1.42
82	AO	301	PEB	C1C-C2C	2.17	1.48	1.42
87	c6	604	CLA	CHC-C1C	2.17	1.42	1.38
87	6N	603	CLA	CHC-C1C	2.17	1.42	1.38
82	A7	201	PEB	CHC-C4C	2.17	1.52	1.49
82	NI	202	PEB	C4A-NA	-2.17	1.32	1.37
87	BL	622	CLA	CMC-C2C	-2.17	1.46	1.50
87	AL	405	CLA	MG-ND	-2.17	2.01	2.05
87	bL	616	CLA	MG-ND	-2.17	2.01	2.05
87	A2	835	CLA	C1B-C2B	2.17	1.48	1.43
87	42	603	CLA	CHC-C1C	2.17	1.42	1.38
82	D7	202	PEB	C4B-C3B	2.17	1.49	1.45
84	L4	1001	CYC	C1A-NA	-2.17	1.33	1.38
87	4N	602	CLA	CMD-C2D	-2.17	1.46	1.50
82	WD	201	PEB	C1B-C2B	2.17	1.50	1.45
82	dM	202	PEB	C1C-C2C	2.17	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	825	CLA	C1B-C2B	2.17	1.48	1.43
82	SJ	202	PEB	C2A-C1A	-2.17	1.50	1.52
82	CD	202	PEB	C4A-NA	-2.17	1.32	1.37
82	UD	201	PEB	C4A-NA	-2.17	1.32	1.37
82	QD	202	PEB	C1C-NC	-2.17	1.34	1.37
87	B2	831	CLA	CMD-C2D	-2.17	1.46	1.50
82	ZO	201	PEB	OD-C4D	2.17	1.27	1.23
84	l3	1001	CYC	OB-C4B	2.17	1.27	1.23
87	BN	806	CLA	MG-ND	-2.17	2.01	2.05
87	A2	834	CLA	C4B-NB	2.17	1.40	1.37
82	BF	202	PEB	C4A-NA	-2.17	1.32	1.37
82	CI	202	PEB	C4A-NA	-2.17	1.32	1.37
82	z8	201	PEB	C4A-NA	-2.17	1.32	1.37
82	a1	201	PEB	C1C-C2C	2.17	1.48	1.42
87	32	309	CLA	CMD-C2D	-2.17	1.46	1.50
82	JI	202	PEB	C4A-NA	-2.17	1.32	1.37
82	HQ	203	PEB	C4A-NA	-2.17	1.32	1.37
82	OJ	203	PEB	C1C-C2C	2.17	1.47	1.42
82	ZF	202	PEB	C2A-C1A	-2.17	1.50	1.52
82	fG	203	PEB	C2A-C1A	-2.17	1.50	1.52
82	Y7	304	PEB	C1D-ND	2.17	1.49	1.45
87	AN	822	CLA	CMB-C2B	-2.17	1.46	1.50
87	B6	608	CLA	CMD-C2D	-2.17	1.46	1.50
87	C6	509	CLA	CMB-C2B	-2.17	1.46	1.50
84	E3	1001	CYC	OB-C4B	2.17	1.27	1.23
82	S1	202	PEB	C1C-C2C	2.17	1.47	1.42
82	eK	201	PEB	C4A-NA	-2.17	1.32	1.37
82	iO	201	PEB	C4A-NA	-2.17	1.32	1.37
82	uC	201	PEB	C1B-C2B	2.17	1.50	1.45
87	b6	614	CLA	CMD-C2D	-2.17	1.46	1.50
82	VJ	201	PEB	CHC-C4C	2.17	1.52	1.49
87	BN	829	CLA	MG-NB	-2.17	2.01	2.05
87	R2	201	CLA	MG-NB	-2.17	2.01	2.05
87	3N	301	CLA	MG-ND	-2.17	2.01	2.05
82	PQ	203	PEB	C1C-NC	-2.17	1.34	1.37
82	O1	201	PEB	C1C-C2C	2.17	1.47	1.42
82	iG	201	PEB	C4A-NA	-2.17	1.32	1.37
87	B2	815	CLA	CMD-C2D	-2.17	1.46	1.50
87	cL	517	CLA	CMC-C2C	-2.17	1.46	1.50
87	BL	623	CLA	C1B-C2B	2.17	1.48	1.43
82	qF	203	PEB	CHC-C4C	2.17	1.52	1.49
82	wK	303	PEB	CHC-C4C	2.17	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	NO	1001	CYC	C4A-C3A	2.17	1.50	1.45
87	32	312	CLA	CMD-C2D	-2.17	1.46	1.50
82	hM	201	PEB	C4B-C3B	2.17	1.49	1.45
82	U9	202	PEB	C1C-C2C	2.17	1.47	1.42
82	Z1	201	PEB	C1A-NA	-2.17	1.34	1.37
87	4N	608	CLA	MG-ND	-2.17	2.01	2.05
87	1N	603	CLA	CMB-C2B	-2.17	1.46	1.50
82	XD	203	PEB	C1C-C2C	2.17	1.47	1.42
82	QM	202	PEB	C1C-C2C	2.17	1.47	1.42
82	LP	201	PEB	C2A-C1A	-2.17	1.50	1.52
82	AE	301	PEB	C4B-C3B	2.17	1.49	1.45
87	B2	833	CLA	CHC-C1C	2.17	1.42	1.38
82	J9	203	PEB	C4A-NA	-2.17	1.32	1.37
87	AN	801	CLA	CMC-C2C	-2.17	1.46	1.50
87	A2	851	CLA	CMB-C2B	-2.17	1.46	1.50
82	WI	203	PEB	C1C-C2C	2.17	1.47	1.42
82	UO	201	PEB	C1C-NC	-2.17	1.34	1.37
82	kE	202	PEB	C1C-NC	-2.17	1.34	1.37
87	B6	614	CLA	CMB-C2B	-2.17	1.46	1.50
82	YF	202	PEB	C4B-C3B	2.17	1.49	1.45
82	XP	201	PEB	C4B-C3B	2.17	1.49	1.45
82	gH	201	PEB	C4B-C3B	2.17	1.49	1.45
82	XI	201	PEB	C1C-C2C	2.17	1.47	1.42
82	MM	203	PEB	C1C-NC	-2.17	1.34	1.37
82	OI	202	PEB	C4A-NA	-2.17	1.32	1.37
82	UQ	201	PEB	C4A-NA	-2.17	1.32	1.37
82	d1	202	PEB	C1B-C2B	2.17	1.50	1.45
87	BN	824	CLA	C1B-NB	-2.17	1.35	1.37
82	a4	202	PEB	C1C-C2C	2.17	1.47	1.42
82	hB	301	PEB	C1C-C2C	2.17	1.47	1.42
87	AN	837	CLA	CMB-C2B	-2.17	1.46	1.50
87	BN	831	CLA	CMD-C2D	-2.17	1.46	1.50
84	KO	1001	CYC	C1B-C2B	2.17	1.49	1.45
84	K4	1001	CYC	C1B-C2B	2.17	1.49	1.45
84	I4	1001	CYC	C4B-NB	-2.17	1.33	1.38
82	Y1	201	PEB	C4B-C3B	2.17	1.49	1.45
82	VQ	201	PEB	C4A-NA	-2.17	1.32	1.37
87	BN	830	CLA	MG-NB	-2.17	2.01	2.05
87	12	606	CLA	MG-NB	-2.17	2.01	2.05
82	EQ	201	PEB	C1B-C2B	2.17	1.50	1.45
82	S4	202	PEB	C1C-C2C	2.17	1.47	1.42
82	lH	201	PEB	C1C-C2C	2.17	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	829	CLA	CMD-C2D	-2.17	1.46	1.50
87	C6	517	CLA	CMB-C2B	-2.17	1.46	1.50
82	JQ	202	PEB	C1D-ND	2.17	1.49	1.45
82	Z1	202	PEB	C4B-C3B	2.17	1.49	1.45
82	gK	202	PEB	C4A-NA	-2.17	1.32	1.37
82	EA	202	PEB	C1C-C2C	2.17	1.47	1.42
87	A2	810	CLA	CHC-C1C	2.17	1.42	1.38
87	ON	203	CLA	MG-NB	-2.17	2.01	2.05
87	12	609	CLA	MG-NB	-2.17	2.01	2.05
87	1N	609	CLA	MG-NB	-2.17	2.01	2.05
87	AN	825	CLA	CMD-C2D	-2.17	1.46	1.50
87	K6	101	CLA	CMC-C2C	-2.17	1.46	1.50
82	P5	202	PEB	C1C-C2C	2.17	1.47	1.42
82	BK	202	PEB	C4A-NA	-2.17	1.32	1.37
87	5N	605	CLA	MG-NB	-2.17	2.01	2.05
87	cL	507	CLA	CMD-C2D	-2.17	1.46	1.50
82	UG	202	PEB	C1C-C2C	2.17	1.47	1.42
82	jK	202	PEB	C1C-C2C	2.17	1.47	1.42
87	CL	511	CLA	C1B-C2B	2.17	1.48	1.43
87	AN	815	CLA	C1B-C2B	2.17	1.48	1.43
82	mE	201	PEB	C4A-NA	-2.17	1.32	1.37
82	eH	203	PEB	C4A-NA	-2.17	1.32	1.37
87	FN	203	CLA	CMC-C2C	-2.17	1.46	1.50
87	FN	203	CLA	CMD-C2D	-2.17	1.46	1.50
87	A2	824	CLA	CMC-C2C	-2.17	1.46	1.50
87	B6	613	CLA	CMB-C2B	-2.17	1.46	1.50
87	ON	201	CLA	MG-NB	-2.17	2.01	2.05
82	sC	201	PEB	C1C-C2C	2.17	1.47	1.42
82	hE	203	PEB	C1C-C2C	2.17	1.47	1.42
82	eM	202	PEB	C1C-C2C	2.17	1.47	1.42
82	KD	202	PEB	C1C-NC	-2.17	1.34	1.37
82	UA	202	PEB	C2A-C1A	-2.17	1.50	1.52
82	AF	201	PEB	C4A-NA	-2.17	1.32	1.37
82	YH	201	PEB	C4A-NA	-2.17	1.32	1.37
82	jO	202	PEB	C4A-NA	-2.17	1.32	1.37
87	ON	201	CLA	CMD-C2D	-2.17	1.46	1.50
87	C6	511	CLA	CMB-C2B	-2.17	1.46	1.50
87	C6	516	CLA	CMD-C2D	-2.17	1.46	1.50
82	CD	201	PEB	C1C-C2C	2.17	1.47	1.42
82	OH	201	PEB	C1C-C2C	2.17	1.47	1.42
82	C5	202	PEB	C1C-C2C	2.17	1.47	1.42
82	IA	201	PEB	C4B-C3B	2.17	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	HA	201	PEB	C4A-NA	-2.17	1.32	1.37
82	EM	201	PEB	C4A-NA	-2.17	1.32	1.37
87	C6	515	CLA	CMC-C2C	-2.17	1.46	1.50
82	PA	203	PEB	C1C-C2C	2.17	1.47	1.42
82	CK	203	PEB	C1C-C2C	2.17	1.47	1.42
82	j1	201	PEB	C1C-C2C	2.17	1.47	1.42
82	sC	202	PEB	C4B-C3B	2.17	1.49	1.45
87	B6	612	CLA	CMB-C2B	-2.17	1.46	1.50
87	B6	615	CLA	CMB-C2B	-2.17	1.46	1.50
87	d6	401	CLA	CMD-C2D	-2.17	1.46	1.50
82	AQ	303	PEB	C1C-NC	-2.17	1.34	1.37
82	V1	203	PEB	C1C-C2C	2.17	1.47	1.42
82	lJ	201	PEB	C1C-C2C	2.17	1.47	1.42
87	RN	201	CLA	MG-NB	-2.17	2.01	2.05
87	B2	833	CLA	MG-ND	-2.17	2.01	2.05
87	B2	836	CLA	C3D-C4D	2.17	1.49	1.44
84	m3	1001	CYC	OB-C4B	2.16	1.27	1.23
82	VA	203	PEB	C4A-NA	-2.16	1.32	1.37
82	DF	202	PEB	C4A-NA	-2.16	1.32	1.37
82	DH	1002	PEB	C4A-NA	-2.16	1.32	1.37
87	A2	818	CLA	CMB-C2B	-2.16	1.46	1.50
87	A2	822	CLA	CMB-C2B	-2.16	1.46	1.50
87	62	312	CLA	CHC-C1C	2.16	1.42	1.38
87	B6	605	CLA	CHC-C1C	2.16	1.42	1.38
82	BA	201	PEB	C1C-C2C	2.16	1.47	1.42
82	kO	202	PEB	C1C-C2C	2.16	1.47	1.42
87	BL	620	CLA	MG-ND	-2.16	2.01	2.05
87	62	310	CLA	MG-NB	-2.16	2.01	2.05
82	H9	203	PEB	C4B-C3B	2.16	1.49	1.45
82	NP	202	PEB	C4A-NA	-2.16	1.32	1.37
87	RN	204	CLA	CMD-C2D	-2.16	1.46	1.50
87	C6	518	CLA	CMD-C2D	-2.16	1.46	1.50
87	b6	604	CLA	CMC-C2C	-2.16	1.46	1.50
87	2N	301	CLA	CMC-C2C	-2.16	1.46	1.50
82	D7	203	PEB	C1C-C2C	2.16	1.47	1.42
87	82	308	CLA	MG-ND	-2.16	2.01	2.05
82	kH	203	PEB	C4B-C3B	2.16	1.49	1.45
82	dM	203	PEB	C4B-C3B	2.16	1.49	1.45
82	ZB	202	PEB	C4A-NA	-2.16	1.32	1.37
82	fF	201	PEB	C1C-C2C	2.16	1.47	1.42
82	aM	204	PEB	C1C-C2C	2.16	1.47	1.42
84	FH	1001	CYC	C4D-C3D	2.16	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	CL	508	CLA	CMD-C2D	-2.16	1.46	1.50
87	BN	814	CLA	CMD-C2D	-2.16	1.46	1.50
87	6N	604	CLA	C3D-C4D	2.16	1.49	1.44
87	KN	102	CLA	C1B-NB	-2.16	1.35	1.37
87	B2	815	CLA	MG-NB	-2.16	2.01	2.05
87	5N	603	CLA	MG-NB	-2.16	2.01	2.05
82	eO	201	PEB	C1B-C2B	2.16	1.50	1.45
82	lK	203	PEB	C1C-C2C	2.16	1.47	1.42
82	O5	202	PEB	C4B-C3B	2.16	1.49	1.45
87	4N	602	CLA	CHC-C1C	2.16	1.42	1.38
87	32	312	CLA	MG-NB	-2.16	2.01	2.05
87	1N	601	CLA	MG-NB	-2.16	2.01	2.05
87	1N	603	CLA	MG-NB	-2.16	2.01	2.05
82	b4	202	PEB	C1C-C2C	2.16	1.47	1.42
82	UK	202	PEB	C4A-NA	-2.16	1.32	1.37
82	LM	201	PEB	C4A-NA	-2.16	1.32	1.37
82	aM	202	PEB	C4A-NA	-2.16	1.32	1.37
96	v6	201	HEM	C3C-C4C	-2.16	1.42	1.46
87	C6	516	CLA	CMB-C2B	-2.16	1.46	1.50
87	D6	402	CLA	CMD-C2D	-2.16	1.46	1.50
87	b6	607	CLA	CMD-C2D	-2.16	1.46	1.50
82	SG	201	PEB	C1C-NC	-2.16	1.34	1.37
87	c6	609	CLA	CHC-C1C	2.16	1.42	1.38
82	BA	202	PEB	C4B-C3B	2.16	1.49	1.45
82	qC	202	PEB	C4B-C3B	2.16	1.49	1.45
82	ZM	202	PEB	C1C-C2C	2.16	1.47	1.42
82	SI	202	PEB	C4A-NA	-2.16	1.32	1.37
87	BN	828	CLA	CMD-C2D	-2.16	1.46	1.50
84	y3	1001	CYC	C1A-C2A	2.16	1.49	1.45
87	32	313	CLA	CMB-C2B	-2.16	1.46	1.50
87	82	308	CLA	CMB-C2B	-2.16	1.46	1.50
87	C6	514	CLA	CMD-C2D	-2.16	1.46	1.50
82	OO	201	PEB	C1C-C2C	2.16	1.47	1.42
82	hG	203	PEB	C1C-C2C	2.16	1.47	1.42
87	82	302	CLA	MG-NB	-2.16	2.01	2.05
87	A2	806	CLA	MG-NB	-2.16	2.01	2.05
87	bL	606	CLA	MG-ND	-2.16	2.01	2.05
82	AK	201	PEB	C4A-NA	-2.16	1.32	1.37
82	FP	202	PEB	C4A-NA	-2.16	1.32	1.37
82	VQ	203	PEB	C4A-NA	-2.16	1.32	1.37
82	eE	203	PEB	C4A-NA	-2.16	1.32	1.37
82	aJ	202	PEB	C4A-NA	-2.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	C6	520	CLA	CMB-C2B	-2.16	1.46	1.50
87	c6	606	CLA	CMD-C2D	-2.16	1.46	1.50
82	M7	202	PEB	C1C-C2C	2.16	1.47	1.42
83	wF	304	PUB	C4B-C3B	2.16	1.47	1.42
82	oF	202	PEB	C1B-C2B	2.16	1.50	1.45
82	OG	203	PEB	C4A-NA	-2.16	1.32	1.37
82	GM	201	PEB	C4A-NA	-2.16	1.32	1.37
82	IM	203	PEB	C4A-NA	-2.16	1.32	1.37
87	AN	840	CLA	CMC-C2C	-2.16	1.46	1.50
82	H9	201	PEB	C1C-NC	-2.16	1.34	1.37
82	LA	202	PEB	C1C-C2C	2.16	1.47	1.42
82	RD	203	PEB	C4A-NA	-2.16	1.32	1.37
82	CP	202	PEB	C4A-NA	-2.16	1.32	1.37
82	RQ	203	PEB	C4A-NA	-2.16	1.32	1.37
82	l4	202	PEB	C4A-NA	-2.16	1.32	1.37
87	6N	609	CLA	MG-NB	-2.16	2.01	2.05
87	C6	512	CLA	CMB-C2B	-2.16	1.46	1.50
82	AH	301	PEB	C1C-NC	-2.16	1.34	1.37
82	X5	202	PEB	C1C-NC	-2.16	1.34	1.37
82	UD	201	PEB	C4B-C3B	2.16	1.49	1.45
84	DG	1001	CYC	C1A-C2A	2.16	1.49	1.45
87	IN	102	CLA	CMC-C2C	-2.16	1.46	1.50
87	A2	838	CLA	CMD-C2D	-2.16	1.46	1.50
87	D6	405	CLA	CMB-C2B	-2.16	1.46	1.50
82	XQ	203	PEB	C1C-C2C	2.16	1.47	1.42
82	W4	201	PEB	CHA-C4A	-2.16	1.32	1.36
87	6N	607	CLA	CHC-C1C	2.16	1.42	1.38
82	UI	202	PEB	C1C-NC	-2.16	1.34	1.37
84	I4	1001	CYC	C1B-NB	-2.16	1.34	1.37
82	TI	201	PEB	C2C-C3C	2.16	1.44	1.38
82	FA	203	PEB	C4A-NA	-2.16	1.32	1.37
82	LM	202	PEB	C4A-NA	-2.16	1.32	1.37
82	D5	202	PEB	C4A-NA	-2.16	1.32	1.37
87	A2	820	CLA	C1B-NB	-2.16	1.35	1.37
87	A2	822	CLA	MG-ND	-2.16	2.01	2.05
82	YK	201	PEB	CHC-C4C	2.16	1.52	1.49
82	ZB	201	PEB	C1C-NC	-2.16	1.34	1.37
82	VE	202	PEB	C1C-NC	-2.16	1.34	1.37
82	HD	201	PEB	C4A-NA	-2.16	1.32	1.37
87	A2	809	CLA	CMB-C2B	-2.16	1.46	1.50
87	K2	106	CLA	CMB-C2B	-2.16	1.46	1.50
87	A2	841	CLA	MG-ND	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mO	202	PEB	C4B-C3B	2.16	1.49	1.45
82	uF	202	PEB	C1C-C2C	2.16	1.47	1.42
82	CJ	202	PEB	C4A-NA	-2.16	1.32	1.37
82	VO	201	PEB	C4A-NA	-2.16	1.32	1.37
82	fE	201	PEB	C4A-NA	-2.16	1.32	1.37
82	iF	203	PEB	C4A-NA	-2.16	1.32	1.37
87	IN	103	CLA	CMD-C2D	-2.16	1.46	1.50
87	A2	821	CLA	CMD-C2D	-2.16	1.46	1.50
87	bL	604	CLA	CMB-C2B	-2.16	1.46	1.50
82	NQ	203	PEB	C1C-NC	-2.16	1.34	1.37
82	rC	201	PEB	C1D-ND	2.16	1.49	1.45
82	PA	202	PEB	C2A-C1A	-2.16	1.50	1.52
82	P7	202	PEB	C2A-C1A	-2.16	1.50	1.52
82	gM	201	PEB	C2A-C1A	-2.16	1.50	1.52
82	JD	201	PEB	C1C-C2C	2.16	1.47	1.42
82	J1	1002	PEB	C1C-C2C	2.16	1.47	1.42
82	V1	201	PEB	C1C-C2C	2.16	1.47	1.42
82	jG	202	PEB	C1C-C2C	2.16	1.47	1.42
87	3N	312	CLA	CMD-C2D	-2.16	1.46	1.50
87	7N	601	CLA	MG-NB	-2.16	2.01	2.05
87	BN	817	CLA	C1B-NB	-2.16	1.35	1.37
82	KJ	203	PEB	C4B-NB	-2.16	1.33	1.38
82	YA	304	PEB	C4A-NA	-2.16	1.32	1.37
82	U5	202	PEB	C4A-NA	-2.16	1.32	1.37
87	BL	604	CLA	CMB-C2B	-2.16	1.46	1.50
87	a6	607	CLA	CMB-C2B	-2.16	1.46	1.50
82	u8	202	PEB	CHC-C4C	2.16	1.52	1.49
82	O4	201	PEB	OD-C4D	2.16	1.27	1.23
82	LM	202	PEB	C1C-C2C	2.16	1.47	1.42
82	R1	201	PEB	C1C-C2C	2.16	1.47	1.42
82	fK	201	PEB	C1C-C2C	2.16	1.47	1.42
82	DB	202	PEB	C1C-NC	-2.16	1.34	1.37
82	K5	202	PEB	C1C-NC	-2.16	1.34	1.37
82	T5	202	PEB	C1C-NC	-2.16	1.34	1.37
82	PQ	201	PEB	C2A-C1A	-2.16	1.50	1.52
87	B6	603	CLA	CHC-C1C	2.16	1.42	1.38
82	YM	203	PEB	C4A-NA	-2.16	1.32	1.37
87	AN	834	CLA	CMD-C2D	-2.16	1.46	1.50
87	BN	802	CLA	CMB-C2B	-2.16	1.46	1.50
87	42	601	CLA	CMB-C2B	-2.16	1.46	1.50
87	B2	812	CLA	CMB-C2B	-2.16	1.46	1.50
87	R2	202	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	b6	606	CLA	CMD-C2D	-2.16	1.46	1.50
84	J1	1001	CYC	C4B-NB	-2.16	1.33	1.38
82	X5	202	PEB	C1C-C2C	2.16	1.47	1.42
87	B6	613	CLA	CHC-C1C	2.16	1.42	1.38
82	RE	202	PEB	C4A-NA	-2.16	1.32	1.37
82	QG	203	PEB	C1C-NC	-2.16	1.34	1.37
87	c6	615	CLA	CMB-C2B	-2.16	1.46	1.50
87	3N	309	CLA	CMD-C2D	-2.16	1.46	1.50
82	a1	202	PEB	C1C-C2C	2.16	1.47	1.42
82	s8	203	PEB	C1C-C2C	2.16	1.47	1.42
87	A2	809	CLA	MG-NB	-2.16	2.01	2.05
87	6N	608	CLA	MG-NB	-2.16	2.01	2.05
82	v8	202	PEB	C1D-ND	2.16	1.49	1.45
82	gF	202	PEB	C4A-NA	-2.16	1.32	1.37
87	B2	832	CLA	CMC-C2C	-2.16	1.46	1.50
87	A6	403	CLA	CMD-C2D	-2.16	1.46	1.50
87	C6	516	CLA	CMC-C2C	-2.16	1.46	1.50
82	QH	202	PEB	C2A-C1A	-2.16	1.50	1.52
82	OG	202	PEB	C1C-NC	-2.16	1.34	1.37
82	N5	202	PEB	C1C-NC	-2.16	1.34	1.37
82	YE	202	PEB	C1C-C2C	2.16	1.47	1.42
84	GO	1001	CYC	C4B-NB	-2.16	1.33	1.38
82	GE	1002	PEB	OD-C4D	2.16	1.27	1.23
82	hE	203	PEB	C4B-C3B	2.16	1.49	1.45
87	BN	832	CLA	CMC-C2C	-2.16	1.46	1.50
87	B2	809	CLA	CMC-C2C	-2.16	1.46	1.50
87	B2	832	CLA	CMB-C2B	-2.16	1.46	1.50
87	b6	611	CLA	CMC-C2C	-2.16	1.46	1.50
82	IJ	203	PEB	C1C-NC	-2.16	1.34	1.37
87	AN	814	CLA	MG-ND	-2.16	2.01	2.05
82	AB	501	PEB	C4A-NA	-2.16	1.32	1.37
87	52	603	CLA	CMB-C2B	-2.16	1.46	1.50
82	PO	202	PEB	C4B-C3B	2.16	1.49	1.45
87	82	304	CLA	MG-NB	-2.15	2.01	2.05
82	QA	202	PEB	C1C-NC	-2.15	1.34	1.37
82	lG	202	PEB	C1C-NC	-2.15	1.34	1.37
84	FE	1002	CYC	C1B-NB	-2.15	1.34	1.37
84	FG	1001	CYC	C1B-NB	-2.15	1.34	1.37
82	V7	203	PEB	C4A-NA	-2.15	1.32	1.37
87	BL	622	CLA	CMB-C2B	-2.15	1.46	1.50
87	BN	833	CLA	CMB-C2B	-2.15	1.46	1.50
82	oF	203	PEB	C4B-C3B	2.15	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	dL	402	CLA	MG-NB	-2.15	2.01	2.05
82	VQ	202	PEB	C1C-C2C	2.15	1.47	1.42
82	R5	202	PEB	C1C-C2C	2.15	1.47	1.42
82	cE	202	PEB	C1C-C2C	2.15	1.47	1.42
82	S9	203	PEB	C4A-NA	-2.15	1.32	1.37
82	ZJ	202	PEB	C1C-NC	-2.15	1.34	1.37
85	K2	102	BCR	C12-C13	2.15	1.50	1.45
82	WK	202	PEB	CHC-C4C	2.15	1.52	1.49
82	FB	201	PEB	C1C-C2C	2.15	1.47	1.42
87	AN	807	CLA	MG-ND	-2.15	2.01	2.05
87	7N	604	CLA	MG-NB	-2.15	2.01	2.05
82	RI	202	PEB	C4A-NA	-2.15	1.32	1.37
87	BN	813	CLA	CMB-C2B	-2.15	1.46	1.50
87	b6	612	CLA	CMC-C2C	-2.15	1.46	1.50
84	FE	1001	CYC	C4B-NB	-2.15	1.33	1.38
84	CG	1001	CYC	C4B-NB	-2.15	1.33	1.38
82	KI	201	PEB	C4D-ND	2.15	1.38	1.35
82	mK	202	PEB	C1C-C2C	2.15	1.47	1.42
87	AN	821	CLA	CMD-C2D	-2.15	1.46	1.50
87	b6	614	CLA	CMB-C2B	-2.15	1.46	1.50
87	c6	611	CLA	CMD-C2D	-2.15	1.46	1.50
82	HI	203	PEB	C1C-NC	-2.15	1.34	1.37
82	sK	201	PEB	C1C-NC	-2.15	1.34	1.37
82	wK	302	PEB	C1C-C2C	2.15	1.47	1.42
82	bO	202	PEB	C1C-C2C	2.15	1.47	1.42
83	xK	301	PUB	C4B-C3B	2.15	1.47	1.42
87	52	605	CLA	MG-NB	-2.15	2.01	2.05
82	GA	202	PEB	C4A-NA	-2.15	1.32	1.37
82	VB	202	PEB	C4A-NA	-2.15	1.32	1.37
87	BN	808	CLA	CMB-C2B	-2.15	1.46	1.50
87	I2	103	CLA	CMB-C2B	-2.15	1.46	1.50
87	O2	201	CLA	CMD-C2D	-2.15	1.46	1.50
87	BL	609	CLA	CHC-C1C	2.15	1.42	1.38
87	AN	810	CLA	CHC-C1C	2.15	1.42	1.38
82	qF	201	PEB	C1B-C2B	2.15	1.50	1.45
82	hK	201	PEB	C1C-NC	-2.15	1.34	1.37
84	DO	1001	CYC	C1B-NB	-2.15	1.34	1.37
82	mH	201	PEB	C4A-NA	-2.15	1.32	1.37
87	CL	505	CLA	MG-NB	-2.15	2.01	2.05
87	AN	806	CLA	MG-NB	-2.15	2.01	2.05
87	82	302	CLA	CMB-C2B	-2.15	1.46	1.50
87	A2	840	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L2	203	CLA	CAC-C3C	-2.15	1.45	1.51
82	OM	201	PEB	C1B-C2B	2.15	1.50	1.45
82	i1	201	PEB	C1B-C2B	2.15	1.50	1.45
82	sK	202	PEB	C1B-C2B	2.15	1.50	1.45
82	CI	201	PEB	C1C-C2C	2.15	1.47	1.42
82	TQ	201	PEB	C1C-C2C	2.15	1.47	1.42
82	pF	201	PEB	C1C-C2C	2.15	1.47	1.42
82	cG	202	PEB	C1C-C2C	2.15	1.47	1.42
87	B2	810	CLA	C1B-NB	-2.15	1.35	1.37
87	BL	608	CLA	CMB-C2B	-2.15	1.46	1.50
87	3N	301	CLA	CMC-C2C	-2.15	1.46	1.50
82	D7	201	PEB	C4A-NA	-2.15	1.32	1.37
82	dO	202	PEB	C4A-NA	-2.15	1.32	1.37
87	BL	601	CLA	CMD-C2D	-2.15	1.46	1.50
87	22	602	CLA	CMC-C2C	-2.15	1.46	1.50
87	F2	205	CLA	CMD-C2D	-2.15	1.46	1.50
87	B6	605	CLA	CMD-C2D	-2.15	1.46	1.50
87	72	607	CLA	C1B-C2B	2.15	1.48	1.43
82	s8	202	PEB	C4B-C3B	2.15	1.49	1.45
82	tK	201	PEB	C4B-C3B	2.15	1.49	1.45
87	22	603	CLA	CMD-C2D	-2.15	1.46	1.50
87	52	611	CLA	CMD-C2D	-2.15	1.46	1.50
87	cL	505	CLA	CMB-C2B	-2.15	1.46	1.50
82	W7	202	PEB	C1C-C2C	2.15	1.47	1.42
87	A2	807	CLA	MG-ND	-2.15	2.01	2.05
95	BL	614	DGD	O5D-C1E	2.15	1.43	1.40
82	YA	303	PEB	C1C-NC	-2.15	1.34	1.37
82	W5	203	PEB	C1C-NC	-2.15	1.34	1.37
87	B2	819	CLA	O2A-CGA	2.15	1.38	1.30
82	NA	201	PEB	C4A-NA	-2.15	1.32	1.37
82	N7	201	PEB	C4A-NA	-2.15	1.32	1.37
84	LO	1001	CYC	C1A-NA	-2.15	1.34	1.38
87	bL	613	CLA	C1B-C2B	2.15	1.48	1.43
82	YQ	202	PEB	C1C-NC	-2.15	1.34	1.37
82	U9	201	PEB	C1C-C2C	2.15	1.47	1.42
82	sC	203	PEB	C1C-C2C	2.15	1.47	1.42
82	DD	202	PEB	OD-C4D	2.15	1.27	1.23
87	1N	607	CLA	CMD-C2D	-2.15	1.46	1.50
87	3N	306	CLA	CMC-C2C	-2.15	1.46	1.50
84	73	1001	CYC	C4A-C3A	2.15	1.50	1.45
87	AN	813	CLA	MG-NB	-2.15	2.01	2.05
87	AN	823	CLA	MG-ND	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	22	604	CLA	MG-ND	-2.15	2.01	2.05
82	nF	202	PEB	C1D-ND	2.15	1.49	1.45
82	XF	203	PEB	C4A-NA	-2.15	1.32	1.37
82	A4	304	PEB	C4A-NA	-2.15	1.32	1.37
87	A2	834	CLA	CMD-C2D	-2.15	1.46	1.50
87	B6	609	CLA	CMD-C2D	-2.15	1.46	1.50
87	2N	303	CLA	CMC-C2C	-2.15	1.46	1.50
87	4N	602	CLA	CMC-C2C	-2.15	1.46	1.50
82	xK	302	PEB	C1C-NC	-2.15	1.34	1.37
82	P7	202	PEB	C4B-C3B	2.15	1.49	1.45
87	BL	608	CLA	MG-NB	-2.15	2.01	2.05
82	QP	203	PEB	C2A-C1A	-2.15	1.50	1.52
82	V5	202	PEB	C2A-C1A	-2.15	1.50	1.52
82	mG	203	PEB	C2A-C1A	-2.15	1.50	1.52
87	AN	803	CLA	CHC-C1C	2.15	1.42	1.38
82	IM	203	PEB	C1C-C2C	2.15	1.47	1.42
82	SQ	202	PEB	C1C-C2C	2.15	1.47	1.42
87	cL	508	CLA	CMC-C2C	-2.15	1.46	1.50
82	u8	201	PEB	C1B-C2B	2.15	1.50	1.45
82	BJ	301	PEB	C1C-NC	-2.15	1.34	1.37
82	eH	202	PEB	CHC-C4C	2.15	1.52	1.49
87	BN	833	CLA	MG-ND	-2.15	2.01	2.05
87	cL	511	CLA	MG-ND	-2.15	2.01	2.05
84	F1	1001	CYC	C4D-C3D	2.15	1.47	1.42
82	ID	201	PEB	C4B-C3B	2.15	1.49	1.45
82	HI	203	PEB	C4A-NA	-2.15	1.32	1.37
87	5N	611	CLA	CMD-C2D	-2.15	1.46	1.50
84	L3	1001	CYC	C4A-C3A	2.15	1.50	1.45
82	VD	202	PEB	C1C-C2C	2.15	1.47	1.42
82	OH	202	PEB	C1C-C2C	2.15	1.47	1.42
83	AO	303	PUB	C4B-C3B	2.15	1.47	1.42
96	v6	201	HEM	C4B-NB	-2.15	1.34	1.38
87	cL	507	CLA	CHC-C1C	2.15	1.42	1.38
82	NI	203	PEB	C2A-C1A	-2.15	1.50	1.52
82	HI	202	PEB	C4A-NA	-2.15	1.32	1.37
82	dH	202	PEB	C4A-NA	-2.15	1.32	1.37
82	cH	202	PEB	C1C-C2C	2.15	1.47	1.42
87	B2	805	CLA	MG-ND	-2.15	2.01	2.05
82	ZG	203	PEB	C1C-NC	-2.15	1.34	1.37
82	mO	201	PEB	C1C-NC	-2.15	1.34	1.37
83	AH	304	PUB	C4B-NB	-2.15	1.34	1.37
82	PI	202	PEB	C4A-NA	-2.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	XI	202	PEB	C4A-NA	-2.15	1.32	1.37
82	m4	201	PEB	C4A-NA	-2.15	1.32	1.37
87	DL	406	CLA	CMB-C2B	-2.15	1.46	1.50
82	O1	202	PEB	C1C-C2C	2.15	1.47	1.42
82	yK	301	PEB	C1C-C2C	2.15	1.47	1.42
87	BL	602	CLA	MG-ND	-2.15	2.01	2.05
82	KD	201	PEB	C4A-NA	-2.15	1.32	1.37
87	B2	829	CLA	CMC-C2C	-2.15	1.46	1.50
87	O2	202	CLA	CMC-C2C	-2.15	1.46	1.50
87	b6	613	CLA	CMB-C2B	-2.15	1.46	1.50
84	D3	1001	CYC	C4A-C3A	2.15	1.50	1.45
82	R5	202	PEB	C2A-C1A	-2.15	1.50	1.52
82	S7	202	PEB	C2A-C1A	-2.15	1.50	1.52
82	QE	203	PEB	C1C-NC	-2.15	1.34	1.37
82	WQ	202	PEB	C4B-C3B	2.15	1.49	1.45
87	AN	809	CLA	CMB-C2B	-2.15	1.46	1.50
87	b6	617	CLA	CMB-C2B	-2.15	1.46	1.50
82	CM	202	PEB	C1C-NC	-2.15	1.34	1.37
87	62	308	CLA	CHC-C1C	2.15	1.42	1.38
87	AN	836	CLA	MG-NB	-2.15	2.01	2.05
87	BN	824	CLA	MG-ND	-2.15	2.01	2.05
87	B6	616	CLA	MG-NB	-2.15	2.01	2.05
82	C7	201	PEB	CHC-C4C	2.15	1.52	1.49
82	vK	201	PEB	CHC-C4C	2.15	1.52	1.49
82	m4	203	PEB	C4A-NA	-2.15	1.32	1.37
84	LO	1001	CYC	C1B-C2B	2.15	1.49	1.45
82	mK	201	PEB	C2A-C1A	-2.15	1.50	1.52
82	QQ	202	PEB	C1C-NC	-2.15	1.34	1.37
82	C9	202	PEB	C1C-NC	-2.15	1.34	1.37
87	A2	813	CLA	MG-NB	-2.15	2.01	2.05
82	YF	201	PEB	C4A-NA	-2.15	1.32	1.37
82	AI	202	PEB	C4A-NA	-2.15	1.32	1.37
82	AP	203	PEB	C4A-NA	-2.15	1.32	1.37
87	A2	807	CLA	CMB-C2B	-2.15	1.46	1.50
82	HD	203	PEB	C4A-NA	-2.15	1.32	1.37
82	uK	201	PEB	C4A-NA	-2.15	1.32	1.37
87	B6	606	CLA	CMD-C2D	-2.15	1.46	1.50
84	BG	1001	CYC	C1B-C2B	2.15	1.49	1.45
87	BN	836	CLA	C3D-C4D	2.15	1.49	1.44
82	c4	203	PEB	C1C-C2C	2.15	1.47	1.42
82	lK	201	PEB	C2A-C1A	-2.14	1.50	1.52
87	CL	504	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AN	835	CLA	CMD-C2D	-2.14	1.46	1.50
87	B2	817	CLA	CMB-C2B	-2.14	1.46	1.50
87	B6	613	CLA	CMD-C2D	-2.14	1.46	1.50
84	F4	1001	CYC	C4C-NC	-2.14	1.32	1.37
82	B7	203	PEB	C1C-NC	-2.14	1.34	1.37
87	bL	616	CLA	C1B-C2B	2.14	1.48	1.43
82	NO	1002	PEB	C1C-C2C	2.14	1.47	1.42
82	V5	202	PEB	C1C-C2C	2.14	1.47	1.42
87	BN	828	CLA	CMC-C2C	-2.14	1.46	1.50
87	A2	803	CLA	CMC-C2C	-2.14	1.46	1.50
82	UP	202	PEB	C4A-NA	-2.14	1.32	1.37
82	fE	202	PEB	C4A-NA	-2.14	1.32	1.37
87	BN	820	CLA	O2A-CGA	2.14	1.37	1.30
82	AE	304	PEB	C1C-C2C	2.14	1.47	1.42
82	T5	202	PEB	C1C-C2C	2.14	1.47	1.42
82	M9	305	PEB	C1C-NC	-2.14	1.34	1.37
84	D4	1001	CYC	C1B-NB	-2.14	1.34	1.37
84	EE	1001	CYC	C1B-C2B	2.14	1.49	1.45
82	iM	201	PEB	C1B-C2B	2.14	1.50	1.45
87	B2	828	CLA	CMD-C2D	-2.14	1.46	1.50
87	62	302	CLA	MG-NB	-2.14	2.01	2.05
87	BL	609	CLA	C1B-C2B	2.14	1.48	1.43
82	W5	202	PEB	CHC-C4C	2.14	1.52	1.49
82	eF	203	PEB	C2A-C1A	-2.14	1.50	1.52
82	lK	202	PEB	C2A-C1A	-2.14	1.50	1.52
82	tK	202	PEB	C1D-ND	2.14	1.49	1.45
82	TI	202	PEB	C1C-C2C	2.14	1.47	1.42
82	CQ	201	PEB	C1C-C2C	2.14	1.47	1.42
82	I5	202	PEB	C1C-C2C	2.14	1.47	1.42
82	L7	203	PEB	C1C-NC	-2.14	1.34	1.37
87	32	306	CLA	CMB-C2B	-2.14	1.46	1.50
82	ZO	201	PEB	CHA-C4A	-2.14	1.32	1.36
87	5N	611	CLA	MG-NB	-2.14	2.01	2.05
87	L2	202	CLA	C3D-C4D	2.14	1.49	1.44
84	IO	1001	CYC	C4B-NB	-2.14	1.33	1.38
82	DD	202	PEB	C4B-NB	-2.14	1.34	1.38
82	XK	203	PEB	C4B-C3B	2.14	1.49	1.45
82	gF	202	PEB	C1C-NC	-2.14	1.34	1.37
87	bL	620	CLA	CMC-C2C	-2.14	1.46	1.50
87	cL	516	CLA	CMC-C2C	-2.14	1.46	1.50
82	fM	203	PEB	C4A-NA	-2.14	1.32	1.37
82	qK	201	PEB	C4B-C3B	2.14	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	M9	304	PEB	C1B-C2B	2.14	1.50	1.45
87	BN	828	CLA	CMB-C2B	-2.14	1.46	1.50
87	A2	806	CLA	CMC-C2C	-2.14	1.46	1.50
87	A6	403	CLA	CHC-C1C	2.14	1.42	1.38
82	e4	202	PEB	C1C-C2C	2.14	1.47	1.42
82	yC	203	PEB	C1C-C2C	2.14	1.47	1.42
82	eO	202	PEB	C1C-C2C	2.14	1.47	1.42
82	DA	202	PEB	C1D-ND	2.14	1.49	1.45
82	kK	203	PEB	C1D-ND	2.14	1.49	1.45
84	KO	1001	CYC	C4B-NB	-2.14	1.33	1.38
82	h4	201	PEB	CHC-C4C	2.14	1.52	1.49
87	C6	517	CLA	CHC-C1C	2.14	1.42	1.38
82	WO	201	PEB	CHA-C4A	-2.14	1.32	1.36
82	dE	203	PEB	C1C-NC	-2.14	1.34	1.37
82	hE	202	PEB	C1D-ND	2.14	1.49	1.45
82	RQ	202	PEB	C1C-C2C	2.14	1.47	1.42
82	m4	202	PEB	C1C-C2C	2.14	1.47	1.42
82	jF	202	PEB	C1C-C2C	2.14	1.47	1.42
82	yF	301	PEB	C1C-C2C	2.14	1.47	1.42
82	jJ	203	PEB	C1C-C2C	2.14	1.47	1.42
87	A2	834	CLA	C3B-C4B	2.14	1.47	1.42
87	RN	202	CLA	CMD-C2D	-2.14	1.46	1.50
82	KD	202	PEB	C2A-C1A	-2.14	1.50	1.52
82	hM	202	PEB	C4A-NA	-2.14	1.32	1.37
87	AN	819	CLA	MG-ND	-2.14	2.01	2.05
82	OE	203	PEB	C4B-C3B	2.14	1.49	1.45
82	O1	202	PEB	C4B-C3B	2.14	1.49	1.45
82	dH	201	PEB	C4B-C3B	2.14	1.49	1.45
82	XA	201	PEB	C1C-NC	-2.14	1.34	1.37
87	DL	406	CLA	CMD-C2D	-2.14	1.46	1.50
82	QI	201	PEB	C4A-NA	-2.14	1.32	1.37
82	H5	203	PEB	C4A-NA	-2.14	1.32	1.37
82	bK	201	PEB	C4A-NA	-2.14	1.32	1.37
87	A2	801	CLA	C1D-C2D	2.14	1.49	1.45
82	SH	202	PEB	C1C-C2C	2.14	1.47	1.42
82	JD	203	PEB	C4B-C3B	2.14	1.49	1.45
82	ZH	202	PEB	C4B-C3B	2.14	1.49	1.45
82	q8	202	PEB	C4B-C3B	2.14	1.49	1.45
82	oK	203	PEB	C4B-C3B	2.14	1.49	1.45
87	3N	313	CLA	CMC-C2C	-2.14	1.46	1.50
82	SO	202	PEB	C4A-NA	-2.14	1.32	1.37
82	gH	201	PEB	C4A-NA	-2.14	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	gB	203	PEB	C2A-C1A	-2.14	1.50	1.52
87	A2	823	CLA	MG-ND	-2.14	2.01	2.05
87	AN	834	CLA	CMC-C2C	-2.14	1.46	1.50
87	7N	603	CLA	CMD-C2D	-2.14	1.46	1.50
82	WK	202	PEB	C4A-NA	-2.14	1.32	1.37
82	Q1	202	PEB	C4A-NA	-2.14	1.32	1.37
82	cJ	201	PEB	C4A-NA	-2.14	1.32	1.37
82	LF	202	PEB	C4B-C3B	2.14	1.49	1.45
82	d1	201	PEB	C4B-C3B	2.14	1.49	1.45
82	OA	202	PEB	C1C-NC	-2.14	1.34	1.37
82	WG	202	PEB	C1C-NC	-2.14	1.34	1.37
82	AK	201	PEB	C1C-NC	-2.14	1.34	1.37
84	LH	1002	CYC	C4D-ND	-2.14	1.34	1.37
87	AN	802	CLA	C1D-C2D	2.14	1.49	1.45
82	kJ	202	PEB	C1C-C2C	2.14	1.47	1.42
87	b6	604	CLA	CMB-C2B	-2.14	1.46	1.50
82	OO	202	PEB	C4A-NA	-2.14	1.32	1.37
82	dE	203	PEB	C4A-NA	-2.14	1.32	1.37
82	C7	201	PEB	C4B-NB	-2.14	1.34	1.38
82	GI	203	PEB	C1C-C2C	2.14	1.47	1.42
82	f1	201	PEB	C2A-C1A	-2.14	1.50	1.52
87	b6	613	CLA	CMD-C2D	-2.14	1.46	1.50
82	s8	201	PEB	C4A-NA	-2.14	1.32	1.37
87	6N	602	CLA	MG-NB	-2.14	2.01	2.05
82	ED	201	PEB	C1B-C2B	2.14	1.50	1.45
82	LA	203	PEB	C1C-NC	-2.14	1.34	1.37
82	AH	305	PEB	C1C-NC	-2.14	1.34	1.37
82	CK	201	PEB	C1C-NC	-2.14	1.34	1.37
82	GM	202	PEB	C4B-C3B	2.14	1.49	1.45
82	XK	203	PEB	C4A-NA	-2.14	1.32	1.37
82	gE	202	PEB	C4A-NA	-2.14	1.32	1.37
82	cH	201	PEB	C4A-NA	-2.14	1.32	1.37
82	WD	202	PEB	C1C-C2C	2.14	1.47	1.42
82	R4	202	PEB	C1C-C2C	2.14	1.47	1.42
84	IO	1001	CYC	C1B-C2B	2.14	1.49	1.45
87	AN	808	CLA	MG-ND	-2.14	2.01	2.05
87	A2	810	CLA	CMB-C2B	-2.14	1.46	1.50
82	LB	201	PEB	C4A-NA	-2.14	1.32	1.37
82	a4	203	PEB	C4A-NA	-2.14	1.32	1.37
82	QE	201	PEB	C1C-C2C	2.14	1.47	1.42
82	C5	202	PEB	C1C-NC	-2.14	1.34	1.37
82	dH	203	PEB	C4B-C3B	2.14	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	62	305	CLA	C3D-C4D	2.14	1.49	1.44
82	mM	202	PEB	C1B-C2B	2.14	1.50	1.45
83	Z5	302	PUB	CAB-C3B	2.14	1.56	1.51
87	52	611	CLA	MG-NB	-2.14	2.01	2.05
87	BN	822	CLA	CMB-C2B	-2.14	1.46	1.50
87	c6	604	CLA	CMB-C2B	-2.14	1.46	1.50
87	c6	611	CLA	CMC-C2C	-2.14	1.46	1.50
82	eA	301	PEB	C1C-C2C	2.14	1.47	1.42
82	lG	202	PEB	C1D-ND	2.14	1.49	1.45
87	AN	823	CLA	C1B-NB	-2.14	1.35	1.37
87	62	304	CLA	CHC-C1C	2.14	1.42	1.38
82	VD	203	PEB	C4B-C3B	2.14	1.49	1.45
82	R4	202	PEB	C4B-C3B	2.14	1.49	1.45
82	VH	202	PEB	C1C-C2C	2.14	1.47	1.42
95	BL	613	DGD	O5D-C1E	2.14	1.43	1.40
87	AL	403	CLA	CMB-C2B	-2.14	1.46	1.50
87	B2	828	CLA	CMB-C2B	-2.14	1.46	1.50
87	3N	303	CLA	CMB-C2B	-2.14	1.46	1.50
82	DQ	202	PEB	C4B-NB	-2.14	1.34	1.38
82	IF	203	PEB	C2C-C3C	2.14	1.44	1.38
82	pK	201	PEB	C2A-C1A	-2.14	1.50	1.52
82	KP	201	PEB	C1C-NC	-2.14	1.34	1.37
82	V1	201	PEB	C1C-NC	-2.14	1.34	1.37
82	I9	202	PEB	C1C-NC	-2.14	1.34	1.37
82	qF	202	PEB	C1B-C2B	2.14	1.50	1.45
87	AN	823	CLA	CMC-C2C	-2.14	1.46	1.50
87	AN	835	CLA	C1B-C2B	2.14	1.48	1.43
82	CA	201	PEB	C1B-C2B	2.14	1.50	1.45
82	WD	202	PEB	C1D-ND	2.14	1.49	1.45
82	CQ	202	PEB	C4A-NA	-2.14	1.32	1.37
82	fJ	203	PEB	C4B-C3B	2.14	1.49	1.45
84	JO	1001	CYC	C1A-NA	-2.14	1.34	1.38
82	Z4	201	PEB	CHA-C4A	-2.14	1.32	1.36
87	AN	830	CLA	CHC-C1C	2.14	1.42	1.38
82	HQ	202	PEB	CHC-C4C	2.14	1.52	1.49
82	J1	1002	PEB	C2A-C1A	-2.14	1.50	1.52
82	X5	202	PEB	C2A-C1A	-2.14	1.50	1.52
87	B2	813	CLA	CMD-C2D	-2.14	1.46	1.50
87	J2	101	CLA	CMD-C2D	-2.14	1.46	1.50
82	WI	203	PEB	C4A-NA	-2.14	1.32	1.37
82	IP	203	PEB	C4A-NA	-2.14	1.32	1.37
82	P5	202	PEB	C1C-NC	-2.14	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	62	307	CLA	MG-NB	-2.14	2.01	2.05
87	1N	606	CLA	MG-NB	-2.14	2.01	2.05
87	3N	312	CLA	MG-NB	-2.14	2.01	2.05
82	II	201	PEB	C1C-C2C	2.14	1.47	1.42
82	PI	201	PEB	C1C-C2C	2.14	1.47	1.42
84	HH	1001	CYC	C4D-C3D	2.14	1.47	1.42
82	w8	204	PEB	C4B-C3B	2.14	1.49	1.45
87	A2	803	CLA	CHC-C1C	2.14	1.42	1.38
87	A2	830	CLA	CMB-C2B	-2.14	1.46	1.50
87	C6	515	CLA	CMB-C2B	-2.14	1.46	1.50
87	BN	813	CLA	MG-ND	-2.14	2.01	2.05
87	B2	809	CLA	MG-NB	-2.14	2.01	2.05
87	LN	203	CLA	CAC-C3C	-2.14	1.45	1.51
82	WQ	202	PEB	C1C-C2C	2.14	1.47	1.42
82	h1	202	PEB	C1D-ND	2.14	1.49	1.45
82	X7	203	PEB	C4B-C3B	2.14	1.49	1.45
87	B6	603	CLA	CMB-C2B	-2.13	1.46	1.50
82	LO	1002	PEB	C4A-NA	-2.13	1.32	1.37
82	y8	203	PEB	C2A-C1A	-2.13	1.50	1.52
87	8N	308	CLA	MG-ND	-2.13	2.01	2.05
82	hG	202	PEB	C1C-NC	-2.13	1.34	1.37
87	72	603	CLA	CMD-C2D	-2.13	1.46	1.50
87	C6	520	CLA	CMC-C2C	-2.13	1.46	1.50
82	P1	201	PEB	C4A-NA	-2.13	1.32	1.37
82	iF	202	PEB	C4A-NA	-2.13	1.32	1.37
82	XK	202	PEB	C4B-C3B	2.13	1.49	1.45
82	c4	202	PEB	C4B-C3B	2.13	1.49	1.45
82	gB	201	PEB	C4B-C3B	2.13	1.49	1.45
82	vK	201	PEB	C1C-C2C	2.13	1.47	1.42
82	JD	202	PEB	CHC-C4C	2.13	1.52	1.49
87	K2	104	CLA	C1B-NB	-2.13	1.35	1.37
82	DM	202	PEB	C1B-C2B	2.13	1.50	1.45
84	CH	1001	CYC	C4A-C3A	2.13	1.50	1.45
87	B2	828	CLA	CMC-C2C	-2.13	1.46	1.50
87	6N	605	CLA	CMD-C2D	-2.13	1.46	1.50
82	DG	1002	PEB	C1C-C2C	2.13	1.47	1.42
82	UM	201	PEB	C4A-NA	-2.13	1.32	1.37
82	b4	201	PEB	C4A-NA	-2.13	1.32	1.37
84	J4	1001	CYC	C1A-NA	-2.13	1.34	1.38
87	12	610	CLA	MG-ND	-2.13	2.01	2.05
82	OD	202	PEB	C1D-ND	2.13	1.49	1.45
82	FD	201	PEB	C1B-C2B	2.13	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Q1	202	PEB	C2A-C1A	-2.13	1.50	1.52
87	AN	806	CLA	CMC-C2C	-2.13	1.46	1.50
87	b6	607	CLA	CMC-C2C	-2.13	1.46	1.50
87	bL	608	CLA	CMC-C2C	-2.13	1.46	1.50
87	BN	834	CLA	C1B-NB	-2.13	1.35	1.37
87	K2	103	CLA	C1B-NB	-2.13	1.35	1.37
82	iE	201	PEB	C1C-NC	-2.13	1.34	1.37
82	dH	202	PEB	C1B-C2B	2.13	1.50	1.45
87	A2	809	CLA	C1B-C2B	2.13	1.48	1.43
87	c6	608	CLA	CHC-C1C	2.13	1.42	1.38
82	wF	302	PEB	C1C-C2C	2.13	1.47	1.42
82	cM	202	PEB	C1C-C2C	2.13	1.47	1.42
82	lF	201	PEB	C1D-ND	2.13	1.49	1.45
82	WA	202	PEB	C4A-NA	-2.13	1.32	1.37
82	O9	201	PEB	C4A-NA	-2.13	1.32	1.37
82	eA	301	PEB	C4A-NA	-2.13	1.32	1.37
82	VI	202	PEB	C1C-NC	-2.13	1.34	1.37
82	X7	201	PEB	C1C-NC	-2.13	1.34	1.37
82	V9	202	PEB	C1C-NC	-2.13	1.34	1.37
84	D1	1001	CYC	C1B-NB	-2.13	1.34	1.37
87	22	609	CLA	MG-ND	-2.13	2.01	2.05
87	AL	403	CLA	C1B-NB	-2.13	1.35	1.37
82	AI	202	PEB	C1C-C2C	2.13	1.47	1.42
84	CH	1001	CYC	C4D-C3D	2.13	1.47	1.42
87	K2	101	CLA	CMB-C2B	-2.13	1.46	1.50
87	b6	604	CLA	CMD-C2D	-2.13	1.46	1.50
87	c6	607	CLA	CMB-C2B	-2.13	1.46	1.50
82	WE	203	PEB	C2A-C1A	-2.13	1.50	1.52
82	1C	203	PEB	C2A-C1A	-2.13	1.50	1.52
82	PM	201	PEB	C4A-NA	-2.13	1.32	1.37
82	cB	402	PEB	C4A-NA	-2.13	1.32	1.37
82	lM	202	PEB	C4A-NA	-2.13	1.32	1.37
82	OG	203	PEB	C4B-C3B	2.13	1.49	1.45
82	iE	202	PEB	C4B-C3B	2.13	1.49	1.45
82	UA	202	PEB	C1C-NC	-2.13	1.34	1.37
87	F2	201	CLA	CMC-C2C	-2.13	1.46	1.50
82	U4	202	PEB	C4A-NA	-2.13	1.32	1.37
82	cB	401	PEB	C4A-NA	-2.13	1.32	1.37
84	D1	1003	CYC	C4C-NC	-2.13	1.32	1.37
96	V6	201	HEM	C4B-NB	-2.13	1.34	1.38
87	B2	835	CLA	C1B-NB	-2.13	1.35	1.37
82	YQ	201	PEB	C4B-C3B	2.13	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	W3	1001	CYC	C1A-C2A	2.13	1.49	1.45
84	O3	1001	CYC	C4A-C3A	2.13	1.50	1.45
82	AH	301	PEB	C1C-C2C	2.13	1.47	1.42
82	lF	203	PEB	C1C-C2C	2.13	1.47	1.42
84	EG	1001	CYC	C1B-C2B	2.13	1.48	1.45
87	FN	205	CLA	CMD-C2D	-2.13	1.46	1.50
82	NJ	202	PEB	C1C-NC	-2.13	1.34	1.37
82	QK	201	PEB	C1C-NC	-2.13	1.34	1.37
82	FQ	203	PEB	C1C-NC	2.13	1.41	1.37
82	BA	201	PEB	C4A-NA	-2.13	1.32	1.37
82	OF	201	PEB	C4A-NA	-2.13	1.32	1.37
82	AO	304	PEB	C4A-NA	-2.13	1.32	1.37
82	SO	201	PEB	C1B-C2B	2.13	1.50	1.45
82	Z4	201	PEB	C1B-C2B	2.13	1.50	1.45
84	B3	1001	CYC	C4A-C3A	2.13	1.50	1.45
82	RJ	202	PEB	C1C-C2C	2.13	1.47	1.42
82	AG	301	PEB	C4B-C3B	2.13	1.49	1.45
87	B2	824	CLA	CMB-C2B	-2.13	1.46	1.50
87	C6	520	CLA	CMD-C2D	-2.13	1.46	1.50
82	iK	201	PEB	C4A-NA	-2.13	1.32	1.37
82	TI	203	PEB	C1C-C2C	2.13	1.47	1.42
82	DO	1002	PEB	C1C-C2C	2.13	1.47	1.42
87	52	603	CLA	MG-NB	-2.13	2.01	2.05
87	2N	309	CLA	MG-ND	-2.13	2.01	2.05
87	62	306	CLA	CMD-C2D	-2.13	1.46	1.50
87	bL	605	CLA	CMB-C2B	-2.13	1.46	1.50
87	8N	308	CLA	C1B-C2B	2.13	1.48	1.43
87	M2	101	CLA	CHC-C1C	2.13	1.42	1.38
82	UB	302	PEB	C4A-NA	-2.13	1.32	1.37
82	mG	203	PEB	C4A-NA	-2.13	1.32	1.37
82	WQ	201	PEB	C1B-C2B	2.13	1.50	1.45
82	vK	202	PEB	C1C-NC	-2.13	1.34	1.37
82	SD	202	PEB	C2A-C1A	-2.13	1.50	1.52
82	sK	202	PEB	C2A-C1A	-2.13	1.50	1.52
87	8N	306	CLA	MG-NB	-2.13	2.01	2.05
87	L2	204	CLA	CMB-C2B	-2.13	1.46	1.50
87	2N	304	CLA	CMD-C2D	-2.13	1.46	1.50
82	a4	203	PEB	O1B-CGB	2.13	1.29	1.22
82	XI	202	PEB	C1C-C2C	2.13	1.47	1.42
82	VB	201	PEB	CHC-C4C	2.13	1.52	1.49
82	WO	201	PEB	C1C-NC	-2.13	1.34	1.37
87	BL	608	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	619	CLA	CMB-C2B	-2.13	1.46	1.50
82	hG	202	PEB	C1C-C2C	2.13	1.47	1.42
82	PH	201	PEB	C4A-NA	-2.13	1.32	1.37
82	EP	203	PEB	C4A-NA	-2.13	1.32	1.37
82	Z9	303	PEB	C1B-C2B	2.13	1.50	1.45
87	CL	515	CLA	CMC-C2C	-2.13	1.46	1.50
87	32	302	CLA	CMB-C2B	-2.13	1.46	1.50
87	4N	611	CLA	CMD-C2D	-2.13	1.46	1.50
82	SP	202	PEB	C1C-NC	-2.13	1.34	1.37
82	dO	202	PEB	C1C-NC	-2.13	1.34	1.37
82	c4	201	PEB	C2A-C1A	-2.13	1.50	1.52
82	RG	202	PEB	C4A-NA	-2.13	1.32	1.37
82	1C	202	PEB	C4A-NA	-2.13	1.32	1.37
87	A6	402	CLA	CHC-C1C	2.13	1.42	1.38
87	D6	403	CLA	CHC-C1C	2.13	1.42	1.38
82	e4	201	PEB	C1B-C2B	2.13	1.50	1.45
87	AN	833	CLA	CMD-C2D	-2.13	1.46	1.50
87	BN	810	CLA	CMC-C2C	-2.13	1.46	1.50
87	12	604	CLA	CMC-C2C	-2.13	1.46	1.50
87	B2	801	CLA	CMB-C2B	-2.13	1.46	1.50
87	b6	605	CLA	CMD-C2D	-2.13	1.46	1.50
87	3N	307	CLA	CMB-C2B	-2.13	1.46	1.50
87	AN	811	CLA	CHC-C4B	-2.13	1.34	1.39
87	A2	825	CLA	MG-ND	-2.13	2.01	2.05
82	U9	203	PEB	C4B-C3B	2.13	1.49	1.45
82	I7	201	PEB	C1D-ND	2.13	1.48	1.45
87	A2	811	CLA	CHC-C4B	-2.13	1.34	1.39
82	DA	201	PEB	C4A-NA	-2.13	1.32	1.37
82	GK	203	PEB	C4A-NA	-2.13	1.32	1.37
82	aF	201	PEB	C4A-NA	-2.13	1.32	1.37
82	OD	202	PEB	C4B-C3B	2.13	1.49	1.45
82	mG	202	PEB	C2A-C1A	-2.13	1.50	1.52
96	E6	101	HEM	C4B-NB	-2.13	1.34	1.38
82	A5	202	PEB	C1C-NC	-2.13	1.34	1.37
82	KI	203	PEB	C1C-C2C	2.13	1.47	1.42
82	VP	202	PEB	C1C-C2C	2.13	1.47	1.42
87	AN	824	CLA	CMC-C2C	-2.13	1.46	1.50
87	D6	402	CLA	CMB-C2B	-2.13	1.46	1.50
83	xK	301	PUB	C1C-NC	-2.13	1.34	1.38
82	GP	201	PEB	C4A-NA	-2.13	1.32	1.37
87	AN	827	CLA	MG-ND	-2.13	2.01	2.05
82	dK	201	PEB	C1C-C2C	2.13	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	XF	203	PEB	CHC-C4C	2.13	1.52	1.49
82	kF	203	PEB	C4B-C3B	2.13	1.49	1.45
82	cG	202	PEB	C4B-C3B	2.13	1.49	1.45
87	AN	838	CLA	CMD-C2D	-2.13	1.46	1.50
87	LN	203	CLA	C3B-C4B	2.13	1.47	1.42
82	UJ	203	PEB	C4A-NA	-2.13	1.32	1.37
82	MP	202	PEB	C4A-NA	-2.13	1.32	1.37
82	M7	202	PEB	C4A-NA	-2.13	1.32	1.37
82	iK	202	PEB	C4A-NA	-2.13	1.32	1.37
82	WA	202	PEB	C1C-C2C	2.13	1.47	1.42
82	PI	202	PEB	C1C-C2C	2.13	1.47	1.42
82	RI	201	PEB	C1C-C2C	2.13	1.47	1.42
82	QJ	202	PEB	C1C-C2C	2.13	1.47	1.42
82	ZH	203	PEB	C2A-C1A	-2.13	1.50	1.52
82	S9	202	PEB	C2A-C1A	-2.13	1.50	1.52
87	KN	102	CLA	CMC-C2C	-2.13	1.46	1.50
87	I2	102	CLA	CMC-C2C	-2.13	1.46	1.50
82	CF	201	PEB	C1C-NC	-2.13	1.34	1.37
82	KF	203	PEB	C1C-NC	-2.13	1.34	1.37
82	jO	202	PEB	C1C-NC	-2.13	1.34	1.37
82	J9	202	PEB	CHC-C4C	2.13	1.52	1.49
82	pF	202	PEB	CHC-C4C	2.13	1.52	1.49
87	AN	803	CLA	CMC-C2C	-2.13	1.46	1.50
87	42	602	CLA	CMC-C2C	-2.13	1.46	1.50
87	B2	814	CLA	CMB-C2B	-2.13	1.46	1.50
82	IA	202	PEB	C1D-ND	2.13	1.48	1.45
82	I7	202	PEB	C1D-ND	2.13	1.48	1.45
82	QP	202	PEB	C4A-NA	-2.13	1.32	1.37
82	O4	202	PEB	C4A-NA	-2.13	1.32	1.37
82	U9	204	PEB	C4A-NA	-2.13	1.32	1.37
82	lG	202	PEB	C4A-NA	-2.13	1.32	1.37
82	gF	202	PEB	C1C-C2C	2.13	1.47	1.42
82	V5	202	PEB	C1C-NC	-2.13	1.34	1.37
84	L1	1001	CYC	C1B-NB	-2.13	1.34	1.37
87	bL	604	CLA	MG-NB	-2.13	2.01	2.05
82	VQ	203	PEB	C4B-C3B	2.13	1.49	1.45
82	x8	201	PEB	C4B-C3B	2.13	1.49	1.45
87	BN	819	CLA	CMD-C2D	-2.13	1.46	1.50
87	BN	825	CLA	CMB-C2B	-2.13	1.46	1.50
87	B6	611	CLA	CMC-C2C	-2.13	1.46	1.50
87	3N	311	CLA	CMD-C2D	-2.13	1.46	1.50
82	DE	1002	PEB	C1C-C2C	2.13	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	XF	203	PEB	C1C-C2C	2.13	1.47	1.42
82	QG	201	PEB	C1C-C2C	2.13	1.47	1.42
82	UG	203	PEB	C1C-C2C	2.13	1.47	1.42
82	K5	202	PEB	C1C-C2C	2.13	1.47	1.42
82	ZF	201	PEB	C2A-C1A	-2.13	1.50	1.52
82	L5	201	PEB	C2A-C1A	-2.13	1.50	1.52
82	yC	203	PEB	C2A-C1A	-2.13	1.50	1.52
87	12	611	CLA	CMD-C2D	-2.13	1.46	1.50
82	H7	201	PEB	C4A-NA	-2.13	1.32	1.37
82	kK	201	PEB	C4A-NA	-2.13	1.32	1.37
84	U3	1001	CYC	C4A-C3A	2.13	1.50	1.45
84	FH	1001	CYC	C4B-NB	-2.13	1.33	1.38
87	22	604	CLA	CMD-C2D	-2.13	1.46	1.50
87	42	602	CLA	CMD-C2D	-2.13	1.46	1.50
96	G2	201	HEM	FE-NA	2.12	2.02	1.95
82	VD	203	PEB	C4A-NA	-2.12	1.32	1.37
82	fG	201	PEB	C4A-NA	-2.12	1.32	1.37
82	wK	303	PEB	C4A-NA	-2.12	1.32	1.37
82	gO	203	PEB	C4A-NA	-2.12	1.32	1.37
82	oF	201	PEB	C1B-C2B	2.12	1.50	1.45
82	EM	203	PEB	C2A-C1A	-2.12	1.50	1.52
82	RG	201	PEB	C1C-C2C	2.12	1.47	1.42
87	AN	809	CLA	CMD-C2D	-2.12	1.46	1.50
87	BN	814	CLA	CMB-C2B	-2.12	1.46	1.50
87	5N	602	CLA	CMC-C2C	-2.12	1.46	1.50
82	FP	201	PEB	C1C-NC	-2.12	1.34	1.37
82	O9	203	PEB	C1C-NC	-2.12	1.34	1.37
82	RF	202	PEB	C4B-C3B	2.12	1.49	1.45
87	AN	830	CLA	CMC-C2C	-2.12	1.46	1.50
87	32	306	CLA	CMC-C2C	-2.12	1.46	1.50
87	52	602	CLA	CMC-C2C	-2.12	1.46	1.50
82	LA	201	PEB	C4A-NA	-2.12	1.32	1.37
82	jM	203	PEB	C4A-NA	-2.12	1.32	1.37
82	AG	301	PEB	C1C-C2C	2.12	1.47	1.42
87	A2	814	CLA	MG-ND	-2.12	2.01	2.05
87	CL	504	CLA	CMD-C2D	-2.12	1.46	1.50
87	72	610	CLA	CMD-C2D	-2.12	1.46	1.50
82	YA	304	PEB	C2A-C1A	-2.12	1.50	1.52
82	OQ	201	PEB	C2A-C1A	-2.12	1.50	1.52
82	IM	202	PEB	C1B-C2B	2.12	1.50	1.45
82	jJ	201	PEB	C4A-NA	-2.12	1.32	1.37
82	VI	201	PEB	C1C-C2C	2.12	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	aH	202	PEB	C1C-C2C	2.12	1.47	1.42
87	5N	602	CLA	CHC-C1C	2.12	1.42	1.38
87	B2	819	CLA	CMB-C2B	-2.12	1.46	1.50
87	1N	611	CLA	CMD-C2D	-2.12	1.46	1.50
82	kK	202	PEB	C1D-ND	2.12	1.48	1.45
82	AM	301	PEB	C4A-NA	-2.12	1.32	1.37
87	A2	823	CLA	C1B-NB	-2.12	1.35	1.37
82	A4	301	PEB	C1C-C2C	2.12	1.47	1.42
96	fL	102	HEM	C4B-NB	-2.12	1.34	1.38
87	BN	819	CLA	MG-ND	-2.12	2.01	2.05
87	8N	306	CLA	MG-ND	-2.12	2.01	2.05
87	AN	810	CLA	CMB-C2B	-2.12	1.46	1.50
87	AN	813	CLA	CMB-C2B	-2.12	1.46	1.50
87	42	611	CLA	CMD-C2D	-2.12	1.46	1.50
82	WE	202	PEB	C1C-NC	-2.12	1.34	1.37
82	A9	202	PEB	C1C-NC	-2.12	1.34	1.37
82	K9	202	PEB	C1C-NC	-2.12	1.34	1.37
87	BN	833	CLA	C1B-C2B	2.12	1.48	1.43
87	cL	508	CLA	C1B-C2B	2.12	1.48	1.43
82	dM	201	PEB	C4A-NA	-2.12	1.32	1.37
82	S4	202	PEB	C2A-C1A	-2.12	1.50	1.52
82	KB	302	PEB	C1C-C2C	2.12	1.47	1.42
82	cJ	201	PEB	CHC-C4C	2.12	1.52	1.49
87	B6	614	CLA	CMD-C2D	-2.12	1.46	1.50
87	b6	615	CLA	CMD-C2D	-2.12	1.46	1.50
87	62	309	CLA	MG-NB	-2.12	2.01	2.05
82	N1	1002	PEB	C1C-C2C	2.12	1.47	1.42
82	F9	203	PEB	C1C-C2C	2.12	1.47	1.42
82	LA	202	PEB	C4B-C3B	2.12	1.49	1.45
82	HI	202	PEB	C2C-C3C	2.12	1.44	1.38
87	AN	825	CLA	MG-ND	-2.12	2.01	2.05
84	o3	1001	CYC	C4A-C3A	2.12	1.50	1.45
82	GI	203	PEB	C4A-NA	-2.12	1.32	1.37
82	gM	201	PEB	C4A-NA	-2.12	1.32	1.37
82	GA	202	PEB	C1C-C2C	2.12	1.47	1.42
82	QK	203	PEB	C1C-C2C	2.12	1.47	1.42
82	HA	202	PEB	CHC-C4C	2.12	1.52	1.49
87	AN	834	CLA	C3B-C4B	2.12	1.47	1.42
82	u8	201	PEB	C2A-C1A	-2.12	1.50	1.52
82	S9	203	PEB	C2A-C1A	-2.12	1.50	1.52
82	hM	203	PEB	C2A-C1A	-2.12	1.50	1.52
82	bO	202	PEB	C2A-C1A	-2.12	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	M3	1001	CYC	C4A-C3A	2.12	1.50	1.45
82	mE	201	PEB	C4B-C3B	2.12	1.49	1.45
87	CL	515	CLA	MG-NB	-2.12	2.01	2.05
82	OG	201	PEB	C1C-C2C	2.12	1.47	1.42
82	lE	201	PEB	C1C-C2C	2.12	1.47	1.42
82	I5	202	PEB	C1C-NC	-2.12	1.34	1.37
87	D6	405	CLA	CHC-C1C	2.12	1.42	1.38
87	b6	615	CLA	CHC-C1C	2.12	1.42	1.38
87	3N	307	CLA	CMC-C2C	-2.12	1.46	1.50
82	lG	201	PEB	C1C-C2C	2.12	1.47	1.42
84	73	1002	CYC	C4D-C3D	2.12	1.47	1.42
87	8N	304	CLA	MG-NB	-2.12	2.01	2.05
82	GD	201	PEB	C4A-NA	-2.12	1.32	1.37
82	QF	201	PEB	C4A-NA	-2.12	1.32	1.37
82	j4	202	PEB	C4A-NA	-2.12	1.32	1.37
82	aJ	203	PEB	C4A-NA	-2.12	1.32	1.37
87	AN	809	CLA	C1B-C2B	2.12	1.48	1.43
87	FN	205	CLA	C4C-C3C	2.12	1.48	1.45
87	42	610	CLA	CMD-C2D	-2.12	1.46	1.50
82	cH	201	PEB	C1C-NC	-2.12	1.34	1.37
82	WQ	202	PEB	C1B-C2B	2.12	1.50	1.45
82	O9	201	PEB	C2A-C1A	-2.12	1.50	1.52
82	wK	301	PEB	C2A-C1A	-2.12	1.50	1.52
82	OM	202	PEB	C4A-NA	-2.12	1.32	1.37
82	U5	203	PEB	C4A-NA	-2.12	1.32	1.37
82	jE	202	PEB	C4A-NA	-2.12	1.32	1.37
87	d6	403	CLA	CHC-C1C	2.12	1.42	1.38
82	BI	202	PEB	C4A-NA	-2.12	1.32	1.37
82	TJ	202	PEB	C4A-NA	-2.12	1.32	1.37
82	lE	203	PEB	C4A-NA	-2.12	1.32	1.37
82	kG	201	PEB	C4A-NA	-2.12	1.32	1.37
82	R5	202	PEB	C1C-NC	-2.12	1.34	1.37
82	mJ	202	PEB	C1C-NC	-2.12	1.34	1.37
82	GP	201	PEB	OD-C4D	2.12	1.27	1.23
82	EI	201	PEB	C1C-C2C	2.12	1.47	1.42
87	BN	822	CLA	CMC-C2C	-2.12	1.46	1.50
87	ON	202	CLA	CMC-C2C	-2.12	1.46	1.50
82	eO	203	PEB	C4B-C3B	2.12	1.49	1.45
82	ZF	202	PEB	C4A-NA	-2.12	1.32	1.37
82	hE	202	PEB	C4A-NA	-2.12	1.32	1.37
87	72	601	CLA	MG-NB	-2.12	2.01	2.05
87	82	305	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	V7	202	PEB	C2A-C1A	-2.12	1.50	1.52
82	N9	202	PEB	C1C-NC	-2.12	1.34	1.37
83	AJ	304	PUB	C4B-NB	-2.12	1.34	1.37
84	FO	1001	CYC	C1B-NB	-2.12	1.34	1.37
82	MK	202	PEB	C1C-C2C	2.12	1.47	1.42
87	22	605	CLA	CMC-C2C	-2.12	1.46	1.50
87	A2	815	CLA	C1B-NB	-2.12	1.35	1.37
87	b6	618	CLA	CHC-C1C	2.12	1.42	1.38
82	AK	202	PEB	C4A-NA	-2.12	1.32	1.37
83	Z5	303	PUB	C4C-NC	2.12	1.38	1.35
82	GJ	202	PEB	C1C-C2C	2.12	1.47	1.42
83	AE	302	PUB	C1C-NC	-2.12	1.34	1.38
87	B2	816	CLA	CMD-C2D	-2.12	1.46	1.50
87	b6	618	CLA	CMB-C2B	-2.12	1.46	1.50
87	cL	510	CLA	CMD-C2D	-2.12	1.46	1.50
84	t3	1001	CYC	C4C-NC	-2.12	1.32	1.37
82	aM	201	PEB	C1C-C2C	2.12	1.47	1.42
87	AN	821	CLA	MG-ND	-2.12	2.01	2.05
82	GI	201	PEB	C2A-C1A	-2.12	1.50	1.52
82	c4	202	PEB	C2A-C1A	-2.12	1.50	1.52
87	AL	404	CLA	CMB-C2B	-2.12	1.46	1.50
87	BN	820	CLA	CMB-C2B	-2.12	1.46	1.50
87	K6	101	CLA	CMD-C2D	-2.12	1.46	1.50
82	WE	201	PEB	C1B-C2B	2.12	1.50	1.45
84	f3	1001	CYC	C4A-C3A	2.12	1.50	1.45
82	M9	301	PEB	C1C-NC	-2.12	1.34	1.37
82	WK	203	PEB	C4A-NA	-2.12	1.32	1.37
82	aO	203	PEB	C1C-C2C	2.12	1.47	1.42
82	lK	201	PEB	C1D-ND	2.12	1.48	1.45
87	82	303	CLA	MG-NB	-2.12	2.01	2.05
84	LE	1001	CYC	OB-C4B	2.12	1.27	1.23
87	C6	518	CLA	CMB-C2B	-2.12	1.46	1.50
87	bL	614	CLA	CMD-C2D	-2.12	1.46	1.50
82	WG	201	PEB	C1B-C2B	2.12	1.50	1.45
82	JD	201	PEB	C4B-C3B	2.12	1.49	1.45
82	VD	202	PEB	C4B-C3B	2.12	1.49	1.45
87	82	302	CLA	MG-NC	2.12	2.11	2.06
82	GQ	202	PEB	C1C-C2C	2.12	1.47	1.42
82	O4	202	PEB	C1C-NC	-2.12	1.34	1.37
82	U7	202	PEB	C1C-NC	-2.12	1.34	1.37
87	bL	616	CLA	C1B-NB	-2.12	1.35	1.37
87	AN	826	CLA	MG-ND	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4N	611	CLA	MG-NB	-2.12	2.01	2.05
87	BN	815	CLA	CMB-C2B	-2.12	1.46	1.50
87	d6	403	CLA	CMB-C2B	-2.12	1.46	1.50
87	7N	610	CLA	CMD-C2D	-2.12	1.46	1.50
82	ZG	202	PEB	C1C-C2C	2.12	1.47	1.42
82	A5	202	PEB	C1C-C2C	2.12	1.47	1.42
82	AJ	301	PEB	C4A-NA	-2.12	1.32	1.37
82	VK	202	PEB	C4A-NA	-2.12	1.32	1.37
84	P3	1001	CYC	C4C-NC	-2.12	1.32	1.37
84	i3	1001	CYC	C4C-NC	-2.12	1.32	1.37
82	P1	202	PEB	C4B-C3B	2.12	1.49	1.45
82	YB	202	PEB	C1C-NC	-2.12	1.34	1.37
84	k3	1001	CYC	C4A-C3A	2.12	1.50	1.45
87	BN	816	CLA	CMD-C2D	-2.12	1.46	1.50
87	B2	821	CLA	CMC-C2C	-2.12	1.46	1.50
87	8N	304	CLA	CMB-C2B	-2.12	1.46	1.50
82	XP	202	PEB	C1C-C2C	2.12	1.47	1.42
87	KN	103	CLA	C1B-NB	-2.12	1.35	1.37
82	YA	303	PEB	C4A-NA	-2.12	1.32	1.37
87	C6	510	CLA	CHC-C1C	2.12	1.42	1.38
82	VH	201	PEB	C1C-NC	-2.12	1.34	1.37
82	fE	203	PEB	C1C-C2C	2.12	1.47	1.42
82	G7	202	PEB	C4A-NA	-2.12	1.32	1.37
87	c6	609	CLA	CMB-C2B	-2.12	1.46	1.50
82	BI	201	PEB	C1C-NC	-2.12	1.34	1.37
82	E5	202	PEB	C1C-NC	-2.12	1.34	1.37
82	QP	203	PEB	C4A-NA	-2.12	1.32	1.37
82	Z9	304	PEB	C4A-NA	-2.12	1.32	1.37
85	KN	101	BCR	C12-C13	2.12	1.50	1.45
82	KB	304	PEB	C1C-C2C	2.12	1.47	1.42
82	I5	201	PEB	C1B-C2B	2.12	1.50	1.45
87	B2	812	CLA	MG-ND	-2.12	2.01	2.05
87	a6	607	CLA	CMC-C2C	-2.12	1.46	1.50
87	a6	609	CLA	CMB-C2B	-2.12	1.46	1.50
87	1N	603	CLA	CMD-C2D	-2.12	1.46	1.50
82	QK	202	PEB	C1D-ND	2.12	1.48	1.45
82	dE	204	PEB	C1D-ND	2.12	1.48	1.45
82	EK	201	PEB	C1C-NC	-2.11	1.34	1.37
82	E9	202	PEB	C1C-NC	-2.11	1.34	1.37
87	nL	101	CLA	C1B-NB	-2.11	1.35	1.37
84	G4	1001	CYC	C4B-NB	-2.11	1.33	1.38
82	KM	201	PEB	C1C-C2C	2.11	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
103	82	309	ZEX	C21-C26	-2.11	1.50	1.53
82	qK	202	PEB	C1B-C2B	2.11	1.50	1.45
87	AN	830	CLA	CMB-C2B	-2.11	1.46	1.50
87	BN	834	CLA	CMC-C2C	-2.11	1.46	1.50
87	B2	813	CLA	CMB-C2B	-2.11	1.46	1.50
82	EA	202	PEB	C2A-C1A	-2.11	1.50	1.52
87	B2	823	CLA	MG-ND	-2.11	2.01	2.05
82	g1	202	PEB	CHC-C4C	2.11	1.52	1.49
82	EF	201	PEB	C4A-NA	-2.11	1.32	1.37
82	UP	203	PEB	C4A-NA	-2.11	1.32	1.37
82	18	202	PEB	C4A-NA	-2.11	1.32	1.37
87	52	607	CLA	CHC-C1C	2.11	1.42	1.38
87	b6	607	CLA	CHC-C1C	2.11	1.42	1.38
82	CP	202	PEB	C1C-C2C	2.11	1.47	1.42
82	Y4	203	PEB	C1C-C2C	2.11	1.47	1.42
82	CI	202	PEB	C1C-NC	-2.11	1.34	1.37
83	M5	303	PUB	C4C-NC	2.11	1.38	1.35
82	qF	201	PEB	C4B-C3B	2.11	1.49	1.45
87	AN	807	CLA	CMB-C2B	-2.11	1.46	1.50
87	42	605	CLA	MG-NB	-2.11	2.01	2.05
82	IF	201	PEB	CBC-CGC	2.11	1.55	1.50
82	aF	203	PEB	C4A-NA	-2.11	1.32	1.37
96	GN	201	HEM	FE-NA	2.11	2.02	1.95
82	PF	201	PEB	C1A-NA	-2.11	1.34	1.37
82	kK	201	PEB	CHC-C4C	2.11	1.52	1.49
87	52	609	CLA	CMC-C2C	-2.11	1.46	1.50
87	B2	825	CLA	CMC-C2C	-2.11	1.46	1.50
87	R2	204	CLA	CMD-C2D	-2.11	1.46	1.50
87	d6	403	CLA	CMC-C2C	-2.11	1.46	1.50
87	2N	305	CLA	CMD-C2D	-2.11	1.46	1.50
82	Y7	303	PEB	C4B-C3B	2.11	1.49	1.45
82	EJ	203	PEB	C4A-NA	-2.11	1.32	1.37
82	kF	201	PEB	C4A-NA	-2.11	1.32	1.37
84	h3	1001	CYC	C4A-C3A	2.11	1.50	1.45
87	82	308	CLA	C1B-C2B	2.11	1.48	1.43
87	BN	830	CLA	CMB-C2B	-2.11	1.46	1.50
87	K2	101	CLA	CMC-C2C	-2.11	1.46	1.50
87	cL	511	CLA	CMB-C2B	-2.11	1.46	1.50
87	LN	202	CLA	C3D-C4D	2.11	1.48	1.44
87	42	611	CLA	MG-NB	-2.11	2.01	2.05
87	62	303	CLA	MG-NB	-2.11	2.01	2.05
87	bL	605	CLA	MG-NB	-2.11	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	w8	201	PEB	C1D-ND	2.11	1.48	1.45
82	dJ	201	PEB	C1C-C2C	2.11	1.47	1.42
82	hJ	201	PEB	C4A-NA	-2.11	1.32	1.37
84	n3	1001	CYC	C4A-C3A	2.11	1.50	1.45
82	Z4	201	PEB	OD-C4D	2.11	1.27	1.23
84	HE	1001	CYC	OB-C4B	2.11	1.27	1.23
87	BL	619	CLA	CMB-C2B	-2.11	1.46	1.50
87	B2	811	CLA	CMD-C2D	-2.11	1.46	1.50
87	A2	826	CLA	MG-ND	-2.11	2.01	2.05
87	2N	305	CLA	MG-ND	-2.11	2.01	2.05
82	dG	203	PEB	C4A-NA	-2.11	1.32	1.37
87	bL	620	CLA	CHC-C1C	2.11	1.42	1.38
82	lF	202	PEB	C1D-ND	2.11	1.48	1.45
82	C5	202	PEB	C2A-C1A	-2.11	1.50	1.52
87	HL	102	CLA	CMD-C2D	-2.11	1.46	1.50
87	32	311	CLA	CMD-C2D	-2.11	1.46	1.50
82	W7	201	PEB	OD-C4D	2.11	1.27	1.23
82	OK	201	PEB	C4A-NA	-2.11	1.32	1.37
82	RK	202	PEB	CHC-C4C	2.11	1.52	1.49
87	BL	619	CLA	CHC-C1C	2.11	1.42	1.38
87	32	308	CLA	CMC-C2C	-2.11	1.46	1.50
87	A2	809	CLA	CMD-C2D	-2.11	1.46	1.50
87	B2	830	CLA	CMB-C2B	-2.11	1.46	1.50
87	a6	608	CLA	CMB-C2B	-2.11	1.46	1.50
82	RG	202	PEB	C1C-C2C	2.11	1.47	1.42
82	NI	201	PEB	C1C-C2C	2.11	1.47	1.42
82	CF	203	PEB	C4A-NA	-2.11	1.32	1.37
87	BN	809	CLA	MG-ND	-2.11	2.01	2.05
87	A2	813	CLA	CMB-C2B	-2.11	1.46	1.50
87	cL	516	CLA	CMB-C2B	-2.11	1.46	1.50
82	aE	201	PEB	C1C-NC	-2.11	1.34	1.37
82	E5	202	PEB	C2A-C1A	-2.11	1.50	1.52
82	gB	202	PEB	C4A-NA	-2.11	1.32	1.37
82	tF	201	PEB	C4B-C3B	2.11	1.49	1.45
87	82	305	CLA	MG-ND	-2.11	2.01	2.05
87	6N	601	CLA	MG-NB	-2.11	2.01	2.05
87	4N	611	CLA	CHC-C1C	2.11	1.42	1.38
82	EI	202	PEB	C1C-C2C	2.11	1.47	1.42
82	WK	203	PEB	C1C-C2C	2.11	1.47	1.42
87	AN	801	CLA	CMD-C2D	-2.11	1.46	1.50
87	AN	812	CLA	CMD-C2D	-2.11	1.46	1.50
87	c6	612	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	cL	511	CLA	CMC-C2C	-2.11	1.46	1.50
82	R9	202	PEB	C1C-NC	-2.11	1.34	1.37
84	S3	1001	CYC	C4A-C3A	2.11	1.50	1.45
84	j3	1001	CYC	C4A-C3A	2.11	1.50	1.45
84	w3	1001	CYC	C4A-C3A	2.11	1.50	1.45
82	eH	203	PEB	C1C-C2C	2.11	1.47	1.42
87	BL	605	CLA	CHC-C1C	2.11	1.42	1.38
82	ZF	201	PEB	C4A-NA	-2.11	1.32	1.37
82	HG	1002	PEB	C4A-NA	-2.11	1.32	1.37
82	W1	201	PEB	C4A-NA	-2.11	1.32	1.37
84	c3	1001	CYC	C4C-NC	-2.11	1.32	1.37
82	GA	202	PEB	C2A-C1A	-2.11	1.50	1.52
82	A5	202	PEB	C2A-C1A	-2.11	1.50	1.52
82	aG	201	PEB	C1C-NC	-2.11	1.34	1.37
87	6N	606	CLA	MG-NB	-2.11	2.01	2.05
82	QF	203	PEB	C1C-C2C	2.11	1.47	1.42
82	AI	201	PEB	C1C-C2C	2.11	1.47	1.42
82	j4	203	PEB	C1C-C2C	2.11	1.47	1.42
82	eF	203	PEB	C1C-NC	-2.11	1.34	1.37
87	12	607	CLA	CHC-C1C	2.11	1.42	1.38
87	BN	835	CLA	CMD-C2D	-2.11	1.46	1.50
82	dE	202	PEB	C4A-NA	-2.11	1.32	1.37
82	jM	201	PEB	C4A-NA	-2.11	1.32	1.37
82	fG	202	PEB	C4B-C3B	2.11	1.49	1.45
82	KI	202	PEB	C1C-C2C	2.11	1.47	1.42
87	AN	815	CLA	C1B-NB	-2.11	1.35	1.37
87	A2	836	CLA	MG-NB	-2.11	2.01	2.05
87	cL	510	CLA	MG-NB	-2.11	2.01	2.05
82	hG	202	PEB	C1D-ND	2.11	1.48	1.45
82	HD	203	PEB	C2A-C1A	-2.11	1.50	1.52
82	JQ	203	PEB	C2A-C1A	-2.11	1.50	1.52
82	O5	203	PEB	C2A-C1A	-2.11	1.50	1.52
87	cL	516	CLA	CMD-C2D	-2.11	1.46	1.50
87	CL	515	CLA	CHC-C1C	2.11	1.42	1.38
87	1N	607	CLA	CHC-C1C	2.11	1.42	1.38
82	CI	202	PEB	C1C-C2C	2.11	1.47	1.42
82	GI	202	PEB	C1C-C2C	2.11	1.47	1.42
82	II	202	PEB	C1C-C2C	2.11	1.47	1.42
82	AJ	302	PEB	C4A-NA	-2.11	1.32	1.37
82	cE	201	PEB	C4A-NA	-2.11	1.32	1.37
82	cG	201	PEB	C4A-NA	-2.11	1.32	1.37
82	YH	201	PEB	C4B-C3B	2.11	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	V4	202	PEB	CHC-C4C	2.11	1.52	1.49
87	CL	518	CLA	CMB-C2B	-2.11	1.46	1.50
87	AN	811	CLA	C3B-C4B	2.11	1.47	1.42
82	RO	202	PEB	C1C-C2C	2.11	1.47	1.42
87	B2	834	CLA	C1B-NB	-2.11	1.35	1.37
82	jH	203	PEB	C4A-NA	-2.11	1.32	1.37
82	fM	201	PEB	C4A-NA	-2.11	1.32	1.37
82	MK	203	PEB	C1B-C2B	2.11	1.50	1.45
87	CL	507	CLA	CMB-C2B	-2.11	1.46	1.50
87	22	607	CLA	CMD-C2D	-2.11	1.46	1.50
87	A2	835	CLA	CMD-C2D	-2.11	1.46	1.50
87	12	603	CLA	CHC-C1C	2.11	1.42	1.38
82	PF	202	PEB	C4B-C3B	2.11	1.49	1.45
82	lG	203	PEB	C4B-C3B	2.11	1.49	1.45
84	C1	1001	CYC	C4D-C3D	2.11	1.47	1.42
82	WF	203	PEB	C4A-NA	-2.11	1.32	1.37
82	L4	1002	PEB	C4A-NA	-2.11	1.32	1.37
87	B2	833	CLA	C1B-C2B	2.11	1.48	1.43
82	f1	202	PEB	CHC-C4C	2.11	1.52	1.49
82	L7	201	PEB	C1C-NC	-2.11	1.34	1.37
82	Z9	304	PEB	C1C-NC	-2.11	1.34	1.37
83	K7	203	PUB	C4B-NB	-2.11	1.34	1.37
87	82	303	CLA	CMB-C2B	-2.11	1.46	1.50
82	dE	204	PEB	C4B-C3B	2.11	1.49	1.45
82	eE	201	PEB	C4B-C3B	2.11	1.49	1.45
82	dG	204	PEB	C4B-C3B	2.11	1.49	1.45
87	B2	835	CLA	CMD-C2D	-2.11	1.46	1.50
87	F2	205	CLA	CMC-C2C	-2.11	1.46	1.50
82	RI	202	PEB	C1C-C2C	2.11	1.47	1.42
82	EM	201	PEB	C1C-C2C	2.11	1.47	1.42
87	1N	610	CLA	MG-ND	-2.11	2.01	2.05
87	8N	306	CLA	O2D-CGD	2.11	1.38	1.33
82	lF	201	PEB	C2A-C1A	-2.11	1.50	1.52
82	CF	203	PEB	C4B-C3B	2.11	1.49	1.45
83	xF	301	PUB	C1C-NC	-2.11	1.34	1.38
87	BN	821	CLA	CMD-C2D	-2.11	1.46	1.50
87	62	301	CLA	CMB-C2B	-2.11	1.46	1.50
87	6N	607	CLA	CMD-C2D	-2.11	1.46	1.50
82	AG	304	PEB	C1C-NC	-2.11	1.34	1.37
82	LJ	202	PEB	C1C-NC	-2.11	1.34	1.37
87	L2	206	CLA	CHC-C1C	2.11	1.42	1.38
87	CL	508	CLA	C1B-C2B	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	O9	202	PEB	C4C-NC	2.11	1.41	1.37
82	lK	203	PEB	C4A-NA	-2.11	1.32	1.37
87	BN	817	CLA	CMD-C2D	-2.11	1.46	1.50
87	AN	809	CLA	MG-NB	-2.11	2.01	2.05
87	72	609	CLA	MG-NB	-2.11	2.01	2.05
82	ZI	401	PEB	C4A-NA	-2.11	1.32	1.37
82	SJ	203	PEB	C4A-NA	-2.11	1.32	1.37
82	QO	201	PEB	C1C-NC	-2.11	1.34	1.37
82	BQ	202	PEB	C1C-NC	-2.11	1.34	1.37
87	BL	606	CLA	C1B-NB	-2.11	1.35	1.37
87	CL	508	CLA	C1B-NB	-2.11	1.35	1.37
82	AG	304	PEB	C1C-C2C	2.11	1.47	1.42
82	P1	201	PEB	C1C-C2C	2.11	1.47	1.42
82	jH	201	PEB	C1C-C2C	2.11	1.47	1.42
82	OH	201	PEB	C1D-ND	2.11	1.48	1.45
82	TK	202	PEB	C1D-ND	2.11	1.48	1.45
82	jH	203	PEB	C2A-C1A	-2.11	1.50	1.52
82	QD	202	PEB	C4A-NA	-2.11	1.32	1.37
87	A2	814	CLA	CMC-C2C	-2.11	1.46	1.50
82	Z1	201	PEB	CHC-C4C	2.11	1.52	1.49
87	CL	505	CLA	CHC-C1C	2.11	1.42	1.38
82	NH	1002	PEB	C4A-NA	-2.10	1.32	1.37
82	Z5	304	PEB	C4A-NA	-2.10	1.32	1.37
82	g4	202	PEB	C1C-C2C	2.10	1.47	1.42
82	UB	301	PEB	OD-C4D	2.10	1.27	1.23
87	BN	831	CLA	CMC-C2C	-2.10	1.46	1.50
87	A2	828	CLA	CMB-C2B	-2.10	1.46	1.50
87	B6	608	CLA	CMC-C2C	-2.10	1.46	1.50
82	UP	202	PEB	C1C-NC	-2.10	1.34	1.37
83	M5	302	PUB	CAB-C3B	2.10	1.56	1.51
87	52	602	CLA	CHC-C1C	2.10	1.42	1.38
82	P7	203	PEB	C1C-C2C	2.10	1.47	1.42
82	eB	201	PEB	C1C-C2C	2.10	1.47	1.42
82	I5	202	PEB	C2A-C1A	-2.10	1.50	1.52
82	m4	202	PEB	C4A-NA	-2.10	1.32	1.37
84	e3	1001	CYC	C4C-NC	-2.10	1.32	1.37
82	aO	203	PEB	O1B-CGB	2.10	1.29	1.22
87	12	607	CLA	CMD-C2D	-2.10	1.46	1.50
87	K2	103	CLA	CMC-C2C	-2.10	1.46	1.50
87	C6	514	CLA	CMC-C2C	-2.10	1.46	1.50
87	H6	102	CLA	CMD-C2D	-2.10	1.46	1.50
87	b6	616	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	d4	202	PEB	C1C-NC	-2.10	1.34	1.37
82	VI	202	PEB	C1C-C2C	2.10	1.47	1.42
82	aM	202	PEB	C1C-C2C	2.10	1.47	1.42
82	mO	202	PEB	C1C-C2C	2.10	1.47	1.42
87	bL	613	CLA	MG-NB	-2.10	2.01	2.05
82	ZK	201	PEB	C4A-NA	-2.10	1.32	1.37
87	LN	206	CLA	CMB-C2B	-2.10	1.46	1.50
87	dL	404	CLA	CMB-C2B	-2.10	1.46	1.50
87	L2	203	CLA	C3B-C4B	2.10	1.47	1.42
82	QD	202	PEB	C4B-C3B	2.10	1.49	1.45
82	xC	201	PEB	C4B-C3B	2.10	1.49	1.45
82	fM	202	PEB	C4B-C3B	2.10	1.49	1.45
82	Q7	201	PEB	C1B-C2B	2.10	1.50	1.45
82	kM	201	PEB	C4A-NA	-2.10	1.32	1.37
87	DL	404	CLA	MG-NB	-2.10	2.01	2.05
87	5N	610	CLA	MG-NB	-2.10	2.01	2.05
87	8N	303	CLA	MG-ND	-2.10	2.01	2.05
87	A2	825	CLA	C1B-NB	-2.10	1.35	1.37
82	N5	202	PEB	C2A-C1A	-2.10	1.50	1.52
87	32	306	CLA	CMD-C2D	-2.10	1.46	1.50
87	6N	610	CLA	CMC-C2C	-2.10	1.46	1.50
82	UH	203	PEB	C1C-C2C	2.10	1.47	1.42
82	U1	203	PEB	C4A-NA	-2.10	1.32	1.37
82	aJ	201	PEB	C4A-NA	-2.10	1.32	1.37
82	cG	201	PEB	C4B-C3B	2.10	1.49	1.45
87	LN	204	CLA	CMB-C2B	-2.10	1.46	1.50
87	B6	608	CLA	CMB-C2B	-2.10	1.46	1.50
87	BL	606	CLA	MG-NB	-2.10	2.01	2.05
87	CL	503	CLA	MG-ND	-2.10	2.01	2.05
82	PA	202	PEB	C1C-C2C	2.10	1.47	1.42
87	A2	837	CLA	CMD-C2D	-2.10	1.46	1.50
82	ZE	203	PEB	C1C-NC	-2.10	1.34	1.37
82	Z4	201	PEB	C1C-NC	-2.10	1.34	1.37
82	eE	201	PEB	C2A-C1A	-2.10	1.50	1.52
84	I3	1001	CYC	C4A-C3A	2.10	1.50	1.45
82	GJ	202	PEB	C4A-NA	-2.10	1.32	1.37
82	SP	201	PEB	C4A-NA	-2.10	1.32	1.37
87	22	601	CLA	MG-NB	-2.10	2.01	2.05
82	j1	202	PEB	C1C-C2C	2.10	1.47	1.42
87	BN	829	CLA	CMB-C2B	-2.10	1.46	1.50
87	FN	205	CLA	CMC-C2C	-2.10	1.46	1.50
87	62	311	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	F2	205	CLA	C4C-C3C	2.10	1.48	1.45
82	lH	201	PEB	CHC-C4C	2.10	1.52	1.49
82	RF	201	PEB	C4B-C3B	2.10	1.49	1.45
82	b4	202	PEB	C4B-C3B	2.10	1.49	1.45
82	GB	202	PEB	C4A-NA	-2.10	1.32	1.37
82	tF	202	PEB	C4A-NA	-2.10	1.32	1.37
83	xF	305	PUB	C4B-C3B	2.10	1.47	1.42
87	cL	507	CLA	MG-NB	-2.10	2.01	2.05
87	8N	305	CLA	MG-NB	-2.10	2.01	2.05
87	32	305	CLA	CMC-C2C	-2.10	1.46	1.50
87	A2	813	CLA	CMC-C2C	-2.10	1.46	1.50
87	4N	610	CLA	CMD-C2D	-2.10	1.46	1.50
82	Q5	202	PEB	C4A-NA	-2.10	1.32	1.37
82	AA	202	PEB	C2A-C1A	-2.10	1.50	1.52
82	TI	201	PEB	C2A-C1A	-2.10	1.50	1.52
82	WQ	201	PEB	C2A-C1A	-2.10	1.50	1.52
82	RJ	202	PEB	C1C-NC	-2.10	1.34	1.37
84	MG	1001	CYC	C4D-ND	-2.10	1.34	1.37
87	5N	607	CLA	CHC-C1C	2.10	1.42	1.38
87	AN	814	CLA	CMC-C2C	-2.10	1.46	1.50
87	BN	801	CLA	CMC-C2C	-2.10	1.46	1.50
87	B6	609	CLA	CMC-C2C	-2.10	1.46	1.50
82	VH	202	PEB	C1B-C2B	2.10	1.50	1.45
82	QK	201	PEB	C4A-NA	-2.10	1.32	1.37
82	d1	202	PEB	C4A-NA	-2.10	1.32	1.37
82	RH	202	PEB	C1C-C2C	2.10	1.47	1.42
83	BM	302	PUB	C4B-C3B	2.10	1.47	1.42
87	C6	511	CLA	CHC-C1C	2.10	1.42	1.38
82	NM	202	PEB	C1C-NC	-2.10	1.34	1.37
87	BN	812	CLA	MG-ND	-2.10	2.01	2.05
87	d6	406	CLA	CMD-C2D	-2.10	1.46	1.50
82	oK	201	PEB	C1B-C2B	2.10	1.50	1.45
82	jF	201	PEB	C1C-C2C	2.10	1.47	1.42
83	AG	303	PUB	C4B-C3B	2.10	1.47	1.42
82	AF	202	PEB	C4A-NA	-2.10	1.32	1.37
87	AN	837	CLA	CMD-C2D	-2.10	1.46	1.50
87	BL	622	CLA	MG-NB	-2.10	2.01	2.05
82	NM	202	PEB	C1B-C2B	2.10	1.50	1.45
82	UE	203	PEB	C1C-C2C	2.10	1.47	1.42
82	dJ	201	PEB	C4B-C3B	2.10	1.49	1.45
82	AH	305	PEB	C4A-NA	-2.10	1.32	1.37
82	k1	201	PEB	C4A-NA	-2.10	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	QP	202	PEB	C1D-ND	2.10	1.48	1.45
87	CL	518	CLA	CMD-C2D	-2.10	1.46	1.50
87	B2	808	CLA	MG-ND	-2.10	2.01	2.05
87	7N	604	CLA	MG-ND	-2.10	2.01	2.05
82	HP	202	PEB	C1C-C2C	2.10	1.47	1.42
82	vF	201	PEB	C1C-C2C	2.10	1.47	1.42
82	MP	201	PEB	C1C-NC	-2.10	1.34	1.37
82	dE	204	PEB	C4A-NA	-2.10	1.32	1.37
82	dG	204	PEB	C4A-NA	-2.10	1.32	1.37
82	uF	203	PEB	C4B-C3B	2.10	1.49	1.45
82	ZH	201	PEB	CHC-C4C	2.10	1.52	1.49
82	Q5	202	PEB	CHC-C4C	2.10	1.52	1.49
87	C6	518	CLA	CMC-C2C	-2.10	1.46	1.50
82	II	203	PEB	C1D-ND	2.10	1.48	1.45
82	ND	202	PEB	C1C-C2C	2.10	1.47	1.42
82	B7	201	PEB	C4A-NA	-2.10	1.32	1.37
87	AL	404	CLA	CMC-C2C	-2.10	1.46	1.50
87	B2	807	CLA	CMC-C2C	-2.10	1.46	1.50
87	B6	613	CLA	CMC-C2C	-2.10	1.46	1.50
87	5N	602	CLA	CMB-C2B	-2.10	1.46	1.50
82	AE	301	PEB	C1C-C2C	2.10	1.47	1.42
82	VF	201	PEB	C1C-C2C	2.10	1.47	1.42
83	xF	301	PUB	C4B-C3B	2.10	1.47	1.42
82	nK	202	PEB	C1D-ND	2.10	1.48	1.45
87	LN	206	CLA	CHC-C1C	2.10	1.42	1.38
87	b6	614	CLA	CHC-C1C	2.10	1.42	1.38
87	B2	813	CLA	CMC-C2C	-2.10	1.46	1.50
82	hF	201	PEB	C1B-C2B	2.10	1.50	1.45
84	L4	1001	CYC	C1B-C2B	2.10	1.48	1.45
82	IA	202	PEB	C4A-NA	-2.10	1.32	1.37
82	mF	201	PEB	C4A-NA	-2.10	1.32	1.37
82	aM	203	PEB	C4A-NA	-2.10	1.32	1.37
82	lM	203	PEB	C4A-NA	-2.10	1.32	1.37
82	FD	202	PEB	C2A-C1A	-2.10	1.50	1.52
82	aM	201	PEB	C2A-C1A	-2.10	1.50	1.52
82	hO	202	PEB	C2A-C1A	-2.10	1.50	1.52
82	a4	203	PEB	C1C-C2C	2.10	1.47	1.42
83	wK	304	PUB	C4B-C3B	2.10	1.47	1.42
87	JN	101	CLA	CMD-C2D	-2.10	1.46	1.50
82	UG	202	PEB	C1C-NC	-2.10	1.34	1.37
82	m4	201	PEB	C1C-NC	-2.10	1.34	1.37
96	vL	201	HEM	C3C-C4C	-2.10	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	GP	203	PEB	C4B-C3B	2.10	1.49	1.45
82	hJ	202	PEB	C4B-C3B	2.10	1.49	1.45
87	LN	202	CLA	CMB-C2B	-2.10	1.46	1.50
87	c6	616	CLA	CMD-C2D	-2.10	1.46	1.50
87	c6	606	CLA	CHC-C1C	2.10	1.42	1.38
87	6N	605	CLA	CHC-C1C	2.10	1.42	1.38
82	IJ	202	PEB	C1C-NC	-2.10	1.34	1.37
82	U4	201	PEB	C1C-NC	-2.10	1.34	1.37
82	M5	304	PEB	C4A-NA	-2.10	1.32	1.37
82	uC	203	PEB	C4A-NA	-2.10	1.32	1.37
87	52	604	CLA	CMD-C2D	-2.10	1.46	1.50
87	4N	611	CLA	CMC-C2C	-2.10	1.46	1.50
82	IB	202	PEB	C4B-C3B	2.10	1.49	1.45
82	H9	203	PEB	C2A-C1A	-2.10	1.50	1.52
82	mF	201	PEB	C2A-C1A	-2.10	1.50	1.52
82	MB	201	PEB	OD-C4D	2.10	1.27	1.23
82	SD	201	PEB	C4A-NA	-2.10	1.32	1.37
82	IF	203	PEB	C4B-NB	-2.10	1.34	1.38
82	XI	202	PEB	C1C-NC	-2.10	1.34	1.37
82	hM	203	PEB	C1C-NC	-2.10	1.34	1.37
87	KN	103	CLA	CMC-C2C	-2.10	1.46	1.50
82	G5	201	PEB	C1B-C2B	2.10	1.50	1.45
87	M2	101	CLA	C1B-NB	-2.10	1.35	1.37
82	W7	201	PEB	C1C-C2C	2.10	1.47	1.42
82	VF	202	PEB	C4A-NA	-2.10	1.32	1.37
82	sF	201	PEB	C1C-NC	-2.10	1.34	1.37
82	lO	201	PEB	C1C-NC	-2.10	1.34	1.37
87	b6	618	CLA	CMC-C2C	-2.10	1.46	1.50
87	3N	311	CLA	CMB-C2B	-2.10	1.46	1.50
84	C4	1001	CYC	C1B-C2B	2.10	1.48	1.45
84	u3	1001	CYC	C4A-C3A	2.10	1.50	1.45
82	sF	202	PEB	C2A-C1A	-2.10	1.50	1.52
82	LE	1002	PEB	C4A-NA	-2.10	1.32	1.37
82	HQ	201	PEB	C4B-C3B	2.10	1.49	1.45
87	12	604	CLA	CMD-C2D	-2.10	1.46	1.50
82	qK	203	PEB	C1B-C2B	2.10	1.50	1.45
87	1N	603	CLA	CHC-C1C	2.10	1.42	1.38
82	PI	202	PEB	C1C-NC	-2.10	1.34	1.37
82	fK	202	PEB	C1C-NC	-2.10	1.34	1.37
82	H7	202	PEB	CHC-C4C	2.09	1.52	1.49
87	62	308	CLA	CMD-C2D	-2.09	1.46	1.50
87	A2	801	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A2	830	CLA	CMC-C2C	-2.09	1.46	1.50
82	UH	203	PEB	C4B-C3B	2.09	1.49	1.45
82	VQ	202	PEB	C4B-C3B	2.09	1.49	1.45
82	B7	202	PEB	C4B-C3B	2.09	1.49	1.45
82	SG	201	PEB	C1C-C2C	2.09	1.47	1.42
82	D4	1002	PEB	C1C-C2C	2.09	1.47	1.42
84	NH	1001	CYC	C4D-C3D	2.09	1.47	1.42
87	KN	102	CLA	CHC-C1C	2.09	1.42	1.38
84	ME	1001	CYC	C1B-C2B	2.09	1.48	1.45
82	hE	202	PEB	C1C-NC	-2.09	1.34	1.37
82	RD	203	PEB	C4B-NB	-2.09	1.34	1.38
82	EK	201	PEB	C4A-NA	-2.09	1.32	1.37
82	QG	203	PEB	C4A-NA	-2.09	1.32	1.37
82	L5	202	PEB	C4A-NA	-2.09	1.32	1.37
84	J3	1001	CYC	C4C-NC	-2.09	1.32	1.37
82	QG	202	PEB	C1C-NC	-2.09	1.34	1.37
83	A1	304	PUB	C4B-NB	-2.09	1.34	1.37
87	BN	818	CLA	CMD-C2D	-2.09	1.46	1.50
87	C6	510	CLA	CMB-C2B	-2.09	1.46	1.50
87	b6	609	CLA	CMC-C2C	-2.09	1.46	1.50
87	c6	604	CLA	CMD-C2D	-2.09	1.46	1.50
87	c6	615	CLA	CMD-C2D	-2.09	1.46	1.50
84	H3	1001	CYC	C4A-C3A	2.09	1.50	1.45
87	52	604	CLA	CHC-C1C	2.09	1.42	1.38
82	HD	202	PEB	C1C-C2C	2.09	1.47	1.42
82	HQ	202	PEB	C1C-C2C	2.09	1.47	1.42
82	kG	202	PEB	C1C-C2C	2.09	1.47	1.42
87	AN	828	CLA	CMB-C2B	-2.09	1.46	1.50
87	BN	821	CLA	CMC-C2C	-2.09	1.46	1.50
87	LN	206	CLA	CMC-C2C	-2.09	1.46	1.50
87	L2	202	CLA	CMB-C2B	-2.09	1.46	1.50
87	D6	402	CLA	CMC-C2C	-2.09	1.46	1.50
87	1N	604	CLA	CMD-C2D	-2.09	1.46	1.50
87	4N	608	CLA	CMD-C2D	-2.09	1.46	1.50
82	G5	202	PEB	C1C-NC	-2.09	1.34	1.37
82	s8	201	PEB	C1C-NC	-2.09	1.34	1.37
84	E1	1001	CYC	C4D-ND	-2.09	1.34	1.37
82	X5	201	PEB	C1B-C2B	2.09	1.50	1.45
82	YJ	203	PEB	C2A-C1A	-2.09	1.50	1.52
82	SQ	202	PEB	C2A-C1A	-2.09	1.50	1.52
82	Q7	201	PEB	C4B-NB	-2.09	1.34	1.38
82	VF	202	PEB	C1C-C2C	2.09	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BQ	201	PEB	C1C-C2C	2.09	1.47	1.42
87	A2	821	CLA	MG-ND	-2.09	2.01	2.05
87	CL	515	CLA	CMB-C2B	-2.09	1.46	1.50
87	b6	614	CLA	CMC-C2C	-2.09	1.46	1.50
82	XD	203	PEB	C4B-C3B	2.09	1.49	1.45
82	XQ	203	PEB	C4B-C3B	2.09	1.49	1.45
82	OE	202	PEB	C1C-NC	-2.09	1.34	1.37
82	wF	303	PEB	C1C-NC	-2.09	1.34	1.37
82	fH	202	PEB	C4A-NA	-2.09	1.33	1.37
82	FH	1002	PEB	C1C-C2C	2.09	1.47	1.42
87	B2	811	CLA	CMB-C2B	-2.09	1.46	1.50
87	B6	604	CLA	CMD-C2D	-2.09	1.46	1.50
82	PD	201	PEB	C1D-ND	2.09	1.48	1.45
82	QP	202	PEB	C4B-C3B	2.09	1.49	1.45
82	mM	201	PEB	CHC-C4C	2.09	1.52	1.49
82	GM	202	PEB	C2A-C1A	-2.09	1.50	1.52
82	PJ	202	PEB	C1C-C2C	2.09	1.47	1.42
82	gK	202	PEB	C1C-C2C	2.09	1.47	1.42
82	EM	203	PEB	C4A-NA	-2.09	1.33	1.37
82	g1	201	PEB	C4A-NA	-2.09	1.33	1.37
82	fJ	202	PEB	C4A-NA	-2.09	1.33	1.37
84	v3	1001	CYC	C4C-NC	-2.09	1.33	1.37
87	ON	203	CLA	MG-NC	2.09	2.11	2.06
87	BN	823	CLA	C1B-C2B	2.09	1.48	1.43
87	B2	814	CLA	MG-ND	-2.09	2.01	2.05
87	5N	604	CLA	CHC-C1C	2.09	1.42	1.38
82	BB	201	PEB	C1C-C2C	2.09	1.47	1.42
82	I7	202	PEB	C1C-C2C	2.09	1.47	1.42
82	jE	201	PEB	C1D-ND	2.09	1.48	1.45
82	QE	203	PEB	C4A-NA	-2.09	1.33	1.37
82	OI	201	PEB	C4A-NA	-2.09	1.33	1.37
82	lG	203	PEB	C4A-NA	-2.09	1.33	1.37
87	22	610	CLA	CMB-C2B	-2.09	1.46	1.50
87	B2	821	CLA	CMB-C2B	-2.09	1.46	1.50
87	A6	403	CLA	CMB-C2B	-2.09	1.46	1.50
87	d6	406	CLA	CMB-C2B	-2.09	1.46	1.50
82	SF	202	PEB	O1C-CGC	2.09	1.29	1.22
87	3N	305	CLA	MG-NB	-2.09	2.01	2.05
87	A2	830	CLA	CHC-C1C	2.09	1.42	1.38
87	MN	101	CLA	C1B-NB	-2.09	1.35	1.37
87	3N	304	CLA	C1B-NB	-2.09	1.35	1.37
82	kM	202	PEB	C4A-NA	-2.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BL	620	CLA	C1B-C2B	2.09	1.48	1.43
82	pF	201	PEB	C2A-C1A	-2.09	1.50	1.52
87	B2	831	CLA	CMC-C2C	-2.09	1.46	1.50
87	H6	102	CLA	CMB-C2B	-2.09	1.46	1.50
82	T5	201	PEB	C1B-C2B	2.09	1.50	1.45
82	EF	201	PEB	C1C-NC	-2.09	1.34	1.37
82	J9	203	PEB	C1C-NC	-2.09	1.34	1.37
82	cM	201	PEB	CHC-C4C	2.09	1.52	1.49
82	GD	201	PEB	C1C-C2C	2.09	1.47	1.42
82	mF	202	PEB	C1C-C2C	2.09	1.47	1.42
87	bL	613	CLA	CHC-C1C	2.09	1.42	1.38
82	SG	203	PEB	C4A-NA	-2.09	1.33	1.37
82	c1	201	PEB	C4A-NA	-2.09	1.33	1.37
82	M9	305	PEB	C4A-NA	-2.09	1.33	1.37
96	VL	201	HEM	C3C-C4C	-2.09	1.42	1.46
87	42	608	CLA	CMD-C2D	-2.09	1.46	1.50
87	4N	601	CLA	CMC-C2C	-2.09	1.46	1.50
87	8N	306	CLA	CMB-C2B	-2.09	1.46	1.50
87	A2	829	CLA	MG-ND	-2.09	2.01	2.05
87	bL	621	CLA	MG-NB	-2.09	2.01	2.05
82	NI	202	PEB	C1C-NC	-2.09	1.34	1.37
82	TI	203	PEB	C1C-NC	-2.09	1.34	1.37
82	mG	201	PEB	C1C-NC	-2.09	1.34	1.37
82	u8	203	PEB	C4A-NA	-2.09	1.33	1.37
82	k1	202	PEB	C4B-C3B	2.09	1.49	1.45
82	DG	1002	PEB	CHC-C4C	2.09	1.52	1.49
82	pK	202	PEB	C1B-C2B	2.09	1.50	1.45
84	d3	1001	CYC	C4A-C3A	2.09	1.50	1.45
87	J2	101	CLA	CMB-C2B	-2.09	1.46	1.50
84	M4	1001	CYC	C4D-C3D	2.09	1.47	1.42
84	HE	1001	CYC	C1B-C2B	2.09	1.48	1.45
84	HG	1001	CYC	C1B-C2B	2.09	1.48	1.45
82	QA	201	PEB	C4B-NB	-2.09	1.34	1.38
82	lM	201	PEB	C4A-NA	-2.09	1.33	1.37
87	C6	512	CLA	CMD-C2D	-2.09	1.46	1.50
87	42	608	CLA	C1B-C2B	2.09	1.48	1.43
82	NI	202	PEB	C1C-C2C	2.09	1.47	1.42
82	EJ	201	PEB	C1C-C2C	2.09	1.47	1.42
82	GQ	201	PEB	C1C-C2C	2.09	1.47	1.42
82	jH	201	PEB	C1B-C2B	2.09	1.50	1.45
87	CL	506	CLA	CMD-C2D	-2.09	1.46	1.50
82	LF	201	PEB	C1C-NC	-2.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	K7	202	PEB	C1C-NC	-2.09	1.34	1.37
82	yF	301	PEB	C1C-NC	-2.09	1.34	1.37
85	a6	605	BCR	C30-C25	-2.09	1.50	1.53
82	d1	203	PEB	C4B-C3B	2.09	1.49	1.45
82	LF	201	PEB	C1A-NA	-2.09	1.34	1.37
87	BN	813	CLA	CMD-C2D	-2.09	1.46	1.50
87	BN	814	CLA	CMC-C2C	-2.09	1.46	1.50
87	12	603	CLA	CMD-C2D	-2.09	1.46	1.50
87	52	607	CLA	CMD-C2D	-2.09	1.46	1.50
87	B2	812	CLA	CMD-C2D	-2.09	1.46	1.50
87	AN	811	CLA	C1B-C2B	2.09	1.48	1.43
82	IB	201	PEB	C1C-NC	-2.09	1.34	1.37
82	DH	1002	PEB	C1C-C2C	2.09	1.47	1.42
82	YD	201	PEB	C4A-NA	-2.09	1.33	1.37
82	L7	203	PEB	C4A-NA	-2.09	1.33	1.37
82	aM	201	PEB	C4A-NA	-2.09	1.33	1.37
84	MO	1001	CYC	C1B-NB	-2.09	1.34	1.37
82	rC	201	PEB	C1B-C2B	2.09	1.50	1.45
82	lJ	202	PEB	C1B-C2B	2.09	1.50	1.45
84	N1	1001	CYC	C4B-NB	-2.09	1.33	1.38
87	C6	519	CLA	CHC-C1C	2.09	1.42	1.38
87	B6	612	CLA	CMC-C2C	-2.09	1.46	1.50
87	5N	607	CLA	CMD-C2D	-2.09	1.46	1.50
82	XF	202	PEB	C4B-C3B	2.09	1.49	1.45
82	gM	201	PEB	CHC-C4C	2.09	1.52	1.49
87	O2	203	CLA	MG-NC	2.09	2.11	2.06
82	dH	202	PEB	C1C-C2C	2.09	1.47	1.42
82	ZO	202	PEB	C4A-NA	-2.09	1.33	1.37
84	C1	1001	CYC	C4C-NC	-2.09	1.33	1.37
87	bL	619	CLA	MG-ND	-2.09	2.01	2.05
87	MN	101	CLA	CHC-C1C	2.09	1.42	1.38
82	GD	202	PEB	C1C-NC	-2.09	1.34	1.37
82	AF	202	PEB	C1C-NC	-2.09	1.34	1.37
82	YH	201	PEB	C1C-NC	-2.09	1.34	1.37
82	LI	202	PEB	C1C-NC	-2.09	1.34	1.37
82	VM	202	PEB	C1C-NC	-2.09	1.34	1.37
82	VP	202	PEB	C1C-NC	-2.09	1.34	1.37
82	GQ	202	PEB	C1C-NC	-2.09	1.34	1.37
84	J4	1001	CYC	C1B-C2B	2.09	1.48	1.45
87	B2	819	CLA	CMC-C2C	-2.09	1.46	1.50
87	B2	818	CLA	C1B-C2B	2.09	1.48	1.43
82	C5	201	PEB	C1B-C2B	2.09	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	72	605	CLA	MG-NB	-2.09	2.01	2.05
87	H6	102	CLA	CHC-C1C	2.09	1.42	1.38
87	52	609	CLA	CMB-C2B	-2.09	1.46	1.50
82	U9	201	PEB	C1C-NC	-2.09	1.34	1.37
82	kG	202	PEB	C1C-NC	-2.09	1.34	1.37
84	EG	1001	CYC	C4D-ND	-2.09	1.34	1.37
87	AN	805	CLA	MG-ND	-2.09	2.01	2.05
87	5N	603	CLA	CMD-C2D	-2.09	1.46	1.50
82	BI	203	PEB	C1C-C2C	2.09	1.47	1.42
82	FJ	202	PEB	C1C-C2C	2.09	1.47	1.42
82	j4	201	PEB	C1C-C2C	2.09	1.47	1.42
82	QD	202	PEB	C1D-ND	2.09	1.48	1.45
82	kF	202	PEB	C1D-ND	2.09	1.48	1.45
82	rF	202	PEB	C1D-ND	2.09	1.48	1.45
82	TD	203	PEB	C1C-NC	-2.09	1.34	1.37
94	d6	408	PL9	C2-C1	-2.09	1.39	1.44
82	dG	202	PEB	C4A-NA	-2.09	1.33	1.37
82	uF	203	PEB	C1B-C2B	2.09	1.50	1.45
84	F3	1001	CYC	C4A-C3A	2.09	1.50	1.45
82	dE	202	PEB	C2A-C1A	-2.09	1.50	1.52
82	HE	1002	PEB	CHC-C4C	2.09	1.52	1.49
82	J7	202	PEB	CHC-C4C	2.09	1.52	1.49
87	52	603	CLA	CMD-C2D	-2.09	1.46	1.50
87	D6	405	CLA	CMD-C2D	-2.09	1.46	1.50
87	5N	609	CLA	CMC-C2C	-2.09	1.46	1.50
82	XD	201	PEB	C4B-C3B	2.09	1.49	1.45
82	QF	201	PEB	C1C-NC	-2.08	1.34	1.37
82	bK	201	PEB	C1C-NC	-2.08	1.34	1.37
87	72	605	CLA	CHC-C1C	2.08	1.42	1.38
87	C6	518	CLA	CHC-C1C	2.08	1.42	1.38
82	JO	1002	PEB	C4B-C3B	2.08	1.49	1.45
82	P4	202	PEB	C4B-C3B	2.08	1.49	1.45
82	I7	202	PEB	C4A-NA	-2.08	1.33	1.37
82	j1	201	PEB	C1B-C2B	2.08	1.50	1.45
82	eJ	202	PEB	C1C-C2C	2.08	1.47	1.42
82	RI	202	PEB	C1C-NC	-2.08	1.34	1.37
87	B2	822	CLA	C1B-C2B	2.08	1.48	1.43
87	7N	607	CLA	CHC-C1C	2.08	1.42	1.38
87	DL	403	CLA	CAC-C3C	-2.08	1.45	1.51
82	jF	201	PEB	C4B-C3B	2.08	1.49	1.45
82	JH	1002	PEB	C4A-NA	-2.08	1.33	1.37
84	m3	1001	CYC	C4C-NC	-2.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	MM	201	PEB	C1C-C2C	2.08	1.47	1.42
82	D1	1002	PEB	C1C-C2C	2.08	1.47	1.42
87	42	602	CLA	CMB-C2B	-2.08	1.46	1.50
82	FF	201	PEB	C1C-NC	-2.08	1.34	1.37
82	Z4	202	PEB	C1C-NC	-2.08	1.34	1.37
82	Y7	303	PEB	C1C-NC	-2.08	1.34	1.37
82	gK	201	PEB	C1C-NC	-2.08	1.34	1.37
82	HH	1002	PEB	CHC-C4C	2.08	1.52	1.49
82	DP	201	PEB	C1C-C2C	2.08	1.47	1.42
84	C3	1001	CYC	C4C-NC	-2.08	1.33	1.37
82	QA	201	PEB	C1B-C2B	2.08	1.50	1.45
87	AN	820	CLA	CMC-C2C	-2.08	1.46	1.50
87	A2	812	CLA	CMD-C2D	-2.08	1.46	1.50
87	C6	517	CLA	CMC-C2C	-2.08	1.46	1.50
87	3N	311	CLA	CMC-C2C	-2.08	1.46	1.50
87	8N	305	CLA	CMB-C2B	-2.08	1.46	1.50
82	iM	202	PEB	C4B-C3B	2.08	1.49	1.45
87	A2	811	CLA	C3B-C4B	2.08	1.47	1.42
87	62	306	CLA	CHC-C1C	2.08	1.42	1.38
82	l4	202	PEB	C1C-C2C	2.08	1.47	1.42
82	uK	201	PEB	C1C-C2C	2.08	1.47	1.42
82	fF	202	PEB	C1C-NC	-2.08	1.34	1.37
82	G5	202	PEB	C2A-C1A	-2.08	1.50	1.52
82	E7	202	PEB	C2A-C1A	-2.08	1.50	1.52
82	Y7	304	PEB	C2A-C1A	-2.08	1.50	1.52
82	EA	202	PEB	C4A-NA	-2.08	1.33	1.37
82	iK	203	PEB	C4A-NA	-2.08	1.33	1.37
87	2N	308	CLA	CMC-C2C	-2.08	1.46	1.50
82	SB	202	PEB	C4B-C3B	2.08	1.49	1.45
82	IA	202	PEB	C1C-C2C	2.08	1.47	1.42
82	gJ	202	PEB	C4A-NA	-2.08	1.33	1.37
84	CH	1001	CYC	C4C-NC	-2.08	1.33	1.37
84	A3	1001	CYC	C4C-NC	-2.08	1.33	1.37
84	l3	1001	CYC	C4C-NC	-2.08	1.33	1.37
84	p3	1001	CYC	C4C-NC	-2.08	1.33	1.37
82	oF	202	PEB	C1C-NC	-2.08	1.34	1.37
87	BN	812	CLA	CMD-C2D	-2.08	1.46	1.50
87	B2	834	CLA	CMC-C2C	-2.08	1.46	1.50
87	62	313	CLA	CHC-C1C	2.08	1.42	1.38
82	JI	202	PEB	C1C-C2C	2.08	1.47	1.42
82	L5	202	PEB	C1C-C2C	2.08	1.47	1.42
82	lE	201	PEB	C1D-ND	2.08	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	810	CLA	MG-NB	-2.08	2.01	2.05
82	DI	201	PEB	C4B-C3B	2.08	1.49	1.45
82	L7	202	PEB	C4B-C3B	2.08	1.49	1.45
82	gB	201	PEB	C4A-NA	-2.08	1.33	1.37
82	gJ	201	PEB	C4A-NA	-2.08	1.33	1.37
82	kJ	202	PEB	C4A-NA	-2.08	1.33	1.37
82	h1	202	PEB	C2A-C1A	-2.08	1.50	1.52
82	e4	202	PEB	C2A-C1A	-2.08	1.50	1.52
87	B6	605	CLA	CMC-C2C	-2.08	1.46	1.50
87	1N	609	CLA	CMD-C2D	-2.08	1.46	1.50
82	AB	501	PEB	C1C-NC	-2.08	1.34	1.37
82	i1	202	PEB	CHC-C4C	2.08	1.52	1.49
82	YP	503	PEB	C1C-C2C	2.08	1.47	1.42
82	WG	202	PEB	C4A-NA	-2.08	1.33	1.37
82	e1	202	PEB	C1D-ND	2.08	1.48	1.45
82	ND	203	PEB	C1C-NC	-2.08	1.34	1.37
82	KI	203	PEB	C1C-NC	-2.08	1.34	1.37
87	MN	101	CLA	MG-ND	-2.08	2.01	2.05
87	32	304	CLA	MG-NB	-2.08	2.01	2.05
82	M5	304	PEB	C1B-C2B	2.08	1.50	1.45
82	N1	1002	PEB	C4A-NA	-2.08	1.33	1.37
82	bF	201	PEB	C4A-NA	-2.08	1.33	1.37
87	K2	104	CLA	CMC-C2C	-2.08	1.46	1.50
87	B6	604	CLA	CMB-C2B	-2.08	1.46	1.50
87	2N	307	CLA	CMD-C2D	-2.08	1.46	1.50
82	YG	202	PEB	C1C-C2C	2.08	1.47	1.42
82	SJ	201	PEB	C1C-C2C	2.08	1.47	1.42
82	NM	202	PEB	C1C-C2C	2.08	1.47	1.42
82	NQ	202	PEB	C1C-C2C	2.08	1.47	1.42
87	J2	101	CLA	CHC-C1C	2.08	1.42	1.38
87	8N	302	CLA	CHC-C1C	2.08	1.42	1.38
87	82	302	CLA	MG-ND	-2.08	2.01	2.05
82	wF	303	PEB	C4A-NA	-2.08	1.33	1.37
87	BN	811	CLA	C1B-NB	-2.08	1.35	1.37
87	AN	813	CLA	CMC-C2C	-2.08	1.46	1.50
87	C6	509	CLA	CMC-C2C	-2.08	1.46	1.50
87	bL	621	CLA	CMD-C2D	-2.08	1.46	1.50
82	lK	201	PEB	C1A-NA	-2.08	1.34	1.37
87	52	603	CLA	CHC-C1C	2.08	1.42	1.38
82	WD	202	PEB	C1B-C2B	2.08	1.50	1.45
82	WB	401	PEB	C4A-NA	-2.08	1.33	1.37
82	g4	203	PEB	C4A-NA	-2.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	aO	203	PEB	C4A-NA	-2.08	1.33	1.37
82	O4	201	PEB	C1C-C2C	2.08	1.47	1.42
82	X9	202	PEB	C1C-NC	-2.08	1.34	1.37
87	BN	818	CLA	CMB-C2B	-2.08	1.46	1.50
82	AJ	301	PEB	C2A-C1A	-2.08	1.50	1.52
82	C9	201	PEB	C2A-C1A	-2.08	1.50	1.52
82	P9	201	PEB	C2A-C1A	-2.08	1.50	1.52
82	FK	202	PEB	C1C-C2C	2.08	1.47	1.42
87	b6	612	CLA	CMD-C2D	-2.08	1.46	1.50
82	ZO	202	PEB	C1C-NC	-2.08	1.34	1.37
87	42	611	CLA	CHC-C1C	2.08	1.42	1.38
82	P5	201	PEB	C1B-C2B	2.08	1.50	1.45
82	aM	204	PEB	C4A-NA	-2.08	1.33	1.37
87	HL	101	CLA	CMD-C2D	-2.08	1.46	1.50
87	B2	810	CLA	C3B-C4B	2.08	1.47	1.42
82	NE	202	PEB	C4B-C3B	2.08	1.49	1.45
82	k4	201	PEB	C1C-NC	-2.08	1.34	1.37
84	L1	1001	CYC	C4D-ND	-2.08	1.34	1.37
82	QF	202	PEB	C1D-ND	2.08	1.48	1.45
84	Q3	1001	CYC	C4A-C3A	2.08	1.50	1.45
84	H4	1001	CYC	C4B-NB	-2.08	1.33	1.38
87	A2	837	CLA	CMC-C2C	-2.08	1.46	1.50
87	C6	510	CLA	CMC-C2C	-2.08	1.46	1.50
87	bL	604	CLA	CMC-C2C	-2.08	1.46	1.50
82	wC	204	PEB	CHC-C4C	2.08	1.52	1.49
82	dB	201	PEB	C1C-C2C	2.08	1.47	1.42
82	dF	201	PEB	C1C-C2C	2.08	1.47	1.42
82	aG	202	PEB	C4B-C3B	2.08	1.49	1.45
87	c6	614	CLA	CHC-C1C	2.08	1.42	1.38
82	GB	201	PEB	C1C-NC	-2.08	1.34	1.37
82	LP	202	PEB	C1C-NC	-2.08	1.34	1.37
82	MM	203	PEB	C4A-NA	-2.08	1.33	1.37
82	AQ	303	PEB	C1D-ND	2.08	1.48	1.45
87	52	610	CLA	MG-NB	-2.08	2.01	2.05
82	pF	201	PEB	C1A-NA	-2.08	1.34	1.37
82	DK	203	PEB	C1C-C2C	2.08	1.47	1.42
82	NP	202	PEB	C1C-C2C	2.08	1.47	1.42
83	A4	303	PUB	C4B-C3B	2.08	1.47	1.42
87	a6	607	CLA	CHC-C1C	2.08	1.42	1.38
96	fL	102	HEM	C3C-C4C	-2.08	1.42	1.46
82	Y9	203	PEB	C1C-NC	-2.08	1.34	1.37
87	AN	802	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	22	611	CLA	CMD-C2D	-2.08	1.46	1.50
87	3N	313	CLA	CMD-C2D	-2.08	1.46	1.50
87	5N	609	CLA	CMB-C2B	-2.08	1.46	1.50
82	JD	202	PEB	C1D-ND	2.08	1.48	1.45
82	pK	202	PEB	CHC-C4C	2.08	1.52	1.49
82	xK	302	PEB	CHC-C4C	2.08	1.52	1.49
87	b6	609	CLA	C1B-C2B	2.08	1.48	1.43
84	E4	1001	CYC	C4A-C3A	2.08	1.50	1.45
82	OQ	202	PEB	C4A-NA	-2.08	1.33	1.37
82	hE	201	PEB	C4A-NA	-2.08	1.33	1.37
87	B2	816	CLA	C1B-NB	-2.08	1.35	1.37
87	12	609	CLA	CMD-C2D	-2.08	1.46	1.50
87	4N	601	CLA	CMD-C2D	-2.08	1.46	1.50
82	QJ	203	PEB	C1C-C2C	2.08	1.47	1.42
82	DP	202	PEB	C1C-C2C	2.08	1.47	1.42
82	AI	202	PEB	C1C-NC	-2.08	1.34	1.37
82	OO	202	PEB	C1C-NC	-2.08	1.34	1.37
82	aB	201	PEB	C1C-NC	-2.08	1.34	1.37
82	b1	203	PEB	C1D-ND	2.08	1.48	1.45
82	O1	201	PEB	C4A-NA	-2.08	1.33	1.37
87	22	603	CLA	CMB-C2B	-2.08	1.46	1.50
87	2N	311	CLA	CMD-C2D	-2.08	1.46	1.50
87	4N	610	CLA	CMB-C2B	-2.08	1.46	1.50
85	cL	504	BCR	C30-C25	-2.08	1.50	1.53
82	XM	202	PEB	C1C-C2C	2.08	1.47	1.42
82	gH	202	PEB	CHC-C4C	2.08	1.52	1.49
87	BN	801	CLA	C1B-C2B	2.08	1.48	1.43
82	FH	1002	PEB	C1C-NC	-2.08	1.34	1.37
84	HH	1001	CYC	C1B-NB	-2.08	1.34	1.37
82	AI	202	PEB	C2A-C1A	-2.08	1.50	1.52
87	12	601	CLA	CMC-C2C	-2.08	1.46	1.50
87	A2	812	CLA	CMC-C2C	-2.08	1.46	1.50
82	HM	202	PEB	C1C-C2C	2.08	1.47	1.42
82	wK	301	PEB	C1C-C2C	2.08	1.47	1.42
82	NH	1002	PEB	C1D-ND	2.08	1.48	1.45
87	BN	826	CLA	C1B-C2B	2.08	1.48	1.43
87	2N	302	CLA	MG-NB	-2.08	2.01	2.05
87	3N	311	CLA	MG-NB	-2.08	2.01	2.05
82	N5	201	PEB	C1B-C2B	2.08	1.50	1.45
82	ZM	202	PEB	C1C-NC	-2.08	1.34	1.37
82	mF	202	PEB	C4A-NA	-2.08	1.33	1.37
82	lJ	201	PEB	C4A-NA	-2.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	NH	1002	PEB	C1C-C2C	2.08	1.47	1.42
82	H5	201	PEB	C1C-C2C	2.08	1.47	1.42
82	PK	202	PEB	C4B-C3B	2.08	1.49	1.45
87	82	304	CLA	CMB-C2B	-2.08	1.46	1.50
87	L2	206	CLA	CMB-C2B	-2.08	1.46	1.50
87	B2	818	CLA	MG-ND	-2.08	2.01	2.05
82	QM	204	PEB	C4A-NA	-2.08	1.33	1.37
82	YO	201	PEB	C4A-NA	-2.08	1.33	1.37
82	KQ	201	PEB	C4A-NA	-2.08	1.33	1.37
87	C6	515	CLA	CHC-C1C	2.08	1.42	1.38
87	AN	808	CLA	CMC-C2C	-2.08	1.46	1.50
87	52	610	CLA	CMC-C2C	-2.08	1.46	1.50
87	72	607	CLA	CMD-C2D	-2.08	1.46	1.50
82	f4	202	PEB	C1C-NC	-2.08	1.34	1.37
82	eG	201	PEB	C2A-C1A	-2.08	1.50	1.52
82	NQ	202	PEB	C4B-C3B	2.08	1.49	1.45
87	A2	808	CLA	MG-ND	-2.08	2.01	2.05
82	ZH	201	PEB	C1A-NA	-2.08	1.34	1.37
82	QP	201	PEB	C1C-C2C	2.08	1.47	1.42
82	mJ	201	PEB	CHC-C4C	2.08	1.52	1.49
82	iO	202	PEB	C4A-NA	-2.08	1.33	1.37
87	A2	811	CLA	C1B-C2B	2.08	1.48	1.43
82	ZM	201	PEB	C1D-ND	2.08	1.48	1.45
87	7N	603	CLA	CHC-C1C	2.07	1.42	1.38
82	P9	202	PEB	C1C-NC	-2.07	1.34	1.37
82	lE	203	PEB	C1C-NC	-2.07	1.34	1.37
82	OQ	202	PEB	C1B-C2B	2.07	1.50	1.45
82	S9	203	PEB	C1C-C2C	2.07	1.47	1.42
82	AH	302	PEB	C4A-NA	-2.07	1.33	1.37
87	AN	820	CLA	CMD-C2D	-2.07	1.46	1.50
82	pF	202	PEB	C1B-C2B	2.07	1.50	1.45
82	II	202	PEB	C1C-NC	-2.07	1.34	1.37
82	eG	203	PEB	C1C-NC	-2.07	1.34	1.37
84	GO	1001	CYC	C1B-NB	-2.07	1.34	1.37
82	l1	202	PEB	C4A-NA	-2.07	1.33	1.37
82	hM	201	PEB	C4A-NA	-2.07	1.33	1.37
84	G3	1001	CYC	C4C-NC	-2.07	1.33	1.37
87	BN	812	CLA	CMB-C2B	-2.07	1.46	1.50
87	1N	601	CLA	CMC-C2C	-2.07	1.46	1.50
87	JN	101	CLA	CHC-C1C	2.07	1.42	1.38
82	EP	201	PEB	C1C-C2C	2.07	1.47	1.42
82	U7	202	PEB	C1C-C2C	2.07	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	62	311	CLA	MG-NB	-2.07	2.01	2.05
87	82	301	CLA	MG-ND	-2.07	2.01	2.05
82	HE	1002	PEB	C4A-NA	-2.07	1.33	1.37
82	OP	203	PEB	C4A-NA	-2.07	1.33	1.37
87	62	301	CLA	CMD-C2D	-2.07	1.46	1.50
87	cL	508	CLA	CMD-C2D	-2.07	1.46	1.50
82	ND	202	PEB	C4B-C3B	2.07	1.49	1.45
82	uK	202	PEB	C1B-C2B	2.07	1.50	1.45
84	EG	1001	CYC	C4A-C3A	2.07	1.50	1.45
82	VH	202	PEB	CHC-C4C	2.07	1.52	1.49
87	BL	602	CLA	C1B-C2B	2.07	1.48	1.43
87	22	610	CLA	C3D-C4D	2.07	1.48	1.44
87	8N	302	CLA	MG-ND	-2.07	2.01	2.05
82	YD	202	PEB	C4A-NA	-2.07	1.33	1.37
87	CL	511	CLA	C3B-C4B	2.07	1.47	1.42
87	72	604	CLA	CMB-C2B	-2.07	1.46	1.50
87	B2	818	CLA	CMD-C2D	-2.07	1.46	1.50
87	7N	606	CLA	CMD-C2D	-2.07	1.46	1.50
82	KM	202	PEB	C2A-C1A	-2.07	1.50	1.52
82	c4	203	PEB	C2A-C1A	-2.07	1.50	1.52
82	uF	201	PEB	C2A-C1A	-2.07	1.50	1.52
82	UF	202	PEB	C1C-NC	-2.07	1.34	1.37
84	EE	1001	CYC	C4D-ND	-2.07	1.34	1.37
82	D5	201	PEB	C1C-C2C	2.07	1.47	1.42
82	W1	202	PEB	C1B-C2B	2.07	1.50	1.45
84	q3	1001	CYC	C4A-C3A	2.07	1.50	1.45
82	TD	201	PEB	C4A-NA	-2.07	1.33	1.37
82	TQ	201	PEB	C4A-NA	-2.07	1.33	1.37
87	BL	601	CLA	CMC-C2C	-2.07	1.46	1.50
87	72	606	CLA	CMD-C2D	-2.07	1.46	1.50
87	A2	836	CLA	CMC-C2C	-2.07	1.46	1.50
87	1N	609	CLA	CMB-C2B	-2.07	1.46	1.50
87	CL	511	CLA	C1B-NB	-2.07	1.35	1.37
82	wF	302	PEB	C1C-NC	-2.07	1.34	1.37
82	kJ	202	PEB	C1C-NC	-2.07	1.34	1.37
82	TH	202	PEB	C1D-ND	2.07	1.48	1.45
87	3N	312	CLA	MG-ND	-2.07	2.01	2.05
82	iM	202	PEB	C4A-NA	-2.07	1.33	1.37
84	E3	1001	CYC	C4C-NC	-2.07	1.33	1.37
87	CL	513	CLA	CMB-C2B	-2.07	1.46	1.50
87	BN	820	CLA	CMC-C2C	-2.07	1.46	1.50
87	3N	307	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	bL	615	CLA	CHC-C1C	2.07	1.42	1.38
82	B9	203	PEB	C1C-NC	-2.07	1.34	1.37
82	wK	303	PEB	C1C-NC	-2.07	1.34	1.37
84	DH	1001	CYC	C1B-NB	-2.07	1.34	1.37
87	4N	609	CLA	MG-ND	-2.07	2.01	2.05
87	32	303	CLA	C1B-NB	-2.07	1.35	1.37
82	LP	201	PEB	C1C-C2C	2.07	1.47	1.42
82	f4	202	PEB	C1D-ND	2.07	1.48	1.45
87	12	609	CLA	CMB-C2B	-2.07	1.46	1.50
82	kF	201	PEB	CHC-C4C	2.07	1.52	1.49
82	QP	203	PEB	C4B-C3B	2.07	1.49	1.45
87	6N	613	CLA	O2A-CGA	2.07	1.37	1.30
82	lO	202	PEB	C1C-C2C	2.07	1.47	1.42
82	WE	202	PEB	C4A-NA	-2.07	1.33	1.37
84	DH	1001	CYC	C4C-NC	-2.07	1.33	1.37
82	YD	202	PEB	C1C-NC	-2.07	1.34	1.37
87	32	310	CLA	CMD-C2D	-2.07	1.46	1.50
82	R5	201	PEB	C1B-C2B	2.07	1.50	1.45
87	AN	835	CLA	CHC-C1C	2.07	1.42	1.38
82	UE	203	PEB	C1D-ND	2.07	1.48	1.45
87	cL	509	CLA	C1B-NB	-2.07	1.35	1.37
82	HE	1002	PEB	C1C-C2C	2.07	1.47	1.42
82	b1	203	PEB	C1C-C2C	2.07	1.47	1.42
82	M9	301	PEB	C2A-C1A	-2.07	1.50	1.52
82	F4	1002	PEB	C4A-NA	-2.07	1.33	1.37
82	mG	202	PEB	C4A-NA	-2.07	1.33	1.37
87	FN	203	CLA	CMB-C2B	-2.07	1.46	1.50
87	5N	610	CLA	CMD-C2D	-2.07	1.46	1.50
84	BE	1001	CYC	C1B-C2B	2.07	1.48	1.45
87	2N	310	CLA	C3D-C4D	2.07	1.48	1.44
82	V5	201	PEB	C1B-C2B	2.07	1.50	1.45
82	QQ	202	PEB	C4A-NA	-2.07	1.33	1.37
82	iH	201	PEB	C4A-NA	-2.07	1.33	1.37
103	82	309	ZEX	C1-C6	-2.07	1.50	1.53
87	HL	102	CLA	CMC-C2C	-2.07	1.46	1.50
87	A2	827	CLA	MG-ND	-2.07	2.01	2.05
84	FG	1001	CYC	C1B-C2B	2.07	1.48	1.45
82	G9	202	PEB	C1C-NC	-2.07	1.34	1.37
87	B2	825	CLA	C1B-C2B	2.07	1.48	1.43
87	8N	303	CLA	MG-NC	2.07	2.11	2.06
87	A2	826	CLA	CMB-C2B	-2.07	1.46	1.50
87	J2	101	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	7N	607	CLA	CMD-C2D	-2.07	1.46	1.50
82	AH	302	PEB	C2A-C1A	-2.07	1.50	1.52
82	R9	201	PEB	C2A-C1A	-2.07	1.50	1.52
82	jH	203	PEB	C4B-NB	-2.07	1.34	1.38
82	DQ	202	PEB	OD-C4D	2.07	1.27	1.23
82	QQ	201	PEB	C1D-ND	2.07	1.48	1.45
82	B5	203	PEB	C1B-C2B	2.07	1.50	1.45
84	LG	1001	CYC	C4A-C3A	2.07	1.50	1.45
82	NF	202	PEB	C1C-C2C	2.07	1.47	1.42
82	WM	201	PEB	C1C-C2C	2.07	1.47	1.42
82	LA	201	PEB	C1C-NC	-2.07	1.34	1.37
82	DI	202	PEB	C1C-NC	-2.07	1.34	1.37
82	MM	202	PEB	C1C-NC	-2.07	1.34	1.37
82	eB	201	PEB	C1C-NC	-2.07	1.34	1.37
87	DL	404	CLA	CMB-C2B	-2.07	1.46	1.50
87	c6	616	CLA	CMB-C2B	-2.07	1.46	1.50
87	72	608	CLA	MG-NB	-2.07	2.01	2.05
87	M2	101	CLA	MG-ND	-2.07	2.01	2.05
87	72	608	CLA	CHC-C1C	2.07	1.42	1.38
82	kJ	201	PEB	C4A-NA	-2.07	1.33	1.37
84	N3	1001	CYC	C4C-NC	-2.07	1.33	1.37
84	N4	1001	CYC	C4D-ND	-2.07	1.34	1.37
82	GI	201	PEB	C2C-C3C	2.07	1.44	1.38
87	82	301	CLA	CHC-C1C	2.07	1.42	1.38
87	7N	606	CLA	CHC-C1C	2.07	1.42	1.38
87	dL	401	CLA	C1B-NB	-2.07	1.35	1.37
82	LA	203	PEB	C4A-NA	-2.07	1.33	1.37
82	AP	202	PEB	C4A-NA	-2.07	1.33	1.37
84	g3	1001	CYC	C4C-NC	-2.07	1.33	1.37
82	jG	201	PEB	C4B-C3B	2.07	1.49	1.45
82	RE	201	PEB	C1C-C2C	2.07	1.47	1.42
82	GI	203	PEB	C1C-NC	-2.07	1.34	1.37
87	3N	311	CLA	CHC-C1C	2.07	1.42	1.38
82	OD	202	PEB	C4A-NA	-2.07	1.33	1.37
82	bH	202	PEB	C4A-NA	-2.07	1.33	1.37
82	PH	202	PEB	C1C-C2C	2.07	1.47	1.42
82	UM	202	PEB	C1B-C2B	2.07	1.50	1.45
82	OQ	202	PEB	C4B-C3B	2.07	1.49	1.45
82	b1	201	PEB	C4B-C3B	2.07	1.49	1.45
82	eB	202	PEB	C1C-NC	-2.07	1.34	1.37
87	5N	605	CLA	CHC-C1C	2.07	1.42	1.38
82	RB	202	PEB	C4A-NA	-2.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	E7	202	PEB	C4A-NA	-2.07	1.33	1.37
82	F9	203	PEB	C4A-NA	-2.07	1.33	1.37
82	hO	201	PEB	C1C-C2C	2.07	1.47	1.42
87	2N	306	CLA	CMB-C2B	-2.07	1.46	1.50
83	Z9	302	PUB	C1C-NC	-2.07	1.34	1.38
82	GK	202	PEB	CHB-C4B	2.07	1.42	1.38
82	dB	201	PEB	C4B-C3B	2.07	1.49	1.45
82	XM	202	PEB	C1C-NC	-2.07	1.34	1.37
82	kM	201	PEB	C1D-ND	2.07	1.48	1.45
82	K5	201	PEB	C1B-C2B	2.07	1.50	1.45
82	fK	201	PEB	C1A-NA	-2.07	1.34	1.37
103	8N	309	ZEX	C21-C26	-2.07	1.50	1.53
87	c6	616	CLA	CHC-C1C	2.07	1.42	1.38
87	6N	612	CLA	CHC-C1C	2.07	1.42	1.38
82	VK	202	PEB	C4B-C3B	2.07	1.49	1.45
82	PQ	201	PEB	C4B-C3B	2.07	1.49	1.45
82	YK	201	PEB	C4A-NA	-2.07	1.33	1.37
87	A2	834	CLA	CMC-C2C	-2.07	1.46	1.50
82	Q5	201	PEB	C1B-C2B	2.07	1.50	1.45
82	Z1	203	PEB	C2A-C1A	-2.07	1.50	1.52
82	P5	202	PEB	C2A-C1A	-2.07	1.50	1.52
82	V9	201	PEB	C2A-C1A	-2.07	1.50	1.52
82	aM	203	PEB	C2A-C1A	-2.07	1.50	1.52
82	O9	202	PEB	C1D-ND	2.07	1.48	1.45
82	rK	202	PEB	C1D-ND	2.07	1.48	1.45
87	A2	801	CLA	MG-NB	-2.07	2.01	2.05
87	2N	307	CLA	MG-ND	-2.07	2.01	2.05
82	ZE	202	PEB	C1C-C2C	2.07	1.47	1.42
82	NG	201	PEB	C1C-C2C	2.07	1.47	1.42
82	rK	202	PEB	C1C-C2C	2.07	1.47	1.42
87	6N	604	CLA	CHC-C1C	2.07	1.42	1.38
96	v6	201	HEM	C1A-C2A	-2.07	1.40	1.44
82	V7	202	PEB	C4B-C3B	2.07	1.49	1.45
82	YP	503	PEB	C1C-NC	-2.07	1.34	1.37
82	S7	202	PEB	C1C-NC	-2.07	1.34	1.37
82	i4	202	PEB	C1C-C2C	2.07	1.47	1.42
87	52	611	CLA	CMB-C2B	-2.07	1.46	1.50
87	c6	610	CLA	CMC-C2C	-2.07	1.46	1.50
94	a6	601	PL9	C2-C1	-2.07	1.39	1.44
84	EG	1001	CYC	C4D-C3D	2.07	1.47	1.42
82	AP	202	PEB	C1C-NC	-2.07	1.34	1.37
82	GP	203	PEB	C1C-NC	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	KM	202	PEB	C4B-C3B	2.07	1.49	1.45
82	lE	203	PEB	C4B-C3B	2.07	1.49	1.45
82	kM	202	PEB	C4B-C3B	2.07	1.49	1.45
82	NI	201	PEB	C2A-C1A	-2.07	1.50	1.52
82	PI	201	PEB	C2A-C1A	-2.07	1.50	1.52
82	G9	201	PEB	C2A-C1A	-2.07	1.50	1.52
82	fE	203	PEB	C2A-C1A	-2.07	1.50	1.52
92	j6	101	LMG	O7-C8	-2.07	1.41	1.46
87	B6	610	CLA	CHC-C1C	2.07	1.42	1.38
87	B2	817	CLA	CMD-C2D	-2.07	1.46	1.50
87	5N	610	CLA	CMC-C2C	-2.07	1.46	1.50
87	7N	606	CLA	CMB-C2B	-2.07	1.46	1.50
82	RQ	203	PEB	C4B-NB	-2.07	1.34	1.38
82	SO	202	PEB	C1C-C2C	2.06	1.47	1.42
82	Y1	202	PEB	C1C-C2C	2.06	1.47	1.42
82	DA	201	PEB	CHC-C4C	2.06	1.52	1.49
82	YF	203	PEB	C4B-C3B	2.06	1.49	1.45
82	J4	1002	PEB	C4B-C3B	2.06	1.49	1.45
82	aM	201	PEB	C4B-C3B	2.06	1.49	1.45
82	MA	202	PEB	C4A-NA	-2.06	1.33	1.37
87	42	610	CLA	CMB-C2B	-2.06	1.46	1.50
87	H6	103	CLA	CMC-C2C	-2.06	1.46	1.50
87	c6	609	CLA	CMD-C2D	-2.06	1.46	1.50
87	6N	603	CLA	CMD-C2D	-2.06	1.46	1.50
87	AN	810	CLA	C3D-C4D	2.06	1.48	1.44
87	62	301	CLA	O2A-CGA	2.06	1.37	1.30
87	BN	832	CLA	MG-ND	-2.06	2.01	2.05
82	CK	203	PEB	C4A-NA	-2.06	1.33	1.37
82	i1	201	PEB	C4A-NA	-2.06	1.33	1.37
84	R3	1001	CYC	C4C-NC	-2.06	1.33	1.37
87	CL	514	CLA	CMB-C2B	-2.06	1.46	1.50
87	c6	605	CLA	CMD-C2D	-2.06	1.46	1.50
87	3N	310	CLA	CMD-C2D	-2.06	1.46	1.50
87	8N	307	CLA	CMD-C2D	-2.06	1.46	1.50
96	GN	201	HEM	CMB-C2B	2.06	1.55	1.50
82	kG	202	PEB	C2A-C1A	-2.06	1.50	1.52
82	gJ	201	PEB	C2A-C1A	-2.06	1.50	1.52
82	EI	202	PEB	C1C-NC	-2.06	1.34	1.37
84	73	1002	CYC	C1B-NB	-2.06	1.34	1.37
82	W1	201	PEB	C1D-ND	2.06	1.48	1.45
82	fO	202	PEB	C1D-ND	2.06	1.48	1.45
82	CM	202	PEB	C4A-NA	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A1	305	PEB	C4A-NA	-2.06	1.33	1.37
87	52	610	CLA	CMD-C2D	-2.06	1.46	1.50
87	bL	615	CLA	CMC-C2C	-2.06	1.46	1.50
96	f6	101	HEM	C4B-NB	-2.06	1.34	1.38
82	PM	202	PEB	C1C-NC	-2.06	1.34	1.37
82	eH	201	PEB	C4B-C3B	2.06	1.49	1.45
82	mK	202	PEB	C4A-NA	-2.06	1.33	1.37
87	CL	505	CLA	CMC-C2C	-2.06	1.46	1.50
82	JA	201	PEB	C1C-C2C	2.06	1.47	1.42
82	nF	201	PEB	CHC-C4C	2.06	1.52	1.49
82	1C	201	PEB	C1D-ND	2.06	1.48	1.45
82	JH	1002	PEB	C2A-C1A	-2.06	1.50	1.52
82	VI	202	PEB	C2A-C1A	-2.06	1.50	1.52
82	SI	201	PEB	C4B-C3B	2.06	1.49	1.45
82	QQ	202	PEB	C4B-C3B	2.06	1.49	1.45
87	R2	203	CLA	CMB-C2B	-2.06	1.46	1.50
87	K2	103	CLA	CHC-C1C	2.06	1.42	1.38
82	YM	201	PEB	C1C-C2C	2.06	1.47	1.42
84	H1	1001	CYC	C1B-NB	-2.06	1.34	1.37
87	52	610	CLA	CMB-C2B	-2.06	1.46	1.50
82	LG	1002	PEB	C4A-NA	-2.06	1.33	1.37
87	72	607	CLA	CHC-C1C	2.06	1.42	1.38
87	B6	614	CLA	CHC-C1C	2.06	1.42	1.38
82	xF	302	PEB	C2A-C1A	-2.06	1.50	1.52
87	A2	826	CLA	CMC-C2C	-2.06	1.46	1.50
87	A6	402	CLA	CMC-C2C	-2.06	1.46	1.50
87	cL	505	CLA	CMC-C2C	-2.06	1.46	1.50
82	FD	201	PEB	C4B-NB	-2.06	1.34	1.38
82	YQ	202	PEB	C4A-NA	-2.06	1.33	1.37
87	CL	507	CLA	CHC-C1C	2.06	1.42	1.38
82	T9	202	PEB	C1C-NC	-2.06	1.34	1.37
82	FD	203	PEB	C1C-NC	2.06	1.41	1.37
82	YM	203	PEB	C1D-ND	2.06	1.48	1.45
82	PH	202	PEB	C4B-C3B	2.06	1.49	1.45
82	GB	201	PEB	C1C-C2C	2.06	1.47	1.42
82	QM	204	PEB	C1C-C2C	2.06	1.47	1.42
82	D7	201	PEB	CHC-C4C	2.06	1.52	1.49
87	B2	832	CLA	MG-ND	-2.06	2.01	2.05
87	BN	835	CLA	C1B-NB	-2.06	1.35	1.37
82	cK	202	PEB	C1C-NC	-2.06	1.34	1.37
82	PO	203	PEB	C1C-C2C	2.06	1.47	1.42
82	M9	301	PEB	C1C-C2C	2.06	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	uK	202	PEB	C4B-C3B	2.06	1.49	1.45
82	CA	201	PEB	C4B-NB	-2.06	1.34	1.38
87	AN	803	CLA	CMD-C2D	-2.06	1.46	1.50
87	82	307	CLA	CMD-C2D	-2.06	1.46	1.50
87	B2	833	CLA	CMC-C2C	-2.06	1.46	1.50
87	H6	103	CLA	CMD-C2D	-2.06	1.46	1.50
87	b6	616	CLA	CMC-C2C	-2.06	1.46	1.50
82	ZO	202	PEB	C2A-C1A	-2.06	1.50	1.52
82	L9	202	PEB	C2A-C1A	-2.06	1.50	1.52
87	A2	831	CLA	CHC-C4B	-2.06	1.34	1.39
82	eG	201	PEB	C1C-NC	-2.06	1.34	1.37
87	C6	512	CLA	CMC-C2C	-2.06	1.46	1.50
87	b6	608	CLA	C1B-NB	-2.06	1.35	1.37
82	LD	201	PEB	C4A-NA	-2.06	1.33	1.37
82	BD	201	PEB	C4B-C3B	2.06	1.49	1.45
87	4N	605	CLA	MG-NB	-2.06	2.01	2.05
87	5N	608	CLA	MG-ND	-2.06	2.01	2.05
82	CM	201	PEB	C1C-NC	-2.06	1.34	1.37
87	CL	515	CLA	CMD-C2D	-2.06	1.46	1.50
87	3N	303	CLA	CMC-C2C	-2.06	1.46	1.50
84	K3	1001	CYC	C4C-NC	-2.06	1.33	1.37
82	AJ	301	PEB	C1C-C2C	2.06	1.47	1.42
82	ZJ	202	PEB	C1C-C2C	2.06	1.47	1.42
87	42	606	CLA	MG-ND	-2.06	2.01	2.05
82	J9	201	PEB	CHC-C4C	2.06	1.52	1.49
82	fE	202	PEB	C4B-C3B	2.06	1.49	1.45
87	42	603	CLA	CMB-C2B	-2.06	1.46	1.50
87	82	305	CLA	CMB-C2B	-2.06	1.46	1.50
87	H6	102	CLA	CMC-C2C	-2.06	1.46	1.50
82	A1	302	PEB	C4A-NA	-2.06	1.33	1.37
82	NE	202	PEB	C1C-C2C	2.06	1.47	1.42
82	lJ	203	PEB	C1C-C2C	2.06	1.47	1.42
87	BN	819	CLA	C1B-C2B	2.06	1.48	1.43
82	SF	203	PEB	C1C-NC	-2.06	1.34	1.37
82	mE	203	PEB	C1C-NC	-2.06	1.34	1.37
82	mG	203	PEB	C1C-NC	-2.06	1.34	1.37
87	H6	103	CLA	CHC-C1C	2.06	1.42	1.38
82	D9	201	PEB	C1D-ND	2.06	1.48	1.45
87	BN	833	CLA	CMC-C2C	-2.06	1.46	1.50
87	82	305	CLA	CMC-C2C	-2.06	1.46	1.50
82	VK	201	PEB	C1C-C2C	2.06	1.47	1.42
82	gG	202	PEB	C4A-NA	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mO	202	PEB	C4A-NA	-2.06	1.33	1.37
87	AN	825	CLA	C1B-NB	-2.06	1.35	1.37
87	AN	834	CLA	CAB-C3B	-2.06	1.41	1.47
82	qF	201	PEB	C2A-C1A	-2.06	1.50	1.52
82	Y7	304	PEB	C1C-C2C	2.06	1.47	1.42
87	b6	605	CLA	CMC-C2C	-2.06	1.46	1.50
82	MD	202	PEB	C4A-NA	-2.06	1.33	1.37
82	d4	201	PEB	C4A-NA	-2.06	1.33	1.37
82	eK	203	PEB	C4A-NA	-2.06	1.33	1.37
87	B6	604	CLA	CHC-C1C	2.06	1.42	1.38
82	EK	202	PEB	C1C-NC	-2.06	1.34	1.37
82	W1	202	PEB	C1C-NC	-2.06	1.34	1.37
82	Q1	203	PEB	C1C-C2C	2.06	1.47	1.42
82	B5	201	PEB	C1C-C2C	2.06	1.47	1.42
87	62	304	CLA	CMB-C2B	-2.06	1.46	1.50
87	A2	820	CLA	CMD-C2D	-2.06	1.46	1.50
87	b6	610	CLA	CMC-C2C	-2.06	1.46	1.50
87	c6	610	CLA	CMB-C2B	-2.06	1.46	1.50
83	wK	304	PUB	C4C-NC	2.06	1.38	1.35
82	q8	202	PEB	C4A-NA	-2.06	1.33	1.37
82	Y9	201	PEB	C4A-NA	-2.06	1.33	1.37
82	kH	201	PEB	C4A-NA	-2.06	1.33	1.37
84	T3	1001	CYC	C4C-NC	-2.06	1.33	1.37
82	vF	201	PEB	CHC-C4C	2.06	1.52	1.49
84	I4	1001	CYC	C1B-C2B	2.06	1.48	1.45
87	12	604	CLA	CHC-C1C	2.06	1.42	1.38
82	tC	201	PEB	C1D-ND	2.06	1.48	1.45
82	jG	201	PEB	C1D-ND	2.06	1.48	1.45
87	72	604	CLA	MG-ND	-2.06	2.01	2.05
87	M2	101	CLA	O2A-CGA	2.06	1.37	1.30
87	b6	606	CLA	CMC-C2C	-2.06	1.46	1.50
87	1N	602	CLA	CMC-C2C	-2.06	1.46	1.50
87	4N	602	CLA	CMB-C2B	-2.06	1.46	1.50
87	4N	603	CLA	CMB-C2B	-2.06	1.46	1.50
82	iG	202	PEB	C1C-NC	-2.06	1.34	1.37
82	j4	203	PEB	C4A-NA	-2.06	1.33	1.37
84	DH	1003	CYC	C4C-NC	-2.06	1.33	1.37
82	fJ	202	PEB	C2A-C1A	-2.06	1.50	1.52
82	bP	501	PEB	C1C-C2C	2.06	1.47	1.42
84	EE	1001	CYC	C4D-C3D	2.06	1.47	1.42
84	N1	1001	CYC	C4D-C3D	2.06	1.47	1.42
87	BN	808	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	62	302	CLA	CMB-C2B	-2.06	1.46	1.50
82	dB	202	PEB	C4A-NA	-2.06	1.33	1.37
84	G4	1001	CYC	C1B-NB	-2.06	1.34	1.37
82	YO	202	PEB	C1C-C2C	2.06	1.47	1.42
82	mG	202	PEB	C1C-C2C	2.06	1.47	1.42
87	7N	605	CLA	CHC-C1C	2.06	1.42	1.38
87	7N	609	CLA	MG-NB	-2.06	2.01	2.05
87	52	604	CLA	CMB-C2B	-2.06	1.46	1.50
87	1N	604	CLA	CMC-C2C	-2.06	1.46	1.50
92	J6	102	LMG	O7-C8	-2.06	1.41	1.46
84	N4	1001	CYC	C4D-C3D	2.06	1.47	1.42
82	TF	202	PEB	C1D-ND	2.06	1.48	1.45
82	N1	1002	PEB	C1D-ND	2.06	1.48	1.45
82	OJ	201	PEB	C1C-NC	-2.06	1.34	1.37
87	1N	604	CLA	CHC-C1C	2.06	1.42	1.38
82	HA	202	PEB	C2A-C1A	-2.06	1.50	1.52
82	VA	202	PEB	C2A-C1A	-2.06	1.50	1.52
82	w8	204	PEB	C2A-C1A	-2.06	1.50	1.52
82	aJ	203	PEB	C2A-C1A	-2.06	1.50	1.52
82	hJ	203	PEB	C2A-C1A	-2.06	1.50	1.52
82	WH	202	PEB	C1B-C2B	2.06	1.50	1.45
87	LN	206	CLA	MG-ND	-2.06	2.01	2.05
87	32	311	CLA	MG-NB	-2.06	2.01	2.05
87	5N	611	CLA	CMB-C2B	-2.06	1.46	1.50
82	B7	202	PEB	C1A-NA	-2.06	1.34	1.37
87	6N	613	CLA	CHC-C1C	2.06	1.42	1.38
82	ZE	202	PEB	C1B-C2B	2.06	1.50	1.45
82	YQ	201	PEB	C1C-NC	-2.06	1.34	1.37
87	72	610	CLA	CMC-C2C	-2.06	1.46	1.50
82	wF	303	PEB	CHC-C4C	2.06	1.52	1.49
82	Z5	304	PEB	C1B-C2B	2.06	1.50	1.45
82	HF	201	PEB	C4B-C3B	2.06	1.49	1.45
82	kH	202	PEB	C4B-C3B	2.06	1.49	1.45
87	C6	519	CLA	CMB-C2B	-2.06	1.46	1.50
82	eK	203	PEB	C2A-C1A	-2.06	1.50	1.52
87	b6	605	CLA	C3B-C2B	-2.06	1.34	1.41
82	SB	202	PEB	C1C-NC	-2.06	1.34	1.37
84	NO	1001	CYC	C4D-ND	-2.06	1.34	1.37
82	HJ	202	PEB	C1C-C2C	2.06	1.47	1.42
82	XM	202	PEB	C1B-C2B	2.05	1.50	1.45
82	sF	201	PEB	C1B-C2B	2.05	1.50	1.45
87	A2	806	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	lJ	202	PEB	C4B-NB	-2.05	1.34	1.38
87	AL	405	CLA	CMC-C2C	-2.05	1.46	1.50
87	82	302	CLA	CMC-C2C	-2.05	1.46	1.50
82	NF	201	PEB	C1C-C2C	2.05	1.47	1.42
82	GM	202	PEB	C4A-NA	-2.05	1.33	1.37
82	dO	201	PEB	C4A-NA	-2.05	1.33	1.37
84	BG	1002	CYC	C1B-C2B	2.05	1.48	1.45
82	KD	201	PEB	C4B-C3B	2.05	1.49	1.45
82	HM	202	PEB	C4B-C3B	2.05	1.49	1.45
82	A1	301	PEB	C1C-NC	-2.05	1.34	1.37
82	SK	202	PEB	C1B-C2B	2.05	1.50	1.45
82	vC	202	PEB	C1D-ND	2.05	1.48	1.45
82	pK	201	PEB	C1A-NA	-2.05	1.34	1.37
96	f6	101	HEM	C1C-NC	-2.05	1.35	1.39
82	k1	202	PEB	C1C-C2C	2.05	1.47	1.42
87	72	605	CLA	CMB-C2B	-2.05	1.46	1.50
82	PQ	201	PEB	C4A-NA	-2.05	1.33	1.37
82	b4	202	PEB	C4A-NA	-2.05	1.33	1.37
82	mE	203	PEB	C4A-NA	-2.05	1.33	1.37
87	62	301	CLA	MG-NB	-2.05	2.01	2.05
82	QE	203	PEB	C2A-C1A	-2.05	1.50	1.52
82	z8	202	PEB	C2A-C1A	-2.05	1.50	1.52
82	dK	202	PEB	C1B-C2B	2.05	1.50	1.45
87	CL	514	CLA	CHC-C1C	2.05	1.42	1.38
83	AE	303	PUB	C4B-C3B	2.05	1.47	1.42
82	gF	203	PEB	C4B-NB	-2.05	1.34	1.38
87	12	605	CLA	CMD-C2D	-2.05	1.46	1.50
87	52	602	CLA	CMB-C2B	-2.05	1.46	1.50
87	A2	818	CLA	CMC-C2C	-2.05	1.46	1.50
87	B6	606	CLA	CMC-C2C	-2.05	1.46	1.50
82	qC	202	PEB	C4A-NA	-2.05	1.33	1.37
87	22	607	CLA	MG-ND	-2.05	2.01	2.05
87	B2	811	CLA	MG-ND	-2.05	2.01	2.05
87	cL	517	CLA	MG-NB	-2.05	2.01	2.05
82	WA	201	PEB	OD-C4D	2.05	1.27	1.23
82	LP	202	PEB	C1C-C2C	2.05	1.47	1.42
82	e4	201	PEB	C1C-C2C	2.05	1.47	1.42
82	S5	201	PEB	C1C-C2C	2.05	1.47	1.42
82	A4	304	PEB	C1C-NC	-2.05	1.34	1.37
87	52	605	CLA	CHC-C1C	2.05	1.42	1.38
87	62	301	CLA	CHC-C1C	2.05	1.42	1.38
82	eG	201	PEB	C4B-C3B	2.05	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	811	CLA	C3B-C4B	2.05	1.47	1.42
87	KN	105	CLA	CMC-C2C	-2.05	1.46	1.50
87	C6	519	CLA	CMC-C2C	-2.05	1.46	1.50
82	TA	202	PEB	CHA-C4A	-2.05	1.32	1.36
82	WH	201	PEB	C4A-NA	-2.05	1.33	1.37
82	eG	203	PEB	C1D-ND	2.05	1.48	1.45
82	WG	201	PEB	C1C-C2C	2.05	1.47	1.42
82	R7	201	PEB	C1C-C2C	2.05	1.47	1.42
84	K1	1001	CYC	C4D-C3D	2.05	1.47	1.42
82	YB	201	PEB	C4B-NB	-2.05	1.34	1.38
87	A2	821	CLA	CHC-C1C	2.05	1.42	1.38
87	4N	607	CLA	CHC-C1C	2.05	1.42	1.38
87	A2	803	CLA	CMD-C2D	-2.05	1.46	1.50
87	B6	604	CLA	CMC-C2C	-2.05	1.46	1.50
82	AD	301	PEB	C4A-NA	-2.05	1.33	1.37
82	S1	202	PEB	C4A-NA	-2.05	1.33	1.37
82	i4	203	PEB	C4A-NA	-2.05	1.33	1.37
82	sC	201	PEB	C1C-NC	-2.05	1.34	1.37
87	A2	803	CLA	MG-ND	-2.05	2.01	2.05
82	YO	203	PEB	C1C-C2C	2.05	1.47	1.42
87	BN	822	CLA	CHC-C1C	2.05	1.42	1.38
82	T1	202	PEB	C1D-ND	2.05	1.48	1.45
82	X9	201	PEB	C1D-ND	2.05	1.48	1.45
87	AN	839	CLA	CMC-C2C	-2.05	1.46	1.50
87	32	311	CLA	CMC-C2C	-2.05	1.46	1.50
87	42	611	CLA	CMC-C2C	-2.05	1.46	1.50
82	SQ	201	PEB	C4A-NA	-2.05	1.33	1.37
82	bO	202	PEB	C4A-NA	-2.05	1.33	1.37
82	WH	202	PEB	C1C-NC	-2.05	1.34	1.37
82	HQ	203	PEB	C4B-C3B	2.05	1.49	1.45
82	e4	203	PEB	C4B-C3B	2.05	1.49	1.45
87	7N	602	CLA	CMB-C2B	-2.05	1.46	1.50
87	8N	303	CLA	CMC-C2C	-2.05	1.46	1.50
87	3N	301	CLA	CHC-C1C	2.05	1.42	1.38
82	T4	201	PEB	C1C-C2C	2.05	1.47	1.42
82	lG	202	PEB	C1C-C2C	2.05	1.47	1.42
82	RD	201	PEB	C1D-ND	2.05	1.48	1.45
82	aJ	201	PEB	C1D-ND	2.05	1.48	1.45
82	JF	201	PEB	C4B-C3B	2.05	1.49	1.45
82	NG	201	PEB	C4B-C3B	2.05	1.49	1.45
87	AN	833	CLA	CMC-C2C	-2.05	1.46	1.50
82	eF	203	PEB	C4A-NA	-2.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	2N	310	CLA	C4D-ND	-2.05	1.34	1.37
87	32	307	CLA	CMD-C2D	-2.05	1.46	1.50
87	1N	606	CLA	CMB-C2B	-2.05	1.46	1.50
87	5N	604	CLA	CMB-C2B	-2.05	1.46	1.50
96	GN	201	HEM	CMC-C2C	2.05	1.55	1.50
87	CL	512	CLA	CHC-C1C	2.05	1.42	1.38
87	72	601	CLA	CHC-C1C	2.05	1.42	1.38
87	cL	511	CLA	CHC-C1C	2.05	1.42	1.38
82	PD	201	PEB	C4A-NA	-2.05	1.33	1.37
82	FA	201	PEB	C2A-C1A	-2.05	1.50	1.52
82	AE	304	PEB	C2A-C1A	-2.05	1.50	1.52
82	qF	203	PEB	C1B-C2B	2.05	1.50	1.45
87	CL	506	CLA	C1B-NB	-2.05	1.35	1.37
87	A2	839	CLA	CMC-C2C	-2.05	1.46	1.50
87	B2	822	CLA	CMC-C2C	-2.05	1.46	1.50
87	A6	403	CLA	CMC-C2C	-2.05	1.46	1.50
87	bL	618	CLA	CMB-C2B	-2.05	1.46	1.50
82	h4	201	PEB	C1C-C2C	2.05	1.47	1.42
82	WH	202	PEB	C4A-NA	-2.05	1.33	1.37
82	Y4	201	PEB	C4A-NA	-2.05	1.33	1.37
82	f1	201	PEB	C1D-ND	2.05	1.48	1.45
82	C9	201	PEB	C1D-ND	2.05	1.48	1.45
82	eH	203	PEB	C1D-ND	2.05	1.48	1.45
82	e1	202	PEB	CHC-C4C	2.05	1.52	1.49
82	EM	201	PEB	C4B-C3B	2.05	1.49	1.45
83	M9	303	PUB	C1C-NC	-2.05	1.34	1.38
82	SO	201	PEB	C1C-C2C	2.05	1.47	1.42
87	52	601	CLA	CMB-C2B	-2.05	1.46	1.50
96	G2	201	HEM	CMB-C2B	2.05	1.55	1.50
87	32	308	CLA	CHC-C1C	2.05	1.42	1.38
82	XB	201	PEB	C1C-NC	-2.05	1.34	1.37
82	sK	201	PEB	C1B-C2B	2.05	1.50	1.45
82	WE	201	PEB	OD-C4D	2.05	1.27	1.23
82	MM	203	PEB	C4B-C3B	2.05	1.49	1.45
87	H6	103	CLA	CMB-C2B	-2.05	1.46	1.50
87	7N	604	CLA	CMB-C2B	-2.05	1.46	1.50
82	aK	201	PEB	CHC-C4C	2.05	1.52	1.49
82	YI	202	PEB	C1C-NC	-2.05	1.34	1.37
82	ZO	201	PEB	C1C-NC	-2.05	1.34	1.37
84	BG	1001	CYC	C4D-ND	-2.05	1.34	1.37
87	A2	805	CLA	MG-ND	-2.05	2.01	2.05
82	UH	203	PEB	C4A-NA	-2.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	E7	201	PEB	C4A-NA	-2.05	1.33	1.37
87	62	305	CLA	CHC-C1C	2.05	1.42	1.38
82	A5	201	PEB	C1B-C2B	2.05	1.50	1.45
82	B7	201	PEB	C1B-C2B	2.05	1.50	1.45
82	U1	202	PEB	C1C-C2C	2.05	1.47	1.42
82	Y5	202	PEB	C1C-C2C	2.05	1.47	1.42
82	hJ	202	PEB	C1C-C2C	2.05	1.47	1.42
82	VD	202	PEB	C1C-NC	-2.05	1.34	1.37
83	yK	303	PUB	C4B-NB	-2.05	1.34	1.37
87	22	608	CLA	CMC-C2C	-2.05	1.46	1.50
82	IJ	202	PEB	C1B-C2B	2.05	1.50	1.45
87	82	305	CLA	O2D-CGD	2.05	1.38	1.33
82	IJ	203	PEB	C4B-C3B	2.05	1.49	1.45
82	pK	201	PEB	C4B-C3B	2.05	1.49	1.45
82	fO	202	PEB	C4B-C3B	2.05	1.49	1.45
82	YJ	203	PEB	C1C-C2C	2.05	1.47	1.42
82	RO	201	PEB	C1C-C2C	2.05	1.47	1.42
82	Y4	202	PEB	C1C-C2C	2.05	1.47	1.42
82	cE	201	PEB	C1C-C2C	2.05	1.47	1.42
82	mE	202	PEB	C1C-C2C	2.05	1.47	1.42
87	A2	802	CLA	CMD-C2D	-2.05	1.46	1.50
82	lO	202	PEB	C4A-NA	-2.05	1.33	1.37
82	GM	202	PEB	C1C-NC	-2.05	1.34	1.37
87	cL	506	CLA	CHC-C1C	2.05	1.42	1.38
87	1N	601	CLA	CHC-C1C	2.05	1.42	1.38
87	5N	608	CLA	CHC-C1C	2.05	1.42	1.38
82	WF	203	PEB	C1C-C2C	2.05	1.47	1.42
82	RO	202	PEB	C4B-C3B	2.05	1.49	1.45
82	NQ	204	PEB	C4B-C3B	2.05	1.49	1.45
82	lM	203	PEB	C4B-C3B	2.05	1.49	1.45
82	Z1	202	PEB	CHC-C4C	2.05	1.52	1.49
87	cL	517	CLA	CMD-C2D	-2.05	1.46	1.50
87	7N	610	CLA	CMC-C2C	-2.05	1.46	1.50
87	BL	605	CLA	MG-ND	-2.05	2.01	2.05
87	AN	815	CLA	MG-ND	-2.05	2.01	2.05
87	F2	201	CLA	CHC-C1C	2.05	1.42	1.38
82	AB	501	PEB	C1C-C2C	2.05	1.47	1.42
82	r8	201	PEB	C1B-C2B	2.05	1.50	1.45
82	hK	201	PEB	C1B-C2B	2.05	1.50	1.45
84	IO	1001	CYC	C4D-ND	-2.05	1.34	1.37
87	BN	826	CLA	C1B-NB	-2.05	1.35	1.37
83	AG	302	PUB	C1C-NC	-2.05	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	32	311	CLA	CMB-C2B	-2.05	1.46	1.50
87	72	604	CLA	CMD-C2D	-2.05	1.46	1.50
87	d6	401	CLA	CMC-C2C	-2.05	1.46	1.50
82	KB	302	PEB	OD-C4D	2.05	1.27	1.23
82	SE	202	PEB	C4A-NA	-2.05	1.33	1.37
82	sC	201	PEB	C4A-NA	-2.05	1.33	1.37
87	7N	608	CLA	MG-NB	-2.05	2.01	2.05
82	KD	202	PEB	C1C-C2C	2.05	1.47	1.42
82	J5	203	PEB	C1C-C2C	2.05	1.47	1.42
82	bE	201	PEB	C1C-C2C	2.05	1.47	1.42
82	OD	202	PEB	C1B-C2B	2.05	1.50	1.45
82	cK	203	PEB	C4B-NB	-2.05	1.34	1.38
82	w8	204	PEB	CHC-C4C	2.05	1.52	1.49
82	OM	202	PEB	C1C-NC	-2.05	1.34	1.37
87	AN	826	CLA	CMB-C2B	-2.05	1.46	1.50
82	OH	201	PEB	C4A-NA	-2.05	1.33	1.37
82	J1	1002	PEB	C4A-NA	-2.05	1.33	1.37
83	AM	303	PUB	C4B-C3B	2.05	1.47	1.42
82	UD	201	PEB	C1B-C2B	2.05	1.50	1.45
84	CO	1001	CYC	C1B-C2B	2.05	1.48	1.45
87	AN	818	CLA	CMC-C2C	-2.05	1.46	1.50
82	EI	202	PEB	C2A-C1A	-2.05	1.50	1.52
82	YO	203	PEB	C2A-C1A	-2.05	1.50	1.52
82	fG	202	PEB	C1C-NC	-2.05	1.34	1.37
82	kH	202	PEB	C1B-C2B	2.05	1.50	1.45
82	dJ	202	PEB	CHC-C4C	2.05	1.52	1.49
87	BN	805	CLA	C1B-C2B	2.05	1.48	1.43
87	4N	608	CLA	C1B-C2B	2.05	1.48	1.43
87	32	313	CLA	CMD-C2D	-2.05	1.46	1.50
87	D6	405	CLA	CMC-C2C	-2.05	1.46	1.50
87	6N	602	CLA	CMB-C2B	-2.05	1.46	1.50
82	DF	203	PEB	C1C-C2C	2.05	1.47	1.42
82	F1	1002	PEB	C1C-NC	-2.05	1.34	1.37
82	SK	202	PEB	O1C-CGC	2.05	1.28	1.22
85	Z6	101	BCR	C1-C6	-2.05	1.51	1.53
87	BN	830	CLA	CHC-C1C	2.05	1.42	1.38
87	b6	611	CLA	CHC-C1C	2.05	1.42	1.38
87	JN	101	CLA	CMB-C2B	-2.05	1.46	1.50
87	cL	514	CLA	CMB-C2B	-2.05	1.46	1.50
87	2N	310	CLA	CMB-C2B	-2.05	1.46	1.50
96	G2	201	HEM	CMC-C2C	2.05	1.55	1.50
82	YD	201	PEB	C4B-C3B	2.05	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	dE	201	PEB	C4A-NA	-2.05	1.33	1.37
82	HG	1002	PEB	CHC-C4C	2.05	1.52	1.49
82	AG	301	PEB	C2A-C1A	-2.05	1.50	1.52
82	cO	203	PEB	C2A-C1A	-2.05	1.50	1.52
87	42	609	CLA	MG-ND	-2.04	2.01	2.05
84	E4	1001	CYC	C4D-ND	-2.04	1.34	1.37
82	SE	201	PEB	C1C-C2C	2.04	1.47	1.42
87	A2	817	CLA	CMB-C2B	-2.04	1.46	1.50
87	BN	815	CLA	MG-ND	-2.04	2.01	2.05
87	4N	606	CLA	MG-ND	-2.04	2.01	2.05
82	QH	203	PEB	C1C-C2C	2.04	1.47	1.42
82	DJ	201	PEB	C1C-C2C	2.04	1.47	1.42
82	A1	301	PEB	C1C-C2C	2.04	1.47	1.42
82	JP	202	PEB	C1C-NC	-2.04	1.34	1.37
82	l4	201	PEB	C1C-NC	-2.04	1.34	1.37
82	mE	201	PEB	C1C-NC	-2.04	1.34	1.37
87	AN	837	CLA	CMC-C2C	-2.04	1.46	1.50
87	RN	203	CLA	CMB-C2B	-2.04	1.46	1.50
82	GF	202	PEB	CHB-C4B	2.04	1.42	1.38
87	BN	801	CLA	C1B-NB	-2.04	1.35	1.37
82	GA	201	PEB	OD-C4D	2.04	1.27	1.23
82	PI	202	PEB	C2A-C1A	-2.04	1.50	1.52
82	fH	201	PEB	C2A-C1A	-2.04	1.50	1.52
82	cO	202	PEB	C2A-C1A	-2.04	1.50	1.52
82	FD	202	PEB	C4B-C3B	2.04	1.49	1.45
87	bL	606	CLA	C3B-C4B	2.04	1.47	1.42
87	AN	812	CLA	CMC-C2C	-2.04	1.46	1.50
87	B2	812	CLA	CMC-C2C	-2.04	1.46	1.50
82	fE	202	PEB	C1D-ND	2.04	1.48	1.45
82	BA	203	PEB	C1C-C2C	2.04	1.47	1.42
82	OE	201	PEB	C1C-C2C	2.04	1.47	1.42
96	V6	201	HEM	C1A-C2A	-2.04	1.40	1.44
87	KN	103	CLA	MG-ND	-2.04	2.01	2.05
87	B6	609	CLA	CHC-C1C	2.04	1.42	1.38
87	72	602	CLA	CMB-C2B	-2.04	1.46	1.50
87	A2	806	CLA	CMB-C2B	-2.04	1.46	1.50
87	6N	613	CLA	CMB-C2B	-2.04	1.46	1.50
82	FF	202	PEB	C4B-C3B	2.04	1.49	1.45
82	YK	202	PEB	C4A-NA	-2.04	1.33	1.37
82	DM	202	PEB	C1C-NC	-2.04	1.34	1.37
82	UO	202	PEB	C1C-NC	-2.04	1.34	1.37
82	S4	201	PEB	C1C-C2C	2.04	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	L5	203	PEB	C1C-C2C	2.04	1.47	1.42
82	j1	203	PEB	C4B-NB	-2.04	1.34	1.38
84	MG	1001	CYC	C1B-C2B	2.04	1.48	1.45
87	A2	808	CLA	CMC-C2C	-2.04	1.46	1.50
87	c6	608	CLA	CMB-C2B	-2.04	1.46	1.50
82	UG	203	PEB	C2A-C1A	-2.04	1.50	1.52
82	A4	301	PEB	C4A-NA	-2.04	1.33	1.37
82	fM	202	PEB	C4A-NA	-2.04	1.33	1.37
82	YE	201	PEB	C1B-C2B	2.04	1.50	1.45
82	kJ	201	PEB	C4B-C3B	2.04	1.49	1.45
87	7N	601	CLA	CHC-C1C	2.04	1.42	1.38
87	7N	608	CLA	CHC-C1C	2.04	1.42	1.38
82	fH	202	PEB	CHC-C4C	2.04	1.52	1.49
87	B2	829	CLA	CMB-C2B	-2.04	1.46	1.50
87	7N	604	CLA	CMD-C2D	-2.04	1.46	1.50
82	N9	201	PEB	C1D-ND	2.04	1.48	1.45
82	a4	201	PEB	C1B-C2B	2.04	1.50	1.45
82	V1	201	PEB	C4A-NA	-2.04	1.33	1.37
82	fO	202	PEB	C4A-NA	-2.04	1.33	1.37
84	HO	1001	CYC	C4B-NB	-2.04	1.33	1.38
82	FQ	202	PEB	C4B-C3B	2.04	1.49	1.45
83	A1	303	PUB	C4B-NB	-2.04	1.34	1.37
87	A2	820	CLA	CMC-C2C	-2.04	1.46	1.50
87	B6	603	CLA	CMC-C2C	-2.04	1.46	1.50
82	OG	203	PEB	C1C-C2C	2.04	1.47	1.42
82	VP	201	PEB	C1C-C2C	2.04	1.47	1.42
82	BA	201	PEB	C1B-C2B	2.04	1.50	1.45
82	eH	201	PEB	C4A-NA	-2.04	1.33	1.37
82	FQ	202	PEB	C2A-C1A	-2.04	1.50	1.52
82	H1	1002	PEB	C2A-C1A	-2.04	1.50	1.52
82	Z9	304	PEB	C2A-C1A	-2.04	1.50	1.52
82	R9	202	PEB	C1D-ND	2.04	1.48	1.45
87	B6	616	CLA	MG-ND	-2.04	2.01	2.05
87	6N	613	CLA	MG-NB	-2.04	2.01	2.05
87	42	601	CLA	CMC-C2C	-2.04	1.46	1.50
87	72	610	CLA	CMB-C2B	-2.04	1.46	1.50
87	4N	606	CLA	CMB-C2B	-2.04	1.46	1.50
87	5N	604	CLA	CMD-C2D	-2.04	1.46	1.50
82	EK	202	PEB	C4B-C3B	2.04	1.49	1.45
82	YJ	203	PEB	C1C-NC	-2.04	1.34	1.37
83	AH	303	PUB	C4B-NB	-2.04	1.34	1.37
82	f1	202	PEB	C4A-NA	-2.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Y5	203	PEB	C4A-NA	-2.04	1.33	1.37
87	CL	513	CLA	C1D-C2D	2.04	1.49	1.45
82	eG	201	PEB	C1C-C2C	2.04	1.47	1.42
82	iO	202	PEB	C1C-C2C	2.04	1.47	1.42
87	32	302	CLA	CMC-C2C	-2.04	1.46	1.50
87	K2	106	CLA	CMC-C2C	-2.04	1.46	1.50
82	QM	204	PEB	C1D-ND	2.04	1.48	1.45
82	hH	201	PEB	C1D-ND	2.04	1.48	1.45
82	GJ	201	PEB	C1C-NC	-2.04	1.34	1.37
82	J9	201	PEB	C1C-NC	-2.04	1.34	1.37
82	J5	202	PEB	C4B-C3B	2.04	1.49	1.45
82	UD	201	PEB	C1C-C2C	2.04	1.47	1.42
82	UQ	201	PEB	C1C-C2C	2.04	1.47	1.42
82	cH	201	PEB	C1C-C2C	2.04	1.47	1.42
82	I9	201	PEB	C2A-C1A	-2.04	1.50	1.52
82	wC	204	PEB	C2A-C1A	-2.04	1.50	1.52
87	O2	203	CLA	CMC-C2C	-2.04	1.46	1.50
87	5N	601	CLA	CMB-C2B	-2.04	1.46	1.50
87	a6	609	CLA	CHC-C1C	2.04	1.42	1.38
82	SF	203	PEB	C1B-C2B	2.04	1.50	1.45
82	BD	201	PEB	C4A-NA	-2.04	1.33	1.37
82	XQ	202	PEB	C4A-NA	-2.04	1.33	1.37
82	A7	202	PEB	C4A-NA	-2.04	1.33	1.37
82	eH	202	PEB	C1D-ND	2.04	1.48	1.45
82	QE	202	PEB	C1C-NC	-2.04	1.34	1.37
82	qC	203	PEB	C1C-NC	-2.04	1.34	1.37
82	wK	302	PEB	C1C-NC	-2.04	1.34	1.37
82	R1	202	PEB	C1C-C2C	2.04	1.47	1.42
82	e1	202	PEB	C1C-C2C	2.04	1.47	1.42
87	42	604	CLA	CHC-C4B	-2.04	1.34	1.39
87	cL	515	CLA	CMC-C2C	-2.04	1.46	1.50
87	5N	605	CLA	CMB-C2B	-2.04	1.46	1.50
87	AN	802	CLA	MG-NB	-2.04	2.01	2.05
82	DA	203	PEB	C4A-NA	-2.04	1.33	1.37
82	D7	203	PEB	C4A-NA	-2.04	1.33	1.37
87	A2	834	CLA	CAB-C3B	-2.04	1.41	1.47
87	A2	810	CLA	C3D-C4D	2.04	1.48	1.44
87	BN	813	CLA	CMC-C2C	-2.04	1.46	1.50
87	72	606	CLA	CHC-C1C	2.04	1.42	1.38
82	CK	203	PEB	C4B-C3B	2.04	1.49	1.45
82	AG	301	PEB	C4A-NA	-2.04	1.33	1.37
82	JQ	203	PEB	C4A-NA	-2.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	k4	201	PEB	C4A-NA	-2.04	1.33	1.37
82	sF	201	PEB	C4A-NA	-2.04	1.33	1.37
82	hO	202	PEB	C4A-NA	-2.04	1.33	1.37
82	mE	202	PEB	C2A-C1A	-2.04	1.50	1.52
87	A2	822	CLA	C1B-NB	-2.04	1.35	1.37
87	A2	839	CLA	C1B-NB	-2.04	1.35	1.37
87	22	606	CLA	CMB-C2B	-2.04	1.46	1.50
87	42	606	CLA	CMB-C2B	-2.04	1.46	1.50
87	nL	101	CLA	CMB-C2B	-2.04	1.46	1.50
87	2N	304	CLA	CMB-C2B	-2.04	1.46	1.50
87	d6	401	CLA	CHC-C1C	2.04	1.42	1.38
82	wC	201	PEB	C1D-ND	2.04	1.48	1.45
85	B6	621	BCR	C1-C6	-2.04	1.51	1.53
82	B5	202	PEB	C4A-NA	-2.04	1.33	1.37
87	B2	819	CLA	MG-ND	-2.04	2.01	2.05
82	YH	202	PEB	C1C-C2C	2.04	1.47	1.42
82	H9	203	PEB	C1C-C2C	2.04	1.47	1.42
82	HA	202	PEB	C4B-C3B	2.04	1.49	1.45
82	H7	202	PEB	C4B-C3B	2.04	1.49	1.45
87	MN	101	CLA	O2A-CGA	2.04	1.37	1.30
87	62	308	CLA	CMB-C2B	-2.04	1.46	1.50
87	4N	605	CLA	CMB-C2B	-2.04	1.46	1.50
82	VB	201	PEB	C1B-C2B	2.04	1.50	1.45
87	A2	835	CLA	CHC-C1C	2.04	1.42	1.38
82	c1	201	PEB	C1C-C2C	2.04	1.47	1.42
82	rC	202	PEB	C1D-ND	2.04	1.48	1.45
85	H6	101	BCR	C30-C25	-2.04	1.51	1.53
82	YK	203	PEB	C4B-C3B	2.04	1.49	1.45
87	32	312	CLA	CMB-C2B	-2.04	1.46	1.50
87	A2	833	CLA	CMC-C2C	-2.04	1.46	1.50
87	1N	601	CLA	CMD-C2D	-2.04	1.46	1.50
84	EH	1001	CYC	C4A-C3A	2.04	1.50	1.45
96	VL	201	HEM	C3B-C4B	2.04	1.48	1.44
87	6N	606	CLA	CHC-C1C	2.04	1.42	1.38
82	WE	202	PEB	C1C-C2C	2.04	1.47	1.42
82	PF	201	PEB	C1C-C2C	2.04	1.47	1.42
82	EM	203	PEB	C1C-C2C	2.04	1.47	1.42
82	O1	202	PEB	C4A-NA	-2.04	1.33	1.37
82	Y9	202	PEB	C4A-NA	-2.04	1.33	1.37
87	CL	518	CLA	CMC-C2C	-2.04	1.46	1.50
87	4N	607	CLA	CMD-C2D	-2.04	1.46	1.50
82	PK	201	PEB	C1C-C2C	2.04	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	820	CLA	MG-ND	-2.04	2.01	2.05
87	72	606	CLA	MG-ND	-2.04	2.01	2.05
87	b6	608	CLA	MG-ND	-2.04	2.01	2.05
87	6N	607	CLA	MG-NB	-2.04	2.01	2.05
84	FE	1002	CYC	C1B-C2B	2.04	1.48	1.45
87	AN	826	CLA	CMC-C2C	-2.04	1.46	1.50
87	1N	609	CLA	CMC-C2C	-2.04	1.46	1.50
82	DH	1002	PEB	C1B-C2B	2.04	1.50	1.45
82	IM	203	PEB	C1C-NC	-2.04	1.34	1.37
82	AE	301	PEB	C2A-C1A	-2.04	1.50	1.52
82	KI	202	PEB	C2A-C1A	-2.04	1.50	1.52
82	KM	203	PEB	C1C-C2C	2.04	1.47	1.42
82	eG	202	PEB	C4A-NA	-2.04	1.33	1.37
82	KD	202	PEB	C1D-ND	2.04	1.48	1.45
87	AN	829	CLA	MG-ND	-2.04	2.01	2.05
87	62	304	CLA	CMD-C2D	-2.04	1.46	1.50
87	c6	606	CLA	CMB-C2B	-2.04	1.46	1.50
82	Z9	303	PEB	C1C-NC	-2.04	1.34	1.37
87	BL	623	CLA	CHC-C1C	2.04	1.42	1.38
82	UQ	202	PEB	CHC-C4C	2.04	1.52	1.49
87	B2	816	CLA	MG-ND	-2.04	2.01	2.05
82	DQ	203	PEB	C4B-C3B	2.04	1.49	1.45
82	E7	202	PEB	C4B-C3B	2.04	1.49	1.45
82	mG	201	PEB	C1D-ND	2.04	1.48	1.45
87	12	602	CLA	CMC-C2C	-2.04	1.46	1.50
87	c6	613	CLA	CMB-C2B	-2.04	1.46	1.50
87	7N	605	CLA	CMB-C2B	-2.04	1.46	1.50
82	nF	202	PEB	C2A-C1A	-2.04	1.50	1.52
82	uK	202	PEB	C2A-C1A	-2.04	1.50	1.52
82	QB	204	PEB	C1C-NC	-2.04	1.34	1.37
82	q8	203	PEB	C1C-NC	-2.04	1.34	1.37
87	32	312	CLA	MG-ND	-2.04	2.01	2.05
82	KQ	202	PEB	C1C-C2C	2.04	1.47	1.42
82	EP	201	PEB	C1B-C2B	2.04	1.50	1.45
87	6N	601	CLA	CMB-C2B	-2.04	1.46	1.50
82	AP	202	PEB	C4B-C3B	2.04	1.49	1.45
82	PM	201	PEB	C1D-ND	2.04	1.48	1.45
82	P7	202	PEB	C1C-C2C	2.04	1.47	1.42
87	CL	504	CLA	MG-ND	-2.04	2.01	2.05
87	cL	515	CLA	MG-NB	-2.04	2.01	2.05
84	NH	1001	CYC	C4B-NB	-2.04	1.33	1.38
87	B2	826	CLA	C1B-C2B	2.04	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B6	615	CLA	CHC-C1C	2.04	1.42	1.38
82	S9	202	PEB	C4B-C3B	2.04	1.49	1.45
82	RA	201	PEB	C1C-C2C	2.04	1.47	1.42
82	UH	202	PEB	C1C-C2C	2.04	1.47	1.42
82	U1	203	PEB	C1C-C2C	2.04	1.47	1.42
82	DA	201	PEB	C1D-ND	2.03	1.48	1.45
82	Z4	202	PEB	C2A-C1A	-2.03	1.50	1.52
87	BN	823	CLA	CMC-C2C	-2.03	1.46	1.50
87	BN	836	CLA	CMB-C2B	-2.03	1.46	1.50
87	ON	203	CLA	CMC-C2C	-2.03	1.46	1.50
87	L2	202	CLA	CMD-C2D	-2.03	1.46	1.50
87	cL	514	CLA	CMC-C2C	-2.03	1.46	1.50
82	OH	202	PEB	C4A-NA	-2.03	1.33	1.37
82	UI	202	PEB	C4A-NA	-2.03	1.33	1.37
82	UJ	202	PEB	OD-C4D	2.03	1.27	1.23
87	BL	621	CLA	MG-ND	-2.03	2.01	2.05
82	S9	201	PEB	C1B-C2B	2.03	1.50	1.45
87	CL	503	CLA	CMC-C2C	-2.03	1.46	1.50
87	22	612	CLA	CMB-C2B	-2.03	1.46	1.50
87	B2	820	CLA	CMC-C2C	-2.03	1.46	1.50
87	3N	312	CLA	CMB-C2B	-2.03	1.46	1.50
87	4N	603	CLA	CMC-C2C	-2.03	1.46	1.50
82	GK	202	PEB	O1C-CGC	2.03	1.28	1.22
82	I9	201	PEB	C4A-NA	-2.03	1.33	1.37
82	gO	201	PEB	C1C-NC	-2.03	1.34	1.37
82	dE	202	PEB	C1C-C2C	2.03	1.47	1.42
82	l1	203	PEB	C4B-NB	-2.03	1.34	1.38
87	FN	203	CLA	CHC-C1C	2.03	1.42	1.38
87	D6	402	CLA	CHC-C1C	2.03	1.42	1.38
96	VL	201	HEM	C1A-C2A	-2.03	1.40	1.44
87	AN	827	CLA	CMC-C2C	-2.03	1.46	1.50
82	PD	201	PEB	C4B-C3B	2.03	1.48	1.45
82	bH	201	PEB	C4B-C3B	2.03	1.48	1.45
82	tC	201	PEB	C2A-C1A	-2.03	1.50	1.52
82	oF	201	PEB	C1D-ND	2.03	1.48	1.45
82	FI	202	PEB	C1C-NC	-2.03	1.34	1.37
87	dL	402	CLA	CMB-C2B	-2.03	1.46	1.50
87	A2	815	CLA	MG-ND	-2.03	2.01	2.05
87	5N	609	CLA	MG-NB	-2.03	2.01	2.05
82	i1	201	PEB	C4B-C3B	2.03	1.48	1.45
82	cO	202	PEB	C4B-C3B	2.03	1.48	1.45
87	62	307	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B6	607	CLA	CHC-C1C	2.03	1.42	1.38
82	eE	203	PEB	C1B-C2B	2.03	1.50	1.45
82	M9	304	PEB	C1C-NC	-2.03	1.34	1.37
82	gJ	201	PEB	C1D-ND	2.03	1.48	1.45
87	72	606	CLA	CMB-C2B	-2.03	1.46	1.50
82	ZK	202	PEB	C4A-NA	-2.03	1.33	1.37
82	mK	201	PEB	C4A-NA	-2.03	1.33	1.37
82	BA	202	PEB	C1A-NA	-2.03	1.35	1.37
82	JF	201	PEB	C1A-NA	-2.03	1.35	1.37
82	Q7	202	PEB	C2A-C1A	-2.03	1.50	1.52
87	42	603	CLA	C1B-NB	-2.03	1.35	1.37
82	BF	201	PEB	C4B-C3B	2.03	1.48	1.45
82	iH	202	PEB	C4B-C3B	2.03	1.48	1.45
82	Q1	203	PEB	C1B-C2B	2.03	1.50	1.45
87	AN	821	CLA	CMC-C2C	-2.03	1.46	1.50
87	cL	517	CLA	CMB-C2B	-2.03	1.46	1.50
82	wC	204	PEB	C1C-C2C	2.03	1.47	1.42
82	kO	202	PEB	C4A-NA	-2.03	1.33	1.37
82	s8	201	PEB	C1D-ND	2.03	1.48	1.45
82	DE	1002	PEB	CHC-C4C	2.03	1.52	1.49
87	52	608	CLA	CHC-C1C	2.03	1.42	1.38
87	d6	406	CLA	CHC-C1C	2.03	1.42	1.38
87	62	313	CLA	CMC-C2C	-2.03	1.46	1.50
87	8N	304	CLA	CAC-C3C	-2.03	1.45	1.51
82	SM	202	PEB	C4A-NA	-2.03	1.33	1.37
83	AM	304	PUB	C4B-NB	-2.03	1.34	1.37
87	32	311	CLA	CHC-C1C	2.03	1.42	1.38
87	5N	603	CLA	CHC-C1C	2.03	1.42	1.38
82	VD	201	PEB	C1D-ND	2.03	1.48	1.45
82	VQ	201	PEB	C1D-ND	2.03	1.48	1.45
82	O1	201	PEB	C1D-ND	2.03	1.48	1.45
82	A1	305	PEB	C1D-ND	2.03	1.48	1.45
82	X9	202	PEB	C1D-ND	2.03	1.48	1.45
82	V1	203	PEB	CHC-C4C	2.03	1.52	1.49
82	AF	201	PEB	C1C-NC	-2.03	1.34	1.37
82	eK	203	PEB	C1C-NC	-2.03	1.34	1.37
82	cM	202	PEB	C1C-NC	-2.03	1.34	1.37
84	EE	1001	CYC	C4A-C3A	2.03	1.50	1.45
87	42	607	CLA	CMB-C2B	-2.03	1.46	1.50
87	A2	819	CLA	CMB-C2B	-2.03	1.46	1.50
87	d6	403	CLA	CMD-C2D	-2.03	1.46	1.50
82	FF	202	PEB	C1C-C2C	2.03	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	ZE	203	PEB	C1B-C2B	2.03	1.50	1.45
82	QF	202	PEB	C4B-C3B	2.03	1.48	1.45
82	iH	201	PEB	C4B-C3B	2.03	1.48	1.45
82	dM	202	PEB	C4B-C3B	2.03	1.48	1.45
82	S4	202	PEB	C1C-NC	-2.03	1.34	1.37
87	62	303	CLA	CMB-C2B	-2.03	1.46	1.50
87	6N	603	CLA	CMB-C2B	-2.03	1.46	1.50
82	QJ	204	PEB	C2A-C1A	-2.03	1.50	1.52
82	QM	204	PEB	C2A-C1A	-2.03	1.50	1.52
82	SH	201	PEB	CHC-C4C	2.03	1.52	1.49
82	hO	201	PEB	CHC-C4C	2.03	1.52	1.49
82	A4	305	PEB	C4A-NA	-2.03	1.33	1.37
83	Z5	302	PUB	CBB-CAB	2.03	1.58	1.52
87	AN	838	CLA	MG-ND	-2.03	2.01	2.05
87	K2	104	CLA	MG-ND	-2.03	2.01	2.05
84	G4	1001	CYC	C4D-C3D	2.03	1.47	1.42
82	WJ	201	PEB	OD-C4D	2.03	1.27	1.23
82	D7	201	PEB	C1B-C2B	2.03	1.50	1.45
82	mG	201	PEB	C1B-C2B	2.03	1.50	1.45
84	LE	1001	CYC	C4A-C3A	2.03	1.50	1.45
87	BL	620	CLA	CHC-C1C	2.03	1.42	1.38
87	B2	836	CLA	CMB-C2B	-2.03	1.46	1.50
82	mG	201	PEB	C4B-C3B	2.03	1.48	1.45
82	SO	202	PEB	C1C-NC	-2.03	1.34	1.37
82	Y1	202	PEB	C1C-NC	-2.03	1.34	1.37
82	Q4	201	PEB	C1C-NC	-2.03	1.34	1.37
82	RE	202	PEB	C1C-C2C	2.03	1.47	1.42
84	FE	1002	CYC	C4B-NB	-2.03	1.33	1.38
87	DL	406	CLA	CHC-C1C	2.03	1.42	1.38
87	A2	808	CLA	CHC-C1C	2.03	1.42	1.38
87	B2	821	CLA	CHC-C1C	2.03	1.42	1.38
82	T9	201	PEB	C1D-ND	2.03	1.48	1.45
82	sK	201	PEB	C4A-NA	-2.03	1.33	1.37
82	C9	201	PEB	C4B-C3B	2.03	1.48	1.45
87	BL	601	CLA	C1B-NB	-2.03	1.35	1.37
82	T5	202	PEB	C2A-C1A	-2.03	1.50	1.52
82	N9	201	PEB	C2A-C1A	-2.03	1.50	1.52
82	MF	203	PEB	C1B-C2B	2.03	1.50	1.45
87	AN	821	CLA	CHC-C1C	2.03	1.42	1.38
87	12	601	CLA	CHC-C1C	2.03	1.42	1.38
87	A2	841	CLA	C1B-C2B	2.03	1.48	1.43
84	MO	1001	CYC	C4D-C3D	2.03	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AA	202	PEB	C4A-NA	-2.03	1.33	1.37
82	c4	203	PEB	C4A-NA	-2.03	1.33	1.37
82	NQ	202	PEB	C1D-ND	2.03	1.48	1.45
87	BN	817	CLA	MG-ND	-2.03	2.01	2.05
82	oK	202	PEB	C1C-NC	-2.03	1.34	1.37
82	jE	202	PEB	C4B-C3B	2.03	1.48	1.45
82	cM	202	PEB	C4B-C3B	2.03	1.48	1.45
82	WF	203	PEB	CHC-C4C	2.03	1.52	1.49
87	BN	824	CLA	CHC-C1C	2.03	1.42	1.38
82	HG	1002	PEB	C1C-C2C	2.03	1.47	1.42
87	AN	831	CLA	CHC-C4B	-2.03	1.34	1.39
82	SJ	202	PEB	C4A-NA	-2.03	1.33	1.37
82	OK	203	PEB	C4A-NA	-2.03	1.33	1.37
87	B2	820	CLA	C2A-C1A	2.03	1.56	1.52
87	AN	836	CLA	CMC-C2C	-2.03	1.46	1.50
87	42	607	CLA	CMD-C2D	-2.03	1.46	1.50
87	B2	815	CLA	CMB-C2B	-2.03	1.46	1.50
83	yF	303	PUB	C4B-NB	-2.03	1.34	1.37
82	CB	202	PEB	C1C-C2C	2.03	1.47	1.42
82	L5	201	PEB	C1C-C2C	2.03	1.47	1.42
82	UH	202	PEB	C2A-C1A	-2.03	1.50	1.52
82	XI	201	PEB	C2A-C1A	-2.03	1.50	1.52
82	DD	203	PEB	C4B-C3B	2.03	1.48	1.45
84	DE	1001	CYC	C1A-C2A	2.03	1.48	1.45
82	h1	201	PEB	C4A-NA	-2.03	1.33	1.37
82	SF	202	PEB	C1B-C2B	2.03	1.50	1.45
82	E5	201	PEB	C1B-C2B	2.03	1.50	1.45
82	PJ	201	PEB	CHC-C4C	2.03	1.52	1.49
87	12	606	CLA	CMB-C2B	-2.03	1.46	1.50
87	BL	604	CLA	CHC-C1C	2.03	1.42	1.38
82	EA	201	PEB	C4A-NA	-2.03	1.33	1.37
82	RD	202	PEB	C4A-NA	-2.03	1.33	1.37
82	XQ	201	PEB	C4A-NA	-2.03	1.33	1.37
82	mM	202	PEB	C4B-C3B	2.03	1.48	1.45
82	V1	203	PEB	C1B-C2B	2.03	1.50	1.45
87	6N	607	CLA	CMB-C2B	-2.03	1.46	1.50
82	S1	201	PEB	C4B-NB	-2.03	1.34	1.38
82	H9	203	PEB	C4A-NA	-2.03	1.33	1.37
82	lF	203	PEB	C4A-NA	-2.03	1.33	1.37
82	I7	201	PEB	CHC-C4C	2.03	1.52	1.49
82	mH	201	PEB	C4B-C3B	2.03	1.48	1.45
87	1N	605	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WD	201	PEB	C4A-NA	-2.03	1.33	1.37
82	Q9	203	PEB	C4A-NA	-2.03	1.33	1.37
82	J9	203	PEB	C1B-C2B	2.03	1.50	1.45
82	dF	202	PEB	C1B-C2B	2.03	1.50	1.45
82	l4	201	PEB	CHA-C4A	-2.03	1.32	1.36
82	OD	202	PEB	C1C-NC	-2.03	1.34	1.37
87	12	604	CLA	CMB-C2B	-2.03	1.46	1.50
82	KQ	202	PEB	C1D-ND	2.03	1.48	1.45
84	GE	1001	CYC	C1B-C2B	2.03	1.48	1.45
87	bL	622	CLA	CHC-C1C	2.03	1.42	1.38
87	B2	833	CLA	C1B-NB	-2.03	1.35	1.37
84	LE	1001	CYC	C1A-NA	-2.03	1.34	1.38
82	uC	202	PEB	C4A-NA	-2.03	1.33	1.37
82	WG	203	PEB	C2A-C1A	-2.03	1.50	1.52
82	lM	203	PEB	C2A-C1A	-2.03	1.50	1.52
87	BN	801	CLA	CMB-C2B	-2.03	1.46	1.50
82	KA	202	PEB	C1C-NC	-2.03	1.34	1.37
82	PO	203	PEB	C1C-NC	-2.03	1.34	1.37
87	cL	506	CLA	C1B-C2B	2.03	1.48	1.43
95	b6	622	DGD	O5D-C1E	2.03	1.43	1.40
82	SH	201	PEB	C4B-NB	-2.03	1.34	1.38
82	gH	203	PEB	C4A-NA	-2.03	1.33	1.37
82	dH	203	PEB	C4A-NA	-2.03	1.33	1.37
82	ZM	202	PEB	C4B-C3B	2.03	1.48	1.45
82	jG	202	PEB	C4B-C3B	2.03	1.48	1.45
82	wF	301	PEB	C1C-C2C	2.03	1.47	1.42
82	YK	203	PEB	C1B-C2B	2.03	1.50	1.45
87	DL	403	CLA	CMC-C2C	-2.03	1.46	1.50
87	B2	817	CLA	CMC-C2C	-2.03	1.46	1.50
87	F2	201	CLA	CMB-C2B	-2.03	1.46	1.50
87	a6	609	CLA	CMC-C2C	-2.03	1.46	1.50
87	AN	822	CLA	C1B-NB	-2.03	1.35	1.37
82	OI	201	PEB	O1B-CGB	2.03	1.28	1.22
82	nK	201	PEB	CHC-C4C	2.03	1.52	1.49
82	LE	1002	PEB	C1C-C2C	2.03	1.47	1.42
82	YB	201	PEB	C1C-NC	-2.03	1.34	1.37
82	KJ	202	PEB	C1C-NC	-2.03	1.34	1.37
82	lG	203	PEB	C1C-NC	-2.03	1.34	1.37
82	iO	201	PEB	C1C-NC	-2.03	1.34	1.37
85	H6	101	BCR	C1-C6	-2.03	1.51	1.53
82	m4	201	PEB	C1B-C2B	2.03	1.50	1.45
82	AI	202	PEB	C4B-C3B	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	l1	201	PEB	C4B-C3B	2.03	1.48	1.45
87	BN	818	CLA	CMC-C2C	-2.02	1.46	1.50
87	A2	827	CLA	CMC-C2C	-2.02	1.46	1.50
87	2N	309	CLA	C1B-C2B	2.02	1.48	1.43
87	bL	608	CLA	MG-NB	-2.02	2.01	2.05
82	DB	202	PEB	C1C-C2C	2.02	1.47	1.42
82	WG	202	PEB	C1C-C2C	2.02	1.47	1.42
82	YQ	201	PEB	C4A-NA	-2.02	1.33	1.37
82	cG	201	PEB	C1C-NC	-2.02	1.34	1.37
84	JH	1003	CYC	C4D-ND	-2.02	1.34	1.37
87	AN	819	CLA	CMB-C2B	-2.02	1.46	1.50
87	1N	611	CLA	CMB-C2B	-2.02	1.46	1.50
82	D9	202	PEB	CHC-C4C	2.02	1.52	1.49
85	B6	601	BCR	C30-C25	-2.02	1.51	1.53
82	YM	203	PEB	C4B-C3B	2.02	1.48	1.45
82	kG	202	PEB	C4B-C3B	2.02	1.48	1.45
82	NB	202	PEB	C1C-C2C	2.02	1.47	1.42
87	52	608	CLA	MG-ND	-2.02	2.01	2.05
82	E9	202	PEB	C1D-ND	2.02	1.48	1.45
87	A2	838	CLA	CHC-C1C	2.02	1.42	1.38
82	AO	305	PEB	C4A-NA	-2.02	1.33	1.37
82	V9	201	PEB	C4A-NA	-2.02	1.33	1.37
87	4N	611	CLA	CMB-C2B	-2.02	1.46	1.50
87	8N	307	CLA	CMC-C2C	-2.02	1.46	1.50
82	J7	201	PEB	C1C-C2C	2.02	1.47	1.42
87	7N	605	CLA	MG-NB	-2.02	2.01	2.05
82	MQ	202	PEB	C4A-NA	-2.02	1.33	1.37
82	IK	201	PEB	CBC-CGC	2.02	1.55	1.50
82	ZG	203	PEB	C1B-C2B	2.02	1.50	1.45
82	Q1	201	PEB	C2A-C1A	-2.02	1.50	1.52
82	JQ	202	PEB	CHC-C4C	2.02	1.52	1.49
82	gB	202	PEB	C1C-C2C	2.02	1.47	1.42
87	82	301	CLA	CMB-C2B	-2.02	1.46	1.50
87	B2	828	CLA	MG-ND	-2.02	2.01	2.05
87	1N	606	CLA	MG-ND	-2.02	2.01	2.05
82	LQ	201	PEB	C4A-NA	-2.02	1.33	1.37
82	R4	201	PEB	C1B-C2B	2.02	1.50	1.45
82	dE	203	PEB	C4B-C3B	2.02	1.48	1.45
82	WB	401	PEB	C1C-C2C	2.02	1.47	1.42
87	62	307	CLA	CMB-C2B	-2.02	1.46	1.50
87	cL	509	CLA	CMB-C2B	-2.02	1.46	1.50
82	JA	202	PEB	CHC-C4C	2.02	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	AL	413	PL9	C2-C1	-2.02	1.39	1.44
82	s8	203	PEB	C2A-C1A	-2.02	1.50	1.52
87	BN	826	CLA	CMC-C2C	-2.02	1.46	1.50
87	42	601	CLA	CMD-C2D	-2.02	1.46	1.50
87	7N	610	CLA	CMB-C2B	-2.02	1.46	1.50
82	gJ	202	PEB	C4B-C3B	2.02	1.48	1.45
82	j1	203	PEB	C4A-NA	-2.02	1.33	1.37
82	AM	301	PEB	C1D-ND	2.02	1.48	1.45
82	P1	202	PEB	C1C-C2C	2.02	1.47	1.42
82	aJ	202	PEB	C1C-NC	-2.02	1.34	1.37
84	EH	1001	CYC	C4D-ND	-2.02	1.34	1.37
87	CL	511	CLA	C4B-NB	2.02	1.40	1.37
87	B2	825	CLA	C1B-NB	-2.02	1.35	1.37
87	12	611	CLA	CMB-C2B	-2.02	1.46	1.50
87	32	312	CLA	CMC-C2C	-2.02	1.46	1.50
82	lH	201	PEB	C4A-NA	-2.02	1.33	1.37
82	DF	203	PEB	CHC-C4C	2.02	1.52	1.49
82	DK	203	PEB	CHC-C4C	2.02	1.52	1.49
82	GA	201	PEB	C1C-C2C	2.02	1.47	1.42
82	GJ	203	PEB	C1C-C2C	2.02	1.47	1.42
87	cL	515	CLA	CHC-C1C	2.02	1.42	1.38
82	IB	203	PEB	C1C-NC	-2.02	1.34	1.37
82	QQ	202	PEB	C1D-ND	2.02	1.48	1.45
82	I9	202	PEB	C1D-ND	2.02	1.48	1.45
87	ON	202	CLA	CMB-C2B	-2.02	1.46	1.50
87	c6	609	CLA	CMC-C2C	-2.02	1.46	1.50
82	g4	202	PEB	C2A-C1A	-2.02	1.50	1.52
87	2N	311	CLA	CMB-C2B	-2.02	1.46	1.50
87	6N	613	CLA	CMD-C2D	-2.02	1.46	1.50
82	QI	201	PEB	C1C-NC	-2.02	1.34	1.37
82	RQ	202	PEB	CHC-C4C	2.02	1.52	1.49
82	hF	202	PEB	C4A-NA	-2.02	1.33	1.37
82	hK	202	PEB	C4A-NA	-2.02	1.33	1.37
82	zK	501	PEB	C4A-NA	-2.02	1.33	1.37
87	52	609	CLA	CMD-C2D	-2.02	1.46	1.50
87	B6	607	CLA	CMC-C2C	-2.02	1.46	1.50
82	I9	201	PEB	C4B-C3B	2.02	1.48	1.45
82	SD	202	PEB	C1B-C2B	2.02	1.50	1.45
82	k1	202	PEB	C1B-C2B	2.02	1.50	1.45
84	I4	1001	CYC	C4D-ND	-2.02	1.34	1.37
82	Q1	203	PEB	C4A-NA	-2.02	1.33	1.37
82	dE	201	PEB	C2A-C1A	-2.02	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	BN	828	CLA	MG-ND	-2.02	2.01	2.05
82	TM	201	PEB	C1D-ND	2.02	1.48	1.45
82	OO	201	PEB	CHA-C4A	-2.02	1.32	1.36
82	IQ	201	PEB	C4B-C3B	2.02	1.48	1.45
87	5N	610	CLA	CMB-C2B	-2.02	1.46	1.50
87	6N	610	CLA	CMB-C2B	-2.02	1.46	1.50
82	eH	202	PEB	C1C-C2C	2.02	1.47	1.42
87	AN	850	CLA	C1B-NB	-2.02	1.35	1.37
82	IK	203	PEB	C4B-NB	-2.02	1.34	1.38
82	FM	202	PEB	C1B-C2B	2.02	1.50	1.45
82	OI	202	PEB	C2C-C3C	2.02	1.44	1.38
87	72	609	CLA	CHC-C1C	2.02	1.42	1.38
87	6N	610	CLA	CHC-C1C	2.02	1.42	1.38
87	2N	311	CLA	MG-NB	-2.02	2.01	2.05
87	L2	206	CLA	CMC-C2C	-2.02	1.46	1.50
82	U4	202	PEB	C1C-NC	-2.02	1.34	1.37
82	aJ	201	PEB	C1C-NC	-2.02	1.34	1.37
82	GI	203	PEB	C2A-C1A	-2.02	1.50	1.52
82	lE	203	PEB	C2A-C1A	-2.02	1.50	1.52
82	gG	202	PEB	C2A-C1A	-2.02	1.50	1.52
82	dH	203	PEB	C2A-C1A	-2.02	1.50	1.52
82	K7	201	PEB	C1B-C2B	2.02	1.50	1.45
82	A1	302	PEB	C1D-ND	2.02	1.48	1.45
87	72	603	CLA	CHC-C1C	2.02	1.42	1.38
82	e1	201	PEB	C4B-C3B	2.02	1.48	1.45
82	JD	201	PEB	C4A-NA	-2.02	1.33	1.37
82	H1	1002	PEB	CHC-C4C	2.02	1.52	1.49
82	bF	202	PEB	C1C-C2C	2.02	1.47	1.42
87	CL	518	CLA	CHC-C1C	2.02	1.42	1.38
82	GD	202	PEB	C2A-C1A	-2.02	1.50	1.52
84	M1	201	CYC	C4D-ND	-2.02	1.34	1.37
87	82	307	CLA	CHC-C1C	2.02	1.42	1.38
87	22	611	CLA	MG-NB	-2.02	2.01	2.05
82	cO	203	PEB	C4A-NA	-2.02	1.33	1.37
84	JH	1003	CYC	C4B-NB	-2.02	1.33	1.38
82	DM	201	PEB	C1C-C2C	2.02	1.47	1.42
82	wF	301	PEB	C1C-NC	-2.02	1.34	1.37
87	dL	401	CLA	CAC-C3C	-2.02	1.45	1.51
87	AN	817	CLA	CMB-C2B	-2.02	1.46	1.50
87	22	611	CLA	CMB-C2B	-2.02	1.46	1.50
87	AN	801	CLA	CHC-C1C	2.02	1.42	1.38
87	12	608	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	CI	201	PEB	C2A-C1A	-2.02	1.50	1.52
82	t8	201	PEB	C2A-C1A	-2.02	1.50	1.52
82	U1	202	PEB	C4B-C3B	2.02	1.48	1.45
82	eM	202	PEB	C4B-C3B	2.02	1.48	1.45
87	B2	806	CLA	MG-ND	-2.02	2.01	2.05
82	NK	201	PEB	C1C-C2C	2.02	1.47	1.42
82	S1	201	PEB	CHC-C4C	2.02	1.52	1.49
82	T9	201	PEB	C4A-NA	-2.02	1.33	1.37
87	AN	808	CLA	CHC-C1C	2.02	1.42	1.38
87	42	607	CLA	CHC-C1C	2.02	1.42	1.38
87	1N	608	CLA	CHC-C1C	2.02	1.42	1.38
82	Z5	301	PEB	C1B-C2B	2.02	1.50	1.45
82	K9	201	PEB	C1D-ND	2.02	1.48	1.45
82	ZB	202	PEB	C1C-C2C	2.02	1.47	1.42
87	6N	610	CLA	MG-NB	-2.02	2.01	2.05
82	AM	301	PEB	C4B-C3B	2.02	1.48	1.45
82	CP	203	PEB	C4B-C3B	2.02	1.48	1.45
87	HL	101	CLA	CMC-C2C	-2.02	1.46	1.50
87	LN	202	CLA	CMD-C2D	-2.02	1.46	1.50
82	M7	202	PEB	C2A-C1A	-2.02	1.50	1.52
82	WK	201	PEB	C4B-NB	-2.02	1.34	1.38
82	lF	202	PEB	C4A-NA	-2.02	1.33	1.37
82	YK	203	PEB	C1D-ND	2.02	1.48	1.45
82	j1	203	PEB	C1D-ND	2.02	1.48	1.45
82	A9	201	PEB	C1D-ND	2.02	1.48	1.45
82	HD	201	PEB	C4B-C3B	2.02	1.48	1.45
82	WF	201	PEB	C4B-C3B	2.02	1.48	1.45
96	vL	201	HEM	C3B-C4B	2.02	1.48	1.44
87	B2	804	CLA	C1B-C2B	2.02	1.48	1.43
87	1N	604	CLA	CMB-C2B	-2.02	1.46	1.50
87	8N	306	CLA	CMC-C2C	-2.02	1.46	1.50
82	pF	202	PEB	C1C-C2C	2.02	1.47	1.42
82	GP	203	PEB	C4A-NA	-2.02	1.33	1.37
82	NQ	204	PEB	C4A-NA	-2.02	1.33	1.37
82	N9	201	PEB	C4A-NA	-2.02	1.33	1.37
82	RQ	202	PEB	C4B-C3B	2.01	1.48	1.45
82	hG	203	PEB	C2A-C1A	-2.01	1.50	1.52
82	O5	202	PEB	C1C-C2C	2.01	1.47	1.42
87	B6	614	CLA	CMC-C2C	-2.01	1.46	1.50
87	AN	806	CLA	CHC-C1C	2.01	1.42	1.38
82	P9	201	PEB	C1D-ND	2.01	1.48	1.45
82	QH	201	PEB	C4A-NA	-2.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S9	202	PEB	C4A-NA	-2.01	1.33	1.37
82	dG	201	PEB	C4A-NA	-2.01	1.33	1.37
82	jG	202	PEB	C4A-NA	-2.01	1.33	1.37
82	kO	201	PEB	C4A-NA	-2.01	1.33	1.37
82	NE	202	PEB	CHC-C4C	2.01	1.52	1.49
87	R2	204	CLA	CMC-C2C	-2.01	1.46	1.50
87	cL	506	CLA	C1B-NB	-2.01	1.35	1.37
87	7N	610	CLA	CHC-C1C	2.01	1.42	1.38
82	zK	501	PEB	C1C-NC	-2.01	1.34	1.37
82	pK	202	PEB	C1C-C2C	2.01	1.47	1.42
82	JD	202	PEB	C4B-C3B	2.01	1.48	1.45
82	UH	202	PEB	C4B-C3B	2.01	1.48	1.45
82	RI	202	PEB	C2A-C1A	-2.01	1.50	1.52
82	z8	202	PEB	C4A-NA	-2.01	1.33	1.37
82	PP	202	PEB	C1C-C2C	2.01	1.47	1.42
87	12	607	CLA	CMB-C2B	-2.01	1.46	1.50
87	42	605	CLA	CMB-C2B	-2.01	1.46	1.50
82	I9	201	PEB	C1D-ND	2.01	1.48	1.45
82	FQ	202	PEB	C4A-NA	-2.01	1.33	1.37
82	t8	201	PEB	C4A-NA	-2.01	1.33	1.37
82	P9	201	PEB	C4A-NA	-2.01	1.33	1.37
82	mE	202	PEB	C4A-NA	-2.01	1.33	1.37
87	BN	807	CLA	MG-ND	-2.01	2.01	2.05
82	GF	202	PEB	O1C-CGC	2.01	1.28	1.22
82	kF	202	PEB	C2A-C1A	-2.01	1.50	1.52
82	MF	203	PEB	C4B-C3B	2.01	1.48	1.45
82	hG	201	PEB	C4A-NA	-2.01	1.33	1.37
87	4N	603	CLA	C1B-NB	-2.01	1.35	1.37
82	AD	303	PEB	C1D-ND	2.01	1.48	1.45
82	jH	203	PEB	C1D-ND	2.01	1.48	1.45
87	B2	835	CLA	CMC-C2C	-2.01	1.46	1.50
87	8N	302	CLA	CMB-C2B	-2.01	1.46	1.50
82	SQ	202	PEB	C1B-C2B	2.01	1.50	1.45
82	UQ	201	PEB	C1B-C2B	2.01	1.50	1.45
84	HH	1001	CYC	C4A-C3A	2.01	1.50	1.45
82	H5	201	PEB	CMD-C2D	2.01	1.53	1.50
82	Y1	201	PEB	C1C-NC	-2.01	1.34	1.37
82	wK	301	PEB	C1C-NC	-2.01	1.34	1.37
87	AN	838	CLA	CHC-C1C	2.01	1.42	1.38
87	L2	206	CLA	MG-ND	-2.01	2.01	2.05
87	62	302	CLA	CMD-C2D	-2.01	1.46	1.50
87	O2	202	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	jM	201	PEB	C1C-C2C	2.01	1.47	1.42
82	vK	202	PEB	C4A-NA	-2.01	1.33	1.37
82	UO	202	PEB	C2A-C1A	-2.01	1.50	1.52
82	Y4	203	PEB	C2A-C1A	-2.01	1.50	1.52
87	12	605	CLA	CMB-C2B	-2.01	1.46	1.50
87	c6	613	CLA	CMC-C2C	-2.01	1.46	1.50
87	AN	803	CLA	MG-ND	-2.01	2.01	2.05
82	VH	201	PEB	C4B-C3B	2.01	1.48	1.45
82	UP	201	PEB	C4B-C3B	2.01	1.48	1.45
82	dH	201	PEB	C1C-C2C	2.01	1.47	1.42
87	C6	513	CLA	CHC-C1C	2.01	1.42	1.38
82	G9	202	PEB	C1D-ND	2.01	1.48	1.45
82	fH	201	PEB	C1D-ND	2.01	1.48	1.45
82	aK	201	PEB	C1D-ND	2.01	1.48	1.45
82	BQ	201	PEB	C4A-NA	-2.01	1.33	1.37
84	DH	1001	CYC	C4B-NB	-2.01	1.33	1.38
82	HA	203	PEB	C1C-NC	-2.01	1.34	1.37
82	TM	202	PEB	C1C-NC	-2.01	1.34	1.37
82	jJ	202	PEB	C1C-NC	-2.01	1.34	1.37
87	AN	809	CLA	CMC-C2C	-2.01	1.46	1.50
87	7N	609	CLA	CMB-C2B	-2.01	1.46	1.50
96	G2	201	HEM	CMA-C3A	2.01	1.55	1.50
82	fE	202	PEB	C1B-C2B	2.01	1.50	1.45
87	BN	833	CLA	C1B-NB	-2.01	1.35	1.37
82	Z5	305	PEB	C4B-C3B	2.01	1.48	1.45
82	aE	202	PEB	C4B-C3B	2.01	1.48	1.45
82	mO	203	PEB	O1B-CGB	2.01	1.28	1.22
82	bG	201	PEB	C1C-C2C	2.01	1.47	1.42
87	12	609	CLA	CMC-C2C	-2.01	1.46	1.50
87	B2	825	CLA	CMB-C2B	-2.01	1.46	1.50
96	GN	201	HEM	CMA-C3A	2.01	1.55	1.50
82	i4	201	PEB	C1C-NC	-2.01	1.34	1.37
84	EO	1001	CYC	C4A-C3A	2.01	1.50	1.45
84	H4	1001	CYC	C4A-C3A	2.01	1.50	1.45
87	52	601	CLA	MG-ND	-2.01	2.01	2.05
82	j1	202	PEB	C4A-NA	-2.01	1.33	1.37
82	SM	202	PEB	C4B-C3B	2.01	1.48	1.45
82	S5	202	PEB	C1C-C2C	2.01	1.47	1.42
84	MG	1001	CYC	C4D-C3D	2.01	1.47	1.42
85	b6	601	BCR	C1-C6	-2.01	1.51	1.53
87	72	609	CLA	CMB-C2B	-2.01	1.46	1.50
82	D1	1002	PEB	C1B-C2B	2.01	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	fG	202	PEB	C1B-C2B	2.01	1.50	1.45
82	SK	201	PEB	C4B-NB	-2.01	1.34	1.38
82	lK	202	PEB	C1D-ND	2.01	1.48	1.45
87	RN	204	CLA	CHC-C1C	2.01	1.42	1.38
87	B2	823	CLA	CHC-C1C	2.01	1.42	1.38
87	B2	830	CLA	CHC-C1C	2.01	1.42	1.38
87	aL	606	CLA	CHC-C1C	2.01	1.42	1.38
82	FD	201	PEB	C1C-C2C	2.01	1.47	1.42
87	DL	406	CLA	CMC-C2C	-2.01	1.46	1.50
87	12	601	CLA	CMD-C2D	-2.01	1.46	1.50
87	82	307	CLA	CMC-C2C	-2.01	1.46	1.50
87	A2	811	CLA	CMC-C2C	-2.01	1.46	1.50
82	HK	201	PEB	C4B-C3B	2.01	1.48	1.45
82	JK	202	PEB	C4B-C3B	2.01	1.48	1.45
82	RK	202	PEB	C4B-C3B	2.01	1.48	1.45
82	M5	305	PEB	C4B-C3B	2.01	1.48	1.45
82	A9	201	PEB	C4B-C3B	2.01	1.48	1.45
87	JN	101	CLA	MG-ND	-2.01	2.01	2.05
87	62	308	CLA	MG-NB	-2.01	2.01	2.05
82	QA	202	PEB	C2A-C1A	-2.01	1.50	1.52
82	X9	201	PEB	C2A-C1A	-2.01	1.50	1.52
82	tK	203	PEB	C2A-C1A	-2.01	1.50	1.52
87	CL	507	CLA	C1B-NB	-2.01	1.35	1.37
82	KE	201	PEB	C1C-NC	-2.01	1.34	1.37
82	E9	201	PEB	C4A-NA	-2.01	1.33	1.37
82	eO	201	PEB	C1C-C2C	2.01	1.47	1.42
87	B2	818	CLA	CHC-C1C	2.01	1.42	1.38
82	OM	202	PEB	C1D-ND	2.01	1.48	1.45
82	g4	201	PEB	C1D-ND	2.01	1.48	1.45
87	AN	811	CLA	CMC-C2C	-2.01	1.46	1.50
87	52	606	CLA	CMB-C2B	-2.01	1.46	1.50
87	6N	602	CLA	CMD-C2D	-2.01	1.46	1.50
87	7N	609	CLA	CMD-C2D	-2.01	1.46	1.50
87	bL	607	CLA	MG-ND	-2.01	2.01	2.05
82	KA	201	PEB	C4B-C3B	2.01	1.48	1.45
82	O5	201	PEB	C4B-C3B	2.01	1.48	1.45
82	AQ	301	PEB	C4A-NA	-2.01	1.33	1.37
82	BQ	202	PEB	C4A-NA	-2.01	1.33	1.37
82	C9	201	PEB	C4A-NA	-2.01	1.33	1.37
82	sC	203	PEB	C4A-NA	-2.01	1.33	1.37
87	22	610	CLA	C4D-ND	-2.01	1.34	1.37
82	MB	202	PEB	C1C-NC	-2.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PP	202	PEB	C1C-NC	-2.01	1.34	1.37
82	g4	201	PEB	C1C-NC	-2.01	1.34	1.37
82	fE	202	PEB	C1C-NC	-2.01	1.34	1.37
87	BN	807	CLA	CHC-C1C	2.01	1.42	1.38
87	c6	612	CLA	CHC-C1C	2.01	1.42	1.38
82	XJ	202	PEB	C1B-C2B	2.01	1.50	1.45
87	52	605	CLA	CMB-C2B	-2.01	1.46	1.50
87	C6	513	CLA	CMC-C2C	-2.01	1.46	1.50
87	BL	604	CLA	MG-ND	-2.01	2.01	2.05
82	EP	202	PEB	C4A-NA	-2.01	1.33	1.37
82	xK	303	PEB	C4A-NA	-2.01	1.33	1.37
87	aL	605	CLA	CHC-C1C	2.01	1.42	1.38
82	A1	302	PEB	C2A-C1A	-2.01	1.50	1.52
82	hM	201	PEB	C2A-C1A	-2.01	1.50	1.52
87	c6	614	CLA	CMB-C2B	-2.01	1.46	1.50
87	6N	606	CLA	CMB-C2B	-2.01	1.46	1.50
82	OE	203	PEB	C1C-C2C	2.01	1.47	1.42
82	GP	202	PEB	C1C-C2C	2.01	1.47	1.42
82	kF	201	PEB	C1C-C2C	2.01	1.47	1.42
87	AN	841	CLA	C1B-C2B	2.01	1.48	1.43
87	A6	404	CLA	CHC-C1C	2.01	1.42	1.38
82	ZM	202	PEB	C1B-C2B	2.01	1.50	1.45
82	dG	203	PEB	C1B-C2B	2.01	1.50	1.45
82	fB	301	PEB	O1B-CGB	2.01	1.28	1.22
87	BN	812	CLA	CMC-C2C	-2.01	1.46	1.50
87	A2	809	CLA	CMC-C2C	-2.01	1.46	1.50
87	6N	612	CLA	CMC-C2C	-2.01	1.46	1.50
82	EF	202	PEB	C4B-C3B	2.01	1.48	1.45
82	KI	203	PEB	C4B-C3B	2.01	1.48	1.45
82	PI	202	PEB	C4B-C3B	2.01	1.48	1.45
82	T7	202	PEB	CHA-C4A	-2.01	1.32	1.36
82	UA	202	PEB	C1C-C2C	2.01	1.47	1.42
82	FO	1002	PEB	C1C-C2C	2.01	1.47	1.42
82	eE	201	PEB	C1C-C2C	2.01	1.47	1.42
82	m1	202	PEB	C1B-C2B	2.01	1.50	1.45
87	B2	816	CLA	CMC-C2C	-2.01	1.46	1.50
87	cL	506	CLA	CMC-C2C	-2.01	1.46	1.50
82	gK	203	PEB	C4B-NB	-2.01	1.34	1.38
82	YB	201	PEB	C1C-C2C	2.01	1.47	1.42
82	TO	201	PEB	C1C-C2C	2.01	1.47	1.42
82	uC	201	PEB	C2A-C1A	-2.01	1.50	1.52
87	B2	810	CLA	CHC-C4B	-2.01	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	i4	202	PEB	C4A-NA	-2.01	1.33	1.37
82	R9	201	PEB	C4A-NA	-2.01	1.33	1.37
87	7N	603	CLA	CMB-C2B	-2.01	1.46	1.50
82	kH	202	PEB	C1C-C2C	2.01	1.47	1.42
87	cL	509	CLA	C3C-C2C	2.01	1.41	1.36
84	M1	201	CYC	C4B-NB	-2.01	1.33	1.38
82	MF	202	PEB	C4A-NA	-2.01	1.33	1.37
82	YG	202	PEB	C1C-NC	-2.01	1.34	1.37
82	IP	201	PEB	C1C-NC	-2.01	1.34	1.37
82	iK	203	PEB	C1C-C2C	2.01	1.47	1.42
87	b6	605	CLA	MG-NA	2.01	2.11	2.06
82	K9	201	PEB	C2A-C1A	-2.01	1.50	1.52
82	rC	201	PEB	C4A-NA	-2.01	1.33	1.37
87	bL	622	CLA	MG-ND	-2.01	2.01	2.05
87	B2	811	CLA	CMC-C2C	-2.01	1.46	1.50
82	MK	203	PEB	C4B-C3B	2.01	1.48	1.45
82	zC	201	PEB	C4B-C3B	2.01	1.48	1.45
87	b6	604	CLA	CHC-C1C	2.01	1.42	1.38
87	2N	306	CLA	CHC-C1C	2.01	1.42	1.38
82	BD	202	PEB	C1C-NC	-2.01	1.34	1.37
84	BE	1001	CYC	C4D-ND	-2.01	1.34	1.37
82	18	203	PEB	C1C-C2C	2.01	1.47	1.42
82	ZO	201	PEB	C1B-C2B	2.01	1.50	1.45
84	x3	1001	CYC	CMA-C3A	-2.01	1.46	1.50
82	RQ	201	PEB	C1D-ND	2.00	1.48	1.45
82	mE	201	PEB	C1D-ND	2.00	1.48	1.45
82	CP	201	PEB	C4B-C3B	2.00	1.48	1.45
82	z8	201	PEB	C4B-C3B	2.00	1.48	1.45
82	TF	201	PEB	C1C-NC	-2.00	1.34	1.37
82	aB	202	PEB	C1C-NC	-2.00	1.34	1.37
82	aE	202	PEB	C1C-NC	-2.00	1.34	1.37
82	f4	201	PEB	CHA-C4A	-2.00	1.32	1.36
82	WE	201	PEB	C1C-C2C	2.00	1.47	1.42
82	PH	201	PEB	C1C-C2C	2.00	1.47	1.42
82	rF	202	PEB	C1C-C2C	2.00	1.47	1.42
82	wK	303	PEB	C1C-C2C	2.00	1.47	1.42
82	JA	201	PEB	C4A-NA	-2.00	1.33	1.37
82	mE	201	PEB	C1B-C2B	2.00	1.50	1.45
87	a6	608	CLA	CMC-C2C	-2.00	1.46	1.50
87	R2	204	CLA	CHC-C1C	2.00	1.42	1.38
82	P7	201	PEB	C1C-NC	-2.00	1.34	1.37
82	D9	201	PEB	C1C-NC	-2.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	mM	202	PEB	C1C-NC	-2.00	1.34	1.37
87	BL	609	CLA	CMC-C2C	-2.00	1.46	1.50
87	62	310	CLA	CMB-C2B	-2.00	1.46	1.50
87	62	311	CLA	CMB-C2B	-2.00	1.46	1.50
82	SF	201	PEB	C4B-NB	-2.00	1.34	1.38
87	3N	305	CLA	O2D-CGD	2.00	1.38	1.33
82	AE	301	PEB	C4A-NA	-2.00	1.33	1.37
82	lM	201	PEB	CHC-C4C	2.00	1.52	1.49
82	MM	202	PEB	C1B-C2B	2.00	1.50	1.45
82	hK	202	PEB	C1C-NC	-2.00	1.34	1.37
82	kO	201	PEB	C1C-NC	-2.00	1.34	1.37
87	cL	507	CLA	CMB-C2B	-2.00	1.46	1.50
82	KF	203	PEB	C4B-C3B	2.00	1.48	1.45
82	K9	201	PEB	C4B-C3B	2.00	1.48	1.45
82	dH	201	PEB	C1D-ND	2.00	1.48	1.45
82	cM	201	PEB	C1D-ND	2.00	1.48	1.45
82	YF	202	PEB	C4A-NA	-2.00	1.33	1.37
82	T4	202	PEB	C4B-NB	-2.00	1.34	1.38
82	R7	202	PEB	C4B-NB	-2.00	1.34	1.38
87	32	310	CLA	CHC-C1C	2.00	1.42	1.38
82	XQ	201	PEB	C4B-C3B	2.00	1.48	1.45
82	G9	201	PEB	C4B-C3B	2.00	1.48	1.45
82	lJ	203	PEB	C4B-C3B	2.00	1.48	1.45
82	hE	201	PEB	C1D-ND	2.00	1.48	1.45
82	W9	203	PEB	C4A-NA	-2.00	1.33	1.37
82	FI	201	PEB	C1B-C2B	2.00	1.50	1.45
84	E1	1001	CYC	C4A-C3A	2.00	1.50	1.45
83	M5	302	PUB	CBB-CAB	2.00	1.58	1.52
82	GM	201	PEB	C1C-C2C	2.00	1.47	1.42
82	cK	202	PEB	C1C-C2C	2.00	1.47	1.42
82	UM	202	PEB	C1C-NC	-2.00	1.34	1.37
82	eE	203	PEB	C1C-NC	-2.00	1.34	1.37
82	XM	202	PEB	C4B-C3B	2.00	1.48	1.45
82	Y4	202	PEB	C4B-C3B	2.00	1.48	1.45
82	bF	202	PEB	C4A-NA	-2.00	1.33	1.37
82	dM	203	PEB	C4A-NA	-2.00	1.33	1.37
82	T9	201	PEB	C2A-C1A	-2.00	1.50	1.52
82	vF	202	PEB	C2A-C1A	-2.00	1.50	1.52
82	eM	201	PEB	C1D-ND	2.00	1.48	1.45
87	5N	609	CLA	CMD-C2D	-2.00	1.46	1.50
87	82	303	CLA	CAC-C3C	-2.00	1.46	1.51
87	DL	403	CLA	MG-ND	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	PM	201	PEB	CHC-C4C	2.00	1.52	1.49
87	7N	609	CLA	CHC-C1C	2.00	1.42	1.38
82	S4	201	PEB	C1C-NC	-2.00	1.34	1.37
87	AN	835	CLA	CMC-C2C	-2.00	1.46	1.50
82	YP	502	PEB	C1C-C2C	2.00	1.47	1.42
82	BQ	202	PEB	C1C-C2C	2.00	1.47	1.42
84	EO	1001	CYC	C4D-C3D	2.00	1.47	1.42
82	lH	201	PEB	C1D-ND	2.00	1.48	1.45
82	mM	201	PEB	C1D-ND	2.00	1.48	1.45
87	22	609	CLA	C1B-C2B	2.00	1.48	1.43
87	32	304	CLA	O2D-CGD	2.00	1.38	1.33
82	KA	201	PEB	C1B-C2B	2.00	1.50	1.45
82	AF	202	PEB	C1C-C2C	2.00	1.47	1.42
87	42	603	CLA	CMC-C2C	-2.00	1.46	1.50
82	LK	201	PEB	C1C-NC	-2.00	1.34	1.37
82	h4	202	PEB	C1C-NC	-2.00	1.34	1.37
82	fG	201	PEB	C1C-NC	-2.00	1.34	1.37
82	CI	202	PEB	C2A-C1A	-2.00	1.50	1.52
82	EA	202	PEB	C4B-C3B	2.00	1.48	1.45
82	CK	201	PEB	C4B-C3B	2.00	1.48	1.45
82	VQ	202	PEB	C1D-ND	2.00	1.48	1.45
87	BL	601	CLA	MG-ND	-2.00	2.01	2.05
87	cL	513	CLA	MG-NB	-2.00	2.01	2.05
82	BK	201	PEB	C4B-C3B	2.00	1.48	1.45
82	YA	304	PEB	C1C-C2C	2.00	1.47	1.42
84	NO	1001	CYC	C4D-C3D	2.00	1.47	1.42
87	A2	835	CLA	CMC-C2C	-2.00	1.46	1.50
87	2N	312	CLA	CMB-C2B	-2.00	1.46	1.50
87	82	305	CLA	O2A-CGA	2.00	1.37	1.30
82	OD	201	PEB	C2A-C1A	-2.00	1.50	1.52
82	VB	202	PEB	C1C-NC	-2.00	1.34	1.37
82	PH	202	PEB	C1C-NC	-2.00	1.34	1.37
82	SK	203	PEB	C1C-NC	-2.00	1.34	1.37
82	HQ	203	PEB	C1C-NC	-2.00	1.34	1.37
87	82	307	CLA	MG-ND	-2.00	2.01	2.05
87	C6	514	CLA	CHC-C1C	2.00	1.42	1.38
82	FP	202	PEB	C1C-C2C	2.00	1.47	1.42

All (38864) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	62	309	CLA	CHB-C4A-NA	-41.83	66.67	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	6N	608	CLA	CHB-C4A-NA	-41.80	66.71	124.51
87	62	309	CLA	C4A-NA-C1A	23.13	117.10	106.71
87	6N	608	CLA	C4A-NA-C1A	22.99	117.04	106.71
87	42	604	CLA	C4D-C3D-CAD	-21.59	82.65	108.10
87	4N	604	CLA	C4D-C3D-CAD	-21.57	82.68	108.10
87	62	309	CLA	C1D-ND-C4D	-19.22	92.68	106.33
87	6N	608	CLA	C1D-ND-C4D	-19.19	92.70	106.33
87	32	307	CLA	CHC-C4B-NB	-18.69	104.47	124.26
87	3N	308	CLA	CHC-C4B-NB	-18.68	104.48	124.26
87	62	309	CLA	CHB-C1B-NB	-17.85	105.36	124.26
87	6N	608	CLA	CHB-C1B-NB	-17.81	105.40	124.26
82	FF	201	PEB	OA-C1A-C2A	-17.66	112.13	126.17
82	FK	201	PEB	OA-C1A-C2A	-17.53	112.24	126.17
82	XK	201	PEB	OA-C1A-C2A	-16.33	113.19	126.17
82	RF	201	PEB	OA-C1A-C2A	-16.31	113.20	126.17
82	XF	201	PEB	OA-C1A-C2A	-16.28	113.23	126.17
82	RK	201	PEB	OA-C1A-C2A	-16.17	113.32	126.17
87	2N	303	CLA	CHD-C1D-ND	-15.26	110.43	124.45
87	22	602	CLA	CHD-C1D-ND	-15.23	110.46	124.45
82	BK	201	PEB	OA-C1A-C2A	-15.18	114.10	126.17
82	BF	201	PEB	OA-C1A-C2A	-14.98	114.26	126.17
94	AL	413	PL9	C7-C3-C4	14.44	128.62	116.88
85	Z6	101	BCR	C40-C30-C25	-13.91	87.74	110.30
82	LF	201	PEB	OA-C1A-C2A	-13.86	115.15	126.17
82	LK	201	PEB	OA-C1A-C2A	-13.78	115.22	126.17
82	PF	201	PEB	OA-C1A-C2A	-13.39	115.53	126.17
82	PK	201	PEB	OA-C1A-C2A	-13.28	115.61	126.17
82	WP	201	PEB	CMC-C3C-C4C	12.81	140.64	127.06
82	nK	201	PEB	OA-C1A-C2A	-12.78	116.01	126.17
84	V3	1001	CYC	C3B-C4B-NB	12.61	116.97	106.78
84	x3	1001	CYC	C3B-C4B-NB	12.57	116.93	106.78
82	nF	201	PEB	OA-C1A-C2A	-12.55	116.20	126.17
82	DK	201	PEB	OA-C1A-C2A	-12.54	116.20	126.17
84	E1	1001	CYC	C3B-C4B-NB	12.53	116.90	106.78
82	NK	201	PEB	OA-C1A-C2A	-12.53	116.21	126.17
82	DF	201	PEB	OA-C1A-C2A	-12.52	116.22	126.17
82	NF	201	PEB	OA-C1A-C2A	-12.50	116.23	126.17
84	EH	1001	CYC	C3B-C4B-NB	12.46	116.85	106.78
82	fK	201	PEB	OA-C1A-C2A	-12.32	116.38	126.17
82	fF	201	PEB	OA-C1A-C2A	-12.30	116.40	126.17
82	KP	201	PEB	CMC-C3C-C4C	12.21	140.00	127.06
82	JF	201	PEB	OA-C1A-C2A	-12.21	116.47	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UP	203	PEB	CMC-C3C-C4C	12.18	139.97	127.06
82	jM	202	PEB	CHC-C1D-ND	-12.05	98.48	113.72
82	JK	201	PEB	OA-C1A-C2A	-12.00	116.63	126.17
82	GP	201	PEB	CMC-C3C-C4C	11.98	139.75	127.06
82	AP	203	PEB	CMC-C3C-C4C	11.95	139.73	127.06
82	IP	203	PEB	CMC-C3C-C4C	11.83	139.60	127.06
84	FO	1001	CYC	C3B-C4B-NB	11.80	116.31	106.78
83	A1	304	PUB	C2A-C1A-NA	11.80	117.67	107.21
83	AH	304	PUB	C2A-C1A-NA	11.78	117.66	107.21
82	TK	201	PEB	OA-C1A-C2A	-11.73	116.85	126.17
84	I1	1001	CYC	C3B-C4B-NB	11.71	116.24	106.78
84	H4	1001	CYC	C3B-C4B-NB	11.70	116.23	106.78
84	HO	1001	CYC	C3B-C4B-NB	11.70	116.23	106.78
84	F4	1001	CYC	C3B-C4B-NB	11.68	116.21	106.78
82	TF	201	PEB	OA-C1A-C2A	-11.67	116.90	126.17
87	4N	604	CLA	CMD-C2D-C1D	-11.66	104.17	124.71
87	42	604	CLA	CMD-C2D-C1D	-11.65	104.17	124.71
84	LH	1001	CYC	C3B-C4B-NB	11.65	116.19	106.78
82	EP	203	PEB	CMC-C3C-C4C	11.61	139.37	127.06
85	B2	802	BCR	C40-C30-C25	-11.56	91.55	110.30
85	BN	803	BCR	C40-C30-C25	-11.56	91.55	110.30
82	MP	203	PEB	CMC-C3C-C4C	11.54	139.30	127.06
82	tF	201	PEB	OA-C1A-C2A	-11.50	117.03	126.17
84	DG	1001	CYC	C3B-C4B-NB	11.49	116.06	106.78
84	DE	1001	CYC	C3B-C4B-NB	11.42	116.01	106.78
84	p3	1001	CYC	C3B-C4B-NB	11.42	116.00	106.78
84	T3	1001	CYC	C3B-C4B-NB	11.42	116.00	106.78
84	FG	1001	CYC	C3B-C4B-NB	11.41	116.00	106.78
82	tK	201	PEB	OA-C1A-C2A	-11.41	117.10	126.17
84	J3	1001	CYC	C3B-C4B-NB	11.40	115.99	106.78
84	e3	1001	CYC	C3B-C4B-NB	11.40	115.99	106.78
84	G3	1001	CYC	C3B-C4B-NB	11.39	115.98	106.78
84	C3	1001	CYC	C3B-C4B-NB	11.38	115.97	106.78
84	v3	1001	CYC	C3B-C4B-NB	11.38	115.97	106.78
84	i3	1001	CYC	C3B-C4B-NB	11.37	115.96	106.78
84	ME	1001	CYC	C3B-C4B-NB	11.35	115.95	106.78
84	P3	1001	CYC	C3B-C4B-NB	11.34	115.94	106.78
84	K3	1001	CYC	C3B-C4B-NB	11.34	115.94	106.78
84	t3	1001	CYC	C3B-C4B-NB	11.34	115.94	106.78
82	QP	203	PEB	CMC-C3C-C4C	11.34	139.08	127.06
84	FE	1002	CYC	C3B-C4B-NB	11.34	115.94	106.78
84	E4	1001	CYC	C3B-C4B-NB	11.33	115.93	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	c3	1001	CYC	C3B-C4B-NB	11.32	115.93	106.78
84	E3	1001	CYC	C3B-C4B-NB	11.32	115.92	106.78
84	l3	1001	CYC	C3B-C4B-NB	11.31	115.92	106.78
84	A3	1001	CYC	C3B-C4B-NB	11.31	115.92	106.78
84	R3	1001	CYC	C3B-C4B-NB	11.31	115.91	106.78
84	g3	1001	CYC	C3B-C4B-NB	11.30	115.91	106.78
84	HE	1001	CYC	C3B-C4B-NB	11.30	115.90	106.78
84	MG	1001	CYC	C3B-C4B-NB	11.29	115.90	106.78
84	HG	1001	CYC	C3B-C4B-NB	11.29	115.90	106.78
84	m3	1001	CYC	C3B-C4B-NB	11.28	115.89	106.78
84	N3	1001	CYC	C3B-C4B-NB	11.27	115.88	106.78
83	BM	302	PUB	C2A-C1A-NA	11.26	117.20	107.21
84	EO	1001	CYC	C3B-C4B-NB	11.24	115.86	106.78
84	C4	1001	CYC	C3B-C4B-NB	11.22	115.85	106.78
84	GO	1001	CYC	C3B-C4B-NB	11.21	115.84	106.78
84	G4	1001	CYC	C3B-C4B-NB	11.18	115.81	106.78
84	DH	1003	CYC	C3B-C4B-NB	11.17	115.81	106.78
84	CO	1001	CYC	C3B-C4B-NB	11.17	115.80	106.78
82	vF	201	PEB	OA-C1A-C2A	-11.16	117.30	126.17
84	D1	1003	CYC	C3B-C4B-NB	11.15	115.78	106.78
83	yF	303	PUB	C2A-C1A-NA	11.12	117.07	107.21
83	BJ	302	PUB	C2A-C1A-NA	11.11	117.07	107.21
83	AE	303	PUB	C2A-C1A-NA	11.10	117.06	107.21
83	AJ	304	PUB	C2A-C1A-NA	11.09	117.05	107.21
83	A4	303	PUB	C2A-C1A-NA	11.09	117.05	107.21
83	AO	303	PUB	C2A-C1A-NA	11.08	117.03	107.21
83	AG	303	PUB	C2A-C1A-NA	11.07	117.03	107.21
84	I4	1001	CYC	C3B-C4B-NB	11.07	115.72	106.78
84	K4	1001	CYC	C3B-C4B-NB	11.04	115.70	106.78
83	NQ	201	PUB	C2A-C1A-NA	11.03	116.99	107.21
84	KO	1001	CYC	C3B-C4B-NB	11.01	115.67	106.78
84	IO	1001	CYC	C3B-C4B-NB	11.00	115.67	106.78
83	Z5	303	PUB	C2A-C1A-NA	11.00	116.97	107.21
83	M5	303	PUB	C2A-C1A-NA	10.99	116.96	107.21
84	IG	1001	CYC	C3B-C4B-NB	10.99	115.65	106.78
84	W3	1001	CYC	C3B-C4B-NB	10.98	115.65	106.78
84	y3	1001	CYC	C3B-C4B-NB	10.95	115.62	106.78
83	yK	303	PUB	C2A-C1A-NA	10.95	116.92	107.21
84	NE	201	CYC	C3B-C4B-NB	10.94	115.62	106.78
83	AH	303	PUB	C2A-C1A-NA	10.94	116.91	107.21
84	GE	1001	CYC	C3B-C4B-NB	10.92	115.60	106.78
83	ND	201	PUB	C2A-C1A-NA	10.92	116.90	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	vK	201	PEB	OA-C1A-C2A	-10.92	117.49	126.17
83	A1	303	PUB	C2A-C1A-NA	10.90	116.88	107.21
84	GG	1001	CYC	C3B-C4B-NB	10.90	115.58	106.78
84	KG	202	CYC	C3B-C4B-NB	10.90	115.58	106.78
84	IE	1001	CYC	C3B-C4B-NB	10.89	115.58	106.78
94	A6	410	PL9	C7-C3-C4	10.89	125.73	116.88
84	K1	1001	CYC	C3B-C4B-NB	10.88	115.57	106.78
84	M4	1001	CYC	C3B-C4B-NB	10.88	115.57	106.78
84	MO	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78
84	j3	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78
83	AM	304	PUB	C2A-C1A-NA	10.86	116.84	107.21
84	H3	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
84	d3	1001	CYC	C3B-C4B-NB	10.85	115.55	106.78
84	h3	1001	CYC	C3B-C4B-NB	10.84	115.53	106.78
84	63	901	CYC	C3B-C4B-NB	10.84	115.53	106.78
84	I3	1001	CYC	C3B-C4B-NB	10.83	115.53	106.78
84	L3	1001	CYC	C3B-C4B-NB	10.83	115.53	106.78
83	AO	302	PUB	C2A-C1A-NA	10.83	116.81	107.21
84	q3	1001	CYC	C3B-C4B-NB	10.83	115.53	106.78
84	Q3	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78
84	o3	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78
83	QM	201	PUB	C2A-C1A-NA	10.82	116.81	107.21
84	D3	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78
84	k3	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78
84	M3	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78
84	KH	1001	CYC	C3B-C4B-NB	10.81	115.51	106.78
84	n3	1001	CYC	C3B-C4B-NB	10.81	115.51	106.78
84	B3	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
84	S3	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
84	EG	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
84	O3	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
84	f3	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
84	F3	1001	CYC	C3B-C4B-NB	10.79	115.50	106.78
84	73	1002	CYC	C3B-C4B-NB	10.79	115.50	106.78
84	U3	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
84	w3	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
84	73	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
84	FE	1001	CYC	C3B-C4B-NB	10.78	115.48	106.78
84	u3	1001	CYC	C3B-C4B-NB	10.75	115.46	106.78
83	Z9	302	PUB	C2A-C1A-NA	10.74	116.73	107.21
83	AM	303	PUB	C2A-C1A-NA	10.73	116.73	107.21
83	A4	302	PUB	C2A-C1A-NA	10.73	116.72	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	EE	1001	CYC	C3B-C4B-NB	10.71	115.43	106.78
83	M9	303	PUB	C2A-C1A-NA	10.70	116.70	107.21
84	M1	201	CYC	C3B-C4B-NB	10.70	115.42	106.78
83	AJ	303	PUB	C2A-C1A-NA	10.70	116.70	107.21
82	hM	203	PEB	CHC-C1D-ND	-10.67	100.22	113.72
83	Z9	305	PUB	C2A-C1A-NA	10.67	116.67	107.21
84	CG	1001	CYC	C3B-C4B-NB	10.66	115.39	106.78
84	JH	1003	CYC	C3B-C4B-NB	10.65	115.38	106.78
82	ZI	401	PEB	OA-C1A-C2A	-10.64	117.71	126.17
84	DO	1001	CYC	C3B-C4B-NB	10.64	115.37	106.78
83	xK	301	PUB	C2A-C1A-NA	10.64	116.64	107.21
83	xF	301	PUB	C2A-C1A-NA	10.62	116.63	107.21
82	Z5	304	PEB	C1D-CHC-C4C	-10.62	97.60	113.26
82	M5	304	PEB	C1D-CHC-C4C	-10.61	97.61	113.26
83	YA	302	PUB	C2A-C1A-NA	10.61	116.62	107.21
84	D4	1001	CYC	C3B-C4B-NB	10.61	115.35	106.78
83	AE	302	PUB	C2A-C1A-NA	10.60	116.61	107.21
83	K7	203	PUB	C2A-C1A-NA	10.59	116.61	107.21
83	xK	305	PUB	C2A-C1A-NA	10.57	116.59	107.21
83	wF	304	PUB	C2A-C1A-NA	10.57	116.58	107.21
83	Y7	302	PUB	C2A-C1A-NA	10.55	116.57	107.21
83	yF	302	PUB	C2A-C1A-NA	10.55	116.57	107.21
83	yK	302	PUB	C2A-C1A-NA	10.54	116.56	107.21
83	AG	302	PUB	C2A-C1A-NA	10.54	116.56	107.21
82	TB	201	PEB	CMB-C2B-C1B	10.54	141.29	125.06
83	KA	203	PUB	C2A-C1A-NA	10.53	116.55	107.21
83	wK	304	PUB	C2A-C1A-NA	10.53	116.55	107.21
83	xF	305	PUB	C2A-C1A-NA	10.53	116.55	107.21
82	JB	201	PEB	CMB-C2B-C1B	10.51	141.24	125.06
84	D1	1001	CYC	C3B-C4B-NB	10.50	115.27	106.78
83	xF	306	PUB	C2A-C1A-NA	10.50	116.52	107.21
84	C1	1001	CYC	C3B-C4B-NB	10.50	115.26	106.78
83	AD	302	PUB	C2A-C1A-NA	10.50	116.52	107.21
83	xK	306	PUB	C2A-C1A-NA	10.48	116.51	107.21
84	FH	1001	CYC	C3B-C4B-NB	10.48	115.24	106.78
85	CL	516	BCR	C40-C30-C39	-10.46	76.42	108.53
84	DH	1001	CYC	C3B-C4B-NB	10.45	115.22	106.78
84	CH	1001	CYC	C3B-C4B-NB	10.43	115.20	106.78
83	Z9	305	PUB	CHC-C1D-ND	-10.42	100.54	113.72
84	F1	1001	CYC	C3B-C4B-NB	10.42	115.19	106.78
82	OJ	202	PEB	CHC-C1D-ND	-10.40	100.57	113.72
83	AQ	302	PUB	C2A-C1A-NA	10.40	116.43	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	J1	1001	CYC	C3B-C4B-NB	10.40	115.18	106.78
82	OP	201	PEB	CMC-C3C-C4C	10.35	138.03	127.06
84	BE	1001	CYC	C3B-C4B-NB	10.32	115.11	106.78
83	QJ	201	PUB	C2A-C1A-NA	10.32	116.36	107.21
83	Z5	302	PUB	C2A-C1A-NA	10.28	116.33	107.21
83	M5	302	PUB	C2A-C1A-NA	10.28	116.32	107.21
85	c6	617	BCR	C20-C21-C22	-10.27	112.65	127.31
84	NO	1001	CYC	C3B-C4B-NB	10.27	115.08	106.78
85	cL	518	BCR	C40-C30-C39	-10.25	77.06	108.53
103	8N	310	ZEX	C27-C28-C29	-10.24	110.77	126.23
103	82	310	ZEX	C27-C28-C29	-10.21	110.80	126.23
84	JH	1001	CYC	C3B-C4B-NB	10.21	115.03	106.78
82	vC	202	PEB	C1D-CHC-C4C	-10.20	98.21	113.26
84	N4	1001	CYC	C3B-C4B-NB	10.20	115.02	106.78
82	v8	202	PEB	C1D-CHC-C4C	-10.20	98.22	113.26
82	SP	201	PEB	CMC-C3C-C4C	10.19	137.86	127.06
84	LE	1001	CYC	C3B-C4B-NB	10.15	114.98	106.78
84	BG	1001	CYC	C3B-C4B-NB	10.15	114.97	106.78
84	LG	1001	CYC	C3B-C4B-NB	10.13	114.96	106.78
84	HH	1001	CYC	C3B-C4B-NB	10.11	114.94	106.78
84	H1	1001	CYC	C3B-C4B-NB	10.10	114.93	106.78
91	DL	405	PHO	C2B-C1B-NB	10.05	116.47	109.53
85	L2	205	BCR	C16-C15-C14	-9.97	103.04	123.47
85	LN	205	BCR	C16-C15-C14	-9.97	103.05	123.47
82	jK	201	PEB	OA-C1A-C2A	-9.87	118.33	126.17
84	JO	1001	CYC	C3B-C4B-NB	9.86	114.74	106.78
84	J4	1001	CYC	C3B-C4B-NB	9.83	114.72	106.78
82	CP	201	PEB	CMC-C3C-C4C	9.81	137.45	127.06
82	jF	201	PEB	OA-C1A-C2A	-9.77	118.41	126.17
85	C6	508	BCR	C20-C21-C22	-9.73	113.42	127.31
84	L1	1001	CYC	C3B-C4B-NB	9.71	114.62	106.78
84	NH	1001	CYC	C3B-C4B-NB	9.57	114.51	106.78
84	LH	1002	CYC	C3B-C4B-NB	9.57	114.51	106.78
91	dL	403	PHO	C2B-C1B-NB	9.56	116.12	109.53
87	42	605	CLA	C4A-NA-C1A	9.55	111.00	106.71
87	4N	605	CLA	C4A-NA-C1A	9.51	110.98	106.71
84	N1	1001	CYC	C3B-C4B-NB	9.50	114.45	106.78
82	O9	202	PEB	C2C-C1C-NC	9.48	120.33	107.57
82	GK	202	PEB	OA-C1A-C2A	9.35	133.61	126.17
82	GF	202	PEB	OA-C1A-C2A	9.33	133.59	126.17
87	B6	616	CLA	CMB-C2B-C1B	-9.31	111.19	125.37
87	A2	829	CLA	C4A-NA-C1A	9.31	110.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	aL	610	PHO	C2B-C1B-NB	9.26	115.92	109.53
82	VK	201	PEB	OA-C1A-C2A	-9.22	118.85	126.17
87	3N	309	CLA	C4A-NA-C1A	9.20	110.84	106.71
87	32	309	CLA	C4A-NA-C1A	9.19	110.84	106.71
87	AN	829	CLA	C4A-NA-C1A	9.16	110.82	106.71
91	D6	404	PHO	C2B-C1B-NB	9.15	115.85	109.53
82	B9	202	PEB	CHC-C4C-NC	9.13	133.51	121.15
82	WJ	202	PEB	CHC-C1D-ND	-9.10	102.21	113.72
82	FA	202	PEB	CHC-C4C-NC	9.06	133.41	121.15
87	F2	205	CLA	C4A-NA-C1A	9.04	110.77	106.71
82	VF	201	PEB	OA-C1A-C2A	-9.03	118.99	126.17
82	HB	201	PEB	CMC-C3C-C4C	9.03	136.63	127.06
87	52	606	CLA	C4A-NA-C1A	9.01	110.76	106.71
85	c6	617	BCR	C24-C23-C22	-8.98	112.66	126.23
91	AL	410	PHO	C2B-C1B-NB	8.98	115.73	109.53
87	b6	605	CLA	C4A-NA-C1A	8.97	110.74	106.71
82	FF	201	PEB	C2A-C1A-NA	8.96	116.00	108.27
82	B7	202	PEB	OA-C1A-C2A	-8.96	119.05	126.17
82	FK	201	PEB	C2A-C1A-NA	8.96	116.00	108.27
82	bF	202	PEB	CMC-C3C-C4C	8.95	136.55	127.06
87	FN	205	CLA	C4A-NA-C1A	8.93	110.72	106.71
82	BA	202	PEB	OA-C1A-C2A	-8.93	119.08	126.17
82	F7	202	PEB	CHC-C4C-NC	8.93	133.23	121.15
85	F6	101	BCR	C16-C17-C18	-8.92	114.58	127.31
87	5N	606	CLA	C4A-NA-C1A	8.90	110.71	106.71
84	L4	1001	CYC	C3B-C4B-NB	8.88	113.95	106.78
82	bK	202	PEB	CMC-C3C-C4C	8.87	136.46	127.06
84	LO	1001	CYC	C3B-C4B-NB	8.85	113.93	106.78
85	KN	101	BCR	C35-C13-C14	-8.81	110.58	122.92
87	O2	202	CLA	C4A-NA-C1A	8.80	110.66	106.71
87	BN	810	CLA	C4A-NA-C1A	8.79	110.66	106.71
87	ON	202	CLA	C4A-NA-C1A	8.77	110.65	106.71
85	K2	102	BCR	C35-C13-C14	-8.76	110.65	122.92
82	HI	202	PEB	CHC-C4C-NC	8.74	132.98	121.15
87	B2	809	CLA	C4A-NA-C1A	8.74	110.64	106.71
87	CL	506	CLA	C4A-NA-C1A	8.73	110.63	106.71
82	XK	201	PEB	C2A-C1A-NA	8.71	115.78	108.27
82	KJ	202	PEB	CHC-C1D-ND	-8.70	102.72	113.72
82	dM	203	PEB	CHC-C1D-ND	-8.69	102.73	113.72
84	BG	1002	CYC	C3B-C4B-NB	8.67	113.78	106.78
85	LN	205	BCR	C15-C14-C13	8.65	139.66	127.31
84	BE	1002	CYC	C3B-C4B-NB	8.65	113.76	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	L2	205	BCR	C15-C14-C13	8.63	139.63	127.31
87	bL	617	CLA	C4A-NA-C1A	8.60	110.57	106.71
82	XF	201	PEB	C2A-C1A-NA	8.60	115.69	108.27
91	A6	407	PHO	C2B-C1B-NB	8.60	115.46	109.53
87	dL	401	CLA	C4A-NA-C1A	8.57	110.56	106.71
82	IK	201	PEB	C2C-C1C-NC	8.57	119.10	107.57
91	d6	404	PHO	C2B-C1B-NB	8.55	115.43	109.53
87	LN	203	CLA	C4A-NA-C1A	8.55	110.55	106.71
82	IF	201	PEB	C2C-C1C-NC	8.55	119.08	107.57
87	L2	203	CLA	C4A-NA-C1A	8.50	110.53	106.71
87	KN	103	CLA	C4A-NA-C1A	8.49	110.52	106.71
82	II	203	PEB	CHA-C1B-NB	-8.46	107.23	124.93
82	lF	201	PEB	OA-C1A-C2A	-8.46	119.45	126.17
85	LN	205	BCR	C35-C13-C14	-8.45	111.08	122.92
87	6N	608	CLA	C5-C3-C4	8.45	133.27	114.60
85	K6	102	BCR	C20-C21-C22	-8.45	115.25	127.31
82	lK	201	PEB	OA-C1A-C2A	-8.45	119.46	126.17
85	L2	205	BCR	C35-C13-C14	-8.44	111.10	122.92
82	RF	201	PEB	C2A-C1A-NA	8.43	115.54	108.27
87	62	309	CLA	C5-C3-C4	8.43	133.21	114.60
87	cL	510	CLA	C4A-NA-C1A	8.42	110.49	106.71
87	BL	605	CLA	C4A-NA-C1A	8.42	110.49	106.71
85	k6	102	BCR	C20-C21-C22	-8.40	115.33	127.31
82	FF	201	PEB	CHA-C4A-NA	8.39	135.18	125.20
87	K2	104	CLA	C4A-NA-C1A	8.38	110.47	106.71
82	OI	202	PEB	CHA-C1B-NB	-8.37	107.43	124.93
82	LO	1002	PEB	CHC-C1D-ND	-8.37	103.14	113.72
87	4N	604	CLA	C4D-CHA-C1A	8.36	131.42	121.25
87	42	604	CLA	C4D-CHA-C1A	8.35	131.41	121.25
87	BL	603	CLA	C4A-NA-C1A	8.35	110.46	106.71
87	82	301	CLA	C4A-NA-C1A	8.34	110.46	106.71
82	fF	202	PEB	CMC-C3C-C4C	8.33	135.89	127.06
82	FK	201	PEB	CHA-C4A-NA	8.33	135.11	125.20
82	XK	201	PEB	CHA-C4A-NA	8.33	135.10	125.20
82	RK	201	PEB	C2A-C1A-NA	8.33	115.45	108.27
85	Z6	101	BCR	C40-C30-C39	-8.32	82.99	108.53
82	UF	201	PEB	C2C-C1C-NC	8.32	118.77	107.57
82	UK	201	PEB	C2C-C1C-NC	8.32	118.77	107.57
82	L4	1002	PEB	CHC-C1D-ND	-8.32	103.20	113.72
82	VI	203	PEB	CHC-C4C-NC	8.31	132.39	121.15
87	12	601	CLA	C4A-NA-C1A	8.31	110.44	106.71
91	a6	613	PHO	C2B-C1B-NB	8.30	115.26	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	32	307	CLA	C1D-ND-C4D	-8.30	100.44	106.33
82	fK	202	PEB	CMC-C3C-C4C	8.29	135.85	127.06
87	1N	601	CLA	C4A-NA-C1A	8.27	110.43	106.71
82	N7	202	PEB	OA-C1A-C2A	-8.27	119.59	126.17
85	BN	803	BCR	C40-C30-C39	-8.27	83.15	108.53
85	B2	802	BCR	C40-C30-C39	-8.27	83.15	108.53
87	3N	308	CLA	C1D-ND-C4D	-8.26	100.47	106.33
87	2N	302	CLA	C4A-NA-C1A	8.25	110.42	106.71
87	AN	836	CLA	C4A-NA-C1A	8.24	110.41	106.71
82	TB	202	PEB	CMC-C3C-C4C	8.23	135.79	127.06
87	8N	302	CLA	C4A-NA-C1A	8.23	110.41	106.71
82	NA	202	PEB	OA-C1A-C2A	-8.23	119.63	126.17
82	JB	202	PEB	CMC-C3C-C4C	8.22	135.78	127.06
82	RI	203	PEB	CHC-C4C-NC	8.22	132.28	121.15
82	XF	201	PEB	CHA-C4A-NA	8.22	134.97	125.20
82	FD	203	PEB	CHB-C1C-C2C	-8.22	108.61	127.15
87	bL	621	CLA	C4A-NA-C1A	8.20	110.39	106.71
82	II	203	PEB	CHC-C4C-NC	8.20	132.25	121.15
82	KI	201	PEB	CHC-C4C-NC	8.20	132.24	121.15
87	22	601	CLA	C4A-NA-C1A	8.19	110.39	106.71
85	K2	105	BCR	C7-C8-C9	8.19	138.61	126.23
87	CL	508	CLA	C4A-NA-C1A	8.18	110.39	106.71
87	bL	607	CLA	C4A-NA-C1A	8.18	110.39	106.71
87	CL	507	CLA	C4A-NA-C1A	8.18	110.38	106.71
87	DL	403	CLA	C4A-NA-C1A	8.17	110.38	106.71
82	sK	203	PEB	CHC-C4C-NC	8.17	132.21	121.15
82	FQ	203	PEB	CHB-C1C-C2C	-8.17	108.72	127.15
82	Z1	201	PEB	OA-C1A-C2A	-8.16	119.68	126.17
82	OI	202	PEB	CHC-C4C-NC	8.16	132.19	121.15
82	sF	203	PEB	CHC-C4C-NC	8.16	132.19	121.15
87	5N	609	CLA	C4A-NA-C1A	8.15	110.37	106.71
85	KN	104	BCR	C7-C8-C9	8.15	138.54	126.23
87	A2	822	CLA	C4A-NA-C1A	8.15	110.37	106.71
82	Y7	303	PEB	CHC-C1D-ND	-8.14	103.42	113.72
87	AN	822	CLA	C4A-NA-C1A	8.14	110.36	106.71
87	6N	608	CLA	C3A-C2A-C1A	-8.13	89.16	101.34
87	62	309	CLA	C3A-C2A-C1A	-8.12	89.18	101.34
82	UK	201	PEB	CMB-C2B-C1B	8.12	137.56	125.06
87	A2	836	CLA	C4A-NA-C1A	8.12	110.36	106.71
82	YA	303	PEB	CHC-C1D-ND	-8.12	103.45	113.72
82	LK	201	PEB	CHA-C4A-NA	8.11	134.85	125.20
87	CL	515	CLA	C4A-NA-C1A	8.11	110.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GF	202	PEB	C2C-C1C-NC	8.11	118.49	107.57
82	UF	201	PEB	CMB-C2B-C1B	8.11	137.55	125.06
82	g1	202	PEB	OA-C1A-C2A	-8.09	119.74	126.17
82	LF	201	PEB	CHA-C4A-NA	8.09	134.83	125.20
103	8N	310	ZEX	C1-C6-C5	-8.09	111.22	122.61
82	GK	202	PEB	C2C-C1C-NC	8.07	118.43	107.57
87	52	609	CLA	C4A-NA-C1A	8.06	110.33	106.71
87	62	311	CLA	C4A-NA-C1A	8.06	110.33	106.71
87	82	303	CLA	C4A-NA-C1A	8.06	110.33	106.71
87	AN	823	CLA	C4A-NA-C1A	8.05	110.33	106.71
103	82	310	ZEX	C1-C6-C5	-8.04	111.29	122.61
87	BL	606	CLA	C4A-NA-C1A	8.04	110.32	106.71
87	AN	810	CLA	C4A-NA-C1A	8.04	110.32	106.71
84	w3	1001	CYC	CHD-C4C-NC	8.04	134.76	125.20
85	cL	518	BCR	C40-C30-C25	-8.03	97.27	110.30
84	d3	1001	CYC	CHD-C4C-NC	8.03	134.75	125.20
87	52	604	CLA	C4A-NA-C1A	8.02	110.31	106.71
82	ZH	201	PEB	OA-C1A-C2A	-8.02	119.80	126.17
83	Z9	305	PUB	CHB-C4B-C3B	-8.02	109.06	127.15
82	gH	202	PEB	OA-C1A-C2A	-8.02	119.80	126.17
87	6N	610	CLA	C4A-NA-C1A	8.01	110.31	106.71
84	U3	1001	CYC	CHD-C4C-NC	8.01	134.72	125.20
87	8N	304	CLA	C4A-NA-C1A	8.00	110.30	106.71
82	RK	201	PEB	CHA-C4A-NA	8.00	134.71	125.20
82	jH	203	PEB	CHC-C4C-NC	8.00	131.97	121.15
84	I3	1001	CYC	CHD-C4C-NC	7.99	134.71	125.20
84	h3	1001	CYC	CHD-C4C-NC	7.99	134.70	125.20
87	B2	810	CLA	C4A-NA-C1A	7.99	110.30	106.71
87	5N	604	CLA	C4A-NA-C1A	7.98	110.29	106.71
84	f3	1001	CYC	CHD-C4C-NC	7.98	134.69	125.20
87	A2	810	CLA	C4A-NA-C1A	7.98	110.29	106.71
82	j1	203	PEB	CHC-C4C-NC	7.98	131.95	121.15
82	YF	203	PEB	CHC-C4C-NC	7.97	131.94	121.15
84	j3	1001	CYC	CHD-C4C-NC	7.97	134.69	125.20
84	O3	1001	CYC	CHD-C4C-NC	7.97	134.68	125.20
84	o3	1001	CYC	CHD-C4C-NC	7.97	134.68	125.20
84	M3	1001	CYC	CHD-C4C-NC	7.97	134.68	125.20
84	D3	1001	CYC	CHD-C4C-NC	7.96	134.67	125.20
84	H3	1001	CYC	CHD-C4C-NC	7.96	134.67	125.20
84	n3	1001	CYC	CHD-C4C-NC	7.96	134.67	125.20
82	H5	201	PEB	CHC-C4C-NC	7.96	131.93	121.15
84	u3	1001	CYC	CHD-C4C-NC	7.96	134.67	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	F3	1001	CYC	CHD-C4C-NC	7.96	134.67	125.20
84	S3	1001	CYC	CHD-C4C-NC	7.96	134.67	125.20
84	B3	1001	CYC	CHD-C4C-NC	7.96	134.66	125.20
84	L3	1001	CYC	CHD-C4C-NC	7.95	134.66	125.20
84	Q3	1001	CYC	CHD-C4C-NC	7.95	134.66	125.20
84	k3	1001	CYC	CHD-C4C-NC	7.95	134.66	125.20
84	q3	1001	CYC	CHD-C4C-NC	7.95	134.66	125.20
87	bL	618	CLA	C4A-NA-C1A	7.95	110.28	106.71
82	RF	201	PEB	CHA-C4A-NA	7.94	134.65	125.20
82	OJ	203	PEB	CHC-C4C-NC	7.94	131.89	121.15
84	73	1001	CYC	CHD-C4C-NC	7.94	134.64	125.20
87	BN	811	CLA	C4A-NA-C1A	7.93	110.27	106.71
87	bL	604	CLA	C4A-NA-C1A	7.92	110.27	106.71
82	QF	203	PEB	CHB-C1C-C2C	-7.92	109.29	127.15
82	LA	202	PEB	OA-C1A-C2A	-7.91	119.88	126.17
82	dF	201	PEB	OA-C1A-C2A	-7.91	119.88	126.17
87	nL	101	CLA	C4A-NA-C1A	7.91	110.26	106.71
82	EJ	201	PEB	CHC-C4C-NC	7.91	131.85	121.15
82	QK	203	PEB	CHB-C1C-C2C	-7.90	109.32	127.15
82	eH	203	PEB	CHC-C4C-NC	7.90	131.84	121.15
82	wC	202	PEB	CHC-C4C-NC	7.90	131.84	121.15
82	w8	202	PEB	CHC-C4C-NC	7.89	131.83	121.15
82	LF	201	PEB	C2A-C1A-NA	7.88	115.07	108.27
87	AN	832	CLA	C4A-NA-C1A	7.88	110.25	106.71
82	LK	201	PEB	C2A-C1A-NA	7.88	115.06	108.27
82	dK	201	PEB	OA-C1A-C2A	-7.88	119.91	126.17
87	A2	832	CLA	C4A-NA-C1A	7.87	110.25	106.71
84	73	1002	CYC	CHB-C4A-NA	-7.85	108.50	124.93
87	A2	812	CLA	C4A-NA-C1A	7.84	110.23	106.71
83	AJ	303	PUB	CHC-C1D-ND	-7.83	103.81	113.72
85	AN	846	BCR	C16-C17-C18	-7.83	116.13	127.31
82	b1	203	PEB	CHC-C4C-NC	7.83	131.75	121.15
82	RA	202	PEB	OA-C1A-C2A	-7.83	119.95	126.17
82	WJ	203	PEB	CHC-C4C-NC	7.83	131.75	121.15
87	BL	622	CLA	C4A-NA-C1A	7.83	110.22	106.71
82	XF	202	PEB	CHC-C4C-NC	7.83	131.74	121.15
87	bL	622	CLA	C4A-NA-C1A	7.83	110.22	106.71
82	YK	203	PEB	CHC-C4C-NC	7.82	131.74	121.15
87	A2	823	CLA	C4A-NA-C1A	7.82	110.22	106.71
87	I2	102	CLA	C4A-NA-C1A	7.82	110.22	106.71
82	R7	202	PEB	OA-C1A-C2A	-7.82	119.96	126.17
84	63	901	CYC	CHB-C4A-NA	-7.81	108.59	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	nF	201	PEB	CHA-C4A-NA	7.80	134.48	125.20
85	A2	846	BCR	C16-C17-C18	-7.80	116.18	127.31
84	L1	1001	CYC	CMA-C3A-C4A	7.80	137.08	125.06
87	2N	309	CLA	CBC-CAC-C3C	-7.80	90.92	112.43
85	CL	516	BCR	C40-C30-C25	-7.80	97.65	110.30
87	32	304	CLA	C4A-NA-C1A	7.79	110.21	106.71
83	Z5	303	PUB	CHC-C1D-ND	-7.79	103.86	113.72
87	22	609	CLA	CBC-CAC-C3C	-7.78	90.97	112.43
87	cL	508	CLA	C4A-NA-C1A	7.78	110.20	106.71
82	X7	202	PEB	OA-C1A-C2A	-7.78	119.99	126.17
85	c6	617	BCR	C15-C14-C13	-7.77	116.22	127.31
87	B2	801	CLA	C4A-NA-C1A	7.77	110.20	106.71
82	O9	202	PEB	CHB-C1C-C2C	-7.77	109.63	127.15
82	pF	201	PEB	OA-C1A-C2A	-7.76	120.00	126.17
83	M5	303	PUB	CHC-C1D-ND	-7.76	103.90	113.72
82	XA	202	PEB	OA-C1A-C2A	-7.76	120.00	126.17
84	BE	1002	CYC	CMA-C3A-C4A	7.76	137.02	125.06
87	5N	601	CLA	C4A-NA-C1A	7.75	110.19	106.71
82	XK	202	PEB	CHC-C4C-NC	7.75	131.64	121.15
87	2N	312	CLA	C4A-NA-C1A	7.75	110.19	106.71
82	BI	202	PEB	CHC-C4C-NC	7.75	131.63	121.15
87	BL	621	CLA	C4A-NA-C1A	7.74	110.19	106.71
87	3N	305	CLA	C4A-NA-C1A	7.74	110.18	106.71
82	NF	201	PEB	CHA-C4A-NA	7.73	134.40	125.20
87	AN	812	CLA	C4A-NA-C1A	7.72	110.18	106.71
82	BK	201	PEB	C2A-C1A-NA	7.72	114.93	108.27
82	CP	201	PEB	C1D-CHC-C4C	7.71	124.63	113.26
82	L7	202	PEB	OA-C1A-C2A	-7.71	120.04	126.17
84	y3	1001	CYC	CMD-C2D-C1D	7.71	136.84	125.56
103	8N	310	ZEX	C7-C8-C9	-7.70	114.60	126.23
84	W3	1001	CYC	CMD-C2D-C1D	7.70	136.83	125.56
84	BG	1002	CYC	CMA-C3A-C4A	7.70	136.92	125.06
87	BN	802	CLA	C4A-NA-C1A	7.70	110.17	106.71
82	pK	201	PEB	OA-C1A-C2A	-7.69	120.06	126.17
87	IN	102	CLA	C4A-NA-C1A	7.69	110.16	106.71
84	LH	1002	CYC	CMA-C3A-C4A	7.69	136.90	125.06
82	BF	201	PEB	C2A-C1A-NA	7.68	114.89	108.27
82	nK	201	PEB	CHA-C4A-NA	7.68	134.33	125.20
83	BM	302	PUB	CAD-C3D-C4D	7.67	133.50	121.38
87	AN	824	CLA	C4A-NA-C1A	7.67	110.16	106.71
87	LN	204	CLA	C4A-NA-C1A	7.67	110.15	106.71
82	HI	202	PEB	CHA-C1B-NB	-7.67	108.89	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	bL	613	CLA	C4A-NA-C1A	7.67	110.15	106.71
87	L2	204	CLA	C4A-NA-C1A	7.66	110.15	106.71
103	82	310	ZEX	C7-C8-C9	-7.65	114.67	126.23
87	BN	836	CLA	C4A-NA-C1A	7.65	110.14	106.71
82	NK	201	PEB	CHA-C4A-NA	7.65	134.30	125.20
87	CL	512	CLA	C4A-NA-C1A	7.64	110.14	106.71
87	A2	852	CLA	CAC-C3C-C4C	7.64	134.72	124.81
87	BN	808	CLA	C4A-NA-C1A	7.63	110.14	106.71
82	KJ	202	PEB	CHC-C4C-NC	7.63	131.47	121.15
82	fM	203	PEB	CHC-C4C-NC	7.63	131.47	121.15
87	B2	814	CLA	C4A-NA-C1A	7.62	110.13	106.71
87	AN	852	CLA	CAC-C3C-C4C	7.62	134.69	124.81
87	42	602	CLA	C4A-NA-C1A	7.62	110.13	106.71
82	QP	203	PEB	C1D-CHC-C4C	7.61	124.48	113.26
87	12	609	CLA	C4A-NA-C1A	7.61	110.13	106.71
87	22	612	CLA	C4A-NA-C1A	7.61	110.13	106.71
87	5N	602	CLA	C4A-NA-C1A	7.61	110.13	106.71
91	DL	405	PHO	C2D-C1D-ND	7.60	114.78	109.53
87	CL	514	CLA	C4A-NA-C1A	7.60	110.12	106.71
87	4N	610	CLA	C4A-NA-C1A	7.60	110.12	106.71
87	7N	602	CLA	CHD-C1D-ND	-7.60	117.47	124.45
82	Y7	301	PEB	CMC-C3C-C4C	7.60	135.11	127.06
87	cL	516	CLA	C4A-NA-C1A	7.60	110.12	106.71
87	B2	836	CLA	C4A-NA-C1A	7.60	110.12	106.71
87	aL	606	CLA	C4A-NA-C1A	7.60	110.12	106.71
82	dM	201	PEB	CHC-C4C-NC	7.60	131.43	121.15
87	52	602	CLA	C4A-NA-C1A	7.59	110.12	106.71
82	WF	201	PEB	CHC-C4C-NC	7.59	131.42	121.15
82	KJ	203	PEB	CHC-C4C-NC	7.59	131.42	121.15
82	tC	202	PEB	C1D-CHC-C4C	-7.59	102.07	113.26
82	ID	201	PEB	CAC-C2C-C1C	7.58	137.84	125.76
83	M9	303	PUB	CHC-C1D-ND	-7.58	104.13	113.72
82	t8	202	PEB	C1D-CHC-C4C	-7.58	102.08	113.26
87	52	601	CLA	C4A-NA-C1A	7.58	110.11	106.71
83	Z9	302	PUB	CHC-C1D-ND	-7.57	104.14	113.72
91	A6	407	PHO	O2D-CGD-CBD	7.57	120.58	111.00
82	IQ	201	PEB	CAC-C2C-C1C	7.57	137.81	125.76
87	BL	620	CLA	C4A-NA-C1A	7.56	110.11	106.71
87	4N	607	CLA	C4A-NA-C1A	7.56	110.11	106.71
82	HF	201	PEB	CHC-C4C-NC	7.56	131.39	121.15
87	bL	608	CLA	C4A-NA-C1A	7.56	110.11	106.71
82	YA	301	PEB	CMC-C3C-C4C	7.56	135.07	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	8N	306	CLA	C4A-NA-C1A	7.56	110.10	106.71
82	BF	201	PEB	CHA-C4A-NA	7.55	134.18	125.20
82	BK	201	PEB	CHA-C4A-NA	7.55	134.18	125.20
82	HK	201	PEB	CHC-C4C-NC	7.54	131.36	121.15
87	A2	824	CLA	C4A-NA-C1A	7.54	110.10	106.71
94	aL	601	PL9	C7-C3-C4	7.54	123.01	116.88
82	QH	201	PEB	CHC-C4C-NC	7.54	131.35	121.15
87	72	602	CLA	CHD-C1D-ND	-7.54	117.53	124.45
82	qK	202	PEB	CHB-C4B-NB	-7.53	108.90	124.58
87	B2	807	CLA	C4A-NA-C1A	7.53	110.09	106.71
87	3N	307	CLA	C4A-NA-C1A	7.53	110.09	106.71
87	B2	815	CLA	C4A-NA-C1A	7.52	110.09	106.71
85	b6	602	BCR	C20-C21-C22	-7.52	116.57	127.31
87	BL	609	CLA	C4A-NA-C1A	7.52	110.09	106.71
82	qF	202	PEB	CHB-C4B-NB	-7.52	108.93	124.58
82	VI	203	PEB	CHA-C1B-NB	-7.52	109.21	124.93
87	1N	609	CLA	C4A-NA-C1A	7.51	110.08	106.71
85	K6	102	BCR	C24-C23-C22	-7.51	114.89	126.23
87	BN	815	CLA	C4A-NA-C1A	7.51	110.08	106.71
87	42	610	CLA	C4A-NA-C1A	7.50	110.08	106.71
82	NI	203	PEB	CHC-C4C-NC	7.49	131.29	121.15
87	cL	511	CLA	C4A-NA-C1A	7.49	110.07	106.71
82	QK	203	PEB	CHA-C1B-NB	-7.49	109.27	124.93
82	Q1	201	PEB	CHC-C4C-NC	7.49	131.28	121.15
87	5N	611	CLA	C4A-NA-C1A	7.48	110.07	106.71
85	k6	102	BCR	C24-C23-C22	-7.48	114.93	126.23
87	BN	816	CLA	C4A-NA-C1A	7.48	110.07	106.71
87	BN	829	CLA	C4A-NA-C1A	7.48	110.07	106.71
87	32	306	CLA	C4A-NA-C1A	7.47	110.07	106.71
87	B2	817	CLA	C4A-NA-C1A	7.47	110.07	106.71
82	WK	201	PEB	CHC-C4C-NC	7.47	131.26	121.15
82	aM	203	PEB	CHC-C1D-ND	-7.47	104.27	113.72
92	J6	102	LMG	C1-C2-C3	-7.47	94.45	110.00
87	BN	818	CLA	C4A-NA-C1A	7.46	110.06	106.71
82	QK	203	PEB	CHC-C4C-NC	7.46	131.25	121.15
87	82	305	CLA	C4A-NA-C1A	7.46	110.06	106.71
87	42	607	CLA	C4A-NA-C1A	7.45	110.06	106.71
87	BL	623	CLA	C4A-NA-C1A	7.45	110.06	106.71
87	4N	602	CLA	C4A-NA-C1A	7.45	110.06	106.71
83	Z9	302	PUB	C1D-CHC-C4C	-7.45	97.16	113.37
82	QF	203	PEB	CHA-C1B-NB	-7.44	109.36	124.93
87	AN	813	CLA	C4A-NA-C1A	7.44	110.05	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BL	602	CLA	C4A-NA-C1A	7.44	110.05	106.71
87	A2	813	CLA	C4A-NA-C1A	7.44	110.05	106.71
87	cL	505	CLA	C4A-NA-C1A	7.43	110.05	106.71
83	M9	303	PUB	C1D-CHC-C4C	-7.43	97.20	113.37
82	LD	201	PEB	CHC-C4C-NC	7.43	131.21	121.15
92	j6	101	LMG	C1-C2-C3	-7.43	94.52	110.00
82	GI	201	PEB	CHA-C1B-NB	-7.43	109.39	124.93
87	42	604	CLA	C4A-NA-C1A	7.43	110.05	106.71
82	gF	203	PEB	CHC-C4C-NC	7.42	131.20	121.15
82	QF	203	PEB	CHC-C4C-NC	7.42	131.20	121.15
82	LQ	201	PEB	CHC-C4C-NC	7.42	131.19	121.15
82	AP	203	PEB	C1D-CHC-C4C	7.42	124.20	113.26
87	cL	509	CLA	C4A-NA-C1A	7.41	110.04	106.71
82	IM	201	PEB	CHC-C4C-NC	7.41	131.18	121.15
82	iF	201	PEB	CHC-C4C-NC	7.41	131.18	121.15
87	b6	608	CLA	C4A-NA-C1A	7.41	110.04	106.71
87	4N	604	CLA	C4A-NA-C1A	7.41	110.04	106.71
87	52	611	CLA	C4A-NA-C1A	7.40	110.03	106.71
84	73	1002	CYC	CMA-C3A-C4A	7.39	136.45	125.06
82	WI	202	PEB	CHC-C4C-NC	7.39	131.16	121.15
87	cL	507	CLA	C4A-NA-C1A	7.39	110.03	106.71
87	cL	512	CLA	C4A-NA-C1A	7.39	110.03	106.71
87	B2	829	CLA	C4A-NA-C1A	7.39	110.03	106.71
87	A2	806	CLA	C4A-NA-C1A	7.38	110.03	106.71
82	iK	201	PEB	CHC-C4C-NC	7.38	131.14	121.15
82	u8	202	PEB	CHC-C4C-NC	7.38	131.14	121.15
82	ID	201	PEB	C1C-C2C-C3C	-7.38	98.90	107.62
103	8N	310	ZEX	C35-C34-C33	-7.38	116.78	127.31
82	uC	202	PEB	CHC-C4C-NC	7.38	131.13	121.15
87	12	602	CLA	C4A-NA-C1A	7.38	110.02	106.71
103	82	310	ZEX	C35-C34-C33	-7.37	116.79	127.31
87	7N	601	CLA	C4A-NA-C1A	7.37	110.02	106.71
87	AN	806	CLA	C4A-NA-C1A	7.37	110.02	106.71
87	B2	813	CLA	C4A-NA-C1A	7.37	110.02	106.71
82	IQ	201	PEB	C1C-C2C-C3C	-7.37	98.91	107.62
82	IP	203	PEB	CMD-C2D-C3D	-7.36	119.68	130.06
87	12	610	CLA	C4A-NA-C1A	7.36	110.02	106.71
85	c6	603	BCR	C7-C8-C9	7.36	137.35	126.23
87	1N	610	CLA	C4A-NA-C1A	7.36	110.01	106.71
82	tK	201	PEB	CHA-C4A-NA	7.35	133.95	125.20
83	Z5	302	PUB	C4B-C3B-C2B	-7.35	98.94	107.62
94	AL	413	PL9	C7-C3-C2	-7.34	113.64	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	841	CLA	C4A-NA-C1A	7.34	110.01	106.71
87	72	601	CLA	C4A-NA-C1A	7.34	110.01	106.71
83	M5	302	PUB	C4B-C3B-C2B	-7.34	98.94	107.62
87	CL	505	CLA	C4A-NA-C1A	7.34	110.00	106.71
82	GI	201	PEB	C2C-C1C-NC	7.33	117.43	107.57
87	1N	602	CLA	C4A-NA-C1A	7.32	110.00	106.71
82	Q5	202	PEB	CHC-C1D-ND	-7.32	104.46	113.72
82	gK	203	PEB	CHC-C4C-NC	7.32	131.05	121.15
87	BN	814	CLA	C4A-NA-C1A	7.32	110.00	106.71
98	BN	837	PQN	C2M-C2-C1	7.31	128.39	116.27
87	2N	303	CLA	C2D-C1D-ND	-7.31	104.72	110.10
87	A2	841	CLA	C4A-NA-C1A	7.31	109.99	106.71
87	7N	606	CLA	C4A-NA-C1A	7.31	109.99	106.71
87	22	606	CLA	C4A-NA-C1A	7.31	109.99	106.71
98	B2	837	PQN	C2M-C2-C1	7.30	128.37	116.27
87	ON	202	CLA	C1D-ND-C4D	-7.30	101.15	106.33
82	1C	202	PEB	CHC-C4C-NC	7.30	131.03	121.15
87	K2	101	CLA	C4A-NA-C1A	7.30	109.99	106.71
98	BN	837	PQN	C2M-C2-C3	-7.28	112.52	124.40
87	AL	405	CLA	C4A-NA-C1A	7.28	109.98	106.71
87	4N	609	CLA	C4A-NA-C1A	7.28	109.98	106.71
87	4N	601	CLA	C4A-NA-C1A	7.28	109.98	106.71
98	B2	837	PQN	C2M-C2-C3	-7.28	112.52	124.40
87	2N	306	CLA	C4A-NA-C1A	7.28	109.98	106.71
82	jM	203	PEB	CHC-C4C-NC	7.28	131.00	121.15
87	BL	608	CLA	C4A-NA-C1A	7.27	109.98	106.71
82	18	202	PEB	CHC-C4C-NC	7.26	130.98	121.15
84	y3	1001	CYC	OC-C1C-C2C	7.26	131.94	126.17
87	2N	311	CLA	C4A-NA-C1A	7.26	109.97	106.71
87	6N	612	CLA	CMD-C2D-C1D	7.26	137.50	124.71
82	O9	202	PEB	C1C-C2C-C3C	-7.26	99.04	107.62
87	cL	517	CLA	C4A-NA-C1A	7.26	109.97	106.71
87	3N	311	CLA	C4A-NA-C1A	7.25	109.97	106.71
87	O2	202	CLA	C1D-ND-C4D	-7.25	101.19	106.33
87	22	602	CLA	C2D-C1D-ND	-7.25	104.76	110.10
82	GI	201	PEB	CHC-C4C-NC	7.25	130.96	121.15
87	B2	830	CLA	C4A-NA-C1A	7.24	109.96	106.71
87	C6	520	CLA	C4A-NA-C1A	7.24	109.96	106.71
87	CL	503	CLA	C4A-NA-C1A	7.24	109.96	106.71
87	12	604	CLA	C4A-NA-C1A	7.24	109.96	106.71
87	22	611	CLA	C4A-NA-C1A	7.24	109.96	106.71
87	62	313	CLA	CMD-C2D-C1D	7.24	137.47	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	W3	1001	CYC	OC-C1C-C2C	7.23	131.92	126.17
82	tF	201	PEB	CHA-C4A-NA	7.23	133.80	125.20
91	d6	404	PHO	O2D-CGD-CBD	7.23	120.15	111.00
87	72	606	CLA	C4A-NA-C1A	7.23	109.95	106.71
87	7N	610	CLA	C4A-NA-C1A	7.23	109.95	106.71
87	42	611	CLA	C4A-NA-C1A	7.22	109.95	106.71
87	A2	805	CLA	C4A-NA-C1A	7.22	109.95	106.71
87	bL	606	CLA	C4A-NA-C1A	7.22	109.95	106.71
82	gF	201	PEB	CMB-C2B-C1B	7.22	136.18	125.06
82	UA	201	PEB	CHA-C1B-NB	-7.22	109.84	124.93
85	kL	100	BCR	C24-C23-C22	-7.21	115.33	126.23
82	TA	202	PEB	C2C-C1C-NC	7.21	117.28	107.57
82	U7	201	PEB	CHA-C1B-NB	-7.21	109.85	124.93
87	BN	830	CLA	C4A-NA-C1A	7.21	109.95	106.71
87	42	609	CLA	C4A-NA-C1A	7.21	109.95	106.71
87	A2	817	CLA	C4A-NA-C1A	7.20	109.94	106.71
87	1N	604	CLA	C4A-NA-C1A	7.20	109.94	106.71
82	T7	202	PEB	C2C-C1C-NC	7.20	117.26	107.57
82	vK	201	PEB	CHA-C4A-NA	7.20	133.76	125.20
87	bL	620	CLA	C4A-NA-C1A	7.20	109.94	106.71
87	4N	611	CLA	C4A-NA-C1A	7.20	109.94	106.71
82	O9	202	PEB	CHC-C4C-NC	7.19	130.89	121.15
87	AN	840	CLA	C4A-NA-C1A	7.19	109.94	106.71
85	KL	100	BCR	C24-C23-C22	-7.19	115.37	126.23
82	SP	201	PEB	C1D-CHC-C4C	7.18	123.85	113.26
87	32	311	CLA	C4A-NA-C1A	7.18	109.93	106.71
82	xC	202	PEB	CHB-C1C-NC	-7.18	108.88	125.32
83	KA	203	PUB	CAD-C3D-C4D	7.17	132.71	121.38
82	FD	201	PEB	CHC-C4C-NC	7.17	130.85	121.15
85	A2	848	BCR	C36-C18-C17	-7.17	112.88	122.92
82	x8	202	PEB	CHB-C1C-NC	-7.17	108.91	125.32
82	TD	201	PEB	CHC-C4C-NC	7.16	130.85	121.15
82	SA	201	PEB	CHA-C1B-NB	-7.16	109.95	124.93
87	4N	604	CLA	CMD-C2D-C3D	7.16	144.08	127.61
82	fJ	203	PEB	CHC-C4C-NC	7.16	130.84	121.15
87	42	604	CLA	CMD-C2D-C3D	7.16	144.07	127.61
85	AN	848	BCR	C36-C18-C17	-7.15	112.90	122.92
82	FQ	201	PEB	CHC-C4C-NC	7.15	130.83	121.15
82	vF	201	PEB	CHA-C4A-NA	7.15	133.71	125.20
87	A2	809	CLA	C4A-NA-C1A	7.15	109.92	106.71
82	QB	201	PEB	CMC-C3C-C4C	7.15	134.64	127.06
82	S7	201	PEB	CHA-C1B-NB	-7.14	109.99	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gK	201	PEB	CMB-C2B-C1B	7.14	136.06	125.06
87	bL	619	CLA	C4A-NA-C1A	7.14	109.92	106.71
87	7N	609	CLA	C4A-NA-C1A	7.14	109.92	106.71
87	DL	406	CLA	C4A-NA-C1A	7.14	109.92	106.71
87	42	601	CLA	C4A-NA-C1A	7.13	109.91	106.71
82	EP	203	PEB	C1D-CHC-C4C	7.13	123.77	113.26
82	LA	202	PEB	CHC-C4C-NC	7.13	130.80	121.15
82	CP	201	PEB	CMD-C2D-C3D	-7.13	120.01	130.06
82	KI	201	PEB	CHA-C1B-NB	-7.13	110.02	124.93
83	K7	203	PUB	CAD-C3D-C4D	7.12	132.63	121.38
91	D6	404	PHO	C2D-C1D-ND	7.12	114.44	109.53
87	72	610	CLA	C4A-NA-C1A	7.12	109.91	106.71
82	L7	202	PEB	CHC-C4C-NC	7.11	130.78	121.15
82	TQ	201	PEB	CHC-C4C-NC	7.11	130.77	121.15
82	NK	202	PEB	CMC-C3C-C4C	7.11	134.60	127.06
82	sF	203	PEB	CHA-C1B-NB	-7.11	110.06	124.93
82	HA	202	PEB	OA-C1A-C2A	-7.11	120.52	126.17
91	dL	403	PHO	C2D-C1D-ND	7.11	114.43	109.53
82	OA	201	PEB	CHA-C1B-NB	-7.10	110.08	124.93
82	Z1	201	PEB	C1C-CHB-C4B	7.10	144.20	128.28
82	QA	201	PEB	CHC-C4C-NC	7.10	130.75	121.15
82	PF	201	PEB	CHA-C4A-NA	7.09	133.64	125.20
87	AN	805	CLA	C4A-NA-C1A	7.09	109.89	106.71
82	hJ	201	PEB	CHC-C4C-NC	7.09	130.75	121.15
82	JK	201	PEB	CHA-C4A-NA	7.09	133.63	125.20
82	Q7	201	PEB	CHC-C4C-NC	7.09	130.74	121.15
82	OA	201	PEB	C2C-C1C-NC	7.09	117.11	107.57
82	JF	201	PEB	CHA-C4A-NA	7.08	133.62	125.20
82	cF	203	PEB	CHA-C1B-NB	-7.08	110.12	124.93
82	ZH	201	PEB	C1C-CHB-C4B	7.08	144.15	128.28
82	KM	203	PEB	CHC-C4C-NC	7.07	130.72	121.15
87	AN	817	CLA	C4A-NA-C1A	7.07	109.89	106.71
82	MP	203	PEB	C1D-CHC-C4C	7.07	123.68	113.26
82	O7	201	PEB	C2C-C1C-NC	7.07	117.08	107.57
87	A2	802	CLA	C4A-NA-C1A	7.07	109.88	106.71
87	A2	840	CLA	C4A-NA-C1A	7.06	109.88	106.71
82	sK	203	PEB	CHA-C1B-NB	-7.06	110.16	124.93
91	a6	613	PHO	O2D-CGD-CBD	7.06	119.94	111.00
87	72	605	CLA	C4A-NA-C1A	7.06	109.88	106.71
87	c6	611	CLA	C4A-NA-C1A	7.06	109.88	106.71
82	BI	202	PEB	CHA-C1B-NB	-7.06	110.17	124.93
82	OI	202	PEB	C2C-C1C-NC	7.05	117.07	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	dL	404	CLA	C4A-NA-C1A	7.05	109.88	106.71
82	MP	203	PEB	CMD-C2D-C3D	-7.05	120.12	130.06
82	NF	202	PEB	CMC-C3C-C4C	7.05	134.53	127.06
82	U5	201	PEB	CHC-C4C-NC	7.05	130.69	121.15
87	72	604	CLA	C4A-NA-C1A	7.05	109.88	106.71
82	DA	202	PEB	OA-C1A-C2A	-7.05	120.57	126.17
82	O7	201	PEB	CHA-C1B-NB	-7.05	110.19	124.93
87	AN	809	CLA	C4A-NA-C1A	7.05	109.87	106.71
87	72	609	CLA	C4A-NA-C1A	7.04	109.87	106.71
82	TI	201	PEB	CHC-C4C-NC	7.04	130.68	121.15
82	II	203	PEB	C2C-C1C-NC	7.04	117.05	107.57
82	cK	203	PEB	CHA-C1B-NB	-7.04	110.21	124.93
87	5N	607	CLA	C4A-NA-C1A	7.04	109.87	106.71
87	7N	605	CLA	C4A-NA-C1A	7.04	109.87	106.71
82	DF	201	PEB	C2A-C1A-NA	7.04	114.34	108.27
87	AN	814	CLA	C4A-NA-C1A	7.03	109.87	106.71
87	C6	512	CLA	C4A-NA-C1A	7.03	109.87	106.71
87	1N	607	CLA	C4A-NA-C1A	7.03	109.87	106.71
82	GK	202	PEB	C4B-C3B-C2B	-7.02	99.01	106.78
85	L2	205	BCR	C15-C16-C17	7.02	137.85	123.47
87	3N	313	CLA	C4A-NA-C1A	7.02	109.86	106.71
85	LN	205	BCR	C15-C16-C17	7.01	137.84	123.47
82	RI	203	PEB	CHA-C1B-NB	-7.01	110.27	124.93
87	A2	838	CLA	C4A-NA-C1A	7.01	109.86	106.71
82	UM	201	PEB	CHC-C4C-NC	7.00	130.63	121.15
84	J4	1001	CYC	CHB-C4A-NA	-7.00	110.29	124.93
87	BN	812	CLA	C4A-NA-C1A	7.00	109.85	106.71
82	JD	203	PEB	CHC-C4C-NC	7.00	130.62	121.15
87	AN	801	CLA	C4A-NA-C1A	7.00	109.85	106.71
82	PK	201	PEB	CHA-C4A-NA	7.00	133.52	125.20
82	JQ	203	PEB	CHC-C4C-NC	6.99	130.61	121.15
82	H7	202	PEB	OA-C1A-C2A	-6.99	120.61	126.17
82	AI	203	PEB	CHC-C4C-NC	6.99	130.61	121.15
82	yC	202	PEB	CHC-C4C-NC	6.98	130.60	121.15
87	B2	811	CLA	C4A-NA-C1A	6.98	109.85	106.71
82	WI	202	PEB	CHA-C1B-NB	-6.98	110.33	124.93
87	3N	308	CLA	C3B-C4B-NB	-6.98	104.04	110.52
87	32	307	CLA	C3B-C4B-NB	-6.98	104.04	110.52
83	Z5	303	PUB	CAD-C3D-C4D	6.98	132.40	121.38
87	AN	838	CLA	C4A-NA-C1A	6.98	109.84	106.71
87	82	308	CLA	C4A-NA-C1A	6.98	109.84	106.71
87	B2	808	CLA	C4A-NA-C1A	6.98	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	b6	617	CLA	C4A-NA-C1A	6.97	109.84	106.71
87	22	602	CLA	CMD-C2D-C1D	6.97	137.00	124.71
82	AI	203	PEB	CHA-C1B-NB	-6.97	110.36	124.93
87	52	607	CLA	C4A-NA-C1A	6.96	109.84	106.71
87	A6	403	CLA	C4A-NA-C1A	6.96	109.84	106.71
87	12	607	CLA	C4A-NA-C1A	6.96	109.83	106.71
87	B2	819	CLA	C4A-NA-C1A	6.96	109.83	106.71
82	D7	202	PEB	OA-C1A-C2A	-6.96	120.64	126.17
85	KN	104	BCR	C24-C23-C22	-6.95	115.73	126.23
84	JO	1001	CYC	CHB-C4A-NA	-6.95	110.39	124.93
83	M5	303	PUB	CAD-C3D-C4D	6.95	132.36	121.38
87	2N	303	CLA	CMD-C2D-C1D	6.95	136.97	124.71
87	B2	806	CLA	C4A-NA-C1A	6.95	109.83	106.71
87	7N	604	CLA	C4A-NA-C1A	6.95	109.83	106.71
82	y8	202	PEB	CHC-C4C-NC	6.95	130.56	121.15
87	c6	607	CLA	C4A-NA-C1A	6.95	109.83	106.71
85	K2	105	BCR	C24-C23-C22	-6.95	115.74	126.23
87	8N	308	CLA	C4A-NA-C1A	6.94	109.83	106.71
82	J9	201	PEB	C4B-C3B-C2B	-6.94	99.10	106.78
87	BN	807	CLA	C4A-NA-C1A	6.94	109.83	106.71
87	R2	201	CLA	C4A-NA-C1A	6.94	109.83	106.71
82	KA	201	PEB	CAC-C2C-C1C	6.94	136.81	125.76
87	32	313	CLA	C4A-NA-C1A	6.93	109.82	106.71
87	52	610	CLA	C4A-NA-C1A	6.93	109.82	106.71
84	IG	1001	CYC	OC-C1C-C2C	-6.93	120.66	126.17
87	A2	816	CLA	C4A-NA-C1A	6.93	109.82	106.71
87	3N	310	CLA	C4A-NA-C1A	6.93	109.82	106.71
85	A2	848	BCR	C36-C18-C19	6.92	128.99	118.08
87	AL	404	CLA	C4A-NA-C1A	6.92	109.82	106.71
85	F2	204	BCR	C24-C23-C22	-6.92	115.78	126.23
87	b6	618	CLA	C4A-NA-C1A	6.92	109.82	106.71
85	AN	848	BCR	C36-C18-C19	6.92	128.98	118.08
82	YM	201	PEB	CHC-C4C-NC	6.92	130.52	121.15
82	GF	202	PEB	C4B-C3B-C2B	-6.92	99.12	106.78
87	bL	614	CLA	C4A-NA-C1A	6.92	109.82	106.71
87	RN	201	CLA	C4A-NA-C1A	6.91	109.81	106.71
87	RN	204	CLA	C4A-NA-C1A	6.91	109.81	106.71
91	dL	403	PHO	O2D-CGD-CBD	6.91	119.75	111.00
87	AN	821	CLA	C4A-NA-C1A	6.90	109.81	106.71
87	B6	607	CLA	C4A-NA-C1A	6.90	109.81	106.71
82	qC	202	PEB	CHC-C4C-NC	6.90	130.49	121.15
87	HL	101	CLA	C4A-NA-C1A	6.90	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	FN	204	BCR	C24-C23-C22	-6.90	115.81	126.23
87	A2	808	CLA	C4A-NA-C1A	6.90	109.81	106.71
87	R2	204	CLA	C4A-NA-C1A	6.89	109.81	106.71
87	F2	202	CLA	C4A-NA-C1A	6.89	109.80	106.71
82	UO	201	PEB	CMB-C2B-C1B	6.89	135.67	125.06
82	q8	202	PEB	CHC-C4C-NC	6.89	130.47	121.15
82	x8	202	PEB	C1D-CHC-C4C	-6.89	103.10	113.26
87	A2	821	CLA	C4A-NA-C1A	6.89	109.80	106.71
87	B6	612	CLA	C4A-NA-C1A	6.89	109.80	106.71
87	b6	616	CLA	C4A-NA-C1A	6.88	109.80	106.71
87	5N	603	CLA	C4A-NA-C1A	6.88	109.80	106.71
82	K7	201	PEB	CAC-C2C-C1C	6.88	136.72	125.76
87	CL	509	CLA	C4A-NA-C1A	6.88	109.80	106.71
87	MN	101	CLA	C4A-NA-C1A	6.88	109.80	106.71
87	B6	610	CLA	C4A-NA-C1A	6.88	109.80	106.71
87	b6	606	CLA	C4A-NA-C1A	6.88	109.80	106.71
87	5N	610	CLA	C4A-NA-C1A	6.88	109.80	106.71
82	IK	201	PEB	C1C-C2C-C3C	-6.88	99.49	107.62
82	xC	202	PEB	C1D-CHC-C4C	-6.87	103.12	113.26
85	K6	102	BCR	C11-C10-C9	-6.87	117.50	127.31
82	GK	201	PEB	CHB-C1C-C2C	-6.87	111.65	127.15
87	dL	409	CLA	C4A-NA-C1A	6.87	109.79	106.71
87	72	603	CLA	C4A-NA-C1A	6.87	109.79	106.71
87	B2	831	CLA	C4A-NA-C1A	6.87	109.79	106.71
87	CL	510	CLA	C4A-NA-C1A	6.86	109.79	106.71
87	AN	834	CLA	C4A-NA-C1A	6.86	109.79	106.71
87	52	603	CLA	C4A-NA-C1A	6.86	109.79	106.71
87	A2	837	CLA	C4A-NA-C1A	6.86	109.79	106.71
82	qF	201	PEB	CHC-C4C-NC	6.86	130.43	121.15
87	b6	609	CLA	C4A-NA-C1A	6.86	109.79	106.71
84	IE	1001	CYC	OC-C1C-C2C	-6.86	120.72	126.17
87	BN	820	CLA	C4A-NA-C1A	6.86	109.79	106.71
82	qK	201	PEB	CHC-C4C-NC	6.86	130.43	121.15
82	MF	203	PEB	CHC-C4C-NC	6.85	130.43	121.15
87	A2	814	CLA	C4A-NA-C1A	6.85	109.79	106.71
87	cL	514	CLA	C4A-NA-C1A	6.85	109.79	106.71
82	OF	202	PEB	CMB-C2B-C1B	6.85	135.61	125.06
82	U4	201	PEB	C2C-C1C-NC	6.85	116.79	107.57
82	GF	201	PEB	CHB-C1C-C2C	-6.85	111.70	127.15
87	A2	851	CLA	C4A-NA-C1A	6.85	109.78	106.71
83	Z9	305	PUB	CAD-C3D-C4D	6.85	132.19	121.38
82	fK	201	PEB	CHA-C4A-NA	6.85	133.34	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	b6	602	BCR	C15-C14-C13	-6.85	117.54	127.31
87	7N	603	CLA	C4A-NA-C1A	6.84	109.78	106.71
82	U4	201	PEB	CMB-C2B-C1B	6.84	135.60	125.06
85	k6	102	BCR	C11-C10-C9	-6.84	117.54	127.31
87	AN	825	CLA	C4A-NA-C1A	6.84	109.78	106.71
87	B2	832	CLA	C4A-NA-C1A	6.84	109.78	106.71
82	DK	201	PEB	C2A-C1A-NA	6.84	114.17	108.27
87	A2	825	CLA	C4A-NA-C1A	6.84	109.78	106.71
82	kF	203	PEB	C1D-CHC-C4C	6.83	123.33	113.26
87	D6	402	CLA	C4A-NA-C1A	6.83	109.78	106.71
82	aJ	204	PEB	CHC-C4C-NC	6.83	130.40	121.15
82	IF	201	PEB	C1C-C2C-C3C	-6.83	99.54	107.62
87	BN	809	CLA	C4A-NA-C1A	6.83	109.78	106.71
82	PA	202	PEB	OA-C1A-C2A	-6.83	120.74	126.17
82	DI	201	PEB	C1C-C2C-C3C	-6.83	99.55	107.62
87	A6	404	CLA	C4A-NA-C1A	6.83	109.78	106.71
82	OK	202	PEB	CMB-C2B-C1B	6.82	135.57	125.06
87	A2	834	CLA	C4A-NA-C1A	6.82	109.77	106.71
82	kK	203	PEB	C1D-CHC-C4C	6.82	123.31	113.26
87	FN	201	CLA	C4A-NA-C1A	6.82	109.77	106.71
87	32	310	CLA	C4A-NA-C1A	6.81	109.77	106.71
87	C6	509	CLA	C4A-NA-C1A	6.81	109.77	106.71
87	CL	518	CLA	C4A-NA-C1A	6.81	109.77	106.71
87	AN	808	CLA	C4A-NA-C1A	6.81	109.77	106.71
82	KP	201	PEB	C1D-CHC-C4C	6.81	123.30	113.26
87	A2	818	CLA	C4A-NA-C1A	6.81	109.77	106.71
87	D6	403	CLA	C4A-NA-C1A	6.81	109.77	106.71
87	22	603	CLA	C4A-NA-C1A	6.80	109.77	106.71
87	B6	605	CLA	C4A-NA-C1A	6.80	109.77	106.71
91	a6	613	PHO	C1C-C2C-C3C	-6.80	102.95	108.61
87	AN	851	CLA	C4A-NA-C1A	6.80	109.76	106.71
87	1N	611	CLA	C4A-NA-C1A	6.80	109.76	106.71
87	3N	303	CLA	CMD-C2D-C1D	6.80	136.69	124.71
87	8N	305	CLA	C4A-NA-C1A	6.79	109.76	106.71
87	32	302	CLA	CMD-C2D-C1D	6.78	136.67	124.71
83	AM	303	PUB	CHC-C1D-ND	-6.78	105.14	113.72
87	32	302	CLA	C4A-NA-C1A	6.78	109.75	106.71
87	82	304	CLA	C4A-NA-C1A	6.78	109.75	106.71
87	C6	518	CLA	C4A-NA-C1A	6.78	109.75	106.71
82	lM	201	PEB	CHC-C4C-NC	6.78	130.32	121.15
87	BN	832	CLA	C4A-NA-C1A	6.78	109.75	106.71
103	8N	310	ZEX	C11-C10-C9	-6.77	117.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	303	CLA	CHD-C1D-ND	-6.77	118.23	124.45
82	MK	203	PEB	CHC-C4C-NC	6.77	130.32	121.15
87	M2	101	CLA	C4A-NA-C1A	6.77	109.75	106.71
87	b6	614	CLA	C4A-NA-C1A	6.77	109.75	106.71
82	fF	201	PEB	CHA-C4A-NA	6.77	133.26	125.20
82	UO	201	PEB	C2C-C1C-NC	6.77	116.69	107.57
87	32	302	CLA	CHD-C1D-ND	-6.77	118.23	124.45
82	P7	202	PEB	OA-C1A-C2A	-6.77	120.79	126.17
84	LO	1001	CYC	CHB-C4A-NA	-6.77	110.78	124.93
87	12	611	CLA	C4A-NA-C1A	6.77	109.75	106.71
82	jF	201	PEB	CHA-C4A-NA	6.76	133.25	125.20
82	cK	203	PEB	CHC-C4C-NC	6.76	130.30	121.15
94	aL	601	PL9	C7-C3-C2	-6.76	114.42	123.30
82	IF	203	PEB	C2C-C1C-NC	6.76	116.67	107.57
87	AN	837	CLA	C4A-NA-C1A	6.76	109.74	106.71
87	A2	811	CLA	C4A-NA-C1A	6.76	109.74	106.71
82	OI	202	PEB	C1C-C2C-C3C	-6.75	99.64	107.62
85	kL	100	BCR	C15-C16-C17	-6.75	109.64	123.47
87	A2	819	CLA	C4A-NA-C1A	6.75	109.74	106.71
91	d6	404	PHO	C2D-C1D-ND	6.75	114.19	109.53
85	KL	100	BCR	C15-C16-C17	-6.75	109.64	123.47
87	AN	811	CLA	C4A-NA-C1A	6.75	109.74	106.71
82	jK	201	PEB	CHA-C4A-NA	6.75	133.23	125.20
82	ZI	401	PEB	C2A-C1A-NA	6.75	114.09	108.27
103	82	310	ZEX	C11-C10-C9	-6.75	117.68	127.31
82	DQ	202	PEB	CHA-C1B-NB	-6.75	110.82	124.93
82	CJ	203	PEB	CHC-C4C-NC	6.75	130.28	121.15
87	b6	604	CLA	C4A-NA-C1A	6.74	109.74	106.71
82	IK	201	PEB	CMB-C2B-C1B	6.74	135.44	125.06
82	qK	202	PEB	CHA-C1B-NB	-6.74	110.84	124.93
87	AN	818	CLA	C4A-NA-C1A	6.74	109.73	106.71
82	IK	203	PEB	C2C-C1C-NC	6.73	116.64	107.57
82	Q9	202	PEB	CHC-C4C-NC	6.73	130.26	121.15
87	6N	607	CLA	C4A-NA-C1A	6.73	109.73	106.71
82	XQ	201	PEB	CHC-C4C-NC	6.73	130.26	121.15
87	3N	306	CLA	C4A-NA-C1A	6.73	109.73	106.71
82	JA	202	PEB	OA-C1A-C2A	-6.73	120.82	126.17
87	AN	816	CLA	C4A-NA-C1A	6.73	109.73	106.71
87	B6	614	CLA	C4A-NA-C1A	6.73	109.73	106.71
82	J7	202	PEB	OA-C1A-C2A	-6.72	120.83	126.17
82	DD	202	PEB	CHA-C1B-NB	-6.72	110.87	124.93
87	32	305	CLA	C4A-NA-C1A	6.72	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	c6	615	CLA	C4A-NA-C1A	6.72	109.73	106.71
82	qF	202	PEB	CHA-C1B-NB	-6.72	110.87	124.93
91	a6	613	PHO	C2D-C1D-ND	6.72	114.17	109.53
87	22	610	CLA	C4A-NA-C1A	6.72	109.73	106.71
87	C6	513	CLA	C4A-NA-C1A	6.72	109.73	106.71
83	Y7	302	PUB	CAD-C3D-C4D	6.72	131.99	121.38
82	SO	201	PEB	CMB-C2B-C1B	6.71	135.40	125.06
84	L4	1001	CYC	CHB-C4A-NA	-6.71	110.89	124.93
82	UF	201	PEB	C1C-C2C-C3C	-6.71	99.68	107.62
87	3N	301	CLA	C4A-NA-C1A	6.71	109.72	106.71
87	IN	103	CLA	C4A-NA-C1A	6.70	109.72	106.71
87	32	308	CLA	C4A-NA-C1A	6.70	109.72	106.71
87	3N	303	CLA	C4A-NA-C1A	6.70	109.72	106.71
82	TF	201	PEB	CHA-C4A-NA	6.69	133.16	125.20
87	HL	102	CLA	C4A-NA-C1A	6.69	109.72	106.71
82	XD	201	PEB	CHC-C4C-NC	6.69	130.21	121.15
82	GF	201	PEB	CHA-C1B-NB	-6.69	110.94	124.93
82	NA	203	PEB	C1D-CHC-C4C	-6.69	103.40	113.26
82	GK	201	PEB	CHA-C1B-NB	-6.69	110.95	124.93
82	OP	201	PEB	C1D-CHC-C4C	6.68	123.11	113.26
82	DK	201	PEB	CHA-C4A-NA	6.68	133.15	125.20
82	S4	201	PEB	CMB-C2B-C1B	6.68	135.35	125.06
91	A6	407	PHO	C2D-C1D-ND	6.67	114.13	109.53
82	TK	201	PEB	CHA-C4A-NA	6.67	133.14	125.20
82	CM	203	PEB	CHC-C4C-NC	6.67	130.18	121.15
82	OF	201	PEB	CHC-C4C-NC	6.67	130.18	121.15
87	6N	605	CLA	C4A-NA-C1A	6.67	109.70	106.71
82	DF	201	PEB	CHA-C4A-NA	6.67	133.13	125.20
87	AN	819	CLA	C4A-NA-C1A	6.67	109.70	106.71
82	IF	201	PEB	CMB-C2B-C1B	6.66	135.32	125.06
83	AM	303	PUB	CAD-C3D-C4D	6.66	131.90	121.38
87	2N	310	CLA	C4A-NA-C1A	6.66	109.70	106.71
87	c6	604	CLA	C4A-NA-C1A	6.66	109.70	106.71
87	2N	307	CLA	C4A-NA-C1A	6.66	109.70	106.71
87	BN	831	CLA	C4A-NA-C1A	6.66	109.70	106.71
87	A2	852	CLA	C2D-C1D-ND	-6.65	105.20	110.10
83	YA	302	PUB	CAD-C3D-C4D	6.65	131.88	121.38
87	BN	826	CLA	C4A-NA-C1A	6.65	109.70	106.71
82	GI	201	PEB	CHB-C1C-C2C	-6.65	112.15	127.15
82	S7	201	PEB	CMB-C2B-C1B	6.65	135.30	125.06
82	SA	201	PEB	CMB-C2B-C1B	6.65	135.30	125.06
87	5N	605	CLA	C4A-NA-C1A	6.65	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	AL	410	PHO	C2D-C1D-ND	6.64	114.11	109.53
82	TK	202	PEB	CMC-C3C-C4C	6.64	134.10	127.06
82	N7	203	PEB	C1D-CHC-C4C	-6.64	103.46	113.26
82	cB	401	PEB	C1D-CHC-C4C	6.64	123.05	113.26
87	c6	606	CLA	C4A-NA-C1A	6.64	109.69	106.71
82	IK	203	PEB	CHC-C1D-ND	-6.64	105.33	113.72
87	12	603	CLA	C4A-NA-C1A	6.64	109.69	106.71
87	62	306	CLA	C4A-NA-C1A	6.64	109.69	106.71
82	TA	202	PEB	OA-C1A-C2A	-6.64	120.90	126.17
87	B6	611	CLA	C4A-NA-C1A	6.64	109.69	106.71
82	cF	203	PEB	CHC-C4C-NC	6.64	130.13	121.15
82	OI	202	PEB	CHB-C1C-C2C	-6.63	112.18	127.15
87	aL	605	CLA	C4A-NA-C1A	6.63	109.69	106.71
82	UK	201	PEB	C1C-C2C-C3C	-6.63	99.78	107.62
82	TI	201	PEB	CHA-C1B-NB	-6.63	111.06	124.93
82	jJ	203	PEB	CHC-C4C-NC	6.63	130.12	121.15
87	c6	616	CLA	C4A-NA-C1A	6.63	109.69	106.71
87	d6	401	CLA	C4A-NA-C1A	6.63	109.69	106.71
87	BN	825	CLA	C4A-NA-C1A	6.62	109.68	106.71
82	DF	202	PEB	CHC-C1D-ND	-6.62	105.34	113.72
87	AN	839	CLA	C4A-NA-C1A	6.62	109.68	106.71
87	2N	304	CLA	C4A-NA-C1A	6.62	109.68	106.71
87	K6	101	CLA	C4A-NA-C1A	6.62	109.68	106.71
87	AN	807	CLA	C4A-NA-C1A	6.62	109.68	106.71
87	b6	615	CLA	C4A-NA-C1A	6.62	109.68	106.71
85	BN	838	BCR	C7-C8-C9	-6.62	116.24	126.23
82	IK	203	PEB	CHB-C1C-C2C	-6.62	112.22	127.15
82	IF	203	PEB	CHB-C1C-C2C	-6.62	112.22	127.15
87	1N	603	CLA	C4A-NA-C1A	6.62	109.68	106.71
87	D6	405	CLA	C4A-NA-C1A	6.61	109.68	106.71
82	OB	201	PEB	CHC-C4C-NC	6.61	130.10	121.15
82	IK	203	PEB	CHC-C4C-NC	6.61	130.10	121.15
83	NQ	201	PUB	CAD-C3D-C4D	6.61	131.82	121.38
85	B2	838	BCR	C7-C8-C9	-6.61	116.25	126.23
87	62	308	CLA	C4A-NA-C1A	6.61	109.68	106.71
87	B2	818	CLA	C4A-NA-C1A	6.61	109.68	106.71
87	C6	511	CLA	C4A-NA-C1A	6.61	109.68	106.71
82	DK	202	PEB	CHC-C1D-ND	-6.60	105.37	113.72
82	SF	202	PEB	CMB-C2B-C1B	6.60	135.23	125.06
82	h1	201	PEB	CHC-C4C-NC	6.60	130.09	121.15
87	B6	604	CLA	C4A-NA-C1A	6.60	109.67	106.71
83	ND	201	PUB	CAD-C3D-C4D	6.60	131.81	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	Z5	303	PUB	C4B-C3B-C2B	-6.60	99.82	107.62
82	OK	201	PEB	CHC-C4C-NC	6.60	130.08	121.15
82	LK	202	PEB	C1C-C2C-C3C	-6.60	99.82	107.62
85	c6	603	BCR	C16-C17-C18	-6.60	117.89	127.31
87	ON	201	CLA	C4A-NA-C1A	6.60	109.67	106.71
87	A2	839	CLA	C4A-NA-C1A	6.59	109.67	106.71
103	8N	310	ZEX	C2-C3-C4	-6.59	101.28	110.30
87	BN	819	CLA	C4A-NA-C1A	6.59	109.67	106.71
87	A2	828	CLA	C4A-NA-C1A	6.59	109.67	106.71
82	gH	203	PEB	CHC-C4C-NC	6.59	130.07	121.15
87	A2	830	CLA	C4A-NA-C1A	6.59	109.67	106.71
87	I2	103	CLA	C4A-NA-C1A	6.59	109.67	106.71
87	b6	613	CLA	C4A-NA-C1A	6.59	109.67	106.71
82	S9	202	PEB	CHC-C4C-NC	6.59	130.07	121.15
82	IF	203	PEB	CHC-C1D-ND	-6.59	105.39	113.72
87	62	313	CLA	CHD-C1D-ND	-6.59	118.40	124.45
87	62	310	CLA	C4A-NA-C1A	6.59	109.67	106.71
87	C6	516	CLA	C4A-NA-C1A	6.59	109.67	106.71
87	6N	609	CLA	C4A-NA-C1A	6.59	109.67	106.71
87	B2	826	CLA	C4A-NA-C1A	6.58	109.67	106.71
87	c6	614	CLA	C4A-NA-C1A	6.58	109.67	106.71
87	AN	835	CLA	C4A-NA-C1A	6.58	109.66	106.71
82	F7	202	PEB	OA-C1A-C2A	-6.58	120.94	126.17
83	BJ	302	PUB	CAD-C3D-C4D	6.58	131.77	121.38
91	D6	404	PHO	C4D-ND-C1D	-6.58	102.14	108.83
103	82	310	ZEX	C2-C3-C4	-6.58	101.30	110.30
82	RA	202	PEB	C2C-C1C-NC	6.57	116.42	107.57
82	TA	202	PEB	CHB-C1C-C2C	-6.57	112.32	127.15
87	62	312	CLA	C4A-NA-C1A	6.57	109.66	106.71
87	AN	852	CLA	C2D-C1D-ND	-6.57	105.26	110.10
83	M5	303	PUB	C4B-C3B-C2B	-6.57	99.85	107.62
87	32	312	CLA	C4A-NA-C1A	6.57	109.66	106.71
87	B6	606	CLA	C4A-NA-C1A	6.57	109.66	106.71
82	T7	202	PEB	CHB-C1C-C2C	-6.57	112.34	127.15
82	IF	203	PEB	CHC-C4C-NC	6.56	130.03	121.15
82	W9	202	PEB	CHC-C4C-NC	6.56	130.03	121.15
83	Z5	303	PUB	C1D-CHC-C4C	-6.55	99.11	113.37
87	B2	824	CLA	C4A-NA-C1A	6.55	109.65	106.71
82	T7	202	PEB	OA-C1A-C2A	-6.55	120.97	126.17
87	A2	820	CLA	C4A-NA-C1A	6.55	109.65	106.71
87	d6	403	CLA	C4A-NA-C1A	6.55	109.65	106.71
87	6N	601	CLA	C4A-NA-C1A	6.55	109.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	R7	202	PEB	C2C-C1C-NC	6.55	116.39	107.57
91	A6	407	PHO	C1C-C2C-C3C	-6.55	103.17	108.61
82	UM	203	PEB	CHC-C4C-NC	6.54	130.01	121.15
87	6N	612	CLA	CHD-C1D-ND	-6.54	118.44	124.45
83	AQ	302	PUB	CAD-C3D-C4D	6.54	131.71	121.38
83	Z9	305	PUB	C3B-C4B-NB	6.54	116.38	107.57
82	LF	202	PEB	C1C-C2C-C3C	-6.54	99.89	107.62
87	AN	830	CLA	C4A-NA-C1A	6.54	109.65	106.71
82	FD	203	PEB	CHC-C4C-NC	6.54	130.00	121.15
87	B6	613	CLA	C4A-NA-C1A	6.53	109.64	106.71
82	RA	202	PEB	CHB-C1C-C2C	-6.53	112.41	127.15
87	12	605	CLA	C4A-NA-C1A	6.53	109.64	106.71
83	M5	303	PUB	C1D-CHC-C4C	-6.53	99.16	113.37
82	EK	201	PEB	CMB-C2B-C1B	6.53	135.12	125.06
87	52	605	CLA	C4A-NA-C1A	6.53	109.64	106.71
82	GP	201	PEB	C1D-CHC-C4C	6.53	122.89	113.26
82	BD	203	PEB	CHC-C4C-NC	6.53	129.99	121.15
87	A2	833	CLA	C4A-NA-C1A	6.53	109.64	106.71
82	H7	202	PEB	CHC-C4C-NC	6.53	129.98	121.15
82	R7	202	PEB	CHB-C1C-C2C	-6.53	112.43	127.15
87	62	302	CLA	C4A-NA-C1A	6.53	109.64	106.71
82	lF	203	PEB	CHC-C4C-NC	6.52	129.98	121.15
87	A2	835	CLA	C4A-NA-C1A	6.52	109.64	106.71
82	D9	202	PEB	CHC-C4C-NC	6.52	129.98	121.15
82	FQ	203	PEB	CHC-C4C-NC	6.52	129.97	121.15
82	qK	202	PEB	CAC-C2C-C1C	6.52	136.15	125.76
82	dJ	201	PEB	CHC-C4C-NC	6.52	129.97	121.15
87	8N	303	CLA	CAC-C3C-C4C	6.52	133.27	124.81
87	B2	835	CLA	C4A-NA-C1A	6.52	109.64	106.71
87	H6	102	CLA	C4A-NA-C1A	6.52	109.64	106.71
87	6N	611	CLA	C4A-NA-C1A	6.52	109.64	106.71
82	CD	201	PEB	C1C-C2C-C3C	-6.51	99.92	107.62
82	UP	203	PEB	C3C-C4C-NC	-6.51	102.48	108.33
82	VI	203	PEB	C2C-C1C-NC	6.51	116.34	107.57
82	II	203	PEB	CHB-C1C-C2C	-6.51	112.46	127.15
82	AP	203	PEB	CMD-C2D-C3D	-6.51	120.88	130.06
87	AN	852	CLA	CAC-C3C-C2C	-6.51	116.39	127.53
82	c1	202	PEB	CMB-C2B-C1B	6.51	135.09	125.06
91	DL	405	PHO	C1C-C2C-C3C	-6.51	103.20	108.61
87	c6	608	CLA	C4A-NA-C1A	6.51	109.63	106.71
82	BQ	203	PEB	CHC-C4C-NC	6.51	129.96	121.15
82	HA	202	PEB	CHC-C4C-NC	6.50	129.95	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	835	CLA	C4A-NA-C1A	6.50	109.63	106.71
87	22	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
87	22	607	CLA	C4A-NA-C1A	6.50	109.63	106.71
87	O2	201	CLA	C4A-NA-C1A	6.50	109.63	106.71
82	FD	201	PEB	CHA-C1B-NB	-6.50	111.33	124.93
87	cL	506	CLA	C4A-NA-C1A	6.50	109.63	106.71
85	CL	502	BCR	C16-C17-C18	-6.50	118.03	127.31
82	FQ	201	PEB	CHA-C1B-NB	-6.50	111.34	124.93
82	XB	202	PEB	CMC-C3C-C4C	6.50	133.95	127.06
82	VA	202	PEB	OA-C1A-C2A	-6.50	121.01	126.17
82	UP	203	PEB	C1D-CHC-C4C	6.50	122.83	113.26
82	GM	203	PEB	CHC-C4C-NC	6.50	129.94	121.15
82	SK	202	PEB	CMB-C2B-C1B	6.49	135.07	125.06
82	Z4	201	PEB	C2C-C1C-NC	6.49	116.31	107.57
82	PK	201	PEB	C2A-C1A-NA	6.49	113.87	108.27
87	B2	812	CLA	C4A-NA-C1A	6.49	109.62	106.71
87	2N	305	CLA	C4A-NA-C1A	6.49	109.62	106.71
82	f1	202	PEB	C1D-CHC-C4C	-6.49	103.69	113.26
85	B2	841	BCR	C7-C8-C9	6.49	136.04	126.23
87	AN	828	CLA	C4A-NA-C1A	6.49	109.62	106.71
82	fH	202	PEB	C1D-CHC-C4C	-6.49	103.69	113.26
85	BN	841	BCR	C7-C8-C9	6.49	136.04	126.23
82	BI	203	PEB	CHC-C1D-ND	-6.49	105.52	113.72
82	qF	202	PEB	CAC-C2C-C1C	6.49	136.09	125.76
91	DL	405	PHO	C4D-ND-C1D	-6.48	102.23	108.83
87	A2	852	CLA	CAC-C3C-C2C	-6.48	116.44	127.53
84	H1	1001	CYC	CAB-C3B-C4B	6.48	131.62	121.38
82	mK	202	PEB	CHA-C4A-NA	-6.48	117.50	125.20
82	TF	202	PEB	CMC-C3C-C4C	6.48	133.93	127.06
84	GG	1001	CYC	OC-C1C-C2C	-6.48	121.02	126.17
82	Z4	201	PEB	CMB-C2B-C1B	6.48	135.04	125.06
82	tK	203	PEB	CHC-C4C-NC	6.48	129.91	121.15
82	AI	203	PEB	C2C-C1C-NC	6.48	116.29	107.57
87	BL	604	CLA	C4A-NA-C1A	6.47	109.62	106.71
82	ZI	401	PEB	C1C-C2C-C3C	-6.47	99.97	107.62
82	IP	203	PEB	C3C-C4C-NC	-6.47	102.51	108.33
87	A2	807	CLA	C4A-NA-C1A	6.47	109.61	106.71
82	lK	203	PEB	CHC-C4C-NC	6.47	129.91	121.15
87	a6	609	CLA	C4A-NA-C1A	6.47	109.61	106.71
87	3N	312	CLA	C4A-NA-C1A	6.47	109.61	106.71
91	D6	404	PHO	O2D-CGD-CBD	6.46	119.19	111.00
87	82	302	CLA	CAC-C3C-C4C	6.46	133.20	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	833	CLA	C4A-NA-C1A	6.46	109.61	106.71
82	UP	203	PEB	CMD-C2D-C3D	-6.46	120.95	130.06
82	Z4	201	PEB	CHB-C4B-C3B	-6.46	110.38	125.32
82	FB	201	PEB	CHC-C4C-NC	6.46	129.89	121.15
87	AN	820	CLA	C4A-NA-C1A	6.46	109.61	106.71
84	BE	1001	CYC	OC-C1C-C2C	-6.46	121.04	126.17
82	ZO	201	PEB	C2C-C1C-NC	6.46	116.26	107.57
82	FA	202	PEB	OA-C1A-C2A	-6.46	121.04	126.17
91	dL	403	PHO	C1C-C2C-C3C	-6.45	103.24	108.61
82	ZO	201	PEB	CHB-C4B-C3B	-6.45	110.39	125.32
82	pF	202	PEB	C1C-CHB-C4B	6.45	142.75	128.28
84	HH	1001	CYC	CAB-C3B-C4B	6.45	131.57	121.38
82	pK	202	PEB	C1C-CHB-C4B	6.45	142.75	128.28
82	GI	201	PEB	C1C-C2C-C3C	-6.45	99.99	107.62
83	Z5	302	PUB	C3B-C4B-NB	6.45	116.25	107.57
82	PF	201	PEB	C2A-C1A-NA	6.45	113.83	108.27
83	A4	302	PUB	CAD-C3D-C4D	6.45	131.56	121.38
87	BN	822	CLA	C4A-NA-C1A	6.45	109.61	106.71
87	bL	615	CLA	C4A-NA-C1A	6.45	109.61	106.71
84	GE	1001	CYC	OC-C1C-C2C	-6.45	121.05	126.17
83	M5	302	PUB	C3B-C4B-NB	6.45	116.25	107.57
82	uF	201	PEB	CHC-C4C-NC	6.45	129.88	121.15
87	AN	803	CLA	C4A-NA-C1A	6.45	109.60	106.71
83	AM	304	PUB	CAD-C3D-C4D	6.45	131.56	121.38
82	hF	201	PEB	OA-C1A-C2A	-6.45	121.05	126.17
87	1N	605	CLA	C4A-NA-C1A	6.44	109.60	106.71
82	KK	201	PEB	CHC-C4C-NC	6.44	129.87	121.15
83	AD	302	PUB	CAD-C3D-C4D	6.44	131.55	121.38
82	V7	202	PEB	OA-C1A-C2A	-6.44	121.05	126.17
82	ZO	201	PEB	CMB-C2B-C1B	6.44	134.98	125.06
82	WP	201	PEB	CMC-C3C-C2C	-6.44	111.68	125.61
82	EF	201	PEB	CMB-C2B-C1B	6.44	134.97	125.06
82	ZG	201	PEB	C2C-C1C-NC	6.44	116.23	107.57
82	mF	202	PEB	CHA-C4A-NA	-6.43	117.56	125.20
82	IJ	202	PEB	CMB-C2B-C1B	6.43	134.97	125.06
82	QA	201	PEB	CHA-C1B-NB	-6.43	111.48	124.93
85	BN	843	BCR	C24-C23-C22	-6.43	116.52	126.23
82	hK	201	PEB	OA-C1A-C2A	-6.43	121.06	126.17
83	AO	302	PUB	CAD-C3D-C4D	6.43	131.53	121.38
87	B6	615	CLA	C4A-NA-C1A	6.43	109.59	106.71
82	cH	202	PEB	CMB-C2B-C1B	6.42	134.96	125.06
85	B2	843	BCR	C24-C23-C22	-6.42	116.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	NO	1001	CYC	OC-C1C-C2C	-6.42	121.07	126.17
82	UP	203	PEB	CMC-C3C-C2C	-6.42	111.73	125.61
91	A6	407	PHO	C4D-ND-C1D	-6.41	102.30	108.83
82	QE	201	PEB	C2C-C1C-NC	6.41	116.20	107.57
82	W1	203	PEB	CHC-C4C-NC	6.41	129.83	121.15
82	Q7	201	PEB	CHA-C1B-NB	-6.41	111.52	124.93
85	cL	504	BCR	C16-C17-C18	-6.41	118.16	127.31
87	BL	601	CLA	C4A-NA-C1A	6.41	109.59	106.71
87	B6	603	CLA	C4A-NA-C1A	6.41	109.59	106.71
82	II	203	PEB	C1C-C2C-C3C	-6.41	100.05	107.62
82	IJ	203	PEB	C1C-C2C-C3C	-6.41	100.05	107.62
82	II	203	PEB	OA-C1A-C2A	-6.41	121.08	126.17
84	N4	1001	CYC	OC-C1C-C2C	-6.40	121.08	126.17
87	B6	608	CLA	C4A-NA-C1A	6.40	109.58	106.71
87	C6	519	CLA	C4A-NA-C1A	6.40	109.58	106.71
82	QG	201	PEB	C2C-C1C-NC	6.40	116.19	107.57
87	8N	307	CLA	C4A-NA-C1A	6.40	109.58	106.71
82	WM	202	PEB	C1C-C2C-C3C	-6.39	100.06	107.62
87	CL	511	CLA	C4A-NA-C1A	6.39	109.58	106.71
85	A6	401	BCR	C15-C14-C13	-6.39	118.19	127.31
87	b6	612	CLA	C4A-NA-C1A	6.39	109.58	106.71
82	GK	203	PEB	CHA-C4A-NA	-6.39	117.61	125.20
82	KF	201	PEB	CHC-C4C-NC	6.39	129.80	121.15
87	32	303	CLA	CMB-C2B-C1B	-6.39	115.64	125.37
87	3N	304	CLA	CMB-C2B-C1B	-6.39	115.64	125.37
87	3N	305	CLA	C20-C18-C19	-6.38	81.07	110.51
87	c6	612	CLA	C4A-NA-C1A	6.38	109.58	106.71
84	BG	1001	CYC	OC-C1C-C2C	-6.38	121.10	126.17
82	QB	201	PEB	C1D-CHC-C4C	6.38	122.66	113.26
87	32	304	CLA	C20-C18-C19	-6.38	81.10	110.51
82	OH	203	PEB	CHC-C4C-NC	6.38	129.78	121.15
87	BN	813	CLA	C4A-NA-C1A	6.38	109.57	106.71
87	bL	616	CLA	C4A-NA-C1A	6.38	109.57	106.71
84	G4	1001	CYC	OC-C1C-C2C	-6.38	121.10	126.17
82	CQ	201	PEB	C1C-C2C-C3C	-6.38	100.08	107.62
87	A2	803	CLA	C4A-NA-C1A	6.37	109.57	106.71
87	a6	607	CLA	C4A-NA-C1A	6.37	109.57	106.71
82	kF	203	PEB	CHC-C4C-NC	6.37	129.78	121.15
82	mG	202	PEB	C1C-CHB-C4B	6.37	142.57	128.28
87	b6	607	CLA	C4A-NA-C1A	6.37	109.57	106.71
82	GF	203	PEB	CHA-C4A-NA	-6.37	117.63	125.20
82	rF	201	PEB	OA-C1A-C2A	-6.37	121.11	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W5	202	PEB	CHC-C4C-NC	6.37	129.76	121.15
87	B2	821	CLA	C4A-NA-C1A	6.36	109.57	106.71
82	WH	203	PEB	CHC-C4C-NC	6.36	129.76	121.15
82	kO	202	PEB	CHC-C4C-NC	6.36	129.76	121.15
82	DQ	202	PEB	CMB-C2B-C1B	6.36	134.86	125.06
82	EP	203	PEB	C3C-C4C-NC	-6.36	102.61	108.33
82	mE	202	PEB	C1C-CHB-C4B	6.36	142.54	128.28
82	ZE	201	PEB	C2C-C1C-NC	6.36	116.13	107.57
91	d6	404	PHO	C1C-C2C-C3C	-6.36	103.33	108.61
82	QA	201	PEB	CMB-C2B-C1B	6.35	134.85	125.06
82	UF	201	PEB	CHC-C1D-ND	-6.35	105.69	113.72
82	MA	201	PEB	CHC-C4C-NC	6.35	129.75	121.15
82	HI	202	PEB	C2C-C1C-NC	6.35	116.12	107.57
82	hG	201	PEB	C1C-CHB-C4B	6.35	142.52	128.28
82	Y5	202	PEB	CHC-C4C-NC	6.34	129.74	121.15
91	a6	613	PHO	C4D-ND-C1D	-6.34	102.38	108.83
83	A1	303	PUB	OD-C4D-C3D	-6.34	121.16	128.04
82	g4	202	PEB	CHC-C4C-NC	6.34	129.73	121.15
85	A2	845	BCR	C24-C23-C22	-6.34	116.66	126.23
83	Z5	302	PUB	CAD-C3D-C4D	6.34	131.39	121.38
87	c6	609	CLA	C4A-NA-C1A	6.34	109.56	106.71
94	A6	410	PL9	C7-C3-C2	-6.33	114.97	123.30
83	xK	301	PUB	CAD-C3D-C4D	6.33	131.38	121.38
87	c6	605	CLA	C4A-NA-C1A	6.33	109.55	106.71
82	UK	201	PEB	CHC-C1D-ND	-6.33	105.71	113.72
82	j4	203	PEB	CHC-C4C-NC	6.33	129.72	121.15
85	AN	845	BCR	C24-C23-C22	-6.33	116.67	126.23
87	52	608	CLA	C4A-NA-C1A	6.33	109.55	106.71
82	rK	201	PEB	OA-C1A-C2A	-6.33	121.14	126.17
83	M5	302	PUB	CAD-C3D-C4D	6.33	131.38	121.38
82	SJ	203	PEB	CHC-C4C-NC	6.33	129.72	121.15
82	m4	202	PEB	CHC-C4C-NC	6.33	129.72	121.15
82	Q1	202	PEB	CHC-C4C-NC	6.33	129.72	121.15
91	AL	410	PHO	O2D-CGD-CBD	6.32	119.01	111.00
87	AN	802	CLA	C4A-NA-C1A	6.32	109.55	106.71
87	62	301	CLA	C4A-NA-C1A	6.32	109.55	106.71
82	hE	201	PEB	C1C-CHB-C4B	6.32	142.45	128.28
85	BN	842	BCR	C7-C8-C9	-6.32	116.69	126.23
82	U1	201	PEB	CHC-C4C-NC	6.32	129.70	121.15
82	M7	201	PEB	CHC-C4C-NC	6.32	129.70	121.15
82	nK	201	PEB	C2A-C1A-NA	6.31	113.72	108.27
84	LE	1001	CYC	CHB-C4A-NA	-6.31	111.73	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QH	202	PEB	CHC-C4C-NC	6.31	129.69	121.15
82	DD	202	PEB	CMB-C2B-C1B	6.31	134.78	125.06
83	AH	303	PUB	OD-C4D-C3D	-6.31	121.19	128.04
82	O1	203	PEB	CHC-C4C-NC	6.31	129.69	121.15
83	QJ	201	PUB	CAD-C3D-C4D	6.31	131.34	121.38
87	6N	613	CLA	C4A-NA-C1A	6.31	109.54	106.71
82	mO	202	PEB	CHC-C4C-NC	6.31	129.69	121.15
87	5N	608	CLA	C4A-NA-C1A	6.31	109.54	106.71
82	KK	201	PEB	C2C-C1C-NC	6.30	116.06	107.57
82	QP	203	PEB	CMD-C2D-C3D	-6.30	121.18	130.06
87	CL	513	CLA	C4A-NA-C1A	6.30	109.54	106.71
82	NA	202	PEB	C2C-C1C-NC	6.30	116.05	107.57
82	B7	202	PEB	CHC-C4C-NC	6.30	129.67	121.15
84	LG	1001	CYC	CHB-C4A-NA	-6.30	111.76	124.93
82	HI	202	PEB	CHB-C1C-C2C	-6.29	112.95	127.15
82	XA	201	PEB	OA-C1A-C2A	-6.29	121.17	126.17
87	C6	514	CLA	C4A-NA-C1A	6.29	109.53	106.71
85	B2	842	BCR	C7-C8-C9	-6.29	116.73	126.23
91	dL	403	PHO	C4D-ND-C1D	-6.29	102.43	108.83
82	WM	202	PEB	CHC-C4C-NC	6.29	129.66	121.15
82	Q7	201	PEB	CMB-C2B-C1B	6.29	134.75	125.06
84	GO	1001	CYC	OC-C1C-C2C	-6.28	121.18	126.17
87	BN	833	CLA	C4A-NA-C1A	6.28	109.53	106.71
82	OA	201	PEB	CHB-C1C-C2C	-6.28	112.98	127.15
87	H6	103	CLA	C4A-NA-C1A	6.28	109.53	106.71
84	LO	1001	CYC	CMA-C3A-C4A	6.28	134.74	125.06
82	SP	201	PEB	CHC-C1D-ND	-6.28	105.78	113.72
82	SM	203	PEB	CHC-C4C-NC	6.28	129.65	121.15
82	GP	201	PEB	CMD-C2D-C3D	-6.28	121.21	130.06
82	O7	201	PEB	CHB-C1C-C2C	-6.28	112.98	127.15
82	OP	201	PEB	CMD-C2D-C3D	-6.28	121.21	130.06
82	X7	202	PEB	C2C-C1C-NC	6.28	116.02	107.57
83	xF	301	PUB	CAD-C3D-C4D	6.28	131.29	121.38
82	gO	202	PEB	CHC-C4C-NC	6.27	129.64	121.15
94	DL	401	PL9	C7-C3-C4	6.27	121.98	116.88
82	KF	201	PEB	C2C-C1C-NC	6.27	116.02	107.57
82	BQ	203	PEB	C2C-C1C-NC	6.27	116.01	107.57
87	6N	603	CLA	C4A-NA-C1A	6.27	109.53	106.71
84	L4	1001	CYC	CMA-C3A-C4A	6.27	134.72	125.06
82	BA	202	PEB	CHC-C4C-NC	6.27	129.63	121.15
87	AN	849	CLA	C4A-NA-C1A	6.27	109.52	106.71
82	KJ	203	PEB	CHC-C1D-ND	-6.26	105.80	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	q3	1001	CYC	CHB-C4A-NA	-6.26	111.83	124.93
82	L9	202	PEB	CHC-C4C-NC	6.26	129.62	121.15
82	N7	202	PEB	C2C-C1C-NC	6.26	116.00	107.57
87	82	307	CLA	C4A-NA-C1A	6.26	109.52	106.71
83	A4	303	PUB	CAD-C3D-C4D	6.26	131.26	121.38
87	aL	606	CLA	O2D-CGD-CBD	6.26	122.39	111.27
82	FQ	203	PEB	CHA-C1B-NB	-6.26	111.84	124.93
84	d3	1001	CYC	CHB-C4A-NA	-6.26	111.84	124.93
84	w3	1001	CYC	CHB-C4A-NA	-6.26	111.84	124.93
82	GF	202	PEB	C2A-C1A-NA	-6.26	102.88	108.27
82	UP	202	PEB	CHC-C4C-NC	6.26	129.62	121.15
82	BD	203	PEB	C2C-C1C-NC	6.26	115.99	107.57
84	Q3	1001	CYC	CHB-C4A-NA	-6.25	111.85	124.93
91	DL	405	PHO	O2D-CGD-CBD	6.25	118.92	111.00
85	KN	101	BCR	C8-C9-C10	-6.25	109.34	118.94
87	JN	101	CLA	C4A-NA-C1A	6.25	109.52	106.71
87	6N	612	CLA	C4A-NA-C1A	6.25	109.52	106.71
82	XA	202	PEB	C2C-C1C-NC	6.25	115.99	107.57
84	h3	1001	CYC	CHB-C4A-NA	-6.25	111.85	124.93
84	F3	1001	CYC	CHB-C4A-NA	-6.25	111.86	124.93
85	K2	102	BCR	C8-C9-C10	-6.25	109.35	118.94
82	X7	201	PEB	OA-C1A-C2A	-6.25	121.20	126.17
82	aJ	203	PEB	CHC-C4C-NC	6.25	129.61	121.15
87	B2	828	CLA	C4A-NA-C1A	6.25	109.52	106.71
82	FD	203	PEB	CHA-C1B-NB	-6.25	111.86	124.93
84	H3	1001	CYC	CHB-C4A-NA	-6.25	111.87	124.93
87	AN	815	CLA	C4A-NA-C1A	6.25	109.51	106.71
84	S3	1001	CYC	CHB-C4A-NA	-6.25	111.87	124.93
84	I3	1001	CYC	CHB-C4A-NA	-6.24	111.87	124.93
91	d6	404	PHO	C4D-ND-C1D	-6.24	102.48	108.83
84	L3	1001	CYC	CHB-C4A-NA	-6.24	111.88	124.93
84	M3	1001	CYC	CHB-C4A-NA	-6.24	111.88	124.93
84	73	1001	CYC	CHB-C4A-NA	-6.24	111.88	124.93
91	aL	610	PHO	C1C-C2C-C3C	-6.24	103.42	108.61
84	U3	1001	CYC	CHB-C4A-NA	-6.24	111.89	124.93
84	f3	1001	CYC	CHB-C4A-NA	-6.24	111.89	124.93
84	n3	1001	CYC	CHB-C4A-NA	-6.24	111.89	124.93
84	u3	1001	CYC	CHB-C4A-NA	-6.24	111.89	124.93
84	o3	1001	CYC	CHB-C4A-NA	-6.24	111.89	124.93
84	B3	1001	CYC	CHB-C4A-NA	-6.23	111.89	124.93
82	S9	201	PEB	CHC-C1D-ND	-6.23	105.84	113.72
82	MM	201	PEB	CHC-C4C-NC	6.23	129.59	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	k3	1001	CYC	CHB-C4A-NA	-6.23	111.90	124.93
82	UH	201	PEB	CHC-C4C-NC	6.23	129.58	121.15
84	O3	1001	CYC	CHB-C4A-NA	-6.23	111.90	124.93
82	IJ	201	PEB	CHC-C4C-NC	6.23	129.58	121.15
82	V1	202	PEB	CHC-C4C-NC	6.23	129.58	121.15
82	GK	202	PEB	C2A-C1A-NA	-6.23	102.91	108.27
84	LH	1001	CYC	CMD-C2D-C1D	6.23	134.67	125.56
84	D3	1001	CYC	CHB-C4A-NA	-6.22	111.91	124.93
84	j3	1001	CYC	CHB-C4A-NA	-6.22	111.91	124.93
87	d6	406	CLA	C4A-NA-C1A	6.22	109.50	106.71
87	22	605	CLA	C4A-NA-C1A	6.22	109.50	106.71
87	42	603	CLA	C4A-NA-C1A	6.22	109.50	106.71
87	62	304	CLA	C4A-NA-C1A	6.22	109.50	106.71
82	IP	203	PEB	CMC-C3C-C2C	-6.22	112.15	125.61
82	KP	201	PEB	CMC-C3C-C2C	-6.22	112.15	125.61
82	BM	301	PEB	CHC-C1D-ND	-6.22	105.85	113.72
87	A2	815	CLA	C4A-NA-C1A	6.22	109.50	106.71
87	B2	833	CLA	C4A-NA-C1A	6.22	109.50	106.71
82	MP	203	PEB	CHC-C1D-ND	-6.22	105.86	113.72
87	BN	806	CLA	C4A-NA-C1A	6.22	109.50	106.71
87	A6	402	CLA	C4A-NA-C1A	6.22	109.50	106.71
87	C6	517	CLA	C4A-NA-C1A	6.22	109.50	106.71
82	KF	202	PEB	CMB-C2B-C1B	6.22	134.64	125.06
82	KK	202	PEB	CMB-C2B-C1B	6.22	134.64	125.06
82	FJ	201	PEB	OA-C1A-C2A	-6.22	121.23	126.17
87	2N	301	CLA	C4A-NA-C1A	6.21	109.50	106.71
82	U4	201	PEB	CHB-C4B-C3B	-6.21	110.95	125.32
82	DD	202	PEB	C2C-C1C-NC	6.21	115.93	107.57
82	ZI	401	PEB	C4B-C3B-C2B	-6.21	99.91	106.78
84	JO	1001	CYC	CMA-C3A-C4A	6.21	134.62	125.06
82	CA	201	PEB	CHA-C1B-NB	-6.21	111.95	124.93
84	I1	1001	CYC	CMD-C2D-C1D	6.20	134.64	125.56
82	hE	201	PEB	CHC-C4C-NC	6.20	129.55	121.15
87	42	608	CLA	C4A-NA-C1A	6.20	109.50	106.71
87	62	313	CLA	C4A-NA-C1A	6.20	109.49	106.71
87	A2	801	CLA	C4A-NA-C1A	6.20	109.49	106.71
83	xF	305	PUB	CAD-C3D-C4D	6.20	131.17	121.38
82	DQ	201	PEB	CHC-C4C-NC	6.20	129.54	121.15
82	zF	501	PEB	C2C-C1C-NC	6.20	115.92	107.57
84	BE	1002	CYC	CHB-C4A-NA	-6.20	111.97	124.93
82	GK	202	PEB	C1C-C2C-C3C	-6.20	100.30	107.62
85	KN	101	BCR	C7-C8-C9	6.20	135.60	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SA	201	PEB	CHC-C4C-NC	6.20	129.53	121.15
91	AL	410	PHO	C1C-C2C-C3C	-6.19	103.46	108.61
82	UO	201	PEB	CHB-C4B-C3B	-6.19	111.00	125.32
87	cL	513	CLA	C4A-NA-C1A	6.19	109.49	106.71
82	SH	203	PEB	CHC-C4C-NC	6.19	129.53	121.15
82	CK	202	PEB	C2C-C1C-NC	6.19	115.90	107.57
82	hG	201	PEB	CHC-C4C-NC	6.19	129.52	121.15
83	AO	303	PUB	CAD-C3D-C4D	6.19	131.15	121.38
82	W4	201	PEB	CMB-C2B-C1B	6.19	134.59	125.06
87	B2	805	CLA	C4A-NA-C1A	6.18	109.49	106.71
82	Y9	202	PEB	CHC-C4C-NC	6.18	129.51	121.15
85	I2	101	BCR	C24-C23-C22	-6.18	116.90	126.23
87	4N	608	CLA	C4A-NA-C1A	6.18	109.48	106.71
85	IN	101	BCR	C24-C23-C22	-6.18	116.90	126.23
84	BG	1002	CYC	CHB-C4A-NA	-6.18	112.01	124.93
87	L2	202	CLA	C4A-NA-C1A	6.18	109.48	106.71
82	S7	201	PEB	CHC-C4C-NC	6.18	129.51	121.15
82	HD	202	PEB	CHA-C1B-NB	-6.18	112.02	124.93
82	S7	201	PEB	C2C-C1C-NC	6.17	115.88	107.57
82	zK	501	PEB	C2C-C1C-NC	6.17	115.88	107.57
83	AH	303	PUB	CAB-C3B-C4B	6.17	135.59	125.76
83	xK	306	PUB	CAD-C3D-C4D	6.17	131.13	121.38
87	BN	828	CLA	C4A-NA-C1A	6.17	109.48	106.71
87	4N	603	CLA	C4A-NA-C1A	6.17	109.48	106.71
82	hM	201	PEB	CHC-C4C-NC	6.17	129.50	121.15
82	TI	201	PEB	C2C-C1C-NC	6.16	115.87	107.57
85	A2	846	BCR	C24-C23-C22	-6.16	116.92	126.23
85	K2	102	BCR	C7-C8-C9	6.16	135.55	126.23
82	DD	201	PEB	CHC-C4C-NC	6.16	129.49	121.15
83	BJ	302	PUB	CHC-C1D-ND	-6.16	105.93	113.72
82	QP	203	PEB	C3C-C4C-NC	-6.16	102.80	108.33
85	Z6	101	BCR	C20-C21-C22	-6.15	118.53	127.31
87	A2	849	CLA	C4A-NA-C1A	6.15	109.47	106.71
87	B2	836	CLA	CMD-C2D-C1D	-6.15	113.87	124.71
82	TB	202	PEB	C1D-CHC-C4C	6.15	122.33	113.26
82	pC	202	PEB	C1D-CHC-C4C	-6.15	104.18	113.26
82	WO	201	PEB	CMB-C2B-C1B	6.15	134.54	125.06
87	BN	836	CLA	CMD-C2D-C1D	-6.15	113.87	124.71
82	gK	201	PEB	C2C-C1C-NC	6.15	115.85	107.57
82	p8	202	PEB	C1D-CHC-C4C	-6.15	104.19	113.26
82	T9	202	PEB	C1D-CHC-C4C	-6.15	104.19	113.26
82	WP	201	PEB	C1D-CHC-C4C	6.15	122.32	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	xK	305	PUB	CAD-C3D-C4D	6.14	131.08	121.38
82	P9	202	PEB	C1D-CHC-C4C	-6.14	104.20	113.26
82	GP	201	PEB	C3C-C4C-NC	-6.14	102.81	108.33
82	R9	202	PEB	C1D-CHC-C4C	-6.14	104.21	113.26
82	I9	202	PEB	C1D-CHC-C4C	-6.14	104.21	113.26
84	F4	1001	CYC	OB-C4B-C3B	-6.14	121.38	128.04
82	SA	201	PEB	C2C-C1C-NC	6.14	115.83	107.57
82	AP	203	PEB	CMC-C3C-C2C	-6.14	112.33	125.61
85	AN	846	BCR	C24-C23-C22	-6.14	116.96	126.23
82	X9	202	PEB	C1D-CHC-C4C	-6.13	104.21	113.26
84	EE	1001	CYC	CAB-C3B-C4B	6.13	131.07	121.38
82	HQ	202	PEB	CHA-C1B-NB	-6.13	112.10	124.93
82	DQ	202	PEB	C2C-C1C-NC	6.13	115.83	107.57
82	G9	202	PEB	C1D-CHC-C4C	-6.13	104.21	113.26
82	K9	202	PEB	C1D-CHC-C4C	-6.13	104.21	113.26
84	EG	1001	CYC	CAB-C3B-C4B	6.13	131.06	121.38
82	OA	201	PEB	CMB-C2B-C1B	6.13	134.50	125.06
82	WE	201	PEB	CMB-C2B-C1B	6.13	134.50	125.06
82	C7	201	PEB	CHA-C1B-NB	-6.13	112.11	124.93
82	MJ	202	PEB	CMB-C2B-C1B	6.13	134.50	125.06
87	LN	202	CLA	C4A-NA-C1A	6.13	109.46	106.71
82	gF	201	PEB	C2C-C1C-NC	6.13	115.82	107.57
83	A1	303	PUB	CAB-C3B-C4B	6.13	135.52	125.76
82	kK	203	PEB	CHC-C4C-NC	6.13	129.44	121.15
82	N9	202	PEB	C1D-CHC-C4C	-6.12	104.23	113.26
87	AN	827	CLA	C4A-NA-C1A	6.12	109.46	106.71
82	JB	202	PEB	C1D-CHC-C4C	6.12	122.28	113.26
82	V9	202	PEB	C1D-CHC-C4C	-6.12	104.23	113.26
82	CF	202	PEB	C2C-C1C-NC	6.12	115.81	107.57
82	EP	203	PEB	CMD-C2D-C3D	-6.12	121.43	130.06
87	32	307	CLA	C4B-CHC-C1C	6.12	140.85	126.34
82	YF	203	PEB	CHA-C1B-NB	-6.12	112.14	124.93
82	Z1	201	PEB	CHB-C1C-C2C	-6.12	113.35	127.15
85	cL	518	BCR	C40-C30-C29	-6.11	84.45	108.91
82	MP	203	PEB	C3C-C4C-NC	-6.11	102.83	108.33
82	E9	202	PEB	C1D-CHC-C4C	-6.11	104.24	113.26
82	C9	202	PEB	C1D-CHC-C4C	-6.11	104.24	113.26
87	C6	515	CLA	C4A-NA-C1A	6.11	109.45	106.71
82	UJ	203	PEB	CHC-C4C-NC	6.11	129.42	121.15
82	UJ	202	PEB	CMB-C2B-C1B	6.11	134.47	125.06
87	3N	308	CLA	C4B-CHC-C1C	6.11	140.83	126.34
83	xF	306	PUB	CAD-C3D-C4D	6.11	131.03	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BM	301	PEB	CAC-C2C-C1C	6.11	135.49	125.76
84	DO	1001	CYC	CMD-C2D-C1D	6.11	134.50	125.56
82	nF	201	PEB	C2A-C1A-NA	6.11	113.54	108.27
84	D4	1001	CYC	CMD-C2D-C1D	6.11	134.50	125.56
82	WI	202	PEB	C2C-C1C-NC	6.11	115.79	107.57
82	GF	202	PEB	C1C-C2C-C3C	-6.11	100.40	107.62
83	M5	302	PUB	OD-C4D-C3D	-6.10	121.42	128.04
83	QM	201	PUB	CAD-C3D-C4D	6.10	131.02	121.38
82	GJ	203	PEB	CHC-C4C-NC	6.10	129.41	121.15
82	O7	201	PEB	CMB-C2B-C1B	6.10	134.46	125.06
82	SK	201	PEB	CHC-C4C-NC	6.10	129.41	121.15
82	ZH	201	PEB	CHB-C1C-C2C	-6.10	113.38	127.15
82	KF	202	PEB	CHA-C1B-NB	-6.10	112.17	124.93
82	HD	203	PEB	CHC-C1D-ND	-6.10	106.00	113.72
82	Q4	201	PEB	C2C-C1C-NC	6.10	115.78	107.57
87	AN	826	CLA	C4A-NA-C1A	6.10	109.45	106.71
82	A9	202	PEB	C1D-CHC-C4C	-6.10	104.27	113.26
87	K2	103	CLA	C4A-NA-C1A	6.10	109.45	106.71
87	6N	606	CLA	C4A-NA-C1A	6.10	109.45	106.71
91	D6	404	PHO	C1C-C2C-C3C	-6.10	103.54	108.61
82	DK	202	PEB	CHC-C4C-NC	6.10	129.40	121.15
82	B9	202	PEB	CHB-C1C-C2C	-6.10	113.40	127.15
85	Z6	101	BCR	C39-C30-C25	6.09	120.19	110.30
82	C7	201	PEB	CMB-C2B-C1B	6.09	134.45	125.06
87	KN	102	CLA	C4A-NA-C1A	6.09	109.45	106.71
87	J2	101	CLA	C4A-NA-C1A	6.09	109.44	106.71
82	H9	202	PEB	C2C-C1C-NC	6.09	115.77	107.57
82	QO	201	PEB	C2C-C1C-NC	6.09	115.77	107.57
85	CL	516	BCR	C40-C30-C29	-6.09	84.55	108.91
87	B2	825	CLA	C4A-NA-C1A	6.09	109.44	106.71
82	tF	202	PEB	C1C-CHB-C4B	6.09	141.93	128.28
87	32	307	CLA	CHB-C1B-NB	6.09	130.70	124.26
82	VA	202	PEB	C2C-C1C-NC	6.09	115.77	107.57
82	GP	201	PEB	CHC-C1D-ND	-6.08	106.03	113.72
82	M5	304	PEB	CHA-C1B-NB	-6.08	112.20	124.93
82	HQ	203	PEB	CHC-C1D-ND	-6.08	106.03	113.72
82	GK	202	PEB	C3B-C4B-NB	6.08	118.90	110.05
82	Z5	304	PEB	CHA-C1B-NB	-6.08	112.21	124.93
82	CA	201	PEB	CMB-C2B-C1B	6.08	134.43	125.06
82	IF	201	PEB	OA-C1A-C2A	6.08	131.01	126.17
82	H9	202	PEB	CHC-C4C-NC	6.08	129.38	121.15
84	J4	1001	CYC	CMA-C3A-C4A	6.08	134.42	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	A2	831	CLA	C4A-NA-C1A	6.08	109.44	106.71
82	KK	202	PEB	CHA-C1B-NB	-6.08	112.22	124.93
82	F9	201	PEB	CHC-C1D-ND	-6.08	106.04	113.72
82	GP	201	PEB	CMC-C3C-C2C	-6.08	112.46	125.61
82	YK	203	PEB	CHA-C1B-NB	-6.07	112.22	124.93
82	DF	202	PEB	CHC-C4C-NC	6.07	129.37	121.15
84	FO	1001	CYC	OB-C4B-C3B	-6.07	121.45	128.04
82	MJ	203	PEB	CHC-C4C-NC	6.07	129.37	121.15
82	WJ	203	PEB	C2C-C1C-NC	6.07	115.74	107.57
83	Z5	302	PUB	OD-C4D-C3D	-6.07	121.45	128.04
82	HK	201	PEB	CHA-C1B-NB	-6.07	112.24	124.93
82	WG	201	PEB	CMB-C2B-C1B	6.07	134.41	125.06
82	V7	202	PEB	C2C-C1C-NC	6.07	115.74	107.57
83	AG	302	PUB	CAD-C3D-C4D	6.07	130.96	121.38
82	MJ	201	PEB	CHC-C4C-NC	6.06	129.36	121.15
82	P7	202	PEB	CHC-C4C-NC	6.06	129.36	121.15
87	8N	303	CLA	C4A-NA-C1A	6.06	109.43	106.71
82	F5	202	PEB	C2C-C1C-NC	6.06	115.73	107.57
82	d1	202	PEB	CHC-C4C-NC	6.06	129.35	121.15
87	R2	202	CLA	C4A-NA-C1A	6.06	109.43	106.71
87	c6	610	CLA	C4A-NA-C1A	6.06	109.43	106.71
82	HF	201	PEB	CHA-C1B-NB	-6.06	112.25	124.93
82	SF	201	PEB	CHC-C4C-NC	6.06	129.35	121.15
82	PA	202	PEB	CHC-C4C-NC	6.06	129.35	121.15
87	C6	510	CLA	C4A-NA-C1A	6.06	109.43	106.71
82	WH	201	PEB	CHC-C4C-NC	6.06	129.35	121.15
82	VA	202	PEB	CHC-C4C-NC	6.06	129.35	121.15
82	JA	202	PEB	CHC-C4C-NC	6.06	129.35	121.15
82	IK	201	PEB	C4B-C3B-C2B	-6.05	100.08	106.78
87	A2	827	CLA	C4A-NA-C1A	6.05	109.43	106.71
82	SF	201	PEB	CHC-C1D-ND	-6.05	106.07	113.72
82	PD	203	PEB	CHC-C1D-ND	-6.05	106.07	113.72
82	F9	202	PEB	CHC-C4C-NC	6.05	129.34	121.15
82	IF	201	PEB	C4B-C3B-C2B	-6.05	100.09	106.78
82	fK	201	PEB	C2A-C1A-NA	6.05	113.49	108.27
82	PQ	203	PEB	CHC-C1D-ND	-6.05	106.07	113.72
82	CM	203	PEB	CHC-C1D-ND	-6.05	106.07	113.72
82	MF	203	PEB	C2C-C1C-NC	6.04	115.70	107.57
87	RN	203	CLA	C4A-NA-C1A	6.04	109.42	106.71
82	HD	201	PEB	CHC-C4C-NC	6.04	129.32	121.15
87	AN	831	CLA	C4A-NA-C1A	6.04	109.42	106.71
82	HQ	201	PEB	CHC-C4C-NC	6.03	129.32	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SK	201	PEB	CHC-C1D-ND	-6.03	106.09	113.72
85	AN	847	BCR	C11-C10-C9	-6.03	118.70	127.31
82	QA	201	PEB	C2C-C1C-NC	6.03	115.69	107.57
82	AF	201	PEB	CMB-C2B-C1B	6.03	134.35	125.06
82	tK	202	PEB	C1C-CHB-C4B	6.03	141.80	128.28
82	lJ	202	PEB	CMB-C2B-C1B	6.03	134.35	125.06
82	H1	1002	PEB	CHC-C1D-ND	-6.03	106.10	113.72
82	V7	202	PEB	CHC-C4C-NC	6.03	129.31	121.15
82	W1	201	PEB	CHC-C4C-NC	6.03	129.31	121.15
82	PD	202	PEB	CMB-C2B-C1B	6.02	134.34	125.06
82	dH	202	PEB	CHC-C4C-NC	6.02	129.30	121.15
87	72	602	CLA	C4D-C3D-CAD	-6.02	101.00	108.10
82	AK	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
82	Q7	201	PEB	C2C-C1C-NC	6.02	115.67	107.57
87	BL	619	CLA	C4A-NA-C1A	6.02	109.41	106.71
82	qK	202	PEB	C1C-C2C-C3C	-6.02	100.51	107.62
85	B2	802	BCR	C40-C30-C29	-6.02	84.84	108.91
87	32	303	CLA	C4A-NA-C1A	6.01	109.41	106.71
83	yF	302	PUB	OD-C4D-C3D	-6.01	121.51	128.04
82	UP	202	PEB	C1C-C2C-C3C	-6.01	100.51	107.62
82	MK	203	PEB	C2C-C1C-NC	6.01	115.67	107.57
85	c6	603	BCR	C20-C21-C22	-6.01	118.73	127.31
87	7N	602	CLA	C4D-C3D-CAD	-6.01	101.01	108.10
87	B6	609	CLA	C4A-NA-C1A	6.01	109.41	106.71
83	AJ	303	PUB	CAD-C3D-C4D	6.01	130.87	121.38
85	BN	803	BCR	C40-C30-C29	-6.01	84.87	108.91
85	BN	803	BCR	C39-C30-C25	6.01	120.05	110.30
87	B2	804	CLA	C4A-NA-C1A	6.01	109.41	106.71
87	b6	611	CLA	C4A-NA-C1A	6.01	109.41	106.71
82	CP	201	PEB	C3C-C4C-NC	-6.01	102.93	108.33
82	PQ	202	PEB	CMB-C2B-C1B	6.01	134.31	125.06
85	fL	101	BCR	C3-C4-C5	-6.01	103.35	114.08
87	62	307	CLA	C4A-NA-C1A	6.01	109.41	106.71
87	3N	308	CLA	CHB-C1B-NB	6.00	130.61	124.26
82	S1	201	PEB	CHA-C1B-NB	-6.00	112.37	124.93
87	bL	605	CLA	C4A-NA-C1A	6.00	109.41	106.71
82	HA	203	PEB	CAB-C3B-C4B	6.00	135.63	125.01
82	VB	201	PEB	CMC-C3C-C4C	6.00	133.42	127.06
85	A2	847	BCR	C11-C10-C9	-6.00	118.74	127.31
82	e4	202	PEB	CHC-C4C-NC	6.00	129.27	121.15
87	AL	403	CLA	C4A-NA-C1A	6.00	109.40	106.71
87	BN	801	CLA	C4A-NA-C1A	6.00	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	J7	202	PEB	CHC-C4C-NC	6.00	129.27	121.15
85	AN	846	BCR	C37-C22-C21	-6.00	114.52	122.92
83	AG	303	PUB	CAD-C3D-C4D	6.00	130.85	121.38
87	BN	805	CLA	C4A-NA-C1A	6.00	109.40	106.71
82	UF	201	PEB	CHB-C4B-C3B	-6.00	111.45	125.32
83	A4	303	PUB	OD-C4D-C3D	-5.99	121.53	128.04
82	UJ	201	PEB	CHC-C4C-NC	5.99	129.26	121.15
87	R2	203	CLA	C4A-NA-C1A	5.99	109.40	106.71
83	AE	302	PUB	CAD-C3D-C4D	5.99	130.84	121.38
103	82	310	ZEX	C11-C12-C13	-5.99	109.59	126.42
82	FQ	201	PEB	CMB-C2B-C1B	5.99	134.28	125.06
83	yK	302	PUB	OD-C4D-C3D	-5.99	121.54	128.04
83	AJ	304	PUB	CAD-C3D-C4D	5.99	130.84	121.38
82	GF	202	PEB	C3B-C4B-NB	5.98	118.75	110.05
84	DG	1001	CYC	OB-C4B-C3B	-5.98	121.55	128.04
103	8N	310	ZEX	C11-C12-C13	-5.98	109.61	126.42
82	W9	201	PEB	C4B-C3B-C2B	-5.98	100.16	106.78
85	B2	802	BCR	C39-C30-C25	5.98	120.00	110.30
82	MP	203	PEB	CMC-C3C-C2C	-5.98	112.67	125.61
82	SG	203	PEB	C2C-C1C-NC	5.98	115.62	107.57
82	eO	202	PEB	CHC-C4C-NC	5.98	129.24	121.15
82	DD	202	PEB	CHB-C1C-C2C	-5.97	113.67	127.15
82	Q4	201	PEB	CHB-C4B-C3B	-5.97	111.50	125.32
83	AE	303	PUB	CAD-C3D-C4D	5.97	130.81	121.38
87	62	303	CLA	C4A-NA-C1A	5.97	109.39	106.71
85	A2	846	BCR	C19-C18-C17	5.97	128.10	118.94
87	4N	606	CLA	C4A-NA-C1A	5.97	109.39	106.71
82	BI	202	PEB	C2C-C1C-NC	5.97	115.61	107.57
82	UK	201	PEB	CHB-C4B-C3B	-5.97	111.51	125.32
83	yF	303	PUB	OD-C4D-C3D	-5.97	121.56	128.04
87	3N	304	CLA	C4A-NA-C1A	5.97	109.39	106.71
82	BK	201	PEB	CHC-C4C-NC	5.97	129.22	121.15
83	AH	304	PUB	OD-C4D-C3D	-5.96	121.57	128.04
82	uC	201	PEB	C1C-C2C-C3C	-5.96	100.57	107.62
82	V4	202	PEB	C2C-C1C-NC	5.96	115.60	107.57
85	A2	846	BCR	C37-C22-C21	-5.96	114.57	122.92
83	AJ	304	PUB	OD-C4D-C3D	-5.96	121.57	128.04
82	qF	202	PEB	C1C-C2C-C3C	-5.96	100.57	107.62
82	AP	203	PEB	C3C-C4C-NC	-5.96	102.97	108.33
82	DQ	202	PEB	CHB-C1C-C2C	-5.96	113.70	127.15
83	AG	302	PUB	CHC-C1D-ND	-5.96	106.18	113.72
82	BF	201	PEB	CHC-C4C-NC	5.96	129.22	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	fF	201	PEB	C2A-C1A-NA	5.96	113.41	108.27
83	A1	304	PUB	OD-C4D-C3D	-5.96	121.57	128.04
82	SP	201	PEB	CMD-C2D-C3D	-5.96	121.66	130.06
82	aK	201	PEB	CHC-C4C-NC	5.96	129.22	121.15
84	DE	1001	CYC	OB-C4B-C3B	-5.96	121.57	128.04
82	QO	201	PEB	CHB-C4B-C3B	-5.96	111.54	125.32
82	H7	203	PEB	CAB-C3B-C4B	5.96	135.55	125.01
84	M4	1001	CYC	OC-C1C-C2C	-5.95	121.44	126.17
82	X7	202	PEB	CHC-C4C-NC	5.95	129.20	121.15
82	SH	201	PEB	CHA-C1B-NB	-5.95	112.48	124.93
82	IP	203	PEB	C1D-CHC-C4C	5.95	122.03	113.26
82	kE	201	PEB	CAC-C2C-C1C	5.95	135.24	125.76
82	hJ	203	PEB	CHC-C1D-ND	-5.95	106.20	113.72
84	W3	1001	CYC	CHD-C1D-ND	-5.94	111.70	125.32
82	SG	203	PEB	CHC-C4C-NC	5.94	129.19	121.15
85	AN	846	BCR	C19-C18-C17	5.94	128.06	118.94
82	aF	201	PEB	CHC-C4C-NC	5.94	129.19	121.15
103	82	310	ZEX	C31-C30-C29	-5.94	118.83	127.31
82	kG	201	PEB	CAC-C2C-C1C	5.94	135.23	125.76
82	cM	201	PEB	C1D-CHC-C4C	5.94	122.01	113.26
84	y3	1001	CYC	CHB-C4A-NA	-5.94	112.51	124.93
103	8N	310	ZEX	C31-C30-C29	-5.93	118.84	127.31
82	XA	202	PEB	CHC-C4C-NC	5.93	129.18	121.15
84	y3	1001	CYC	CHD-C1D-ND	-5.93	111.73	125.32
82	WP	201	PEB	CMD-C2D-C3D	-5.93	121.70	130.06
82	IK	201	PEB	OA-C1A-C2A	5.93	130.89	126.17
83	yF	303	PUB	CAD-C3D-C4D	5.93	130.75	121.38
82	EP	203	PEB	CMC-C3C-C2C	-5.93	112.78	125.61
84	W3	1001	CYC	CHB-C4A-NA	-5.93	112.53	124.93
83	xK	306	PUB	OD-C4D-C3D	-5.93	121.61	128.04
82	FD	201	PEB	CMB-C2B-C1B	5.93	134.19	125.06
85	LN	205	BCR	C7-C8-C9	-5.93	117.28	126.23
82	VO	202	PEB	C2C-C1C-NC	5.93	115.55	107.57
84	C1	1001	CYC	CMD-C2D-C1D	5.92	134.23	125.56
83	wF	304	PUB	CAD-C3D-C4D	5.92	130.73	121.38
82	HH	1002	PEB	CHC-C1D-ND	-5.92	106.23	113.72
84	73	1002	CYC	CHB-C4A-C3A	5.92	140.12	124.90
83	AO	302	PUB	OD-C4D-C3D	-5.91	121.62	128.04
87	4N	604	CLA	C3D-C4D-ND	5.91	119.81	110.24
85	L2	205	BCR	C7-C8-C9	-5.91	117.30	126.23
82	SE	202	PEB	CHC-C4C-NC	5.91	129.15	121.15
83	xF	305	PUB	OD-C4D-C3D	-5.91	121.62	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lJ	201	PEB	CHC-C4C-NC	5.91	129.15	121.15
87	RN	202	CLA	C4A-NA-C1A	5.91	109.36	106.71
83	xF	306	PUB	OD-C4D-C3D	-5.91	121.63	128.04
84	LE	1001	CYC	CMA-C3A-C4A	5.91	134.16	125.06
87	42	604	CLA	C3D-C4D-ND	5.91	119.80	110.24
83	AE	302	PUB	CHC-C1D-ND	-5.91	106.25	113.72
83	yK	303	PUB	OD-C4D-C3D	-5.90	121.63	128.04
82	SE	202	PEB	C2C-C1C-NC	5.90	115.52	107.57
82	u8	201	PEB	C1C-C2C-C3C	-5.90	100.65	107.62
82	UA	201	PEB	C2C-C1C-NC	5.90	115.51	107.57
87	A2	850	CLA	C4A-NA-C1A	5.90	109.36	106.71
82	R4	202	PEB	C2C-C1C-NC	5.89	115.51	107.57
82	xF	302	PEB	C1C-CHB-C4B	-5.89	115.07	128.28
82	JF	201	PEB	C2A-C1A-NA	5.89	113.35	108.27
82	QP	203	PEB	CMC-C3C-C2C	-5.89	112.86	125.61
82	XA	202	PEB	CHB-C1C-C2C	-5.89	113.86	127.15
87	42	606	CLA	C4A-NA-C1A	5.89	109.35	106.71
83	BJ	302	PUB	OD-C4D-C3D	-5.89	121.65	128.04
82	WF	202	PEB	CMB-C2B-C1B	5.89	134.13	125.06
84	CH	1001	CYC	CMD-C2D-C1D	5.89	134.18	125.56
84	LG	1001	CYC	CMA-C3A-C4A	5.89	134.13	125.06
84	MO	1001	CYC	OC-C1C-C2C	-5.88	121.50	126.17
87	82	302	CLA	C4A-NA-C1A	5.88	109.35	106.71
83	wK	304	PUB	CAD-C3D-C4D	5.88	130.67	121.38
83	A4	302	PUB	OD-C4D-C3D	-5.88	121.66	128.04
85	b6	603	BCR	C11-C10-C9	-5.88	118.92	127.31
87	6N	602	CLA	C4A-NA-C1A	5.88	109.35	106.71
84	f3	1001	CYC	CMB-C2B-C1B	5.88	131.51	124.17
82	oK	203	PEB	OA-C1A-C2A	-5.88	121.50	126.17
87	c6	613	CLA	C4A-NA-C1A	5.87	109.35	106.71
84	S3	1001	CYC	CMB-C2B-C1B	5.87	131.50	124.17
84	u3	1001	CYC	CMB-C2B-C1B	5.87	131.50	124.17
87	A2	826	CLA	C4A-NA-C1A	5.87	109.35	106.71
82	xK	302	PEB	C1C-CHB-C4B	-5.87	115.11	128.28
82	U7	201	PEB	C2C-C1C-NC	5.87	115.47	107.57
82	OH	201	PEB	CHC-C4C-NC	5.87	129.09	121.15
87	BN	824	CLA	C4A-NA-C1A	5.86	109.34	106.71
82	W4	201	PEB	C2C-C1C-NC	5.86	115.47	107.57
84	h3	1001	CYC	CMB-C2B-C1B	5.86	131.49	124.17
82	N7	201	PEB	OA-C1A-C2A	-5.86	121.51	126.17
82	RO	202	PEB	C2C-C1C-NC	5.86	115.46	107.57
82	F9	201	PEB	C1C-C2C-C3C	-5.85	100.70	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RI	203	PEB	C2C-C1C-NC	5.85	115.45	107.57
84	F3	1001	CYC	CMB-C2B-C1B	5.85	131.48	124.17
82	TA	202	PEB	CHC-C4C-NC	5.85	129.07	121.15
82	NI	203	PEB	CHA-C1B-NB	-5.85	112.69	124.93
82	BJ	301	PEB	CAC-C2C-C1C	5.85	135.08	125.76
82	R7	202	PEB	CHC-C4C-NC	5.85	129.06	121.15
84	73	1001	CYC	CMB-C2B-C1B	5.85	131.47	124.17
85	b6	602	BCR	C24-C23-C22	-5.85	117.40	126.23
82	qF	202	PEB	CHB-C1C-NC	-5.85	111.93	125.32
87	a6	608	CLA	C4A-NA-C1A	5.85	109.33	106.71
82	T7	202	PEB	C2A-C1A-NA	5.85	113.31	108.27
83	Z9	305	PUB	C1C-C2C-C3C	-5.84	100.31	106.78
83	QM	201	PUB	OD-C4D-C3D	-5.84	121.70	128.04
83	AO	303	PUB	OD-C4D-C3D	-5.84	121.70	128.04
82	X7	202	PEB	CHB-C1C-C2C	-5.84	113.97	127.15
84	D3	1001	CYC	CMB-C2B-C1B	5.84	131.46	124.17
83	xK	305	PUB	OD-C4D-C3D	-5.84	121.70	128.04
84	H3	1001	CYC	CMB-C2B-C1B	5.84	131.46	124.17
84	L3	1001	CYC	CMB-C2B-C1B	5.84	131.46	124.17
82	lH	202	PEB	CHA-C1B-NB	-5.84	112.72	124.93
87	b6	610	CLA	C4A-NA-C1A	5.84	109.33	106.71
83	AQ	302	PUB	OD-C4D-C3D	-5.84	121.70	128.04
85	d6	405	BCR	C16-C17-C18	-5.84	118.98	127.31
91	AL	410	PHO	C4D-ND-C1D	-5.84	102.89	108.83
87	cL	515	CLA	C4A-NA-C1A	5.84	109.33	106.71
82	WM	203	PEB	C2C-C1C-NC	5.84	115.43	107.57
82	JK	201	PEB	C2A-C1A-NA	5.84	113.30	108.27
82	SK	202	PEB	CHA-C1B-NB	-5.84	112.73	124.93
82	oF	203	PEB	OA-C1A-C2A	-5.83	121.53	126.17
84	q3	1001	CYC	CMB-C2B-C1B	5.83	131.45	124.17
84	w3	1001	CYC	CMB-C2B-C1B	5.83	131.45	124.17
82	RA	202	PEB	CHC-C4C-NC	5.83	129.04	121.15
84	d3	1001	CYC	CMB-C2B-C1B	5.83	131.45	124.17
82	YM	201	PEB	C2C-C1C-NC	5.83	115.42	107.57
84	n3	1001	CYC	CMB-C2B-C1B	5.83	131.45	124.17
84	o3	1001	CYC	CMB-C2B-C1B	5.83	131.45	124.17
82	WM	202	PEB	CMC-C3C-C4C	-5.83	120.88	127.06
82	l1	203	PEB	CHA-C1B-NB	-5.83	112.74	124.93
84	M3	1001	CYC	CMB-C2B-C1B	5.83	131.44	124.17
84	j3	1001	CYC	CMB-C2B-C1B	5.83	131.44	124.17
84	k3	1001	CYC	CMB-C2B-C1B	5.83	131.44	124.17
84	O3	1001	CYC	CMB-C2B-C1B	5.82	131.44	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	KO	1001	CYC	OC-C1C-C2C	-5.82	121.54	126.17
82	YM	203	PEB	CHC-C4C-NC	5.82	129.03	121.15
84	I3	1001	CYC	CMB-C2B-C1B	5.82	131.44	124.17
84	Q3	1001	CYC	CMB-C2B-C1B	5.82	131.44	124.17
82	WO	201	PEB	C2C-C1C-NC	5.82	115.41	107.57
82	O1	201	PEB	CHC-C4C-NC	5.82	129.03	121.15
84	GO	1001	CYC	CAB-C3B-C4B	5.82	130.56	121.38
83	AH	304	PUB	CAD-C3D-C4D	5.81	130.56	121.38
87	AN	850	CLA	C4A-NA-C1A	5.81	109.32	106.71
84	U3	1001	CYC	CMB-C2B-C1B	5.81	131.43	124.17
82	eE	203	PEB	C1C-C2C-C3C	-5.81	100.75	107.62
84	JH	1001	CYC	CMA-C3A-C4A	5.81	134.01	125.06
82	TA	202	PEB	C2A-C1A-NA	5.81	113.28	108.27
83	yK	303	PUB	CAD-C3D-C4D	5.81	130.55	121.38
84	B3	1001	CYC	CMB-C2B-C1B	5.81	131.42	124.17
82	WK	202	PEB	CMB-C2B-C1B	5.81	134.01	125.06
82	SH	203	PEB	OA-C1A-C2A	-5.81	121.56	126.17
82	eK	202	PEB	C2C-C1C-NC	5.81	115.39	107.57
82	SA	201	PEB	CHB-C1C-C2C	-5.80	114.06	127.15
82	T7	202	PEB	CHC-C4C-NC	5.80	129.00	121.15
85	C6	508	BCR	C24-C23-C22	5.80	135.00	126.23
82	eF	202	PEB	C2C-C1C-NC	5.80	115.38	107.57
82	EF	201	PEB	C2C-C1C-NC	5.80	115.38	107.57
82	SF	202	PEB	CHA-C1B-NB	-5.80	112.81	124.93
91	aL	610	PHO	C2D-C1D-ND	5.79	113.53	109.53
84	G4	1001	CYC	CAB-C3B-C4B	5.79	130.53	121.38
87	2N	308	CLA	C4A-NA-C1A	5.79	109.31	106.71
82	qK	202	PEB	CHB-C1C-NC	-5.79	112.05	125.32
82	MM	201	PEB	CHC-C1D-ND	-5.79	106.40	113.72
82	T7	203	PEB	CHC-C1D-ND	-5.79	106.40	113.72
82	YG	201	PEB	C1C-C2C-C3C	-5.79	100.78	107.62
82	d1	203	PEB	CHA-C1B-NB	-5.79	112.83	124.93
82	TA	203	PEB	CHC-C1D-ND	-5.79	106.40	113.72
83	xK	301	PUB	C1D-CHC-C4C	-5.79	100.78	113.37
85	c6	602	BCR	C11-C10-C9	-5.78	119.06	127.31
82	eG	203	PEB	C1C-C2C-C3C	-5.78	100.79	107.62
83	A1	303	PUB	CAD-C3D-C4D	5.78	130.51	121.38
82	WP	201	PEB	C3C-C4C-NC	-5.78	103.14	108.33
84	K4	1001	CYC	OC-C1C-C2C	-5.78	121.58	126.17
82	YE	201	PEB	C1C-C2C-C3C	-5.78	100.79	107.62
83	AD	302	PUB	OD-C4D-C3D	-5.78	121.77	128.04
82	Y5	203	PEB	CHC-C1D-ND	-5.78	106.41	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NA	201	PEB	OA-C1A-C2A	-5.78	121.58	126.17
87	aL	606	CLA	CMD-C2D-C1D	5.78	134.90	124.71
82	s8	201	PEB	CMB-C2B-C1B	5.78	133.96	125.06
84	BE	1001	CYC	CAB-C3B-C4B	5.78	130.50	121.38
82	HD	202	PEB	CHC-C4C-NC	5.77	128.96	121.15
85	A2	848	BCR	C7-C8-C9	-5.77	117.51	126.23
82	S7	201	PEB	CHB-C1C-C2C	-5.77	114.12	127.15
84	D1	1001	CYC	OC-C1C-C2C	-5.77	121.58	126.17
85	bL	602	BCR	C7-C8-C9	5.77	134.96	126.23
82	rC	202	PEB	C1D-CHC-C4C	-5.77	104.75	113.26
83	AH	303	PUB	CAD-C3D-C4D	5.77	130.49	121.38
82	TB	201	PEB	CHA-C1B-NB	-5.77	112.86	124.93
82	HD	202	PEB	CMB-C2B-C1B	5.77	133.95	125.06
82	HQ	202	PEB	CMB-C2B-C1B	5.77	133.95	125.06
82	D9	201	PEB	C4B-C3B-C2B	-5.77	100.40	106.78
83	A1	304	PUB	CAD-C3D-C4D	5.77	130.49	121.38
82	r8	202	PEB	C1D-CHC-C4C	-5.77	104.75	113.26
85	AN	804	BCR	C3-C4-C5	-5.77	103.78	114.08
85	AN	848	BCR	C7-C8-C9	-5.77	117.52	126.23
82	R7	202	PEB	CHC-C1D-ND	-5.77	106.43	113.72
83	AM	304	PUB	OD-C4D-C3D	-5.77	121.78	128.04
87	22	609	CLA	C4A-NA-C1A	5.77	109.30	106.71
84	EH	1001	CYC	OB-C4B-C3B	-5.76	121.79	128.04
82	JB	201	PEB	CHA-C1B-NB	-5.76	112.88	124.93
82	VO	202	PEB	CHB-C1C-C2C	-5.76	114.15	127.15
82	F1	1002	PEB	OA-C1A-C2A	-5.76	121.59	126.17
82	J9	202	PEB	CHC-C4C-NC	5.76	128.95	121.15
82	HK	201	PEB	C2C-C1C-NC	5.76	115.32	107.57
82	gF	203	PEB	CHA-C1B-NB	-5.76	112.89	124.93
82	lK	203	PEB	CHA-C1B-NB	-5.76	112.89	124.93
85	A2	804	BCR	C3-C4-C5	-5.76	103.80	114.08
82	TQ	203	PEB	CHC-C1D-ND	-5.76	106.44	113.72
87	B2	823	CLA	C4A-NA-C1A	5.75	109.29	106.71
82	OP	201	PEB	C3C-C4C-NC	-5.75	103.16	108.33
82	Z9	303	PEB	OA-C1A-C2A	-5.75	121.60	126.17
85	cL	504	BCR	C24-C23-C22	5.75	134.93	126.23
82	ZH	201	PEB	C2C-C1C-NC	5.75	115.31	107.57
82	HF	201	PEB	C2C-C1C-NC	5.75	115.31	107.57
82	V4	202	PEB	CHB-C1C-C2C	-5.75	114.18	127.15
87	CL	504	CLA	C4A-NA-C1A	5.75	109.29	106.71
84	E1	1001	CYC	OB-C4B-C3B	-5.75	121.80	128.04
85	FL	101	BCR	C3-C4-C5	-5.75	103.82	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YJ	203	PEB	CHC-C4C-NC	5.74	128.93	121.15
82	YA	303	PEB	C1C-CHB-C4B	-5.74	115.40	128.28
83	xF	301	PUB	C1D-CHC-C4C	-5.74	100.87	113.37
82	lJ	202	PEB	CHA-C1B-NB	-5.74	112.92	124.93
84	DH	1001	CYC	OC-C1C-C2C	-5.74	121.61	126.17
82	EK	201	PEB	C2C-C1C-NC	5.74	115.30	107.57
82	K7	201	PEB	C1C-C2C-C3C	-5.74	100.83	107.62
82	EA	201	PEB	CHC-C4C-NC	5.74	128.92	121.15
82	QM	202	PEB	CHC-C4C-NC	5.74	128.92	121.15
82	AI	203	PEB	C1C-C2C-C3C	-5.74	100.84	107.62
85	F2	203	BCR	C3-C4-C5	-5.74	103.83	114.08
85	FN	202	BCR	C3-C4-C5	-5.74	103.83	114.08
82	RA	202	PEB	CHC-C1D-ND	-5.74	106.47	113.72
82	MJ	202	PEB	C2C-C1C-NC	5.74	115.29	107.57
82	TK	201	PEB	C2A-C1A-NA	5.73	113.22	108.27
82	U9	202	PEB	CHC-C4C-NC	5.73	128.91	121.15
82	gK	203	PEB	CHA-C1B-NB	-5.73	112.94	124.93
82	P7	202	PEB	C2C-C1C-NC	5.73	115.29	107.57
82	HQ	202	PEB	CHC-C4C-NC	5.73	128.91	121.15
82	Z1	201	PEB	C2C-C1C-NC	5.73	115.29	107.57
82	dH	203	PEB	CHA-C1B-NB	-5.73	112.95	124.93
82	NA	202	PEB	C2A-C1A-NA	5.73	113.21	108.27
82	kH	203	PEB	C1D-CHC-C4C	5.73	121.70	113.26
82	OM	201	PEB	CHA-C1B-NB	-5.73	112.95	124.93
82	LD	202	PEB	CHA-C1B-NB	-5.73	112.95	124.93
84	BG	1001	CYC	CAB-C3B-C4B	5.73	130.42	121.38
82	KA	201	PEB	C1C-C2C-C3C	-5.72	100.85	107.62
85	B2	841	BCR	C34-C9-C8	5.72	127.10	118.08
82	zF	501	PEB	C1C-C2C-C3C	-5.72	100.86	107.62
82	CK	202	PEB	C1C-C2C-C3C	-5.72	100.86	107.62
85	BN	841	BCR	C34-C9-C8	5.72	127.09	118.08
82	rF	202	PEB	CMC-C3C-C4C	5.72	133.12	127.06
82	sC	201	PEB	CMB-C2B-C1B	5.72	133.87	125.06
82	N7	202	PEB	CHC-C4C-NC	5.72	128.89	121.15
84	LG	1001	CYC	C3D-C4D-ND	5.72	115.27	107.57
82	MJ	201	PEB	C2C-C1C-NC	5.72	115.27	107.57
83	Z9	305	PUB	CAC-C2C-C1C	5.72	135.12	125.01
82	FF	201	PEB	OA-C1A-NA	5.72	131.86	124.94
82	D9	201	PEB	C1C-C2C-C3C	-5.72	100.86	107.62
84	H4	1001	CYC	OB-C4B-C3B	-5.71	121.84	128.04
82	zK	501	PEB	C1C-C2C-C3C	-5.71	100.86	107.62
82	WP	201	PEB	CHC-C1D-ND	-5.71	106.49	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	l1	201	PEB	C1D-CHC-C4C	5.71	121.68	113.26
84	J1	1001	CYC	CMA-C3A-C4A	5.71	133.86	125.06
82	Z4	201	PEB	C1C-C2C-C3C	-5.71	100.87	107.62
82	F9	201	PEB	C2C-C1C-NC	5.71	115.26	107.57
82	E7	201	PEB	CHC-C4C-NC	5.71	128.88	121.15
82	rK	202	PEB	CMC-C3C-C4C	5.71	133.11	127.06
82	B9	202	PEB	C2C-C1C-NC	5.71	115.26	107.57
82	Y7	303	PEB	C1C-CHB-C4B	-5.71	115.48	128.28
82	GJ	203	PEB	CHC-C1D-ND	-5.71	106.50	113.72
82	PA	202	PEB	C2C-C1C-NC	5.71	115.25	107.57
82	dF	202	PEB	C1D-CHC-C4C	5.71	121.67	113.26
82	pC	202	PEB	CHB-C1C-NC	-5.71	112.25	125.32
87	22	608	CLA	C4A-NA-C1A	5.71	109.27	106.71
82	s8	202	PEB	CHC-C4C-NC	5.70	128.87	121.15
82	TD	203	PEB	CHC-C1D-ND	-5.70	106.51	113.72
82	lF	203	PEB	CHA-C1B-NB	-5.70	113.01	124.93
82	N7	202	PEB	C2A-C1A-NA	5.70	113.19	108.27
82	EM	203	PEB	CHC-C4C-NC	5.70	128.86	121.15
82	CB	202	PEB	CHC-C1D-ND	-5.70	106.52	113.72
82	WD	201	PEB	C1C-C2C-C3C	-5.69	100.89	107.62
82	p8	202	PEB	CHB-C1C-NC	-5.69	112.28	125.32
84	DH	1003	CYC	OB-C4B-C3B	-5.69	121.86	128.04
82	RO	201	PEB	CHC-C1D-ND	-5.69	106.52	113.72
84	FE	1002	CYC	CMD-C2D-C1D	5.69	133.89	125.56
82	CJ	203	PEB	C2C-C1C-NC	5.69	115.23	107.57
103	8N	310	ZEX	C28-C29-C30	5.69	127.67	118.94
82	HI	202	PEB	C1C-C2C-C3C	-5.69	100.90	107.62
84	LE	1001	CYC	C3D-C4D-ND	5.69	115.23	107.57
82	sC	202	PEB	CHC-C4C-NC	5.69	128.85	121.15
82	KF	201	PEB	CHB-C1C-C2C	-5.69	114.32	127.15
82	LQ	202	PEB	CHA-C1B-NB	-5.69	113.04	124.93
82	i4	202	PEB	CHC-C4C-NC	5.68	128.84	121.15
82	MQ	201	PEB	C1C-C2C-C3C	-5.68	100.90	107.62
83	NQ	201	PUB	C1D-CHC-C4C	-5.68	101.00	113.37
82	S9	201	PEB	CAA-C3A-C2A	-5.68	100.06	114.26
82	SP	201	PEB	C3C-C4C-NC	-5.68	103.22	108.33
103	82	310	ZEX	C28-C29-C30	5.68	127.66	118.94
84	HO	1001	CYC	OB-C4B-C3B	-5.68	121.87	128.04
82	M9	304	PEB	OA-C1A-C2A	-5.68	121.66	126.17
84	FG	1001	CYC	CMD-C2D-C1D	5.68	133.88	125.56
82	aM	203	PEB	C1C-C2C-C3C	-5.68	100.91	107.62
82	YJ	201	PEB	CHC-C4C-NC	5.68	128.83	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QF	201	PEB	CMB-C2B-C1B	5.68	133.81	125.06
82	lF	201	PEB	CHA-C4A-NA	5.68	131.96	125.20
82	TF	201	PEB	C2A-C1A-NA	5.68	113.17	108.27
85	KN	101	BCR	C16-C15-C14	-5.68	111.84	123.47
82	WI	202	PEB	C1C-C2C-C3C	-5.67	100.91	107.62
82	MM	202	PEB	CMB-C2B-C1B	5.67	133.80	125.06
85	A2	848	BCR	C37-C22-C21	-5.67	114.98	122.92
82	S5	202	PEB	CHC-C4C-NC	5.67	128.82	121.15
83	QJ	201	PUB	OD-C4D-C3D	-5.67	121.89	128.04
84	D3	1001	CYC	OB-C4B-C3B	-5.67	121.89	128.04
84	Q3	1001	CYC	OB-C4B-C3B	-5.67	121.89	128.04
82	MD	201	PEB	C1C-C2C-C3C	-5.67	100.92	107.62
87	B2	816	CLA	C4A-NA-C1A	5.67	109.25	106.71
82	I7	201	PEB	CHC-C4C-NC	5.67	128.82	121.15
84	LH	1002	CYC	CMB-C2B-C1B	5.66	131.24	124.17
85	AN	848	BCR	C37-C22-C21	-5.66	114.99	122.92
82	EM	201	PEB	CHC-C4C-NC	5.66	128.81	121.15
85	K2	102	BCR	C16-C15-C14	-5.66	111.88	123.47
84	k3	1001	CYC	OB-C4B-C3B	-5.66	121.90	128.04
84	o3	1001	CYC	OB-C4B-C3B	-5.66	121.90	128.04
82	NA	202	PEB	CHC-C4C-NC	5.66	128.81	121.15
82	ED	201	PEB	C1C-C2C-C3C	-5.66	100.94	107.62
84	I3	1001	CYC	OB-C4B-C3B	-5.65	121.90	128.04
84	L3	1001	CYC	OB-C4B-C3B	-5.65	121.91	128.04
85	Z6	101	BCR	C40-C30-C29	-5.65	86.30	108.91
85	B2	842	BCR	C35-C13-C12	5.65	126.98	118.08
83	ND	201	PUB	C1D-CHC-C4C	-5.65	101.07	113.37
82	FK	202	PEB	C1C-C2C-C3C	-5.65	100.94	107.62
82	FH	1002	PEB	OA-C1A-C2A	-5.65	121.68	126.17
82	SH	201	PEB	CHC-C4C-NC	5.65	128.79	121.15
87	AN	852	CLA	CMD-C2D-C1D	5.65	134.67	124.71
82	R4	201	PEB	CHC-C1D-ND	-5.65	106.58	113.72
84	JH	1001	CYC	CHB-C4A-NA	-5.65	113.12	124.93
83	AE	303	PUB	OD-C4D-C3D	-5.65	121.91	128.04
84	d3	1001	CYC	OB-C4B-C3B	-5.65	121.91	128.04
82	UJ	202	PEB	C2C-C1C-NC	5.65	115.17	107.57
84	j3	1001	CYC	OB-C4B-C3B	-5.65	121.91	128.04
83	AG	303	PUB	OD-C4D-C3D	-5.65	121.91	128.04
82	S1	201	PEB	CHC-C4C-NC	5.64	128.79	121.15
82	EQ	201	PEB	C1C-C2C-C3C	-5.64	100.95	107.62
84	H3	1001	CYC	OB-C4B-C3B	-5.64	121.92	128.04
82	ZO	201	PEB	C1C-C2C-C3C	-5.64	100.95	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dK	202	PEB	C1D-CHC-C4C	5.64	121.57	113.26
85	BN	842	BCR	C35-C13-C12	5.64	126.96	118.08
82	jM	202	PEB	C1C-C2C-C3C	-5.64	100.95	107.62
82	DQ	201	PEB	C2C-C1C-NC	5.64	115.16	107.57
82	QA	201	PEB	CHB-C1C-C2C	-5.64	114.43	127.15
82	DD	201	PEB	C2C-C1C-NC	5.64	115.16	107.57
82	WQ	201	PEB	C1C-C2C-C3C	-5.64	100.96	107.62
82	qK	202	PEB	CMB-C2B-C1B	5.64	133.74	125.06
82	FD	203	PEB	C2C-C1C-NC	5.63	115.16	107.57
82	FK	201	PEB	OA-C1A-NA	5.63	131.77	124.94
84	n3	1001	CYC	OB-C4B-C3B	-5.63	121.92	128.04
84	KH	1001	CYC	CMD-C2D-C1D	5.63	133.81	125.56
82	qF	202	PEB	CMB-C2B-C1B	5.63	133.74	125.06
82	CM	203	PEB	C2C-C1C-NC	5.63	115.16	107.57
84	F3	1001	CYC	OB-C4B-C3B	-5.63	121.93	128.04
82	YO	202	PEB	C2C-C1C-NC	5.63	115.16	107.57
82	iO	202	PEB	CHC-C4C-NC	5.63	128.77	121.15
82	KK	201	PEB	CHB-C1C-C2C	-5.63	114.44	127.15
84	w3	1001	CYC	OB-C4B-C3B	-5.63	121.93	128.04
82	P7	201	PEB	CMB-C2B-C1B	5.63	133.74	125.06
83	AD	302	PUB	CHA-C1B-NB	5.63	128.77	121.15
82	DF	202	PEB	OA-C1A-C2A	-5.63	121.70	126.17
82	pK	202	PEB	OA-C1A-C2A	-5.63	121.70	126.17
84	E4	1001	CYC	CAB-C3B-C4B	5.63	130.27	121.38
84	h3	1001	CYC	OB-C4B-C3B	-5.63	121.93	128.04
84	u3	1001	CYC	OB-C4B-C3B	-5.63	121.93	128.04
82	RF	201	PEB	CHC-C4C-NC	5.63	128.77	121.15
82	CD	201	PEB	C2C-C1C-NC	5.63	115.15	107.57
83	AQ	302	PUB	CHA-C1B-NB	5.63	128.77	121.15
82	OF	201	PEB	OA-C1A-C2A	-5.63	121.70	126.17
84	B3	1001	CYC	OB-C4B-C3B	-5.63	121.94	128.04
87	DL	404	CLA	C4A-NA-C1A	5.63	109.23	106.71
82	TH	201	PEB	C1D-CHC-C4C	-5.62	104.96	113.26
84	M3	1001	CYC	OB-C4B-C3B	-5.62	121.94	128.04
85	CL	516	BCR	C39-C30-C25	5.62	119.42	110.30
85	J2	103	BCR	C24-C23-C22	-5.62	117.74	126.23
84	FE	1001	CYC	CAB-C3B-C4B	5.62	130.26	121.38
84	O3	1001	CYC	OB-C4B-C3B	-5.62	121.94	128.04
84	J1	1001	CYC	CHB-C4A-NA	-5.62	113.17	124.93
87	A2	852	CLA	CMD-C2D-C1D	5.62	134.62	124.71
83	xF	306	PUB	C4A-CHA-C1B	-5.62	104.97	113.26
83	NQ	201	PUB	OD-C4D-C3D	-5.62	121.94	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U4	201	PEB	C1C-C2C-C3C	-5.62	100.98	107.62
82	LF	202	PEB	C1C-CHB-C4B	5.62	140.88	128.28
82	OJ	202	PEB	C1C-C2C-C3C	-5.62	100.98	107.62
84	K1	1001	CYC	CMD-C2D-C1D	5.62	133.78	125.56
82	lK	201	PEB	CHA-C4A-NA	5.62	131.88	125.20
82	Q7	201	PEB	CHB-C1C-C2C	-5.62	114.48	127.15
82	RK	201	PEB	CHC-C4C-NC	5.62	128.75	121.15
82	DK	202	PEB	OA-C1A-C2A	-5.62	121.71	126.17
82	QH	202	PEB	CHA-C1B-NB	-5.62	113.19	124.93
84	L1	1001	CYC	CMB-C2B-C1B	5.61	131.18	124.17
82	T1	201	PEB	C1D-CHC-C4C	-5.61	104.98	113.26
82	Q1	202	PEB	CHA-C1B-NB	-5.61	113.19	124.93
84	q3	1001	CYC	OB-C4B-C3B	-5.61	121.95	128.04
84	CG	1001	CYC	CAB-C3B-C4B	5.61	130.25	121.38
84	EO	1001	CYC	CAB-C3B-C4B	5.61	130.24	121.38
82	U7	201	PEB	CHC-C4C-NC	5.61	128.75	121.15
84	FH	1001	CYC	CMB-C2B-C1B	5.61	131.18	124.17
82	NI	203	PEB	C2C-C1C-NC	5.61	115.13	107.57
91	aL	610	PHO	O2D-CGD-CBD	5.61	118.11	111.00
82	PM	201	PEB	CHC-C1D-ND	5.61	120.83	113.72
82	KJ	203	PEB	C2C-C1C-NC	5.61	115.12	107.57
84	U3	1001	CYC	OB-C4B-C3B	-5.61	121.95	128.04
82	UA	201	PEB	CHC-C4C-NC	5.61	128.74	121.15
84	D1	1003	CYC	OB-C4B-C3B	-5.61	121.96	128.04
84	S3	1001	CYC	OB-C4B-C3B	-5.61	121.96	128.04
84	NH	1001	CYC	OC-C1C-C2C	-5.61	121.72	126.17
84	f3	1001	CYC	OB-C4B-C3B	-5.60	121.96	128.04
85	CL	502	BCR	C24-C23-C22	5.60	134.70	126.23
82	eF	202	PEB	CMB-C2B-C1B	5.60	133.69	125.06
82	FF	202	PEB	C1C-C2C-C3C	-5.60	101.00	107.62
83	QJ	201	PUB	CHC-C1D-ND	-5.60	106.64	113.72
84	F1	1001	CYC	CMB-C2B-C1B	5.60	131.16	124.17
82	UG	201	PEB	CHB-C1C-C2C	-5.60	114.51	127.15
82	QK	203	PEB	C1C-CHB-C4B	5.60	140.84	128.28
82	aF	203	PEB	CMB-C2B-C1B	5.60	133.69	125.06
82	yC	202	PEB	CHB-C1C-C2C	-5.60	114.52	127.15
82	mG	203	PEB	C1C-C2C-C3C	-5.60	101.00	107.62
87	AN	852	CLA	C3C-C4C-NC	-5.60	104.29	110.57
82	aK	203	PEB	CMB-C2B-C1B	5.60	133.68	125.06
85	L2	205	BCR	C34-C9-C10	-5.60	115.08	122.92
82	y8	202	PEB	CHB-C1C-C2C	-5.59	114.53	127.15
82	QK	201	PEB	CMB-C2B-C1B	5.59	133.68	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jJ	202	PEB	CHC-C4C-NC	5.59	128.72	121.15
82	eK	202	PEB	CMB-C2B-C1B	5.59	133.68	125.06
83	Z9	302	PUB	CHA-C4A-NA	-5.59	106.65	113.72
82	WI	201	PEB	CHC-C1D-ND	-5.59	106.65	113.72
84	HG	1001	CYC	OB-C4B-C3B	-5.59	121.97	128.04
82	mE	203	PEB	C1C-C2C-C3C	-5.59	101.01	107.62
82	QG	201	PEB	CHC-C1D-ND	-5.59	106.65	113.72
94	D6	408	PL9	C7-C3-C4	5.59	121.42	116.88
82	OJ	203	PEB	C2C-C1C-NC	5.59	115.10	107.57
82	O4	201	PEB	C2C-C1C-NC	5.59	115.10	107.57
82	jH	201	PEB	C2C-C1C-NC	5.59	115.10	107.57
82	aK	202	PEB	CMB-C2B-C1B	5.59	133.67	125.06
83	M9	303	PUB	CHA-C4A-NA	-5.59	106.65	113.72
84	73	1001	CYC	OB-C4B-C3B	-5.59	121.98	128.04
82	UO	201	PEB	C1C-C2C-C3C	-5.59	101.02	107.62
82	lG	201	PEB	CHC-C4C-NC	5.58	128.71	121.15
82	U9	201	PEB	C4B-C3B-C2B	-5.58	100.60	106.78
85	KN	101	BCR	C34-C9-C8	5.58	126.87	118.08
82	HD	201	PEB	C2C-C1C-NC	5.58	115.09	107.57
82	KP	201	PEB	CMD-C2D-C3D	-5.58	122.19	130.06
82	aF	202	PEB	CMB-C2B-C1B	5.58	133.66	125.06
82	V1	202	PEB	OA-C1A-C2A	-5.58	121.73	126.17
84	HE	1001	CYC	OB-C4B-C3B	-5.58	121.99	128.04
83	A1	304	PUB	C4B-C3B-C2B	-5.58	101.03	107.62
85	KN	104	BCR	C37-C22-C21	-5.58	115.11	122.92
85	LN	205	BCR	C34-C9-C10	-5.58	115.11	122.92
85	B6	602	BCR	C11-C10-C9	-5.58	119.35	127.31
83	xK	306	PUB	C4A-CHA-C1B	-5.58	105.03	113.26
82	PA	201	PEB	CMB-C2B-C1B	5.58	133.65	125.06
82	U7	201	PEB	CMB-C2B-C1B	5.58	133.65	125.06
87	A2	852	CLA	C3C-C4C-NC	-5.58	104.32	110.57
82	UA	201	PEB	CMB-C2B-C1B	5.58	133.65	125.06
82	W1	202	PEB	C1C-C2C-C3C	-5.58	101.03	107.62
82	HF	201	PEB	CHB-C1C-C2C	-5.57	114.58	127.15
82	QE	201	PEB	CHC-C1D-ND	-5.57	106.67	113.72
82	LK	202	PEB	C1C-CHB-C4B	5.57	140.78	128.28
82	V1	203	PEB	OA-C1A-C2A	-5.57	121.74	126.17
85	K2	102	BCR	C34-C9-C8	5.57	126.86	118.08
82	BD	201	PEB	CHC-C4C-NC	5.57	128.69	121.15
82	BQ	201	PEB	CHC-C4C-NC	5.57	128.69	121.15
82	eF	201	PEB	CHC-C4C-NC	5.57	128.69	121.15
85	JN	103	BCR	C24-C23-C22	-5.57	117.82	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UE	201	PEB	CHB-C1C-C2C	-5.57	114.59	127.15
82	IA	201	PEB	CHC-C4C-NC	5.57	128.68	121.15
82	Y4	202	PEB	C2C-C1C-NC	5.57	115.06	107.57
82	fM	202	PEB	CHC-C1D-ND	-5.56	106.68	113.72
82	WH	202	PEB	C1C-C2C-C3C	-5.56	101.04	107.62
82	x8	202	PEB	C1C-C2C-C3C	-5.56	101.05	107.62
82	xC	202	PEB	C1C-C2C-C3C	-5.56	101.05	107.62
82	S9	201	PEB	C2C-C1C-NC	5.56	115.06	107.57
82	QJ	202	PEB	CHC-C4C-NC	5.56	128.67	121.15
84	FE	1002	CYC	CAB-C3B-C4B	5.56	130.16	121.38
82	GK	201	PEB	C2C-C1C-NC	5.56	115.05	107.57
85	K2	105	BCR	C37-C22-C21	-5.56	115.14	122.92
85	h6	102	BCR	C7-C8-C9	-5.56	117.84	126.23
82	FQ	203	PEB	C2C-C1C-NC	5.55	115.05	107.57
82	DI	201	PEB	CHB-C1C-NC	-5.55	112.60	125.32
82	wF	303	PEB	CHA-C1B-NB	-5.55	113.31	124.93
87	6N	608	CLA	CHD-C1D-ND	5.55	129.56	124.45
82	DJ	201	PEB	OA-C1A-C2A	-5.55	121.76	126.17
82	R7	203	PEB	C1C-C2C-C3C	-5.55	101.06	107.62
85	BN	803	BCR	C19-C18-C17	-5.55	110.42	118.94
87	62	309	CLA	C2D-C1D-ND	5.55	114.20	110.10
82	Y7	301	PEB	OA-C1A-C2A	-5.55	121.76	126.17
82	NQ	204	PEB	CHC-C4C-NC	5.55	128.66	121.15
103	8N	310	ZEX	C19-C9-C10	-5.55	115.15	122.92
82	RB	201	PEB	C1D-CHC-C4C	5.55	121.44	113.26
84	N1	1001	CYC	OC-C1C-C2C	-5.55	121.76	126.17
87	BN	817	CLA	C4A-NA-C1A	5.55	109.20	106.71
82	IM	202	PEB	CMB-C2B-C1B	5.55	133.61	125.06
82	QF	203	PEB	C1C-CHB-C4B	5.55	140.72	128.28
103	82	310	ZEX	C19-C9-C10	-5.55	115.15	122.92
85	B2	802	BCR	C19-C18-C17	-5.55	110.43	118.94
82	O9	201	PEB	C4B-C3B-C2B	-5.55	100.64	106.78
85	cL	518	BCR	C39-C30-C25	5.55	119.29	110.30
82	DF	202	PEB	C2C-C1C-NC	5.54	115.04	107.57
83	YA	302	PUB	OD-C4D-C3D	-5.54	122.03	128.04
84	E1	1001	CYC	CMD-C2D-C1D	5.54	133.68	125.56
82	j1	201	PEB	C2C-C1C-NC	5.54	115.03	107.57
82	R5	201	PEB	CMB-C2B-C1B	5.54	133.60	125.06
82	CF	202	PEB	C1C-C2C-C3C	-5.54	101.07	107.62
84	FG	1001	CYC	CAB-C3B-C4B	5.54	130.13	121.38
82	O9	202	PEB	C1D-CHC-C4C	5.54	121.43	113.26
83	Z5	302	PUB	CHC-C1D-ND	-5.54	106.71	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gJ	201	PEB	C1C-CHB-C4B	-5.54	115.86	128.28
82	WJ	201	PEB	CMB-C2B-C1B	5.54	133.60	125.06
82	eK	201	PEB	CHC-C4C-NC	5.54	128.65	121.15
84	EH	1001	CYC	CMD-C2D-C1D	5.54	133.67	125.56
87	2N	303	CLA	CMD-C2D-C3D	-5.54	114.87	127.61
82	WO	201	PEB	CHB-C4B-C3B	-5.54	112.51	125.32
87	8N	308	CLA	CAC-C3C-C2C	5.54	137.00	127.53
92	mL	101	LMG	O7-C10-C11	5.53	123.43	111.50
82	OK	201	PEB	OA-C1A-C2A	-5.53	121.77	126.17
82	YJ	202	PEB	CMB-C2B-C1B	5.53	133.58	125.06
82	QF	201	PEB	C2C-C1C-NC	5.53	115.02	107.57
82	WI	202	PEB	CHC-C1D-ND	5.53	120.72	113.72
82	G5	201	PEB	CMB-C2B-C1B	5.53	133.57	125.06
87	82	308	CLA	CAC-C3C-C2C	5.53	136.98	127.53
82	B9	202	PEB	CHA-C1B-NB	-5.53	113.37	124.93
83	ND	201	PUB	C4B-C3B-C2B	-5.53	101.09	107.62
82	WB	402	PEB	C2C-C1C-NC	5.52	115.01	107.57
85	I2	101	BCR	C3-C4-C5	-5.52	104.21	114.08
82	CQ	201	PEB	C2C-C1C-NC	5.52	115.01	107.57
82	HK	201	PEB	CHB-C1C-C2C	-5.52	114.69	127.15
82	N5	201	PEB	CMB-C2B-C1B	5.52	133.57	125.06
83	NQ	201	PUB	C4B-C3B-C2B	-5.52	101.09	107.62
87	22	602	CLA	CMD-C2D-C3D	-5.52	114.91	127.61
87	62	309	CLA	CHD-C1D-ND	5.52	129.53	124.45
83	wF	304	PUB	C1D-CHC-C4C	-5.52	101.36	113.37
84	V3	1001	CYC	OB-C4B-C3B	-5.52	122.05	128.04
82	X5	201	PEB	CMB-C2B-C1B	5.52	133.56	125.06
82	W4	201	PEB	CHB-C4B-C3B	-5.52	112.56	125.32
82	UP	202	PEB	CMC-C3C-C4C	-5.52	121.21	127.06
83	AH	304	PUB	C4B-C3B-C2B	-5.52	101.10	107.62
85	IN	101	BCR	C3-C4-C5	-5.52	104.23	114.08
87	2N	309	CLA	C4A-NA-C1A	5.52	109.19	106.71
83	M5	302	PUB	CHC-C1D-ND	-5.52	106.75	113.72
82	O5	202	PEB	C2C-C1C-NC	5.52	115.00	107.57
82	YA	304	PEB	C1D-CHC-C4C	-5.51	105.13	113.26
82	A5	201	PEB	CMB-C2B-C1B	5.51	133.55	125.06
82	GF	201	PEB	C2C-C1C-NC	5.51	114.99	107.57
82	HQ	201	PEB	C2C-C1C-NC	5.51	114.99	107.57
82	QK	201	PEB	C2C-C1C-NC	5.51	114.99	107.57
82	K5	201	PEB	CMB-C2B-C1B	5.51	133.55	125.06
87	7N	608	CLA	C4A-NA-C1A	5.51	109.18	106.71
82	E5	201	PEB	CMB-C2B-C1B	5.51	133.55	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UB	301	PEB	CHC-C1D-ND	-5.51	106.75	113.72
87	72	602	CLA	C4A-NA-C1A	5.51	109.18	106.71
82	NE	202	PEB	OA-C1A-C2A	-5.51	121.80	126.17
85	F6	101	BCR	C7-C8-C9	-5.51	117.92	126.23
87	6N	608	CLA	C2D-C1D-ND	5.51	114.16	110.10
82	WJ	202	PEB	CHC-C4C-NC	5.50	128.60	121.15
82	WE	203	PEB	C2C-C1C-NC	5.50	114.98	107.57
82	pF	202	PEB	OA-C1A-C2A	-5.50	121.80	126.17
82	C5	201	PEB	CMB-C2B-C1B	5.50	133.54	125.06
82	YG	201	PEB	C2C-C1C-NC	5.50	114.98	107.57
82	MM	202	PEB	C1C-C2C-C3C	-5.50	101.12	107.62
82	sK	201	PEB	C2C-C1C-NC	5.50	114.98	107.57
82	V5	201	PEB	CMB-C2B-C1B	5.50	133.53	125.06
83	ND	201	PUB	OD-C4D-C3D	-5.50	122.07	128.04
84	T3	1001	CYC	OB-C4B-C3B	-5.50	122.07	128.04
82	KI	201	PEB	C2C-C1C-NC	5.50	114.97	107.57
85	B2	842	BCR	C24-C23-C22	-5.50	117.93	126.23
82	wK	303	PEB	CHA-C1B-NB	-5.50	113.43	124.93
82	AI	203	PEB	CHB-C1C-C2C	-5.50	114.75	127.15
82	OO	201	PEB	C2C-C1C-NC	5.50	114.97	107.57
82	NG	201	PEB	OA-C1A-C2A	-5.50	121.80	126.17
82	VA	202	PEB	CHB-C1C-C2C	-5.50	114.75	127.15
82	I5	201	PEB	CMB-C2B-C1B	5.50	133.53	125.06
85	BN	842	BCR	C24-C23-C22	-5.50	117.93	126.23
103	8N	310	ZEX	C18-C5-C4	5.50	124.54	114.36
82	BA	202	PEB	CHA-C4A-NA	5.49	131.74	125.20
83	Y7	302	PUB	OD-C4D-C3D	-5.49	122.08	128.04
82	UJ	201	PEB	C2C-C1C-NC	5.49	114.97	107.57
82	V7	202	PEB	CHB-C1C-C2C	-5.49	114.76	127.15
82	MM	202	PEB	C2C-C1C-NC	5.49	114.97	107.57
103	82	310	ZEX	C18-C5-C4	5.49	124.53	114.36
82	DK	202	PEB	C2C-C1C-NC	5.49	114.96	107.57
82	P5	201	PEB	CMB-C2B-C1B	5.49	133.51	125.06
82	WJ	201	PEB	CHA-C1B-NB	-5.49	113.45	124.93
85	JN	103	BCR	C20-C21-C22	-5.49	119.48	127.31
85	B2	838	BCR	C16-C17-C18	-5.49	119.48	127.31
82	GK	201	PEB	CHC-C4C-NC	5.49	128.58	121.15
82	SK	201	PEB	CHB-C1C-C2C	-5.49	114.77	127.15
82	Y7	304	PEB	C1D-CHC-C4C	-5.49	105.17	113.26
82	B7	202	PEB	CHA-C4A-NA	5.49	131.73	125.20
82	RI	203	PEB	CHB-C1C-C2C	-5.49	114.77	127.15
84	m3	1001	CYC	CHB-C4A-NA	-5.49	113.46	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	NQ	201	PUB	CHA-C4A-NA	-5.49	106.78	113.72
82	iF	202	PEB	C2C-C1C-NC	5.48	114.95	107.57
84	J3	1001	CYC	OB-C4B-C3B	-5.48	122.09	128.04
82	NF	201	PEB	C2A-C1A-NA	5.48	113.00	108.27
84	i3	1001	CYC	CHB-C4A-NA	-5.48	113.47	124.93
84	HO	1001	CYC	CMD-C2D-C1D	5.48	133.58	125.56
84	G3	1001	CYC	CHD-C1D-ND	-5.48	112.77	125.32
82	RA	203	PEB	CHC-C1D-ND	-5.48	106.79	113.72
82	L7	202	PEB	C2C-C1C-NC	5.48	114.95	107.57
82	HB	201	PEB	C1D-CHC-C4C	5.48	121.33	113.26
84	CO	1001	CYC	OC-C1C-C2C	-5.48	121.82	126.17
84	p3	1001	CYC	CHD-C1D-ND	-5.48	112.77	125.32
83	wK	304	PUB	C1D-CHC-C4C	-5.48	101.45	113.37
84	K3	1001	CYC	OB-C4B-C3B	-5.48	122.10	128.04
82	LA	202	PEB	C2C-C1C-NC	5.48	114.94	107.57
82	YE	201	PEB	C2C-C1C-NC	5.48	114.94	107.57
84	JH	1001	CYC	C3D-C4D-ND	5.48	114.94	107.57
84	J1	1001	CYC	C3D-C4D-ND	5.48	114.94	107.57
82	T5	201	PEB	CMB-C2B-C1B	5.48	133.50	125.06
84	x3	1001	CYC	OB-C4B-C3B	-5.48	122.10	128.04
84	K3	1001	CYC	CHD-C1D-ND	-5.47	112.78	125.32
82	LO	1002	PEB	OA-C1A-C2A	-5.47	121.82	126.17
84	K3	1001	CYC	CHB-C4A-NA	-5.47	113.48	124.93
85	BN	838	BCR	C16-C17-C18	-5.47	119.50	127.31
82	EJ	201	PEB	C2C-C1C-NC	5.47	114.94	107.57
82	NK	201	PEB	C2A-C1A-NA	5.47	112.99	108.27
84	i3	1001	CYC	CHD-C1D-ND	-5.47	112.78	125.32
84	t3	1001	CYC	CHD-C1D-ND	-5.47	112.78	125.32
85	J2	103	BCR	C20-C21-C22	-5.47	119.50	127.31
82	WG	203	PEB	C2C-C1C-NC	5.47	114.94	107.57
84	A3	1001	CYC	CHD-C1D-ND	-5.47	112.79	125.32
84	m3	1001	CYC	CHD-C1D-ND	-5.47	112.79	125.32
84	C4	1001	CYC	OC-C1C-C2C	-5.47	121.82	126.17
84	R3	1001	CYC	CHD-C1D-ND	-5.47	112.79	125.32
85	KL	100	BCR	C20-C21-C22	-5.47	119.50	127.31
84	G3	1001	CYC	OB-C4B-C3B	-5.47	122.11	128.04
82	R7	203	PEB	CHC-C1D-ND	-5.47	106.81	113.72
84	R3	1001	CYC	CHB-C4A-NA	-5.47	113.49	124.93
84	c3	1001	CYC	CHD-C1D-ND	-5.47	112.79	125.32
82	PF	202	PEB	CMC-C3C-C4C	5.47	132.85	127.06
82	aO	202	PEB	CHB-C1C-C2C	-5.47	114.82	127.15
85	kL	100	BCR	C20-C21-C22	-5.47	119.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	P3	1001	CYC	CHD-C1D-ND	-5.47	112.80	125.32
84	E3	1001	CYC	CHB-C4A-NA	-5.47	113.50	124.93
84	l3	1001	CYC	CHB-C4A-NA	-5.47	113.50	124.93
82	UM	202	PEB	CMB-C2B-C1B	5.47	133.48	125.06
84	BE	1002	CYC	C3D-C4D-ND	5.47	114.93	107.57
84	A3	1001	CYC	CHB-C4A-NA	-5.47	113.50	124.93
82	aM	204	PEB	CHC-C4C-NC	5.46	128.55	121.15
82	GF	201	PEB	CHC-C4C-NC	5.46	128.54	121.15
84	e3	1001	CYC	CHD-C1D-ND	-5.46	112.80	125.32
84	BG	1002	CYC	C3D-C4D-ND	5.46	114.93	107.57
84	g3	1001	CYC	CHD-C1D-ND	-5.46	112.80	125.32
82	QO	201	PEB	CMB-C2B-C1B	5.46	133.48	125.06
92	ML	101	LMG	O7-C10-C11	5.46	123.28	111.50
82	WF	202	PEB	C2C-C1C-NC	5.46	114.93	107.57
84	e3	1001	CYC	CHB-C4A-NA	-5.46	113.51	124.93
92	J6	102	LMG	O7-C10-C11	5.46	123.27	111.50
84	N3	1001	CYC	CHD-C1D-ND	-5.46	112.81	125.32
84	T3	1001	CYC	CHB-C4A-NA	-5.46	113.51	124.93
84	J3	1001	CYC	CHD-C1D-ND	-5.46	112.81	125.32
83	AJ	303	PUB	C4B-C3B-C2B	-5.46	101.17	107.62
82	GA	201	PEB	C2C-C1C-NC	5.46	114.92	107.57
82	Q4	201	PEB	CMB-C2B-C1B	5.46	133.47	125.06
84	J3	1001	CYC	CHB-C4A-NA	-5.46	113.52	124.93
84	T3	1001	CYC	CHD-C1D-ND	-5.46	112.82	125.32
84	v3	1001	CYC	CHB-C4A-NA	-5.46	113.52	124.93
84	e3	1001	CYC	OB-C4B-C3B	-5.46	122.12	128.04
84	63	901	CYC	CHB-C4A-C3A	5.46	138.93	124.90
84	H4	1001	CYC	CMD-C2D-C1D	5.46	133.55	125.56
84	C3	1001	CYC	CHD-C1D-ND	-5.46	112.82	125.32
84	C3	1001	CYC	OB-C4B-C3B	-5.46	122.12	128.04
84	P3	1001	CYC	CHB-C4A-NA	-5.46	113.52	124.93
84	c3	1001	CYC	CHB-C4A-NA	-5.46	113.52	124.93
84	g3	1001	CYC	CHB-C4A-NA	-5.46	113.52	124.93
82	Y7	304	PEB	CHA-C1B-NB	-5.45	113.52	124.93
84	G3	1001	CYC	CHB-C4A-NA	-5.45	113.52	124.93
84	v3	1001	CYC	CHD-C1D-ND	-5.45	112.83	125.32
82	RJ	201	PEB	C1D-CHC-C4C	5.45	121.30	113.26
84	l3	1001	CYC	CHD-C1D-ND	-5.45	112.83	125.32
84	t3	1001	CYC	CHB-C4A-NA	-5.45	113.53	124.93
82	lO	201	PEB	C2C-C1C-NC	5.45	114.91	107.57
82	bF	202	PEB	OA-C1A-C2A	-5.45	121.84	126.17
85	B2	802	BCR	C20-C21-C22	-5.45	119.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	E3	1001	CYC	CHD-C1D-ND	-5.45	112.83	125.32
84	C3	1001	CYC	CHB-C4A-NA	-5.45	113.53	124.93
83	ND	201	PUB	CHA-C4A-NA	-5.45	106.83	113.72
82	eH	203	PEB	OA-C1A-C2A	-5.45	121.84	126.17
82	qF	202	PEB	CHB-C4B-C3B	5.45	137.92	125.32
84	p3	1001	CYC	CHB-C4A-NA	-5.45	113.54	124.93
83	Z9	302	PUB	CAD-C3D-C4D	5.45	129.98	121.38
82	G7	201	PEB	C2C-C1C-NC	5.45	114.91	107.57
82	YA	304	PEB	CHA-C1B-NB	-5.45	113.54	124.93
82	UJ	203	PEB	C1C-C2C-C3C	-5.45	101.18	107.62
82	OM	202	PEB	CMC-C3C-C4C	-5.45	121.29	127.06
82	TI	201	PEB	OA-C1A-C2A	-5.44	121.84	126.17
82	RI	203	PEB	C1D-CHC-C4C	-5.44	105.23	113.26
82	WM	203	PEB	CHC-C4C-NC	5.44	128.52	121.15
82	RA	203	PEB	C1C-C2C-C3C	-5.44	101.19	107.62
87	B2	822	CLA	C4A-NA-C1A	5.44	109.15	106.71
83	M9	303	PUB	CAD-C3D-C4D	5.44	129.97	121.38
87	B6	616	CLA	CMB-C2B-C3B	5.44	139.77	126.59
82	CA	201	PEB	C2C-C1C-NC	5.44	114.90	107.57
85	I2	101	BCR	C4-C5-C6	-5.44	114.83	122.73
82	MB	202	PEB	C2C-C1C-NC	5.44	114.90	107.57
82	N1	1002	PEB	CHC-C4C-NC	5.44	128.51	121.15
82	SF	201	PEB	CHB-C1C-C2C	-5.44	114.88	127.15
84	N3	1001	CYC	CHB-C4A-NA	-5.44	113.55	124.93
82	GI	201	PEB	OA-C1A-C2A	-5.44	121.85	126.17
82	NH	1002	PEB	CHC-C4C-NC	5.44	128.51	121.15
82	J1	1002	PEB	CHC-C1D-ND	-5.44	106.84	113.72
84	v3	1001	CYC	OB-C4B-C3B	-5.44	122.14	128.04
82	U9	202	PEB	C2C-C1C-NC	5.44	114.89	107.57
84	T3	1001	CYC	CMB-C2B-C1B	5.44	130.96	124.17
85	A6	401	BCR	C16-C17-C18	-5.44	119.55	127.31
85	KL	100	BCR	C36-C18-C17	-5.44	115.31	122.92
84	HH	1001	CYC	OC-C1C-C2C	-5.44	121.85	126.17
84	p3	1001	CYC	OB-C4B-C3B	-5.44	122.14	128.04
93	d6	410	BCT	O2-C-O1	5.43	133.64	119.55
82	qK	202	PEB	CHB-C4B-C3B	5.43	137.89	125.32
85	C6	508	BCR	C15-C14-C13	-5.43	119.56	127.31
92	j6	101	LMG	O7-C10-C11	5.43	123.21	111.50
82	m4	202	PEB	C2C-C1C-NC	5.43	114.88	107.57
82	a4	202	PEB	CHB-C1C-C2C	-5.43	114.90	127.15
82	ND	204	PEB	CHC-C4C-NC	5.43	128.50	121.15
85	BL	617	BCR	C7-C8-C9	5.43	134.44	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	DH	1003	CYC	C3D-C4D-ND	5.43	114.88	107.57
85	kL	100	BCR	C36-C18-C17	-5.43	115.32	122.92
82	IF	201	PEB	CHB-C4B-C3B	-5.43	112.76	125.32
82	QP	202	PEB	C1D-CHC-C4C	-5.43	105.25	113.26
82	lE	201	PEB	CHC-C4C-NC	5.43	128.50	121.15
84	g3	1001	CYC	OB-C4B-C3B	-5.43	122.15	128.04
84	i3	1001	CYC	OB-C4B-C3B	-5.43	122.15	128.04
82	W7	201	PEB	C2C-C1C-NC	5.43	114.88	107.57
82	RH	201	PEB	CHC-C1D-ND	-5.43	106.86	113.72
82	KM	203	PEB	C2C-C1C-NC	5.43	114.88	107.57
82	YA	301	PEB	OA-C1A-C2A	-5.43	121.86	126.17
82	L4	1002	PEB	OA-C1A-C2A	-5.43	121.86	126.17
82	FJ	201	PEB	C3D-C4D-ND	5.43	117.91	107.26
83	AG	302	PUB	OD-C4D-C3D	-5.42	122.15	128.04
84	t3	1001	CYC	OB-C4B-C3B	-5.42	122.15	128.04
84	E1	1001	CYC	CHB-C4A-NA	-5.42	113.58	124.93
84	JO	1001	CYC	CMD-C2D-C1D	5.42	133.50	125.56
85	B6	602	BCR	C7-C8-C9	-5.42	118.04	126.23
84	m3	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
82	FD	201	PEB	C2C-C1C-NC	5.42	114.87	107.57
82	IK	201	PEB	CHB-C4B-C3B	-5.42	112.78	125.32
85	Z6	101	BCR	C24-C23-C22	-5.42	118.04	126.23
82	B7	201	PEB	C1C-C2C-C3C	-5.42	101.21	107.62
84	l3	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
84	EH	1001	CYC	CHB-C4A-NA	-5.42	113.59	124.93
87	BN	827	CLA	C4A-NA-C1A	5.42	109.14	106.71
87	4N	604	CLA	CHA-C4D-ND	-5.42	121.16	132.50
85	CL	516	BCR	C20-C21-C22	-5.42	119.58	127.31
82	R1	201	PEB	CHC-C1D-ND	-5.42	106.87	113.72
84	P3	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
82	UJ	201	PEB	CHC-C1D-ND	-5.42	106.87	113.72
82	S9	201	PEB	C1C-C2C-C3C	-5.42	101.22	107.62
82	l4	201	PEB	C2C-C1C-NC	5.42	114.86	107.57
82	JH	1002	PEB	CHC-C1D-ND	-5.42	106.87	113.72
82	PK	202	PEB	CMC-C3C-C4C	5.42	132.80	127.06
82	FQ	201	PEB	C2C-C1C-NC	5.42	114.86	107.57
82	P4	201	PEB	OA-C1A-C2A	-5.42	121.87	126.17
84	E3	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
84	D1	1003	CYC	C3D-C4D-ND	5.41	114.86	107.57
84	G3	1001	CYC	CMB-C2B-C1B	5.41	130.93	124.17
87	BN	823	CLA	C4A-NA-C1A	5.41	109.14	106.71
82	IJ	201	PEB	C2C-C1C-NC	5.41	114.86	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FI	202	PEB	OA-C1A-C2A	-5.41	121.87	126.17
88	C6	522	LHG	O7-C7-C8	5.41	123.16	111.50
84	N3	1001	CYC	CMB-C2B-C1B	5.41	130.92	124.17
84	R3	1001	CYC	CMB-C2B-C1B	5.41	130.92	124.17
82	VI	203	PEB	OA-C1A-C2A	-5.41	121.87	126.17
84	J4	1001	CYC	CMD-C2D-C1D	5.41	133.48	125.56
82	WH	202	PEB	C2C-C1C-NC	5.41	114.86	107.57
98	BN	837	PQN	O1-C1-C10	-5.41	112.80	121.56
85	IN	101	BCR	C4-C5-C6	-5.41	114.88	122.73
82	ID	201	PEB	CMB-C2B-C1B	5.41	133.39	125.06
84	t3	1001	CYC	CMB-C2B-C1B	5.41	130.92	124.17
84	A3	1001	CYC	OB-C4B-C3B	-5.41	122.17	128.04
82	WA	201	PEB	CHC-C4C-NC	5.41	128.47	121.15
82	W7	201	PEB	CHC-C4C-NC	5.41	128.47	121.15
82	WK	202	PEB	C2C-C1C-NC	5.41	114.85	107.57
85	BN	803	BCR	C20-C21-C22	-5.41	119.59	127.31
84	c3	1001	CYC	OB-C4B-C3B	-5.41	122.17	128.04
82	RO	201	PEB	OA-C1A-C2A	-5.41	121.87	126.17
82	aO	202	PEB	C2C-C1C-NC	5.41	114.85	107.57
82	Z4	201	PEB	C3B-C4B-NB	5.41	117.91	110.05
82	OK	202	PEB	C2C-C1C-NC	5.41	114.85	107.57
87	42	604	CLA	CHA-C4D-ND	-5.41	121.19	132.50
84	MG	1001	CYC	OC-C1C-C2C	-5.41	121.88	126.17
84	K3	1001	CYC	CMB-C2B-C1B	5.40	130.91	124.17
84	E3	1001	CYC	CMB-C2B-C1B	5.40	130.91	124.17
82	b1	203	PEB	OA-C1A-C2A	-5.40	121.88	126.17
84	R3	1001	CYC	OB-C4B-C3B	-5.40	122.18	128.04
82	sF	201	PEB	C2C-C1C-NC	5.40	114.84	107.57
82	mO	202	PEB	C2C-C1C-NC	5.40	114.84	107.57
82	UE	203	PEB	C1C-C2C-C3C	-5.40	101.24	107.62
84	J3	1001	CYC	CMB-C2B-C1B	5.40	130.91	124.17
82	WM	201	PEB	CMB-C2B-C1B	5.40	133.38	125.06
82	BQ	201	PEB	C2C-C1C-NC	5.40	114.84	107.57
82	iK	202	PEB	C2C-C1C-NC	5.40	114.84	107.57
84	N3	1001	CYC	OB-C4B-C3B	-5.40	122.18	128.04
84	P3	1001	CYC	CMB-C2B-C1B	5.40	130.91	124.17
83	Z9	305	PUB	CMB-C2B-C1B	5.40	132.78	127.06
82	OF	202	PEB	C2C-C1C-NC	5.39	114.83	107.57
82	F9	202	PEB	C2C-C1C-NC	5.39	114.83	107.57
84	e3	1001	CYC	CMB-C2B-C1B	5.39	130.90	124.17
82	WJ	202	PEB	C1C-C2C-C3C	-5.39	101.25	107.62
98	B2	837	PQN	O1-C1-C10	-5.39	112.84	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	A3	1001	CYC	CMB-C2B-C1B	5.39	130.89	124.17
82	a4	202	PEB	C2C-C1C-NC	5.39	114.82	107.57
82	Z5	301	PEB	C2C-C1C-NC	5.39	114.82	107.57
82	YO	201	PEB	OA-C1A-C2A	-5.39	121.89	126.17
82	F5	202	PEB	CHC-C4C-NC	5.39	128.44	121.15
82	BA	201	PEB	C1C-C2C-C3C	-5.39	101.25	107.62
82	A7	202	PEB	C1C-C2C-C3C	-5.38	101.25	107.62
82	M5	301	PEB	C2C-C1C-NC	5.38	114.82	107.57
84	HE	1001	CYC	CMD-C2D-C1D	5.38	133.44	125.56
84	M4	1001	CYC	CAB-C3B-C4B	5.38	129.88	121.38
84	v3	1001	CYC	CMB-C2B-C1B	5.38	130.89	124.17
85	Z6	101	BCR	C16-C17-C18	-5.38	119.63	127.31
84	l3	1001	CYC	CMB-C2B-C1B	5.38	130.89	124.17
84	E1	1001	CYC	CMA-C3A-C4A	5.38	133.35	125.06
82	AP	201	PEB	CHC-C4C-NC	5.38	128.43	121.15
82	XK	203	PEB	C1C-C2C-C3C	-5.38	101.26	107.62
84	EH	1001	CYC	CMA-C3A-C4A	5.38	133.35	125.06
82	BD	201	PEB	C2C-C1C-NC	5.38	114.81	107.57
84	MO	1001	CYC	CAB-C3B-C4B	5.38	129.87	121.38
82	VH	202	PEB	OA-C1A-C2A	-5.38	121.90	126.17
82	GJ	203	PEB	C2C-C1C-NC	5.38	114.81	107.57
82	T4	202	PEB	C2C-C1C-NC	5.38	114.81	107.57
82	WG	201	PEB	CHA-C1B-NB	-5.38	113.68	124.93
84	NE	201	CYC	CAB-C3B-C4B	5.38	129.87	121.38
82	SO	201	PEB	C2C-C1C-NC	5.38	114.81	107.57
84	H1	1001	CYC	OC-C1C-C2C	-5.38	121.90	126.17
84	i3	1001	CYC	CMB-C2B-C1B	5.38	130.88	124.17
84	C3	1001	CYC	CMB-C2B-C1B	5.37	130.88	124.17
82	F7	202	PEB	C2C-C1C-NC	5.37	114.81	107.57
82	H5	202	PEB	CHC-C4C-NC	5.37	128.42	121.15
84	E4	1001	CYC	OC-C1C-C2C	-5.37	121.90	126.17
82	W1	202	PEB	C2C-C1C-NC	5.37	114.80	107.57
82	OI	202	PEB	CAC-C2C-C1C	5.37	134.32	125.76
84	m3	1001	CYC	CMB-C2B-C1B	5.37	130.87	124.17
84	g3	1001	CYC	CMB-C2B-C1B	5.37	130.87	124.17
82	lF	203	PEB	CHB-C1C-C2C	-5.37	115.04	127.15
82	J5	202	PEB	CHC-C4C-NC	5.37	128.41	121.15
82	R4	201	PEB	OA-C1A-C2A	-5.37	121.91	126.17
82	f1	203	PEB	CHC-C4C-NC	5.37	128.41	121.15
84	c3	1001	CYC	CMB-C2B-C1B	5.37	130.87	124.17
84	p3	1001	CYC	CMB-C2B-C1B	5.36	130.87	124.17
103	8N	310	ZEX	C23-C24-C25	5.36	116.97	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FA	202	PEB	C2C-C1C-NC	5.36	114.79	107.57
82	WA	201	PEB	C2C-C1C-NC	5.36	114.79	107.57
82	f4	201	PEB	C2C-C1C-NC	5.36	114.79	107.57
82	IQ	201	PEB	CMB-C2B-C1B	5.36	133.32	125.06
82	hH	201	PEB	CHC-C4C-NC	5.36	128.41	121.15
83	AE	302	PUB	OD-C4D-C3D	-5.36	122.22	128.04
82	S4	201	PEB	C2C-C1C-NC	5.36	114.79	107.57
82	D7	202	PEB	CHC-C4C-NC	5.36	128.40	121.15
82	TO	202	PEB	C2C-C1C-NC	5.36	114.79	107.57
82	OB	201	PEB	C1D-CHC-C4C	5.36	121.16	113.26
82	D5	202	PEB	CHC-C4C-NC	5.36	128.40	121.15
82	cB	403	PEB	C2C-C1C-NC	5.36	114.78	107.57
82	QK	203	PEB	OA-C1A-C2A	-5.36	121.91	126.17
82	Y4	201	PEB	OA-C1A-C2A	-5.36	121.91	126.17
85	L2	201	BCR	C7-C8-C9	-5.36	118.14	126.23
82	VI	203	PEB	CHB-C1C-C2C	-5.35	115.07	127.15
82	YJ	202	PEB	C2C-C1C-NC	5.35	114.78	107.57
82	L1	1002	PEB	OA-C1A-C2A	-5.35	121.92	126.17
84	E1	1001	CYC	OC-C1C-C2C	-5.35	121.92	126.17
82	XF	203	PEB	C1C-C2C-C3C	-5.35	101.29	107.62
82	QK	203	PEB	C2C-C1C-NC	5.35	114.78	107.57
82	WJ	203	PEB	CHB-C1C-C2C	-5.35	115.08	127.15
82	OP	203	PEB	C2C-C1C-NC	5.35	114.78	107.57
95	C6	503	DGD	O2G-C1B-C2B	5.35	123.03	111.50
82	N7	203	PEB	CHC-C1D-ND	-5.35	106.96	113.72
82	P4	202	PEB	C2C-C1C-NC	5.35	114.77	107.57
82	C7	201	PEB	C2C-C1C-NC	5.35	114.77	107.57
82	MB	202	PEB	C1C-C2C-C3C	-5.35	101.30	107.62
82	l1	203	PEB	CHC-C4C-NC	5.35	128.38	121.15
82	JA	202	PEB	C1C-CHB-C4B	5.35	140.27	128.28
82	WE	201	PEB	CHA-C1B-NB	-5.34	113.75	124.93
84	IE	1001	CYC	C3D-C4D-ND	5.34	114.77	107.57
84	IG	1001	CYC	C3D-C4D-ND	5.34	114.77	107.57
82	ZG	202	PEB	CMB-C2B-C1B	5.34	133.29	125.06
87	72	608	CLA	C4A-NA-C1A	5.34	109.11	106.71
84	IO	1001	CYC	OC-C1C-C2C	-5.34	121.92	126.17
82	D5	201	PEB	C1C-C2C-C3C	-5.34	101.31	107.62
85	LN	205	BCR	C12-C13-C14	5.34	127.14	118.94
85	L2	205	BCR	C12-C13-C14	5.34	127.14	118.94
84	HG	1001	CYC	CMD-C2D-C1D	5.34	133.38	125.56
82	M9	302	PEB	C2C-C1C-NC	5.34	114.76	107.57
82	MJ	202	PEB	C1C-C2C-C3C	-5.34	101.31	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	7N	602	CLA	C4A-NA-C1A	5.34	109.11	106.71
85	LN	201	BCR	C7-C8-C9	-5.34	118.17	126.23
82	ZO	201	PEB	C3B-C4B-NB	5.34	117.82	110.05
82	UG	203	PEB	C1C-C2C-C3C	-5.34	101.31	107.62
82	ZG	201	PEB	CHB-C1C-C2C	-5.34	115.11	127.15
82	UO	201	PEB	C3B-C4B-NB	5.34	117.81	110.05
82	U4	201	PEB	C3B-C4B-NB	5.34	117.81	110.05
82	PO	202	PEB	CHC-C4C-NC	5.34	128.38	121.15
85	B2	842	BCR	C11-C10-C9	-5.34	119.69	127.31
82	SH	202	PEB	C2C-C1C-NC	5.34	114.76	107.57
87	32	307	CLA	CHC-C4B-C3B	5.34	151.46	127.71
82	U5	202	PEB	C2C-C1C-NC	5.34	114.76	107.57
82	NA	202	PEB	CHB-C1C-C2C	-5.33	115.11	127.15
87	3N	308	CLA	CHC-C4B-C3B	5.33	151.44	127.71
82	AF	201	PEB	C2C-C1C-NC	5.33	114.75	107.57
84	EH	1001	CYC	C3D-C4D-ND	5.33	114.75	107.57
82	qK	202	PEB	CAB-C3B-C4B	5.33	134.44	125.01
82	M9	302	PEB	C1D-CHC-C4C	-5.33	105.39	113.26
82	fO	201	PEB	C2C-C1C-NC	5.33	114.75	107.57
82	lK	203	PEB	CHB-C1C-C2C	-5.33	115.12	127.15
82	c4	202	PEB	CHC-C4C-NC	5.33	128.37	121.15
84	D1	1001	CYC	CAB-C3B-C4B	5.33	129.80	121.38
82	N7	202	PEB	CHB-C1C-C2C	-5.33	115.12	127.15
84	I1	1001	CYC	OB-C4B-C3B	-5.33	122.25	128.04
82	bK	202	PEB	OA-C1A-C2A	-5.33	121.94	126.17
82	MM	201	PEB	C2C-C1C-NC	5.33	114.75	107.57
82	Z9	301	PEB	C1D-CHC-C4C	-5.33	105.40	113.26
82	J7	202	PEB	C1C-CHB-C4B	5.33	140.23	128.28
82	ZJ	201	PEB	OA-C1A-C2A	-5.33	121.94	126.17
82	NA	203	PEB	CHC-C1D-ND	-5.33	106.98	113.72
82	ZE	202	PEB	CMB-C2B-C1B	5.33	133.27	125.06
84	KG	202	CYC	CAB-C3B-C4B	5.33	129.79	121.38
82	TI	201	PEB	CHB-C1C-C2C	-5.33	115.13	127.15
85	A2	846	BCR	C21-C20-C19	-5.33	106.59	123.22
82	AA	202	PEB	C1C-C2C-C3C	-5.33	101.32	107.62
82	AH	305	PEB	C1C-C2C-C3C	-5.33	101.32	107.62
82	VD	203	PEB	CHC-C4C-NC	5.33	128.36	121.15
82	ZE	203	PEB	CMB-C2B-C1B	5.33	133.27	125.06
85	BN	842	BCR	C11-C10-C9	-5.33	119.71	127.31
82	OG	201	PEB	CMB-C2B-C1B	5.33	133.27	125.06
82	h1	202	PEB	CHC-C4C-NC	5.33	128.36	121.15
82	Z9	304	PEB	CHA-C1B-NB	-5.33	113.79	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	DH	1001	CYC	CAB-C3B-C4B	5.33	129.79	121.38
85	B2	839	BCR	C7-C8-C9	-5.32	118.19	126.23
85	H6	101	BCR	C16-C17-C18	-5.32	119.71	127.31
82	O5	203	PEB	C2C-C1C-NC	5.32	114.74	107.57
82	NA	202	PEB	C1C-CHB-C4B	5.32	140.22	128.28
83	Z9	305	PUB	OD-C4D-ND	-5.32	118.04	125.93
103	82	310	ZEX	C23-C24-C25	5.32	116.91	109.33
84	EO	1001	CYC	OC-C1C-C2C	-5.32	121.94	126.17
82	SO	201	PEB	CHB-C4B-C3B	-5.32	113.01	125.32
82	OM	202	PEB	CHC-C4C-NC	5.32	128.35	121.15
82	aG	201	PEB	C1C-C2C-C3C	-5.32	101.33	107.62
82	H5	202	PEB	C2C-C1C-NC	5.32	114.74	107.57
82	MP	201	PEB	CMB-C2B-C1B	5.32	133.26	125.06
82	qF	202	PEB	CAB-C3B-C4B	5.32	134.42	125.01
82	VK	202	PEB	C1C-C2C-C3C	-5.32	101.33	107.62
83	KA	203	PUB	OD-C4D-C3D	-5.32	122.27	128.04
82	OM	201	PEB	CMB-C2B-C1B	5.32	133.26	125.06
82	j1	202	PEB	CHC-C4C-NC	5.32	128.35	121.15
82	LK	202	PEB	C2C-C1C-NC	5.32	114.73	107.57
82	B5	202	PEB	CHC-C4C-NC	5.32	128.35	121.15
82	iH	201	PEB	C1C-C2C-C3C	-5.32	101.33	107.62
82	cO	202	PEB	CHC-C4C-NC	5.32	128.35	121.15
85	AN	846	BCR	C21-C20-C19	-5.32	106.62	123.22
82	RA	202	PEB	C2A-C1A-NA	5.32	112.86	108.27
82	M9	305	PEB	CHA-C1B-NB	-5.32	113.81	124.93
82	lH	202	PEB	CHC-C4C-NC	5.32	128.34	121.15
82	Z9	301	PEB	C2C-C1C-NC	5.32	114.73	107.57
82	SD	201	PEB	CHC-C1D-ND	-5.32	107.00	113.72
82	S4	201	PEB	CHB-C4B-C3B	-5.32	113.02	125.32
82	mJ	201	PEB	CHC-C1D-ND	5.31	120.45	113.72
84	H1	1001	CYC	C3D-C4D-ND	5.31	114.72	107.57
82	KM	202	PEB	CHC-C4C-NC	5.31	128.34	121.15
83	M9	303	PUB	C4B-C3B-C2B	-5.31	101.34	107.62
82	kK	201	PEB	CMB-C2B-C1B	5.31	133.24	125.06
82	U1	203	PEB	C2C-C1C-NC	5.31	114.72	107.57
82	i4	202	PEB	C2C-C1C-NC	5.31	114.72	107.57
82	AK	201	PEB	C2C-C1C-NC	5.31	114.72	107.57
82	A1	305	PEB	C1C-C2C-C3C	-5.31	101.34	107.62
103	82	309	ZEX	C31-C30-C29	-5.31	119.73	127.31
82	ZE	201	PEB	CHB-C1C-C2C	-5.31	115.17	127.15
83	AJ	304	PUB	CHC-C1D-ND	-5.31	107.01	113.72
82	R7	203	PEB	C2C-C1C-NC	5.31	114.72	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OP	201	PEB	CMC-C3C-C2C	-5.31	114.12	125.61
84	LH	1002	CYC	C3D-C4D-ND	5.31	114.72	107.57
82	N7	202	PEB	C1C-CHB-C4B	5.31	140.18	128.28
82	eE	202	PEB	CHC-C4C-NC	5.31	128.33	121.15
82	SK	201	PEB	C2C-C1C-NC	5.31	114.71	107.57
82	dE	202	PEB	CHC-C1D-ND	-5.30	107.01	113.72
87	2N	303	CLA	C4A-NA-C1A	5.30	109.09	106.71
82	OP	203	PEB	CMC-C3C-C4C	5.30	132.68	127.06
82	PO	201	PEB	OA-C1A-C2A	-5.30	121.96	126.17
82	QO	201	PEB	C3B-C4B-NB	5.30	117.76	110.05
85	c6	602	BCR	C7-C8-C9	-5.30	118.22	126.23
82	KI	201	PEB	CHB-C1C-C2C	-5.30	115.19	127.15
103	8N	309	ZEX	C31-C30-C29	-5.30	119.74	127.31
82	SM	202	PEB	CHC-C4C-NC	5.30	128.32	121.15
84	HH	1001	CYC	C3D-C4D-ND	5.30	114.71	107.57
82	P4	202	PEB	CHC-C4C-NC	5.30	128.32	121.15
84	ME	1001	CYC	OC-C1C-C2C	-5.30	121.96	126.17
84	I4	1001	CYC	OC-C1C-C2C	-5.30	121.96	126.17
83	AM	304	PUB	C4B-C3B-C2B	-5.30	101.36	107.62
82	WD	201	PEB	C2C-C1C-NC	5.30	114.70	107.57
82	VQ	203	PEB	CHC-C4C-NC	5.30	128.32	121.15
84	E1	1001	CYC	C3D-C4D-ND	5.30	114.70	107.57
82	QJ	204	PEB	C1D-CHC-C4C	-5.30	105.45	113.26
82	kF	201	PEB	CMB-C2B-C1B	5.30	133.22	125.06
87	7N	607	CLA	C4A-NA-C1A	5.30	109.09	106.71
82	jH	202	PEB	CHC-C4C-NC	5.30	128.32	121.15
82	dE	202	PEB	CHC-C4C-NC	5.29	128.32	121.15
84	63	901	CYC	OB-C4B-C3B	-5.29	122.30	128.04
82	S5	201	PEB	C4C-C3C-C2C	-5.29	102.61	107.50
82	i1	201	PEB	C1C-C2C-C3C	-5.29	101.36	107.62
83	Z9	302	PUB	C4B-C3B-C2B	-5.29	101.36	107.62
84	FE	1002	CYC	OB-C4B-C3B	-5.29	122.30	128.04
82	SF	201	PEB	C2C-C1C-NC	5.29	114.69	107.57
82	lJ	203	PEB	C1C-C2C-C3C	-5.29	101.37	107.62
82	IF	201	PEB	C3B-C4B-NB	5.29	117.74	110.05
85	BN	839	BCR	C7-C8-C9	-5.29	118.24	126.23
82	LH	1003	PEB	OA-C1A-C2A	-5.29	121.97	126.17
91	aL	610	PHO	C4D-ND-C1D	-5.29	103.45	108.83
82	aJ	204	PEB	C2C-C1C-NC	5.29	114.69	107.57
82	cK	203	PEB	C2C-C1C-NC	5.29	114.69	107.57
82	eO	202	PEB	C2C-C1C-NC	5.29	114.69	107.57
84	x3	1001	CYC	CHD-C4C-NC	5.29	131.49	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QF	203	PEB	C2C-C1C-NC	5.29	114.69	107.57
84	KG	202	CYC	C3D-C4D-ND	5.29	114.69	107.57
95	c6	601	DGD	C1D-O6D-C5D	-5.29	103.31	113.69
82	d4	201	PEB	C2C-C1C-NC	5.28	114.69	107.57
82	LF	202	PEB	C2C-C1C-NC	5.28	114.69	107.57
82	EA	201	PEB	CHA-C1B-NB	-5.28	113.88	124.93
82	IK	201	PEB	C3B-C4B-NB	5.28	117.73	110.05
82	FK	202	PEB	C2C-C1C-NC	5.28	114.68	107.57
87	dL	402	CLA	C4A-NA-C1A	5.28	109.08	106.71
82	PO	202	PEB	C2C-C1C-NC	5.28	114.68	107.57
94	dL	406	PL9	C7-C3-C4	5.28	121.17	116.88
95	C6	502	DGD	C1D-O6D-C5D	-5.28	103.33	113.69
84	DG	1001	CYC	C2B-C1B-NB	5.28	114.71	106.99
84	L1	1001	CYC	C3D-C4D-ND	5.27	114.67	107.57
82	CP	202	PEB	CMB-C2B-C1B	5.27	133.19	125.06
82	Q4	201	PEB	C3B-C4B-NB	5.27	117.72	110.05
82	VF	202	PEB	C1C-CHB-C4B	5.27	140.11	128.28
82	S1	202	PEB	C2C-C1C-NC	5.27	114.67	107.57
82	dG	202	PEB	CHC-C4C-NC	5.27	128.28	121.15
82	B5	202	PEB	CHB-C1C-C2C	-5.27	115.26	127.15
87	L2	206	CLA	C4A-NA-C1A	5.27	109.08	106.71
82	iO	202	PEB	C2C-C1C-NC	5.27	114.67	107.57
82	O5	201	PEB	C1C-C2C-C3C	-5.27	101.39	107.62
82	FF	202	PEB	C2C-C1C-NC	5.27	114.67	107.57
84	V3	1001	CYC	CHD-C4C-NC	5.27	131.47	125.20
82	a4	202	PEB	CHC-C4C-NC	5.27	128.28	121.15
82	aE	201	PEB	C1C-C2C-C3C	-5.27	101.39	107.62
82	SQ	201	PEB	CHC-C1D-ND	-5.27	107.06	113.72
82	cF	203	PEB	C2C-C1C-NC	5.27	114.66	107.57
82	OO	201	PEB	CMB-C2B-C1B	5.27	133.18	125.06
82	IJ	202	PEB	C2C-C1C-NC	5.27	114.66	107.57
82	KJ	203	PEB	CHB-C1C-C2C	-5.27	115.27	127.15
87	LN	206	CLA	C4A-NA-C1A	5.26	109.07	106.71
82	E7	201	PEB	CHA-C1B-NB	-5.26	113.92	124.93
85	cL	518	BCR	C20-C21-C22	-5.26	119.80	127.31
82	GM	203	PEB	C2C-C1C-NC	5.26	114.66	107.57
82	S9	202	PEB	C2C-C1C-NC	5.26	114.66	107.57
82	p8	202	PEB	C1C-C2C-C3C	-5.26	101.40	107.62
82	OE	201	PEB	CMB-C2B-C1B	5.26	133.17	125.06
82	VK	202	PEB	C1C-CHB-C4B	5.26	140.08	128.28
82	JA	201	PEB	C1C-C2C-C3C	-5.26	101.40	107.62
84	NE	201	CYC	C3D-C4D-ND	5.26	114.66	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	K7	203	PUB	OD-C4D-C3D	-5.26	122.33	128.04
82	WB	402	PEB	C1C-C2C-C3C	-5.26	101.40	107.62
82	VF	202	PEB	C1C-C2C-C3C	-5.26	101.40	107.62
82	JK	202	PEB	CMC-C3C-C4C	5.26	132.64	127.06
82	IM	201	PEB	C2C-C1C-NC	5.26	114.65	107.57
87	B2	834	CLA	C4A-NA-C1A	5.26	109.07	106.71
82	VF	201	PEB	CHA-C4A-NA	5.26	131.46	125.20
82	RK	202	PEB	C2C-C1C-NC	5.26	114.65	107.57
82	xK	304	PEB	OA-C1A-C2A	-5.25	122.00	126.17
82	lJ	202	PEB	C2C-C1C-NC	5.25	114.65	107.57
82	AI	203	PEB	OA-C1A-C2A	-5.25	122.00	126.17
82	dK	201	PEB	CHA-C4A-NA	5.25	131.45	125.20
82	VD	201	PEB	C2C-C1C-NC	5.25	114.64	107.57
82	a4	201	PEB	C1C-C2C-C3C	-5.25	101.41	107.62
82	DA	202	PEB	CHC-C4C-NC	5.25	128.25	121.15
87	B2	827	CLA	C4A-NA-C1A	5.25	109.07	106.71
82	e4	202	PEB	C2C-C1C-NC	5.25	114.64	107.57
82	kO	202	PEB	C2C-C1C-NC	5.25	114.64	107.57
82	R7	202	PEB	C2A-C1A-NA	5.25	112.80	108.27
82	eG	202	PEB	CHC-C4C-NC	5.25	128.25	121.15
82	fH	203	PEB	CHC-C4C-NC	5.25	128.25	121.15
82	VK	202	PEB	CHB-C4B-C3B	-5.25	113.18	125.32
84	x3	1001	CYC	CHD-C1D-ND	-5.25	113.30	125.32
82	VQ	202	PEB	CHC-C1D-ND	-5.25	107.09	113.72
82	VQ	201	PEB	C2C-C1C-NC	5.25	114.64	107.57
82	WQ	201	PEB	C2C-C1C-NC	5.25	114.64	107.57
82	ZB	203	PEB	CMC-C3C-C4C	5.25	132.62	127.06
82	YG	202	PEB	C1C-C2C-C3C	-5.25	101.42	107.62
82	pC	202	PEB	C1C-C2C-C3C	-5.25	101.42	107.62
82	H7	201	PEB	OA-C1A-C2A	-5.25	122.00	126.17
82	gO	202	PEB	C2C-C1C-NC	5.24	114.63	107.57
82	J7	201	PEB	C1C-C2C-C3C	-5.24	101.42	107.62
94	AL	413	PL9	O1-C4-C3	5.24	126.50	120.72
82	H5	201	PEB	CAA-C3A-C2A	-5.24	101.16	114.26
82	aO	201	PEB	C1C-C2C-C3C	-5.24	101.42	107.62
83	M5	302	PUB	CBB-CAB-C3B	5.24	127.19	112.63
84	C1	1001	CYC	OB-C4B-C3B	-5.24	122.35	128.04
82	O4	201	PEB	CMB-C2B-C1B	5.24	133.13	125.06
82	UH	203	PEB	C2C-C1C-NC	5.24	114.63	107.57
82	LQ	202	PEB	CHC-C4C-NC	5.24	128.24	121.15
82	d1	201	PEB	C2C-C1C-NC	5.24	114.62	107.57
82	jO	201	PEB	C2C-C1C-NC	5.24	114.62	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dE	201	PEB	C1C-C2C-C3C	-5.24	101.43	107.62
82	VI	203	PEB	C3C-C4C-NC	5.24	113.05	108.33
82	BB	203	PEB	CHC-C1D-ND	-5.24	107.10	113.72
82	dG	201	PEB	C1C-C2C-C3C	-5.24	101.43	107.62
82	RA	203	PEB	C2C-C1C-NC	5.24	114.62	107.57
82	AA	202	PEB	C2C-C1C-NC	5.24	114.62	107.57
82	U5	202	PEB	CHC-C4C-NC	5.24	128.24	121.15
82	CB	201	PEB	CHC-C1D-ND	-5.23	107.10	113.72
82	YA	303	PEB	C1C-C2C-C3C	-5.23	101.43	107.62
82	BB	201	PEB	CHC-C4C-NC	5.23	128.23	121.15
82	b1	201	PEB	CHC-C4C-NC	5.23	128.23	121.15
82	PG	202	PEB	C2C-C1C-NC	5.23	114.62	107.57
85	B2	838	BCR	C3-C4-C5	-5.23	104.73	114.08
82	GK	202	PEB	CMB-C2B-C1B	5.23	133.12	125.06
85	B6	621	BCR	C16-C17-C18	-5.23	119.84	127.31
82	aO	201	PEB	OA-C1A-C2A	-5.23	122.01	126.17
85	AN	846	BCR	C16-C15-C14	-5.23	112.76	123.47
82	QF	203	PEB	OA-C1A-C2A	-5.23	122.01	126.17
83	Z5	302	PUB	C4A-CHA-C1B	-5.23	105.54	113.26
84	V3	1001	CYC	CHD-C1D-ND	-5.23	113.34	125.32
82	TO	201	PEB	OA-C1A-C2A	-5.23	122.02	126.17
85	A2	846	BCR	C16-C15-C14	-5.23	112.76	123.47
82	WF	201	PEB	C2C-C1C-NC	5.23	114.61	107.57
82	CA	201	PEB	CHB-C1C-C2C	-5.23	115.35	127.15
84	LH	1001	CYC	OB-C4B-C3B	-5.23	122.37	128.04
83	Z5	302	PUB	CBB-CAB-C3B	5.23	127.15	112.63
82	VK	201	PEB	CHA-C4A-NA	5.23	131.42	125.20
85	B2	838	BCR	C11-C10-C9	-5.23	119.85	127.31
82	PG	202	PEB	C1C-C2C-C3C	-5.23	101.44	107.62
82	NM	201	PEB	CMC-C3C-C4C	5.23	132.60	127.06
82	Q1	201	PEB	C2C-C1C-NC	5.23	114.61	107.57
82	C7	201	PEB	CHB-C1C-C2C	-5.22	115.36	127.15
82	bH	201	PEB	CHC-C4C-NC	5.22	128.22	121.15
82	O1	203	PEB	C2C-C1C-NC	5.22	114.60	107.57
85	BN	838	BCR	C11-C10-C9	-5.22	119.86	127.31
82	ZG	203	PEB	CMB-C2B-C1B	5.22	133.11	125.06
82	LD	202	PEB	CHC-C4C-NC	5.22	128.22	121.15
85	BN	838	BCR	C3-C4-C5	-5.22	104.75	114.08
82	VF	202	PEB	CHB-C4B-C3B	-5.22	113.24	125.32
82	WK	201	PEB	C2C-C1C-NC	5.22	114.60	107.57
87	22	602	CLA	C4A-NA-C1A	5.22	109.05	106.71
82	dO	201	PEB	C2C-C1C-NC	5.22	114.59	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CP	201	PEB	CMC-C3C-C2C	-5.22	114.32	125.61
85	A6	401	BCR	C20-C21-C22	-5.22	119.87	127.31
82	YE	202	PEB	C1C-C2C-C3C	-5.22	101.45	107.62
84	FG	1001	CYC	OB-C4B-C3B	-5.22	122.38	128.04
82	KB	302	PEB	CHC-C1D-ND	-5.21	107.13	113.72
82	KP	201	PEB	C3C-C4C-NC	-5.21	103.64	108.33
82	NB	203	PEB	CHC-C1D-ND	-5.21	107.13	113.72
82	OG	203	PEB	C2C-C1C-NC	5.21	114.59	107.57
83	AH	304	PUB	C4B-CHB-C1C	-5.21	116.59	128.28
82	PE	202	PEB	C2C-C1C-NC	5.21	114.59	107.57
82	J7	201	PEB	C2C-C1C-NC	5.21	114.59	107.57
82	g4	202	PEB	C2C-C1C-NC	5.21	114.59	107.57
82	SP	202	PEB	CMB-C2B-C1B	5.21	133.09	125.06
82	FK	202	PEB	C1C-CHB-C4B	5.21	139.97	128.28
82	M5	304	PEB	C2C-C1C-NC	5.21	114.58	107.57
84	KH	1001	CYC	CAB-C3B-C4B	5.21	129.61	121.38
84	K1	1001	CYC	CAB-C3B-C4B	5.21	129.60	121.38
84	EH	1001	CYC	OC-C1C-C2C	-5.21	122.03	126.17
82	OM	203	PEB	CHC-C4C-NC	5.21	128.19	121.15
82	aO	202	PEB	CHC-C4C-NC	5.21	128.19	121.15
82	j4	201	PEB	C2C-C1C-NC	5.21	114.58	107.57
84	DG	1001	CYC	CMD-C2D-C1D	5.20	133.18	125.56
82	xF	304	PEB	OA-C1A-C2A	-5.20	122.03	126.17
82	Z5	304	PEB	C2C-C1C-NC	5.20	114.58	107.57
82	RF	202	PEB	C2C-C1C-NC	5.20	114.58	107.57
82	O4	201	PEB	CHB-C4B-C3B	-5.20	113.28	125.32
82	dG	202	PEB	CHC-C1D-ND	-5.20	107.14	113.72
82	B7	202	PEB	C1C-CHB-C4B	5.20	139.95	128.28
82	DA	202	PEB	C2C-C1C-NC	5.20	114.57	107.57
82	UG	201	PEB	C2C-C1C-NC	5.20	114.57	107.57
82	YG	202	PEB	OA-C1A-C2A	-5.20	122.04	126.17
87	O2	203	CLA	C4A-NA-C1A	5.20	109.04	106.71
85	B2	802	BCR	C16-C17-C18	5.20	134.73	127.31
87	1N	606	CLA	C4A-NA-C1A	5.20	109.04	106.71
82	OO	201	PEB	CHB-C4B-C3B	-5.20	113.29	125.32
82	tF	201	PEB	C2A-C1A-NA	5.20	112.75	108.27
83	A1	304	PUB	C4B-CHB-C1C	-5.20	116.63	128.28
82	RF	201	PEB	OA-C1A-NA	5.20	131.24	124.94
82	PG	201	PEB	C1C-C2C-C3C	-5.20	101.48	107.62
82	hM	203	PEB	C1C-C2C-C3C	-5.20	101.48	107.62
82	OH	203	PEB	C2C-C1C-NC	5.20	114.57	107.57
82	lJ	201	PEB	C2C-C1C-NC	5.20	114.57	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	tK	201	PEB	C2A-C1A-NA	5.20	112.75	108.27
82	ID	201	PEB	CHB-C1C-NC	-5.20	113.42	125.32
82	WI	202	PEB	C1B-C2B-C3B	-5.19	100.55	106.51
82	FF	202	PEB	C1C-CHB-C4B	5.19	139.93	128.28
82	CJ	201	PEB	OA-C1A-C2A	-5.19	122.04	126.17
82	V1	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
82	Z1	203	PEB	CMB-C2B-C1B	5.19	133.06	125.06
82	jM	201	PEB	C1C-C2C-C3C	-5.19	101.48	107.62
82	GF	202	PEB	CMB-C2B-C1B	5.19	133.06	125.06
82	b1	203	PEB	C2C-C1C-NC	5.19	114.56	107.57
82	gE	201	PEB	C1C-C2C-C3C	-5.19	101.48	107.62
82	JA	201	PEB	C2C-C1C-NC	5.19	114.56	107.57
82	R4	201	PEB	C1C-C2C-C3C	-5.19	101.48	107.62
82	UE	203	PEB	C2C-C1C-NC	5.19	114.56	107.57
84	L3	1001	CYC	C4D-C3D-C2D	-5.19	101.49	107.62
82	Y4	202	PEB	CHC-C4C-NC	5.19	128.17	121.15
82	LF	202	PEB	CMB-C2B-C1B	5.19	133.06	125.06
103	82	309	ZEX	C11-C10-C9	-5.19	119.91	127.31
82	UK	201	PEB	C3B-C4B-NB	5.19	117.60	110.05
82	HA	201	PEB	OA-C1A-C2A	-5.19	122.05	126.17
93	AL	412	BCT	O2-C-O1	5.19	133.00	119.55
82	kG	202	PEB	C1C-C2C-C3C	-5.19	101.49	107.62
88	CL	522	LHG	O7-C7-C8	5.18	122.67	111.50
84	CH	1001	CYC	OB-C4B-C3B	-5.18	122.42	128.04
82	YE	202	PEB	OA-C1A-C2A	-5.18	122.05	126.17
82	ZG	201	PEB	CHC-C4C-NC	5.18	128.16	121.15
84	S3	1001	CYC	C4D-C3D-C2D	-5.18	101.50	107.62
82	LB	201	PEB	OA-C1A-C2A	-5.18	122.05	126.17
87	BN	836	CLA	CMD-C2D-C3D	5.18	139.53	127.61
82	XF	203	PEB	C2C-C1C-NC	5.18	114.55	107.57
82	a4	201	PEB	OA-C1A-C2A	-5.18	122.05	126.17
84	DE	1001	CYC	C2B-C1B-NB	5.18	114.57	106.99
82	VE	202	PEB	C1C-C2C-C3C	-5.18	101.50	107.62
85	BN	803	BCR	C16-C17-C18	5.18	134.70	127.31
83	M5	302	PUB	C4A-CHA-C1B	-5.18	105.62	113.26
82	D9	201	PEB	C2C-C1C-NC	5.18	114.54	107.57
82	QH	201	PEB	C2C-C1C-NC	5.18	114.54	107.57
82	RK	201	PEB	OA-C1A-NA	5.18	131.21	124.94
82	A9	202	PEB	CHB-C4B-NB	-5.18	113.80	124.58
82	G9	202	PEB	CHB-C4B-NB	-5.18	113.81	124.58
82	K9	202	PEB	CHB-C4B-NB	-5.18	113.81	124.58
82	VD	202	PEB	CHC-C1D-ND	-5.18	107.18	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NI	203	PEB	OA-C1A-C2A	-5.18	122.06	126.17
82	m4	201	PEB	OA-C1A-C2A	-5.18	122.06	126.17
84	w3	1001	CYC	C3D-C4D-ND	5.17	114.54	107.57
84	73	1001	CYC	C3D-C4D-ND	5.17	114.54	107.57
82	PE	202	PEB	C1C-C2C-C3C	-5.17	101.50	107.62
82	W4	201	PEB	C1C-C2C-C3C	-5.17	101.50	107.62
82	aJ	203	PEB	C1C-C2C-C3C	-5.17	101.50	107.62
82	VH	201	PEB	CMB-C2B-C1B	5.17	133.03	125.06
84	L1	1001	CYC	CMD-C2D-C1D	5.17	133.13	125.56
84	f3	1001	CYC	C4D-C3D-C2D	-5.17	101.51	107.62
82	V9	202	PEB	CHB-C4B-NB	-5.17	113.82	124.58
82	YE	201	PEB	OA-C1A-C2A	-5.17	122.06	126.17
82	LJ	201	PEB	OA-C1A-C2A	-5.17	122.06	126.17
82	IQ	201	PEB	CHB-C1C-NC	-5.17	113.48	125.32
82	JF	202	PEB	CMC-C3C-C4C	5.17	132.54	127.06
84	I3	1001	CYC	C3D-C4D-ND	5.17	114.53	107.57
84	o3	1001	CYC	C4D-C3D-C2D	-5.17	101.51	107.62
84	u3	1001	CYC	C3D-C4D-ND	5.17	114.53	107.57
82	IJ	203	PEB	CHC-C4C-NC	5.17	128.14	121.15
82	eG	203	PEB	CHA-C1B-NB	-5.17	114.12	124.93
82	D5	201	PEB	C2C-C1C-NC	5.17	114.53	107.57
84	M3	1001	CYC	C4D-C3D-C2D	-5.17	101.51	107.62
87	B2	836	CLA	CMD-C2D-C3D	5.17	139.50	127.61
82	EQ	201	PEB	CAC-C2C-C1C	5.17	133.99	125.76
82	Q5	203	PEB	C2C-C1C-NC	5.17	114.53	107.57
82	R9	202	PEB	CHB-C4B-NB	-5.17	113.83	124.58
85	BN	839	BCR	C30-C25-C26	-5.17	115.34	122.61
84	q3	1001	CYC	C3D-C4D-ND	5.17	114.53	107.57
82	VF	202	PEB	C2C-C1C-NC	5.16	114.53	107.57
82	wF	301	PEB	C1D-CHC-C4C	-5.16	105.64	113.26
84	Q3	1001	CYC	C3D-C4D-ND	5.16	114.52	107.57
82	LK	202	PEB	CMB-C2B-C1B	5.16	133.02	125.06
82	BA	202	PEB	C1C-CHB-C4B	5.16	139.86	128.28
82	I9	202	PEB	CHB-C4B-NB	-5.16	113.83	124.58
84	H3	1001	CYC	C3D-C4D-ND	5.16	114.52	107.57
82	UI	202	PEB	OA-C1A-C2A	-5.16	122.07	126.17
87	FN	203	CLA	C4A-NA-C1A	5.16	109.03	106.71
87	72	607	CLA	C4A-NA-C1A	5.16	109.03	106.71
82	lJ	202	PEB	CHC-C4C-NC	5.16	128.13	121.15
85	k6	102	BCR	C15-C14-C13	-5.16	119.94	127.31
82	WG	203	PEB	CHC-C4C-NC	5.16	128.13	121.15
82	ZH	203	PEB	CMB-C2B-C1B	5.16	133.01	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	H3	1001	CYC	C4D-C3D-C2D	-5.16	101.52	107.62
82	hG	201	PEB	CHB-C1C-C2C	-5.16	115.51	127.15
82	D7	202	PEB	C2C-C1C-NC	5.16	114.52	107.57
82	S7	202	PEB	C2C-C1C-NC	5.16	114.52	107.57
84	D3	1001	CYC	C4D-C3D-C2D	-5.16	101.52	107.62
82	A7	202	PEB	C2C-C1C-NC	5.16	114.52	107.57
87	AN	849	CLA	CMB-C2B-C1B	-5.16	117.51	125.37
82	RO	201	PEB	C1C-C2C-C3C	-5.16	101.52	107.62
84	u3	1001	CYC	C4D-C3D-C2D	-5.16	101.52	107.62
82	Y7	303	PEB	C1C-C2C-C3C	-5.16	101.52	107.62
84	L3	1001	CYC	C3D-C4D-ND	5.16	114.52	107.57
84	o3	1001	CYC	C3D-C4D-ND	5.16	114.52	107.57
82	DQ	202	PEB	CHC-C4C-NC	5.16	128.13	121.15
84	73	1001	CYC	C4D-C3D-C2D	-5.16	101.53	107.62
87	A2	849	CLA	CMB-C2B-C1B	-5.16	117.52	125.37
82	S1	202	PEB	C1D-CHC-C4C	-5.16	105.65	113.26
87	BN	834	CLA	C4A-NA-C1A	5.16	109.02	106.71
82	SA	202	PEB	C2C-C1C-NC	5.16	114.51	107.57
82	gG	201	PEB	C1C-C2C-C3C	-5.16	101.53	107.62
82	P9	202	PEB	CHB-C4B-NB	-5.16	113.85	124.58
82	VG	202	PEB	C1C-C2C-C3C	-5.15	101.53	107.62
84	Q3	1001	CYC	C4D-C3D-C2D	-5.15	101.53	107.62
84	d3	1001	CYC	C4D-C3D-C2D	-5.15	101.53	107.62
82	E9	202	PEB	CHB-C4B-NB	-5.15	113.85	124.58
82	T9	202	PEB	CHB-C4B-NB	-5.15	113.85	124.58
103	8N	309	ZEX	C11-C10-C9	-5.15	119.95	127.31
82	KB	301	PEB	C2C-C1C-NC	5.15	114.51	107.57
82	eE	203	PEB	OA-C1A-C2A	-5.15	122.08	126.17
84	U3	1001	CYC	C3D-C4D-ND	5.15	114.51	107.57
85	B6	621	BCR	C28-C27-C26	-5.15	104.88	114.08
82	eH	203	PEB	C2C-C1C-NC	5.15	114.51	107.57
85	K6	102	BCR	C15-C14-C13	-5.15	119.96	127.31
82	OE	203	PEB	C2C-C1C-NC	5.15	114.51	107.57
82	j4	203	PEB	C2C-C1C-NC	5.15	114.51	107.57
82	MM	203	PEB	CHC-C4C-NC	5.15	128.12	121.15
83	AM	303	PUB	C4B-C3B-C2B	-5.15	101.53	107.62
87	62	305	CLA	C4A-NA-C1A	5.15	109.02	106.71
84	L4	1001	CYC	C3D-C4D-ND	5.15	114.50	107.57
84	f3	1001	CYC	C3D-C4D-ND	5.15	114.50	107.57
84	LH	1001	CYC	CHD-C1D-ND	-5.15	113.53	125.32
82	KI	201	PEB	OA-C1A-C2A	-5.15	122.08	126.17
84	J4	1001	CYC	C3D-C4D-ND	5.15	114.50	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	N9	202	PEB	CHB-C4B-NB	-5.15	113.86	124.58
96	fL	102	HEM	CHD-C1D-ND	5.15	130.01	124.42
82	p8	201	PEB	C1C-C2C-C3C	-5.15	101.54	107.62
82	UF	201	PEB	C4B-C3B-C2B	-5.15	101.09	106.78
82	XF	202	PEB	C2C-C1C-NC	5.15	114.50	107.57
84	F3	1001	CYC	C3D-C4D-ND	5.15	114.50	107.57
82	sK	201	PEB	C1C-C2C-C3C	-5.15	101.54	107.62
84	ME	1001	CYC	OB-C4B-C3B	-5.14	122.46	128.04
82	bB	201	PEB	C2C-C1C-NC	5.14	114.50	107.57
85	B6	621	BCR	C15-C14-C13	-5.14	119.97	127.31
84	j3	1001	CYC	C4D-C3D-C2D	-5.14	101.54	107.62
82	TH	201	PEB	C2C-C1C-NC	5.14	114.50	107.57
82	cK	201	PEB	C2C-C1C-NC	5.14	114.50	107.57
84	B3	1001	CYC	C3D-C4D-ND	5.14	114.50	107.57
82	aK	203	PEB	CHA-C1B-NB	-5.14	114.18	124.93
83	KA	203	PUB	C4B-C3B-C2B	-5.14	101.54	107.62
84	d3	1001	CYC	C3D-C4D-ND	5.14	114.49	107.57
83	BM	302	PUB	CHC-C1D-ND	-5.14	107.22	113.72
84	I1	1001	CYC	CHD-C1D-ND	-5.14	113.54	125.32
84	h3	1001	CYC	C4D-C3D-C2D	-5.14	101.54	107.62
82	IP	202	PEB	C2C-C1C-NC	5.14	114.49	107.57
84	p3	1001	CYC	CMD-C2D-C1D	5.14	133.09	125.56
84	F3	1001	CYC	C4D-C3D-C2D	-5.14	101.55	107.62
82	R4	201	PEB	C2C-C1C-NC	5.14	114.49	107.57
82	JB	201	PEB	CHA-C1B-C2B	5.14	138.11	124.90
82	wK	301	PEB	C1D-CHC-C4C	-5.14	105.68	113.26
84	k3	1001	CYC	C4D-C3D-C2D	-5.14	101.55	107.62
84	h3	1001	CYC	C3D-C4D-ND	5.14	114.49	107.57
82	DD	202	PEB	CHC-C4C-NC	5.14	128.10	121.15
82	UE	201	PEB	C2C-C1C-NC	5.14	114.49	107.57
84	k3	1001	CYC	C3D-C4D-ND	5.14	114.49	107.57
82	MJ	203	PEB	C1C-C2C-C3C	-5.14	101.55	107.62
82	wK	302	PEB	C1C-C2C-C3C	-5.14	101.55	107.62
84	j3	1001	CYC	C3D-C4D-ND	5.14	114.49	107.57
82	TB	201	PEB	CHA-C1B-C2B	5.14	138.11	124.90
84	B3	1001	CYC	C4D-C3D-C2D	-5.14	101.55	107.62
82	X9	202	PEB	CHB-C4B-NB	-5.14	113.89	124.58
82	BI	202	PEB	C3C-C4C-NC	5.14	112.95	108.33
84	M3	1001	CYC	C3D-C4D-ND	5.14	114.49	107.57
84	q3	1001	CYC	C4D-C3D-C2D	-5.14	101.55	107.62
82	C9	202	PEB	CHB-C4B-NB	-5.14	113.89	124.58
82	UM	202	PEB	CHA-C1B-NB	-5.13	114.19	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iH	201	PEB	C2C-C1C-NC	5.13	114.48	107.57
82	X7	201	PEB	C1C-C2C-C3C	-5.13	101.55	107.62
82	b4	201	PEB	C2C-C1C-NC	5.13	114.48	107.57
84	I1	1001	CYC	OC-C1C-C2C	-5.13	122.09	126.17
87	F2	201	CLA	C4A-NA-C1A	5.13	109.01	106.71
84	t3	1001	CYC	CMD-C2D-C1D	5.13	133.08	125.56
82	SJ	203	PEB	C2C-C1C-NC	5.13	114.48	107.57
82	XK	203	PEB	C2C-C1C-NC	5.13	114.48	107.57
85	B2	839	BCR	C30-C25-C26	-5.13	115.38	122.61
82	fF	201	PEB	CHC-C4C-NC	5.13	128.10	121.15
84	O3	1001	CYC	C3D-C4D-ND	5.13	114.48	107.57
82	SH	202	PEB	C1D-CHC-C4C	-5.13	105.69	113.26
82	pC	201	PEB	C1C-C2C-C3C	-5.13	101.56	107.62
84	I3	1001	CYC	C4D-C3D-C2D	-5.13	101.56	107.62
82	BI	203	PEB	OA-C1A-C2A	-5.13	122.09	126.17
82	UF	201	PEB	C3B-C4B-NB	5.13	117.51	110.05
84	D3	1001	CYC	C3D-C4D-ND	5.13	114.48	107.57
84	K3	1001	CYC	CMD-C2D-C1D	5.13	133.07	125.56
82	TO	201	PEB	C1C-C2C-C3C	-5.13	101.56	107.62
82	VQ	203	PEB	C2C-C1C-NC	5.13	114.48	107.57
84	K1	1001	CYC	OB-C4B-C3B	-5.13	122.47	128.04
82	hE	201	PEB	CHB-C1C-C2C	-5.13	115.58	127.15
84	w3	1001	CYC	C4D-C3D-C2D	-5.13	101.56	107.62
82	WM	201	PEB	CHA-C1B-NB	-5.13	114.21	124.93
82	dG	203	PEB	CMB-C2B-C1B	5.13	132.96	125.06
84	S3	1001	CYC	C3D-C4D-ND	5.13	114.47	107.57
82	dH	201	PEB	CHC-C4C-NC	5.13	128.09	121.15
82	PB	201	PEB	CHC-C1D-ND	-5.13	107.24	113.72
82	O5	202	PEB	CHB-C1C-C2C	-5.13	115.59	127.15
82	S5	202	PEB	C2C-C1C-NC	5.13	114.47	107.57
82	tK	202	PEB	C1C-C2C-C3C	-5.12	101.56	107.62
84	U3	1001	CYC	C4D-C3D-C2D	-5.12	101.56	107.62
82	T7	202	PEB	C1C-C2C-C3C	-5.12	101.56	107.62
84	O3	1001	CYC	C4D-C3D-C2D	-5.12	101.56	107.62
82	TB	201	PEB	C2C-C1C-NC	5.12	114.47	107.57
82	WE	203	PEB	CHC-C4C-NC	5.12	128.08	121.15
87	82	308	CLA	CAC-C3C-C4C	-5.12	118.16	124.81
82	YO	202	PEB	CHC-C4C-NC	5.12	128.08	121.15
82	xK	302	PEB	C1C-C2C-C3C	-5.12	101.57	107.62
84	MG	1001	CYC	OB-C4B-C3B	-5.12	122.48	128.04
82	kE	202	PEB	C2C-C1C-NC	5.12	114.47	107.57
84	e3	1001	CYC	CMD-C2D-C1D	5.12	133.06	125.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YB	201	PEB	OA-C1A-C2A	-5.12	122.10	126.17
82	JA	203	PEB	C2C-C1C-NC	5.12	114.47	107.57
82	kE	202	PEB	C1C-C2C-C3C	-5.12	101.57	107.62
84	R3	1001	CYC	CMD-C2D-C1D	5.12	133.06	125.56
84	N3	1001	CYC	CMD-C2D-C1D	5.12	133.06	125.56
103	8N	309	ZEX	C35-C34-C33	-5.12	120.00	127.31
82	tF	202	PEB	C1C-C2C-C3C	-5.12	101.57	107.62
82	MJ	201	PEB	CHB-C1C-C2C	-5.12	115.60	127.15
85	B2	842	BCR	C16-C15-C14	-5.12	112.99	123.47
82	MJ	201	PEB	CHC-C1D-ND	-5.12	107.25	113.72
85	BN	842	BCR	C16-C15-C14	-5.12	112.99	123.47
82	eE	203	PEB	CHA-C1B-NB	-5.12	114.23	124.93
96	FL	102	HEM	CHC-C4B-NB	5.12	129.98	124.42
82	fK	201	PEB	CHC-C4C-NC	5.12	128.07	121.15
83	A4	302	PUB	C4B-C3B-C2B	-5.12	101.57	107.62
84	LO	1001	CYC	C3D-C4D-ND	5.12	114.46	107.57
87	2N	303	CLA	C1D-ND-C4D	5.12	109.97	106.33
82	F5	202	PEB	C1C-C2C-C3C	-5.12	101.57	107.62
82	UK	201	PEB	C4B-C3B-C2B	-5.11	101.12	106.78
82	Q9	202	PEB	C2C-C1C-NC	5.11	114.46	107.57
83	AO	302	PUB	C4B-C3B-C2B	-5.11	101.58	107.62
82	IM	202	PEB	CHA-C1B-NB	-5.11	114.24	124.93
84	n3	1001	CYC	C4D-C3D-C2D	-5.11	101.58	107.62
98	B2	837	PQN	O1-C1-C2	5.11	126.89	120.25
82	T1	201	PEB	C2C-C1C-NC	5.11	114.45	107.57
82	J7	203	PEB	C2C-C1C-NC	5.11	114.45	107.57
84	LH	1002	CYC	CMD-C2D-C1D	5.11	133.04	125.56
82	KP	202	PEB	C1C-C2C-C3C	-5.11	101.58	107.62
82	aF	203	PEB	CHA-C1B-NB	-5.11	114.24	124.93
103	82	309	ZEX	C35-C34-C33	-5.11	120.02	127.31
84	E3	1001	CYC	CMD-C2D-C1D	5.11	133.04	125.56
82	JB	201	PEB	C2C-C1C-NC	5.11	114.45	107.57
82	QD	201	PEB	OA-C1A-C2A	-5.11	122.11	126.17
84	73	1002	CYC	OB-C4B-C3B	-5.11	122.50	128.04
82	WO	201	PEB	C1C-C2C-C3C	-5.11	101.58	107.62
87	22	602	CLA	C1D-ND-C4D	5.11	109.96	106.33
87	12	606	CLA	C4A-NA-C1A	5.11	109.00	106.71
82	JH	1002	PEB	C2C-C1C-NC	5.11	114.45	107.57
82	lF	203	PEB	C2C-C1C-NC	5.11	114.45	107.57
84	DE	1001	CYC	CMD-C2D-C1D	5.10	133.03	125.56
82	L9	203	PEB	OA-C1A-C2A	-5.10	122.11	126.17
95	lL	101	DGD	C1D-O6D-C5D	5.10	123.71	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	T4	201	PEB	C1C-C2C-C3C	-5.10	101.59	107.62
82	TA	202	PEB	C1C-C2C-C3C	-5.10	101.59	107.62
82	bO	201	PEB	C2C-C1C-NC	5.10	114.44	107.57
84	m3	1001	CYC	CMD-C2D-C1D	5.10	133.03	125.56
82	i1	201	PEB	C2C-C1C-NC	5.10	114.44	107.57
82	fE	203	PEB	CHC-C4C-NC	5.10	128.05	121.15
82	l1	201	PEB	C2C-C1C-NC	5.10	114.44	107.57
87	8N	308	CLA	CAC-C3C-C4C	-5.10	118.19	124.81
82	T4	201	PEB	OA-C1A-C2A	-5.10	122.12	126.17
82	SP	201	PEB	CMC-C3C-C2C	-5.10	114.57	125.61
82	NA	203	PEB	C2C-C1C-NC	5.10	114.44	107.57
82	PB	201	PEB	C2C-C1C-NC	5.10	114.44	107.57
82	BQ	203	PEB	CHB-C1C-C2C	-5.10	115.65	127.15
82	kK	203	PEB	C2C-C1C-NC	5.10	114.44	107.57
84	GG	1001	CYC	CAB-C3B-C4B	5.10	129.43	121.38
82	XA	201	PEB	C1C-C2C-C3C	-5.10	101.60	107.62
98	BN	837	PQN	O1-C1-C2	5.10	126.87	120.25
87	ON	203	CLA	C4A-NA-C1A	5.10	109.00	106.71
82	SG	203	PEB	CHC-C1D-ND	-5.10	107.28	113.72
82	ZH	203	PEB	CHC-C1D-ND	-5.09	107.28	113.72
84	G3	1001	CYC	CMD-C2D-C1D	5.09	133.02	125.56
91	D6	404	PHO	C3D-C4D-ND	5.09	114.66	107.72
83	AO	303	PUB	C4B-C3B-C2B	-5.09	101.60	107.62
87	42	604	CLA	CAD-C3D-C2D	5.09	165.38	140.80
87	6N	604	CLA	C4A-NA-C1A	5.09	109.00	106.71
84	i3	1001	CYC	CMD-C2D-C1D	5.09	133.01	125.56
87	4N	604	CLA	CAD-C3D-C2D	5.09	165.37	140.80
82	YG	201	PEB	OA-C1A-C2A	-5.09	122.12	126.17
82	NK	202	PEB	C2C-C1C-NC	5.09	114.43	107.57
84	v3	1001	CYC	CMD-C2D-C1D	5.09	133.01	125.56
82	VD	203	PEB	C2C-C1C-NC	5.09	114.42	107.57
84	n3	1001	CYC	C3D-C4D-ND	5.09	114.42	107.57
82	H9	202	PEB	CHB-C1C-C2C	-5.09	115.67	127.15
84	A3	1001	CYC	CMD-C2D-C1D	5.09	133.01	125.56
84	l3	1001	CYC	CMD-C2D-C1D	5.09	133.01	125.56
84	GE	1001	CYC	CAB-C3B-C4B	5.09	129.42	121.38
82	DB	203	PEB	CHC-C1D-ND	-5.09	107.29	113.72
82	VK	202	PEB	C2C-C1C-NC	5.09	114.42	107.57
84	P3	1001	CYC	CMD-C2D-C1D	5.09	133.01	125.56
82	L1	1002	PEB	C2C-C1C-NC	5.09	114.42	107.57
82	J1	1002	PEB	C2C-C1C-NC	5.09	114.42	107.57
82	PE	201	PEB	C1C-C2C-C3C	-5.09	101.61	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mO	201	PEB	C1C-C2C-C3C	-5.08	101.61	107.62
82	ZE	201	PEB	CHC-C4C-NC	5.08	128.03	121.15
91	a6	613	PHO	C3D-C4D-ND	5.08	114.65	107.72
84	T3	1001	CYC	CMD-C2D-C1D	5.08	133.00	125.56
82	dD	401	PEB	C2C-C1C-NC	5.08	114.42	107.57
82	dE	203	PEB	CMB-C2B-C1B	5.08	132.89	125.06
82	ED	201	PEB	CAC-C2C-C1C	5.08	133.86	125.76
82	dH	201	PEB	C2C-C1C-NC	5.08	114.42	107.57
85	b6	601	BCR	C20-C21-C22	-5.08	120.06	127.31
85	B6	601	BCR	C15-C14-C13	-5.08	120.06	127.31
82	KM	203	PEB	CHB-C1C-C2C	-5.08	115.69	127.15
82	DI	201	PEB	C2C-C1C-NC	5.08	114.41	107.57
82	Y5	202	PEB	C2C-C1C-NC	5.08	114.41	107.57
82	z8	202	PEB	C1D-CHC-C4C	-5.08	105.77	113.26
82	xF	302	PEB	C1C-C2C-C3C	-5.08	101.62	107.62
82	BD	203	PEB	CHB-C1C-C2C	-5.08	115.69	127.15
82	jM	201	PEB	CHA-C1B-NB	-5.08	114.31	124.93
93	aL	612	BCT	O2-C-O1	5.08	132.72	119.55
83	Z9	305	PUB	C1D-CHC-C4C	-5.08	102.32	113.37
84	LE	1001	CYC	OC-C1C-C2C	-5.08	122.14	126.17
82	RO	201	PEB	C2C-C1C-NC	5.08	114.41	107.57
82	hF	201	PEB	CHA-C4A-NA	5.08	131.24	125.20
82	UM	203	PEB	C1C-C2C-C3C	-5.08	101.62	107.62
82	NB	203	PEB	OA-C1A-C2A	-5.08	122.14	126.17
82	iK	201	PEB	CHA-C1B-NB	-5.08	114.31	124.93
83	M5	302	PUB	CHB-C4B-NB	-5.08	113.69	125.32
82	N7	203	PEB	C2C-C1C-NC	5.08	114.41	107.57
84	KO	1001	CYC	CAB-C3B-C4B	5.07	129.39	121.38
84	C3	1001	CYC	CMD-C2D-C1D	5.07	132.99	125.56
84	LH	1001	CYC	OC-C1C-C2C	-5.07	122.14	126.17
82	UM	201	PEB	C2C-C1C-NC	5.07	114.40	107.57
82	Q7	202	PEB	C2C-C1C-NC	5.07	114.40	107.57
82	zC	202	PEB	C1D-CHC-C4C	-5.07	105.78	113.26
82	fG	203	PEB	CHC-C4C-NC	5.07	128.01	121.15
82	iF	201	PEB	CHA-C1B-NB	-5.07	114.33	124.93
84	KH	1001	CYC	C3D-C4D-ND	5.07	114.40	107.57
82	KB	301	PEB	C1C-C2C-C3C	-5.07	101.63	107.62
85	L2	205	BCR	C16-C17-C18	5.07	134.54	127.31
82	AD	301	PEB	C1C-C2C-C3C	-5.07	101.63	107.62
82	UG	203	PEB	C2C-C1C-NC	5.07	114.39	107.57
82	kG	202	PEB	C2C-C1C-NC	5.07	114.39	107.57
82	LH	1003	PEB	C1C-C2C-C3C	-5.07	101.63	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O5	203	PEB	C1C-C2C-C3C	-5.07	101.63	107.62
82	J5	202	PEB	C2C-C1C-NC	5.07	114.39	107.57
82	NJ	201	PEB	CMC-C3C-C4C	5.07	132.43	127.06
82	WI	202	PEB	CHB-C1C-C2C	-5.07	115.72	127.15
82	CM	202	PEB	CHC-C4C-NC	5.07	128.00	121.15
82	J9	203	PEB	OA-C1A-C2A	-5.06	122.15	126.17
82	G7	201	PEB	CHC-C4C-NC	5.06	128.00	121.15
84	J3	1001	CYC	CMD-C2D-C1D	5.06	132.97	125.56
82	d1	201	PEB	CHC-C4C-NC	5.06	128.00	121.15
82	IJ	203	PEB	C2C-C1C-NC	5.06	114.39	107.57
82	Q5	202	PEB	C3D-C4D-ND	5.06	117.19	107.26
85	d6	405	BCR	C38-C26-C25	-5.06	118.84	124.53
84	V3	1001	CYC	CMD-C2D-C1D	5.06	132.97	125.56
82	SB	202	PEB	OA-C1A-C2A	-5.06	122.15	126.17
84	LG	1001	CYC	OC-C1C-C2C	-5.06	122.15	126.17
82	B7	201	PEB	C2C-C1C-NC	5.06	114.39	107.57
82	kH	203	PEB	C2C-C1C-NC	5.06	114.39	107.57
82	OM	202	PEB	C1C-C2C-C3C	-5.06	101.64	107.62
82	YM	202	PEB	CMB-C2B-C1B	5.06	132.86	125.06
82	XF	201	PEB	OA-C1A-NA	5.06	131.07	124.94
82	QA	202	PEB	C2C-C1C-NC	5.06	114.38	107.57
82	KJ	202	PEB	C2C-C1C-NC	5.06	114.38	107.57
82	D5	203	PEB	C2C-C1C-NC	5.06	114.38	107.57
85	cL	504	BCR	C38-C26-C25	-5.06	118.85	124.53
83	Z5	302	PUB	CHB-C4B-NB	-5.06	113.73	125.32
82	XK	202	PEB	C2C-C1C-NC	5.06	114.38	107.57
82	EM	201	PEB	C2C-C1C-NC	5.06	114.38	107.57
85	CL	502	BCR	C7-C8-C9	-5.06	118.59	126.23
84	x3	1001	CYC	CMD-C2D-C1D	5.06	132.96	125.56
82	CJ	202	PEB	CHC-C4C-NC	5.05	127.99	121.15
84	N4	1001	CYC	C2C-C1C-NC	5.05	112.63	108.27
82	YG	202	PEB	C2C-C1C-NC	5.05	114.38	107.57
82	cF	201	PEB	C2C-C1C-NC	5.05	114.38	107.57
82	gB	203	PEB	CMC-C3C-C4C	5.05	132.42	127.06
84	g3	1001	CYC	CMD-C2D-C1D	5.05	132.96	125.56
82	kG	201	PEB	OA-C1A-C2A	-5.05	122.16	126.17
82	RD	203	PEB	CHC-C4C-NC	5.05	127.99	121.15
82	UJ	202	PEB	C1C-C2C-C3C	-5.05	101.65	107.62
84	c3	1001	CYC	CMD-C2D-C1D	5.05	132.96	125.56
82	SH	202	PEB	C1C-C2C-C3C	-5.05	101.65	107.62
82	NJ	201	PEB	OA-C1A-C2A	-5.05	122.16	126.17
82	F7	201	PEB	OA-C1A-C2A	-5.05	122.16	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LH	1003	PEB	C2C-C1C-NC	5.05	114.37	107.57
82	Z4	202	PEB	C1C-C2C-C3C	-5.05	101.65	107.62
82	SE	202	PEB	CHC-C1D-ND	-5.05	107.34	113.72
82	V4	202	PEB	CHC-C4C-NC	5.05	127.98	121.15
82	jM	201	PEB	C2C-C1C-NC	5.05	114.37	107.57
82	UF	201	PEB	CHB-C1C-C2C	-5.05	115.76	127.15
82	FK	202	PEB	CMB-C2B-C1B	5.05	132.84	125.06
82	Z1	203	PEB	CHC-C1D-ND	-5.05	107.34	113.72
83	A1	304	PUB	CBA-CAA-C3A	5.05	120.63	112.98
82	m4	201	PEB	C1C-C2C-C3C	-5.05	101.66	107.62
82	B5	203	PEB	C2C-C1C-NC	5.05	114.37	107.57
82	D7	203	PEB	C2C-C1C-NC	5.04	114.36	107.57
87	62	309	CLA	CHB-C1B-C2B	5.04	141.48	127.24
82	uK	201	PEB	CHA-C1B-NB	-5.04	114.38	124.93
82	EP	202	PEB	C1C-C2C-C3C	-5.04	101.66	107.62
82	UK	201	PEB	CHB-C1C-C2C	-5.04	115.77	127.15
82	RF	202	PEB	C1C-C2C-C3C	-5.04	101.66	107.62
82	dD	401	PEB	C1C-C2C-C3C	-5.04	101.66	107.62
82	PQ	202	PEB	CHA-C1B-NB	-5.04	114.39	124.93
82	dF	201	PEB	CHA-C4A-NA	5.04	131.20	125.20
82	CB	201	PEB	C2C-C1C-NC	5.04	114.36	107.57
85	LN	205	BCR	C16-C17-C18	5.04	134.50	127.31
82	BM	301	PEB	C1C-C2C-C3C	-5.04	101.66	107.62
84	ME	1001	CYC	CMD-C2D-C1D	5.04	132.94	125.56
82	RD	203	PEB	CHA-C1B-NB	-5.04	114.39	124.93
84	K4	1001	CYC	CAB-C3B-C4B	5.04	129.34	121.38
82	KJ	202	PEB	C1C-C2C-C3C	-5.04	101.66	107.62
82	lJ	202	PEB	C1C-C2C-C3C	-5.04	101.67	107.62
82	RQ	203	PEB	CHA-C1B-NB	-5.04	114.39	124.93
82	NF	202	PEB	C2C-C1C-NC	5.04	114.35	107.57
82	QO	201	PEB	C1C-C2C-C3C	-5.04	101.67	107.62
82	BJ	301	PEB	CHC-C1D-ND	-5.04	107.35	113.72
82	cJ	201	PEB	C1D-CHC-C4C	5.04	120.68	113.26
82	XF	202	PEB	CHA-C1B-NB	-5.04	114.40	124.93
85	KN	101	BCR	C30-C25-C26	-5.04	115.52	122.61
82	BA	201	PEB	C2C-C1C-NC	5.04	114.35	107.57
84	NO	1001	CYC	CAB-C3B-C4B	5.03	129.33	121.38
82	UI	202	PEB	C2C-C1C-NC	5.03	114.35	107.57
85	K2	102	BCR	C30-C25-C26	-5.03	115.52	122.61
82	DA	203	PEB	C2C-C1C-NC	5.03	114.35	107.57
82	Q5	202	PEB	C2C-C1C-NC	5.03	114.35	107.57
82	dQ	401	PEB	C2C-C1C-NC	5.03	114.35	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OA	201	PEB	C1C-C2C-C3C	-5.03	101.67	107.62
82	wF	302	PEB	C1C-C2C-C3C	-5.03	101.67	107.62
82	PD	202	PEB	CHA-C1B-NB	-5.03	114.41	124.93
82	EM	202	PEB	C2C-C1C-NC	5.03	114.35	107.57
82	NA	202	PEB	CHC-C1D-ND	-5.03	107.36	113.72
82	G5	201	PEB	C1C-C2C-C3C	-5.03	101.67	107.62
84	E4	1001	CYC	CMA-C3A-C4A	5.03	132.81	125.06
82	XD	201	PEB	C2C-C1C-NC	5.03	114.34	107.57
82	U5	202	PEB	CHB-C1C-C2C	-5.03	115.80	127.15
82	iF	202	PEB	CHB-C1C-C2C	-5.03	115.80	127.15
82	T4	202	PEB	CHC-C4C-NC	5.03	127.96	121.15
82	I5	201	PEB	C1C-C2C-C3C	-5.03	101.68	107.62
82	sF	201	PEB	C1C-C2C-C3C	-5.03	101.68	107.62
82	RO	202	PEB	CHC-C4C-NC	5.03	127.95	121.15
82	FF	202	PEB	CMB-C2B-C1B	5.03	132.81	125.06
82	M9	305	PEB	CMB-C2B-C1B	5.03	132.81	125.06
82	hJ	203	PEB	CHC-C4C-NC	5.03	127.95	121.15
82	YJ	201	PEB	CHC-C1D-ND	-5.03	107.36	113.72
82	yC	202	PEB	C2C-C1C-NC	5.03	114.34	107.57
84	EO	1001	CYC	CMA-C3A-C4A	5.03	132.80	125.06
82	BF	202	PEB	C1C-CHB-C4B	5.02	139.55	128.28
82	XQ	201	PEB	C2C-C1C-NC	5.02	114.34	107.57
82	dM	201	PEB	C2C-C1C-NC	5.02	114.34	107.57
82	RQ	203	PEB	CHC-C4C-NC	5.02	127.95	121.15
82	eJ	202	PEB	C1C-C2C-C3C	-5.02	101.68	107.62
84	BG	1002	CYC	OC-C1C-C2C	-5.02	122.18	126.17
82	C7	201	PEB	CHC-C4C-NC	5.02	127.95	121.15
82	P1	201	PEB	CHC-C1D-ND	-5.02	107.37	113.72
83	K7	203	PUB	C4B-C3B-C2B	-5.02	101.68	107.62
82	Z1	201	PEB	CMC-C3C-C4C	5.02	132.38	127.06
82	b1	202	PEB	C1C-C2C-C3C	-5.02	101.68	107.62
83	xK	301	PUB	C4B-C3B-C2B	-5.02	101.68	107.62
85	B2	841	BCR	C28-C27-C26	-5.02	105.11	114.08
84	NO	1001	CYC	C2C-C1C-NC	5.02	112.60	108.27
82	E5	201	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
82	OM	203	PEB	C2C-C1C-NC	5.02	114.33	107.57
82	lK	203	PEB	C2C-C1C-NC	5.02	114.33	107.57
84	N4	1001	CYC	CAB-C3B-C4B	5.02	129.31	121.38
82	C5	201	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
87	6N	608	CLA	CHB-C1B-C2B	5.02	141.41	127.24
82	W5	201	PEB	C2C-C1C-NC	5.02	114.33	107.57
82	GA	201	PEB	CHC-C4C-NC	5.02	127.94	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RK	202	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
82	FJ	201	PEB	CHA-C1B-NB	-5.02	114.44	124.93
82	iK	202	PEB	CHB-C1C-C2C	-5.02	115.83	127.15
82	XK	201	PEB	OA-C1A-NA	5.02	131.02	124.94
82	mO	201	PEB	OA-C1A-C2A	-5.02	122.18	126.17
82	NF	202	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
82	Q4	201	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
82	MK	203	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
82	dG	201	PEB	C1D-CHC-C4C	-5.02	105.86	113.26
82	IB	202	PEB	OA-C1A-C2A	-5.02	122.19	126.17
82	P5	201	PEB	C1C-C2C-C3C	-5.02	101.69	107.62
82	XK	202	PEB	CHA-C1B-NB	-5.01	114.44	124.93
84	N1	1001	CYC	CAB-C3B-C4B	5.01	129.30	121.38
82	dQ	401	PEB	C1C-C2C-C3C	-5.01	101.69	107.62
82	HK	202	PEB	C1C-C2C-C3C	-5.01	101.69	107.62
82	X7	203	PEB	C1C-C2C-C3C	-5.01	101.69	107.62
85	BN	841	BCR	C28-C27-C26	-5.01	105.12	114.08
82	GB	203	PEB	OA-C1A-C2A	-5.01	122.19	126.17
82	K5	201	PEB	C1C-C2C-C3C	-5.01	101.69	107.62
82	T5	201	PEB	C1C-C2C-C3C	-5.01	101.69	107.62
82	AJ	301	PEB	C1C-C2C-C3C	-5.01	101.70	107.62
82	X5	201	PEB	C1C-C2C-C3C	-5.01	101.70	107.62
82	pK	201	PEB	C1C-C2C-C3C	-5.01	101.70	107.62
82	v8	201	PEB	OA-C1A-C2A	-5.01	122.19	126.17
82	QE	201	PEB	C1C-C2C-C3C	-5.01	101.70	107.62
82	Q9	201	PEB	C4B-C3B-C2B	-5.01	101.24	106.78
82	y8	202	PEB	C2C-C1C-NC	5.01	114.31	107.57
83	A4	303	PUB	C4B-C3B-C2B	-5.01	101.70	107.62
82	CA	201	PEB	CHC-C4C-NC	5.01	127.92	121.15
82	HI	202	PEB	OA-C1A-C2A	-5.01	122.19	126.17
82	LD	202	PEB	C2C-C1C-NC	5.01	114.31	107.57
84	K1	1001	CYC	C3D-C4D-ND	5.01	114.31	107.57
82	L1	1002	PEB	C1C-C2C-C3C	-5.01	101.70	107.62
84	JO	1001	CYC	C3D-C4D-ND	5.00	114.31	107.57
82	W5	201	PEB	C1C-C2C-C3C	-5.00	101.71	107.62
82	Z9	304	PEB	CMB-C2B-C1B	5.00	132.77	125.06
82	TF	202	PEB	C2C-C1C-NC	5.00	114.31	107.57
85	BN	803	BCR	C7-C8-C9	-5.00	118.68	126.23
82	N7	202	PEB	CHC-C1D-ND	-5.00	107.39	113.72
82	HM	201	PEB	C1D-CHC-C4C	5.00	120.63	113.26
82	MP	202	PEB	C1C-C2C-C3C	-5.00	101.71	107.62
82	A5	201	PEB	C1C-C2C-C3C	-5.00	101.71	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CM	203	PEB	CHB-C1C-C2C	-5.00	115.87	127.15
93	A6	409	BCT	O2-C-O1	5.00	132.52	119.55
82	V5	201	PEB	C1C-C2C-C3C	-5.00	101.71	107.62
82	Y5	201	PEB	C1C-C2C-C3C	-5.00	101.71	107.62
82	cK	201	PEB	CHA-C1B-NB	-5.00	114.47	124.93
82	UB	301	PEB	C2C-C1C-NC	5.00	114.30	107.57
82	M7	201	PEB	C2C-C1C-NC	5.00	114.30	107.57
84	EE	1001	CYC	C3D-C4D-ND	5.00	114.30	107.57
84	EG	1001	CYC	C3D-C4D-ND	5.00	114.30	107.57
85	I2	101	BCR	C15-C16-C17	-5.00	113.23	123.47
82	RO	201	PEB	CMB-C2B-C1B	5.00	132.76	125.06
84	NH	1001	CYC	CAB-C3B-C4B	5.00	129.27	121.38
94	d6	408	PL9	C7-C3-C4	5.00	120.94	116.88
82	DA	201	PEB	CHA-C1B-NB	-5.00	114.48	124.93
82	BK	202	PEB	C1C-CHB-C4B	5.00	139.49	128.28
82	ZH	201	PEB	CMC-C3C-C4C	5.00	132.36	127.06
84	MG	1001	CYC	CMD-C2D-C1D	5.00	132.88	125.56
82	R5	201	PEB	C1C-C2C-C3C	-5.00	101.71	107.62
82	YJ	201	PEB	C2C-C1C-NC	5.00	114.30	107.57
82	kF	203	PEB	C2C-C1C-NC	5.00	114.30	107.57
82	S1	202	PEB	C1C-C2C-C3C	-5.00	101.72	107.62
82	iM	201	PEB	CMB-C2B-C1B	5.00	132.76	125.06
82	YM	201	PEB	CHB-C1C-C2C	-5.00	115.88	127.15
82	NJ	202	PEB	C1C-C2C-C3C	-4.99	101.72	107.62
85	IN	101	BCR	C15-C16-C17	-4.99	113.24	123.47
82	NK	202	PEB	C1C-C2C-C3C	-4.99	101.72	107.62
82	P4	202	PEB	CHB-C1C-C2C	-4.99	115.88	127.15
82	QM	202	PEB	C2C-C1C-NC	4.99	114.30	107.57
83	wF	304	PUB	OD-C4D-C3D	-4.99	122.62	128.04
82	PQ	203	PEB	C1C-C2C-C3C	-4.99	101.72	107.62
82	VO	202	PEB	CHC-C4C-NC	4.99	127.91	121.15
82	Z4	202	PEB	C2C-C1C-NC	4.99	114.29	107.57
82	N5	201	PEB	C1C-C2C-C3C	-4.99	101.72	107.62
85	B6	621	BCR	C7-C8-C9	-4.99	118.69	126.23
82	WK	201	PEB	CHA-C1B-NB	-4.99	114.49	124.93
84	C3	1001	CYC	CHD-C4C-NC	4.99	131.14	125.20
82	R4	202	PEB	CHC-C4C-NC	4.99	127.90	121.15
82	bP	502	PEB	CHC-C4C-NC	4.99	127.90	121.15
82	J1	1002	PEB	C1C-C2C-C3C	-4.99	101.72	107.62
82	q8	202	PEB	C2C-C1C-NC	4.99	114.29	107.57
82	hK	201	PEB	CHA-C4A-NA	4.99	131.14	125.20
82	dJ	202	PEB	C1C-C2C-C3C	-4.99	101.72	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
94	DL	401	PL9	C7-C3-C2	-4.99	116.74	123.30
82	DA	201	PEB	OA-C1A-C2A	-4.99	122.21	126.17
82	QG	201	PEB	C1C-C2C-C3C	-4.99	101.72	107.62
84	DO	1001	CYC	OB-C4B-C3B	-4.99	122.63	128.04
103	8N	309	ZEX	C15-C14-C13	-4.99	120.19	127.31
82	vC	201	PEB	OA-C1A-C2A	-4.99	122.21	126.17
84	g3	1001	CYC	CHD-C4C-NC	4.99	131.13	125.20
82	LQ	202	PEB	CMB-C2B-C1B	4.99	132.74	125.06
82	PO	202	PEB	CHB-C1C-C2C	-4.99	115.90	127.15
82	WB	402	PEB	CHC-C1D-ND	-4.99	107.42	113.72
82	WI	203	PEB	C2C-C1C-NC	4.99	114.28	107.57
82	R4	201	PEB	CMB-C2B-C1B	4.98	132.74	125.06
82	T7	201	PEB	CHC-C4C-NC	4.98	127.89	121.15
82	j1	201	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
84	D4	1001	CYC	OB-C4B-C3B	-4.98	122.63	128.04
82	dE	201	PEB	C1D-CHC-C4C	-4.98	105.91	113.26
82	O7	201	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
83	M5	303	PUB	CAB-C3B-C4B	4.98	133.70	125.76
85	B2	802	BCR	C7-C8-C9	-4.98	118.71	126.23
85	cL	504	BCR	C7-C8-C9	-4.98	118.71	126.23
82	DD	202	PEB	CHC-C1D-ND	-4.98	107.42	113.72
82	XA	203	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
82	yK	301	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
82	EF	201	PEB	CHB-C1C-C2C	-4.98	115.91	127.15
83	AJ	303	PUB	C3B-C4B-NB	4.98	114.28	107.57
83	Z5	303	PUB	CAB-C3B-C4B	4.98	133.70	125.76
82	j4	202	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
84	t3	1001	CYC	CHD-C4C-NC	4.98	131.13	125.20
82	SM	202	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
82	yF	301	PEB	C1C-C2C-C3C	-4.98	101.73	107.62
85	BN	838	BCR	C35-C13-C12	4.98	125.92	118.08
82	DQ	202	PEB	CHC-C1D-ND	-4.98	107.42	113.72
84	T3	1001	CYC	CHD-C4C-NC	4.98	131.13	125.20
83	xK	301	PUB	OD-C4D-C3D	-4.98	122.64	128.04
84	FE	1001	CYC	C3D-C4D-ND	4.98	114.28	107.57
82	PB	201	PEB	OA-C1A-C2A	-4.98	122.21	126.17
82	dJ	202	PEB	CHC-C4C-NC	4.98	127.89	121.15
82	cF	201	PEB	CHA-C1B-NB	-4.98	114.52	124.93
82	LD	202	PEB	CMB-C2B-C1B	4.98	132.73	125.06
82	BK	202	PEB	C2C-C1C-NC	4.98	114.27	107.57
84	CG	1001	CYC	C3D-C4D-ND	4.98	114.27	107.57
82	PH	201	PEB	CHC-C1D-ND	-4.98	107.43	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O7	202	PEB	C2C-C1C-NC	4.98	114.27	107.57
82	ZO	202	PEB	C1C-C2C-C3C	-4.98	101.74	107.62
82	mJ	202	PEB	C1C-C2C-C3C	-4.98	101.74	107.62
82	YM	201	PEB	CHC-C1D-ND	-4.98	107.43	113.72
84	63	901	CYC	CAB-C3B-C4B	4.97	129.24	121.38
82	EK	201	PEB	CHB-C1C-C2C	-4.97	115.93	127.15
82	KA	201	PEB	C2C-C1C-NC	4.97	114.27	107.57
82	BK	201	PEB	OA-C1A-NA	4.97	130.97	124.94
84	A3	1001	CYC	CHD-C4C-NC	4.97	131.12	125.20
82	MA	201	PEB	C2C-C1C-NC	4.97	114.27	107.57
83	AH	304	PUB	CBA-CAA-C3A	4.97	120.52	112.98
82	QQ	201	PEB	OA-C1A-C2A	-4.97	122.22	126.17
82	pF	201	PEB	C1C-C2C-C3C	-4.97	101.74	107.62
84	P3	1001	CYC	CHD-C4C-NC	4.97	131.12	125.20
82	LQ	202	PEB	C2C-C1C-NC	4.97	114.26	107.57
84	i3	1001	CYC	CHD-C4C-NC	4.97	131.11	125.20
82	FQ	203	PEB	C1C-CHB-C4B	4.97	139.43	128.28
82	K7	201	PEB	C2C-C1C-NC	4.97	114.26	107.57
82	F4	1002	PEB	OA-C1A-C2A	-4.97	122.22	126.17
82	aB	201	PEB	OA-C1A-C2A	-4.97	122.22	126.17
82	IP	202	PEB	C1D-CHC-C4C	-4.97	105.93	113.26
82	GK	203	PEB	CAB-C3B-C4B	4.97	133.80	125.01
83	xF	306	PUB	C4B-C3B-C2B	-4.97	101.75	107.62
82	kE	201	PEB	OA-C1A-C2A	-4.97	122.22	126.17
82	qC	202	PEB	C2C-C1C-NC	4.97	114.26	107.57
82	HF	202	PEB	C1C-C2C-C3C	-4.97	101.75	107.62
91	A6	407	PHO	C3D-C4D-ND	4.97	114.49	107.72
82	L7	202	PEB	CHB-C1C-C2C	-4.97	115.94	127.15
82	AO	304	PEB	C1C-C2C-C3C	-4.97	101.75	107.62
82	HA	202	PEB	C2A-C1A-NA	4.97	112.55	108.27
82	OI	202	PEB	C1B-C2B-C3B	-4.97	100.81	106.51
84	c3	1001	CYC	CHD-C4C-NC	4.97	131.11	125.20
82	cB	403	PEB	C1C-C2C-C3C	-4.97	101.75	107.62
82	F5	201	PEB	C4C-C3C-C2C	-4.97	102.92	107.50
82	WQ	201	PEB	CMB-C2B-C1B	4.97	132.71	125.06
82	CM	201	PEB	C2C-C1C-NC	4.96	114.26	107.57
82	SO	201	PEB	C1C-C2C-C3C	-4.96	101.75	107.62
82	TM	202	PEB	OA-C1A-C2A	-4.96	122.23	126.17
84	KH	1001	CYC	OB-C4B-C3B	-4.96	122.65	128.04
82	LB	201	PEB	C2C-C1C-NC	4.96	114.25	107.57
84	K3	1001	CYC	CHD-C4C-NC	4.96	131.11	125.20
84	l3	1001	CYC	CHD-C4C-NC	4.96	131.11	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	yK	303	PUB	CHA-C4A-NA	-4.96	107.44	113.72
82	HB	203	PEB	C2C-C1C-NC	4.96	114.25	107.57
82	ZO	202	PEB	C2C-C1C-NC	4.96	114.25	107.57
82	CF	202	PEB	C1D-CHC-C4C	-4.96	105.94	113.26
82	fJ	202	PEB	CHC-C1D-ND	-4.96	107.45	113.72
84	CO	1001	CYC	CAB-C3B-C4B	4.96	129.22	121.38
82	BJ	301	PEB	C1C-C2C-C3C	-4.96	101.75	107.62
83	KA	203	PUB	C3B-C4B-NB	4.96	114.25	107.57
82	bH	202	PEB	C1C-C2C-C3C	-4.96	101.76	107.62
82	IM	202	PEB	C2C-C1C-NC	4.96	114.25	107.57
96	G2	201	HEM	C4D-ND-C1D	4.96	110.20	105.07
85	IN	101	BCR	C1-C6-C5	-4.96	115.63	122.61
82	PE	201	PEB	OA-C1A-C2A	-4.96	122.23	126.17
83	yK	303	PUB	C3B-C4B-NB	4.96	114.25	107.57
82	YE	202	PEB	C2C-C1C-NC	4.96	114.25	107.57
82	I5	201	PEB	C2C-C1C-NC	4.96	114.25	107.57
82	mG	203	PEB	C2C-C1C-NC	4.96	114.25	107.57
82	qF	201	PEB	CMB-C2B-C1B	4.96	132.70	125.06
82	F5	201	PEB	CAA-C3A-C2A	-4.96	101.87	114.26
82	LA	202	PEB	CHB-C1C-C2C	-4.96	115.97	127.15
83	xK	306	PUB	C4B-C3B-C2B	-4.96	101.76	107.62
82	AQ	301	PEB	C1C-C2C-C3C	-4.96	101.76	107.62
82	ZK	201	PEB	CHA-C1B-NB	-4.96	114.56	124.93
82	D7	201	PEB	CHA-C1B-NB	-4.96	114.56	124.93
82	QE	203	PEB	C2C-C1C-NC	4.96	114.25	107.57
84	HH	1001	CYC	CMB-C2B-C1B	4.96	130.36	124.17
82	VI	203	PEB	C1C-C2C-C3C	-4.96	101.76	107.62
82	KP	202	PEB	CMB-C2B-C1B	4.96	132.69	125.06
103	82	309	ZEX	C15-C14-C13	-4.96	120.24	127.31
82	uF	202	PEB	CHA-C1B-NB	-4.96	114.57	124.93
82	NJ	201	PEB	C4B-C3B-C2B	-4.95	101.30	106.78
82	TO	202	PEB	CHC-C4C-NC	4.95	127.86	121.15
83	AJ	304	PUB	C4B-C3B-C2B	-4.95	101.76	107.62
82	JI	202	PEB	C2C-C1C-NC	4.95	114.24	107.57
82	GF	203	PEB	CAB-C3B-C4B	4.95	133.78	125.01
82	OJ	202	PEB	CHC-C4C-NC	4.95	127.85	121.15
84	e3	1001	CYC	CHD-C4C-NC	4.95	131.09	125.20
84	m3	1001	CYC	CHD-C4C-NC	4.95	131.09	125.20
84	v3	1001	CYC	CHD-C4C-NC	4.95	131.09	125.20
85	I2	101	BCR	C1-C6-C5	-4.95	115.64	122.61
82	JH	1002	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
82	IM	203	PEB	C1C-C2C-C3C	-4.95	101.77	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	KA	203	PUB	CHC-C1D-ND	-4.95	107.46	113.72
82	NM	202	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
82	S4	201	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
85	B2	838	BCR	C35-C13-C12	4.95	125.88	118.08
82	YG	201	PEB	CHC-C1D-ND	-4.95	107.46	113.72
82	MK	201	PEB	C2C-C1C-NC	4.95	114.24	107.57
82	mE	203	PEB	C2C-C1C-NC	4.95	114.24	107.57
82	MF	203	PEB	CHA-C1B-NB	-4.95	114.58	124.93
82	A4	304	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
96	GN	201	HEM	C4D-ND-C1D	4.95	110.19	105.07
82	SB	201	PEB	C2C-C1C-NC	4.95	114.23	107.57
82	jO	202	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
84	CH	1001	CYC	CMA-C3A-C4A	4.95	132.68	125.06
82	r8	201	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
82	AD	301	PEB	C2C-C1C-NC	4.95	114.23	107.57
82	T5	201	PEB	C2C-C1C-NC	4.95	114.23	107.57
82	P7	203	PEB	C2C-C1C-NC	4.95	114.23	107.57
84	KG	202	CYC	CMA-C3A-C4A	4.95	132.68	125.06
82	eM	201	PEB	C1D-CHC-C4C	4.95	120.55	113.26
83	K7	203	PUB	CHC-C1D-ND	-4.95	107.47	113.72
82	MF	203	PEB	C1C-C2C-C3C	-4.95	101.77	107.62
82	TK	202	PEB	C2C-C1C-NC	4.95	114.23	107.57
82	UH	201	PEB	C1C-CHB-C4B	4.94	139.37	128.28
82	qK	201	PEB	CMB-C2B-C1B	4.94	132.68	125.06
84	F4	1001	CYC	C2B-C1B-NB	4.94	114.23	106.99
85	FN	202	BCR	C15-C14-C13	-4.94	120.25	127.31
82	D7	201	PEB	OA-C1A-C2A	-4.94	122.24	126.17
84	J3	1001	CYC	CHD-C4C-NC	4.94	131.08	125.20
82	QK	203	PEB	C2A-C1A-NA	4.94	112.53	108.27
85	F2	203	BCR	C15-C14-C13	-4.94	120.26	127.31
87	8N	308	CLA	CBC-CAC-C3C	4.94	126.06	112.43
82	IP	202	PEB	C1C-C2C-C3C	-4.94	101.78	107.62
82	eB	201	PEB	C1C-C2C-C3C	-4.94	101.78	107.62
84	GE	1001	CYC	C3D-C4D-ND	4.94	114.23	107.57
85	b6	601	BCR	C15-C14-C13	-4.94	120.26	127.31
82	RP	202	PEB	CHC-C4C-NC	4.94	127.84	121.15
84	I4	1001	CYC	CAB-C3B-C4B	4.94	129.18	121.38
82	H9	202	PEB	C3C-C4C-NC	4.94	112.78	108.33
82	RA	201	PEB	CHC-C1D-ND	-4.94	107.47	113.72
82	QG	203	PEB	C2C-C1C-NC	4.94	114.22	107.57
82	KP	202	PEB	C2C-C1C-NC	4.94	114.22	107.57
82	jJ	201	PEB	C2C-C1C-NC	4.94	114.22	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HH	1002	PEB	CHA-C1B-NB	-4.94	114.60	124.93
84	C1	1001	CYC	CAB-C3B-C4B	4.94	129.18	121.38
82	B9	203	PEB	OA-C1A-C2A	-4.94	122.25	126.17
85	cL	504	BCR	C16-C15-C14	-4.94	113.36	123.47
84	C4	1001	CYC	CAB-C3B-C4B	4.94	129.18	121.38
84	HE	1001	CYC	C3D-C4D-ND	4.94	114.22	107.57
85	AN	845	BCR	C15-C14-C13	-4.94	120.26	127.31
84	N3	1001	CYC	CHD-C4C-NC	4.94	131.07	125.20
82	FM	202	PEB	C1C-C2C-C3C	-4.94	101.78	107.62
83	AG	302	PUB	C3B-C4B-NB	4.94	114.22	107.57
82	AP	201	PEB	C1C-C2C-C3C	-4.94	101.79	107.62
84	R3	1001	CYC	CHD-C4C-NC	4.94	131.07	125.20
85	A2	845	BCR	C15-C14-C13	-4.93	120.27	127.31
82	B9	201	PEB	C4B-C3B-C2B	-4.93	101.32	106.78
82	WK	202	PEB	CHA-C1B-NB	-4.93	114.61	124.93
82	PQ	201	PEB	CHC-C4C-NC	4.93	127.83	121.15
84	G3	1001	CYC	CHD-C4C-NC	4.93	131.07	125.20
84	p3	1001	CYC	CHD-C4C-NC	4.93	131.07	125.20
82	B9	203	PEB	C2C-C1C-NC	4.93	114.22	107.57
82	U9	204	PEB	CHA-C1B-NB	-4.93	114.61	124.93
82	gB	201	PEB	OA-C1A-C2A	-4.93	122.25	126.17
83	xF	301	PUB	CHC-C1D-ND	-4.93	107.48	113.72
87	82	308	CLA	CBC-CAC-C3C	4.93	126.03	112.43
82	C5	201	PEB	C2C-C1C-NC	4.93	114.21	107.57
83	QM	201	PUB	C4B-C3B-C2B	-4.93	101.79	107.62
84	LO	1001	CYC	C1B-C2B-C3B	-4.93	102.72	107.87
82	UB	303	PEB	C1C-C2C-C3C	-4.93	101.79	107.62
84	FH	1001	CYC	CHB-C1B-NB	-4.93	115.47	126.06
82	OJ	201	PEB	C2C-C1C-NC	4.93	114.21	107.57
83	xK	301	PUB	CHC-C1D-ND	-4.93	107.48	113.72
82	TA	201	PEB	CHC-C4C-NC	4.93	127.82	121.15
82	FD	203	PEB	C1C-CHB-C4B	4.93	139.34	128.28
82	CM	201	PEB	CMB-C2B-C1B	4.93	132.66	125.06
84	BG	1001	CYC	C3D-C4D-ND	4.93	114.21	107.57
82	OA	202	PEB	C2C-C1C-NC	4.93	114.21	107.57
87	82	302	CLA	CHD-C4C-C3C	4.93	132.09	124.84
82	PA	203	PEB	C2C-C1C-NC	4.93	114.21	107.57
82	s8	202	PEB	C1D-CHC-C4C	4.93	120.52	113.26
82	hJ	203	PEB	C1C-C2C-C3C	-4.93	101.79	107.62
82	sC	202	PEB	OA-C1A-C2A	-4.93	122.25	126.17
82	KI	201	PEB	C1C-C2C-C3C	-4.93	101.80	107.62
82	WD	201	PEB	CMB-C2B-C1B	4.93	132.65	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	AE	302	PUB	C3B-C4B-NB	4.93	114.21	107.57
82	H5	202	PEB	CHB-C1C-C2C	-4.93	116.03	127.15
84	H1	1001	CYC	CMB-C2B-C1B	4.93	130.32	124.17
83	AH	304	PUB	C1C-C2C-C3C	-4.93	101.33	106.78
85	bL	602	BCR	C36-C18-C19	4.93	125.84	118.08
82	WF	201	PEB	CHA-C1B-NB	-4.93	114.63	124.93
82	TO	202	PEB	C1C-C2C-C3C	-4.93	101.80	107.62
82	jH	201	PEB	C1C-C2C-C3C	-4.93	101.80	107.62
82	H7	202	PEB	C2A-C1A-NA	4.93	112.52	108.27
82	m1	201	PEB	C2C-C1C-NC	4.93	114.20	107.57
82	IF	201	PEB	CHC-C1D-ND	-4.92	107.49	113.72
82	lO	201	PEB	C1C-C2C-C3C	-4.92	101.80	107.62
82	MK	203	PEB	CHA-C1B-NB	-4.92	114.63	124.93
85	F6	101	BCR	C38-C26-C25	-4.92	119.00	124.53
84	LG	1001	CYC	CAB-C3B-C4B	4.92	129.16	121.38
82	gM	202	PEB	C1C-C2C-C3C	-4.92	101.80	107.62
82	UD	201	PEB	OA-C1A-C2A	-4.92	122.26	126.17
82	FO	1002	PEB	OA-C1A-C2A	-4.92	122.26	126.17
82	V5	201	PEB	C2C-C1C-NC	4.92	114.20	107.57
84	x3	1001	CYC	CHB-C4A-NA	-4.92	114.63	124.93
82	tC	202	PEB	CHA-C4A-NA	-4.92	119.35	125.20
82	F9	203	PEB	C1C-C2C-C3C	-4.92	101.80	107.62
82	P7	201	PEB	OA-C1A-C2A	-4.92	122.26	126.17
82	OI	201	PEB	CHC-C1D-ND	-4.92	107.50	113.72
92	j6	101	LMG	O1-C1-C2	4.92	115.99	108.30
82	YE	201	PEB	CHC-C1D-ND	-4.92	107.50	113.72
82	eG	202	PEB	CHB-C1C-C2C	-4.92	116.05	127.15
82	QB	202	PEB	C1C-C2C-C3C	-4.92	101.80	107.62
82	lG	201	PEB	OA-C1A-C2A	-4.92	122.26	126.17
82	R7	203	PEB	CAB-CBB-CGB	-4.92	103.01	113.60
82	fJ	202	PEB	C1D-CHC-C4C	-4.92	106.00	113.26
82	RA	203	PEB	CAB-CBB-CGB	-4.92	103.01	113.60
82	t8	202	PEB	CHA-C4A-NA	-4.92	119.36	125.20
84	ME	1001	CYC	C3D-C4D-ND	4.92	114.20	107.57
82	M5	304	PEB	OA-C1A-C2A	-4.92	122.26	126.17
85	k6	102	BCR	C3-C4-C5	-4.92	105.29	114.08
82	H1	1002	PEB	CHA-C1B-NB	-4.92	114.64	124.93
84	C4	1001	CYC	CMD-C2D-C1D	4.92	132.76	125.56
82	AM	301	PEB	C1C-C2C-C3C	-4.92	101.81	107.62
82	TQ	203	PEB	C1C-C2C-C3C	-4.92	101.81	107.62
82	KJ	201	PEB	C2C-C1C-NC	4.92	114.19	107.57
82	dB	202	PEB	C2C-C1C-NC	4.92	114.19	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	K6	102	BCR	C3-C4-C5	-4.92	105.30	114.08
82	L5	202	PEB	C2C-C1C-NC	4.92	114.19	107.57
82	P5	201	PEB	C2C-C1C-NC	4.92	114.19	107.57
84	M1	201	CYC	C2D-C1D-ND	4.92	114.31	107.40
82	WF	202	PEB	CHA-C1B-NB	-4.92	114.65	124.93
82	PD	203	PEB	C1C-C2C-C3C	-4.92	101.81	107.62
82	BF	202	PEB	C2C-C1C-NC	4.92	114.19	107.57
84	F4	1001	CYC	CMD-C2D-C1D	4.92	132.76	125.56
82	zK	501	PEB	C1D-CHC-C4C	-4.92	106.01	113.26
82	ZE	202	PEB	C1C-C2C-C3C	-4.92	101.81	107.62
82	T4	202	PEB	C1C-C2C-C3C	-4.92	101.81	107.62
85	AL	401	BCR	C15-C14-C13	-4.92	120.30	127.31
82	rC	202	PEB	CHB-C1C-NC	-4.91	114.06	125.32
82	r8	202	PEB	CHB-C1C-NC	-4.91	114.06	125.32
83	A1	304	PUB	C1C-C2C-C3C	-4.91	101.34	106.78
82	W4	201	PEB	C3B-C4B-NB	4.91	117.20	110.05
82	c1	202	PEB	CHA-C1B-NB	-4.91	114.66	124.93
82	FP	202	PEB	CHC-C4C-NC	4.91	127.80	121.15
82	BI	202	PEB	OA-C1A-C2A	-4.91	122.27	126.17
82	UA	201	PEB	CHB-C1C-C2C	-4.91	116.07	127.15
82	XI	201	PEB	C1C-C2C-C3C	-4.91	101.81	107.62
82	A5	201	PEB	C2C-C1C-NC	4.91	114.19	107.57
84	CH	1001	CYC	CAB-C3B-C4B	4.91	129.14	121.38
82	RG	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
84	V3	1001	CYC	CHB-C4A-NA	-4.91	114.66	124.93
82	RM	201	PEB	CMB-C2B-C1B	4.91	132.63	125.06
82	D5	202	PEB	C2C-C1C-NC	4.91	114.18	107.57
82	U1	201	PEB	C1C-CHB-C4B	4.91	139.29	128.28
82	BI	202	PEB	CHB-C1C-C2C	-4.91	116.07	127.15
82	W7	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
82	M5	301	PEB	C1C-C2C-C3C	-4.91	101.82	107.62
82	sC	202	PEB	C1D-CHC-C4C	4.91	120.50	113.26
82	E5	201	PEB	C2C-C1C-NC	4.91	114.18	107.57
82	s8	202	PEB	OA-C1A-C2A	-4.91	122.27	126.17
85	fL	101	BCR	C36-C18-C19	4.91	125.81	118.08
82	PD	202	PEB	C2C-C1C-NC	4.91	114.18	107.57
82	K5	201	PEB	C2C-C1C-NC	4.91	114.18	107.57
82	H7	201	PEB	CHC-C4C-NC	4.91	127.79	121.15
82	qF	201	PEB	CHA-C1B-NB	-4.91	114.67	124.93
82	Z5	301	PEB	C1C-C2C-C3C	-4.91	101.82	107.62
82	FM	201	PEB	C4B-C3B-C2B	-4.91	101.35	106.78
82	RG	202	PEB	OA-C1A-C2A	-4.91	122.27	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cJ	202	PEB	OA-C1A-C2A	-4.91	122.27	126.17
84	FO	1001	CYC	C2B-C1B-NB	4.91	114.17	106.99
84	BE	1001	CYC	C3D-C4D-ND	4.90	114.17	107.57
82	Q1	201	PEB	CHB-C1C-C2C	-4.90	116.08	127.15
82	DD	203	PEB	C2C-C1C-NC	4.90	114.17	107.57
82	HK	202	PEB	C2C-C1C-NC	4.90	114.17	107.57
82	ZF	201	PEB	CHA-C1B-NB	-4.90	114.67	124.93
82	aJ	204	PEB	CHC-C1D-ND	-4.90	107.52	113.72
82	JK	202	PEB	CMB-C2B-C1B	4.90	132.62	125.06
82	W9	201	PEB	C3B-C4B-NB	4.90	117.18	110.05
85	KL	100	BCR	C16-C15-C14	4.90	133.52	123.47
84	LE	1001	CYC	CAB-C3B-C4B	4.90	129.12	121.38
82	vF	201	PEB	C2A-C1A-NA	4.90	112.50	108.27
83	yF	303	PUB	CHA-C4A-NA	-4.90	107.52	113.72
82	wC	202	PEB	CHB-C1C-C2C	-4.90	116.09	127.15
84	FO	1001	CYC	CMD-C2D-C1D	4.90	132.74	125.56
82	eG	203	PEB	OA-C1A-C2A	-4.90	122.28	126.17
84	IO	1001	CYC	CAB-C3B-C4B	4.90	129.12	121.38
82	QF	203	PEB	C2A-C1A-NA	4.90	112.50	108.27
84	GG	1001	CYC	C3D-C4D-ND	4.90	114.17	107.57
82	m1	201	PEB	C1C-C2C-C3C	-4.90	101.83	107.62
84	NE	201	CYC	CMA-C3A-C4A	4.90	132.61	125.06
82	SM	203	PEB	C2C-C1C-NC	4.90	114.17	107.57
82	Z5	304	PEB	OA-C1A-C2A	-4.90	122.28	126.17
82	EJ	202	PEB	C2C-C1C-NC	4.90	114.17	107.57
84	F1	1001	CYC	CHB-C1B-NB	-4.90	115.54	126.06
82	QM	202	PEB	C1D-CHC-C4C	-4.90	106.03	113.26
82	X5	201	PEB	C2C-C1C-NC	4.90	114.17	107.57
82	UH	203	PEB	C1C-C2C-C3C	-4.90	101.83	107.62
82	R7	201	PEB	CHC-C1D-ND	-4.90	107.53	113.72
82	LQ	203	PEB	C2C-C1C-NC	4.90	114.17	107.57
82	DF	202	PEB	CHB-C1C-C2C	-4.90	116.10	127.15
82	IJ	202	PEB	C1C-C2C-C3C	-4.90	101.83	107.62
82	EJ	201	PEB	CHB-C1C-C2C	-4.90	116.10	127.15
95	BL	613	DGD	O2G-C1B-C2B	4.90	122.05	111.50
84	E3	1001	CYC	CHD-C4C-NC	4.90	131.03	125.20
82	S7	202	PEB	C1C-C2C-C3C	-4.90	101.83	107.62
82	lM	202	PEB	C2C-C1C-NC	4.89	114.16	107.57
82	DQ	203	PEB	C2C-C1C-NC	4.89	114.16	107.57
82	dJ	201	PEB	C2C-C1C-NC	4.89	114.16	107.57
82	cB	402	PEB	OA-C1A-C2A	-4.89	122.28	126.17
82	G5	201	PEB	C2C-C1C-NC	4.89	114.16	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mH	201	PEB	C2C-C1C-NC	4.89	114.16	107.57
84	IG	1001	CYC	CAB-C3B-C4B	4.89	129.10	121.38
82	RH	202	PEB	C1D-CHC-C4C	4.89	120.47	113.26
82	N5	201	PEB	C2C-C1C-NC	4.89	114.16	107.57
82	DD	203	PEB	CMC-C3C-C4C	4.89	132.24	127.06
82	R5	201	PEB	C2C-C1C-NC	4.89	114.16	107.57
82	eE	202	PEB	CHB-C1C-C2C	-4.89	116.12	127.15
82	CK	202	PEB	C1D-CHC-C4C	-4.89	106.05	113.26
82	F7	202	PEB	C1C-C2C-C3C	-4.89	101.84	107.62
82	vC	202	PEB	C1C-C2C-C3C	-4.89	101.84	107.62
82	a4	201	PEB	C2C-C1C-NC	4.89	114.16	107.57
82	U7	201	PEB	CHB-C1C-C2C	-4.89	116.12	127.15
82	Q5	203	PEB	CMB-C2B-C1B	4.89	132.59	125.06
84	W3	1001	CYC	C3D-C4D-ND	4.89	114.15	107.57
87	8N	303	CLA	CHD-C4C-C3C	4.89	132.03	124.84
83	AE	303	PUB	CHA-C1B-NB	4.89	127.77	121.15
82	RI	201	PEB	C1C-C2C-C3C	-4.89	101.84	107.62
85	B6	621	BCR	C20-C21-C22	-4.89	120.33	127.31
82	ND	203	PEB	CHC-C1D-ND	-4.89	107.54	113.72
82	w8	202	PEB	C1C-CHB-C4B	4.89	139.24	128.28
82	O5	201	PEB	C2C-C1C-NC	4.89	114.15	107.57
84	DE	1001	CYC	C1B-C2B-C3B	-4.89	102.77	107.87
82	PE	201	PEB	CMB-C2B-C1B	4.89	132.59	125.06
82	w8	202	PEB	CHB-C1C-C2C	-4.89	116.13	127.15
82	YP	502	PEB	C2C-C1C-NC	4.89	114.15	107.57
85	K2	102	BCR	C11-C10-C9	4.89	134.28	127.31
82	OF	201	PEB	CHB-C1C-C2C	-4.89	116.13	127.15
82	DQ	202	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
82	R1	202	PEB	C1D-CHC-C4C	4.88	120.46	113.26
82	wC	202	PEB	C1C-CHB-C4B	4.88	139.24	128.28
82	EI	201	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
85	c6	617	BCR	C16-C17-C18	-4.88	120.34	127.31
82	YJ	202	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
82	CJ	202	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
82	FA	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
82	F4	1002	PEB	C2C-C1C-NC	4.88	114.14	107.57
82	NQ	203	PEB	CHC-C1D-ND	-4.88	107.55	113.72
82	TJ	202	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
82	V9	201	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
82	AJ	301	PEB	C2C-C1C-NC	4.88	114.14	107.57
82	WO	201	PEB	C3B-C4B-NB	4.88	117.15	110.05
82	MJ	202	PEB	CHA-C1B-NB	-4.88	114.72	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	yK	302	PUB	C1D-CHC-C4C	-4.88	102.75	113.37
82	YF	203	PEB	OA-C1A-C2A	-4.88	122.29	126.17
85	KN	101	BCR	C11-C10-C9	4.88	134.27	127.31
82	HB	202	PEB	C2C-C1C-NC	4.88	114.14	107.57
82	SA	202	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
82	EM	202	PEB	C1C-C2C-C3C	-4.88	101.85	107.62
83	yF	302	PUB	C1D-CHC-C4C	-4.88	102.75	113.37
82	MF	201	PEB	C2C-C1C-NC	4.88	114.14	107.57
82	cB	402	PEB	CHC-C4C-NC	4.88	127.75	121.15
84	N1	1001	CYC	CMB-C2B-C1B	4.88	130.26	124.17
82	TD	203	PEB	C1C-C2C-C3C	-4.88	101.86	107.62
82	U1	203	PEB	C1C-C2C-C3C	-4.88	101.86	107.62
82	B9	203	PEB	C1C-C2C-C3C	-4.88	101.86	107.62
82	SF	203	PEB	C2C-C1C-NC	4.88	114.14	107.57
82	B9	202	PEB	C1C-C2C-C3C	-4.88	101.86	107.62
82	I9	201	PEB	C1C-C2C-C3C	-4.88	101.86	107.62
82	HA	201	PEB	CHC-C4C-NC	4.88	127.75	121.15
82	GD	202	PEB	C2C-C1C-NC	4.88	114.14	107.57
83	wK	304	PUB	OD-C4D-C3D	-4.88	122.75	128.04
82	YG	201	PEB	CMB-C2B-C1B	4.88	132.57	125.06
103	8N	310	ZEX	C39-C29-C30	-4.88	116.09	122.92
82	C9	201	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	F9	203	PEB	C2C-C1C-NC	4.87	114.14	107.57
84	DG	1001	CYC	C1B-C2B-C3B	-4.87	102.78	107.87
103	82	310	ZEX	C39-C29-C30	-4.87	116.09	122.92
82	KI	202	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	DO	1002	PEB	OA-C1A-C2A	-4.87	122.30	126.17
82	GQ	202	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	OG	201	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	DK	202	PEB	CHB-C1C-C2C	-4.87	116.16	127.15
85	k6	102	BCR	C7-C8-C9	-4.87	118.87	126.23
82	BF	201	PEB	OA-C1A-NA	4.87	130.84	124.94
82	TI	202	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	K9	201	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	R9	201	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	YE	201	PEB	C3B-C4B-NB	4.87	117.14	110.05
82	LD	203	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	AQ	301	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	bG	201	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	DD	202	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	FM	202	PEB	OA-C1A-C2A	-4.87	122.30	126.17
84	CO	1001	CYC	OB-C4B-C3B	-4.87	122.75	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	C4	1001	CYC	OB-C4B-C3B	-4.87	122.75	128.04
82	F5	203	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	N9	201	PEB	C1C-C2C-C3C	-4.87	101.86	107.62
82	KF	202	PEB	C2C-C1C-NC	4.87	114.13	107.57
84	F3	1001	CYC	CMA-C3A-C4A	4.87	132.56	125.06
82	EM	201	PEB	CHC-C1D-ND	-4.87	107.56	113.72
84	h3	1001	CYC	CMA-C3A-C4A	4.87	132.56	125.06
82	dG	201	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	dG	202	PEB	C2C-C1C-NC	4.87	114.13	107.57
82	LK	202	PEB	OA-C1A-C2A	-4.87	122.30	126.17
92	J6	102	LMG	O1-C1-C2	4.87	115.90	108.30
82	VI	201	PEB	C1C-C2C-C3C	-4.87	101.87	107.62
84	L4	1001	CYC	C1B-C2B-C3B	-4.87	102.79	107.87
82	gF	203	PEB	C2C-C1C-NC	4.87	114.12	107.57
84	KG	202	CYC	OC-C1C-C2C	-4.87	122.30	126.17
82	FA	202	PEB	C1C-C2C-C3C	-4.87	101.87	107.62
82	eG	203	PEB	C2C-C1C-NC	4.87	114.12	107.57
82	WP	202	PEB	C1C-C2C-C3C	-4.87	101.87	107.62
83	xF	301	PUB	OD-C4D-C3D	-4.87	122.76	128.04
82	JF	202	PEB	CMB-C2B-C1B	4.87	132.56	125.06
84	n3	1001	CYC	CMA-C3A-C4A	4.87	132.56	125.06
83	BJ	302	PUB	C4B-C3B-C2B	-4.86	101.87	107.62
83	xF	301	PUB	C4B-C3B-C2B	-4.86	101.87	107.62
82	FO	1002	PEB	C2C-C1C-NC	4.86	114.12	107.57
82	QH	202	PEB	CMB-C2B-C1B	4.86	132.55	125.06
82	dE	202	PEB	C2C-C1C-NC	4.86	114.12	107.57
82	D9	201	PEB	C3B-C4B-NB	4.86	117.12	110.05
82	PI	201	PEB	C1C-C2C-C3C	-4.86	101.87	107.62
82	18	201	PEB	C1C-C2C-C3C	-4.86	101.87	107.62
84	Q3	1001	CYC	CMA-C3A-C4A	4.86	132.55	125.06
82	kJ	201	PEB	OA-C1A-C2A	-4.86	122.31	126.17
82	zF	501	PEB	C1D-CHC-C4C	-4.86	106.09	113.26
82	SK	203	PEB	C2C-C1C-NC	4.86	114.12	107.57
82	DF	203	PEB	C1C-C2C-C3C	-4.86	101.87	107.62
82	GI	202	PEB	C1C-C2C-C3C	-4.86	101.87	107.62
82	IM	202	PEB	C1C-C2C-C3C	-4.86	101.87	107.62
82	PG	201	PEB	CMB-C2B-C1B	4.86	132.55	125.06
84	B3	1001	CYC	CMA-C3A-C4A	4.86	132.55	125.06
82	IP	201	PEB	CMB-C2B-C1B	4.86	132.55	125.06
82	AH	305	PEB	C2C-C1C-NC	4.86	114.11	107.57
84	CO	1001	CYC	CMD-C2D-C1D	4.86	132.68	125.56
82	AI	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CI	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
84	M1	201	CYC	CAB-C3B-C4B	4.86	129.05	121.38
82	CQ	201	PEB	C3B-C4B-NB	4.86	117.12	110.05
82	A9	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
82	rC	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
82	YE	201	PEB	CMB-C2B-C1B	4.86	132.55	125.06
83	Z9	302	PUB	CAC-CBC-CGC	-4.86	103.15	113.60
82	vK	201	PEB	C2A-C1A-NA	4.86	112.46	108.27
84	k3	1001	CYC	CMA-C3A-C4A	4.86	132.54	125.06
82	hM	201	PEB	C2C-C1C-NC	4.86	114.11	107.57
82	KM	201	PEB	CHC-C4C-NC	4.86	127.72	121.15
85	kL	100	BCR	C16-C15-C14	4.86	133.42	123.47
82	II	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
82	P9	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
82	IK	201	PEB	CHC-C1D-ND	-4.86	107.58	113.72
82	B7	202	PEB	C2A-C1A-NA	4.86	112.46	108.27
84	NH	1001	CYC	CMB-C2B-C1B	4.86	130.23	124.17
85	K6	102	BCR	C7-C8-C9	-4.86	118.90	126.23
82	gK	203	PEB	C2C-C1C-NC	4.86	114.11	107.57
83	K7	203	PUB	C3B-C4B-NB	4.86	114.11	107.57
82	mH	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
83	M9	303	PUB	CAC-CBC-CGC	-4.86	103.15	113.60
82	cH	202	PEB	CHA-C1B-NB	-4.86	114.78	124.93
82	AH	302	PEB	C2C-C1C-NC	4.86	114.11	107.57
82	O5	202	PEB	CHC-C4C-NC	4.86	127.72	121.15
82	VE	201	PEB	C1C-C2C-C3C	-4.86	101.88	107.62
82	QH	201	PEB	CHB-C1C-C2C	-4.86	116.20	127.15
82	jK	202	PEB	C2C-C1C-NC	4.85	114.11	107.57
82	XA	203	PEB	CAB-CBB-CGB	-4.85	103.16	113.60
82	ZG	202	PEB	C1C-C2C-C3C	-4.85	101.88	107.62
82	OH	202	PEB	C1C-C2C-C3C	-4.85	101.88	107.62
83	AQ	302	PUB	C4B-C3B-C2B	-4.85	101.88	107.62
82	IJ	201	PEB	CHB-C1C-C2C	-4.85	116.20	127.15
103	82	310	ZEX	C18-C5-C6	-4.85	119.08	124.53
82	NI	201	PEB	C1C-C2C-C3C	-4.85	101.88	107.62
82	cF	203	PEB	CHB-C1C-C2C	-4.85	116.20	127.15
83	AG	303	PUB	CHA-C1B-NB	4.85	127.72	121.15
82	aJ	202	PEB	C2C-C1C-NC	4.85	114.11	107.57
82	WF	202	PEB	C1C-C2C-C3C	-4.85	101.89	107.62
85	BN	803	BCR	C4-C5-C6	-4.85	115.69	122.73
82	G9	201	PEB	C1C-C2C-C3C	-4.85	101.89	107.62
82	iG	202	PEB	C1C-C2C-C3C	-4.85	101.89	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eE	203	PEB	C2C-C1C-NC	4.85	114.10	107.57
82	Z9	303	PEB	CHA-C1B-NB	-4.85	114.79	124.93
82	qF	202	PEB	C1D-CHC-C4C	-4.85	106.10	113.26
82	fM	203	PEB	C2C-C1C-NC	4.85	114.10	107.57
82	PD	201	PEB	CHC-C4C-NC	4.85	127.71	121.15
82	OK	201	PEB	CHB-C1C-C2C	-4.85	116.21	127.15
83	BM	302	PUB	C4B-C3B-C2B	-4.85	101.89	107.62
84	f3	1001	CYC	CMA-C3A-C4A	4.85	132.53	125.06
82	II	203	PEB	CAC-C2C-C1C	4.85	133.49	125.76
82	T9	201	PEB	C1C-C2C-C3C	-4.85	101.89	107.62
82	X9	201	PEB	C1C-C2C-C3C	-4.85	101.89	107.62
82	a4	202	PEB	OA-C1A-C2A	-4.85	122.32	126.17
84	U3	1001	CYC	CMA-C3A-C4A	4.85	132.53	125.06
82	A1	302	PEB	C2C-C1C-NC	4.85	114.10	107.57
84	HO	1001	CYC	C3D-C4D-ND	4.85	114.10	107.57
82	cK	203	PEB	CHB-C1C-C2C	-4.85	116.21	127.15
88	cL	501	LHG	O7-C7-C8	4.85	121.95	111.50
82	jF	202	PEB	C2C-C1C-NC	4.85	114.10	107.57
82	v8	202	PEB	C1C-C2C-C3C	-4.85	101.89	107.62
87	F2	205	CLA	C1D-ND-C4D	-4.85	102.89	106.33
83	AM	304	PUB	C3B-C4B-NB	4.85	114.10	107.57
82	P7	202	PEB	CHB-C1C-C2C	-4.85	116.22	127.15
87	b6	605	CLA	C2B-C1B-NB	4.85	113.48	110.23
84	o3	1001	CYC	CMA-C3A-C4A	4.85	132.53	125.06
84	q3	1001	CYC	CMA-C3A-C4A	4.85	132.53	125.06
82	OB	201	PEB	OA-C1A-C2A	-4.85	122.32	126.17
82	WI	201	PEB	C4B-C3B-C2B	-4.85	101.42	106.78
82	PG	201	PEB	C2C-C1C-NC	4.85	114.09	107.57
82	QP	202	PEB	C2C-C1C-NC	4.85	114.09	107.57
82	Y9	203	PEB	OA-C1A-C2A	-4.84	122.32	126.17
82	E9	201	PEB	C1C-C2C-C3C	-4.84	101.89	107.62
82	1C	201	PEB	C1C-C2C-C3C	-4.84	101.89	107.62
85	B2	802	BCR	C4-C5-C6	-4.84	115.70	122.73
84	I3	1001	CYC	CMA-C3A-C4A	4.84	132.52	125.06
82	aO	201	PEB	C2C-C1C-NC	4.84	114.09	107.57
84	MG	1001	CYC	C3D-C4D-ND	4.84	114.09	107.57
82	DA	203	PEB	C1C-C2C-C3C	-4.84	101.89	107.62
82	AB	501	PEB	CHC-C4C-NC	4.84	127.70	121.15
82	h1	202	PEB	C2C-C1C-NC	4.84	114.09	107.57
84	y3	1001	CYC	C3D-C4D-ND	4.84	114.09	107.57
82	VG	201	PEB	C1C-C2C-C3C	-4.84	101.90	107.62
85	c6	617	BCR	C23-C22-C21	4.84	126.37	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gK	202	PEB	OA-C1A-C2A	-4.84	122.32	126.17
82	aE	202	PEB	C1C-C2C-C3C	-4.84	101.90	107.62
82	kO	202	PEB	CHB-C1C-C2C	-4.84	116.23	127.15
84	d3	1001	CYC	CMA-C3A-C4A	4.84	132.52	125.06
84	j3	1001	CYC	CMA-C3A-C4A	4.84	132.52	125.06
82	OJ	203	PEB	CHB-C1C-C2C	-4.84	116.23	127.15
82	WJ	202	PEB	C2C-C1C-NC	4.84	114.09	107.57
82	HM	201	PEB	C2C-C1C-NC	4.84	114.09	107.57
84	IE	1001	CYC	CAB-C3B-C4B	4.84	129.02	121.38
82	YG	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
82	CJ	203	PEB	CHB-C1C-C2C	-4.84	116.23	127.15
82	sC	201	PEB	CHA-C1B-NB	-4.84	114.81	124.93
82	qK	203	PEB	C1C-CHB-C4B	4.84	139.13	128.28
82	j4	202	PEB	C2C-C1C-NC	4.84	114.09	107.57
82	r8	202	PEB	CHB-C4B-NB	-4.84	114.51	124.58
84	w3	1001	CYC	CMA-C3A-C4A	4.84	132.52	125.06
83	M5	303	PUB	OD-C4D-ND	-4.84	118.76	125.93
82	CK	202	PEB	CHB-C1C-C2C	-4.84	116.23	127.15
82	zF	501	PEB	CHB-C1C-C2C	-4.84	116.23	127.15
82	OD	201	PEB	C1C-C2C-C3C	-4.84	101.90	107.62
82	M9	304	PEB	CHA-C1B-NB	-4.84	114.81	124.93
82	PQ	202	PEB	C2C-C1C-NC	4.84	114.08	107.57
82	aB	201	PEB	C2C-C1C-NC	4.84	114.08	107.57
82	zK	501	PEB	CHB-C1C-C2C	-4.84	116.24	127.15
84	O3	1001	CYC	CMA-C3A-C4A	4.84	132.51	125.06
84	73	1001	CYC	CMA-C3A-C4A	4.84	132.51	125.06
82	EP	202	PEB	C2C-C1C-NC	4.84	114.08	107.57
82	C9	202	PEB	C1C-C2C-C3C	-4.84	101.90	107.62
82	KB	302	PEB	C1C-C2C-C3C	-4.84	101.90	107.62
82	A9	202	PEB	C1C-C2C-C3C	-4.84	101.90	107.62
84	H3	1001	CYC	CMA-C3A-C4A	4.84	132.51	125.06
85	A6	401	BCR	C24-C23-C22	-4.84	118.93	126.23
83	AO	303	PUB	C3B-C4B-NB	4.84	114.08	107.57
82	PA	202	PEB	CHB-C1C-C2C	-4.83	116.24	127.15
82	g4	203	PEB	C4B-C3B-C2B	-4.83	101.43	106.78
82	bE	201	PEB	C1C-C2C-C3C	-4.83	101.91	107.62
82	VQ	201	PEB	CHC-C4C-NC	4.83	127.69	121.15
82	O4	201	PEB	C1C-C2C-C3C	-4.83	101.91	107.62
82	D4	1002	PEB	OA-C1A-C2A	-4.83	122.33	126.17
82	VB	201	PEB	C2C-C1C-NC	4.83	114.08	107.57
84	u3	1001	CYC	CMA-C3A-C4A	4.83	132.51	125.06
84	D3	1001	CYC	CMA-C3A-C4A	4.83	132.50	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O9	202	PEB	C1C-NC-C4C	-4.83	101.00	109.60
82	dM	203	PEB	C1C-C2C-C3C	-4.83	101.91	107.62
82	TO	203	PEB	CHC-C4C-NC	4.83	127.69	121.15
83	Z9	302	PUB	C1C-C2C-C3C	-4.83	101.44	106.78
85	JN	103	BCR	C16-C17-C18	-4.83	120.42	127.31
82	xC	202	PEB	CHB-C4B-NB	-4.83	114.52	124.58
82	WG	202	PEB	C2C-C1C-NC	4.83	114.08	107.57
82	FH	1002	PEB	C2C-C1C-NC	4.83	114.07	107.57
83	Z5	303	PUB	OD-C4D-ND	-4.83	118.78	125.93
103	8N	310	ZEX	C18-C5-C6	-4.83	119.11	124.53
82	BA	202	PEB	C2A-C1A-NA	4.83	112.44	108.27
84	C1	1001	CYC	CMA-C3A-C4A	4.83	132.50	125.06
82	QE	201	PEB	CHB-C1C-C2C	-4.83	116.26	127.15
82	VQ	203	PEB	CHB-C1C-C2C	-4.83	116.26	127.15
82	WE	202	PEB	C2C-C1C-NC	4.83	114.07	107.57
82	A1	305	PEB	C2C-C1C-NC	4.83	114.07	107.57
82	DM	202	PEB	C1C-C2C-C3C	-4.83	101.92	107.62
82	U4	202	PEB	C1C-C2C-C3C	-4.83	101.92	107.62
82	bG	201	PEB	C1C-C2C-C3C	-4.83	101.92	107.62
82	bE	201	PEB	C2C-C1C-NC	4.83	114.07	107.57
85	J2	103	BCR	C16-C17-C18	-4.83	120.42	127.31
82	A1	301	PEB	C2C-C1C-NC	4.83	114.07	107.57
82	GD	202	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	YD	201	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	R9	202	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
83	M9	303	PUB	C1C-C2C-C3C	-4.82	101.44	106.78
84	L3	1001	CYC	CMA-C3A-C4A	4.82	132.49	125.06
84	S3	1001	CYC	CMA-C3A-C4A	4.82	132.49	125.06
91	d6	404	PHO	C3D-C4D-ND	4.82	114.29	107.72
82	XJ	202	PEB	C2C-C1C-NC	4.82	114.06	107.57
82	qK	202	PEB	C1D-CHC-C4C	-4.82	106.14	113.26
82	iJ	202	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	dE	201	PEB	C2C-C1C-NC	4.82	114.06	107.57
82	IJ	203	PEB	CAC-C2C-C1C	4.82	133.44	125.76
82	E9	202	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	hH	201	PEB	C2C-C1C-NC	4.82	114.06	107.57
82	WP	202	PEB	CMB-C2B-C1B	4.82	132.49	125.06
84	M3	1001	CYC	CMA-C3A-C4A	4.82	132.49	125.06
82	DJ	202	PEB	CHC-C4C-NC	4.82	127.67	121.15
82	HB	203	PEB	OA-C1A-C2A	-4.82	122.34	126.17
82	OI	203	PEB	OA-C1A-C2A	-4.82	122.34	126.17
82	OB	201	PEB	C1C-C2C-C3C	-4.82	101.92	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	I9	202	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	II	203	PEB	C1B-C2B-C3B	-4.82	100.97	106.51
82	X7	203	PEB	CAB-CBB-CGB	-4.82	103.23	113.60
82	m4	202	PEB	CHB-C1C-C2C	-4.82	116.28	127.15
82	UQ	201	PEB	OA-C1A-C2A	-4.82	122.34	126.17
82	rF	201	PEB	CHC-C4C-NC	4.82	127.67	121.15
82	GB	201	PEB	C2C-C1C-NC	4.82	114.06	107.57
82	WM	202	PEB	C2C-C1C-NC	4.82	114.06	107.57
82	EJ	203	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	R1	201	PEB	C1C-C2C-C3C	-4.82	101.92	107.62
82	KK	202	PEB	C2C-C1C-NC	4.82	114.06	107.57
82	CD	201	PEB	C3B-C4B-NB	4.82	117.06	110.05
84	BE	1002	CYC	OC-C1C-C2C	-4.82	122.34	126.17
82	qF	201	PEB	CHC-C1D-ND	-4.82	107.63	113.72
82	PA	201	PEB	OA-C1A-C2A	-4.82	122.34	126.17
82	N7	202	PEB	C1C-C2C-C3C	-4.82	101.93	107.62
96	fL	102	HEM	CHC-C4B-NB	4.82	129.65	124.42
82	NA	202	PEB	C1C-C2C-C3C	-4.82	101.93	107.62
82	F1	1002	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	z8	202	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	x8	202	PEB	CHB-C4B-NB	-4.81	114.56	124.58
84	HG	1001	CYC	CMA-C3A-C4A	4.81	132.48	125.06
82	YP	502	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	eM	202	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	AH	301	PEB	C2C-C1C-NC	4.81	114.05	107.57
82	qF	203	PEB	C1C-CHB-C4B	4.81	139.08	128.28
82	BD	203	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
84	HE	1001	CYC	CMA-C3A-C4A	4.81	132.48	125.06
82	cF	203	PEB	CHA-C1B-C2B	4.81	137.28	124.90
82	RJ	202	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	B5	201	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	Y1	201	PEB	OA-C1A-C2A	-4.81	122.35	126.17
82	OQ	201	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	G9	202	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	K9	202	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
82	jJ	201	PEB	C1C-C2C-C3C	-4.81	101.93	107.62
84	I4	1001	CYC	OB-C4B-C3B	-4.81	122.82	128.04
82	eH	203	PEB	CHB-C1C-C2C	-4.81	116.30	127.15
84	JH	1003	CYC	C2D-C1D-ND	4.81	114.16	107.40
82	kF	201	PEB	CHA-C1B-NB	-4.81	114.87	124.93
82	JD	201	PEB	CHA-C1B-NB	-4.81	114.87	124.93
83	wK	304	PUB	C4B-C3B-C2B	-4.81	101.94	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	b1	203	PEB	CHB-C1C-C2C	-4.81	116.30	127.15
82	Q1	202	PEB	CMB-C2B-C1B	4.81	132.47	125.06
82	UO	201	PEB	CHA-C4A-NA	4.81	130.92	125.20
82	N9	202	PEB	C1C-C2C-C3C	-4.81	101.94	107.62
82	L9	201	PEB	C1C-C2C-C3C	-4.81	101.94	107.62
85	IN	101	BCR	C30-C25-C26	-4.81	115.84	122.61
82	QG	201	PEB	CHB-C1C-C2C	-4.81	116.30	127.15
82	aO	202	PEB	OA-C1A-C2A	-4.81	122.35	126.17
82	Y9	203	PEB	C2C-C1C-NC	4.81	114.04	107.57
82	UB	302	PEB	CAC-C2C-C3C	4.81	138.08	127.07
82	PG	201	PEB	OA-C1A-C2A	-4.81	122.35	126.17
82	gH	203	PEB	OA-C1A-C2A	-4.81	122.35	126.17
87	72	608	CLA	CHD-C1D-ND	-4.81	120.04	124.45
84	FE	1001	CYC	CMA-C3A-C4A	4.81	132.46	125.06
82	kK	201	PEB	CHA-C1B-NB	-4.80	114.88	124.93
82	CM	201	PEB	C1C-C2C-C3C	-4.80	101.94	107.62
82	QJ	202	PEB	C2C-C1C-NC	4.80	114.04	107.57
82	PQ	203	PEB	C2C-C1C-NC	4.80	114.04	107.57
82	bH	201	PEB	C2C-C1C-NC	4.80	114.04	107.57
83	yF	303	PUB	C3B-C4B-NB	4.80	114.04	107.57
84	CH	1001	CYC	C3D-C4D-ND	4.80	114.04	107.57
82	mO	202	PEB	CHB-C1C-C2C	-4.80	116.31	127.15
85	AN	846	BCR	C36-C18-C19	-4.80	110.51	118.08
87	FN	205	CLA	C1D-ND-C4D	-4.80	102.92	106.33
82	zC	202	PEB	C1C-C2C-C3C	-4.80	101.94	107.62
84	HG	1001	CYC	C3D-C4D-ND	4.80	114.04	107.57
82	iE	202	PEB	C1C-C2C-C3C	-4.80	101.94	107.62
82	c1	201	PEB	C2C-C1C-NC	4.80	114.04	107.57
85	I2	101	BCR	C30-C25-C26	-4.80	115.85	122.61
82	rC	202	PEB	CHB-C4B-NB	-4.80	114.59	124.58
82	UO	202	PEB	C1C-C2C-C3C	-4.80	101.95	107.62
82	GP	203	PEB	C1C-C2C-C3C	-4.80	101.95	107.62
82	FM	201	PEB	CMC-C3C-C4C	4.80	132.15	127.06
82	JD	203	PEB	C2C-C1C-NC	4.80	114.03	107.57
82	T7	202	PEB	C3B-C4B-NB	4.80	117.03	110.05
82	Y9	203	PEB	C1C-C2C-C3C	-4.80	101.95	107.62
82	LK	202	PEB	CHB-C4B-C3B	-4.80	114.22	125.32
82	LJ	202	PEB	C1C-C2C-C3C	-4.80	101.95	107.62
84	C1	1001	CYC	C3D-C4D-ND	4.80	114.03	107.57
82	PD	203	PEB	C2C-C1C-NC	4.80	114.03	107.57
84	LH	1001	CYC	C3D-C4D-ND	4.80	114.03	107.57
82	BQ	203	PEB	C1C-C2C-C3C	-4.80	101.95	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HF	202	PEB	C2C-C1C-NC	4.80	114.03	107.57
82	AG	301	PEB	C1C-C2C-C3C	-4.80	101.95	107.62
82	Z9	303	PEB	C2C-C1C-NC	4.80	114.03	107.57
82	gO	203	PEB	C4B-C3B-C2B	-4.79	101.47	106.78
84	M1	201	CYC	C3D-C4D-ND	4.79	114.03	107.57
84	I1	1001	CYC	C3D-C4D-ND	4.79	114.03	107.57
82	OO	201	PEB	C1C-C2C-C3C	-4.79	101.95	107.62
82	YO	201	PEB	C1C-C2C-C3C	-4.79	101.95	107.62
82	mG	202	PEB	CHC-C4C-NC	4.79	127.64	121.15
82	F1	1002	PEB	C2C-C1C-NC	4.79	114.03	107.57
82	FO	1002	PEB	C1C-C2C-C3C	-4.79	101.95	107.62
82	JJ	201	PEB	OA-C1A-C2A	-4.79	122.36	126.17
84	EE	1001	CYC	OC-C1C-C2C	-4.79	122.36	126.17
82	GK	202	PEB	CHB-C1C-C2C	-4.79	116.34	127.15
82	J5	203	PEB	C2C-C1C-NC	4.79	114.02	107.57
84	JH	1003	CYC	CAB-C3B-C4B	4.79	128.95	121.38
82	AH	302	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	V9	202	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	QE	201	PEB	OA-C1A-C2A	-4.79	122.36	126.17
82	SH	203	PEB	C1C-CHB-C4B	4.79	139.03	128.28
82	IA	201	PEB	C2C-C1C-NC	4.79	114.02	107.57
82	uC	202	PEB	CHC-C1D-ND	-4.79	107.66	113.72
84	IO	1001	CYC	OB-C4B-C3B	-4.79	122.84	128.04
82	rF	202	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	qK	201	PEB	CHA-C1B-NB	-4.79	114.92	124.93
82	GP	202	PEB	C2C-C1C-NC	4.79	114.02	107.57
82	JQ	203	PEB	C2C-C1C-NC	4.79	114.02	107.57
82	DD	201	PEB	CHB-C1C-C2C	-4.79	116.35	127.15
82	GJ	201	PEB	C2C-C1C-NC	4.79	114.02	107.57
82	JA	203	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	IK	203	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	PP	201	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	vC	201	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	gE	202	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	P9	202	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	HM	201	PEB	CMC-C3C-C4C	4.79	132.13	127.06
82	lM	201	PEB	C2C-C1C-NC	4.79	114.02	107.57
96	f6	101	HEM	C4B-C3B-C2B	-4.79	103.31	107.11
82	rK	201	PEB	CHC-C4C-NC	4.79	127.63	121.15
87	7N	608	CLA	CHD-C1D-ND	-4.79	120.06	124.45
82	HI	203	PEB	C2C-C1C-NC	4.79	114.02	107.57
82	IJ	202	PEB	CHA-C1B-NB	-4.79	114.92	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A2	846	BCR	C36-C18-C19	-4.79	110.54	118.08
82	YA	304	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	aG	202	PEB	C1C-C2C-C3C	-4.79	101.96	107.62
82	JQ	201	PEB	CHA-C1B-NB	-4.79	114.92	124.93
82	WI	203	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	SQ	201	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	T9	202	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	s8	201	PEB	CHA-C1B-NB	-4.78	114.92	124.93
82	D7	203	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	dQ	401	PEB	OA-C1A-C2A	-4.78	122.37	126.17
82	W9	201	PEB	C2C-C1C-NC	4.78	114.01	107.57
82	jO	202	PEB	C2C-C1C-NC	4.78	114.01	107.57
82	A1	302	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
87	CL	510	CLA	CMB-C2B-C1B	-4.78	118.09	125.37
82	TA	203	PEB	C2C-C1C-NC	4.78	114.01	107.57
82	iK	201	PEB	C2C-C1C-NC	4.78	114.01	107.57
82	vF	202	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	UG	202	PEB	OA-C1A-C2A	-4.78	122.37	126.17
82	PE	201	PEB	C2C-C1C-NC	4.78	114.01	107.57
83	A4	303	PUB	C3B-C4B-NB	4.78	114.01	107.57
82	cK	203	PEB	CHA-C1B-C2B	4.78	137.19	124.90
82	NK	201	PEB	OA-C1A-NA	4.78	130.73	124.94
82	GF	202	PEB	CHB-C1C-C2C	-4.78	116.36	127.15
84	F4	1001	CYC	C1B-C2B-C3B	-4.78	102.88	107.87
84	C1	1001	CYC	CHD-C1D-ND	-4.78	114.37	125.32
82	U4	202	PEB	C2C-C1C-NC	4.78	114.01	107.57
82	CB	201	PEB	CMB-C2B-C1B	4.78	132.43	125.06
82	j4	203	PEB	CHB-C1C-C2C	-4.78	116.37	127.15
82	TE	201	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	l4	201	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	X9	202	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	CJ	203	PEB	OA-C1A-C2A	-4.78	122.37	126.17
82	UO	202	PEB	C2C-C1C-NC	4.78	114.01	107.57
82	BK	202	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	F4	1002	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
82	UB	303	PEB	C2C-C1C-NC	4.78	114.00	107.57
82	gG	202	PEB	C2C-C1C-NC	4.78	114.00	107.57
82	mO	201	PEB	C2C-C1C-NC	4.78	114.00	107.57
95	AL	416	DGD	O2G-C1B-C2B	4.78	121.80	111.50
82	lE	201	PEB	OA-C1A-C2A	-4.78	122.37	126.17
82	SG	203	PEB	CHB-C1C-C2C	-4.78	116.37	127.15
82	dB	202	PEB	CMC-C3C-C4C	4.78	132.12	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GG	1002	PEB	OA-C1A-C2A	-4.78	122.38	126.17
82	QE	201	PEB	CHC-C4C-NC	4.78	127.61	121.15
82	CF	202	PEB	CHB-C1C-C2C	-4.78	116.37	127.15
82	U4	201	PEB	CHA-C4A-NA	4.78	130.88	125.20
82	qF	201	PEB	C2C-C1C-NC	4.78	114.00	107.57
82	gB	201	PEB	C1C-C2C-C3C	-4.78	101.97	107.62
85	CL	502	BCR	C38-C26-C25	-4.78	119.17	124.53
103	8N	310	ZEX	C40-C33-C34	-4.78	116.23	122.92
82	wK	302	PEB	C2C-C1C-NC	4.78	114.00	107.57
82	gF	201	PEB	C1C-C2C-C3C	-4.78	101.98	107.62
82	XB	202	PEB	C2C-C1C-NC	4.77	114.00	107.57
82	V1	202	PEB	C1C-CHB-C4B	4.77	138.99	128.28
82	RE	201	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
83	AD	302	PUB	C4B-C3B-C2B	-4.77	101.98	107.62
82	OI	202	PEB	OA-C1A-C2A	-4.77	122.38	126.17
82	BI	201	PEB	C4B-C3B-C2B	-4.77	101.50	106.78
82	mE	202	PEB	CHC-C4C-NC	4.77	127.61	121.15
82	YB	201	PEB	C2A-C1A-NA	4.77	112.39	108.27
82	OQ	202	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
83	AE	302	PUB	CHA-C1B-NB	4.77	127.61	121.15
91	DL	405	PHO	C3D-C4D-ND	4.77	114.22	107.72
84	CH	1001	CYC	CHD-C1D-ND	-4.77	114.39	125.32
82	AP	202	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
82	GP	202	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
82	OI	201	PEB	C4B-C3B-C2B	-4.77	101.50	106.78
82	h4	201	PEB	C2C-C1C-NC	4.77	114.00	107.57
82	Z5	305	PEB	C2C-C1C-NC	4.77	114.00	107.57
82	I7	201	PEB	C2C-C1C-NC	4.77	114.00	107.57
82	gF	202	PEB	OA-C1A-C2A	-4.77	122.38	126.17
82	AE	304	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
103	82	310	ZEX	C40-C33-C34	-4.77	116.24	122.92
82	XF	202	PEB	CHB-C1C-C2C	-4.77	116.39	127.15
82	LF	202	PEB	CHB-C4B-C3B	-4.77	114.28	125.32
82	PF	202	PEB	C1D-CHC-C4C	4.77	120.29	113.26
82	Y7	304	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
83	M9	303	PUB	C3B-C4B-NB	4.77	114.00	107.57
82	HM	201	PEB	C4B-C3B-C2B	-4.77	101.50	106.78
82	M9	305	PEB	C2C-C1C-NC	4.77	113.99	107.57
84	D4	1001	CYC	C3D-C4D-ND	4.77	113.99	107.57
82	CP	202	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
82	lG	202	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
82	DQ	201	PEB	CHB-C1C-C2C	-4.77	116.39	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YQ	201	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
82	iF	201	PEB	C2C-C1C-NC	4.77	113.99	107.57
82	Y1	202	PEB	CMB-C2B-C1B	4.77	132.41	125.06
83	Z9	302	PUB	C3B-C4B-NB	4.77	113.99	107.57
82	ZI	401	PEB	CHB-C1C-NC	-4.77	114.40	125.32
82	J9	201	PEB	C3B-C4B-NB	4.77	116.98	110.05
82	RI	203	PEB	C1C-C2C-C3C	-4.77	101.98	107.62
82	U7	201	PEB	C3D-C4D-ND	4.77	116.61	107.26
84	FH	1001	CYC	OB-C4B-C3B	-4.77	122.87	128.04
82	GB	202	PEB	OA-C1A-C2A	-4.77	122.38	126.17
82	VM	202	PEB	C1C-C2C-C3C	-4.77	101.99	107.62
82	HP	202	PEB	C2C-C1C-NC	4.77	113.99	107.57
82	T7	203	PEB	C2C-C1C-NC	4.77	113.99	107.57
82	WA	201	PEB	OA-C1A-C2A	-4.77	122.38	126.17
82	S7	201	PEB	C3D-C4D-ND	4.77	116.61	107.26
82	AP	201	PEB	CMB-C2B-C1B	4.77	132.40	125.06
82	GB	201	PEB	C1C-C2C-C3C	-4.76	101.99	107.62
82	b1	201	PEB	C2C-C1C-NC	4.76	113.99	107.57
82	KB	304	PEB	CHC-C4C-NC	4.76	127.60	121.15
82	dF	201	PEB	CHC-C4C-NC	4.76	127.60	121.15
82	W9	201	PEB	CHC-C1D-ND	-4.76	107.70	113.72
82	ND	203	PEB	C2C-C1C-NC	4.76	113.98	107.57
82	UM	202	PEB	C2C-C1C-NC	4.76	113.98	107.57
82	FP	202	PEB	C2C-C1C-NC	4.76	113.98	107.57
84	JH	1003	CYC	C3D-C4D-ND	4.76	113.98	107.57
83	yK	303	PUB	C4B-C3B-C2B	-4.76	101.99	107.62
84	CG	1001	CYC	CMA-C3A-C4A	4.76	132.40	125.06
82	a4	201	PEB	CHC-C1D-ND	-4.76	107.70	113.72
82	GQ	202	PEB	C1C-C2C-C3C	-4.76	101.99	107.62
82	FQ	203	PEB	CHB-C1C-NC	4.76	136.23	125.32
82	UJ	202	PEB	CHA-C1B-NB	-4.76	114.97	124.93
82	cB	402	PEB	CHC-C1D-ND	-4.76	107.70	113.72
82	FD	203	PEB	CHB-C1C-NC	4.76	136.23	125.32
82	ZB	203	PEB	CMB-C2B-C1B	4.76	132.40	125.06
82	JJ	202	PEB	C1C-C2C-C3C	-4.76	101.99	107.62
82	QQ	201	PEB	C1C-C2C-C3C	-4.76	101.99	107.62
82	J7	203	PEB	C1C-C2C-C3C	-4.76	101.99	107.62
84	FE	1002	CYC	C3D-C4D-ND	4.76	113.98	107.57
83	Z9	305	PUB	C4B-CHB-C1C	4.76	138.96	128.28
82	z8	202	PEB	CHB-C1C-NC	-4.76	114.42	125.32
82	VA	202	PEB	C3C-C4C-NC	4.76	112.62	108.33
85	B6	602	BCR	C15-C14-C13	-4.76	120.52	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aM	203	PEB	CHC-C4C-NC	4.76	127.59	121.15
82	Z4	201	PEB	CMA-C2A-C1A	-4.76	102.15	112.40
82	BI	201	PEB	OA-C1A-C2A	-4.76	122.39	126.17
82	N4	1002	PEB	C1C-C2C-C3C	-4.76	102.00	107.62
82	WM	201	PEB	CHC-C4C-NC	4.76	127.59	121.15
82	NF	201	PEB	OA-C1A-NA	4.76	130.70	124.94
82	l1	202	PEB	OA-C1A-C2A	-4.76	122.39	126.17
84	I4	1001	CYC	CMD-C2D-C1D	4.76	132.53	125.56
82	AE	301	PEB	C1C-C2C-C3C	-4.76	102.00	107.62
82	rK	202	PEB	C1C-C2C-C3C	-4.76	102.00	107.62
82	SE	202	PEB	CHB-C1C-C2C	-4.76	116.42	127.15
82	zC	202	PEB	CHB-C1C-NC	-4.76	114.42	125.32
82	AB	501	PEB	C2C-C1C-NC	4.76	113.97	107.57
82	KM	202	PEB	C1C-C2C-C3C	-4.76	102.00	107.62
82	jJ	203	PEB	CHC-C1D-ND	-4.75	107.71	113.72
82	TJ	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	tK	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
87	32	310	CLA	CAA-C2A-C3A	-4.75	105.01	116.10
82	TG	201	PEB	CMB-C2B-C1B	4.75	132.38	125.06
82	CM	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	Y9	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	M9	304	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	O1	202	PEB	C1C-C2C-C3C	-4.75	102.00	107.62
82	BB	203	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	mF	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	mE	202	PEB	OA-C1A-C2A	-4.75	122.39	126.17
84	F1	1001	CYC	CAB-C3B-C4B	4.75	128.88	121.38
82	kJ	202	PEB	C1C-C2C-C3C	-4.75	102.00	107.62
82	hO	201	PEB	CHC-C4C-NC	4.75	127.58	121.15
84	NE	201	CYC	OC-C1C-C2C	-4.75	122.39	126.17
82	FI	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	AJ	302	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	cB	401	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	UB	302	PEB	C1C-C2C-C3C	-4.75	102.00	107.62
82	BF	202	PEB	C1C-C2C-C3C	-4.75	102.00	107.62
82	QF	203	PEB	CHA-C1B-C2B	4.75	137.12	124.90
82	VI	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	lG	201	PEB	C2C-C1C-NC	4.75	113.97	107.57
82	RG	201	PEB	C1C-C2C-C3C	-4.75	102.00	107.62
82	WG	201	PEB	C1C-C2C-C3C	-4.75	102.00	107.62
82	VD	203	PEB	CHB-C1C-C2C	-4.75	116.43	127.15
82	MF	201	PEB	CMB-C2B-C1B	4.75	132.38	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	IG	1001	CYC	CMA-C3A-C4A	4.75	132.38	125.06
82	RH	201	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	gF	201	PEB	CHB-C1C-C2C	-4.75	116.44	127.15
82	QK	203	PEB	CHA-C1B-C2B	4.75	137.11	124.90
87	12	608	CLA	C4A-NA-C1A	4.75	108.84	106.71
82	NI	202	PEB	C2C-C1C-NC	4.75	113.97	107.57
84	DO	1001	CYC	C3D-C4D-ND	4.75	113.97	107.57
82	OE	201	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	AG	304	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	FJ	202	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	J5	201	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	mG	202	PEB	CHB-C1C-C2C	-4.75	116.44	127.15
82	HI	201	PEB	C4B-C3B-C2B	-4.75	101.53	106.78
84	H4	1001	CYC	C3D-C4D-ND	4.75	113.96	107.57
82	YK	203	PEB	OA-C1A-C2A	-4.75	122.40	126.17
82	XA	202	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	CB	202	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	bB	201	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	L5	203	PEB	C2C-C1C-NC	4.75	113.96	107.57
82	wF	302	PEB	C2C-C1C-NC	4.75	113.96	107.57
82	O7	201	PEB	CHC-C4C-NC	4.75	127.57	121.15
82	JF	202	PEB	C2C-C1C-NC	4.75	113.96	107.57
82	qK	201	PEB	CHC-C1D-ND	-4.75	107.72	113.72
82	OD	202	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	DK	203	PEB	C1C-C2C-C3C	-4.75	102.01	107.62
82	Y9	201	PEB	C4B-C3B-C2B	-4.75	101.53	106.78
82	UB	302	PEB	OA-C1A-C2A	-4.75	122.40	126.17
82	K7	202	PEB	C2C-C1C-NC	4.74	113.96	107.57
82	D5	203	PEB	C1C-C2C-C3C	-4.74	102.01	107.62
82	nK	202	PEB	C1C-C2C-C3C	-4.74	102.01	107.62
82	aM	201	PEB	C1C-C2C-C3C	-4.74	102.01	107.62
82	QG	201	PEB	CHC-C4C-NC	4.74	127.57	121.15
82	WK	202	PEB	C1C-C2C-C3C	-4.74	102.01	107.62
82	Y4	201	PEB	C1C-C2C-C3C	-4.74	102.01	107.62
82	UA	201	PEB	C3D-C4D-ND	4.74	116.57	107.26
82	XI	202	PEB	C2C-C1C-NC	4.74	113.96	107.57
82	W7	202	PEB	C2C-C1C-NC	4.74	113.96	107.57
82	cH	202	PEB	C2C-C1C-NC	4.74	113.96	107.57
82	U9	202	PEB	CHB-C1C-C2C	-4.74	116.45	127.15
82	z8	202	PEB	CHB-C4B-NB	-4.74	114.71	124.58
82	nF	202	PEB	C1C-C2C-C3C	-4.74	102.01	107.62
82	CJ	201	PEB	C2C-C1C-NC	4.74	113.96	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mK	202	PEB	C2C-C1C-NC	4.74	113.96	107.57
82	VK	202	PEB	CMB-C2B-C1B	4.74	132.37	125.06
82	Y1	201	PEB	CMB-C2B-C1B	4.74	132.37	125.06
84	F1	1001	CYC	CMD-C2D-C1D	4.74	132.50	125.56
82	CI	202	PEB	C2C-C1C-NC	4.74	113.96	107.57
82	VD	201	PEB	CHC-C4C-NC	4.74	127.57	121.15
82	HI	203	PEB	OA-C1A-C2A	-4.74	122.40	126.17
82	mG	202	PEB	OA-C1A-C2A	-4.74	122.40	126.17
82	GB	203	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	MJ	203	PEB	C2C-C1C-NC	4.74	113.95	107.57
84	FH	1001	CYC	CAB-C3B-C4B	4.74	128.87	121.38
82	JP	202	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	wC	202	PEB	C2C-C1C-NC	4.74	113.95	107.57
84	EH	1001	CYC	CHD-C1D-ND	-4.74	114.46	125.32
85	C6	507	BCR	C7-C8-C9	-4.74	119.07	126.23
82	gE	202	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	yF	301	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	MM	202	PEB	CHC-C4C-NC	4.74	127.56	121.15
82	LI	202	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	T4	203	PEB	CHC-C4C-NC	4.74	127.56	121.15
83	wF	304	PUB	C4B-C3B-C2B	-4.74	102.02	107.62
82	VJ	202	PEB	CHC-C1D-ND	-4.74	107.73	113.72
82	MK	203	PEB	CHB-C1C-C2C	-4.74	116.46	127.15
84	HE	1001	CYC	CAB-C3B-C4B	4.74	128.86	121.38
82	SE	201	PEB	C1C-C2C-C3C	-4.74	102.02	107.62
87	3N	310	CLA	CAA-C2A-C3A	-4.74	105.04	116.10
82	aJ	202	PEB	OA-C1A-C2A	-4.74	122.41	126.17
82	NQ	203	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	OA	201	PEB	CHC-C4C-NC	4.74	127.56	121.15
82	jF	202	PEB	CMB-C2B-C1B	4.74	132.36	125.06
82	VB	202	PEB	C2C-C1C-NC	4.74	113.95	107.57
84	F1	1001	CYC	OB-C4B-C3B	-4.74	122.90	128.04
82	aB	201	PEB	C1C-C2C-C3C	-4.74	102.02	107.62
82	rC	202	PEB	C1C-C2C-C3C	-4.74	102.02	107.62
82	u8	202	PEB	CHC-C1D-ND	-4.74	107.73	113.72
82	M5	305	PEB	C2C-C1C-NC	4.74	113.95	107.57
82	SA	201	PEB	C3D-C4D-ND	4.74	116.55	107.26
87	1N	608	CLA	C4A-NA-C1A	4.74	108.83	106.71
82	SP	203	PEB	CHC-C1D-ND	-4.74	107.73	113.72
82	aH	201	PEB	C1D-CHC-C4C	-4.74	106.27	113.26
83	YA	302	PUB	C4A-CHA-C1B	-4.74	106.27	113.26
82	U4	201	PEB	CHA-C1B-NB	-4.73	115.03	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MF	203	PEB	CHB-C1C-C2C	-4.73	116.47	127.15
84	E1	1001	CYC	CHD-C1D-ND	-4.73	114.47	125.32
82	hM	203	PEB	C2C-C1C-NC	4.73	113.95	107.57
82	LF	202	PEB	OA-C1A-C2A	-4.73	122.41	126.17
82	gJ	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	TE	201	PEB	CMB-C2B-C1B	4.73	132.35	125.06
82	YH	202	PEB	CMB-C2B-C1B	4.73	132.35	125.06
82	XI	202	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	Q5	202	PEB	CHB-C1C-C2C	-4.73	116.47	127.15
82	EJ	202	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	TA	202	PEB	C3B-C4B-NB	4.73	116.93	110.05
82	FM	202	PEB	C2C-C1C-NC	4.73	113.94	107.57
82	UP	202	PEB	C2C-C1C-NC	4.73	113.94	107.57
82	TG	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	B5	203	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	JD	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	QM	202	PEB	OA-C1A-C2A	-4.73	122.41	126.17
82	II	202	PEB	C2C-C1C-NC	4.73	113.94	107.57
82	qK	201	PEB	C2C-C1C-NC	4.73	113.94	107.57
82	IP	202	PEB	CMC-C3C-C4C	4.73	132.07	127.06
82	SF	201	PEB	CHA-C1B-NB	-4.73	115.04	124.93
82	K7	202	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
84	FG	1001	CYC	C3D-C4D-ND	4.73	113.94	107.57
82	SA	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	UB	301	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	IF	203	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	lM	203	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	lF	203	PEB	OA-C1A-C2A	-4.73	122.41	126.17
82	YG	202	PEB	CHC-C4C-NC	4.73	127.55	121.15
82	SG	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	DM	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
85	cL	518	BCR	C24-C23-C22	-4.73	119.09	126.23
84	BG	1002	CYC	CMD-C2D-C1D	4.73	132.48	125.56
82	UB	302	PEB	C2C-C1C-NC	4.73	113.94	107.57
82	Q5	203	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	v8	201	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	dK	202	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	RI	202	PEB	C2C-C1C-NC	4.73	113.93	107.57
82	YH	201	PEB	CMB-C2B-C1B	4.73	132.34	125.06
82	DQ	203	PEB	CMC-C3C-C4C	4.73	132.07	127.06
82	NO	1002	PEB	C1C-C2C-C3C	-4.73	102.03	107.62
82	b1	203	PEB	C1C-C2C-C3C	-4.73	102.03	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	AH	303	PUB	C4B-C3B-C2B	-4.73	102.03	107.62
82	qK	203	PEB	CHB-C1C-C2C	-4.73	116.49	127.15
87	42	604	CLA	CAA-C2A-C3A	-4.72	102.45	114.26
82	FH	1002	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	eO	201	PEB	CMB-C2B-C1B	4.72	132.34	125.06
82	Z1	203	PEB	CHA-C1B-NB	-4.72	115.05	124.93
82	CB	202	PEB	C2C-C1C-NC	4.72	113.93	107.57
82	KM	203	PEB	CHC-C1D-ND	-4.72	107.75	113.72
82	QB	204	PEB	C2C-C1C-NC	4.72	113.93	107.57
82	hO	201	PEB	C2C-C1C-NC	4.72	113.93	107.57
82	VB	202	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	JI	202	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	vK	202	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	tF	202	PEB	C2C-C1C-NC	4.72	113.93	107.57
82	h1	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
82	D5	202	PEB	CHB-C1C-C2C	-4.72	116.50	127.15
82	SK	201	PEB	CHA-C1B-NB	-4.72	115.06	124.93
82	CP	203	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	EP	201	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	B9	201	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	HF	202	PEB	C1C-CHB-C4B	4.72	138.87	128.28
84	LO	1001	CYC	CBB-CAB-C3B	-4.72	99.42	112.43
82	YK	201	PEB	C2C-C1C-NC	4.72	113.93	107.57
83	Y7	302	PUB	C4A-CHA-C1B	-4.72	106.30	113.26
83	Z5	303	PUB	CHA-C1B-NB	4.72	127.53	121.15
82	KI	203	PEB	C2C-C1C-NC	4.72	113.92	107.57
82	SJ	201	PEB	C2C-C1C-NC	4.72	113.92	107.57
82	aJ	201	PEB	C2C-C1C-NC	4.72	113.92	107.57
87	4N	604	CLA	CAA-C2A-C3A	-4.72	102.47	114.26
82	O7	202	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	wF	301	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	eH	203	PEB	C1C-C2C-C3C	-4.72	102.04	107.62
82	NB	201	PEB	C2C-C1C-NC	4.72	113.92	107.57
84	HG	1001	CYC	CAB-C3B-C4B	4.72	128.83	121.38
82	WG	202	PEB	C1C-C2C-C3C	-4.72	102.05	107.62
82	L5	202	PEB	CHC-C4C-NC	4.72	127.53	121.15
82	YF	201	PEB	C2C-C1C-NC	4.72	113.92	107.57
82	HK	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
84	FH	1001	CYC	CMD-C2D-C1D	4.72	132.47	125.56
82	M5	305	PEB	C1C-CHB-C4B	-4.72	117.71	128.28
82	jJ	202	PEB	C1C-C2C-C3C	-4.72	102.05	107.62
84	BE	1002	CYC	CMD-C2D-C1D	4.72	132.47	125.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	AG	302	PUB	CHA-C1B-NB	4.72	127.53	121.15
92	B6	618	LMG	O7-C10-C11	4.72	121.66	111.50
82	MJ	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
82	DB	203	PEB	C2C-C1C-NC	4.72	113.92	107.57
82	PJ	202	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	EQ	201	PEB	CMB-C2B-C1B	4.71	132.32	125.06
82	NA	203	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	wK	301	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	Z5	305	PEB	C1C-CHB-C4B	-4.71	117.71	128.28
82	HG	1002	PEB	C4B-C3B-C2B	-4.71	101.56	106.78
82	ZB	202	PEB	C2C-C1C-NC	4.71	113.92	107.57
82	EK	202	PEB	C2C-C1C-NC	4.71	113.92	107.57
82	EQ	202	PEB	C2C-C1C-NC	4.71	113.92	107.57
82	ZB	202	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	JF	202	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	N7	203	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	Y9	201	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
82	XB	201	PEB	C2C-C1C-NC	4.71	113.92	107.57
84	MO	1001	CYC	C3D-C4D-ND	4.71	113.92	107.57
82	h4	201	PEB	CHC-C4C-NC	4.71	127.53	121.15
82	OK	203	PEB	C2C-C1C-NC	4.71	113.92	107.57
82	ZO	201	PEB	CMA-C2A-C1A	-4.71	102.25	112.40
82	CF	202	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
84	IE	1001	CYC	CMA-C3A-C4A	4.71	132.32	125.06
82	O9	203	PEB	C2C-C1C-NC	4.71	113.92	107.57
82	yK	301	PEB	C2C-C1C-NC	4.71	113.92	107.57
82	wC	203	PEB	OA-C1A-C2A	-4.71	122.43	126.17
82	aO	201	PEB	CMB-C2B-C1B	4.71	132.32	125.06
85	fL	101	BCR	C20-C21-C22	-4.71	120.59	127.31
82	AD	304	PEB	C1C-CHB-C4B	-4.71	117.72	128.28
84	LH	1002	CYC	OC-C1C-C2C	-4.71	122.43	126.17
82	BI	203	PEB	CHC-C4C-NC	4.71	127.52	121.15
82	lJ	201	PEB	CHC-C1D-ND	-4.71	107.77	113.72
82	gG	202	PEB	C1C-C2C-C3C	-4.71	102.05	107.62
83	yF	303	PUB	C4B-C3B-C2B	-4.71	102.05	107.62
82	ZE	203	PEB	C2C-C1C-NC	4.71	113.91	107.57
82	HF	201	PEB	OA-C1A-C2A	-4.71	122.43	126.17
82	BA	202	PEB	C2C-C1C-NC	4.71	113.91	107.57
82	r8	202	PEB	C1C-C2C-C3C	-4.71	102.06	107.62
82	gK	201	PEB	C1C-C2C-C3C	-4.71	102.06	107.62
92	b6	619	LMG	O7-C10-C11	4.71	121.65	111.50
82	UK	202	PEB	C2C-C1C-NC	4.71	113.91	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lH	201	PEB	OA-C1A-C2A	-4.71	122.43	126.17
82	PH	202	PEB	C1C-C2C-C3C	-4.71	102.06	107.62
82	B7	202	PEB	C2C-C1C-NC	4.71	113.91	107.57
82	Z9	304	PEB	C2C-C1C-NC	4.71	113.91	107.57
82	UB	302	PEB	CMC-C3C-C4C	-4.71	122.07	127.06
82	JJ	202	PEB	OA-C1A-C2A	-4.71	122.43	126.17
82	PI	202	PEB	C2C-C1C-NC	4.71	113.91	107.57
82	RI	202	PEB	C1C-C2C-C3C	-4.71	102.06	107.62
82	OD	201	PEB	C2C-C1C-NC	4.71	113.91	107.57
85	A2	848	BCR	C24-C23-C22	4.71	133.34	126.23
84	L4	1001	CYC	CBB-CAB-C3B	-4.71	99.46	112.43
82	aM	202	PEB	C1C-C2C-C3C	-4.70	102.06	107.62
82	ED	202	PEB	C2C-C1C-NC	4.70	113.91	107.57
82	eF	201	PEB	C2C-C1C-NC	4.70	113.91	107.57
82	QD	201	PEB	C1C-C2C-C3C	-4.70	102.06	107.62
82	CI	202	PEB	C1C-C2C-C3C	-4.70	102.06	107.62
82	II	202	PEB	C1C-C2C-C3C	-4.70	102.06	107.62
82	M5	304	PEB	CMB-C2B-C1B	4.70	132.31	125.06
82	YB	202	PEB	C2C-C1C-NC	4.70	113.91	107.57
82	SJ	203	PEB	OA-C1A-C2A	-4.70	122.43	126.17
82	XA	203	PEB	CAC-C2C-C1C	4.70	133.25	125.76
84	GG	1001	CYC	OB-C4B-C3B	-4.70	122.94	128.04
82	EM	203	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	m4	201	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	S7	201	PEB	C1C-C2C-C3C	-4.70	102.06	107.62
85	b6	603	BCR	C7-C8-C9	-4.70	119.13	126.23
82	Z5	304	PEB	CMB-C2B-C1B	4.70	132.31	125.06
82	WJ	201	PEB	CHC-C4C-NC	4.70	127.51	121.15
84	K4	1001	CYC	CMD-C2D-C1D	4.70	132.45	125.56
82	V7	202	PEB	C3C-C4C-NC	4.70	112.56	108.33
82	EP	201	PEB	CMB-C2B-C1B	4.70	132.31	125.06
82	a4	201	PEB	CMB-C2B-C1B	4.70	132.31	125.06
82	XK	202	PEB	CHB-C1C-C2C	-4.70	116.54	127.15
83	Z9	305	PUB	CHA-C1B-NB	4.70	127.51	121.15
82	lG	202	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	hK	202	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	AQ	304	PEB	C1C-CHB-C4B	-4.70	117.74	128.28
82	Z5	305	PEB	C1C-C2C-C3C	-4.70	102.06	107.62
83	M5	303	PUB	CHA-C1B-NB	4.70	127.51	121.15
82	NB	203	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	PB	201	PEB	C2A-C1A-NA	4.70	112.32	108.27
82	PA	202	PEB	C3C-C4C-NC	4.70	112.56	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IK	201	PEB	CAC-CBC-CGC	4.70	123.72	113.60
82	HK	202	PEB	C1C-CHB-C4B	4.70	138.82	128.28
82	CF	201	PEB	C1C-C2C-C3C	-4.70	102.07	107.62
82	PK	202	PEB	C1C-C2C-C3C	-4.70	102.07	107.62
82	ZM	202	PEB	C1C-C2C-C3C	-4.70	102.07	107.62
82	TK	201	PEB	CHC-C4C-NC	4.70	127.51	121.15
82	MK	201	PEB	CMB-C2B-C1B	4.70	132.30	125.06
82	QG	201	PEB	OA-C1A-C2A	-4.70	122.44	126.17
82	ZG	203	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	w8	202	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	lM	202	PEB	C1C-C2C-C3C	-4.70	102.07	107.62
82	UO	201	PEB	CHA-C1B-NB	-4.70	115.11	124.93
82	lJ	203	PEB	C2C-C1C-NC	4.70	113.90	107.57
84	GE	1001	CYC	OB-C4B-C3B	-4.70	122.94	128.04
82	uF	201	PEB	OA-C1A-C2A	-4.70	122.44	126.17
82	EI	202	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	TI	203	PEB	C2C-C1C-NC	4.70	113.90	107.57
82	gB	202	PEB	C2C-C1C-NC	4.70	113.90	107.57
85	B2	802	BCR	C1-C6-C5	-4.70	116.00	122.61
82	P7	202	PEB	C3C-C4C-NC	4.70	112.56	108.33
82	NJ	202	PEB	C2C-C1C-NC	4.70	113.89	107.57
82	X7	202	PEB	C1C-C2C-C3C	-4.70	102.07	107.62
85	BN	803	BCR	C1-C6-C5	-4.70	116.00	122.61
82	CJ	202	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	kE	201	PEB	C1C-C2C-C3C	-4.69	102.07	107.62
82	cH	201	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	KA	202	PEB	C1C-C2C-C3C	-4.69	102.07	107.62
82	LD	202	PEB	C1C-C2C-C3C	-4.69	102.07	107.62
82	hK	201	PEB	C1C-C2C-C3C	-4.69	102.07	107.62
82	PE	202	PEB	OA-C1A-C2A	-4.69	122.44	126.17
84	KO	1001	CYC	CMD-C2D-C1D	4.69	132.43	125.56
87	6N	608	CLA	CHD-C1D-C2D	-4.69	115.64	125.48
82	AI	202	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	mE	202	PEB	CHB-C1C-C2C	-4.69	116.56	127.15
82	a1	201	PEB	C1D-CHC-C4C	-4.69	106.34	113.26
82	U7	201	PEB	CHA-C1B-C2B	4.69	136.97	124.90
82	p8	202	PEB	CHB-C4B-NB	-4.69	114.81	124.58
82	mG	202	PEB	C2C-C1C-NC	4.69	113.89	107.57
85	h6	102	BCR	C11-C10-C9	-4.69	120.61	127.31
82	VM	201	PEB	C1D-CHC-C4C	4.69	120.17	113.26
82	TO	202	PEB	CHB-C1C-C2C	-4.69	116.57	127.15
82	SD	201	PEB	C1C-C2C-C3C	-4.69	102.08	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B7	203	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	eB	202	PEB	OA-C1A-C2A	-4.69	122.44	126.17
82	OJ	202	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	IB	202	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	GI	203	PEB	C2C-C1C-NC	4.69	113.89	107.57
82	AD	303	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	NI	202	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	d4	202	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	ZI	401	PEB	CAA-C3A-C2A	-4.69	102.54	114.26
84	KH	1001	CYC	C2B-C1B-NB	4.69	113.85	106.99
82	IK	201	PEB	C1D-CHC-C4C	-4.69	106.34	113.26
84	IO	1001	CYC	CMD-C2D-C1D	4.69	132.43	125.56
82	kG	201	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	T4	202	PEB	CHB-C1C-C2C	-4.69	116.57	127.15
82	PG	202	PEB	OA-C1A-C2A	-4.69	122.44	126.17
82	BA	203	PEB	C2C-C1C-NC	4.69	113.88	107.57
82	OF	203	PEB	C2C-C1C-NC	4.69	113.88	107.57
82	PK	202	PEB	C1D-CHC-C4C	4.69	120.17	113.26
82	gK	201	PEB	CHB-C1C-C2C	-4.69	116.57	127.15
87	62	309	CLA	CHD-C1D-C2D	-4.69	115.65	125.48
82	TI	203	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	cB	401	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
85	L2	201	BCR	C20-C21-C22	-4.69	120.62	127.31
85	b6	603	BCR	C16-C17-C18	-4.69	120.62	127.31
82	KK	203	PEB	C2C-C1C-NC	4.69	113.88	107.57
82	WP	202	PEB	C2C-C1C-NC	4.69	113.88	107.57
82	eB	201	PEB	C2C-C1C-NC	4.69	113.88	107.57
82	YH	201	PEB	OA-C1A-C2A	-4.69	122.45	126.17
82	qC	201	PEB	OA-C1A-C2A	-4.69	122.45	126.17
82	IF	201	PEB	CAC-CBC-CGC	4.69	123.69	113.60
82	KI	203	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	AO	305	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	NA	202	PEB	CHA-C1B-NB	-4.69	115.13	124.93
82	pC	202	PEB	CHB-C4B-NB	-4.69	114.82	124.58
82	TF	201	PEB	CHC-C4C-NC	4.69	127.49	121.15
82	jO	201	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	HJ	201	PEB	C1D-CHC-C4C	4.69	120.17	113.26
87	A2	802	CLA	CAA-C2A-C3A	-4.69	99.95	112.78
82	R4	202	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
82	O9	203	PEB	C1C-C2C-C3C	-4.69	102.08	107.62
83	AM	303	PUB	C3B-C4B-NB	4.69	113.88	107.57
82	UE	202	PEB	OA-C1A-C2A	-4.68	122.45	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OG	201	PEB	C2C-C1C-NC	4.68	113.88	107.57
82	aM	203	PEB	C2C-C1C-NC	4.68	113.88	107.57
82	f1	202	PEB	C1C-C2C-C3C	-4.68	102.08	107.62
84	K1	1001	CYC	C2B-C1B-NB	4.68	113.85	106.99
87	32	307	CLA	C4A-NA-C1A	4.68	108.81	106.71
82	UE	201	PEB	CHC-C4C-NC	4.68	127.49	121.15
82	zC	202	PEB	CHB-C4B-NB	-4.68	114.83	124.58
92	j6	101	LMG	C9-C8-C7	-4.68	100.71	111.79
82	ND	203	PEB	C1C-C2C-C3C	-4.68	102.08	107.62
82	GI	203	PEB	C1C-C2C-C3C	-4.68	102.08	107.62
84	EE	1001	CYC	CMD-C2D-C1D	4.68	132.42	125.56
82	KF	203	PEB	C2C-C1C-NC	4.68	113.88	107.57
82	X7	203	PEB	CAC-C2C-C1C	4.68	133.22	125.76
82	EI	202	PEB	C1C-C2C-C3C	-4.68	102.08	107.62
82	AJ	302	PEB	C1C-C2C-C3C	-4.68	102.08	107.62
82	W1	201	PEB	C1C-C2C-C3C	-4.68	102.08	107.62
103	82	310	ZEX	C28-C27-C26	4.68	135.09	127.09
85	BL	617	BCR	C36-C18-C19	4.68	125.45	118.08
82	KA	202	PEB	C2C-C1C-NC	4.68	113.88	107.57
82	PD	202	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	XM	202	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	LJ	201	PEB	CMC-C3C-C4C	4.68	132.02	127.06
82	HF	201	PEB	C2A-C1A-NA	4.68	112.31	108.27
82	JQ	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	NQ	203	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	qF	203	PEB	CHB-C1C-C2C	-4.68	116.59	127.15
96	V6	201	HEM	CHC-C4B-NB	4.68	129.50	124.42
82	EP	201	PEB	C2C-C1C-NC	4.68	113.87	107.57
82	VI	202	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	LQ	202	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	M5	305	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	RE	202	PEB	OA-C1A-C2A	-4.68	122.45	126.17
85	B2	840	BCR	C24-C23-C22	-4.68	119.16	126.23
82	lF	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	ED	201	PEB	CMB-C2B-C1B	4.68	132.27	125.06
87	32	302	CLA	CMD-C2D-C3D	-4.68	116.85	127.61
82	LP	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	R7	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	M9	304	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	AI	202	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	KM	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
92	b6	620	LMG	O7-C10-C11	4.68	121.58	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jK	202	PEB	CMB-C2B-C1B	4.68	132.27	125.06
82	XB	202	PEB	OA-C1A-C2A	-4.68	122.45	126.17
82	W1	201	PEB	C2C-C1C-NC	4.68	113.87	107.57
82	RA	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	W9	201	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	lE	201	PEB	C2C-C1C-NC	4.68	113.87	107.57
85	bL	602	BCR	C15-C14-C13	-4.68	120.64	127.31
82	WE	202	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	AQ	303	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	Z9	303	PEB	C1C-C2C-C3C	-4.68	102.09	107.62
82	QJ	203	PEB	CHC-C4C-NC	4.68	127.48	121.15
82	Z1	201	PEB	CHC-C1D-ND	-4.68	107.81	113.72
83	xK	305	PUB	C1C-C2C-C3C	-4.68	101.61	106.78
87	3N	308	CLA	C4A-NA-C1A	4.68	108.81	106.71
82	QG	203	PEB	C1D-CHC-C4C	-4.68	106.36	113.26
82	YK	203	PEB	C2C-C1C-NC	4.67	113.87	107.57
82	aM	201	PEB	C2C-C1C-NC	4.67	113.87	107.57
82	dD	401	PEB	OA-C1A-C2A	-4.67	122.46	126.17
82	c1	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	O9	202	PEB	C4B-C3B-C2B	-4.67	101.61	106.78
85	LN	201	BCR	C20-C21-C22	-4.67	120.64	127.31
82	hF	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	e4	201	PEB	CMB-C2B-C1B	4.67	132.26	125.06
82	WA	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	QA	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	HK	201	PEB	C2A-C1A-NA	4.67	112.30	108.27
82	ZH	203	PEB	CHA-C1B-NB	-4.67	115.16	124.93
87	3N	308	CLA	C2B-C1B-NB	4.67	113.36	110.23
82	PI	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	SJ	201	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	aJ	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	QF	203	PEB	CHB-C1C-NC	4.67	136.02	125.32
82	O9	201	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	hG	203	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	aK	203	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	ZH	201	PEB	CHC-C1D-ND	-4.67	107.81	113.72
82	XM	201	PEB	OA-C1A-C2A	-4.67	122.46	126.17
82	e1	201	PEB	OA-C1A-C2A	-4.67	122.46	126.17
82	fM	201	PEB	OA-C1A-C2A	-4.67	122.46	126.17
102	32	301	BGC	C1-O5-C5	4.67	118.52	112.19
82	UG	201	PEB	CHC-C4C-NC	4.67	127.47	121.15
82	UD	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QQ	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	LA	202	PEB	C1C-CHB-C4B	4.67	138.75	128.28
82	aF	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	gM	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	WE	203	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	mM	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	XK	201	PEB	CHC-C4C-NC	4.67	127.47	121.15
103	8N	310	ZEX	C28-C27-C26	4.67	135.06	127.09
82	NM	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
85	AN	848	BCR	C24-C23-C22	4.67	133.29	126.23
82	PF	201	PEB	OA-C1A-NA	4.67	130.59	124.94
82	wF	303	PEB	CMC-C3C-C4C	4.67	132.01	127.06
82	OA	202	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	QA	201	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	A4	305	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	xK	303	PEB	C1C-C2C-C3C	-4.67	102.10	107.62
82	SF	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	J9	202	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	hK	201	PEB	C2C-C1C-NC	4.67	113.86	107.57
82	cK	201	PEB	CHB-C1C-C2C	-4.67	116.62	127.15
102	3N	302	BGC	C1-O5-C5	4.67	118.51	112.19
82	HJ	201	PEB	C2C-C1C-NC	4.67	113.85	107.57
82	eK	201	PEB	C2C-C1C-NC	4.67	113.85	107.57
82	JM	202	PEB	C1C-C2C-C3C	-4.67	102.11	107.62
82	LO	1002	PEB	C1C-C2C-C3C	-4.67	102.11	107.62
82	bG	201	PEB	CMB-C2B-C1B	4.67	132.25	125.06
84	BE	1001	CYC	C2C-C1C-NC	4.67	112.30	108.27
82	UE	202	PEB	C1C-C2C-C3C	-4.67	102.11	107.62
82	w8	203	PEB	OA-C1A-C2A	-4.66	122.46	126.17
87	AN	801	CLA	CAA-C2A-C3A	-4.66	100.00	112.78
83	BJ	302	PUB	C3B-C4B-NB	4.66	113.85	107.57
82	FB	201	PEB	C1D-CHC-C4C	4.66	120.13	113.26
82	jH	202	PEB	CHB-C4B-NB	-4.66	114.87	124.58
84	EG	1001	CYC	OC-C1C-C2C	-4.66	122.47	126.17
82	VJ	202	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	lF	202	PEB	C2C-C1C-NC	4.66	113.85	107.57
82	UG	202	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	UA	201	PEB	CHA-C1B-C2B	4.66	136.89	124.90
82	GM	202	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	UQ	202	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
85	BN	840	BCR	C24-C23-C22	-4.66	119.19	126.23
82	hJ	201	PEB	C2C-C1C-NC	4.66	113.85	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	zF	501	PEB	C4B-C3B-C2B	-4.66	101.62	106.78
82	FP	202	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	aJ	201	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	fJ	203	PEB	C2C-C1C-NC	4.66	113.85	107.57
82	dJ	201	PEB	CHB-C1C-C2C	-4.66	116.64	127.15
87	32	310	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
82	HI	202	PEB	C1D-CHC-C4C	-4.66	106.38	113.26
82	BD	201	PEB	CHA-C1B-NB	-4.66	115.18	124.93
82	AG	304	PEB	C2C-C1C-NC	4.66	113.85	107.57
82	UQ	202	PEB	C2C-C1C-NC	4.66	113.85	107.57
82	eO	201	PEB	C2C-C1C-NC	4.66	113.85	107.57
82	fM	202	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	B5	203	PEB	CMB-C2B-C1B	4.66	132.24	125.06
87	3N	310	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
83	xF	305	PUB	C1C-C2C-C3C	-4.66	101.62	106.78
82	N7	202	PEB	CHA-C1B-NB	-4.66	115.19	124.93
92	J6	102	LMG	C9-C8-C7	-4.66	100.77	111.79
82	QM	203	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	r8	201	PEB	C2C-C1C-NC	4.66	113.84	107.57
82	GE	1002	PEB	C4B-C3B-C2B	-4.66	101.63	106.78
82	PA	202	PEB	C2A-C1A-NA	4.66	112.29	108.27
82	IB	203	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	AQ	304	PEB	C1C-C2C-C3C	-4.66	102.11	107.62
82	U1	201	PEB	CHC-C1D-ND	-4.66	107.83	113.72
84	EE	1001	CYC	CHD-C1D-ND	-4.66	114.65	125.32
82	DJ	201	PEB	C1C-C2C-C3C	-4.66	102.12	107.62
82	WJ	203	PEB	C1C-C2C-C3C	-4.66	102.12	107.62
85	c6	617	BCR	C38-C26-C25	-4.66	119.30	124.53
84	EG	1001	CYC	CHD-C1D-ND	-4.66	114.65	125.32
82	FD	203	PEB	C2A-C1A-NA	4.66	112.29	108.27
82	dM	201	PEB	CHC-C1D-ND	-4.66	107.83	113.72
82	RQ	201	PEB	CHC-C4C-NC	4.66	127.45	121.15
82	ZG	202	PEB	CHA-C1B-NB	-4.66	115.19	124.93
82	EQ	202	PEB	OA-C1A-C2A	-4.66	122.47	126.17
82	LM	201	PEB	C1C-C2C-C3C	-4.66	102.12	107.62
82	AG	301	PEB	C2C-C1C-NC	4.66	113.84	107.57
82	JJ	202	PEB	C2C-C1C-NC	4.66	113.84	107.57
82	LI	201	PEB	CHC-C1D-ND	-4.66	107.83	113.72
84	BG	1002	CYC	C1B-C2B-C3B	-4.66	103.01	107.87
82	c1	202	PEB	OA-C1A-C2A	-4.65	122.47	126.17
87	3N	303	CLA	CMD-C2D-C3D	-4.65	116.91	127.61
82	O4	202	PEB	C1C-C2C-C3C	-4.65	102.12	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	L7	202	PEB	C1C-CHB-C4B	4.65	138.72	128.28
82	RD	201	PEB	CHC-C4C-NC	4.65	127.45	121.15
82	BQ	201	PEB	CHA-C1B-NB	-4.65	115.20	124.93
82	kF	203	PEB	C1C-CHB-C4B	4.65	138.72	128.28
82	kH	202	PEB	OA-C1A-C2A	-4.65	122.47	126.17
82	N4	1002	PEB	C2C-C1C-NC	4.65	113.84	107.57
82	DP	202	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
87	8N	301	CLA	C4A-NA-C1A	4.65	108.80	106.71
82	HG	1002	PEB	CHC-C4C-NC	4.65	127.45	121.15
82	GP	202	PEB	CMB-C2B-C1B	4.65	132.23	125.06
82	EF	202	PEB	C2C-C1C-NC	4.65	113.84	107.57
82	JK	202	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
83	Z5	302	PUB	CHB-C1C-C2C	-4.65	114.56	125.32
82	ZE	203	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
82	XJ	202	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
82	JK	202	PEB	C2C-C1C-NC	4.65	113.83	107.57
84	I4	1001	CYC	C3D-C4D-ND	4.65	113.83	107.57
83	M5	302	PUB	CHB-C1C-C2C	-4.65	114.56	125.32
82	CM	202	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
83	A1	303	PUB	C4B-C3B-C2B	-4.65	102.12	107.62
82	ZE	202	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	DP	202	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	jJ	203	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	j1	202	PEB	CHB-C4B-NB	-4.65	114.90	124.58
82	YM	202	PEB	CHC-C4C-NC	4.65	127.44	121.15
87	4N	605	CLA	C2A-C1A-CHA	4.65	131.99	123.86
82	OO	202	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
82	fK	201	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
82	t8	202	PEB	CHA-C1B-NB	-4.65	115.21	124.93
82	kJ	202	PEB	C2C-C1C-NC	4.65	113.83	107.57
84	M4	1001	CYC	C3D-C4D-ND	4.65	113.83	107.57
82	VH	201	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
82	Q9	203	PEB	C1C-C2C-C3C	-4.65	102.12	107.62
82	gG	202	PEB	C1C-CHB-C4B	-4.65	117.86	128.28
82	BB	203	PEB	OA-C1A-C2A	-4.65	122.48	126.17
82	GJ	202	PEB	OA-C1A-C2A	-4.65	122.48	126.17
82	V1	203	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	bK	201	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	S5	203	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	Q7	201	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	QE	203	PEB	C1D-CHC-C4C	-4.65	106.40	113.26
82	q8	203	PEB	OA-C1A-C2A	-4.65	122.48	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HB	202	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	CK	201	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	SH	201	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	aM	202	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	aM	204	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	L4	1002	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	Q7	202	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	fJ	202	PEB	C1C-C2C-C3C	-4.65	102.13	107.62
82	SB	203	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	GM	201	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	RP	202	PEB	C2C-C1C-NC	4.65	113.83	107.57
82	a1	202	PEB	C1C-C2C-C3C	-4.64	102.13	107.62
82	KA	201	PEB	C1C-CHB-C4B	4.64	138.70	128.28
82	OJ	202	PEB	CAC-C2C-C1C	4.64	133.16	125.76
82	FD	203	PEB	OA-C1A-C2A	-4.64	122.48	126.17
82	OJ	203	PEB	C1C-C2C-C3C	-4.64	102.13	107.62
95	C6	502	DGD	O2E-C2E-C3E	-4.64	99.62	110.35
82	VF	202	PEB	CMB-C2B-C1B	4.64	132.21	125.06
82	aF	203	PEB	C2C-C1C-NC	4.64	113.82	107.57
82	RE	201	PEB	OA-C1A-C2A	-4.64	122.48	126.17
82	aO	201	PEB	CHC-C1D-ND	-4.64	107.85	113.72
84	EG	1001	CYC	CMD-C2D-C1D	4.64	132.36	125.56
95	c6	601	DGD	O2E-C2E-C3E	-4.64	99.62	110.35
82	uC	201	PEB	C2C-C1C-NC	4.64	113.82	107.57
82	WE	201	PEB	C1C-C2C-C3C	-4.64	102.13	107.62
82	EF	201	PEB	C1C-C2C-C3C	-4.64	102.13	107.62
82	ZE	202	PEB	CHA-C1B-NB	-4.64	115.22	124.93
82	XP	202	PEB	CHA-C1B-NB	-4.64	115.22	124.93
82	K7	201	PEB	C1C-CHB-C4B	4.64	138.69	128.28
82	R4	202	PEB	CHB-C1C-C2C	-4.64	116.68	127.15
82	ZH	202	PEB	C2C-C1C-NC	4.64	113.82	107.57
82	gF	202	PEB	C2C-C1C-NC	4.64	113.82	107.57
82	U5	202	PEB	C1C-C2C-C3C	-4.64	102.14	107.62
82	YE	202	PEB	CHC-C4C-NC	4.64	127.43	121.15
82	MQ	202	PEB	C1C-C2C-C3C	-4.64	102.14	107.62
82	GG	1002	PEB	C4B-C3B-C2B	-4.64	101.65	106.78
82	QB	202	PEB	C2C-C1C-NC	4.64	113.82	107.57
82	JD	201	PEB	C2C-C1C-NC	4.64	113.82	107.57
82	bE	201	PEB	CMB-C2B-C1B	4.64	132.21	125.06
94	D6	408	PL9	C7-C3-C2	-4.64	117.20	123.30
82	H9	202	PEB	C4B-C3B-C2B	-4.64	101.65	106.78
82	QB	202	PEB	OA-C1A-C2A	-4.64	122.48	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RO	202	PEB	CHB-C1C-C2C	-4.64	116.69	127.15
82	UH	201	PEB	CHC-C1D-ND	-4.64	107.86	113.72
82	q8	203	PEB	C1C-C2C-C3C	-4.64	102.14	107.62
82	fJ	201	PEB	C2C-C1C-NC	4.64	113.81	107.57
82	WM	203	PEB	CHB-C1C-C2C	-4.64	116.69	127.15
82	NJ	201	PEB	C1C-CHB-C4B	-4.64	117.88	128.28
82	WM	201	PEB	C1C-C2C-C3C	-4.64	102.14	107.62
82	RB	202	PEB	C2C-C1C-NC	4.64	113.81	107.57
82	Y5	203	PEB	C2C-C1C-NC	4.64	113.81	107.57
82	WE	202	PEB	OA-C1A-C2A	-4.64	122.49	126.17
82	PJ	201	PEB	OA-C1A-C2A	-4.64	122.49	126.17
82	oF	202	PEB	C1C-C2C-C3C	-4.64	102.14	107.62
82	JA	202	PEB	C2C-C1C-NC	4.63	113.81	107.57
85	FL	101	BCR	C1-C6-C5	-4.63	116.08	122.61
82	dO	202	PEB	C1C-C2C-C3C	-4.63	102.14	107.62
82	cF	201	PEB	CHB-C1C-C2C	-4.63	116.69	127.15
82	GE	1002	PEB	OA-C1A-C2A	-4.63	122.49	126.17
82	ZM	201	PEB	OA-C1A-C2A	-4.63	122.49	126.17
84	HE	1001	CYC	OC-C1C-C2C	-4.63	122.49	126.17
82	VI	203	PEB	OD-C4D-ND	-4.63	119.06	125.93
82	BI	201	PEB	C3B-C4B-NB	4.63	116.79	110.05
82	IM	203	PEB	C2C-C1C-NC	4.63	113.81	107.57
82	RQ	201	PEB	OA-C1A-C2A	-4.63	122.49	126.17
82	Y1	202	PEB	C2C-C1C-NC	4.63	113.81	107.57
82	aJ	201	PEB	OA-C1A-C2A	-4.63	122.49	126.17
85	c6	603	BCR	C34-C9-C8	4.63	125.38	118.08
82	wF	301	PEB	C2C-C1C-NC	4.63	113.81	107.57
82	eJ	202	PEB	C2C-C1C-NC	4.63	113.81	107.57
84	FE	1002	CYC	C2B-C1B-NB	4.63	113.77	106.99
82	CP	202	PEB	C2C-C1C-NC	4.63	113.81	107.57
84	DG	1001	CYC	C1B-NB-C4B	-4.63	104.77	110.67
82	qC	203	PEB	OA-C1A-C2A	-4.63	122.49	126.17
82	zK	501	PEB	C4B-C3B-C2B	-4.63	101.66	106.78
82	xF	303	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	jK	202	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	PJ	202	PEB	C2C-C1C-NC	4.63	113.81	107.57
82	m4	203	PEB	C4B-C3B-C2B	-4.63	101.66	106.78
82	ZG	202	PEB	C2C-C1C-NC	4.63	113.81	107.57
84	IO	1001	CYC	C3D-C4D-ND	4.63	113.81	107.57
82	EA	202	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	RO	202	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	wK	303	PEB	CMC-C3C-C4C	4.63	131.97	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ZM	201	PEB	CHA-C1B-NB	-4.63	115.25	124.93
82	E7	202	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	uF	202	PEB	CMB-C2B-C1B	4.63	132.19	125.06
82	AP	203	PEB	CHC-C1D-ND	-4.63	107.87	113.72
82	FB	201	PEB	OA-C1A-C2A	-4.63	122.49	126.17
82	NO	1002	PEB	OA-C1A-C2A	-4.63	122.49	126.17
82	WG	201	PEB	C2C-C1C-NC	4.63	113.80	107.57
82	ZG	203	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	qC	203	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	z8	201	PEB	CHB-C4B-C3B	-4.63	114.61	125.32
84	E1	1001	CYC	CAB-C3B-C4B	4.63	128.69	121.38
82	OQ	201	PEB	C2C-C1C-NC	4.63	113.80	107.57
82	q8	201	PEB	OA-C1A-C2A	-4.63	122.49	126.17
82	dF	202	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	mO	203	PEB	C4B-C3B-C2B	-4.63	101.66	106.78
82	I7	202	PEB	C2C-C1C-NC	4.63	113.80	107.57
82	sC	202	PEB	C2C-C1C-NC	4.63	113.80	107.57
82	eO	202	PEB	CHB-C1C-C2C	-4.63	116.71	127.15
82	KE	201	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	R1	201	PEB	C2C-C1C-NC	4.63	113.80	107.57
84	L1	1001	CYC	OC-C1C-C2C	-4.63	122.50	126.17
82	jF	202	PEB	C1C-C2C-C3C	-4.63	102.15	107.62
82	u8	201	PEB	C2C-C1C-NC	4.63	113.80	107.57
82	CK	202	PEB	C4B-C3B-C2B	-4.63	101.66	106.78
82	DI	201	PEB	OA-C1A-C2A	-4.62	122.50	126.17
82	VP	202	PEB	C1C-C2C-C3C	-4.62	102.15	107.62
87	42	605	CLA	C2A-C1A-CHA	4.62	131.94	123.86
82	DE	1002	PEB	CHC-C4C-NC	4.62	127.41	121.15
82	UF	202	PEB	CHA-C1B-NB	-4.62	115.26	124.93
85	Z6	101	BCR	C7-C8-C9	-4.62	119.25	126.23
82	EJ	203	PEB	C2C-C1C-NC	4.62	113.80	107.57
82	K5	202	PEB	C2C-C1C-NC	4.62	113.80	107.57
82	mJ	202	PEB	C2C-C1C-NC	4.62	113.80	107.57
82	AM	302	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	PM	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	WF	201	PEB	CHB-C1C-C2C	-4.62	116.72	127.15
84	MG	1001	CYC	CAB-C3B-C4B	4.62	128.68	121.38
82	PA	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	F5	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	L7	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	J9	203	PEB	C2C-C1C-NC	4.62	113.80	107.57
82	gK	203	PEB	CMB-C2B-C1B	4.62	132.18	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
96	FL	102	HEM	CHD-C1D-ND	4.62	129.44	124.42
84	ME	1001	CYC	CAB-C3B-C4B	4.62	128.68	121.38
82	HE	1002	PEB	CHC-C4C-NC	4.62	127.41	121.15
82	lK	203	PEB	OA-C1A-C2A	-4.62	122.50	126.17
82	j4	201	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	fM	201	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
84	FO	1001	CYC	C1B-C2B-C3B	-4.62	103.05	107.87
82	O4	201	PEB	C3B-C4B-NB	4.62	116.77	110.05
82	B5	201	PEB	C4B-C3B-C2B	-4.62	101.67	106.78
84	DG	1001	CYC	C3D-C4D-ND	4.62	113.79	107.57
82	gE	202	PEB	C1C-CHB-C4B	-4.62	117.92	128.28
96	v6	201	HEM	CHC-C4B-NB	4.62	129.44	124.42
82	ZK	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	Y5	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	ND	204	PEB	C2C-C1C-NC	4.62	113.79	107.57
83	yK	302	PUB	CHC-C1D-ND	-4.62	107.88	113.72
82	T7	202	PEB	C4B-C3B-C2B	-4.62	101.67	106.78
82	KJ	201	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	RM	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	GJ	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
82	vF	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	IP	201	PEB	CHC-C4C-NC	4.62	127.40	121.15
82	dJ	202	PEB	CAC-C2C-C1C	4.62	133.12	125.76
82	QK	203	PEB	CHB-C1C-NC	4.62	135.90	125.32
82	QJ	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
85	BN	803	BCR	C36-C18-C19	4.62	125.35	118.08
82	PK	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	SK	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	NQ	204	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	aE	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	e4	202	PEB	CHB-C1C-C2C	-4.62	116.73	127.15
92	A6	408	LMG	O7-C10-C11	4.62	121.45	111.50
82	jF	201	PEB	CHA-C1B-NB	-4.62	115.27	124.93
82	J7	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	aK	201	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	WG	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	TI	201	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	P7	203	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
87	82	306	CLA	C4A-NA-C1A	4.62	108.78	106.71
82	XM	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
84	NO	1001	CYC	C3D-C4D-ND	4.62	113.79	107.57
84	BE	1002	CYC	C1B-C2B-C3B	-4.62	103.05	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PF	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	TK	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	P1	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
82	XF	201	PEB	CHC-C4C-NC	4.62	127.40	121.15
82	P7	202	PEB	C2A-C1A-NA	4.62	112.25	108.27
82	AE	301	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	rF	202	PEB	C2C-C1C-NC	4.62	113.79	107.57
82	QD	202	PEB	C1C-C2C-C3C	-4.62	102.16	107.62
84	L1	1001	CYC	C4D-CHA-C1A	4.62	138.63	128.28
82	cG	201	PEB	OA-C1A-C2A	-4.62	122.50	126.17
82	zC	201	PEB	CHB-C4B-C3B	-4.62	114.64	125.32
82	IF	201	PEB	C1D-CHC-C4C	-4.62	106.45	113.26
82	H1	1002	PEB	C1D-CHC-C4C	4.62	120.06	113.26
82	F9	203	PEB	CHA-C1B-NB	-4.62	115.28	124.93
82	fH	202	PEB	C1C-C2C-C3C	-4.62	102.17	107.62
82	VH	202	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	O9	203	PEB	OA-C1A-C2A	-4.61	122.50	126.17
84	EH	1001	CYC	CAB-C3B-C4B	4.61	128.67	121.38
84	CG	1001	CYC	C2D-C1D-ND	4.61	113.89	107.40
85	B2	802	BCR	C36-C18-C19	4.61	125.35	118.08
82	MD	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	TF	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	kK	203	PEB	C1C-CHB-C4B	4.61	138.63	128.28
82	FM	201	PEB	C3D-C4D-ND	4.61	116.31	107.26
82	IP	201	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	oF	201	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	aK	201	PEB	CHA-C1B-NB	-4.61	115.28	124.93
85	B6	621	BCR	C11-C10-C9	-4.61	120.73	127.31
82	SJ	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	P1	201	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	M7	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	D9	202	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	Y5	202	PEB	CHB-C1C-C2C	-4.61	116.75	127.15
84	FG	1001	CYC	C2B-C1B-NB	4.61	113.74	106.99
82	IA	202	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	DG	1002	PEB	CHC-C4C-NC	4.61	127.39	121.15
82	A7	201	PEB	CHC-C4C-NC	4.61	127.39	121.15
82	a1	202	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	hE	203	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	gO	202	PEB	CHB-C1C-C2C	-4.61	116.75	127.15
82	gF	203	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
87	32	307	CLA	C2B-C1B-NB	4.61	113.32	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DB	202	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	OE	201	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	tC	202	PEB	CHA-C1B-NB	-4.61	115.29	124.93
82	V1	203	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
82	R7	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
84	L4	1001	CYC	OC-C1C-C2C	-4.61	122.51	126.17
82	UD	202	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	UJ	203	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	NO	1002	PEB	C2C-C1C-NC	4.61	113.78	107.57
82	t8	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
84	MO	1001	CYC	OB-C4B-C3B	-4.61	123.04	128.04
82	F9	202	PEB	CHB-C1C-C2C	-4.61	116.76	127.15
82	UM	202	PEB	C1C-C2C-C3C	-4.61	102.17	107.62
85	J2	103	BCR	C33-C5-C6	-4.61	119.36	124.53
82	EB	501	PEB	C2C-C1C-NC	4.61	113.77	107.57
82	RE	201	PEB	C2C-C1C-NC	4.61	113.77	107.57
82	TJ	201	PEB	C2C-C1C-NC	4.61	113.77	107.57
82	U5	203	PEB	C2C-C1C-NC	4.61	113.77	107.57
82	NB	202	PEB	CHC-C4C-NC	4.61	127.38	121.15
82	aJ	204	PEB	CHA-C1B-NB	-4.61	115.30	124.93
82	Q1	203	PEB	C2C-C1C-NC	4.61	113.77	107.57
84	M4	1001	CYC	OB-C4B-C3B	-4.60	123.04	128.04
82	AE	304	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	WE	201	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	oK	201	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	E7	202	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	dK	201	PEB	CHC-C4C-NC	4.60	127.38	121.15
82	QM	204	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	JP	201	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	gK	203	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	iJ	202	PEB	OA-C1A-C2A	-4.60	122.51	126.17
82	IB	201	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	mE	202	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	OP	202	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	WK	201	PEB	CHB-C1C-C2C	-4.60	116.77	127.15
82	aG	202	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	tC	202	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	MA	202	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	KD	202	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	EM	203	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	HE	1002	PEB	C4B-C3B-C2B	-4.60	101.69	106.78
82	qC	203	PEB	C2C-C1C-NC	4.60	113.77	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	L2	204	CLA	C3C-C4C-NC	-4.60	105.41	110.57
82	N1	1002	PEB	C1C-C2C-C3C	-4.60	102.18	107.62
82	N5	202	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	aK	202	PEB	C2C-C1C-NC	4.60	113.77	107.57
82	jK	201	PEB	CHA-C1B-NB	-4.60	115.31	124.93
82	AO	305	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	AP	201	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	vK	202	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	cJ	202	PEB	C1C-C2C-C3C	-4.60	102.19	107.62
83	AG	303	PUB	C4B-C3B-C2B	-4.60	102.19	107.62
82	JQ	201	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	jM	202	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	QP	201	PEB	C1C-C2C-C3C	-4.60	102.19	107.62
82	mK	202	PEB	C1C-C2C-C3C	-4.60	102.19	107.62
82	dM	203	PEB	CHC-C4C-NC	4.60	127.37	121.15
82	TG	201	PEB	OA-C1A-C2A	-4.60	122.52	126.17
82	lM	202	PEB	OA-C1A-C2A	-4.60	122.52	126.17
82	VM	202	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	Z1	202	PEB	C2C-C1C-NC	4.60	113.76	107.57
82	lK	201	PEB	C2A-C1A-NA	4.60	112.23	108.27
82	HJ	201	PEB	OA-C1A-C2A	-4.60	122.52	126.17
82	lJ	201	PEB	OA-C1A-C2A	-4.60	122.52	126.17
82	V5	202	PEB	C2C-C1C-NC	4.59	113.76	107.57
84	D1	1001	CYC	CMD-C2D-C1D	4.59	132.29	125.56
82	aM	202	PEB	OA-C1A-C2A	-4.59	122.52	126.17
82	FD	203	PEB	CMC-C3C-C4C	4.59	131.93	127.06
82	m1	202	PEB	C1C-C2C-C3C	-4.59	102.19	107.62
84	LH	1002	CYC	C4D-CHA-C1A	4.59	138.58	128.28
85	C6	507	BCR	C11-C10-C9	-4.59	120.75	127.31
82	OE	203	PEB	CHC-C4C-NC	4.59	127.37	121.15
82	RO	203	PEB	CHC-C4C-NC	4.59	127.37	121.15
82	aG	201	PEB	C2C-C1C-NC	4.59	113.76	107.57
82	R4	203	PEB	CHC-C4C-NC	4.59	127.36	121.15
82	RJ	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	aF	201	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	lK	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	cK	201	PEB	CHC-C4C-NC	4.59	127.36	121.15
82	X5	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	rC	201	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	gK	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
83	AE	303	PUB	C4B-C3B-C2B	-4.59	102.19	107.62
82	JQ	202	PEB	C2C-C1C-NC	4.59	113.75	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	wK	301	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	TA	201	PEB	OA-C1A-C2A	-4.59	122.52	126.17
82	VK	201	PEB	CHC-C4C-NC	4.59	127.36	121.15
82	UF	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	PQ	201	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	UO	201	PEB	C3D-C4D-ND	4.59	116.26	107.26
82	CQ	201	PEB	CMB-C2B-C1B	4.59	132.13	125.06
82	EA	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	RD	201	PEB	OA-C1A-C2A	-4.59	122.52	126.17
82	BD	201	PEB	C1C-C2C-C3C	-4.59	102.20	107.62
82	KG	201	PEB	C1C-C2C-C3C	-4.59	102.20	107.62
82	cM	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
84	D4	1001	CYC	CAB-C3B-C4B	4.59	128.63	121.38
82	QF	202	PEB	CHC-C4C-NC	4.59	127.36	121.15
84	N4	1001	CYC	CMD-C2D-C1D	4.59	132.28	125.56
82	YJ	201	PEB	CHB-C1C-C2C	-4.59	116.80	127.15
85	IN	101	BCR	C27-C26-C25	-4.59	116.07	122.73
82	f4	202	PEB	C1C-C2C-C3C	-4.59	102.20	107.62
84	x3	1001	CYC	C3D-C4D-ND	4.59	113.75	107.57
82	O7	201	PEB	C3D-C4D-ND	4.59	116.26	107.26
82	T1	201	PEB	C1C-C2C-C3C	-4.59	102.20	107.62
82	oK	202	PEB	C1C-C2C-C3C	-4.59	102.20	107.62
82	WI	201	PEB	OA-C1A-C2A	-4.59	122.53	126.17
82	SO	201	PEB	C3B-C4B-NB	4.59	116.72	110.05
82	OQ	202	PEB	C2C-C1C-NC	4.59	113.75	107.57
82	eF	202	PEB	C4B-C3B-C2B	-4.58	101.71	106.78
82	A4	305	PEB	C2C-C1C-NC	4.58	113.74	107.57
84	V3	1001	CYC	C3D-C4D-ND	4.58	113.74	107.57
82	fF	201	PEB	C1C-C2C-C3C	-4.58	102.20	107.62
82	cJ	202	PEB	C2C-C1C-NC	4.58	113.74	107.57
82	SB	201	PEB	C1C-C2C-C3C	-4.58	102.20	107.62
85	FL	101	BCR	C36-C18-C19	4.58	125.30	118.08
82	UK	202	PEB	CHA-C1B-NB	-4.58	115.35	124.93
84	NO	1001	CYC	CMD-C2D-C1D	4.58	132.27	125.56
82	PF	202	PEB	C2C-C1C-NC	4.58	113.74	107.57
82	NH	1002	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	VH	202	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	AM	302	PEB	C2C-C1C-NC	4.58	113.74	107.57
82	G5	202	PEB	C2C-C1C-NC	4.58	113.74	107.57
82	AH	301	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	XQ	203	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
84	FE	1001	CYC	C2D-C1D-ND	4.58	113.84	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LF	202	PEB	CHB-C1C-NC	-4.58	114.83	125.32
82	YH	202	PEB	C2C-C1C-NC	4.58	113.74	107.57
85	BN	803	BCR	C16-C15-C14	-4.58	114.10	123.47
82	gJ	202	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
83	A4	302	PUB	CHA-C1B-NB	4.58	127.34	121.15
82	Y5	201	PEB	C2C-C1C-NC	4.58	113.73	107.57
82	eK	202	PEB	C4B-C3B-C2B	-4.58	101.72	106.78
82	MK	201	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	L5	201	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	g4	202	PEB	CHB-C1C-C2C	-4.58	116.82	127.15
82	LP	202	PEB	C2C-C1C-NC	4.58	113.73	107.57
82	S1	201	PEB	C2C-C1C-NC	4.58	113.73	107.57
82	bF	201	PEB	C2C-C1C-NC	4.58	113.73	107.57
84	DH	1003	CYC	C2B-C1B-NB	4.58	113.69	106.99
82	YP	501	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	IM	203	PEB	CHC-C4C-NC	4.58	127.34	121.15
82	z8	202	PEB	CHA-C4A-NA	-4.58	119.76	125.20
82	e4	201	PEB	C2C-C1C-NC	4.58	113.73	107.57
82	fE	203	PEB	C2C-C1C-NC	4.58	113.73	107.57
85	B2	802	BCR	C16-C15-C14	-4.58	114.10	123.47
82	gB	202	PEB	C1C-C2C-C3C	-4.58	102.21	107.62
82	DF	203	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	QH	203	PEB	C2C-C1C-NC	4.57	113.73	107.57
83	AJ	304	PUB	C3B-C4B-NB	4.57	113.73	107.57
82	OF	202	PEB	C1C-C2C-C3C	-4.57	102.21	107.62
82	W7	201	PEB	C1C-C2C-C3C	-4.57	102.21	107.62
82	iM	201	PEB	CMC-C3C-C4C	4.57	131.91	127.06
82	N4	1002	PEB	OA-C1A-C2A	-4.57	122.54	126.17
82	aH	202	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	D7	202	PEB	C2A-C1A-NA	4.57	112.22	108.27
92	mL	101	LMG	O1-C1-C2	4.57	115.44	108.30
82	HP	202	PEB	C1C-C2C-C3C	-4.57	102.21	107.62
82	H4	1002	PEB	C1C-C2C-C3C	-4.57	102.21	107.62
82	T9	201	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	T7	201	PEB	OA-C1A-C2A	-4.57	122.54	126.17
82	PQ	202	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
84	E4	1001	CYC	CMD-C2D-C1D	4.57	132.26	125.56
82	q8	203	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	HO	1002	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	V1	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	s8	202	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	xC	202	PEB	CHB-C1C-C2C	4.57	137.46	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	LN	204	CLA	C3C-C4C-NC	-4.57	105.44	110.57
82	gF	203	PEB	CMB-C2B-C1B	4.57	132.10	125.06
82	U5	203	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	P7	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
85	JN	103	BCR	C33-C5-C6	-4.57	119.39	124.53
82	OD	202	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	BP	202	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	aE	201	PEB	C2C-C1C-NC	4.57	113.73	107.57
82	L7	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
82	KD	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	PK	201	PEB	OA-C1A-NA	4.57	130.48	124.94
82	i1	202	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	vC	202	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	KK	201	PEB	CHC-C1D-ND	-4.57	107.94	113.72
82	gF	201	PEB	CHA-C1B-NB	-4.57	115.37	124.93
82	SA	201	PEB	CHA-C1B-C2B	4.57	136.65	124.90
82	SK	203	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	YM	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	G9	201	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	K9	201	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	V9	201	PEB	C2C-C1C-NC	4.57	113.72	107.57
83	AG	303	PUB	C3B-C4B-NB	4.57	113.72	107.57
82	DA	202	PEB	C2A-C1A-NA	4.57	112.21	108.27
82	DG	1002	PEB	C4B-C3B-C2B	-4.57	101.72	106.78
82	iH	202	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	IM	201	PEB	CHB-C1C-C2C	-4.57	116.84	127.15
82	PD	201	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	LK	202	PEB	CHB-C1C-NC	-4.57	114.86	125.32
85	I2	101	BCR	C27-C26-C25	-4.57	116.10	122.73
82	LA	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
82	AP	202	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	TH	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	eJ	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	SJ	202	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	MM	203	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	EQ	201	PEB	C2C-C1C-NC	4.57	113.72	107.57
82	uK	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
82	MD	201	PEB	CAC-C2C-C1C	4.57	133.03	125.76
82	HJ	201	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
84	73	1002	CYC	CHD-C4C-NC	4.57	130.63	125.20
82	x8	202	PEB	CHB-C1C-C2C	4.57	137.45	127.15
82	KM	201	PEB	C2C-C1C-NC	4.57	113.72	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	N4	1001	CYC	C3D-C4D-ND	4.57	113.72	107.57
85	AL	401	BCR	C16-C17-C18	-4.57	120.79	127.31
84	LO	1001	CYC	OC-C1C-C2C	-4.57	122.54	126.17
82	S7	201	PEB	CHA-C1B-C2B	4.57	136.64	124.90
82	Y5	202	PEB	C1C-C2C-C3C	-4.57	102.22	107.62
82	iM	201	PEB	CHA-C1B-NB	-4.57	115.38	124.93
82	OK	201	PEB	C2C-C1C-NC	4.56	113.72	107.57
82	OA	201	PEB	C3D-C4D-ND	4.56	116.22	107.26
82	LA	203	PEB	C1C-C2C-C3C	-4.56	102.22	107.62
82	SE	202	PEB	C1C-C2C-C3C	-4.56	102.22	107.62
82	GE	1002	PEB	C2C-C1C-NC	4.56	113.72	107.57
82	IQ	202	PEB	CHC-C1D-ND	-4.56	107.95	113.72
84	HG	1001	CYC	C2B-C1B-NB	4.56	113.67	106.99
82	SG	203	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	DJ	202	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	OM	201	PEB	C2C-C1C-NC	4.56	113.72	107.57
82	lK	201	PEB	CHC-C4C-NC	4.56	127.33	121.15
82	AH	301	PEB	OA-C1A-C2A	-4.56	122.55	126.17
82	dM	202	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	eO	201	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	P5	202	PEB	C2C-C1C-NC	4.56	113.72	107.57
82	gB	201	PEB	C2C-C1C-NC	4.56	113.72	107.57
84	DE	1001	CYC	C3D-C4D-ND	4.56	113.72	107.57
84	DO	1001	CYC	CAB-C3B-C4B	4.56	128.58	121.38
82	OP	203	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	gK	201	PEB	CHA-C1B-NB	-4.56	115.39	124.93
87	3N	304	CLA	CMB-C2B-C3B	4.56	137.64	126.59
84	J1	1001	CYC	CAB-C3B-C4B	4.56	128.58	121.38
82	IB	203	PEB	C2C-C1C-NC	4.56	113.71	107.57
82	JD	202	PEB	C2C-C1C-NC	4.56	113.71	107.57
82	XP	201	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	A5	202	PEB	C2C-C1C-NC	4.56	113.71	107.57
82	eG	202	PEB	C2C-C1C-NC	4.56	113.71	107.57
85	KN	104	BCR	C8-C7-C6	4.56	140.01	127.20
82	cH	202	PEB	OA-C1A-C2A	-4.56	122.55	126.17
82	YB	202	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	HP	201	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	l1	201	PEB	CHC-C4C-NC	4.56	127.32	121.15
84	HG	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
82	RA	201	PEB	C2C-C1C-NC	4.56	113.71	107.57
84	x3	1001	CYC	CAB-C3B-C4B	4.56	128.58	121.38
82	mG	201	PEB	C1C-C2C-C3C	-4.56	102.23	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eH	201	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	GB	201	PEB	OA-C1A-C2A	-4.56	122.55	126.17
82	AD	304	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	OK	202	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	KQ	202	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	GG	1002	PEB	C2C-C1C-NC	4.56	113.71	107.57
82	gF	203	PEB	CHC-C1D-ND	-4.56	107.96	113.72
82	SB	202	PEB	CHC-C4C-NC	4.56	127.32	121.15
82	BA	203	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	UA	201	PEB	C1C-C2C-C3C	-4.56	102.23	107.62
82	w8	204	PEB	C2C-C1C-NC	4.56	113.71	107.57
82	wC	204	PEB	C2C-C1C-NC	4.56	113.71	107.57
82	GK	203	PEB	OA-C1A-C2A	-4.56	122.55	126.17
82	NB	201	PEB	CMB-C2B-C1B	4.56	132.08	125.06
83	yK	302	PUB	CMD-C2D-C3D	4.56	134.61	127.77
85	FL	101	BCR	C4-C5-C6	-4.56	116.12	122.73
82	I5	202	PEB	C2C-C1C-NC	4.56	113.71	107.57
84	LH	1001	CYC	CMA-C3A-C4A	4.56	132.08	125.06
82	TM	201	PEB	CMC-C3C-C4C	4.56	131.89	127.06
84	DH	1001	CYC	CMD-C2D-C1D	4.56	132.23	125.56
84	EO	1001	CYC	CMD-C2D-C1D	4.56	132.23	125.56
82	eH	201	PEB	OA-C1A-C2A	-4.56	122.55	126.17
82	I7	201	PEB	C1C-C2C-C3C	-4.56	102.24	107.62
82	kM	202	PEB	C1C-C2C-C3C	-4.56	102.24	107.62
82	fO	202	PEB	C1C-C2C-C3C	-4.56	102.24	107.62
84	V3	1001	CYC	CAB-C3B-C4B	4.55	128.57	121.38
82	MQ	201	PEB	CAC-C2C-C1C	4.55	133.02	125.76
82	jM	203	PEB	C2C-C1C-NC	4.55	113.70	107.57
84	E4	1001	CYC	C3D-C4D-ND	4.55	113.70	107.57
82	XD	203	PEB	C1C-C2C-C3C	-4.55	102.24	107.62
82	YM	202	PEB	CHA-C1B-NB	-4.55	115.41	124.93
82	W5	203	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	R9	201	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	uK	201	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	ID	202	PEB	CHC-C1D-ND	-4.55	107.97	113.72
82	AA	201	PEB	CHC-C4C-NC	4.55	127.31	121.15
87	32	303	CLA	CMB-C2B-C3B	4.55	137.61	126.59
94	d6	408	PL9	C22-C23-C24	-4.55	116.70	127.66
82	GK	201	PEB	C3D-C4D-ND	4.55	116.19	107.26
85	J2	102	BCR	C15-C14-C13	-4.55	120.81	127.31
82	M5	304	PEB	C1C-C2C-C3C	-4.55	102.24	107.62
82	QJ	203	PEB	C2C-C1C-NC	4.55	113.70	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	I9	201	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	P9	201	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	bP	502	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	W1	203	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	C5	202	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	E5	202	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	R5	202	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	S5	203	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	T5	202	PEB	C2C-C1C-NC	4.55	113.70	107.57
82	NI	203	PEB	C3C-C4C-NC	4.55	112.43	108.33
82	hK	202	PEB	C1C-C2C-C3C	-4.55	102.24	107.62
82	A9	201	PEB	C2C-C1C-NC	4.55	113.70	107.57
84	HE	1001	CYC	C2B-C1B-NB	4.55	113.65	106.99
82	DP	201	PEB	C1C-C2C-C3C	-4.55	102.24	107.62
82	XP	202	PEB	C1C-C2C-C3C	-4.55	102.24	107.62
82	Z5	304	PEB	C1C-C2C-C3C	-4.55	102.24	107.62
82	u8	203	PEB	OA-C1A-C2A	-4.55	122.56	126.17
84	HO	1001	CYC	CHB-C4A-NA	-4.55	115.42	124.93
82	IJ	202	PEB	CHC-C4C-NC	4.55	127.31	121.15
82	j1	201	PEB	CMB-C2B-C1B	4.55	132.07	125.06
82	aF	201	PEB	CHA-C1B-NB	-4.55	115.42	124.93
82	U4	201	PEB	C3D-C4D-ND	4.55	116.18	107.26
82	gK	203	PEB	CHC-C1D-ND	-4.55	107.97	113.72
82	E9	201	PEB	C2C-C1C-NC	4.55	113.69	107.57
82	pK	201	PEB	C2C-C1C-NC	4.55	113.69	107.57
82	TA	202	PEB	C4B-C3B-C2B	-4.55	101.75	106.78
82	RH	201	PEB	C2C-C1C-NC	4.55	113.69	107.57
82	VP	202	PEB	C2C-C1C-NC	4.55	113.69	107.57
82	fG	203	PEB	C2C-C1C-NC	4.55	113.69	107.57
84	D1	1003	CYC	C2B-C1B-NB	4.55	113.64	106.99
82	DE	1002	PEB	C4B-C3B-C2B	-4.55	101.75	106.78
82	VE	202	PEB	C2C-C1C-NC	4.55	113.69	107.57
82	C9	201	PEB	C2C-C1C-NC	4.55	113.69	107.57
82	JJ	202	PEB	CHC-C1D-ND	-4.55	107.97	113.72
85	K2	105	BCR	C8-C7-C6	4.55	139.97	127.20
82	MA	201	PEB	OA-C1A-C2A	-4.55	122.56	126.17
82	A1	301	PEB	OA-C1A-C2A	-4.55	122.56	126.17
82	ZF	202	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	YM	202	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	VQ	201	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	A1	301	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	N9	201	PEB	C2C-C1C-NC	4.54	113.69	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QK	202	PEB	CHC-C4C-NC	4.54	127.30	121.15
82	B7	203	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
88	M6	101	LHG	O7-C7-C8	4.54	121.29	111.50
82	V4	201	PEB	CMB-C2B-C1B	4.54	132.06	125.06
82	S9	203	PEB	C2C-C1C-NC	4.54	113.69	107.57
82	MM	203	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	lO	202	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	mJ	201	PEB	OA-C1A-C2A	-4.54	122.56	126.17
82	WH	201	PEB	C2C-C1C-NC	4.54	113.69	107.57
82	SF	203	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	xF	302	PEB	CHC-C4C-NC	4.54	127.30	121.15
82	ED	201	PEB	C2C-C1C-NC	4.54	113.69	107.57
82	SO	202	PEB	C2C-C1C-NC	4.54	113.69	107.57
85	c6	602	BCR	C20-C21-C22	-4.54	120.83	127.31
82	CD	202	PEB	C1C-C2C-C3C	-4.54	102.25	107.62
82	aJ	203	PEB	C2C-C1C-NC	4.54	113.68	107.57
82	OA	201	PEB	CHA-C1B-C2B	4.54	136.57	124.90
82	DD	203	PEB	OA-C1A-C2A	-4.54	122.56	126.17
82	MP	202	PEB	C2C-C1C-NC	4.54	113.68	107.57
82	O7	201	PEB	CHA-C1B-C2B	4.54	136.57	124.90
82	RA	202	PEB	C1C-C2C-C3C	-4.54	102.26	107.62
82	v8	202	PEB	C2C-C1C-NC	4.54	113.68	107.57
82	ZM	201	PEB	CMB-C2B-C1B	4.54	132.05	125.06
83	QJ	201	PUB	C3B-C4B-NB	4.54	113.68	107.57
82	YQ	202	PEB	C1C-C2C-C3C	-4.54	102.26	107.62
82	S4	201	PEB	C3B-C4B-NB	4.54	116.65	110.05
82	KM	202	PEB	C2C-C1C-NC	4.54	113.68	107.57
91	dL	403	PHO	C3D-C4D-ND	4.54	113.90	107.72
82	PM	201	PEB	C1D-CHC-C4C	4.54	119.94	113.26
82	eE	202	PEB	C2C-C1C-NC	4.54	113.68	107.57
84	DE	1001	CYC	C1B-NB-C4B	-4.54	104.89	110.67
82	TB	201	PEB	CMB-C2B-C3B	-4.54	113.80	126.12
82	h1	201	PEB	C1C-C2C-C3C	-4.54	102.26	107.62
82	SB	202	PEB	C2C-C1C-NC	4.54	113.68	107.57
82	X9	201	PEB	C2C-C1C-NC	4.54	113.68	107.57
82	rK	202	PEB	C2C-C1C-NC	4.54	113.68	107.57
82	kH	203	PEB	CHC-C4C-NC	4.53	127.29	121.15
82	UJ	201	PEB	CHB-C1C-C2C	-4.53	116.92	127.15
82	KF	201	PEB	C1C-C2C-C3C	-4.53	102.26	107.62
82	PP	202	PEB	C2C-C1C-NC	4.53	113.68	107.57
82	qF	203	PEB	C2C-C1C-NC	4.53	113.68	107.57
83	yF	302	PUB	CHC-C1D-ND	-4.53	107.99	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B5	201	PEB	C3B-C4B-NB	4.53	116.64	110.05
82	zC	202	PEB	CHA-C4A-NA	-4.53	119.81	125.20
84	H4	1001	CYC	CHB-C4A-NA	-4.53	115.45	124.93
82	RP	201	PEB	C1C-C2C-C3C	-4.53	102.26	107.62
82	IF	201	PEB	CHB-C1C-C2C	-4.53	116.92	127.15
82	LO	1002	PEB	C2C-C1C-NC	4.53	113.68	107.57
82	HQ	201	PEB	CHB-C1C-C2C	-4.53	116.92	127.15
82	lK	201	PEB	C1C-C2C-C3C	-4.53	102.26	107.62
82	fE	201	PEB	C2C-C1C-NC	4.53	113.67	107.57
82	YA	301	PEB	C1C-CHB-C4B	-4.53	118.12	128.28
82	LE	1002	PEB	C1C-C2C-C3C	-4.53	102.26	107.62
82	pF	201	PEB	C2C-C1C-NC	4.53	113.67	107.57
84	JH	1001	CYC	CAB-C3B-C4B	4.53	128.54	121.38
82	GK	201	PEB	CMA-C2A-C1A	-4.53	102.63	112.40
82	FQ	203	PEB	CMC-C3C-C4C	4.53	131.86	127.06
82	WA	201	PEB	C1C-C2C-C3C	-4.53	102.26	107.62
85	FL	101	BCR	C20-C21-C22	-4.53	120.84	127.31
85	JN	102	BCR	C15-C14-C13	-4.53	120.84	127.31
82	NB	203	PEB	CMB-C2B-C1B	4.53	132.04	125.06
82	gB	203	PEB	CHA-C1B-NB	-4.53	115.45	124.93
82	qK	202	PEB	CHC-C4C-NC	4.53	127.28	121.15
82	V4	201	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
82	UM	201	PEB	CHC-C1D-ND	-4.53	107.99	113.72
82	FI	201	PEB	C4B-C3B-C2B	-4.53	101.77	106.78
82	DB	202	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
82	YF	203	PEB	C2C-C1C-NC	4.53	113.67	107.57
82	AM	301	PEB	C2C-C1C-NC	4.53	113.67	107.57
82	QQ	202	PEB	C2C-C1C-NC	4.53	113.67	107.57
82	kG	202	PEB	CHC-C4C-NC	4.53	127.28	121.15
82	d4	201	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
82	TF	201	PEB	C2C-C1C-NC	4.53	113.67	107.57
83	AE	303	PUB	C3B-C4B-NB	4.53	113.67	107.57
82	N1	1002	PEB	C4B-C3B-C2B	-4.53	101.77	106.78
82	eK	202	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
82	CJ	203	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
82	BQ	201	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
82	jJ	201	PEB	CHC-C4C-NC	4.53	127.28	121.15
82	JP	202	PEB	C1C-C2C-C3C	-4.53	102.27	107.62
84	L4	1001	CYC	CMD-C2D-C1D	4.53	132.19	125.56
82	qK	202	PEB	CHA-C1B-C2B	4.53	136.54	124.90
82	QM	203	PEB	C2C-C1C-NC	4.53	113.67	107.57
82	xK	304	PEB	C1C-C2C-C3C	-4.53	102.27	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	I1	1001	CYC	CMA-C3A-C4A	4.53	132.03	125.06
82	dB	202	PEB	OA-C1A-C2A	-4.53	122.58	126.17
87	aL	606	CLA	C1-C2-C3	-4.52	118.22	126.04
82	CD	201	PEB	CMB-C2B-C1B	4.52	132.03	125.06
82	VD	201	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	XD	201	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	L5	203	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	U7	201	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	eA	301	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
85	CL	502	BCR	C19-C18-C17	4.52	125.88	118.94
82	EB	501	PEB	CHC-C4C-NC	4.52	127.27	121.15
85	b6	603	BCR	C15-C14-C13	-4.52	120.85	127.31
82	cE	201	PEB	OA-C1A-C2A	-4.52	122.58	126.17
82	tK	203	PEB	OA-C1A-C2A	-4.52	122.58	126.17
82	eF	202	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	OO	201	PEB	C3B-C4B-NB	4.52	116.63	110.05
82	LG	1002	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	e4	201	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	rK	201	PEB	C1C-C2C-C3C	-4.52	102.27	107.62
82	NE	202	PEB	C2A-C1A-NA	4.52	112.17	108.27
82	TE	201	PEB	OA-C1A-C2A	-4.52	122.58	126.17
82	EK	201	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
82	W5	203	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
82	j1	203	PEB	C2C-C1C-NC	4.52	113.66	107.57
82	d4	202	PEB	C2C-C1C-NC	4.52	113.66	107.57
82	k1	202	PEB	OA-C1A-C2A	-4.52	122.58	126.17
82	AB	501	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
95	C6	504	DGD	O2G-C1B-C2B	4.52	121.25	111.50
82	cO	202	PEB	C2C-C1C-NC	4.52	113.66	107.57
82	SF	203	PEB	CMB-C2B-C1B	4.52	132.03	125.06
82	RJ	201	PEB	CMC-C3C-C4C	4.52	131.85	127.06
82	SO	202	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
82	aH	202	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
82	XP	202	PEB	C2C-C1C-NC	4.52	113.66	107.57
84	x3	1001	CYC	C1D-C2D-C3D	-4.52	102.03	107.79
82	IQ	201	PEB	C2C-C1C-NC	4.52	113.66	107.57
82	hF	201	PEB	C2C-C1C-NC	4.52	113.66	107.57
82	QP	203	PEB	CHC-C1D-ND	-4.52	108.01	113.72
83	AO	302	PUB	CHA-C1B-NB	4.52	127.27	121.15
82	qF	202	PEB	CHA-C1B-C2B	4.52	136.52	124.90
82	GA	201	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
82	lF	201	PEB	CHC-C4C-NC	4.52	127.26	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	BE	1001	CYC	CHB-C4A-NA	-4.52	115.48	124.93
82	UG	201	PEB	OA-C1A-C2A	-4.52	122.58	126.17
84	BG	1001	CYC	C2C-C1C-NC	4.52	112.17	108.27
82	YB	201	PEB	C2C-C1C-NC	4.52	113.65	107.57
82	GF	203	PEB	OA-C1A-C2A	-4.52	122.58	126.17
82	pC	202	PEB	OA-C1A-C2A	-4.52	122.58	126.17
82	yF	301	PEB	OA-C1A-C2A	-4.52	122.58	126.17
83	A1	304	PUB	CHA-C4A-NA	-4.52	108.01	113.72
82	OG	202	PEB	C1C-C2C-C3C	-4.52	102.28	107.62
84	J4	1001	CYC	CHB-C4A-C3A	4.52	136.51	124.90
82	ID	201	PEB	C2C-C1C-NC	4.52	113.65	107.57
82	V1	202	PEB	C2C-C1C-NC	4.52	113.65	107.57
85	cL	518	BCR	C30-C25-C26	-4.52	116.25	122.61
82	IJ	203	PEB	CHB-C1C-NC	-4.51	114.98	125.32
82	yC	203	PEB	C1C-C2C-C3C	-4.51	102.28	107.62
82	JB	201	PEB	CMB-C2B-C3B	-4.51	113.86	126.12
82	PM	201	PEB	CMC-C3C-C4C	4.51	131.84	127.06
82	eF	203	PEB	CHC-C1D-ND	-4.51	108.01	113.72
82	F9	203	PEB	CMB-C2B-C1B	4.51	132.01	125.06
82	SM	201	PEB	C1C-C2C-C3C	-4.51	102.28	107.62
82	LA	201	PEB	CHA-C1B-NB	-4.51	115.49	124.93
82	GJ	202	PEB	CHC-C4C-NC	4.51	127.26	121.15
82	OP	202	PEB	CHC-C4C-NC	4.51	127.26	121.15
82	fG	201	PEB	C2C-C1C-NC	4.51	113.65	107.57
82	M7	201	PEB	OA-C1A-C2A	-4.51	122.58	126.17
82	YP	501	PEB	CHC-C1D-ND	-4.51	108.02	113.72
82	N1	1002	PEB	C2C-C1C-NC	4.51	113.65	107.57
82	fM	201	PEB	C2C-C1C-NC	4.51	113.65	107.57
84	BG	1001	CYC	CHB-C4A-NA	-4.51	115.49	124.93
82	TB	201	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	mE	201	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	mM	201	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	EQ	202	PEB	CHC-C1D-ND	-4.51	108.02	113.72
82	jG	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
84	J4	1001	CYC	CAB-C3B-C4B	4.51	128.50	121.38
82	HH	1002	PEB	C1D-CHC-C4C	4.51	119.91	113.26
82	Z1	203	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	mF	202	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	RM	201	PEB	C2C-C1C-NC	4.51	113.64	107.57
85	hL	102	BCR	C3-C4-C5	-4.51	106.02	114.08
82	XP	202	PEB	CMB-C2B-C1B	4.51	132.01	125.06
82	NI	203	PEB	CHB-C1C-C2C	-4.51	116.97	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	b1	202	PEB	CHA-C1B-NB	-4.51	115.50	124.93
82	PA	201	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	LH	1003	PEB	CHA-C1B-NB	-4.51	115.50	124.93
82	SE	201	PEB	C2C-C1C-NC	4.51	113.64	107.57
83	QM	201	PUB	C3B-C4B-NB	4.51	113.64	107.57
82	kE	202	PEB	CHC-C4C-NC	4.51	127.25	121.15
82	V4	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
82	VG	202	PEB	C2C-C1C-NC	4.51	113.64	107.57
84	JO	1001	CYC	CAB-C3B-C4B	4.51	128.50	121.38
82	LP	202	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	OE	202	PEB	C2C-C1C-NC	4.51	113.64	107.57
82	SG	201	PEB	C2C-C1C-NC	4.51	113.64	107.57
82	TQ	203	PEB	C2C-C1C-NC	4.51	113.64	107.57
82	GF	201	PEB	C3D-C4D-ND	4.51	116.10	107.26
82	VO	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
82	L4	1002	PEB	CHC-C4C-NC	4.51	127.25	121.15
82	BB	202	PEB	C2C-C1C-NC	4.51	113.64	107.57
82	XB	201	PEB	CHC-C4C-NC	4.51	127.25	121.15
82	bP	501	PEB	C2C-C1C-NC	4.51	113.64	107.57
82	EB	501	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	KK	201	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	e1	201	PEB	C1C-C2C-C3C	-4.51	102.29	107.62
82	J7	203	PEB	C4B-C3B-C2B	-4.51	101.80	106.78
82	ZB	201	PEB	C2C-C1C-NC	4.51	113.64	107.57
82	BI	202	PEB	C1C-C2C-C3C	-4.51	102.30	107.62
82	Y7	301	PEB	C1C-CHB-C4B	-4.50	118.18	128.28
84	MO	1001	CYC	C2B-C1B-NB	4.50	113.58	106.99
82	qK	201	PEB	C1C-CHB-C4B	4.50	138.38	128.28
82	c4	202	PEB	C2C-C1C-NC	4.50	113.64	107.57
82	qK	203	PEB	C2C-C1C-NC	4.50	113.64	107.57
82	cF	201	PEB	CHC-C4C-NC	4.50	127.25	121.15
82	JB	201	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	MF	201	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	rF	201	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	L9	201	PEB	C2C-C1C-NC	4.50	113.64	107.57
82	dO	202	PEB	C2C-C1C-NC	4.50	113.64	107.57
82	GF	201	PEB	CMA-C2A-C1A	-4.50	102.70	112.40
82	OP	203	PEB	C1D-CHC-C4C	-4.50	106.62	113.26
82	JJ	201	PEB	CHA-C1B-NB	-4.50	115.51	124.93
82	eB	202	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	iO	202	PEB	CHB-C1C-C2C	-4.50	116.99	127.15
82	bB	201	PEB	CMB-C2B-C1B	4.50	132.00	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YD	202	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	NE	202	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	PH	201	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	YA	301	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	GA	201	PEB	C3D-C4D-ND	4.50	116.09	107.26
82	W9	203	PEB	OA-C1A-C2A	-4.50	122.59	126.17
82	Q7	201	PEB	C3D-C4D-ND	4.50	116.09	107.26
82	GM	201	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	XD	203	PEB	OA-C1A-C2A	-4.50	122.59	126.17
82	JJ	201	PEB	CMC-C3C-C4C	4.50	131.83	127.06
82	JA	202	PEB	C2A-C1A-NA	4.50	112.15	108.27
82	FQ	203	PEB	C2A-C1A-NA	4.50	112.15	108.27
82	V7	201	PEB	CAC-CBC-CGC	-4.50	103.92	113.60
82	O7	201	PEB	C3C-C4C-NC	4.50	112.38	108.33
82	pC	202	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	VP	202	PEB	OA-C1A-C2A	-4.50	122.60	126.17
82	qF	201	PEB	C1C-CHB-C4B	4.50	138.37	128.28
84	J1	1001	CYC	CMD-C2D-C1D	4.50	132.15	125.56
84	V3	1001	CYC	C1D-C2D-C3D	-4.50	102.06	107.79
82	OJ	201	PEB	C1C-C2C-C3C	-4.50	102.30	107.62
82	NA	203	PEB	OA-C1A-C2A	-4.50	122.60	126.17
82	QD	202	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	DK	201	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	Y7	301	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	hG	202	PEB	C2C-C1C-NC	4.50	113.63	107.57
82	eJ	201	PEB	C2C-C1C-NC	4.50	113.63	107.57
84	S3	1001	CYC	CHB-C4A-C3A	4.50	136.47	124.90
82	fG	202	PEB	C2C-C1C-NC	4.50	113.63	107.57
85	h6	102	BCR	C16-C17-C18	-4.50	120.89	127.31
82	XA	202	PEB	C2A-C1A-NA	4.50	112.15	108.27
82	BB	203	PEB	C2A-C1A-NA	4.50	112.15	108.27
83	M5	303	PUB	C3B-C4B-NB	4.50	113.62	107.57
82	KI	201	PEB	C3C-C4C-NC	4.50	112.38	108.33
82	W9	202	PEB	CAB-C3B-C4B	4.50	132.96	125.01
82	OE	202	PEB	C1C-C2C-C3C	-4.50	102.31	107.62
82	IK	201	PEB	CHB-C1C-C2C	-4.49	117.01	127.15
87	62	309	CLA	C2A-C3A-C4A	4.49	109.13	101.87
82	QF	203	PEB	C3C-C4C-NC	4.49	112.38	108.33
82	L7	201	PEB	CHA-C1B-NB	-4.49	115.53	124.93
82	WM	203	PEB	CMB-C2B-C1B	4.49	131.99	125.06
82	TF	201	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	NG	201	PEB	C1C-C2C-C3C	-4.49	102.31	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PP	202	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
83	Z5	303	PUB	C3B-C4B-NB	4.49	113.62	107.57
82	W7	201	PEB	C3D-C4D-ND	4.49	116.07	107.26
82	Y5	203	PEB	CAC-C2C-C1C	4.49	132.92	125.76
82	WH	202	PEB	CHC-C1D-ND	-4.49	108.04	113.72
82	cO	201	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	P1	202	PEB	C2C-C1C-NC	4.49	113.62	107.57
82	YO	202	PEB	CHB-C1C-C2C	-4.49	117.02	127.15
83	yF	302	PUB	CMD-C2D-C3D	4.49	134.51	127.77
82	KJ	203	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	y8	203	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	m1	201	PEB	CMB-C2B-C1B	4.49	131.98	125.06
82	L1	1002	PEB	CHA-C1B-NB	-4.49	115.54	124.93
82	h4	202	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	R7	201	PEB	C2C-C1C-NC	4.49	113.62	107.57
82	i4	202	PEB	CHB-C1C-C2C	-4.49	117.02	127.15
82	WH	201	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	UJ	201	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	S9	202	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	UM	203	PEB	C2C-C1C-NC	4.49	113.62	107.57
83	BM	302	PUB	C3B-C4B-NB	4.49	113.62	107.57
82	cE	202	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
82	dG	203	PEB	C1C-C2C-C3C	-4.49	102.31	107.62
84	M3	1001	CYC	CHB-C4A-C3A	4.49	136.44	124.90
82	NM	202	PEB	CMB-C2B-C1B	4.49	131.98	125.06
82	H5	201	PEB	OA-C1A-C2A	-4.49	122.60	126.17
82	LD	201	PEB	C2C-C1C-NC	4.49	113.61	107.57
82	SH	203	PEB	C2C-C1C-NC	4.49	113.61	107.57
82	kK	201	PEB	C2C-C1C-NC	4.49	113.61	107.57
82	OG	203	PEB	CHC-C4C-NC	4.49	127.22	121.15
82	ZM	202	PEB	C2C-C1C-NC	4.49	113.61	107.57
83	AO	302	PUB	C3B-C4B-NB	4.49	113.61	107.57
82	W7	202	PEB	OA-C1A-C2A	-4.49	122.61	126.17
82	uC	203	PEB	OA-C1A-C2A	-4.49	122.61	126.17
84	63	901	CYC	CHD-C4C-NC	4.49	130.54	125.20
82	RG	201	PEB	C2C-C1C-NC	4.49	113.61	107.57
82	B5	202	PEB	C2C-C1C-NC	4.49	113.61	107.57
85	JN	102	BCR	C7-C8-C9	-4.49	119.46	126.23
83	M5	302	PUB	CHA-C4A-NA	-4.49	108.05	113.72
82	OF	201	PEB	C2C-C1C-NC	4.49	113.61	107.57
82	HD	201	PEB	CHB-C1C-C2C	-4.49	117.03	127.15
82	VO	201	PEB	CMB-C2B-C1B	4.49	131.97	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TK	201	PEB	C1C-C2C-C3C	-4.49	102.32	107.62
82	uK	202	PEB	C1C-C2C-C3C	-4.49	102.32	107.62
82	h1	201	PEB	C2C-C1C-NC	4.49	113.61	107.57
82	k1	201	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
82	c4	201	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
83	QJ	201	PUB	C4B-C3B-C2B	-4.48	102.32	107.62
82	QI	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
82	xK	302	PEB	CHC-C4C-NC	4.48	127.22	121.15
84	H3	1001	CYC	CHB-C4A-C3A	4.48	136.43	124.90
85	B2	843	BCR	C20-C21-C22	-4.48	120.91	127.31
82	A4	304	PEB	C2C-C1C-NC	4.48	113.61	107.57
82	KJ	203	PEB	CHA-C1B-NB	-4.48	115.55	124.93
82	RI	203	PEB	CHC-C1D-ND	-4.48	108.05	113.72
82	mH	202	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
82	YI	202	PEB	C2C-C1C-NC	4.48	113.61	107.57
82	SQ	202	PEB	C2C-C1C-NC	4.48	113.61	107.57
85	B2	839	BCR	C27-C26-C25	-4.48	116.22	122.73
82	mJ	201	PEB	CHA-C1B-NB	-4.48	115.56	124.93
84	o3	1001	CYC	CHB-C4A-C3A	4.48	136.43	124.90
82	TE	201	PEB	C2C-C1C-NC	4.48	113.61	107.57
82	L4	1002	PEB	C2C-C1C-NC	4.48	113.61	107.57
82	D7	201	PEB	CHC-C4C-NC	4.48	127.22	121.15
82	YI	202	PEB	OA-C1A-C2A	-4.48	122.61	126.17
84	CG	1001	CYC	OC-C1C-C2C	-4.48	122.61	126.17
82	IA	201	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
82	NF	201	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
82	UI	202	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
82	OG	201	PEB	CHC-C1D-ND	-4.48	108.05	113.72
82	PH	202	PEB	C2C-C1C-NC	4.48	113.61	107.57
82	uF	202	PEB	C2C-C1C-NC	4.48	113.61	107.57
82	S4	202	PEB	C1C-C2C-C3C	-4.48	102.32	107.62
82	H9	201	PEB	C4B-C3B-C2B	-4.48	101.82	106.78
84	u3	1001	CYC	CHB-C4A-C3A	4.48	136.42	124.90
82	GB	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	OG	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	YP	503	PEB	C2C-C1C-NC	4.48	113.60	107.57
85	BN	843	BCR	C20-C21-C22	-4.48	120.92	127.31
84	d3	1001	CYC	CHB-C4A-C3A	4.48	136.42	124.90
84	h3	1001	CYC	CHB-C4A-C3A	4.48	136.42	124.90
84	w3	1001	CYC	CHB-C4A-C3A	4.48	136.42	124.90
82	ED	202	PEB	OA-C1A-C2A	-4.48	122.61	126.17
82	gJ	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YM	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	gJ	201	PEB	C2C-C1C-NC	4.48	113.60	107.57
84	O3	1001	CYC	CHB-C4A-C3A	4.48	136.42	124.90
82	LJ	202	PEB	CMB-C2B-C1B	4.48	131.96	125.06
82	NM	201	PEB	C1C-C2C-C3C	-4.48	102.33	107.62
82	JO	1002	PEB	C1C-C2C-C3C	-4.48	102.33	107.62
82	DB	201	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	NM	201	PEB	C2C-C1C-NC	4.48	113.60	107.57
83	BJ	302	PUB	CMA-C2A-C1A	4.48	131.92	121.39
84	LO	1001	CYC	CMD-C2D-C1D	4.48	132.12	125.56
84	L3	1001	CYC	CHB-C4A-C3A	4.48	136.42	124.90
85	B6	601	BCR	C28-C27-C26	-4.48	106.08	114.08
82	CK	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
82	VM	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
82	NH	1002	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	DM	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	p8	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
82	L9	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
85	K2	102	BCR	C28-C27-C26	-4.48	106.08	114.08
82	ZB	201	PEB	C1C-C2C-C3C	-4.48	102.33	107.62
82	NJ	201	PEB	C1C-C2C-C3C	-4.48	102.33	107.62
84	Q3	1001	CYC	CHB-C4A-C3A	4.48	136.41	124.90
85	J2	102	BCR	C16-C17-C18	-4.48	120.92	127.31
82	lJ	203	PEB	CHC-C4C-NC	4.48	127.21	121.15
82	T5	202	PEB	C1D-CHC-C4C	-4.48	106.66	113.26
84	q3	1001	CYC	CHB-C4A-C3A	4.48	136.41	124.90
84	73	1001	CYC	CHB-C4A-C3A	4.48	136.41	124.90
82	eM	202	PEB	C2C-C1C-NC	4.48	113.60	107.57
87	6N	608	CLA	C2A-C3A-C4A	4.47	109.10	101.87
82	AO	304	PEB	C2C-C1C-NC	4.47	113.60	107.57
84	EO	1001	CYC	C3D-C4D-ND	4.47	113.60	107.57
82	OP	202	PEB	CMB-C2B-C1B	4.47	131.95	125.06
82	U9	203	PEB	C1C-C2C-C3C	-4.47	102.33	107.62
82	YE	201	PEB	CHA-C1B-NB	-4.47	115.57	124.93
82	IP	203	PEB	CHC-C1D-ND	-4.47	108.06	113.72
82	DH	1002	PEB	C1C-C2C-C3C	-4.47	102.33	107.62
83	AM	303	PUB	CMA-C2A-C1A	4.47	131.91	121.39
82	WG	202	PEB	OA-C1A-C2A	-4.47	122.62	126.17
82	OA	201	PEB	C3C-C4C-NC	4.47	112.36	108.33
82	NF	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	fM	202	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	VF	201	PEB	CHC-C4C-NC	4.47	127.20	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	D3	1001	CYC	CHB-C4A-C3A	4.47	136.40	124.90
84	I3	1001	CYC	CHB-C4A-C3A	4.47	136.40	124.90
84	M4	1001	CYC	C2B-C1B-NB	4.47	113.53	106.99
82	SH	201	PEB	C1C-C2C-C3C	-4.47	102.33	107.62
82	HJ	202	PEB	C1C-C2C-C3C	-4.47	102.33	107.62
82	DF	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	WM	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
84	63	901	CYC	C3D-C4D-ND	4.47	113.59	107.57
82	DB	202	PEB	OA-C1A-C2A	-4.47	122.62	126.17
82	F5	202	PEB	CHB-C1C-C2C	-4.47	117.06	127.15
82	jH	201	PEB	CMB-C2B-C1B	4.47	131.95	125.06
82	X7	202	PEB	C2A-C1A-NA	4.47	112.13	108.27
84	D1	1003	CYC	C4D-C3D-C2D	-4.47	102.34	107.62
82	Y4	202	PEB	CHB-C1C-C2C	-4.47	117.06	127.15
82	Q4	201	PEB	C3D-C4D-ND	4.47	116.03	107.26
82	LO	1002	PEB	CHC-C4C-NC	4.47	127.20	121.15
87	AN	852	CLA	CHD-C4C-C3C	4.47	131.41	124.84
83	AH	304	PUB	CHA-C4A-NA	-4.47	108.07	113.72
84	j3	1001	CYC	CHB-C4A-C3A	4.47	136.39	124.90
82	PK	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	F5	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	fE	202	PEB	C2C-C1C-NC	4.47	113.59	107.57
85	J2	102	BCR	C7-C8-C9	-4.47	119.48	126.23
84	F3	1001	CYC	CHB-C4A-C3A	4.47	136.39	124.90
82	hF	201	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	cG	202	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
84	DH	1003	CYC	C4D-C3D-C2D	-4.47	102.34	107.62
84	HH	1001	CYC	C2D-C1D-ND	4.47	113.68	107.40
83	wK	304	PUB	CHA-C1B-NB	4.47	127.20	121.15
82	YI	201	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	PF	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	TK	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	TP	202	PEB	C2C-C1C-NC	4.47	113.59	107.57
85	FN	204	BCR	C20-C21-C22	-4.47	120.93	127.31
82	dH	201	PEB	OA-C1A-C2A	-4.47	122.62	126.17
82	YO	202	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	iM	202	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	SK	203	PEB	CMB-C2B-C1B	4.47	131.94	125.06
82	RB	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	SI	202	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	Y1	201	PEB	C2C-C1C-NC	4.47	113.59	107.57
82	V1	201	PEB	CHA-C1B-NB	-4.47	115.59	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	c1	202	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	dO	201	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	DQ	201	PEB	OA-C1A-C2A	-4.47	122.62	126.17
84	JO	1001	CYC	CHB-C4A-C3A	4.47	136.38	124.90
82	D1	1002	PEB	CHA-C1B-NB	-4.47	115.59	124.93
82	KB	304	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	TP	202	PEB	C1C-C2C-C3C	-4.47	102.34	107.62
82	SJ	203	PEB	CHC-C1D-ND	-4.46	108.08	113.72
82	SP	203	PEB	C1C-C2C-C3C	-4.46	102.34	107.62
82	gH	203	PEB	C1C-C2C-C3C	-4.46	102.34	107.62
82	R5	202	PEB	C1D-CHC-C4C	-4.46	106.67	113.26
84	k3	1001	CYC	CHB-C4A-C3A	4.46	136.38	124.90
82	IM	202	PEB	CHC-C4C-NC	4.46	127.19	121.15
82	q8	202	PEB	CHB-C1C-C2C	-4.46	117.08	127.15
82	YD	201	PEB	C2C-C1C-NC	4.46	113.58	107.57
84	B3	1001	CYC	CHB-C4A-C3A	4.46	136.38	124.90
84	f3	1001	CYC	CHB-C4A-C3A	4.46	136.38	124.90
82	MD	202	PEB	CHC-C1D-ND	-4.46	108.08	113.72
82	NK	201	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	uK	202	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	WE	201	PEB	C3D-C4D-ND	4.46	116.02	107.26
82	W1	202	PEB	CHC-C1D-ND	-4.46	108.08	113.72
82	KB	304	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	YH	201	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	GM	202	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	S4	202	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	cG	201	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	YP	501	PEB	OA-C1A-C2A	-4.46	122.62	126.17
84	DH	1003	CYC	OC-C1C-C2C	-4.46	122.62	126.17
82	cM	202	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
84	FO	1001	CYC	C1B-NB-C4B	-4.46	104.99	110.67
82	MQ	202	PEB	CHC-C1D-ND	-4.46	108.08	113.72
82	RD	203	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	LJ	201	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	NJ	201	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	DK	203	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	QG	201	PEB	C4B-C3B-C2B	-4.46	101.84	106.78
82	VA	201	PEB	CAC-CBC-CGC	-4.46	104.00	113.60
84	F4	1001	CYC	OC-C1C-C2C	-4.46	122.63	126.17
82	eK	203	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	NB	201	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
82	kH	201	PEB	C1C-C2C-C3C	-4.46	102.35	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KF	201	PEB	CHC-C1D-ND	-4.46	108.08	113.72
83	Z5	302	PUB	CHA-C4A-NA	-4.46	108.08	113.72
82	aB	202	PEB	C2C-C1C-NC	4.46	113.58	107.57
85	KN	101	BCR	C28-C27-C26	-4.46	106.11	114.08
82	BB	203	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
82	TH	202	PEB	C2C-C1C-NC	4.46	113.58	107.57
82	J7	202	PEB	C2A-C1A-NA	4.46	112.12	108.27
82	ZH	203	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
95	C6	521	DGD	O2G-C1B-C2B	4.46	121.11	111.50
82	bH	202	PEB	CHA-C1B-NB	-4.46	115.61	124.93
82	MD	202	PEB	C2C-C1C-NC	4.46	113.57	107.57
84	DH	1001	CYC	C3D-C4D-ND	4.46	113.57	107.57
82	VO	201	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
82	Q1	203	PEB	CMB-C2B-C1B	4.46	131.93	125.06
82	UK	201	PEB	CAC-CBC-CGC	4.46	123.20	113.60
82	NP	202	PEB	CHC-C4C-NC	4.46	127.18	121.15
82	U1	202	PEB	C2C-C1C-NC	4.46	113.57	107.57
82	iG	202	PEB	C2C-C1C-NC	4.46	113.57	107.57
82	Q5	202	PEB	C4B-C3B-C2B	-4.46	101.85	106.78
82	YO	201	PEB	CHC-C1D-ND	-4.46	108.08	113.72
82	GJ	203	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
82	AK	201	PEB	CHA-C1B-NB	-4.46	115.61	124.93
82	lO	201	PEB	CMB-C2B-C1B	4.46	131.93	125.06
82	eF	203	PEB	C2C-C1C-NC	4.46	113.57	107.57
82	KI	201	PEB	C1B-C2B-C3B	-4.46	101.39	106.51
82	NH	1002	PEB	C4B-C3B-C2B	-4.46	101.85	106.78
82	XQ	201	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
84	FH	1001	CYC	C3D-C4D-ND	4.46	113.57	107.57
82	DH	1002	PEB	CHA-C1B-NB	-4.46	115.61	124.93
82	oK	201	PEB	CHA-C1B-NB	-4.46	115.61	124.93
82	FA	201	PEB	C1C-C2C-C3C	-4.46	102.35	107.62
82	SH	201	PEB	CMB-C2B-C1B	4.46	131.93	125.06
82	qF	202	PEB	CHC-C4C-NC	4.46	127.18	121.15
82	MD	201	PEB	CMB-C2B-C1B	4.45	131.92	125.06
82	QP	201	PEB	CMB-C2B-C1B	4.45	131.92	125.06
92	x6	601	LMG	O7-C10-C11	4.45	121.10	111.50
82	KQ	201	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
84	D1	1001	CYC	C3D-C4D-ND	4.45	113.57	107.57
82	WA	202	PEB	OA-C1A-C2A	-4.45	122.63	126.17
83	KA	203	PUB	C4B-CHB-C1C	-4.45	118.30	128.28
82	fK	202	PEB	C1D-CHC-C4C	4.45	119.82	113.26
82	SF	202	PEB	C1C-C2C-C3C	-4.45	102.36	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UH	202	PEB	C2C-C1C-NC	4.45	113.57	107.57
82	WH	203	PEB	C2C-C1C-NC	4.45	113.57	107.57
82	WA	201	PEB	C3D-C4D-ND	4.45	116.00	107.26
84	n3	1001	CYC	CHB-C4A-C3A	4.45	136.35	124.90
84	U3	1001	CYC	CHB-C4A-C3A	4.45	136.35	124.90
82	PP	201	PEB	C2C-C1C-NC	4.45	113.57	107.57
82	cH	202	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
95	cL	502	DGD	C4E-C3E-C2E	4.45	118.59	110.82
82	M7	202	PEB	C2C-C1C-NC	4.45	113.56	107.57
83	A4	302	PUB	C3B-C4B-NB	4.45	113.56	107.57
83	NQ	201	PUB	CMA-C2A-C1A	4.45	131.86	121.39
84	LO	1001	CYC	CHB-C4A-C3A	4.45	136.35	124.90
83	AJ	303	PUB	CMA-C2A-C1A	4.45	131.86	121.39
82	NA	203	PEB	CAC-CBC-CGC	-4.45	104.03	113.60
82	I5	202	PEB	C1D-CHC-C4C	-4.45	106.69	113.26
82	mH	201	PEB	CMB-C2B-C1B	4.45	131.92	125.06
85	JN	102	BCR	C16-C17-C18	-4.45	120.96	127.31
82	BB	202	PEB	CHC-C4C-NC	4.45	127.17	121.15
82	OH	202	PEB	C2C-C1C-NC	4.45	113.56	107.57
82	jH	203	PEB	C2C-C1C-NC	4.45	113.56	107.57
82	cO	201	PEB	C2C-C1C-NC	4.45	113.56	107.57
82	VF	202	PEB	OA-C1A-C2A	-4.45	122.64	126.17
82	MJ	201	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
82	hM	202	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
83	yK	302	PUB	C4B-C3B-C2B	-4.45	102.36	107.62
85	BL	617	BCR	C15-C14-C13	-4.45	120.96	127.31
84	F1	1001	CYC	C3D-C4D-ND	4.45	113.56	107.57
82	CP	201	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
82	G7	201	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
82	dE	203	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
82	OP	203	PEB	OA-C1A-C2A	-4.45	122.64	126.17
82	J9	202	PEB	CHC-C1D-ND	-4.45	108.10	113.72
82	j1	203	PEB	CHB-C1C-C2C	-4.45	117.11	127.15
82	PO	201	PEB	C1C-C2C-C3C	-4.45	102.36	107.62
82	GF	203	PEB	C2C-C1C-NC	4.45	113.56	107.57
85	F2	204	BCR	C20-C21-C22	-4.45	120.96	127.31
82	BD	202	PEB	C2C-C1C-NC	4.45	113.56	107.57
82	X5	202	PEB	C1D-CHC-C4C	-4.45	106.70	113.26
85	C6	507	BCR	C24-C23-C22	-4.45	119.52	126.23
82	fM	202	PEB	CHC-C4C-NC	4.45	127.17	121.15
82	qC	202	PEB	CHB-C1C-C2C	-4.45	117.12	127.15
82	aJ	204	PEB	CHB-C1C-C2C	-4.45	117.12	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	BN	839	BCR	C27-C26-C25	-4.45	116.28	122.73
82	A7	201	PEB	CAB-C3B-C4B	4.45	132.88	125.01
82	uC	201	PEB	CHC-C4C-NC	4.45	127.17	121.15
82	hM	203	PEB	CHC-C4C-NC	4.45	127.17	121.15
82	lM	202	PEB	CHC-C4C-NC	4.45	127.17	121.15
82	E5	202	PEB	C1D-CHC-C4C	-4.45	106.70	113.26
82	IF	203	PEB	C4B-C3B-C2B	-4.45	101.86	106.78
82	DI	202	PEB	C2C-C1C-NC	4.45	113.56	107.57
82	RI	203	PEB	C1B-C2B-C3B	-4.45	101.40	106.51
82	p8	202	PEB	OA-C1A-C2A	-4.44	122.64	126.17
82	HB	201	PEB	C2C-C1C-NC	4.44	113.56	107.57
82	KE	201	PEB	C2C-C1C-NC	4.44	113.56	107.57
82	PM	202	PEB	C2C-C1C-NC	4.44	113.56	107.57
82	Q9	201	PEB	C1C-C2C-C3C	-4.44	102.37	107.62
82	iJ	202	PEB	C2C-C1C-NC	4.44	113.55	107.57
82	c4	202	PEB	CHB-C1C-C2C	-4.44	117.13	127.15
82	KF	202	PEB	C1C-C2C-C3C	-4.44	102.37	107.62
82	QA	201	PEB	C3D-C4D-ND	4.44	115.97	107.26
82	G7	201	PEB	C3D-C4D-ND	4.44	115.97	107.26
82	P7	201	PEB	C2C-C1C-NC	4.44	113.55	107.57
83	xK	301	PUB	C3B-C4B-NB	4.44	113.55	107.57
84	H1	1001	CYC	C2D-C1D-ND	4.44	113.64	107.40
82	VO	201	PEB	CHC-C1D-ND	-4.44	108.10	113.72
82	iJ	202	PEB	CHC-C1D-ND	-4.44	108.10	113.72
82	qC	201	PEB	C1C-C2C-C3C	-4.44	102.37	107.62
82	DA	201	PEB	CHC-C4C-NC	4.44	127.16	121.15
82	MQ	201	PEB	CMB-C2B-C1B	4.44	131.90	125.06
82	mO	202	PEB	C1C-C2C-C3C	-4.44	102.37	107.62
82	GJ	201	PEB	CHA-C1B-NB	-4.44	115.64	124.93
82	hE	202	PEB	C2C-C1C-NC	4.44	113.55	107.57
82	uF	203	PEB	C2C-C1C-NC	4.44	113.55	107.57
82	fF	202	PEB	C1D-CHC-C4C	4.44	119.80	113.26
83	yF	302	PUB	C4B-C3B-C2B	-4.44	102.37	107.62
82	V5	202	PEB	C1D-CHC-C4C	-4.44	106.71	113.26
82	A1	305	PEB	C1C-CHB-C4B	-4.44	118.33	128.28
82	V4	201	PEB	CHC-C1D-ND	-4.44	108.11	113.72
82	SD	202	PEB	C1D-CHC-C4C	4.44	119.80	113.26
82	G5	202	PEB	C1D-CHC-C4C	-4.44	106.71	113.26
82	lF	201	PEB	C2A-C1A-NA	4.44	112.10	108.27
82	c1	201	PEB	C1C-C2C-C3C	-4.44	102.37	107.62
82	AJ	301	PEB	CHC-C4C-NC	4.44	127.16	121.15
82	hF	202	PEB	C1C-C2C-C3C	-4.44	102.37	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	oK	203	PEB	C1C-C2C-C3C	-4.44	102.37	107.62
82	N5	202	PEB	C1D-CHC-C4C	-4.44	106.71	113.26
82	VJ	202	PEB	C2C-C1C-NC	4.44	113.55	107.57
85	FN	202	BCR	C4-C5-C6	-4.44	116.29	122.73
82	OE	201	PEB	CHC-C1D-ND	-4.44	108.11	113.72
82	SD	202	PEB	C2C-C1C-NC	4.44	113.55	107.57
82	WJ	203	PEB	OA-C1A-C2A	-4.44	122.64	126.17
82	JI	201	PEB	C1C-C2C-C3C	-4.44	102.38	107.62
83	ND	201	PUB	CMA-C2A-C1A	4.44	131.82	121.39
82	AF	201	PEB	C1C-C2C-C3C	-4.44	102.38	107.62
82	ZF	202	PEB	OA-C1A-C2A	-4.44	122.65	126.17
82	KB	302	PEB	C2C-C1C-NC	4.44	113.54	107.57
82	YQ	201	PEB	C2C-C1C-NC	4.44	113.54	107.57
84	MO	1001	CYC	CMD-C2D-C1D	4.44	132.06	125.56
82	KJ	201	PEB	CHC-C4C-NC	4.44	127.15	121.15
82	GJ	202	PEB	C1C-C2C-C3C	-4.44	102.38	107.62
82	N7	203	PEB	CAC-CBC-CGC	-4.44	104.06	113.60
82	RQ	203	PEB	C2C-C1C-NC	4.43	113.54	107.57
84	IG	1001	CYC	CHD-C1D-ND	-4.43	115.16	125.32
82	RJ	202	PEB	CMB-C2B-C1B	4.43	131.89	125.06
82	O1	202	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	EJ	201	PEB	C1C-C2C-C3C	-4.43	102.38	107.62
82	H9	202	PEB	C1C-C2C-C3C	-4.43	102.38	107.62
82	P5	202	PEB	C1D-CHC-C4C	-4.43	106.72	113.26
82	MQ	202	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	p8	201	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	cB	402	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	gH	203	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	J4	1002	PEB	C1C-C2C-C3C	-4.43	102.38	107.62
82	YG	201	PEB	CHA-C1B-NB	-4.43	115.66	124.93
82	C5	202	PEB	C1D-CHC-C4C	-4.43	106.72	113.26
82	lM	201	PEB	C1C-CHB-C4B	4.43	138.22	128.28
82	TD	203	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	Z1	203	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	YB	201	PEB	C1C-C2C-C3C	-4.43	102.38	107.62
82	CK	201	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	HI	202	PEB	C1B-C2B-C3B	-4.43	101.42	106.51
82	WB	401	PEB	OA-C1A-C2A	-4.43	122.65	126.17
82	UM	201	PEB	OA-C1A-C2A	-4.43	122.65	126.17
82	O5	202	PEB	OA-C1A-C2A	-4.43	122.65	126.17
84	FE	1001	CYC	OC-C1C-C2C	-4.43	122.65	126.17
82	LK	202	PEB	C3D-C4D-ND	4.43	115.95	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	K7	203	PUB	C4B-CHB-C1C	-4.43	118.35	128.28
84	L4	1001	CYC	CHB-C4A-C3A	4.43	136.29	124.90
82	RM	201	PEB	CHA-C1B-NB	-4.43	115.67	124.93
82	GM	203	PEB	CHB-C1C-C2C	-4.43	117.16	127.15
82	NK	202	PEB	CHC-C4C-NC	-4.43	115.15	121.15
82	HB	203	PEB	C1C-C2C-C3C	-4.43	102.38	107.62
82	HM	201	PEB	C1C-C2C-C3C	-4.43	102.38	107.62
82	N7	201	PEB	CMB-C2B-C1B	4.43	131.89	125.06
84	ME	1001	CYC	CHD-C1D-ND	-4.43	115.17	125.32
82	XQ	203	PEB	C2C-C1C-NC	4.43	113.54	107.57
82	d1	201	PEB	OA-C1A-C2A	-4.43	122.65	126.17
82	QH	203	PEB	CMB-C2B-C1B	4.43	131.88	125.06
82	IQ	202	PEB	CAB-C3B-C4B	4.43	132.85	125.01
82	J5	201	PEB	CAA-C3A-C2A	-4.43	103.19	114.26
82	A5	202	PEB	C1D-CHC-C4C	-4.43	106.73	113.26
82	GJ	203	PEB	CHB-C1C-C2C	-4.43	117.16	127.15
82	GI	201	PEB	CAC-C2C-C1C	4.43	132.81	125.76
82	AA	201	PEB	CAB-C3B-C4B	4.43	132.84	125.01
82	ED	202	PEB	CHC-C1D-ND	-4.43	108.12	113.72
84	JH	1001	CYC	CMD-C2D-C1D	4.43	132.04	125.56
82	AD	303	PEB	C2C-C1C-NC	4.43	113.53	107.57
82	VG	201	PEB	C2C-C1C-NC	4.43	113.53	107.57
82	JA	203	PEB	C4B-C3B-C2B	-4.43	101.88	106.78
84	M1	201	CYC	OC-C1C-C2C	-4.43	122.65	126.17
83	wF	304	PUB	CMA-C2A-C1A	4.43	131.80	121.39
82	eJ	202	PEB	C1C-CHB-C4B	-4.43	118.36	128.28
82	w8	201	PEB	CHC-C4C-NC	4.43	127.14	121.15
82	Y4	201	PEB	C2C-C1C-NC	4.43	113.53	107.57
82	ID	202	PEB	CAB-C3B-C4B	4.43	132.84	125.01
82	AK	201	PEB	C1C-C2C-C3C	-4.43	102.39	107.62
82	PK	201	PEB	C1C-C2C-C3C	-4.43	102.39	107.62
82	h4	201	PEB	C1C-C2C-C3C	-4.43	102.39	107.62
82	iH	202	PEB	C1C-C2C-C3C	-4.43	102.39	107.62
84	IE	1001	CYC	CHD-C1D-ND	-4.43	115.18	125.32
82	eK	203	PEB	CHC-C1D-ND	-4.43	108.12	113.72
82	NK	201	PEB	C1C-C2C-C3C	-4.42	102.39	107.62
82	kF	203	PEB	C1C-C2C-C3C	-4.42	102.39	107.62
82	kK	203	PEB	C1C-C2C-C3C	-4.42	102.39	107.62
82	QO	201	PEB	C3D-C4D-ND	4.42	115.94	107.26
82	FM	201	PEB	C2C-C1C-NC	4.42	113.53	107.57
82	PF	201	PEB	C1C-C2C-C3C	-4.42	102.39	107.62
82	S9	203	PEB	C1C-C2C-C3C	-4.42	102.39	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iE	202	PEB	C2C-C1C-NC	4.42	113.53	107.57
82	NA	201	PEB	CMB-C2B-C1B	4.42	131.88	125.06
82	dM	202	PEB	CHC-C4C-NC	4.42	127.14	121.15
82	NB	202	PEB	OA-C1A-C2A	-4.42	122.66	126.17
82	FQ	203	PEB	OA-C1A-C2A	-4.42	122.66	126.17
82	FD	201	PEB	C1C-C2C-C3C	-4.42	102.39	107.62
82	K5	202	PEB	C1D-CHC-C4C	-4.42	106.73	113.26
82	YJ	203	PEB	C2C-C1C-NC	4.42	113.53	107.57
82	LF	202	PEB	C3D-C4D-ND	4.42	115.94	107.26
82	CD	202	PEB	C2C-C1C-NC	4.42	113.53	107.57
82	LQ	201	PEB	C2C-C1C-NC	4.42	113.53	107.57
82	CP	202	PEB	CHA-C1B-NB	-4.42	115.68	124.93
82	uF	203	PEB	C1C-C2C-C3C	-4.42	102.39	107.62
82	XJ	202	PEB	CMB-C2B-C1B	4.42	131.87	125.06
82	bF	202	PEB	CHC-C1D-ND	4.42	119.32	113.72
82	cM	201	PEB	CHC-C1D-ND	4.42	119.32	113.72
82	lF	201	PEB	C4B-C3B-C2B	-4.42	101.89	106.78
84	I4	1001	CYC	C2D-C1D-ND	4.42	113.61	107.40
82	BI	201	PEB	CHC-C1D-ND	-4.42	108.13	113.72
84	M1	201	CYC	OB-C4B-C3B	-4.42	123.24	128.04
82	Z9	301	PEB	C3B-C4B-NB	4.42	116.48	110.05
87	72	602	CLA	CAA-C2A-C3A	-4.42	100.67	112.78
82	J9	201	PEB	CHC-C1D-ND	-4.42	108.13	113.72
82	GE	1002	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
82	HI	203	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
85	B6	621	BCR	C33-C5-C6	-4.42	119.56	124.53
82	MM	203	PEB	OA-C1A-C2A	-4.42	122.66	126.17
82	jE	201	PEB	OA-C1A-C2A	-4.42	122.66	126.17
82	pC	201	PEB	C2C-C1C-NC	4.42	113.52	107.57
87	7N	602	CLA	CAA-C2A-C3A	-4.42	100.68	112.78
82	GG	1002	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
82	oF	201	PEB	CHA-C1B-NB	-4.42	115.69	124.93
82	pC	202	PEB	CHA-C4A-NA	-4.42	119.95	125.20
82	dM	202	PEB	C2C-C1C-NC	4.42	113.52	107.57
85	F2	203	BCR	C4-C5-C6	-4.42	116.32	122.73
82	HI	201	PEB	CHC-C1D-ND	-4.42	108.13	113.72
82	GB	203	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
82	QK	201	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
82	D1	1002	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
82	hO	201	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
84	C4	1001	CYC	C2D-C1D-ND	4.42	113.61	107.40
82	TP	201	PEB	C1C-C2C-C3C	-4.42	102.40	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	BG	1001	CYC	C4D-C3D-C2D	-4.42	102.40	107.62
82	jK	201	PEB	C2A-C1A-NA	4.42	112.08	108.27
84	IE	1001	CYC	C2C-C1C-NC	4.42	112.08	108.27
82	eF	201	PEB	CHB-C1C-C2C	-4.42	117.19	127.15
82	YP	503	PEB	C1C-C2C-C3C	-4.42	102.40	107.62
82	XP	201	PEB	C2C-C1C-NC	4.42	113.52	107.57
91	aL	610	PHO	C4A-C3A-C2A	-4.42	98.64	102.84
82	UE	201	PEB	OA-C1A-C2A	-4.42	122.66	126.17
82	gG	201	PEB	C2C-C1C-NC	4.42	113.52	107.57
82	WG	201	PEB	C3D-C4D-ND	4.42	115.92	107.26
82	WF	201	PEB	C1C-C2C-C3C	-4.41	102.40	107.62
82	FQ	201	PEB	CHB-C1C-C2C	-4.41	117.19	127.15
85	L2	205	BCR	C3-C4-C5	-4.41	106.19	114.08
82	XB	201	PEB	C1C-C2C-C3C	-4.41	102.40	107.62
82	BP	202	PEB	C1C-C2C-C3C	-4.41	102.40	107.62
82	m4	202	PEB	C1C-C2C-C3C	-4.41	102.40	107.62
82	xF	304	PEB	C1C-C2C-C3C	-4.41	102.40	107.62
84	IG	1001	CYC	C2C-C1C-NC	4.41	112.08	108.27
82	QM	204	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	VK	202	PEB	OA-C1A-C2A	-4.41	122.66	126.17
82	RG	201	PEB	CMB-C2B-C1B	4.41	131.86	125.06
82	hO	202	PEB	C1C-C2C-C3C	-4.41	102.40	107.62
83	wF	304	PUB	CHA-C1B-NB	4.41	127.12	121.15
82	YJ	202	PEB	CHA-C1B-NB	-4.41	115.70	124.93
82	j1	202	PEB	CHA-C1B-NB	-4.41	115.70	124.93
82	S1	201	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
84	JH	1003	CYC	OB-C4B-C3B	-4.41	123.25	128.04
82	YP	503	PEB	OA-C1A-C2A	-4.41	122.67	126.17
82	L5	203	PEB	OA-C1A-C2A	-4.41	122.67	126.17
82	CQ	202	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	hG	203	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	bP	501	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	VH	201	PEB	CHA-C1B-NB	-4.41	115.70	124.93
82	YD	202	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	YQ	202	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	aO	203	PEB	C4B-C3B-C2B	-4.41	101.90	106.78
87	A2	852	CLA	CHD-C4C-C3C	4.41	131.32	124.84
82	SB	203	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
95	a6	604	DGD	O2G-C1B-C2B	4.41	121.01	111.50
82	RE	202	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	L7	202	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	TQ	202	PEB	OA-C1A-C2A	-4.41	122.67	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	H4	1002	PEB	OA-C1A-C2A	-4.41	122.67	126.17
82	fO	201	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	TQ	201	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	oF	202	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	nK	202	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	CF	201	PEB	OA-C1A-C2A	-4.41	122.67	126.17
82	cO	202	PEB	CHB-C1C-C2C	-4.41	117.20	127.15
82	L1	1002	PEB	C2A-C1A-NA	4.41	112.07	108.27
82	TQ	202	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	D9	203	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	T4	201	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	G7	202	PEB	C2C-C1C-NC	4.41	113.51	107.57
82	vC	202	PEB	CHB-C4B-NB	-4.41	115.41	124.58
84	N1	1001	CYC	C4D-CHA-C1A	4.41	138.16	128.28
82	KD	202	PEB	C2C-C1C-NC	4.41	113.50	107.57
82	XI	201	PEB	C2C-C1C-NC	4.41	113.50	107.57
82	AF	201	PEB	CHA-C1B-NB	-4.41	115.72	124.93
82	CJ	201	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
91	AL	410	PHO	C4A-C3A-C2A	-4.41	98.65	102.84
82	MA	202	PEB	C2C-C1C-NC	4.41	113.50	107.57
82	JP	201	PEB	OA-C1A-C2A	-4.41	122.67	126.17
82	WE	202	PEB	CHC-C4C-NC	4.41	127.11	121.15
82	QK	203	PEB	C3C-C4C-NC	4.41	112.30	108.33
82	SK	202	PEB	C1C-C2C-C3C	-4.41	102.41	107.62
82	SJ	203	PEB	CHB-C1C-C2C	-4.40	117.21	127.15
82	L9	201	PEB	C4B-C3B-C2B	-4.40	101.91	106.78
84	N1	1001	CYC	OB-C4B-C3B	-4.40	123.26	128.04
82	RM	202	PEB	CMB-C2B-C1B	4.40	131.85	125.06
82	S5	202	PEB	C1C-C2C-C3C	-4.40	102.41	107.62
84	FO	1001	CYC	OC-C1C-C2C	-4.40	122.67	126.17
82	RM	201	PEB	CHC-C4C-NC	4.40	127.11	121.15
82	N5	201	PEB	CHA-C1B-NB	-4.40	115.72	124.93
82	RI	201	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	jH	203	PEB	CHB-C1C-C2C	-4.40	117.22	127.15
82	dK	202	PEB	CMC-C3C-C4C	4.40	131.73	127.06
82	P4	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	cG	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	U1	201	PEB	CMB-C2B-C1B	4.40	131.84	125.06
82	E7	202	PEB	CHC-C4C-NC	4.40	127.11	121.15
82	NF	202	PEB	CHC-C4C-NC	-4.40	115.19	121.15
82	H5	203	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	eA	301	PEB	C2C-C1C-NC	4.40	113.50	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IJ	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	HQ	203	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	e4	203	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	QE	201	PEB	C4B-C3B-C2B	-4.40	101.91	106.78
82	u8	201	PEB	CHC-C4C-NC	4.40	127.11	121.15
82	nK	201	PEB	OA-C1A-NA	4.40	130.27	124.94
82	RM	202	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	Q9	203	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	cE	201	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	cJ	201	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	hH	201	PEB	CHA-C1B-NB	-4.40	115.73	124.93
82	D7	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	TI	201	PEB	C3C-C4C-NC	4.40	112.29	108.33
82	VQ	203	PEB	CHA-C1B-NB	-4.40	115.73	124.93
82	UH	201	PEB	C1D-CHC-C4C	4.40	119.75	113.26
92	m6	103	LMG	O7-C10-C11	4.40	120.98	111.50
82	IK	203	PEB	C4B-C3B-C2B	-4.40	101.91	106.78
82	TO	201	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	WG	202	PEB	CHC-C4C-NC	4.40	127.10	121.15
82	OM	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	l4	201	PEB	CMB-C2B-C1B	4.40	131.84	125.06
82	RH	202	PEB	OA-C1A-C2A	-4.40	122.67	126.17
82	U1	203	PEB	CHC-C1D-ND	-4.40	108.16	113.72
82	A5	201	PEB	CHA-C1B-NB	-4.40	115.73	124.93
82	PA	201	PEB	C2C-C1C-NC	4.40	113.50	107.57
82	e4	203	PEB	C2C-C1C-NC	4.40	113.50	107.57
84	F4	1001	CYC	C1B-NB-C4B	-4.40	105.07	110.67
82	MJ	202	PEB	C3D-C4D-ND	4.40	115.89	107.26
82	v8	202	PEB	CHB-C4B-NB	-4.40	115.42	124.58
82	MJ	202	PEB	CHC-C4C-NC	4.40	127.10	121.15
82	LB	201	PEB	CMC-C3C-C4C	4.40	131.72	127.06
83	wK	304	PUB	CMA-C2A-C1A	4.40	131.74	121.39
82	V5	201	PEB	CHA-C1B-NB	-4.40	115.73	124.93
82	l4	202	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	f4	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	lJ	201	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	dH	201	PEB	CHB-C1C-C2C	-4.40	117.23	127.15
82	K5	201	PEB	CHA-C1B-NB	-4.40	115.73	124.93
83	M5	303	PUB	CAC-CBC-CGC	-4.40	104.14	113.60
82	GI	202	PEB	C2C-C1C-NC	4.40	113.49	107.57
82	NG	201	PEB	C2A-C1A-NA	4.40	112.06	108.27
82	S1	201	PEB	CMB-C2B-C1B	4.40	131.84	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	GG	1001	CYC	CMA-C3A-C4A	4.40	131.84	125.06
82	AH	305	PEB	C1C-CHB-C4B	-4.40	118.42	128.28
82	MD	201	PEB	CHC-C1D-ND	-4.40	108.16	113.72
82	E5	201	PEB	CHA-C1B-NB	-4.40	115.73	124.93
82	UH	201	PEB	CMB-C2B-C1B	4.40	131.84	125.06
87	8N	303	CLA	CAC-C3C-C2C	-4.40	120.01	127.53
82	dK	202	PEB	C2C-C1C-NC	4.40	113.49	107.57
82	R7	201	PEB	CMB-C2B-C1B	4.40	131.83	125.06
82	eE	202	PEB	C1C-CHB-C4B	4.40	138.14	128.28
82	nF	201	PEB	OA-C1A-NA	4.40	130.27	124.94
82	eK	201	PEB	CHB-C1C-C2C	-4.40	117.23	127.15
82	jH	202	PEB	CHA-C1B-NB	-4.40	115.74	124.93
82	TD	202	PEB	C1C-C2C-C3C	-4.40	102.42	107.62
82	DM	201	PEB	C2C-C1C-NC	4.39	113.49	107.57
82	gE	201	PEB	C2C-C1C-NC	4.39	113.49	107.57
82	EA	202	PEB	CHC-C4C-NC	4.39	127.10	121.15
82	a4	202	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	aO	202	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	Y5	202	PEB	OA-C1A-C2A	-4.39	122.68	126.17
82	N7	203	PEB	OA-C1A-C2A	-4.39	122.68	126.17
82	u8	202	PEB	OA-C1A-C2A	-4.39	122.68	126.17
82	RA	201	PEB	CMB-C2B-C1B	4.39	131.83	125.06
84	NH	1001	CYC	CMA-C3A-C4A	4.39	131.83	125.06
82	kF	201	PEB	C2C-C1C-NC	4.39	113.49	107.57
85	a6	605	BCR	C15-C14-C13	-4.39	121.04	127.31
82	MQ	201	PEB	CHC-C1D-ND	-4.39	108.17	113.72
82	jM	203	PEB	CHC-C1D-ND	-4.39	108.17	113.72
82	p8	202	PEB	CHA-C4A-NA	-4.39	119.98	125.20
82	NI	203	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	i1	202	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	T1	202	PEB	C2C-C1C-NC	4.39	113.49	107.57
82	QB	203	PEB	OA-C1A-C2A	-4.39	122.68	126.17
84	JH	1003	CYC	OC-C1C-C2C	-4.39	122.68	126.17
82	A7	201	PEB	C2C-C1C-NC	4.39	113.49	107.57
82	dM	201	PEB	CHB-C1C-C2C	-4.39	117.24	127.15
82	KB	302	PEB	C3D-C4D-ND	4.39	115.88	107.26
82	B7	202	PEB	CHC-C1D-ND	-4.39	108.17	113.72
82	W5	201	PEB	C3B-C4B-NB	4.39	116.44	110.05
82	BQ	202	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	LB	201	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	FQ	201	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	q8	201	PEB	C1C-C2C-C3C	-4.39	102.43	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	C5	201	PEB	CHA-C1B-NB	-4.39	115.75	124.93
82	KE	201	PEB	OA-C1A-C2A	-4.39	122.68	126.17
82	JF	202	PEB	OA-C1A-C2A	-4.39	122.68	126.17
82	VE	201	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	JI	201	PEB	C4B-C3B-C2B	-4.39	101.92	106.78
82	SI	201	PEB	C4B-C3B-C2B	-4.39	101.92	106.78
84	K1	1001	CYC	CHD-C1D-ND	-4.39	115.26	125.32
82	M9	302	PEB	C3B-C4B-NB	4.39	116.44	110.05
82	YP	501	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	FD	201	PEB	CHB-C1C-C2C	-4.39	117.25	127.15
82	F7	201	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
82	wC	204	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
87	BN	802	CLA	C1D-ND-C4D	-4.39	103.22	106.33
82	TG	201	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	IB	202	PEB	CHC-C4C-NC	4.39	127.09	121.15
82	SB	203	PEB	CHC-C4C-NC	4.39	127.09	121.15
82	fJ	201	PEB	C1C-C2C-C3C	-4.39	102.43	107.62
84	N1	1001	CYC	CMA-C3A-C4A	4.39	131.82	125.06
84	FG	1001	CYC	C1B-NB-C4B	-4.39	105.08	110.67
82	KP	202	PEB	C3D-C4D-ND	4.39	115.87	107.26
84	y3	1001	CYC	CMA-C3A-C4A	4.39	131.82	125.06
82	d1	201	PEB	CHB-C1C-C2C	-4.39	117.25	127.15
84	NH	1001	CYC	C3D-C4D-ND	4.39	113.48	107.57
82	ZK	202	PEB	CMC-C3C-C4C	4.39	131.71	127.06
82	RE	201	PEB	CMB-C2B-C1B	4.39	131.82	125.06
82	GP	202	PEB	CHC-C4C-NC	4.39	127.09	121.15
82	wC	203	PEB	C1C-C2C-C3C	-4.39	102.44	107.62
82	EI	201	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	YO	201	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	kM	202	PEB	C2C-C1C-NC	4.39	113.48	107.57
84	F4	1001	CYC	C3D-C4D-ND	4.39	113.48	107.57
82	d1	203	PEB	C1D-CHC-C4C	-4.39	106.79	113.26
82	mJ	201	PEB	CMC-C3C-C4C	4.39	131.71	127.06
82	TM	201	PEB	OA-C1A-C2A	-4.39	122.69	126.17
84	LH	1002	CYC	CHD-C1D-ND	-4.39	115.27	125.32
82	KG	201	PEB	C2C-C1C-NC	4.39	113.48	107.57
82	U1	202	PEB	C1C-C2C-C3C	-4.39	102.44	107.62
82	X7	202	PEB	C1D-CHC-C4C	-4.39	106.79	113.26
82	KJ	201	PEB	CHA-C1B-NB	-4.38	115.76	124.93
82	hB	301	PEB	CHC-C4C-NC	4.38	127.08	121.15
82	BF	202	PEB	CMC-C3C-C4C	4.38	131.71	127.06
82	OP	202	PEB	C2C-C1C-NC	4.38	113.47	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gB	203	PEB	C2C-C1C-NC	4.38	113.47	107.57
84	CO	1001	CYC	C3D-C4D-ND	4.38	113.47	107.57
82	VG	202	PEB	OA-C1A-C2A	-4.38	122.69	126.17
82	lO	202	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	YO	203	PEB	CHC-C4C-NC	4.38	127.08	121.15
82	UF	201	PEB	CAC-CBC-CGC	4.38	123.04	113.60
82	XD	203	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	KI	202	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	QJ	204	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	c4	201	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	jJ	202	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	DJ	201	PEB	C1C-CHB-C4B	-4.38	118.45	128.28
82	G5	201	PEB	CHA-C1B-NB	-4.38	115.77	124.93
84	L1	1001	CYC	CAB-C3B-C4B	4.38	128.30	121.38
82	Z5	301	PEB	CHA-C1B-NB	-4.38	115.77	124.93
82	KK	202	PEB	C1C-C2C-C3C	-4.38	102.44	107.62
83	Z5	303	PUB	CAC-CBC-CGC	-4.38	104.17	113.60
84	73	1002	CYC	C3D-C4D-ND	4.38	113.47	107.57
82	QF	201	PEB	C1C-C2C-C3C	-4.38	102.44	107.62
82	ZH	203	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	OM	202	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	AQ	303	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	KQ	202	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	GF	203	PEB	C1C-C2C-C3C	-4.38	102.44	107.62
82	AA	201	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	FJ	202	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	sC	201	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	I5	201	PEB	CHA-C1B-NB	-4.38	115.77	124.93
82	X5	201	PEB	CHA-C1B-NB	-4.38	115.77	124.93
85	HL	103	BCR	C7-C8-C9	-4.38	119.62	126.23
82	WA	202	PEB	CHC-C4C-NC	4.38	127.08	121.15
82	SM	201	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	DB	203	PEB	C1C-C2C-C3C	-4.38	102.44	107.62
82	YH	201	PEB	C1C-C2C-C3C	-4.38	102.44	107.62
82	YM	203	PEB	C1C-C2C-C3C	-4.38	102.44	107.62
82	UM	203	PEB	OA-C1A-C2A	-4.38	122.69	126.17
82	M5	301	PEB	CHA-C1B-NB	-4.38	115.78	124.93
82	NI	201	PEB	C2C-C1C-NC	4.38	113.47	107.57
82	D4	1002	PEB	C1C-C2C-C3C	-4.38	102.45	107.62
82	wC	201	PEB	CHC-C4C-NC	4.38	127.07	121.15
84	LG	1001	CYC	CAD-C3D-C2D	4.38	137.09	127.07
84	MG	1001	CYC	CHD-C1D-ND	-4.38	115.29	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	C6	522	LHG	C5-O7-C7	-4.38	107.02	117.79
82	JM	202	PEB	C2C-C1C-NC	4.38	113.46	107.57
82	YJ	201	PEB	C1C-CHB-C4B	4.38	138.10	128.28
82	T5	201	PEB	CHA-C1B-NB	-4.38	115.78	124.93
82	VP	201	PEB	C1C-C2C-C3C	-4.38	102.45	107.62
82	AI	201	PEB	C2C-C1C-NC	4.38	113.46	107.57
85	cL	504	BCR	C37-C22-C23	4.38	124.97	118.08
84	IO	1001	CYC	C2D-C1D-ND	4.38	113.55	107.40
82	HK	202	PEB	CMB-C2B-C1B	4.38	131.80	125.06
82	eO	203	PEB	C1C-C2C-C3C	-4.38	102.45	107.62
84	KH	1001	CYC	CHD-C1D-ND	-4.37	115.30	125.32
82	oF	203	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	QE	202	PEB	CMB-C2B-C1B	4.37	131.80	125.06
82	FF	202	PEB	CHB-C4B-C3B	-4.37	115.20	125.32
82	VD	203	PEB	CHA-C1B-NB	-4.37	115.78	124.93
82	tC	201	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	iE	201	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	HM	202	PEB	C4B-C3B-C2B	-4.37	101.94	106.78
82	eO	203	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	TD	201	PEB	CHB-C1C-C2C	-4.37	117.28	127.15
82	dB	202	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	O9	201	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	WI	202	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	rF	202	PEB	CMB-C2B-C1B	4.37	131.80	125.06
82	HK	202	PEB	CHB-C4B-C3B	-4.37	115.20	125.32
82	H9	201	PEB	C2C-C1C-NC	4.37	113.46	107.57
84	K4	1001	CYC	C3D-C4D-ND	4.37	113.46	107.57
82	WK	201	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	TI	201	PEB	C1D-CHC-C4C	-4.37	106.81	113.26
82	VI	201	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	JA	203	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	CF	203	PEB	C1D-CHC-C4C	-4.37	106.81	113.26
84	L1	1001	CYC	CHD-C1D-ND	-4.37	115.31	125.32
82	TJ	201	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	Q9	202	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
84	BE	1001	CYC	C4D-C3D-C2D	-4.37	102.45	107.62
95	c6	601	DGD	O3E-C3E-C2E	-4.37	100.25	110.35
82	HD	203	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	ZF	202	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	iM	201	PEB	C2C-C1C-NC	4.37	113.46	107.57
82	SQ	202	PEB	C1D-CHC-C4C	4.37	119.70	113.26
82	HF	202	PEB	CHB-C4B-C3B	-4.37	115.21	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TH	202	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	cE	201	PEB	C1C-C2C-C3C	-4.37	102.45	107.62
82	TI	202	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	xF	303	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	xK	302	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	VQ	201	PEB	C4B-C3B-C2B	-4.37	101.95	106.78
85	LN	205	BCR	C3-C4-C5	-4.37	106.28	114.08
82	P5	201	PEB	CHA-C1B-NB	-4.37	115.79	124.93
82	R5	201	PEB	CHA-C1B-NB	-4.37	115.79	124.93
82	TD	202	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	yK	301	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	FB	201	PEB	C1C-C2C-C3C	-4.37	102.46	107.62
84	W3	1001	CYC	CMA-C3A-C4A	4.37	131.79	125.06
82	dF	202	PEB	CMC-C3C-C4C	4.37	131.69	127.06
82	J5	202	PEB	CHB-C1C-C2C	-4.37	117.29	127.15
82	SI	201	PEB	CHC-C1D-ND	-4.37	108.20	113.72
82	HQ	203	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	J5	201	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	BA	202	PEB	CHC-C1D-ND	-4.37	108.20	113.72
82	bK	201	PEB	CMB-C2B-C1B	4.37	131.79	125.06
95	C6	502	DGD	O3E-C3E-C2E	-4.37	100.25	110.35
82	LH	1003	PEB	C2A-C1A-NA	4.37	112.04	108.27
82	L7	203	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	UH	203	PEB	CHC-C1D-ND	-4.37	108.20	113.72
84	HG	1001	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
82	DD	201	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	tK	203	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	ZJ	202	PEB	C1C-C2C-C3C	-4.37	102.46	107.62
84	LH	1002	CYC	CAB-C3B-C4B	4.37	128.28	121.38
82	YI	201	PEB	CHC-C1D-ND	-4.37	108.20	113.72
82	SM	202	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	WM	203	PEB	C1C-C2C-C3C	-4.37	102.46	107.62
82	iO	201	PEB	C1C-C2C-C3C	-4.37	102.46	107.62
82	SO	202	PEB	C3D-C4D-ND	4.37	115.82	107.26
82	TJ	201	PEB	OA-C1A-C2A	-4.37	122.70	126.17
82	jJ	203	PEB	OA-C1A-C2A	-4.37	122.70	126.17
103	8N	310	ZEX	C1-C6-C7	4.37	128.13	115.78
82	QP	201	PEB	C2C-C1C-NC	4.37	113.45	107.57
82	OI	202	PEB	CHA-C1B-C2B	4.37	136.12	124.90
82	g4	201	PEB	C1C-C2C-C3C	-4.36	102.46	107.62
82	GK	203	PEB	C2C-C1C-NC	4.36	113.45	107.57
83	Z9	305	PUB	OD-C4D-C3D	-4.36	123.30	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	f1	202	PEB	C1C-CHB-C4B	-4.36	118.50	128.28
84	DO	1001	CYC	CMA-C3A-C4A	4.36	131.78	125.06
82	hJ	203	PEB	C2C-C1C-NC	4.36	113.45	107.57
82	bO	202	PEB	C2C-C1C-NC	4.36	113.45	107.57
84	CG	1001	CYC	CMD-C2D-C1D	4.36	131.95	125.56
82	XQ	203	PEB	OA-C1A-C2A	-4.36	122.70	126.17
82	GA	202	PEB	C2C-C1C-NC	4.36	113.45	107.57
82	IQ	202	PEB	C2C-C1C-NC	4.36	113.45	107.57
82	O4	202	PEB	C2C-C1C-NC	4.36	113.45	107.57
85	c6	602	BCR	C3-C4-C5	-4.36	106.29	114.08
82	ZK	202	PEB	C2C-C1C-NC	4.36	113.44	107.57
83	xF	301	PUB	C3B-C4B-NB	4.36	113.44	107.57
82	eG	202	PEB	C1C-CHB-C4B	4.36	138.06	128.28
82	CB	201	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	IB	202	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	UH	202	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	UK	202	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	SD	201	PEB	C4B-C3B-C2B	-4.36	101.95	106.78
82	NB	202	PEB	C2C-C1C-NC	4.36	113.44	107.57
82	II	201	PEB	C2C-C1C-NC	4.36	113.44	107.57
82	AP	201	PEB	C3D-C4D-ND	4.36	115.82	107.26
82	mM	202	PEB	CMB-C2B-C1B	4.36	131.78	125.06
84	JO	1001	CYC	C1B-C2B-C3B	-4.36	103.32	107.87
82	nF	202	PEB	C2C-C1C-NC	4.36	113.44	107.57
82	z8	201	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	oF	203	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	FJ	201	PEB	OD-C4D-ND	-4.36	119.47	125.93
82	QB	204	PEB	CMC-C3C-C4C	4.36	131.68	127.06
82	XA	203	PEB	CHC-C1D-ND	-4.36	108.21	113.72
85	aL	604	BCR	C15-C14-C13	-4.36	121.09	127.31
82	cJ	202	PEB	C1C-CHB-C4B	-4.36	118.50	128.28
84	J1	1001	CYC	OB-C4B-C3B	-4.36	123.31	128.04
82	TD	201	PEB	C2C-C1C-NC	4.36	113.44	107.57
82	PM	201	PEB	C2C-C1C-NC	4.36	113.44	107.57
82	MK	201	PEB	CHC-C4C-NC	4.36	127.05	121.15
82	SQ	201	PEB	C4B-C3B-C2B	-4.36	101.96	106.78
82	OH	203	PEB	CHC-C1D-ND	-4.36	108.21	113.72
87	B2	801	CLA	C1D-ND-C4D	-4.36	103.24	106.33
82	F1	1002	PEB	C2A-C1A-NA	4.36	112.03	108.27
82	H9	201	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
83	AQ	302	PUB	CMA-C2A-C1A	4.36	131.64	121.39
82	lK	201	PEB	C4B-C3B-C2B	-4.36	101.96	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WJ	203	PEB	C3C-C4C-NC	4.36	112.25	108.33
82	DH	1002	PEB	C2C-C1C-NC	4.36	113.44	107.57
82	Y1	201	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	dH	203	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
85	FN	204	BCR	C3-C4-C5	-4.36	106.30	114.08
82	HD	203	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	w8	203	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
82	bK	201	PEB	C1C-C2C-C3C	-4.36	102.47	107.62
84	CO	1001	CYC	C2D-C1D-ND	4.36	113.52	107.40
82	OI	203	PEB	C2C-C1C-NC	4.36	113.44	107.57
84	GE	1001	CYC	CMA-C3A-C4A	4.36	131.77	125.06
84	JH	1001	CYC	OB-C4B-C3B	-4.36	123.31	128.04
82	h1	202	PEB	CHA-C1B-NB	-4.36	115.82	124.93
82	hJ	202	PEB	CHC-C4C-NC	4.36	127.04	121.15
82	KF	201	PEB	OA-C1A-C2A	-4.36	122.71	126.17
84	FE	1002	CYC	OC-C1C-C2C	-4.36	122.71	126.17
82	S4	202	PEB	C3D-C4D-ND	4.36	115.80	107.26
83	BM	302	PUB	OD-C4D-C3D	-4.35	123.31	128.04
82	DQ	201	PEB	C1C-C2C-C3C	-4.35	102.47	107.62
82	A7	201	PEB	C1C-C2C-C3C	-4.35	102.47	107.62
84	CO	1001	CYC	C1D-C2D-C3D	-4.35	102.25	107.79
82	s8	201	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	cF	203	PEB	C3D-C4D-ND	4.35	115.80	107.26
94	D6	408	PL9	C10-C9-C11	4.35	122.59	115.27
82	LA	202	PEB	C1C-C2C-C3C	-4.35	102.47	107.62
82	J5	203	PEB	C1C-C2C-C3C	-4.35	102.47	107.62
82	II	201	PEB	CMB-C2B-C1B	4.35	131.77	125.06
84	M4	1001	CYC	CMD-C2D-C1D	4.35	131.93	125.56
82	cK	203	PEB	C3D-C4D-ND	4.35	115.80	107.26
82	eB	202	PEB	CHC-C1D-ND	-4.35	108.22	113.72
84	DH	1003	CYC	C1B-C2B-C3B	-4.35	103.33	107.87
82	tF	201	PEB	OA-C1A-NA	4.35	130.21	124.94
82	EJ	202	PEB	CMB-C2B-C1B	4.35	131.76	125.06
82	EF	202	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
84	C1	1001	CYC	CHB-C4A-NA	-4.35	115.83	124.93
82	PI	201	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	MJ	203	PEB	OA-C1A-C2A	-4.35	122.71	126.17
82	ZB	203	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	FD	202	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	p8	202	PEB	CBA-CAA-C3A	-4.35	103.78	113.47
85	H6	101	BCR	C3-C4-C5	-4.35	106.31	114.08
82	YJ	203	PEB	C1C-C2C-C3C	-4.35	102.48	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	H5	203	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
82	t8	201	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
82	MM	202	PEB	CHA-C1B-NB	-4.35	115.83	124.93
82	TG	201	PEB	CHC-C1D-ND	-4.35	108.22	113.72
82	Y4	201	PEB	CHC-C1D-ND	-4.35	108.22	113.72
84	C4	1001	CYC	C3D-C4D-ND	4.35	113.43	107.57
82	VI	203	PEB	C1B-C2B-C3B	-4.35	101.51	106.51
82	uC	202	PEB	OA-C1A-C2A	-4.35	122.72	126.17
82	DA	201	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
103	82	310	ZEX	C1-C6-C7	4.35	128.08	115.78
82	CI	201	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	GJ	202	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	P1	201	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	iO	201	PEB	C2C-C1C-NC	4.35	113.43	107.57
82	cB	402	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
82	gO	201	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
82	jM	203	PEB	OA-C1A-C2A	-4.35	122.72	126.17
82	VJ	201	PEB	C3D-C4D-ND	4.35	115.79	107.26
82	QG	202	PEB	CMB-C2B-C1B	4.35	131.76	125.06
82	F9	201	PEB	C3B-C4B-NB	4.35	116.37	110.05
82	TK	202	PEB	CMB-C2B-C1B	4.35	131.76	125.06
82	AI	203	PEB	C3C-C4C-NC	4.35	112.25	108.33
82	M7	201	PEB	C3D-C4D-ND	4.35	115.79	107.26
82	MB	201	PEB	C2C-C1C-NC	4.35	113.42	107.57
82	fB	301	PEB	CHC-C4C-NC	4.35	127.03	121.15
82	lM	202	PEB	CHA-C1B-NB	-4.35	115.84	124.93
82	FI	202	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
82	gF	202	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
82	lO	201	PEB	C3B-C4B-NB	4.35	116.37	110.05
87	82	302	CLA	CAC-C3C-C2C	-4.35	120.10	127.53
82	IF	203	PEB	C3D-C4D-ND	4.35	115.78	107.26
82	N5	202	PEB	C1C-C2C-C3C	-4.35	102.48	107.62
85	bL	602	BCR	C24-C23-C22	-4.35	119.67	126.23
82	FH	1002	PEB	C2A-C1A-NA	4.35	112.02	108.27
82	JK	202	PEB	OA-C1A-C2A	-4.35	122.72	126.17
82	dF	202	PEB	OA-C1A-C2A	-4.35	122.72	126.17
82	NM	201	PEB	C4B-C3B-C2B	-4.35	101.97	106.78
82	II	203	PEB	CHA-C1B-C2B	4.34	136.07	124.90
82	hJ	202	PEB	C2C-C1C-NC	4.34	113.42	107.57
82	oK	202	PEB	C2C-C1C-NC	4.34	113.42	107.57
82	pK	201	PEB	CHA-C4A-NA	4.34	130.37	125.20
82	iF	201	PEB	C3D-C4D-ND	4.34	115.78	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DI	202	PEB	OA-C1A-C2A	-4.34	122.72	126.17
84	G4	1001	CYC	C2B-C1B-NB	4.34	113.35	106.99
85	H6	101	BCR	C28-C27-C26	-4.34	106.32	114.08
82	xK	303	PEB	C2C-C1C-NC	4.34	113.42	107.57
82	DI	201	PEB	CAC-C2C-C1C	4.34	132.68	125.76
82	JQ	202	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	JQ	203	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
84	N4	1001	CYC	CHB-C4A-NA	-4.34	115.85	124.93
82	bK	202	PEB	CHC-C1D-ND	4.34	119.22	113.72
82	MP	203	PEB	OA-C1A-C2A	-4.34	122.72	126.17
82	RI	203	PEB	OD-C4D-ND	-4.34	119.50	125.93
82	Q1	202	PEB	C2C-C1C-NC	4.34	113.42	107.57
82	D5	201	PEB	C3B-C4B-NB	4.34	116.36	110.05
82	Y4	202	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
84	CH	1001	CYC	CHB-C4A-NA	-4.34	115.85	124.93
85	F2	204	BCR	C3-C4-C5	-4.34	106.33	114.08
82	AI	203	PEB	C1B-C2B-C3B	-4.34	101.52	106.51
82	FA	201	PEB	C2C-C1C-NC	4.34	113.42	107.57
82	IK	203	PEB	C3D-C4D-ND	4.34	115.78	107.26
82	RP	202	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	J4	1002	PEB	OA-C1A-C2A	-4.34	122.72	126.17
82	UM	201	PEB	CHB-C1C-C2C	-4.34	117.36	127.15
85	BL	617	BCR	C24-C23-C22	-4.34	119.68	126.23
82	HA	203	PEB	C4B-C3B-C2B	-4.34	101.98	106.78
83	A4	302	PUB	C1C-C2C-C3C	-4.34	101.98	106.78
82	RE	202	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	U9	204	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	mO	203	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	Y7	303	PEB	CHB-C4B-NB	-4.34	115.55	124.58
82	RQ	202	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	XQ	201	PEB	C1C-CHB-C4B	4.34	138.01	128.28
82	AI	201	PEB	CMB-C2B-C1B	4.34	131.75	125.06
82	VI	201	PEB	CMB-C2B-C1B	4.34	131.75	125.06
84	MG	1001	CYC	CMA-C3A-C4A	4.34	131.75	125.06
82	ZG	201	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	i4	201	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	X7	203	PEB	CHC-C1D-ND	-4.34	108.23	113.72
82	CF	201	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	f4	202	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	U7	202	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	JJ	201	PEB	C1D-CHC-C4C	4.34	119.65	113.26
82	EI	201	PEB	CMB-C2B-C1B	4.34	131.74	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WJ	201	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	FK	202	PEB	CHB-C4B-C3B	-4.34	115.28	125.32
87	32	304	CLA	CED-O2D-CGD	4.34	125.75	115.94
82	CI	201	PEB	CMB-C2B-C1B	4.34	131.74	125.06
82	YK	203	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	HM	202	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	O1	203	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	hG	202	PEB	C1C-C2C-C3C	-4.34	102.49	107.62
82	NM	201	PEB	CHC-C1D-ND	4.34	119.21	113.72
95	C6	503	DGD	O6D-C1D-C2D	-4.34	101.17	110.35
83	M5	302	PUB	CMA-C2A-C1A	4.34	131.59	121.39
82	RG	202	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	eH	201	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	RG	202	PEB	C1C-C2C-C3C	-4.34	102.50	107.62
82	J9	201	PEB	C1C-C2C-C3C	-4.34	102.50	107.62
82	Z1	201	PEB	C2A-C1A-NA	4.34	112.01	108.27
82	Q5	202	PEB	C1C-CHB-C4B	4.34	138.01	128.28
82	CK	202	PEB	CMB-C2B-C1B	4.34	131.74	125.06
82	F7	202	PEB	CHB-C1C-C2C	-4.34	117.37	127.15
82	FQ	202	PEB	C2C-C1C-NC	4.34	113.41	107.57
82	lM	203	PEB	OA-C1A-C2A	-4.34	122.73	126.17
82	WP	202	PEB	C3D-C4D-ND	4.33	115.76	107.26
84	LH	1002	CYC	CHB-C1B-NB	-4.33	116.75	126.06
82	bF	202	PEB	C1C-CHB-C4B	4.33	138.00	128.28
82	GI	202	PEB	CMB-C2B-C1B	4.33	131.74	125.06
82	zF	501	PEB	CMB-C2B-C1B	4.33	131.74	125.06
82	g1	201	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	CJ	201	PEB	CHA-C1B-NB	-4.33	115.87	124.93
82	s8	202	PEB	CHB-C1C-C2C	-4.33	117.37	127.15
82	KI	202	PEB	CMB-C2B-C1B	4.33	131.74	125.06
83	Z5	302	PUB	CMA-C2A-C1A	4.33	131.58	121.39
82	DQ	203	PEB	CHC-C1D-ND	-4.33	108.24	113.72
82	DM	201	PEB	OA-C1A-C2A	-4.33	122.73	126.17
82	m4	203	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	mJ	201	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
84	FO	1001	CYC	C3D-C4D-ND	4.33	113.41	107.57
84	NH	1001	CYC	C4D-CHA-C1A	4.33	138.00	128.28
82	YF	202	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	g4	203	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	jO	201	PEB	C3B-C4B-NB	4.33	116.35	110.05
82	pC	202	PEB	CBA-CAA-C3A	-4.33	103.82	113.47
82	BB	201	PEB	C1C-C2C-C3C	-4.33	102.50	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	d1	203	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	w8	204	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	iG	201	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	e1	201	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	W1	202	PEB	CHA-C1B-NB	-4.33	115.87	124.93
82	H9	203	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	IP	203	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	V5	202	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
84	FE	1002	CYC	C1B-NB-C4B	-4.33	105.16	110.67
82	HF	202	PEB	CMB-C2B-C1B	4.33	131.73	125.06
82	XK	203	PEB	CMB-C2B-C1B	4.33	131.73	125.06
82	zK	501	PEB	CMB-C2B-C1B	4.33	131.73	125.06
82	l1	201	PEB	CHB-C1C-C2C	-4.33	117.38	127.15
82	cE	202	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	TQ	201	PEB	CHB-C1C-C2C	-4.33	117.38	127.15
82	eH	202	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	FA	202	PEB	CHB-C1C-C2C	-4.33	117.39	127.15
82	D1	1002	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	N7	201	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	cG	202	PEB	C2C-C1C-NC	4.33	113.40	107.57
84	DH	1003	CYC	C2D-C1D-ND	4.33	113.48	107.40
85	AN	846	BCR	C23-C22-C21	4.33	125.58	118.94
82	HD	201	PEB	OA-C1A-C2A	-4.33	122.73	126.17
82	K5	202	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
82	P5	202	PEB	C1C-C2C-C3C	-4.33	102.50	107.62
83	AE	302	PUB	C4B-C3B-C2B	-4.33	102.50	107.62
84	C4	1001	CYC	C1D-C2D-C3D	-4.33	102.28	107.79
82	XI	201	PEB	CMB-C2B-C1B	4.33	131.73	125.06
82	Z1	202	PEB	CHC-C4C-NC	4.33	127.01	121.15
82	W7	202	PEB	CHC-C4C-NC	4.33	127.01	121.15
82	JD	202	PEB	C1C-C2C-C3C	-4.33	102.51	107.62
82	cK	203	PEB	C1C-C2C-C3C	-4.33	102.51	107.62
82	JF	201	PEB	CHC-C4C-NC	4.33	127.00	121.15
82	eB	201	PEB	CHC-C4C-NC	4.33	127.00	121.15
82	HM	202	PEB	C2C-C1C-NC	4.33	113.40	107.57
84	LE	1001	CYC	CAD-C3D-C2D	4.33	136.98	127.07
82	I7	202	PEB	C1C-C2C-C3C	-4.33	102.51	107.62
82	UA	202	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	RD	202	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	B5	201	PEB	C2C-C1C-NC	4.33	113.40	107.57
82	l4	201	PEB	CHB-C4B-C3B	-4.33	115.31	125.32
82	BB	202	PEB	C1C-C2C-C3C	-4.33	102.51	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bF	201	PEB	C1C-C2C-C3C	-4.33	102.51	107.62
82	wC	203	PEB	C2C-C1C-NC	4.32	113.39	107.57
83	AD	302	PUB	CMA-C2A-C1A	4.32	131.56	121.39
82	OH	203	PEB	C1C-C2C-C3C	-4.32	102.51	107.62
82	KM	203	PEB	C1C-C2C-C3C	-4.32	102.51	107.62
82	hJ	202	PEB	C1C-C2C-C3C	-4.32	102.51	107.62
82	YK	202	PEB	C2C-C1C-NC	4.32	113.39	107.57
82	OO	202	PEB	C2C-C1C-NC	4.32	113.39	107.57
82	bK	202	PEB	C1C-CHB-C4B	4.32	137.98	128.28
82	KG	201	PEB	OA-C1A-C2A	-4.32	122.73	126.17
82	fG	203	PEB	OA-C1A-C2A	-4.32	122.73	126.17
82	CQ	202	PEB	C2C-C1C-NC	4.32	113.39	107.57
87	3N	305	CLA	CED-O2D-CGD	4.32	125.72	115.94
82	OA	202	PEB	CHC-C4C-NC	4.32	127.00	121.15
82	WH	202	PEB	CHA-C1B-NB	-4.32	115.89	124.93
82	PI	201	PEB	CMB-C2B-C1B	4.32	131.72	125.06
82	mM	201	PEB	C2C-C1C-NC	4.32	113.39	107.57
82	TE	201	PEB	CHC-C1D-ND	-4.32	108.25	113.72
82	P4	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
82	kF	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
82	j4	201	PEB	C3B-C4B-NB	4.32	116.34	110.05
82	QK	201	PEB	CHB-C1C-C2C	-4.32	117.40	127.15
82	sC	202	PEB	C1C-CHB-C4B	4.32	137.97	128.28
82	hE	203	PEB	C1C-C2C-C3C	-4.32	102.51	107.62
82	a4	203	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
82	ZJ	201	PEB	CMC-C3C-C4C	4.32	131.64	127.06
82	DD	203	PEB	CHC-C1D-ND	-4.32	108.26	113.72
82	WJ	201	PEB	C3D-C4D-ND	4.32	115.74	107.26
82	zC	201	PEB	C1C-C2C-C3C	-4.32	102.51	107.62
82	M9	305	PEB	C1C-C2C-C3C	-4.32	102.51	107.62
84	HE	1001	CYC	C1B-C2B-C3B	-4.32	103.36	107.87
84	D4	1001	CYC	CMA-C3A-C4A	4.32	131.72	125.06
94	dL	406	PL9	C7-C3-C2	-4.32	117.62	123.30
82	aB	201	PEB	CHC-C4C-NC	4.32	127.00	121.15
82	xF	302	PEB	C2C-C1C-NC	4.32	113.39	107.57
82	TI	202	PEB	CMB-C2B-C1B	4.32	131.72	125.06
82	bB	201	PEB	CHC-C1D-ND	-4.32	108.26	113.72
82	GB	202	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
82	MM	201	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
82	J9	203	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
87	b6	605	CLA	CHB-C1B-NB	4.32	128.83	124.26
82	tK	203	PEB	C1C-C2C-C3C	-4.32	102.52	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lM	203	PEB	C2C-C1C-NC	4.32	113.39	107.57
82	eH	202	PEB	CHA-C1B-NB	-4.32	115.90	124.93
82	NA	201	PEB	C2C-C1C-NC	4.32	113.39	107.57
82	HE	1002	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
82	RM	201	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
82	hE	202	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
82	MA	201	PEB	C3D-C4D-ND	4.32	115.73	107.26
82	lO	201	PEB	CHB-C4B-C3B	-4.32	115.33	125.32
85	c6	617	BCR	C35-C13-C14	-4.32	116.88	122.92
82	PH	201	PEB	C2C-C1C-NC	4.32	113.38	107.57
82	G5	202	PEB	C1C-C2C-C3C	-4.32	102.52	107.62
82	eM	201	PEB	CHA-C1B-NB	-4.32	115.90	124.93
82	bF	202	PEB	C3D-C4D-ND	4.32	115.73	107.26
82	VE	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
82	RI	201	PEB	CMB-C2B-C1B	4.32	131.71	125.06
83	QJ	201	PUB	C1C-C2C-C3C	-4.32	102.00	106.78
82	CJ	201	PEB	CHC-C4C-NC	4.32	126.99	121.15
82	gB	202	PEB	CHC-C4C-NC	4.32	126.99	121.15
83	yK	302	PUB	CHA-C1B-NB	4.32	126.99	121.15
82	e1	202	PEB	C2C-C1C-NC	4.32	113.38	107.57
82	aE	201	PEB	CAC-C2C-C1C	4.32	132.64	125.76
82	OB	201	PEB	C2C-C1C-NC	4.32	113.38	107.57
82	18	203	PEB	C2C-C1C-NC	4.32	113.38	107.57
82	fF	201	PEB	CHA-C1B-NB	-4.32	115.91	124.93
82	l4	201	PEB	C3B-C4B-NB	4.32	116.33	110.05
82	OI	201	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	YK	202	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	GM	203	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	cH	201	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	dH	203	PEB	C1D-CHC-C4C	-4.31	106.89	113.26
82	FJ	202	PEB	CMB-C2B-C1B	4.31	131.71	125.06
82	UF	202	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	X5	202	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	T7	201	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	fE	202	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	gO	203	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
82	PA	202	PEB	CHC-C1D-ND	-4.31	108.27	113.72
82	JB	202	PEB	C2C-C1C-NC	4.31	113.38	107.57
84	GO	1001	CYC	C2B-C1B-NB	4.31	113.30	106.99
92	B6	619	LMG	O7-C10-C11	4.31	120.80	111.50
82	e1	202	PEB	CHA-C1B-NB	-4.31	115.91	124.93
82	cO	202	PEB	C1C-CHB-C4B	4.31	137.95	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VH	201	PEB	C2C-C1C-NC	4.31	113.38	107.57
82	vF	201	PEB	OA-C1A-NA	4.31	130.16	124.94
82	WP	202	PEB	CHC-C4C-NC	4.31	126.98	121.15
82	LI	201	PEB	C1C-C2C-C3C	-4.31	102.52	107.62
85	B2	838	BCR	C20-C21-C22	-4.31	121.16	127.31
84	I1	1001	CYC	CAB-C3B-C4B	4.31	128.19	121.38
82	ZH	202	PEB	CHC-C4C-NC	4.31	126.98	121.15
84	L1	1001	CYC	CHB-C1B-NB	-4.31	116.80	126.06
82	DO	1002	PEB	C1C-C2C-C3C	-4.31	102.53	107.62
82	QB	204	PEB	OA-C1A-C2A	-4.31	122.75	126.17
82	fE	203	PEB	OA-C1A-C2A	-4.31	122.75	126.17
82	AA	201	PEB	C1C-C2C-C3C	-4.31	102.53	107.62
83	Y7	302	PUB	C4B-C3B-C2B	-4.31	102.53	107.62
84	NH	1001	CYC	OB-C4B-C3B	-4.31	123.36	128.04
95	O6	301	DGD	O2G-C1B-C2B	4.31	120.79	111.50
95	C6	502	DGD	C3G-O3G-C1D	-4.31	105.32	113.74
82	iK	201	PEB	CHB-C1C-C2C	-4.31	117.43	127.15
82	DD	201	PEB	C1C-C2C-C3C	-4.31	102.53	107.62
82	aG	201	PEB	CAC-C2C-C1C	4.31	132.62	125.76
82	fM	201	PEB	CHC-C4C-NC	4.31	126.98	121.15
82	FQ	203	PEB	CHA-C1B-C2B	4.31	135.98	124.90
82	rK	202	PEB	CMB-C2B-C1B	4.31	131.70	125.06
84	LH	1001	CYC	CHB-C4A-NA	-4.31	115.92	124.93
82	bP	502	PEB	C1C-C2C-C3C	-4.31	102.53	107.62
87	6N	612	CLA	CMD-C2D-C3D	-4.31	117.70	127.61
84	EE	1001	CYC	CMA-C3A-C4A	4.31	131.70	125.06
82	U1	201	PEB	C1D-CHC-C4C	4.31	119.61	113.26
82	O1	203	PEB	CHC-C1D-ND	-4.31	108.27	113.72
82	VB	201	PEB	OA-C1A-C2A	-4.31	122.75	126.17
82	kJ	202	PEB	OA-C1A-C2A	-4.31	122.75	126.17
84	FE	1001	CYC	CMD-C2D-C1D	4.31	131.87	125.56
82	IB	201	PEB	C1C-C2C-C3C	-4.31	102.53	107.62
82	NI	201	PEB	CMB-C2B-C1B	4.31	131.70	125.06
82	F7	201	PEB	C2C-C1C-NC	4.31	113.37	107.57
82	Y7	303	PEB	CHA-C1B-NB	-4.31	115.92	124.93
82	MM	201	PEB	CHB-C1C-C2C	-4.31	117.43	127.15
85	BN	838	BCR	C20-C21-C22	-4.31	121.16	127.31
83	AQ	302	PUB	C3B-C4B-NB	4.31	113.37	107.57
82	NP	202	PEB	CHA-C1B-NB	-4.31	115.92	124.93
82	D7	202	PEB	CHA-C1B-NB	-4.31	115.92	124.93
84	J1	1001	CYC	C2D-C1D-ND	4.31	113.45	107.40
82	bH	202	PEB	C1D-CHC-C4C	-4.31	106.91	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gO	203	PEB	C2C-C1C-NC	4.31	113.37	107.57
83	yK	302	PUB	C3B-C4B-NB	4.31	113.37	107.57
84	J4	1001	CYC	C1B-C2B-C3B	-4.31	103.38	107.87
82	NB	201	PEB	CHC-C1D-ND	-4.31	108.28	113.72
82	BF	201	PEB	OD-C4D-C3D	-4.31	119.70	129.46
82	QI	201	PEB	C2C-C1C-NC	4.30	113.37	107.57
82	ZO	201	PEB	C3D-C4D-ND	4.30	115.70	107.26
82	VB	201	PEB	C1C-C2C-C3C	-4.30	102.53	107.62
82	ZH	201	PEB	C2A-C1A-NA	4.30	111.98	108.27
82	XA	202	PEB	C1D-CHC-C4C	-4.30	106.91	113.26
82	BA	202	PEB	CHB-C1C-C2C	-4.30	117.44	127.15
82	fH	202	PEB	C1C-CHB-C4B	-4.30	118.63	128.28
82	GJ	201	PEB	C1C-C2C-C3C	-4.30	102.53	107.62
82	lG	201	PEB	C1C-C2C-C3C	-4.30	102.53	107.62
82	KB	302	PEB	CHC-C4C-NC	4.30	126.97	121.15
85	A2	846	BCR	C23-C22-C21	4.30	125.55	118.94
87	62	313	CLA	CMD-C2D-C3D	-4.30	117.71	127.61
82	WB	401	PEB	C2C-C1C-NC	4.30	113.37	107.57
82	dF	202	PEB	C2C-C1C-NC	4.30	113.37	107.57
85	A2	804	BCR	C11-C10-C9	-4.30	121.17	127.31
82	fK	201	PEB	CHA-C1B-NB	-4.30	115.93	124.93
82	LA	203	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	GF	201	PEB	CMC-C3C-C4C	4.30	131.62	127.06
82	FJ	201	PEB	C2A-C1A-NA	4.30	111.98	108.27
82	DQ	202	PEB	OD-C4D-ND	-4.30	119.56	125.93
84	I1	1001	CYC	CHB-C4A-NA	-4.30	115.93	124.93
82	QB	204	PEB	C1C-C2C-C3C	-4.30	102.53	107.62
84	HO	1001	CYC	C2B-C1B-NB	4.30	113.29	106.99
82	GP	203	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	UJ	202	PEB	C3D-C4D-ND	4.30	115.70	107.26
83	M9	303	PUB	OD-C4D-C3D	-4.30	123.37	128.04
82	lE	201	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	O9	202	PEB	CHA-C1B-NB	-4.30	115.94	124.93
82	ID	202	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	hK	201	PEB	C1D-CHC-C4C	-4.30	106.91	113.26
82	Y4	203	PEB	CHC-C4C-NC	4.30	126.97	121.15
87	6N	608	CLA	CMA-C3A-C4A	4.30	123.33	111.77
82	LI	202	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	ZK	201	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	w8	203	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	fF	201	PEB	OA-C1A-NA	4.30	130.15	124.94
82	YM	203	PEB	OA-C1A-C2A	-4.30	122.75	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	F7	203	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	g4	203	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	GE	1002	PEB	C3D-C4D-ND	4.30	115.69	107.26
82	iF	201	PEB	CHB-C1C-C2C	-4.30	117.45	127.15
82	mM	202	PEB	C2C-C1C-NC	4.30	113.36	107.57
82	MP	203	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	MK	203	PEB	C3C-C4C-NC	4.30	112.20	108.33
82	VJ	202	PEB	CMB-C2B-C1B	4.30	131.68	125.06
83	AD	302	PUB	C3B-C4B-NB	4.30	113.36	107.57
82	Y7	303	PEB	CHB-C1C-NC	-4.30	115.47	125.32
82	LQ	203	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	C5	202	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	F9	202	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	uF	201	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
83	AG	302	PUB	C4B-C3B-C2B	-4.30	102.54	107.62
95	c6	601	DGD	O5D-C1E-C2E	4.30	115.01	108.30
82	QF	201	PEB	CHB-C1C-C2C	-4.30	117.45	127.15
82	sC	202	PEB	CHB-C1C-C2C	-4.30	117.45	127.15
82	bF	201	PEB	CMB-C2B-C1B	4.30	131.68	125.06
82	RA	202	PEB	C4B-C3B-C2B	-4.30	102.03	106.78
82	ZI	401	PEB	C3B-C4B-NB	4.30	116.30	110.05
82	iK	201	PEB	C3D-C4D-ND	4.30	115.69	107.26
82	pC	202	PEB	CHA-C1B-NB	-4.30	115.94	124.93
84	63	901	CYC	CMA-C3A-C4A	4.30	131.68	125.06
82	fM	203	PEB	CHB-C1C-C2C	-4.30	117.46	127.15
82	YA	303	PEB	CHB-C4B-NB	-4.30	115.64	124.58
82	WF	203	PEB	CHA-C1B-NB	-4.30	115.94	124.93
82	SD	202	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	TF	202	PEB	CMB-C2B-C1B	4.30	131.68	125.06
82	U9	201	PEB	C2C-C1C-NC	4.30	113.36	107.57
85	kL	100	BCR	C33-C5-C6	-4.30	119.70	124.53
82	s8	202	PEB	C1C-CHB-C4B	4.30	137.92	128.28
82	MA	201	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	iF	202	PEB	C1C-C2C-C3C	-4.30	102.54	107.62
82	tK	201	PEB	OA-C1A-NA	4.30	130.14	124.94
82	i4	201	PEB	C2C-C1C-NC	4.30	113.36	107.57
85	AN	804	BCR	C11-C10-C9	-4.30	121.18	127.31
82	B7	202	PEB	CHB-C1C-C2C	-4.30	117.46	127.15
82	FM	201	PEB	OA-C1A-C2A	-4.30	122.76	126.17
82	gJ	202	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	b1	202	PEB	C1D-CHC-C4C	-4.29	106.92	113.26
83	Z9	302	PUB	OD-C4D-C3D	-4.29	123.38	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WK	203	PEB	CHA-C1B-NB	-4.29	115.95	124.93
82	Q7	201	PEB	CHA-C1B-C2B	4.29	135.94	124.90
82	TA	201	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	gH	201	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	kH	203	PEB	CHB-C1C-C2C	-4.29	117.46	127.15
82	KJ	201	PEB	CMB-C2B-C1B	4.29	131.68	125.06
82	UP	201	PEB	OD-C4D-ND	-4.29	119.57	125.93
82	V1	201	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	k1	201	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	uF	201	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	GK	203	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	L9	203	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	dG	204	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	aJ	204	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	B7	203	PEB	CHC-C1D-ND	-4.29	108.29	113.72
82	MP	202	PEB	CHC-C4C-NC	4.29	126.96	121.15
82	e4	201	PEB	OA-C1A-C2A	-4.29	122.76	126.17
82	XA	201	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	iF	203	PEB	C2C-C1C-NC	4.29	113.35	107.57
87	62	309	CLA	CMA-C3A-C4A	4.29	123.31	111.77
82	TM	202	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	OG	201	PEB	C3D-C4D-ND	4.29	115.68	107.26
82	QJ	202	PEB	C1C-CHB-C4B	4.29	137.91	128.28
82	bK	202	PEB	C3D-C4D-ND	4.29	115.68	107.26
82	QH	202	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	fO	202	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	eO	201	PEB	OA-C1A-C2A	-4.29	122.76	126.17
83	AH	304	PUB	C3B-C4B-NB	4.29	113.35	107.57
82	H9	203	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	S9	201	PEB	C3B-C4B-NB	4.29	116.29	110.05
84	NO	1001	CYC	CHB-C4A-NA	-4.29	115.96	124.93
82	NK	202	PEB	C1D-CHC-C4C	4.29	119.58	113.26
82	kH	202	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	iK	203	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	bH	201	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	LE	1002	PEB	CMC-C3C-C4C	4.29	131.61	127.06
82	BK	201	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	mK	201	PEB	C2C-C1C-NC	4.29	113.35	107.57
82	FD	203	PEB	CHA-C1B-C2B	4.29	135.93	124.90
82	LM	202	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	I5	202	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
82	r8	202	PEB	OA-C1A-C2A	-4.29	122.76	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iJ	201	PEB	OA-C1A-C2A	-4.29	122.76	126.17
82	dM	201	PEB	C1C-CHB-C4B	4.29	137.90	128.28
82	OM	201	PEB	CHC-C4C-NC	4.29	126.95	121.15
83	yF	302	PUB	CHA-C1B-NB	4.29	126.95	121.15
82	TB	202	PEB	C2C-C1C-NC	4.29	113.34	107.57
95	c6	601	DGD	C3G-O3G-C1D	-4.29	105.36	113.74
82	oK	203	PEB	C2C-C1C-NC	4.29	113.34	107.57
82	fG	202	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
85	AN	804	BCR	C7-C8-C9	-4.29	119.76	126.23
82	LP	201	PEB	C2C-C1C-NC	4.29	113.34	107.57
82	CM	203	PEB	OA-C1A-C2A	-4.29	122.77	126.17
82	tC	202	PEB	OA-C1A-C2A	-4.29	122.77	126.17
82	ZH	202	PEB	C1C-C2C-C3C	-4.29	102.55	107.62
87	B6	606	CLA	C1-C2-C3	-4.29	118.63	126.04
82	FJ	201	PEB	C1D-CHC-C4C	4.29	119.58	113.26
82	DA	202	PEB	CHA-C1B-NB	-4.29	115.97	124.93
82	IM	201	PEB	C1C-C2C-C3C	-4.29	102.56	107.62
82	fE	201	PEB	C1C-C2C-C3C	-4.29	102.56	107.62
82	O7	202	PEB	CHC-C4C-NC	4.29	126.95	121.15
82	RO	203	PEB	CAB-C3B-C4B	4.29	132.59	125.01
82	ZJ	201	PEB	C2C-C1C-NC	4.28	113.34	107.57
82	R5	202	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	WQ	202	PEB	C2C-C1C-NC	4.28	113.34	107.57
82	X7	201	PEB	C2C-C1C-NC	4.28	113.34	107.57
84	LH	1001	CYC	CAB-C3B-C4B	4.28	128.15	121.38
82	MF	203	PEB	CHC-C1D-ND	-4.28	108.30	113.72
82	T5	202	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	Z9	304	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
84	LH	1002	CYC	C4D-C3D-C2D	-4.28	102.56	107.62
82	Z4	201	PEB	C3D-C4D-ND	4.28	115.66	107.26
82	BF	201	PEB	C2C-C1C-NC	4.28	113.34	107.57
82	PD	201	PEB	C1C-CHB-C4B	4.28	137.89	128.28
82	E5	202	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	V4	201	PEB	C2C-C1C-NC	4.28	113.34	107.57
82	SB	203	PEB	OA-C1A-C2A	-4.28	122.77	126.17
82	Q5	202	PEB	OD-C4D-ND	-4.28	119.59	125.93
82	YF	202	PEB	C2C-C1C-NC	4.28	113.34	107.57
82	GG	1002	PEB	C3D-C4D-ND	4.28	115.66	107.26
82	R4	203	PEB	CAB-C3B-C4B	4.28	132.59	125.01
82	qC	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
82	dM	203	PEB	C2C-C1C-NC	4.28	113.34	107.57
82	GF	202	PEB	CHB-C4B-C3B	-4.28	115.42	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VD	201	PEB	C4B-C3B-C2B	-4.28	102.04	106.78
82	WJ	202	PEB	CMB-C2B-C1B	4.28	131.66	125.06
82	j1	202	PEB	C2C-C1C-NC	4.28	113.33	107.57
82	D9	203	PEB	C2C-C1C-NC	4.28	113.33	107.57
84	GG	1001	CYC	C2C-C1C-NC	4.28	111.96	108.27
83	Z9	305	PUB	C4B-C3B-C2B	-4.28	102.56	107.62
83	AE	302	PUB	C1C-C2C-C3C	-4.28	102.05	106.78
83	AG	302	PUB	C1C-C2C-C3C	-4.28	102.05	106.78
82	UP	201	PEB	C3B-C4B-NB	4.28	116.28	110.05
82	XD	201	PEB	C1C-CHB-C4B	4.28	137.88	128.28
84	D1	1003	CYC	C2D-C1D-ND	4.28	113.42	107.40
82	EK	202	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	OJ	202	PEB	CHB-C1C-NC	-4.28	115.52	125.32
82	KK	203	PEB	CHC-C1D-ND	-4.28	108.31	113.72
83	BM	302	PUB	CMA-C2A-C1A	4.28	131.46	121.39
82	l1	202	PEB	C2C-C1C-NC	4.28	113.33	107.57
82	c4	202	PEB	C1C-CHB-C4B	4.28	137.88	128.28
82	aJ	204	PEB	CMB-C2B-C1B	4.28	131.65	125.06
82	RI	203	PEB	OA-C1A-C2A	-4.28	122.77	126.17
82	NB	202	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	WI	201	PEB	C3B-C4B-NB	4.28	116.27	110.05
82	OK	203	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	HB	201	PEB	OA-C1A-C2A	-4.28	122.77	126.17
84	EG	1001	CYC	CMA-C3A-C4A	4.28	131.65	125.06
82	OF	203	PEB	C1C-C2C-C3C	-4.28	102.56	107.62
82	MK	203	PEB	CHC-C1D-ND	-4.28	108.31	113.72
82	g4	201	PEB	C2C-C1C-NC	4.28	113.33	107.57
82	fH	202	PEB	C2C-C1C-NC	4.28	113.33	107.57
82	gO	201	PEB	C2C-C1C-NC	4.28	113.33	107.57
83	AO	302	PUB	C1C-C2C-C3C	-4.28	102.05	106.78
82	YB	201	PEB	CHA-C1B-NB	-4.28	115.99	124.93
82	f1	203	PEB	OA-C1A-C2A	-4.28	122.77	126.17
82	MP	201	PEB	C1C-C2C-C3C	-4.28	102.57	107.62
82	QA	201	PEB	CHA-C1B-C2B	4.28	135.90	124.90
88	CL	522	LHG	C5-O7-C7	-4.28	107.26	117.79
82	RB	201	PEB	CMC-C3C-C4C	4.28	131.59	127.06
82	HJ	202	PEB	C2C-C1C-NC	4.28	113.33	107.57
82	oF	201	PEB	C1C-C2C-C3C	-4.28	102.57	107.62
82	YA	303	PEB	CHA-C1B-NB	-4.28	115.99	124.93
94	DL	401	PL9	C15-C14-C16	4.27	122.46	115.27
82	EJ	201	PEB	CHC-C1D-ND	-4.27	108.32	113.72
87	2N	301	CLA	CMB-C2B-C1B	-4.27	118.86	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ZF	202	PEB	CMC-C3C-C4C	4.27	131.59	127.06
82	JK	201	PEB	CHC-C4C-NC	4.27	126.93	121.15
82	WD	202	PEB	C2C-C1C-NC	4.27	113.33	107.57
82	DG	1002	PEB	OA-C1A-C2A	-4.27	122.78	126.17
82	J7	203	PEB	OA-C1A-C2A	-4.27	122.78	126.17
82	eG	202	PEB	OA-C1A-C2A	-4.27	122.78	126.17
82	SQ	202	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
85	h6	102	BCR	C38-C26-C25	-4.27	119.73	124.53
82	SP	202	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
82	uK	201	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
82	q8	202	PEB	OA-C1A-C2A	-4.27	122.78	126.17
82	DJ	201	PEB	C2A-C1A-NA	4.27	111.96	108.27
84	D1	1001	CYC	C2B-C1B-NB	4.27	113.24	106.99
82	JD	203	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
82	PQ	201	PEB	C1C-CHB-C4B	4.27	137.86	128.28
82	HO	1002	PEB	C2C-C1C-NC	4.27	113.32	107.57
87	AN	828	CLA	CHB-C1B-NB	4.27	128.78	124.26
82	DQ	202	PEB	C3D-C4D-ND	4.27	115.64	107.26
82	HA	201	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
82	QE	202	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
82	b1	203	PEB	C1C-CHB-C4B	4.27	137.86	128.28
84	ME	1001	CYC	CMA-C3A-C4A	4.27	131.64	125.06
82	xK	303	PEB	CHC-C4C-NC	4.27	126.93	121.15
82	UP	203	PEB	C1C-C2C-C3C	-4.27	102.57	107.62
82	jF	201	PEB	C2A-C1A-NA	4.27	111.95	108.27
82	VI	203	PEB	C3B-C4B-NB	4.27	116.26	110.05
82	LF	201	PEB	CHC-C1D-ND	-4.27	108.32	113.72
95	C6	502	DGD	O5D-C1E-C2E	4.27	114.97	108.30
82	b1	203	PEB	C2A-C1A-NA	4.27	111.95	108.27
82	CP	203	PEB	C2C-C1C-NC	4.27	113.32	107.57
84	N1	1001	CYC	C3D-C4D-ND	4.27	113.32	107.57
82	IA	202	PEB	C1C-C2C-C3C	-4.27	102.58	107.62
82	O9	203	PEB	C2A-C1A-NA	4.27	111.95	108.27
84	GE	1001	CYC	C2C-C1C-NC	4.27	111.95	108.27
82	YA	303	PEB	CHB-C1C-NC	-4.27	115.54	125.32
82	eM	201	PEB	C2C-C1C-NC	4.27	113.32	107.57
82	FP	201	PEB	C1C-C2C-C3C	-4.27	102.58	107.62
83	xF	301	PUB	C1C-C2C-C3C	-4.27	102.06	106.78
82	HQ	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
82	BI	202	PEB	C1B-C2B-C3B	-4.27	101.61	106.51
84	DG	1001	CYC	OC-C1C-C2C	-4.27	122.78	126.17
84	D1	1003	CYC	OC-C1C-C2C	-4.27	122.78	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hM	202	PEB	C2C-C1C-NC	4.27	113.31	107.57
82	bO	202	PEB	C1C-C2C-C3C	-4.27	102.58	107.62
82	SJ	201	PEB	CHA-C1B-NB	-4.27	116.01	124.93
82	BK	202	PEB	CMC-C3C-C4C	4.26	131.58	127.06
82	lH	202	PEB	C2C-C1C-NC	4.26	113.31	107.57
82	DD	201	PEB	C4B-C3B-C2B	-4.26	102.06	106.78
84	JH	1001	CYC	C2D-C1D-ND	4.26	113.39	107.40
82	lF	201	PEB	C2C-C1C-NC	4.26	113.31	107.57
83	A4	303	PUB	C1C-C2C-C3C	-4.26	102.06	106.78
82	WB	401	PEB	CHC-C4C-NC	4.26	126.92	121.15
82	d1	203	PEB	OA-C1A-C2A	-4.26	122.78	126.17
82	W7	202	PEB	C1C-C2C-C3C	-4.26	102.58	107.62
82	YP	502	PEB	CMB-C2B-C1B	4.26	131.63	125.06
82	LG	1002	PEB	CMC-C3C-C4C	4.26	131.58	127.06
82	JA	202	PEB	CHB-C1C-C2C	-4.26	117.53	127.15
82	VM	201	PEB	C1C-C2C-C3C	-4.26	102.58	107.62
82	H5	202	PEB	C1C-C2C-C3C	-4.26	102.58	107.62
82	CF	202	PEB	CMB-C2B-C1B	4.26	131.63	125.06
82	ZK	202	PEB	OA-C1A-C2A	-4.26	122.78	126.17
82	PM	201	PEB	OA-C1A-C2A	-4.26	122.78	126.17
84	LG	1001	CYC	C4D-C3D-C2D	-4.26	102.58	107.62
85	bL	602	BCR	C20-C21-C22	-4.26	121.23	127.31
88	c6	619	LHG	O7-C7-C8	4.26	120.69	111.50
82	cJ	201	PEB	CHC-C1D-ND	4.26	119.12	113.72
82	eH	203	PEB	C1C-CHB-C4B	4.26	137.84	128.28
82	W9	203	PEB	C1C-C2C-C3C	-4.26	102.58	107.62
82	BK	201	PEB	OD-C4D-C3D	-4.26	119.81	129.46
87	22	605	CLA	CMB-C2B-C1B	-4.26	118.88	125.37
87	dL	402	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
82	mJ	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
82	VO	201	PEB	C2C-C1C-NC	4.26	113.31	107.57
84	L1	1001	CYC	C4D-C3D-C2D	-4.26	102.58	107.62
82	IK	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
82	YP	501	PEB	CHC-C4C-NC	4.26	126.91	121.15
82	A5	202	PEB	C1C-C2C-C3C	-4.26	102.59	107.62
82	iM	202	PEB	C2C-C1C-NC	4.26	113.31	107.57
82	FQ	203	PEB	CHB-C4B-NB	-4.26	115.71	124.58
84	D1	1003	CYC	C1B-C2B-C3B	-4.26	103.43	107.87
83	AM	304	PUB	CMA-C2A-C1A	4.26	131.41	121.39
82	B9	201	PEB	OA-C1A-C2A	-4.26	122.79	126.17
82	jH	203	PEB	OA-C1A-C2A	-4.26	122.79	126.17
84	K1	1001	CYC	OC-C1C-C2C	-4.26	122.79	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U9	202	PEB	C1C-C2C-C3C	-4.26	102.59	107.62
82	CK	203	PEB	C1D-CHC-C4C	-4.26	106.98	113.26
82	P7	202	PEB	CHC-C1D-ND	-4.26	108.34	113.72
82	WJ	201	PEB	C1C-C2C-C3C	-4.26	102.59	107.62
82	ZF	201	PEB	C2C-C1C-NC	4.26	113.30	107.57
82	k1	202	PEB	C2C-C1C-NC	4.26	113.30	107.57
82	vK	201	PEB	C2C-C1C-NC	4.26	113.30	107.57
82	JO	1002	PEB	OA-C1A-C2A	-4.26	122.79	126.17
82	II	203	PEB	C2A-C1A-NA	4.26	111.94	108.27
82	FD	203	PEB	CHB-C4B-NB	-4.26	115.72	124.58
82	OG	203	PEB	C1C-C2C-C3C	-4.26	102.59	107.62
82	dE	204	PEB	C1C-C2C-C3C	-4.26	102.59	107.62
82	KF	203	PEB	CHC-C1D-ND	-4.26	108.34	113.72
82	eH	203	PEB	C2A-C1A-NA	4.26	111.94	108.27
82	HO	1002	PEB	OA-C1A-C2A	-4.26	122.79	126.17
82	j1	203	PEB	OA-C1A-C2A	-4.26	122.79	126.17
82	HM	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
82	tK	202	PEB	C3D-C4D-ND	4.26	115.61	107.26
85	BL	618	BCR	C7-C8-C9	-4.26	119.81	126.23
82	qK	203	PEB	CHC-C4C-NC	4.25	126.91	121.15
83	AM	304	PUB	CHC-C1D-ND	-4.25	108.34	113.72
82	TJ	201	PEB	C4B-C3B-C2B	-4.25	102.07	106.78
83	M9	303	PUB	C4B-CHB-C1C	-4.25	118.74	128.28
82	fJ	202	PEB	C2C-C1C-NC	4.25	113.30	107.57
82	p8	202	PEB	CHA-C1B-NB	-4.25	116.03	124.93
82	R1	202	PEB	OA-C1A-C2A	-4.25	122.79	126.17
82	S9	202	PEB	CHB-C1C-C2C	-4.25	117.55	127.15
82	fK	201	PEB	OA-C1A-NA	4.25	130.09	124.94
83	wK	304	PUB	C3B-C4B-NB	4.25	113.30	107.57
82	L5	201	PEB	C1B-C2B-C3B	-4.25	101.62	106.51
82	FJ	202	PEB	CHC-C1D-ND	-4.25	108.34	113.72
82	ZE	201	PEB	C1C-C2C-C3C	-4.25	102.59	107.62
82	HF	201	PEB	C1D-CHC-C4C	-4.25	106.99	113.26
82	VJ	201	PEB	C2C-C1C-NC	4.25	113.30	107.57
82	XF	203	PEB	CMB-C2B-C1B	4.25	131.61	125.06
82	VJ	202	PEB	OA-C1A-C2A	-4.25	122.79	126.17
82	RP	202	PEB	CHC-C1D-ND	-4.25	108.35	113.72
82	vC	202	PEB	CHA-C4A-NA	-4.25	120.15	125.20
82	OE	201	PEB	C3D-C4D-ND	4.25	115.60	107.26
82	J7	202	PEB	CHB-C1C-C2C	-4.25	117.56	127.15
82	DQ	203	PEB	OA-C1A-C2A	-4.25	122.79	126.17
82	FK	202	PEB	C3D-C4D-ND	4.25	115.60	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	c1	201	PEB	CHC-C1D-ND	-4.25	108.35	113.72
82	H4	1002	PEB	C2C-C1C-NC	4.25	113.29	107.57
82	JF	201	PEB	OA-C1A-NA	4.25	130.09	124.94
82	QG	203	PEB	C1C-C2C-C3C	-4.25	102.60	107.62
84	H4	1001	CYC	C2B-C1B-NB	4.25	113.21	106.99
82	HK	201	PEB	C1D-CHC-C4C	-4.25	106.99	113.26
82	iO	201	PEB	OA-C1A-C2A	-4.25	122.80	126.17
82	QG	202	PEB	C1C-C2C-C3C	-4.25	102.60	107.62
82	iM	201	PEB	C1C-C2C-C3C	-4.25	102.60	107.62
82	M7	202	PEB	OA-C1A-C2A	-4.25	122.80	126.17
82	BA	203	PEB	CHC-C1D-ND	-4.25	108.35	113.72
84	K1	1001	CYC	C1B-NB-C4B	-4.25	105.26	110.67
82	FM	201	PEB	C1C-C2C-C3C	-4.25	102.60	107.62
82	oK	201	PEB	C1C-C2C-C3C	-4.25	102.60	107.62
82	jH	202	PEB	C2C-C1C-NC	4.25	113.29	107.57
87	AN	850	CLA	CMB-C2B-C1B	-4.25	118.90	125.37
82	KB	302	PEB	CMB-C2B-C1B	4.25	131.60	125.06
82	GK	202	PEB	CHB-C4B-C3B	-4.25	115.50	125.32
82	D9	203	PEB	OA-C1A-C2A	-4.25	122.80	126.17
82	FF	202	PEB	C3D-C4D-ND	4.25	115.59	107.26
82	b4	202	PEB	C2C-C1C-NC	4.25	113.29	107.57
87	A2	828	CLA	CHB-C1B-NB	4.25	128.75	124.26
82	QB	203	PEB	C2C-C1C-NC	4.24	113.29	107.57
82	lO	202	PEB	C1D-CHC-C4C	4.24	119.51	113.26
82	H7	203	PEB	C4B-C3B-C2B	-4.24	102.08	106.78
82	lH	201	PEB	C2C-C1C-NC	4.24	113.29	107.57
83	yF	302	PUB	C3B-C4B-NB	4.24	113.29	107.57
82	SM	203	PEB	C1C-C2C-C3C	-4.24	102.60	107.62
82	VM	201	PEB	C3D-C4D-ND	4.24	115.58	107.26
82	T1	202	PEB	C1C-C2C-C3C	-4.24	102.61	107.62
82	JM	201	PEB	CHA-C1B-NB	-4.24	116.06	124.93
82	NM	201	PEB	C1C-CHB-C4B	-4.24	118.77	128.28
82	NF	202	PEB	C1D-CHC-C4C	4.24	119.51	113.26
83	A1	304	PUB	C3B-C4B-NB	4.24	113.28	107.57
82	CA	201	PEB	C1C-C2C-C3C	-4.24	102.61	107.62
82	S5	202	PEB	CHB-C1C-C2C	-4.24	117.58	127.15
92	BL	612	LMG	O7-C10-C11	4.24	120.64	111.50
95	BL	614	DGD	C1E-O6E-C5E	4.24	122.01	113.69
85	A2	804	BCR	C7-C8-C9	-4.24	119.83	126.23
82	FJ	201	PEB	CMB-C2B-C1B	4.24	131.59	125.06
82	ZJ	201	PEB	CMB-C2B-C1B	4.24	131.59	125.06
82	KP	201	PEB	C1C-C2C-C3C	-4.24	102.61	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	tF	201	PEB	C1C-C2C-C3C	-4.24	102.61	107.62
82	KK	201	PEB	OA-C1A-C2A	-4.24	122.80	126.17
87	A2	850	CLA	CMB-C2B-C1B	-4.24	118.91	125.37
82	eJ	202	PEB	C4B-C3B-C2B	-4.24	102.09	106.78
82	kM	201	PEB	CMC-C3C-C4C	4.24	131.55	127.06
82	SJ	201	PEB	CHC-C4C-NC	4.24	126.89	121.15
88	a6	610	LHG	O7-C7-C8	4.24	120.64	111.50
84	DH	1003	CYC	C1B-NB-C4B	-4.24	105.27	110.67
82	TA	202	PEB	C3C-C4C-NC	4.24	112.15	108.33
82	T7	202	PEB	C3C-C4C-NC	4.24	112.15	108.33
82	DD	202	PEB	C3D-C4D-ND	4.24	115.58	107.26
82	QE	203	PEB	C1C-C2C-C3C	-4.24	102.61	107.62
82	QH	203	PEB	C1D-CHC-C4C	-4.24	107.01	113.26
82	VI	203	PEB	C2A-C1A-NA	4.24	111.93	108.27
82	LK	201	PEB	CHC-C1D-ND	-4.24	108.36	113.72
82	Q1	203	PEB	C1D-CHC-C4C	-4.24	107.01	113.26
82	v8	202	PEB	CHA-C4A-NA	-4.24	120.17	125.20
82	TD	202	PEB	CHC-C4C-NC	4.24	126.88	121.15
82	RM	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
82	QQ	201	PEB	C2C-C1C-NC	4.24	113.28	107.57
82	jF	201	PEB	C2C-C1C-NC	4.24	113.28	107.57
82	WI	203	PEB	CMB-C2B-C1B	4.24	131.59	125.06
82	M9	305	PEB	OA-C1A-C2A	-4.24	122.81	126.17
82	ZH	201	PEB	CHB-C4B-C3B	-4.24	115.52	125.32
85	C6	507	BCR	C15-C14-C13	-4.24	121.27	127.31
82	lE	203	PEB	C1C-C2C-C3C	-4.24	102.61	107.62
82	LJ	201	PEB	C2A-C1A-NA	4.24	111.92	108.27
82	bF	202	PEB	C2C-C1C-NC	4.24	113.27	107.57
84	FH	1001	CYC	C1B-CHB-C4A	-4.23	117.73	128.08
82	BI	201	PEB	C1C-C2C-C3C	-4.23	102.61	107.62
82	OP	201	PEB	CHC-C1D-ND	-4.23	108.37	113.72
82	NP	202	PEB	C1C-C2C-C3C	-4.23	102.62	107.62
82	cF	203	PEB	C1C-C2C-C3C	-4.23	102.62	107.62
82	f1	202	PEB	C2C-C1C-NC	4.23	113.27	107.57
84	D1	1003	CYC	C1B-NB-C4B	-4.23	105.28	110.67
94	DL	401	PL9	C10-C9-C11	4.23	122.39	115.27
82	ID	201	PEB	CAB-C3B-C4B	4.23	132.50	125.01
82	QE	202	PEB	CHA-C1B-NB	-4.23	116.08	124.93
82	OH	201	PEB	CHA-C1B-NB	-4.23	116.08	124.93
84	IO	1001	CYC	C1D-C2D-C3D	-4.23	102.40	107.79
82	DD	202	PEB	OD-C4D-ND	-4.23	119.66	125.93
82	LJ	202	PEB	C2C-C1C-NC	4.23	113.27	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	YA	302	PUB	C4B-C3B-C2B	-4.23	102.62	107.62
95	AL	414	DGD	C4E-C3E-C2E	4.23	118.21	110.82
82	RJ	201	PEB	C3D-C4D-ND	4.23	115.56	107.26
82	OP	202	PEB	C3D-C4D-ND	4.23	115.56	107.26
82	VH	202	PEB	CMB-C2B-C1B	4.23	131.58	125.06
82	ZI	401	PEB	CBB-CAB-C3B	4.23	124.38	112.63
82	MJ	201	PEB	C4B-C3B-C2B	-4.23	102.10	106.78
82	H7	201	PEB	C1C-C2C-C3C	-4.23	102.62	107.62
82	W5	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
82	eE	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
82	bO	201	PEB	C1C-CHB-C4B	4.23	137.77	128.28
84	W3	1001	CYC	OB-C4B-C3B	-4.23	123.45	128.04
82	R7	202	PEB	C4B-C3B-C2B	-4.23	102.10	106.78
82	GA	201	PEB	CHA-C1B-NB	-4.23	116.08	124.93
82	H7	203	PEB	C2C-C1C-NC	4.23	113.27	107.57
82	L9	203	PEB	C2C-C1C-NC	4.23	113.27	107.57
82	gF	201	PEB	C4B-C3B-C2B	-4.23	102.10	106.78
82	GA	201	PEB	CHB-C1C-C2C	-4.23	117.61	127.15
82	KM	203	PEB	C1C-CHB-C4B	4.23	137.77	128.28
82	kH	201	PEB	C3D-C4D-ND	4.23	115.56	107.26
82	QG	202	PEB	CHA-C1B-NB	-4.23	116.09	124.93
82	T7	201	PEB	CHA-C1B-NB	-4.23	116.09	124.93
82	hF	201	PEB	CHA-C1B-NB	-4.23	116.09	124.93
82	I7	202	PEB	CHC-C4C-NC	4.23	126.87	121.15
82	e1	202	PEB	C1C-C2C-C3C	-4.23	102.62	107.62
82	TM	201	PEB	C4B-C3B-C2B	-4.23	102.10	106.78
84	DE	1001	CYC	OC-C1C-C2C	-4.23	122.81	126.17
82	TA	201	PEB	CHA-C1B-NB	-4.23	116.09	124.93
85	KL	100	BCR	C33-C5-C6	-4.23	119.78	124.53
84	y3	1001	CYC	OB-C4B-C3B	-4.23	123.45	128.04
82	Z1	201	PEB	CHB-C4B-C3B	-4.23	115.54	125.32
82	IP	203	PEB	OA-C1A-C2A	-4.23	122.81	126.17
82	mE	203	PEB	OA-C1A-C2A	-4.23	122.81	126.17
82	aH	201	PEB	C2C-C1C-NC	4.23	113.26	107.57
83	Z9	302	PUB	C4B-CHB-C1C	-4.23	118.80	128.28
84	DH	1003	CYC	CAB-C3B-C4B	4.23	128.05	121.38
82	D9	202	PEB	CHB-C1C-C2C	-4.23	117.61	127.15
82	H7	202	PEB	C2C-C1C-NC	4.23	113.26	107.57
82	M7	201	PEB	C1C-C2C-C3C	-4.23	102.62	107.62
82	jJ	203	PEB	C1C-C2C-C3C	-4.23	102.62	107.62
82	IQ	201	PEB	CAB-C3B-C4B	4.23	132.49	125.01
82	cH	201	PEB	CHC-C1D-ND	-4.23	108.38	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	GG	1001	CYC	CMD-C2D-C1D	4.23	131.75	125.56
82	KD	201	PEB	C2C-C1C-NC	4.23	113.26	107.57
82	jK	201	PEB	C2C-C1C-NC	4.23	113.26	107.57
82	mJ	201	PEB	CMB-C2B-C1B	4.23	131.57	125.06
82	YF	203	PEB	C1C-C2C-C3C	-4.23	102.63	107.62
82	uF	202	PEB	C1C-C2C-C3C	-4.23	102.63	107.62
87	BN	827	CLA	CHB-C1B-NB	4.23	128.73	124.26
103	8N	310	ZEX	C15-C14-C13	-4.23	121.28	127.31
82	xF	303	PEB	CHC-C4C-NC	4.22	126.87	121.15
82	QJ	204	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	k4	201	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
103	82	310	ZEX	C15-C14-C13	-4.22	121.28	127.31
82	TI	201	PEB	C3B-C4B-NB	4.22	116.19	110.05
84	DH	1001	CYC	C2B-C1B-NB	4.22	113.17	106.99
84	DO	1001	CYC	C2B-C1B-NB	4.22	113.17	106.99
83	AH	303	PUB	CMA-C2A-C1A	4.22	131.33	121.39
84	KG	202	CYC	CMD-C2D-C1D	4.22	131.75	125.56
82	1C	203	PEB	C2C-C1C-NC	4.22	113.26	107.57
82	mF	201	PEB	C2C-C1C-NC	4.22	113.26	107.57
82	lH	202	PEB	CHB-C4B-NB	-4.22	115.79	124.58
85	CL	502	BCR	C16-C15-C14	-4.22	114.82	123.47
82	HG	1002	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	OM	203	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
85	cL	503	BCR	C24-C23-C22	-4.22	119.85	126.23
82	GF	201	PEB	C2A-C1A-NA	4.22	111.91	108.27
84	KO	1001	CYC	C3D-C4D-ND	4.22	113.26	107.57
82	YA	301	PEB	CHC-C4C-NC	-4.22	115.43	121.15
85	Z6	101	BCR	C11-C10-C9	-4.22	121.28	127.31
82	NB	203	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	ZJ	201	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	KK	203	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	a1	201	PEB	C2C-C1C-NC	4.22	113.26	107.57
82	h4	202	PEB	C2C-C1C-NC	4.22	113.26	107.57
82	TQ	202	PEB	CHC-C4C-NC	4.22	126.86	121.15
82	eO	203	PEB	CHC-C4C-NC	4.22	126.86	121.15
82	MA	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	LM	201	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	Z9	304	PEB	OA-C1A-C2A	-4.22	122.82	126.17
84	F1	1001	CYC	C1B-CHB-C4A	-4.22	117.77	128.08
82	b4	201	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	TJ	201	PEB	CMC-C3C-C4C	4.22	131.53	127.06
82	cO	203	PEB	C4B-C3B-C2B	-4.22	102.11	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CM	203	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	l4	202	PEB	C2C-C1C-NC	4.22	113.25	107.57
82	I7	201	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	rC	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	kK	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	IF	201	PEB	C3D-C4D-ND	4.22	115.54	107.26
82	YK	203	PEB	CMB-C2B-C1B	4.22	131.56	125.06
82	ZJ	201	PEB	C2A-C1A-NA	4.22	111.91	108.27
82	B9	203	PEB	C2A-C1A-NA	4.22	111.91	108.27
85	A2	845	BCR	C16-C15-C14	-4.22	114.83	123.47
82	DK	202	PEB	C1D-CHC-C4C	-4.22	107.03	113.26
82	i4	201	PEB	OA-C1A-C2A	-4.22	122.82	126.17
87	3N	305	CLA	CAA-C2A-C3A	-4.22	101.22	112.78
82	jM	202	PEB	CHC-C4C-NC	4.22	126.86	121.15
84	I4	1001	CYC	C2B-C1B-NB	4.22	113.17	106.99
82	LD	203	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	VJ	201	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
82	UB	301	PEB	C3D-C4D-ND	4.22	115.54	107.26
82	HD	201	PEB	C3D-C4D-ND	4.22	115.54	107.26
82	SQ	201	PEB	C2C-C1C-NC	4.22	113.25	107.57
82	Y7	301	PEB	CHC-C4C-NC	-4.22	115.44	121.15
82	H5	201	PEB	C1C-C2C-C3C	-4.22	102.63	107.62
85	a6	605	BCR	C38-C26-C25	-4.22	119.79	124.53
83	Z9	305	PUB	CHB-C1C-NC	-4.22	115.80	124.58
82	HB	203	PEB	CMC-C3C-C4C	4.22	131.53	127.06
82	ZM	201	PEB	C1C-C2C-C3C	-4.22	102.64	107.62
82	MB	201	PEB	CHA-C1B-NB	-4.22	116.11	124.93
82	aB	201	PEB	CHA-C1B-NB	-4.22	116.11	124.93
82	DD	202	PEB	CHA-C1B-C2B	4.22	135.75	124.90
83	A1	303	PUB	CMA-C2A-C1A	4.22	131.31	121.39
82	j4	202	PEB	C3D-C4D-ND	4.22	115.53	107.26
82	kO	201	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	r8	201	PEB	CAA-C3A-C2A	-4.22	103.72	114.26
84	E1	1001	CYC	C2B-C1B-NB	4.22	113.16	106.99
82	pF	201	PEB	C2A-C1A-NA	4.22	111.91	108.27
82	m1	202	PEB	C2C-C1C-NC	4.22	113.25	107.57
82	rC	201	PEB	CAA-C3A-C2A	-4.22	103.72	114.26
82	V1	201	PEB	OA-C1A-C2A	-4.22	122.82	126.17
82	hO	202	PEB	C2C-C1C-NC	4.22	113.25	107.57
85	kL	100	BCR	C35-C13-C14	-4.22	117.02	122.92
82	jH	202	PEB	C1C-C2C-C3C	-4.22	102.64	107.62
82	bK	202	PEB	C2C-C1C-NC	4.22	113.25	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MF	201	PEB	CHC-C4C-NC	4.22	126.85	121.15
87	IN	103	CLA	CAA-C2A-C3A	-4.21	101.24	112.78
84	E1	1001	CYC	C1B-NB-C4B	-4.21	105.30	110.67
82	XJ	201	PEB	OA-C1A-C2A	-4.21	122.82	126.17
82	Z1	202	PEB	C1C-C2C-C3C	-4.21	102.64	107.62
82	kH	201	PEB	C2C-C1C-NC	4.21	113.25	107.57
82	pF	201	PEB	CHA-C4A-NA	4.21	130.22	125.20
82	B9	201	PEB	C2C-C1C-NC	4.21	113.25	107.57
82	JA	202	PEB	C1C-C2C-C3C	-4.21	102.64	107.62
82	FI	201	PEB	C3D-C4D-ND	4.21	115.53	107.26
87	I2	103	CLA	CAA-C2A-C3A	-4.21	101.24	112.78
82	SK	203	PEB	CHC-C1D-ND	-4.21	108.39	113.72
82	xC	202	PEB	C2C-C1C-NC	4.21	113.24	107.57
82	cJ	202	PEB	CAB-C3B-C4B	4.21	132.46	125.01
82	aF	201	PEB	CHB-C1C-C2C	-4.21	117.65	127.15
82	tF	201	PEB	CHC-C4C-NC	4.21	126.85	121.15
82	IK	203	PEB	OA-C1A-C2A	-4.21	122.82	126.17
84	IO	1001	CYC	C2B-C1B-NB	4.21	113.15	106.99
82	eH	202	PEB	C1C-C2C-C3C	-4.21	102.64	107.62
83	AJ	304	PUB	C1C-C2C-C3C	-4.21	102.12	106.78
82	lE	203	PEB	C2C-C1C-NC	4.21	113.24	107.57
82	QJ	202	PEB	C1C-C2C-C3C	-4.21	102.64	107.62
82	HQ	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	hG	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	X9	202	PEB	CHB-C1C-NC	-4.21	115.67	125.32
82	ID	201	PEB	CMC-C3C-C4C	-4.21	122.60	127.06
84	d3	1001	CYC	CHD-C1D-ND	-4.21	115.68	125.32
82	lG	203	PEB	C2C-C1C-NC	4.21	113.24	107.57
84	D1	1003	CYC	CAB-C3B-C4B	4.21	128.03	121.38
82	xK	302	PEB	CHB-C4B-NB	-4.21	115.82	124.58
82	NJ	202	PEB	CMB-C2B-C1B	4.21	131.55	125.06
82	P4	201	PEB	C2C-C1C-NC	4.21	113.24	107.57
85	KL	100	BCR	C35-C13-C14	-4.21	117.03	122.92
82	Y1	201	PEB	CHC-C1D-ND	-4.21	108.40	113.72
82	IF	203	PEB	C3B-C4B-NB	4.21	116.17	110.05
82	FA	203	PEB	C1C-C2C-C3C	-4.21	102.65	107.62
82	gK	202	PEB	C1C-C2C-C3C	-4.21	102.65	107.62
82	VP	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	OQ	202	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	S5	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
82	i4	203	PEB	C4B-C3B-C2B	-4.21	102.12	106.78
82	JM	201	PEB	C1C-C2C-C3C	-4.21	102.65	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iJ	201	PEB	C1C-C2C-C3C	-4.21	102.65	107.62
82	iK	202	PEB	C1C-C2C-C3C	-4.21	102.65	107.62
82	G7	201	PEB	CHA-C1B-NB	-4.21	116.13	124.93
82	b4	201	PEB	C1C-CHB-C4B	4.21	137.72	128.28
82	M5	304	PEB	CHA-C4A-NA	4.21	130.21	125.20
82	IA	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	TA	202	PEB	CHC-C1D-ND	-4.21	108.40	113.72
82	k1	201	PEB	C3D-C4D-ND	4.21	115.51	107.26
82	KJ	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	B5	202	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	jK	202	PEB	OA-C1A-C2A	-4.21	122.83	126.17
82	QB	203	PEB	CHC-C4C-NC	4.21	126.84	121.15
82	EJ	203	PEB	CHC-C4C-NC	4.21	126.84	121.15
82	HJ	201	PEB	C3D-C4D-ND	4.21	115.51	107.26
82	IJ	202	PEB	C3D-C4D-ND	4.21	115.51	107.26
82	d1	203	PEB	CHB-C4B-NB	-4.21	115.83	124.58
82	sK	203	PEB	C2C-C1C-NC	4.21	113.23	107.57
85	AN	845	BCR	C16-C15-C14	-4.21	114.86	123.47
82	U9	201	PEB	C1C-C2C-C3C	-4.21	102.65	107.62
82	DF	202	PEB	C1D-CHC-C4C	-4.20	107.06	113.26
84	HG	1001	CYC	C1B-NB-C4B	-4.20	105.32	110.67
82	FK	201	PEB	CHC-C1D-ND	-4.20	108.41	113.72
82	s8	201	PEB	C1C-C2C-C3C	-4.20	102.65	107.62
82	WO	201	PEB	C3D-C4D-ND	4.20	115.51	107.26
82	O1	201	PEB	CHA-C1B-NB	-4.20	116.14	124.93
91	AL	410	PHO	C3D-C4D-ND	4.20	113.45	107.72
87	32	304	CLA	CAA-C2A-C3A	-4.20	101.27	112.78
83	xK	301	PUB	C1C-C2C-C3C	-4.20	102.13	106.78
82	J5	202	PEB	C1C-C2C-C3C	-4.20	102.65	107.62
82	nF	202	PEB	OA-C1A-C2A	-4.20	122.83	126.17
84	I4	1001	CYC	CHD-C1D-ND	-4.20	115.69	125.32
84	LE	1001	CYC	C4D-C3D-C2D	-4.20	102.65	107.62
82	C9	202	PEB	CHB-C1C-NC	-4.20	115.69	125.32
84	KO	1001	CYC	CMA-C3A-C4A	4.20	131.53	125.06
82	IF	203	PEB	OA-C1A-C2A	-4.20	122.83	126.17
82	BK	202	PEB	OA-C1A-C2A	-4.20	122.83	126.17
82	fG	201	PEB	C1C-C2C-C3C	-4.20	102.65	107.62
82	SO	201	PEB	C1D-CHC-C4C	-4.20	107.06	113.26
84	KH	1001	CYC	C1B-NB-C4B	-4.20	105.32	110.67
82	mH	202	PEB	C2C-C1C-NC	4.20	113.23	107.57
82	C7	201	PEB	C1C-C2C-C3C	-4.20	102.66	107.62
82	OI	201	PEB	OA-C1A-C2A	-4.20	122.83	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	F5	202	PEB	C1C-CHB-C4B	4.20	137.70	128.28
82	GB	201	PEB	C2A-C1A-NA	4.20	111.89	108.27
82	rK	201	PEB	C2C-C1C-NC	4.20	113.23	107.57
85	AN	804	BCR	C4-C5-C6	-4.20	116.63	122.73
85	H6	101	BCR	C20-C21-C22	-4.20	121.32	127.31
82	P9	202	PEB	CHB-C1C-NC	-4.20	115.70	125.32
85	bL	603	BCR	C7-C8-C9	-4.20	119.89	126.23
82	cJ	202	PEB	C4B-C3B-C2B	-4.20	102.13	106.78
82	a4	202	PEB	C1C-CHB-C4B	4.20	137.70	128.28
82	LH	1003	PEB	CHC-C4C-NC	4.20	126.83	121.15
82	x8	202	PEB	C2C-C1C-NC	4.20	113.23	107.57
82	W9	202	PEB	C2C-C1C-NC	4.20	113.23	107.57
82	cO	203	PEB	C2C-C1C-NC	4.20	113.23	107.57
82	hF	201	PEB	C1D-CHC-C4C	-4.20	107.06	113.26
82	LA	202	PEB	C2A-C1A-NA	4.20	111.89	108.27
84	U3	1001	CYC	CHD-C1D-ND	-4.20	115.70	125.32
82	sC	201	PEB	C1C-C2C-C3C	-4.20	102.66	107.62
82	bF	201	PEB	OA-C1A-C2A	-4.20	122.83	126.17
84	FG	1001	CYC	OC-C1C-C2C	-4.20	122.83	126.17
82	V1	203	PEB	CMB-C2B-C1B	4.20	131.53	125.06
84	o3	1001	CYC	CHD-C1D-ND	-4.20	115.70	125.32
82	PO	201	PEB	C2C-C1C-NC	4.20	113.22	107.57
84	f3	1001	CYC	CHD-C1D-ND	-4.20	115.70	125.32
94	d6	408	PL9	C7-C3-C2	-4.20	117.78	123.30
82	KP	202	PEB	CHC-C4C-NC	4.20	126.83	121.15
82	ZK	202	PEB	C3D-C4D-ND	4.20	115.49	107.26
82	c4	203	PEB	C2C-C1C-NC	4.20	113.22	107.57
82	z8	202	PEB	C2C-C1C-NC	4.20	113.22	107.57
82	TG	201	PEB	CHA-C1B-NB	-4.20	116.15	124.93
82	J7	201	PEB	C4B-C3B-C2B	-4.20	102.14	106.78
82	eM	201	PEB	OA-C1A-C2A	-4.20	122.84	126.17
95	AL	414	DGD	O2G-C1B-C2B	4.20	120.55	111.50
84	B3	1001	CYC	CHD-C1D-ND	-4.20	115.71	125.32
82	tK	201	PEB	C1C-C2C-C3C	-4.20	102.66	107.62
82	NP	202	PEB	C2C-C1C-NC	4.20	113.22	107.57
82	l4	202	PEB	C1D-CHC-C4C	4.20	119.44	113.26
82	ZI	401	PEB	CAC-C2C-C1C	4.20	132.44	125.76
82	dM	201	PEB	C1C-C2C-C3C	-4.20	102.66	107.62
82	V9	202	PEB	CHB-C1C-NC	-4.20	115.71	125.32
85	B2	841	BCR	C33-C5-C6	-4.20	119.82	124.53
82	e4	203	PEB	CHC-C4C-NC	4.20	126.83	121.15
82	MD	201	PEB	C2C-C1C-NC	4.19	113.22	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y9	201	PEB	C2C-C1C-NC	4.19	113.22	107.57
83	A1	304	PUB	CAC-C2C-C1C	4.19	132.43	125.01
84	u3	1001	CYC	CHD-C1D-ND	-4.19	115.71	125.32
82	IB	203	PEB	OA-C1A-C2A	-4.19	122.84	126.17
82	U9	204	PEB	OA-C1A-C2A	-4.19	122.84	126.17
82	JI	202	PEB	CMB-C2B-C1B	4.19	131.52	125.06
82	HA	202	PEB	C2C-C1C-NC	4.19	113.22	107.57
82	X7	203	PEB	C2C-C1C-NC	4.19	113.22	107.57
82	IQ	201	PEB	CMC-C3C-C4C	-4.19	122.62	127.06
82	LJ	201	PEB	CHC-C1D-ND	4.19	119.03	113.72
82	NA	203	PEB	CAB-CBB-CGB	-4.19	104.58	113.60
82	tF	202	PEB	C3D-C4D-ND	4.19	115.49	107.26
82	gK	201	PEB	C4B-C3B-C2B	-4.19	102.14	106.78
84	BG	1002	CYC	C2D-C1D-ND	4.19	113.29	107.40
82	RF	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
82	i4	202	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
82	dH	203	PEB	CHB-C4B-NB	-4.19	115.85	124.58
82	nF	201	PEB	CHA-C1B-NB	-4.19	116.16	124.93
82	BJ	301	PEB	OA-C1A-C2A	-4.19	122.84	126.17
82	cK	203	PEB	CMB-C2B-C1B	4.19	131.52	125.06
82	gB	203	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
82	bO	201	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
82	XA	203	PEB	C2C-C1C-NC	4.19	113.22	107.57
82	aJ	204	PEB	C3D-C4D-ND	4.19	115.48	107.26
84	I4	1001	CYC	C1D-C2D-C3D	-4.19	102.45	107.79
82	OE	203	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
84	GE	1001	CYC	CMD-C2D-C1D	4.19	131.70	125.56
82	YA	304	PEB	C2C-C1C-NC	4.19	113.21	107.57
82	DE	1002	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
82	DM	202	PEB	CMB-C2B-C1B	4.19	131.52	125.06
83	KA	203	PUB	CMA-C2A-C1A	4.19	131.25	121.39
83	Y7	302	PUB	CMA-C2A-C1A	4.19	131.24	121.39
82	mJ	201	PEB	C2C-C1C-NC	4.19	113.21	107.57
82	a4	202	PEB	CHA-C1B-NB	-4.19	116.17	124.93
84	w3	1001	CYC	CHD-C1D-ND	-4.19	115.72	125.32
82	EM	201	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
84	n3	1001	CYC	CHD-C1D-ND	-4.19	115.72	125.32
82	tK	201	PEB	CHC-C4C-NC	4.19	126.82	121.15
82	RF	202	PEB	C1C-CHB-C4B	4.19	137.68	128.28
82	DQ	202	PEB	CHA-C1B-C2B	4.19	135.67	124.90
84	I3	1001	CYC	CHD-C1D-ND	-4.19	115.73	125.32
82	RB	202	PEB	C1C-C2C-C3C	-4.19	102.67	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TE	201	PEB	CHA-C1B-NB	-4.19	116.17	124.93
82	XM	201	PEB	CHA-C1B-NB	-4.19	116.17	124.93
82	PM	201	PEB	C4B-C3B-C2B	-4.19	102.15	106.78
103	82	309	ZEX	C27-C28-C29	-4.19	119.91	126.23
82	MF	203	PEB	C3C-C4C-NC	4.19	112.10	108.33
82	Z5	304	PEB	CHA-C4A-NA	4.19	130.18	125.20
82	LJ	202	PEB	CHC-C1D-ND	-4.19	108.43	113.72
87	B2	827	CLA	CHB-C1B-NB	4.19	128.69	124.26
84	Q3	1001	CYC	CHD-C1D-ND	-4.19	115.73	125.32
82	D4	1002	PEB	CHC-C4C-NC	4.19	126.82	121.15
82	IP	201	PEB	C2C-C1C-NC	4.19	113.21	107.57
82	l1	203	PEB	C2C-C1C-NC	4.19	113.21	107.57
82	T9	202	PEB	CHB-C1C-NC	-4.19	115.73	125.32
82	ZE	201	PEB	C3C-C4C-NC	4.19	112.10	108.33
103	8N	309	ZEX	C27-C28-C29	-4.19	119.91	126.23
82	oF	202	PEB	CMB-C2B-C1B	4.19	131.51	125.06
82	b4	202	PEB	C1C-C2C-C3C	-4.19	102.67	107.62
82	FD	201	PEB	CHA-C1B-C2B	4.19	135.66	124.90
82	TM	202	PEB	C2C-C1C-NC	4.19	113.21	107.57
82	G7	201	PEB	CHB-C1C-C2C	-4.19	117.71	127.15
95	AL	415	DGD	O2G-C1B-C2B	4.19	120.52	111.50
82	T7	202	PEB	CHC-C1D-ND	-4.19	108.43	113.72
82	vK	201	PEB	OA-C1A-NA	4.18	130.01	124.94
82	L5	202	PEB	CHB-C1C-C2C	-4.18	117.71	127.15
84	D3	1001	CYC	CHD-C1D-ND	-4.18	115.73	125.32
82	cH	201	PEB	OA-C1A-C2A	-4.18	122.85	126.17
82	cM	201	PEB	OA-C1A-C2A	-4.18	122.85	126.17
82	PF	201	PEB	CHC-C4C-NC	4.18	126.81	121.15
95	CL	517	DGD	O2G-C1B-C2B	4.18	120.52	111.50
84	j3	1001	CYC	CHD-C1D-ND	-4.18	115.74	125.32
82	YH	201	PEB	CHC-C1D-ND	-4.18	108.43	113.72
85	A2	804	BCR	C4-C5-C6	-4.18	116.66	122.73
82	WM	201	PEB	C3D-C4D-ND	4.18	115.47	107.26
82	N9	202	PEB	CHB-C1C-NC	-4.18	115.74	125.32
82	DE	1002	PEB	OA-C1A-C2A	-4.18	122.85	126.17
84	NE	201	CYC	CMD-C2D-C1D	4.18	131.69	125.56
83	K7	203	PUB	CMA-C2A-C1A	4.18	131.23	121.39
82	IB	201	PEB	CHC-C1D-ND	-4.18	108.43	113.72
82	L1	1002	PEB	C3D-C4D-ND	4.18	115.47	107.26
85	LN	205	BCR	C8-C9-C10	4.18	125.36	118.94
84	L3	1001	CYC	CHD-C1D-ND	-4.18	115.74	125.32
82	KQ	201	PEB	C2C-C1C-NC	4.18	113.20	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MQ	201	PEB	C2C-C1C-NC	4.18	113.20	107.57
82	vF	201	PEB	C2C-C1C-NC	4.18	113.20	107.57
82	iK	203	PEB	C1C-C2C-C3C	-4.18	102.68	107.62
82	E9	202	PEB	CHB-C1C-NC	-4.18	115.74	125.32
82	PO	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
82	JA	201	PEB	C4B-C3B-C2B	-4.18	102.15	106.78
95	c6	618	DGD	O2G-C1B-C2B	4.18	120.51	111.50
84	H3	1001	CYC	CHD-C1D-ND	-4.18	115.74	125.32
85	L2	205	BCR	C8-C9-C10	4.18	125.36	118.94
84	A3	1001	CYC	CHB-C4A-C3A	4.18	135.65	124.90
82	cJ	201	PEB	C3D-C4D-ND	4.18	115.46	107.26
82	sF	202	PEB	C2C-C1C-NC	4.18	113.20	107.57
82	B9	202	PEB	C4B-C3B-C2B	-4.18	102.16	106.78
82	lM	201	PEB	CHB-C1C-C2C	-4.18	117.72	127.15
84	k3	1001	CYC	CHD-C1D-ND	-4.18	115.74	125.32
82	lG	203	PEB	C1C-C2C-C3C	-4.18	102.68	107.62
82	eM	201	PEB	C1C-C2C-C3C	-4.18	102.68	107.62
82	kO	201	PEB	C1C-C2C-C3C	-4.18	102.68	107.62
83	wF	304	PUB	C3B-C4B-NB	4.18	113.20	107.57
82	b1	201	PEB	C1C-C2C-C3C	-4.18	102.68	107.62
82	i4	203	PEB	C1C-C2C-C3C	-4.18	102.68	107.62
85	Z6	101	BCR	C15-C14-C13	-4.18	121.34	127.31
82	L7	202	PEB	C2A-C1A-NA	4.18	111.88	108.27
84	S3	1001	CYC	CHD-C1D-ND	-4.18	115.75	125.32
82	c1	201	PEB	OA-C1A-C2A	-4.18	122.85	126.17
82	IK	203	PEB	C3B-C4B-NB	4.18	116.13	110.05
82	I9	202	PEB	CHB-C1C-NC	-4.18	115.75	125.32
82	K9	202	PEB	CHB-C1C-NC	-4.18	115.75	125.32
82	R9	202	PEB	CHB-C1C-NC	-4.18	115.75	125.32
82	ZI	401	PEB	C3D-C4D-ND	4.18	115.46	107.26
82	IA	202	PEB	CHC-C4C-NC	4.18	126.81	121.15
82	FI	201	PEB	C3B-C4B-NB	4.18	116.13	110.05
82	oF	203	PEB	C1D-CHC-C4C	4.18	119.42	113.26
82	Z5	305	PEB	CHA-C1B-NB	-4.18	116.19	124.93
82	dK	202	PEB	CMB-C2B-C1B	4.18	131.50	125.06
84	D4	1001	CYC	C2B-C1B-NB	4.18	113.10	106.99
82	dG	204	PEB	CHC-C4C-NC	4.18	126.80	121.15
82	XJ	201	PEB	CHA-C1B-NB	-4.18	116.19	124.93
82	iG	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
82	O9	202	PEB	CHA-C4A-NA	-4.18	120.24	125.20
82	U1	201	PEB	CHA-C1B-NB	-4.18	116.20	124.93
84	h3	1001	CYC	CHD-C1D-ND	-4.18	115.75	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hK	201	PEB	CHA-C1B-NB	-4.18	116.20	124.93
82	P1	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
82	KF	203	PEB	C1C-C2C-C3C	-4.18	102.69	107.62
82	N7	201	PEB	C1C-C2C-C3C	-4.18	102.69	107.62
83	KA	203	PUB	C1C-C2C-C3C	-4.18	102.16	106.78
83	K7	203	PUB	C1C-C2C-C3C	-4.18	102.16	106.78
82	fE	203	PEB	CHB-C1C-C2C	-4.17	117.73	127.15
82	zC	202	PEB	C2C-C1C-NC	4.17	113.19	107.57
96	VL	201	HEM	CHA-C4D-ND	4.17	129.52	124.37
82	OO	201	PEB	C3D-C4D-ND	4.17	115.45	107.26
82	BF	202	PEB	OA-C1A-C2A	-4.17	122.85	126.17
82	xF	302	PEB	CHB-C4B-NB	-4.17	115.89	124.58
82	jO	202	PEB	C3D-C4D-ND	4.17	115.45	107.26
84	q3	1001	CYC	CHD-C1D-ND	-4.17	115.76	125.32
84	K4	1001	CYC	C2B-C1B-NB	4.17	113.10	106.99
82	BK	202	PEB	C3D-C4D-ND	4.17	115.45	107.26
82	fG	203	PEB	CHB-C1C-C2C	-4.17	117.73	127.15
82	KB	304	PEB	OA-C1A-C2A	-4.17	122.86	126.17
82	IB	203	PEB	CHC-C4C-NC	4.17	126.80	121.15
82	DO	1002	PEB	CHC-C4C-NC	4.17	126.80	121.15
82	y8	202	PEB	C1C-C2C-C3C	-4.17	102.69	107.62
82	A9	202	PEB	CHB-C1C-NC	-4.17	115.76	125.32
82	aO	202	PEB	CHA-C1B-NB	-4.17	116.20	124.93
84	m3	1001	CYC	CHB-C4A-C3A	4.17	135.63	124.90
82	lH	201	PEB	CHC-C4C-NC	4.17	126.80	121.15
82	G9	202	PEB	CHB-C1C-NC	-4.17	115.76	125.32
82	RK	202	PEB	C1C-CHB-C4B	4.17	137.64	128.28
82	LH	1003	PEB	C3D-C4D-ND	4.17	115.44	107.26
85	A6	401	BCR	C3-C4-C5	-4.17	106.63	114.08
87	B6	616	CLA	C4A-NA-C1A	4.17	108.58	106.71
82	mG	203	PEB	OA-C1A-C2A	-4.17	122.86	126.17
82	pF	202	PEB	C2C-C1C-NC	4.17	113.19	107.57
84	e3	1001	CYC	CHB-C4A-C3A	4.17	135.62	124.90
82	cM	201	PEB	C2A-C1A-NA	4.17	111.87	108.27
82	LK	201	PEB	C4B-C3B-C2B	-4.17	102.17	106.78
84	BE	1002	CYC	C2D-C1D-ND	4.17	113.26	107.40
84	HE	1001	CYC	C1B-NB-C4B	-4.17	105.36	110.67
82	QK	202	PEB	C2C-C1C-NC	4.17	113.19	107.57
82	EM	201	PEB	CHB-C1C-C2C	-4.17	117.74	127.15
82	aK	201	PEB	CHB-C1C-C2C	-4.17	117.74	127.15
82	Y9	201	PEB	CHC-C1D-ND	-4.17	108.45	113.72
82	bK	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	J5	201	PEB	C2C-C1C-NC	4.17	113.19	107.57
84	GO	1001	CYC	OB-C4B-C3B	-4.17	123.52	128.04
84	73	1001	CYC	CHD-C1D-ND	-4.17	115.77	125.32
83	YA	302	PUB	CMA-C2A-C1A	4.17	131.20	121.39
82	i1	201	PEB	C3B-C4B-NB	4.17	116.11	110.05
82	DQ	201	PEB	C4B-C3B-C2B	-4.17	102.17	106.78
82	L4	1002	PEB	CMD-C2D-C3D	4.17	135.94	130.06
84	O3	1001	CYC	CHD-C1D-ND	-4.17	115.77	125.32
82	UJ	203	PEB	OA-C1A-C2A	-4.17	122.86	126.17
82	V7	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17
83	wK	304	PUB	CHC-C1D-ND	-4.17	108.45	113.72
82	WB	401	PEB	C1C-C2C-C3C	-4.17	102.69	107.62
82	yC	202	PEB	C1C-C2C-C3C	-4.17	102.69	107.62
82	bG	201	PEB	C3D-C4D-ND	4.17	115.44	107.26
84	M3	1001	CYC	CHD-C1D-ND	-4.17	115.77	125.32
84	G3	1001	CYC	CHB-C4A-C3A	4.17	135.62	124.90
82	HA	203	PEB	C2C-C1C-NC	4.17	113.18	107.57
82	SD	201	PEB	C2C-C1C-NC	4.17	113.18	107.57
82	OM	203	PEB	CMB-C2B-C1B	4.17	131.48	125.06
82	GG	1002	PEB	CAB-C3B-C2B	4.17	135.64	127.88
82	GF	201	PEB	C1B-C2B-C3B	-4.17	101.72	106.51
82	T7	201	PEB	CMB-C2B-C1B	4.17	131.48	125.06
82	L1	1002	PEB	CHC-C4C-NC	4.17	126.79	121.15
82	kJ	202	PEB	CHC-C1D-ND	-4.17	108.45	113.72
82	J7	202	PEB	C1C-C2C-C3C	-4.17	102.70	107.62
84	F3	1001	CYC	CHD-C1D-ND	-4.17	115.78	125.32
82	GE	1002	PEB	CAB-C3B-C2B	4.17	135.64	127.88
82	ID	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17
82	YJ	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17
96	v6	201	HEM	CHD-C1D-ND	4.16	128.94	124.42
82	iO	203	PEB	C4B-C3B-C2B	-4.16	102.17	106.78
82	IF	201	PEB	C2A-C1A-NA	-4.16	104.68	108.27
92	b6	624	LMG	O7-C10-C11	4.16	120.48	111.50
82	XD	202	PEB	OA-C1A-C2A	-4.16	122.86	126.17
84	KO	1001	CYC	C2B-C1B-NB	4.16	113.08	106.99
82	DJ	202	PEB	C2C-C1C-NC	4.16	113.18	107.57
82	rF	201	PEB	C2C-C1C-NC	4.16	113.18	107.57
84	K3	1001	CYC	CHB-C4A-C3A	4.16	135.61	124.90
84	E3	1001	CYC	CHB-C4A-C3A	4.16	135.61	124.90
85	b6	601	BCR	C33-C5-C6	-4.16	119.85	124.53
82	sF	203	PEB	C2C-C1C-NC	4.16	113.18	107.57
82	WA	202	PEB	C1C-C2C-C3C	-4.16	102.70	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	F9	201	PEB	C4B-C3B-C2B	-4.16	102.17	106.78
82	TA	201	PEB	CMB-C2B-C1B	4.16	131.47	125.06
82	LP	201	PEB	CHC-C1D-ND	-4.16	108.46	113.72
82	X7	203	PEB	CAC-CBC-CGC	-4.16	104.65	113.60
84	T3	1001	CYC	CHB-C4A-C3A	4.16	135.60	124.90
82	VO	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
82	Z4	201	PEB	C4B-NB-C1B	-4.16	98.67	106.51
82	dE	202	PEB	CHB-C1C-C2C	-4.16	117.76	127.15
82	pK	202	PEB	C2C-C1C-NC	4.16	113.17	107.57
82	g1	202	PEB	C1C-C2C-C3C	-4.16	102.70	107.62
82	ZJ	202	PEB	C2C-C1C-NC	4.16	113.17	107.57
84	P3	1001	CYC	CHB-C4A-C3A	4.16	135.60	124.90
84	t3	1001	CYC	CHB-C4A-C3A	4.16	135.60	124.90
82	Q1	203	PEB	C1C-C2C-C3C	-4.16	102.70	107.62
82	lF	203	PEB	C1C-C2C-C3C	-4.16	102.70	107.62
82	dJ	202	PEB	C2C-C1C-NC	4.16	113.17	107.57
82	gM	201	PEB	C2C-C1C-NC	4.16	113.17	107.57
82	M5	305	PEB	CHA-C1B-NB	-4.16	116.23	124.93
84	R3	1001	CYC	CHB-C4A-C3A	4.16	135.60	124.90
82	hE	201	PEB	OA-C1A-C2A	-4.16	122.87	126.17
82	QO	201	PEB	CMA-C2A-C1A	-4.16	103.44	112.40
82	PD	201	PEB	C1C-C2C-C3C	-4.16	102.70	107.62
82	iF	203	PEB	CHC-C1D-ND	-4.16	108.46	113.72
82	UE	201	PEB	CMC-C3C-C4C	4.16	131.47	127.06
82	eA	301	PEB	C3D-C4D-ND	4.16	115.42	107.26
82	R4	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
82	oK	202	PEB	CMB-C2B-C1B	4.16	131.47	125.06
84	c3	1001	CYC	CHB-C4A-C3A	4.16	135.59	124.90
82	oK	203	PEB	C1D-CHC-C4C	4.16	119.39	113.26
84	g3	1001	CYC	CHB-C4A-C3A	4.16	135.59	124.90
96	vL	201	HEM	CHA-C4D-ND	4.16	129.50	124.37
82	EK	201	PEB	CHC-C4C-NC	4.16	126.78	121.15
84	i3	1001	CYC	CHB-C4A-C3A	4.16	135.59	124.90
85	b6	601	BCR	C16-C17-C18	-4.16	121.38	127.31
82	V4	202	PEB	C4B-C3B-C2B	-4.16	102.18	106.78
82	IK	201	PEB	C2A-C1A-NA	-4.16	104.69	108.27
82	IQ	201	PEB	CAB-CBB-CGB	-4.16	104.66	113.60
82	SF	203	PEB	CHC-C1D-ND	-4.16	108.47	113.72
82	O4	201	PEB	C3D-C4D-ND	4.16	115.41	107.26
82	PQ	201	PEB	C1C-C2C-C3C	-4.16	102.71	107.62
82	qF	201	PEB	C1C-C2C-C3C	-4.16	102.71	107.62
83	Z9	305	PUB	C4A-CHA-C1B	4.16	119.38	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iG	201	PEB	C2C-C1C-NC	4.16	113.17	107.57
82	BQ	203	PEB	C3C-C4C-NC	4.16	112.07	108.33
82	L5	202	PEB	CHC-C1D-ND	-4.16	108.47	113.72
82	DG	1002	PEB	C1C-C2C-C3C	-4.16	102.71	107.62
82	TI	201	PEB	C1B-C2B-C3B	-4.16	101.74	106.51
82	cF	203	PEB	CMB-C2B-C1B	4.15	131.46	125.06
82	GK	201	PEB	CMC-C3C-C4C	4.15	131.46	127.06
82	vF	201	PEB	C1C-C2C-C3C	-4.15	102.71	107.62
82	dK	202	PEB	OA-C1A-C2A	-4.15	122.87	126.17
87	32	304	CLA	C20-C18-C17	-4.15	85.87	111.54
82	YA	303	PEB	C2C-C1C-NC	4.15	113.17	107.57
82	DJ	201	PEB	C2C-C1C-NC	4.15	113.17	107.57
83	QJ	201	PUB	CMA-C2A-C1A	4.15	131.16	121.39
82	mM	201	PEB	C4B-C3B-C2B	-4.15	102.19	106.78
84	l3	1001	CYC	CHB-C4A-C3A	4.15	135.58	124.90
87	3N	305	CLA	C20-C18-C17	-4.15	85.87	111.54
82	lF	202	PEB	C1C-C2C-C3C	-4.15	102.71	107.62
82	gH	202	PEB	C1C-C2C-C3C	-4.15	102.71	107.62
82	vK	201	PEB	C1C-C2C-C3C	-4.15	102.71	107.62
84	IO	1001	CYC	CHD-C1D-ND	-4.15	115.81	125.32
82	ZB	202	PEB	OA-C1A-C2A	-4.15	122.87	126.17
83	AO	303	PUB	C1C-C2C-C3C	-4.15	102.19	106.78
84	J3	1001	CYC	CHB-C4A-C3A	4.15	135.58	124.90
82	LM	202	PEB	CMB-C2B-C1B	4.15	131.46	125.06
85	BN	841	BCR	C33-C5-C6	-4.15	119.86	124.53
82	YK	201	PEB	CHB-C1C-C2C	-4.15	117.78	127.15
85	A2	845	BCR	C11-C12-C13	-4.15	114.75	126.42
82	KB	302	PEB	OA-C1A-C2A	-4.15	122.87	126.17
82	HJ	202	PEB	CHC-C4C-NC	4.15	126.77	121.15
85	AN	845	BCR	C11-C12-C13	-4.15	114.75	126.42
84	C3	1001	CYC	CHB-C4A-C3A	4.15	135.57	124.90
82	sF	203	PEB	C1B-C2B-C3B	-4.15	101.74	106.51
84	IG	1001	CYC	C2D-C1D-ND	4.15	113.23	107.40
82	eB	202	PEB	C1C-C2C-C3C	-4.15	102.72	107.62
82	cK	201	PEB	C1C-C2C-C3C	-4.15	102.72	107.62
82	l1	202	PEB	CHC-C4C-NC	4.15	126.77	121.15
82	ZG	203	PEB	CHA-C1B-NB	-4.15	116.25	124.93
84	EH	1001	CYC	C2B-C1B-NB	4.15	113.06	106.99
82	C9	202	PEB	C2C-C1C-NC	4.15	113.16	107.57
85	b6	603	BCR	C24-C23-C22	-4.15	119.97	126.23
82	BB	202	PEB	OA-C1A-C2A	-4.15	122.87	126.17
82	ZO	201	PEB	C4B-NB-C1B	-4.15	98.69	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NM	201	PEB	C1D-CHC-C4C	4.15	119.37	113.26
82	BM	301	PEB	C2C-C1C-NC	4.15	113.16	107.57
82	TJ	202	PEB	CHC-C1D-ND	-4.15	108.48	113.72
82	iH	201	PEB	C3B-C4B-NB	4.15	116.08	110.05
82	XQ	202	PEB	OA-C1A-C2A	-4.15	122.88	126.17
91	dL	403	PHO	CMB-C2B-C3B	4.15	132.44	124.68
84	F1	1001	CYC	C1B-C2B-C3B	-4.15	103.54	107.87
82	GD	201	PEB	C1C-C2C-C3C	-4.15	102.72	107.62
82	eG	201	PEB	C1C-C2C-C3C	-4.15	102.72	107.62
82	hH	201	PEB	C1C-C2C-C3C	-4.15	102.72	107.62
82	EB	501	PEB	C3D-C4D-ND	4.15	115.39	107.26
82	mM	201	PEB	C3D-C4D-ND	4.15	115.39	107.26
82	dO	202	PEB	C3D-C4D-ND	4.15	115.39	107.26
82	Y7	303	PEB	C2C-C1C-NC	4.15	113.15	107.57
82	Y7	304	PEB	C2C-C1C-NC	4.15	113.15	107.57
82	JK	201	PEB	OA-C1A-NA	4.15	129.96	124.94
84	p3	1001	CYC	CHB-C4A-C3A	4.14	135.56	124.90
82	SI	202	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
87	F2	202	CLA	CAA-C2A-C3A	-4.14	106.43	116.10
82	TQ	202	PEB	C2C-C1C-NC	4.14	113.15	107.57
94	a6	601	PL9	C32-C33-C34	-4.14	117.68	127.66
82	YI	202	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	HK	201	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	D5	202	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	LO	1002	PEB	CMD-C2D-C3D	4.14	135.91	130.06
82	l1	203	PEB	CHB-C4B-NB	-4.14	115.95	124.58
84	v3	1001	CYC	CHB-C4A-C3A	4.14	135.56	124.90
82	LM	202	PEB	C2C-C1C-NC	4.14	113.15	107.57
82	cM	201	PEB	C2C-C1C-NC	4.14	113.15	107.57
82	OK	201	PEB	CHA-C1B-NB	-4.14	116.27	124.93
82	OI	203	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	LJ	201	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	HQ	202	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	iE	201	PEB	C2C-C1C-NC	4.14	113.15	107.57
87	CL	503	CLA	CAA-C2A-C3A	-4.14	101.43	112.78
82	JA	202	PEB	C3D-C4D-ND	4.14	115.39	107.26
82	Q7	202	PEB	CHC-C4C-NC	4.14	126.76	121.15
82	UP	201	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	xC	201	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	pK	201	PEB	C2A-C1A-NA	4.14	111.84	108.27
82	SE	202	PEB	CHA-C1B-NB	-4.14	116.27	124.93
82	ZE	203	PEB	CHA-C1B-NB	-4.14	116.27	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gK	203	PEB	C3D-C4D-ND	4.14	115.39	107.26
82	YF	203	PEB	CMB-C2B-C1B	4.14	131.44	125.06
82	VA	202	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	BK	201	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	iO	202	PEB	C1C-C2C-C3C	-4.14	102.72	107.62
82	IB	201	PEB	OA-C1A-C2A	-4.14	122.88	126.17
82	aJ	204	PEB	OA-C1A-C2A	-4.14	122.88	126.17
82	SP	202	PEB	C2C-C1C-NC	4.14	113.15	107.57
82	YJ	201	PEB	C1C-C2C-C3C	-4.14	102.73	107.62
82	AH	301	PEB	C3D-C4D-ND	4.14	115.38	107.26
82	V7	203	PEB	OA-C1A-C2A	-4.14	122.88	126.17
82	V4	202	PEB	C3D-C4D-ND	4.14	115.38	107.26
82	OF	201	PEB	C2A-C1A-NA	4.14	111.84	108.27
82	V9	202	PEB	C2C-C1C-NC	4.14	113.15	107.57
82	jE	202	PEB	C1C-C2C-C3C	-4.14	102.73	107.62
84	MO	1001	CYC	CHD-C1D-ND	-4.14	115.84	125.32
82	XD	202	PEB	C1D-CHC-C4C	4.14	119.36	113.26
85	FN	202	BCR	C7-C8-C9	4.14	132.49	126.23
84	N3	1001	CYC	CHB-C4A-C3A	4.14	135.54	124.90
82	1C	201	PEB	C2C-C1C-NC	4.14	113.14	107.57
82	Z4	202	PEB	C3D-C4D-ND	4.14	115.38	107.26
85	b6	603	BCR	C38-C26-C25	-4.14	119.88	124.53
82	dH	203	PEB	OA-C1A-C2A	-4.14	122.88	126.17
83	AG	302	PUB	CMA-C2A-C1A	4.14	131.13	121.39
82	DA	202	PEB	C1C-C2C-C3C	-4.14	102.73	107.62
82	O5	202	PEB	C1C-C2C-C3C	-4.14	102.73	107.62
82	iF	203	PEB	C1C-C2C-C3C	-4.14	102.73	107.62
82	lK	203	PEB	C2A-C1A-NA	4.14	111.84	108.27
82	IK	201	PEB	CAC-C2C-C3C	4.14	136.55	127.07
82	FQ	201	PEB	CHA-C1B-C2B	4.14	135.54	124.90
82	SG	203	PEB	CHA-C1B-NB	-4.14	116.28	124.93
82	fE	201	PEB	OA-C1A-C2A	-4.14	122.88	126.17
82	BB	201	PEB	C2C-C1C-NC	4.14	113.14	107.57
85	F6	101	BCR	C15-C14-C13	-4.14	121.41	127.31
88	AN	844	LHG	O7-C7-C8	4.14	120.42	111.50
82	ID	201	PEB	CAB-CBB-CGB	-4.14	104.70	113.60
82	UF	201	PEB	C1D-CHC-C4C	-4.14	107.16	113.26
82	QA	202	PEB	CHC-C4C-NC	4.14	126.75	121.15
82	KB	301	PEB	OA-C1A-C2A	-4.14	122.88	126.17
82	QK	202	PEB	C1C-C2C-C3C	-4.14	102.73	107.62
82	sF	203	PEB	CHB-C1C-C2C	-4.14	117.82	127.15
82	v8	202	PEB	CHB-C1C-NC	-4.14	115.85	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VB	201	PEB	C3D-C4D-ND	4.14	115.37	107.26
82	I9	202	PEB	C2C-C1C-NC	4.14	113.14	107.57
82	UH	201	PEB	CHA-C1B-NB	-4.14	116.28	124.93
95	BL	614	DGD	C4D-C3D-C2D	4.14	118.04	110.82
88	A2	844	LHG	O7-C7-C8	4.14	120.41	111.50
82	F9	201	PEB	C3D-C4D-ND	4.14	115.37	107.26
82	x8	201	PEB	C1C-C2C-C3C	-4.13	102.73	107.62
82	iO	203	PEB	C1C-C2C-C3C	-4.13	102.73	107.62
82	RJ	201	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	ZM	201	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	DP	201	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	dB	201	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	YI	202	PEB	CMB-C2B-C1B	4.13	131.43	125.06
82	EJ	203	PEB	OA-C1A-C2A	-4.13	122.89	126.17
82	MB	201	PEB	C1C-C2C-C3C	-4.13	102.73	107.62
88	cL	501	LHG	C5-O7-C7	-4.13	107.61	117.79
82	OP	203	PEB	C3B-C4B-NB	4.13	116.06	110.05
82	U1	201	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	18	201	PEB	C2C-C1C-NC	4.13	113.14	107.57
83	AH	304	PUB	CAC-C2C-C1C	4.13	132.32	125.01
82	QH	203	PEB	C1C-C2C-C3C	-4.13	102.73	107.62
82	YF	201	PEB	CHB-C1C-C2C	-4.13	117.83	127.15
82	iE	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
82	E9	202	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	j1	201	PEB	C3B-C4B-NB	4.13	116.06	110.05
82	S4	201	PEB	C1D-CHC-C4C	-4.13	107.16	113.26
82	Q4	201	PEB	CMA-C2A-C1A	-4.13	103.50	112.40
87	FN	201	CLA	CAA-C2A-C3A	-4.13	106.46	116.10
85	BL	616	BCR	C15-C14-C13	-4.13	121.41	127.31
82	AQ	304	PEB	C2C-C1C-NC	4.13	113.14	107.57
82	QJ	204	PEB	OA-C1A-C2A	-4.13	122.89	126.17
82	TI	201	PEB	C3D-C4D-ND	4.13	115.36	107.26
82	ZE	202	PEB	CHC-C1D-ND	-4.13	108.50	113.72
84	K4	1001	CYC	CMA-C3A-C4A	4.13	131.43	125.06
82	dQ	401	PEB	CHA-C1B-NB	-4.13	116.29	124.93
84	IG	1001	CYC	CMD-C2D-C1D	4.13	131.61	125.56
82	JJ	201	PEB	C2C-C1C-NC	4.13	113.13	107.57
82	U9	203	PEB	C2C-C1C-NC	4.13	113.13	107.57
82	UG	201	PEB	CMC-C3C-C4C	4.13	131.44	127.06
82	OK	201	PEB	C2A-C1A-NA	4.13	111.83	108.27
82	QF	202	PEB	C1C-C2C-C3C	-4.13	102.74	107.62
96	VL	201	HEM	CHD-C1D-ND	4.13	128.91	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GJ	203	PEB	C1C-CHB-C4B	4.13	137.54	128.28
84	BG	1002	CYC	CHB-C4A-C3A	4.13	135.52	124.90
82	a4	201	PEB	C3D-C4D-ND	4.13	115.36	107.26
82	WD	201	PEB	CHB-C4B-C3B	-4.13	115.77	125.32
82	GQ	201	PEB	C1C-C2C-C3C	-4.13	102.74	107.62
82	dH	202	PEB	C1C-C2C-C3C	-4.13	102.74	107.62
82	vC	202	PEB	CHB-C1C-NC	-4.13	115.86	125.32
82	U9	204	PEB	CHB-C4B-NB	-4.13	115.98	124.58
82	cB	403	PEB	CMB-C2B-C1B	4.13	131.42	125.06
82	iJ	201	PEB	CMB-C2B-C1B	4.13	131.42	125.06
84	IG	1001	CYC	OB-C4B-C3B	-4.13	123.56	128.04
82	bE	201	PEB	CHA-C1B-NB	-4.13	116.30	124.93
92	BL	611	LMG	O7-C10-C11	4.13	120.40	111.50
82	ZF	202	PEB	C3D-C4D-ND	4.13	115.36	107.26
85	BN	843	BCR	C11-C10-C9	-4.13	121.42	127.31
82	NA	201	PEB	C1C-C2C-C3C	-4.13	102.74	107.62
82	U7	202	PEB	C1C-C2C-C3C	-4.13	102.74	107.62
82	mK	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
84	EH	1001	CYC	C1B-NB-C4B	-4.13	105.41	110.67
82	BF	202	PEB	C3D-C4D-ND	4.13	115.36	107.26
82	hK	201	PEB	C3D-C4D-ND	4.13	115.36	107.26
94	d6	408	PL9	C7-C8-C9	-4.13	119.92	126.79
82	lM	201	PEB	C1C-C2C-C3C	-4.13	102.74	107.62
82	UI	201	PEB	CHC-C1D-ND	-4.13	108.50	113.72
82	XQ	202	PEB	C1D-CHC-C4C	4.13	119.34	113.26
82	UH	201	PEB	C2C-C1C-NC	4.13	113.13	107.57
82	PO	203	PEB	C2C-C1C-NC	4.13	113.13	107.57
82	LB	201	PEB	C3D-C4D-ND	4.13	115.36	107.26
84	FH	1001	CYC	C1B-C2B-C3B	-4.13	103.56	107.87
82	UG	202	PEB	C3D-C4D-ND	4.13	115.35	107.26
82	Z1	202	PEB	C4B-C3B-C2B	-4.13	102.22	106.78
82	BB	201	PEB	CHA-C1B-NB	-4.13	116.30	124.93
82	PF	202	PEB	CMB-C2B-C1B	4.13	131.42	125.06
82	IP	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
84	LG	1001	CYC	CHB-C4A-C3A	4.12	135.51	124.90
82	SI	201	PEB	C3B-C4B-NB	4.12	116.05	110.05
82	K9	202	PEB	C2C-C1C-NC	4.12	113.12	107.57
82	XF	203	PEB	C3D-C4D-ND	4.12	115.35	107.26
85	C6	507	BCR	C20-C21-C22	-4.12	121.42	127.31
82	MB	201	PEB	CMB-C2B-C1B	4.12	131.41	125.06
82	F5	203	PEB	CMB-C2B-C1B	4.12	131.41	125.06
82	nK	201	PEB	CHA-C1B-NB	-4.12	116.31	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JF	202	PEB	C1D-CHC-C4C	4.12	119.34	113.26
82	OF	201	PEB	C3D-C4D-ND	4.12	115.35	107.26
82	eO	202	PEB	C3D-C4D-ND	4.12	115.35	107.26
82	l4	202	PEB	CHC-C4C-NC	4.12	126.73	121.15
82	aO	202	PEB	C1C-CHB-C4B	4.12	137.53	128.28
82	LF	201	PEB	C4B-C3B-C2B	-4.12	102.22	106.78
83	xK	305	PUB	CMA-C2A-C1A	4.12	131.09	121.39
82	HB	201	PEB	C3D-C4D-ND	4.12	115.35	107.26
82	ZJ	201	PEB	C3D-C4D-ND	4.12	115.35	107.26
82	t8	202	PEB	OA-C1A-C2A	-4.12	122.89	126.17
82	TD	202	PEB	C3D-C4D-ND	4.12	115.35	107.26
82	S9	201	PEB	C3D-C4D-ND	4.12	115.35	107.26
82	N7	203	PEB	CAB-CBB-CGB	-4.12	104.73	113.60
82	KB	301	PEB	CHA-C1B-NB	-4.12	116.31	124.93
82	Y9	202	PEB	CHB-C1C-C2C	-4.12	117.85	127.15
82	YE	202	PEB	C2A-C1A-NA	4.12	111.83	108.27
82	QB	201	PEB	C1C-C2C-C3C	-4.12	102.75	107.62
82	FA	201	PEB	CHC-C4C-NC	4.12	126.73	121.15
82	dE	204	PEB	CHC-C4C-NC	4.12	126.73	121.15
82	jK	202	PEB	CHB-C4B-C3B	-4.12	115.78	125.32
85	CL	501	BCR	C24-C23-C22	-4.12	120.01	126.23
82	VJ	201	PEB	CMC-C3C-C4C	4.12	131.43	127.06
82	W1	201	PEB	CHB-C1C-C2C	-4.12	117.85	127.15
82	UG	202	PEB	C2A-C1A-NA	4.12	111.83	108.27
82	N9	202	PEB	C2C-C1C-NC	4.12	113.12	107.57
82	l1	203	PEB	C1C-C2C-C3C	-4.12	102.75	107.62
82	gH	201	PEB	C1D-CHC-C4C	4.12	119.33	113.26
84	M1	201	CYC	C1D-C2D-C3D	-4.12	102.54	107.79
82	GI	201	PEB	C1B-C2B-C3B	-4.12	101.78	106.51
82	NQ	202	PEB	C2C-C1C-NC	4.12	113.12	107.57
82	qC	202	PEB	C1C-CHB-C4B	4.12	137.52	128.28
82	dG	202	PEB	CHB-C1C-C2C	-4.12	117.86	127.15
82	YQ	201	PEB	CHC-C1D-ND	-4.12	108.51	113.72
85	F6	101	BCR	C11-C10-C9	-4.12	121.43	127.31
82	VF	202	PEB	C3B-C4B-NB	4.12	116.04	110.05
82	dD	401	PEB	CHA-C1B-NB	-4.12	116.32	124.93
96	vL	201	HEM	CHC-C4B-NB	4.12	128.89	124.42
82	P9	202	PEB	C2C-C1C-NC	4.12	113.12	107.57
82	X9	202	PEB	C2C-C1C-NC	4.12	113.12	107.57
82	aM	201	PEB	OA-C1A-C2A	-4.12	122.90	126.17
82	FM	201	PEB	OD-C4D-ND	-4.12	119.83	125.93
84	E4	1001	CYC	OB-C4B-C3B	-4.12	123.57	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UE	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
82	OK	201	PEB	C3D-C4D-ND	4.12	115.34	107.26
82	XJ	201	PEB	CBC-CAC-C2C	-4.12	101.19	112.63
82	iK	201	PEB	C1C-C2C-C3C	-4.12	102.75	107.62
82	qK	201	PEB	C1C-C2C-C3C	-4.12	102.75	107.62
82	sK	201	PEB	CMB-C2B-C1B	4.12	131.40	125.06
82	J7	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
82	FF	201	PEB	CHC-C1D-ND	-4.12	108.52	113.72
82	aK	202	PEB	C1C-C2C-C3C	-4.12	102.75	107.62
92	m6	101	LMG	O7-C10-C11	4.12	120.37	111.50
82	RO	201	PEB	C2A-C1A-NA	4.12	111.82	108.27
82	T4	201	PEB	CMB-C2B-C1B	4.12	131.40	125.06
82	sK	203	PEB	CHB-C1C-C2C	-4.12	117.86	127.15
82	AD	304	PEB	C2C-C1C-NC	4.12	113.11	107.57
82	QD	201	PEB	C2C-C1C-NC	4.12	113.11	107.57
82	lK	201	PEB	C2C-C1C-NC	4.12	113.11	107.57
82	sK	203	PEB	CHA-C1B-C2B	4.12	135.48	124.90
83	yF	302	PUB	CMA-C2A-C1A	4.12	131.07	121.39
82	DB	203	PEB	OA-C1A-C2A	-4.12	122.90	126.17
82	BD	203	PEB	C4B-C3B-C2B	-4.11	102.23	106.78
92	dL	407	LMG	O1-C7-C8	-4.11	100.97	110.90
82	q8	202	PEB	C1C-CHB-C4B	4.11	137.51	128.28
82	bP	502	PEB	OA-C1A-C2A	-4.11	122.90	126.17
84	LE	1001	CYC	CHB-C4A-C3A	4.11	135.48	124.90
82	TO	201	PEB	CMB-C2B-C1B	4.11	131.40	125.06
82	kF	201	PEB	C3D-C4D-ND	4.11	115.33	107.26
91	aL	610	PHO	C3D-C4D-ND	4.11	113.33	107.72
82	cF	201	PEB	C1C-C2C-C3C	-4.11	102.76	107.62
82	s8	203	PEB	C2C-C1C-NC	4.11	113.11	107.57
82	W9	203	PEB	C2C-C1C-NC	4.11	113.11	107.57
82	TP	202	PEB	CHA-C1B-NB	-4.11	116.33	124.93
82	UP	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
82	RM	201	PEB	OA-C1A-C2A	-4.11	122.90	126.17
82	lK	202	PEB	OA-C1A-C2A	-4.11	122.90	126.17
82	PJ	202	PEB	CHC-C1D-ND	-4.11	108.52	113.72
82	qF	203	PEB	CHC-C4C-NC	4.11	126.71	121.15
82	WF	203	PEB	C1C-C2C-C3C	-4.11	102.76	107.62
82	sK	202	PEB	C2C-C1C-NC	4.11	113.11	107.57
82	cK	202	PEB	CMC-C3C-C4C	4.11	131.42	127.06
82	XQ	201	PEB	CHC-C1D-ND	-4.11	108.52	113.72
85	h6	102	BCR	C20-C21-C22	-4.11	121.44	127.31
82	sF	203	PEB	CHA-C1B-C2B	4.11	135.47	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	BE	1002	CYC	CHB-C4A-C3A	4.11	135.47	124.90
82	CM	201	PEB	CHA-C1B-NB	-4.11	116.34	124.93
82	jH	203	PEB	CHA-C1B-NB	-4.11	116.34	124.93
82	qK	203	PEB	CMB-C2B-C1B	4.11	131.39	125.06
82	A4	305	PEB	OA-C1A-C2A	-4.11	122.91	126.17
82	OD	201	PEB	C3B-C4B-NB	4.11	116.03	110.05
83	AE	302	PUB	CMA-C2A-C1A	4.11	131.06	121.39
82	DD	201	PEB	C3C-C4C-NC	4.11	112.03	108.33
82	J9	203	PEB	C2A-C1A-NA	4.11	111.81	108.27
82	j1	202	PEB	C1C-C2C-C3C	-4.11	102.76	107.62
82	lH	202	PEB	C1C-C2C-C3C	-4.11	102.76	107.62
82	iJ	201	PEB	C3D-C4D-ND	4.11	115.32	107.26
84	K4	1001	CYC	OB-C4B-C3B	-4.11	123.58	128.04
82	UP	201	PEB	CHC-C4C-NC	4.11	126.71	121.15
95	b6	621	DGD	O2G-C1B-C2B	4.11	120.35	111.50
82	S9	201	PEB	C4B-C3B-C2B	-4.11	102.24	106.78
82	CD	202	PEB	OA-C1A-C2A	-4.11	122.91	126.17
84	x3	1001	CYC	C2D-C1D-ND	4.11	113.17	107.40
82	VJ	201	PEB	CHA-C1B-NB	-4.11	116.34	124.93
87	b6	605	CLA	CHC-C4B-NB	4.11	128.60	124.26
82	DK	202	PEB	C1C-C2C-C3C	-4.11	102.77	107.62
82	KM	201	PEB	CHA-C1B-NB	-4.11	116.34	124.93
96	V6	201	HEM	CHD-C1D-ND	4.11	128.88	124.42
82	XK	203	PEB	C3D-C4D-ND	4.11	115.32	107.26
82	l1	201	PEB	OA-C1A-C2A	-4.11	122.91	126.17
82	aK	201	PEB	C1B-C2B-C3B	-4.11	101.79	106.51
82	aO	201	PEB	C3D-C4D-ND	4.11	115.31	107.26
82	F7	201	PEB	CHC-C4C-NC	4.11	126.71	121.15
82	ZG	201	PEB	C3C-C4C-NC	4.11	112.03	108.33
82	PK	202	PEB	CMB-C2B-C1B	4.11	131.39	125.06
82	p8	201	PEB	OA-C1A-C2A	-4.11	122.91	126.17
82	QB	201	PEB	C2C-C1C-NC	4.11	113.10	107.57
82	bE	201	PEB	C3D-C4D-ND	4.10	115.31	107.26
82	gF	203	PEB	C3D-C4D-ND	4.10	115.31	107.26
82	jH	201	PEB	C3B-C4B-NB	4.10	116.02	110.05
82	A9	202	PEB	C2C-C1C-NC	4.10	113.10	107.57
82	sC	203	PEB	C2C-C1C-NC	4.10	113.10	107.57
82	OF	201	PEB	CHA-C1B-NB	-4.10	116.35	124.93
82	WQ	201	PEB	CHB-C4B-C3B	-4.10	115.83	125.32
82	kH	203	PEB	OA-C1A-C2A	-4.10	122.91	126.17
95	b6	622	DGD	O2G-C1B-C2B	4.10	120.34	111.50
82	QM	202	PEB	C1C-C2C-C3C	-4.10	102.77	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MF	203	PEB	C3D-C4D-ND	4.10	115.31	107.26
82	XM	202	PEB	CMB-C2B-C1B	4.10	131.38	125.06
95	BL	607	DGD	O2G-C1B-C2B	4.10	120.34	111.50
82	ZJ	201	PEB	C1D-CHC-C4C	4.10	119.31	113.26
82	VK	202	PEB	C3B-C4B-NB	4.10	116.02	110.05
82	j1	203	PEB	CHA-C1B-NB	-4.10	116.35	124.93
82	A1	301	PEB	C3D-C4D-ND	4.10	115.31	107.26
82	UM	201	PEB	C1C-C2C-C3C	-4.10	102.77	107.62
85	B2	843	BCR	C11-C10-C9	-4.10	121.46	127.31
85	F2	203	BCR	C7-C8-C9	4.10	132.43	126.23
85	C6	508	BCR	C7-C8-C9	-4.10	120.04	126.23
82	JK	202	PEB	C1D-CHC-C4C	4.10	119.30	113.26
84	LG	1001	CYC	C1B-C2B-C3B	-4.10	103.59	107.87
82	TD	202	PEB	C2C-C1C-NC	4.10	113.09	107.57
82	c4	203	PEB	C4B-C3B-C2B	-4.10	102.24	106.78
82	OP	203	PEB	C3D-C4D-ND	4.10	115.31	107.26
82	sF	201	PEB	CMB-C2B-C1B	4.10	131.38	125.06
82	hF	201	PEB	C3D-C4D-ND	4.10	115.30	107.26
84	MO	1001	CYC	C2D-C1D-ND	4.10	113.16	107.40
82	HA	203	PEB	C1C-C2C-C3C	-4.10	102.77	107.62
82	PO	203	PEB	C1C-C2C-C3C	-4.10	102.77	107.62
82	WH	202	PEB	CMB-C2B-C1B	4.10	131.38	125.06
82	UB	301	PEB	OA-C1A-C2A	-4.10	122.91	126.17
82	NQ	204	PEB	OA-C1A-C2A	-4.10	122.91	126.17
82	b1	202	PEB	C2C-C1C-NC	4.10	113.09	107.57
82	M9	301	PEB	C2C-C1C-NC	4.10	113.09	107.57
82	GQ	201	PEB	CHC-C1D-ND	-4.10	108.54	113.72
82	JP	201	PEB	C4B-C3B-C2B	-4.10	102.25	106.78
84	HE	1001	CYC	CMB-C2B-C1B	4.10	129.29	124.17
82	OE	203	PEB	CHB-C1C-C2C	-4.10	117.90	127.15
82	cB	401	PEB	C3D-C4D-ND	4.10	115.30	107.26
82	eF	203	PEB	CMC-C3C-C4C	4.10	131.41	127.06
82	GD	202	PEB	OA-C1A-C2A	-4.10	122.91	126.17
84	HG	1001	CYC	CMB-C2B-C1B	4.10	129.28	124.17
84	CO	1001	CYC	C2B-C1B-NB	4.10	112.99	106.99
82	TM	201	PEB	C2C-C1C-NC	4.10	113.09	107.57
82	CM	203	PEB	CHA-C1B-NB	-4.10	116.36	124.93
82	aM	204	PEB	C1C-CHB-C4B	4.10	137.47	128.28
82	VA	203	PEB	OA-C1A-C2A	-4.10	122.92	126.17
82	W5	201	PEB	OA-C1A-C2A	-4.10	122.92	126.17
84	M4	1001	CYC	CHD-C1D-ND	-4.10	115.93	125.32
82	i4	203	PEB	C2C-C1C-NC	4.10	113.09	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QF	201	PEB	C4B-C3B-C2B	-4.10	102.25	106.78
82	V7	202	PEB	C1C-C2C-C3C	-4.10	102.78	107.62
82	UP	201	PEB	CMB-C2B-C1B	4.10	131.37	125.06
82	AP	203	PEB	C1C-C2C-C3C	-4.10	102.78	107.62
103	82	309	ZEX	C28-C27-C26	-4.10	120.09	127.09
82	CK	203	PEB	C2C-C1C-NC	4.10	113.09	107.57
82	xK	304	PEB	C2C-C1C-NC	4.10	113.09	107.57
82	BJ	301	PEB	C3D-C4D-ND	4.10	115.29	107.26
82	d4	202	PEB	C3D-C4D-ND	4.10	115.29	107.26
82	H7	203	PEB	C1C-C2C-C3C	-4.10	102.78	107.62
82	aF	202	PEB	C1C-C2C-C3C	-4.10	102.78	107.62
82	TQ	202	PEB	C3D-C4D-ND	4.09	115.29	107.26
82	G9	202	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	R9	202	PEB	C2C-C1C-NC	4.09	113.08	107.57
103	8N	309	ZEX	C28-C27-C26	-4.09	120.09	127.09
82	cJ	201	PEB	C1C-C2C-C3C	-4.09	102.78	107.62
82	S5	202	PEB	C4B-C3B-C2B	-4.09	102.25	106.78
82	T9	202	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	ND	204	PEB	OA-C1A-C2A	-4.09	122.92	126.17
82	W4	201	PEB	C3D-C4D-ND	4.09	115.29	107.26
82	kK	201	PEB	C3D-C4D-ND	4.09	115.29	107.26
84	MG	1001	CYC	C2B-C1B-NB	4.09	112.98	106.99
82	OQ	201	PEB	C3B-C4B-NB	4.09	116.00	110.05
87	A2	852	CLA	CMD-C2D-C3D	-4.09	118.20	127.61
82	WK	203	PEB	C1C-C2C-C3C	-4.09	102.78	107.62
82	jG	202	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	BF	201	PEB	C3D-C4D-ND	4.09	115.29	107.26
82	J9	201	PEB	C2C-C1C-NC	4.09	113.08	107.57
84	G4	1001	CYC	OB-C4B-C3B	-4.09	123.60	128.04
82	O9	201	PEB	C3B-C4B-NB	4.09	116.00	110.05
82	OG	203	PEB	CHB-C1C-C2C	-4.09	117.92	127.15
82	PB	201	PEB	C3D-C4D-ND	4.09	115.29	107.26
82	PF	202	PEB	C3D-C4D-ND	4.09	115.29	107.26
82	lO	202	PEB	CHC-C4C-NC	4.09	126.69	121.15
95	J6	101	DGD	O2G-C1B-C2B	4.09	120.32	111.50
95	a6	602	DGD	O2G-C1B-C2B	4.09	120.32	111.50
83	xF	305	PUB	CMA-C2A-C1A	4.09	131.01	121.39
82	KM	203	PEB	OA-C1A-C2A	-4.09	122.92	126.17
92	a6	614	LMG	O7-C10-C11	4.09	120.32	111.50
85	kL	100	BCR	C16-C17-C18	4.09	133.15	127.31
85	CL	516	BCR	C3-C4-C5	-4.09	106.77	114.08
82	Z9	304	PEB	C4B-C3B-C2B	-4.09	102.25	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lJ	201	PEB	CHB-C1C-C2C	-4.09	117.92	127.15
82	wK	303	PEB	C3D-C4D-ND	4.09	115.28	107.26
82	CF	203	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	bP	501	PEB	OA-C1A-C2A	-4.09	122.92	126.17
82	Q1	201	PEB	C1C-C2C-C3C	-4.09	102.79	107.62
82	eJ	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
82	dF	202	PEB	CMB-C2B-C1B	4.09	131.36	125.06
82	GD	201	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	mO	203	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	BF	201	PEB	C1C-C2C-C3C	-4.09	102.79	107.62
82	fM	203	PEB	C1C-C2C-C3C	-4.09	102.79	107.62
85	K2	105	BCR	C21-C20-C19	-4.09	110.46	123.22
82	QF	202	PEB	C2C-C1C-NC	4.09	113.08	107.57
82	LD	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
82	IF	201	PEB	CAC-C2C-C3C	4.09	136.43	127.07
85	KL	100	BCR	C11-C10-C9	-4.09	121.47	127.31
82	V1	202	PEB	CHB-C1C-C2C	-4.09	117.93	127.15
82	lF	203	PEB	C2A-C1A-NA	4.09	111.80	108.27
82	xK	304	PEB	C2A-C1A-NA	4.09	111.80	108.27
82	HD	202	PEB	CHA-C1B-C2B	4.09	135.41	124.90
82	dO	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
87	AL	403	CLA	CMB-C2B-C1B	-4.09	119.14	125.37
82	dF	201	PEB	C1C-C2C-C3C	-4.09	102.79	107.62
82	PA	201	PEB	CHC-C4C-NC	4.09	126.68	121.15
82	S9	203	PEB	CMB-C2B-C1B	4.09	131.36	125.06
84	C4	1001	CYC	C2B-C1B-NB	4.09	112.97	106.99
84	F1	1001	CYC	OC-C1C-C2C	-4.09	122.92	126.17
87	AN	852	CLA	CMD-C2D-C3D	-4.09	118.21	127.61
82	d4	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
82	lO	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
82	PK	201	PEB	CHC-C4C-NC	4.09	126.68	121.15
82	fJ	201	PEB	CHC-C4C-NC	4.09	126.68	121.15
82	A4	301	PEB	C2C-C1C-NC	4.09	113.07	107.57
82	BD	203	PEB	C3C-C4C-NC	4.09	112.01	108.33
84	DO	1001	CYC	C1B-C2B-C3B	-4.09	103.61	107.87
82	pF	202	PEB	C3D-C4D-ND	4.09	115.27	107.26
82	pK	202	PEB	C3D-C4D-ND	4.09	115.27	107.26
82	VO	202	PEB	C4B-C3B-C2B	-4.09	102.26	106.78
83	AE	303	PUB	CMA-C2A-C1A	4.09	131.00	121.39
82	BQ	202	PEB	C1C-C2C-C3C	-4.08	102.79	107.62
82	w8	204	PEB	CHC-C1D-ND	-4.08	108.56	113.72
82	WG	203	PEB	OA-C1A-C2A	-4.08	122.93	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UI	201	PEB	OA-C1A-C2A	-4.08	122.93	126.17
82	NM	201	PEB	OA-C1A-C2A	-4.08	122.93	126.17
88	bL	612	LHG	O7-C7-C8	4.08	120.30	111.50
82	LJ	201	PEB	C3D-C4D-ND	4.08	115.27	107.26
82	aO	203	PEB	CAC-CBC-CGC	-4.08	104.82	113.60
82	GM	203	PEB	C1C-CHB-C4B	4.08	137.44	128.28
82	MM	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
82	aM	203	PEB	OA-C1A-C2A	-4.08	122.93	126.17
82	Z5	304	PEB	C3D-C4D-ND	4.08	115.27	107.26
82	ND	202	PEB	C2C-C1C-NC	4.08	113.07	107.57
84	BG	1002	CYC	CHD-C1D-ND	-4.08	115.97	125.32
82	VA	201	PEB	CHA-C1B-NB	-4.08	116.39	124.93
95	a6	603	DGD	O2G-C1B-C2B	4.08	120.30	111.50
85	KN	104	BCR	C21-C20-C19	-4.08	110.48	123.22
82	a1	202	PEB	OA-C1A-C2A	-4.08	122.93	126.17
84	LG	1001	CYC	CHD-C1D-ND	-4.08	115.97	125.32
82	GK	201	PEB	C1B-C2B-C3B	-4.08	101.82	106.51
82	PE	202	PEB	CHA-C1B-NB	-4.08	116.40	124.93
82	fH	202	PEB	CHC-C1D-ND	-4.08	108.56	113.72
83	AD	302	PUB	CHA-C4A-NA	-4.08	108.56	113.72
82	D7	202	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
82	l4	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
82	V7	201	PEB	CHA-C1B-NB	-4.08	116.40	124.93
83	yK	302	PUB	CMA-C2A-C1A	4.08	130.99	121.39
84	LE	1001	CYC	CHD-C1D-ND	-4.08	115.97	125.32
82	HM	202	PEB	CHA-C1B-NB	-4.08	116.40	124.93
82	ZO	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
82	OD	202	PEB	OA-C1A-C2A	-4.08	122.93	126.17
82	VG	201	PEB	OA-C1A-C2A	-4.08	122.93	126.17
82	jG	202	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
82	bH	202	PEB	C2C-C1C-NC	4.08	113.06	107.57
82	S4	201	PEB	CHA-C1B-NB	-4.08	116.40	124.93
82	lJ	201	PEB	C1C-CHB-C4B	4.08	137.43	128.28
82	OK	203	PEB	OA-C1A-C2A	-4.08	122.93	126.17
84	FH	1001	CYC	OC-C1C-C2C	-4.08	122.93	126.17
82	lG	201	PEB	C2A-C1A-NA	4.08	111.79	108.27
82	SB	202	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
84	BE	1002	CYC	CHD-C1D-ND	-4.08	115.98	125.32
82	g1	201	PEB	C1D-CHC-C4C	4.08	119.27	113.26
95	B2	844	DGD	O2G-C1B-C2B	4.08	120.29	111.50
82	mG	201	PEB	C2C-C1C-NC	4.08	113.06	107.57
82	M9	301	PEB	C1C-C2C-C3C	-4.08	102.80	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ZM	202	PEB	C1C-CHB-C4B	-4.08	119.14	128.28
82	fK	201	PEB	C2C-C1C-NC	4.08	113.06	107.57
83	xF	306	PUB	C3B-C4B-NB	4.08	113.06	107.57
83	xK	305	PUB	C3B-C4B-NB	4.08	113.06	107.57
85	A2	846	BCR	C20-C21-C22	4.08	133.13	127.31
82	UA	202	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
82	XB	202	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
82	V7	201	PEB	CHC-C4C-NC	4.08	126.67	121.15
82	YA	301	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
82	HD	202	PEB	C1C-C2C-C3C	-4.08	102.80	107.62
82	eB	201	PEB	CMB-C2B-C1B	4.08	131.34	125.06
103	8N	309	ZEX	C7-C8-C9	-4.08	120.08	126.23
85	KL	100	BCR	C16-C17-C18	4.08	133.13	127.31
82	ED	201	PEB	C3B-C4B-NB	4.08	115.98	110.05
82	NA	201	PEB	C2A-C1A-NA	4.08	111.79	108.27
82	qF	203	PEB	CMB-C2B-C1B	4.07	131.34	125.06
82	XA	201	PEB	CHC-C1D-ND	-4.07	108.57	113.72
85	kL	100	BCR	C11-C10-C9	-4.07	121.50	127.31
82	XA	203	PEB	CAC-CBC-CGC	-4.07	104.83	113.60
85	AN	804	BCR	C28-C27-C26	-4.07	106.80	114.08
82	eE	201	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	M9	302	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	jE	202	PEB	C2C-C1C-NC	4.07	113.06	107.57
82	D9	202	PEB	C1C-CHB-C4B	4.07	137.42	128.28
82	f1	202	PEB	CHC-C1D-ND	-4.07	108.57	113.72
82	RJ	201	PEB	OA-C1A-C2A	-4.07	122.93	126.17
82	Z9	303	PEB	CMB-C2B-C1B	4.07	131.34	125.06
82	RB	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	KJ	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	NJ	202	PEB	C4B-C3B-C2B	-4.07	102.27	106.78
82	kK	203	PEB	C3C-C4C-NC	4.07	112.00	108.33
82	GQ	201	PEB	C2C-C1C-NC	4.07	113.06	107.57
82	h1	202	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	wC	204	PEB	CHC-C1D-ND	-4.07	108.57	113.72
82	UF	201	PEB	CAC-C2C-C3C	4.07	136.40	127.07
82	GD	201	PEB	C1C-CHB-C4B	4.07	137.42	128.28
82	JA	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	AJ	302	PEB	CHA-C1B-NB	-4.07	116.41	124.93
96	VL	201	HEM	CHC-C4B-NB	4.07	128.84	124.42
84	EO	1001	CYC	C2B-C1B-NB	4.07	112.95	106.99
84	V3	1001	CYC	C2D-C1D-ND	4.07	113.12	107.40
82	QK	201	PEB	C4B-C3B-C2B	-4.07	102.28	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	KH	1001	CYC	OC-C1C-C2C	-4.07	122.94	126.17
82	NA	201	PEB	CHA-C1B-NB	-4.07	116.41	124.93
82	DK	202	PEB	CHA-C1B-NB	-4.07	116.41	124.93
82	YM	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	H5	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	c4	202	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	T5	201	PEB	CHC-C1D-ND	-4.07	108.57	113.72
82	O1	203	PEB	CHB-C1C-C2C	-4.07	117.96	127.15
82	PA	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	QG	201	PEB	C1D-CHC-C4C	-4.07	107.25	113.26
85	c6	603	BCR	C15-C14-C13	-4.07	121.50	127.31
82	yC	203	PEB	C2C-C1C-NC	4.07	113.05	107.57
82	F4	1002	PEB	C2A-C1A-NA	4.07	111.78	108.27
83	AQ	302	PUB	CHA-C4A-NA	-4.07	108.57	113.72
82	PP	202	PEB	OA-C1A-C2A	-4.07	122.94	126.17
82	nK	202	PEB	OA-C1A-C2A	-4.07	122.94	126.17
95	CL	520	DGD	O2G-C1B-C2B	4.07	120.28	111.50
82	jH	203	PEB	C1D-CHC-C4C	-4.07	107.25	113.26
82	HF	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	VK	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
82	M9	305	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
82	DF	202	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	bG	201	PEB	CHA-C1B-NB	-4.07	116.42	124.93
82	V1	202	PEB	C1D-CHC-C4C	4.07	119.26	113.26
82	gB	203	PEB	CMB-C2B-C1B	4.07	131.33	125.06
82	e4	202	PEB	C3D-C4D-ND	4.07	115.24	107.26
82	M5	304	PEB	C3D-C4D-ND	4.07	115.24	107.26
84	LE	1001	CYC	C1B-C2B-C3B	-4.07	103.62	107.87
82	ZH	202	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
82	HB	203	PEB	CMB-C2B-C1B	4.07	131.33	125.06
82	HQ	202	PEB	CHA-C1B-C2B	4.07	135.37	124.90
87	8N	308	CLA	CMC-C2C-C1C	-4.07	118.84	125.04
82	Q4	201	PEB	C1D-CHC-C4C	-4.07	107.26	113.26
82	WH	203	PEB	C1C-CHB-C4B	4.07	137.41	128.28
82	JK	201	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	TI	201	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
82	HA	201	PEB	C2C-C1C-NC	4.07	113.05	107.57
82	SO	201	PEB	CHA-C1B-NB	-4.07	116.42	124.93
82	VA	201	PEB	CHC-C4C-NC	4.07	126.66	121.15
82	QH	201	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	UP	201	PEB	CHB-C4B-C3B	-4.07	115.91	125.32
84	ME	1001	CYC	C2B-C1B-NB	4.07	112.94	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CB	202	PEB	CHA-C1B-NB	-4.07	116.42	124.93
85	AN	846	BCR	C20-C21-C22	4.07	133.12	127.31
82	VH	201	PEB	OA-C1A-C2A	-4.07	122.94	126.17
82	PK	202	PEB	C3D-C4D-ND	4.07	115.24	107.26
82	dM	202	PEB	C3D-C4D-ND	4.07	115.24	107.26
82	YM	203	PEB	C2C-C1C-NC	4.07	113.05	107.57
82	BD	202	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
82	GQ	201	PEB	C1C-CHB-C4B	4.07	137.40	128.28
82	N7	201	PEB	C2A-C1A-NA	4.07	111.78	108.27
82	p8	202	PEB	C3D-C4D-ND	4.07	115.24	107.26
83	wF	304	PUB	CHC-C1D-ND	-4.07	108.58	113.72
82	fE	201	PEB	CHC-C4C-NC	4.07	126.65	121.15
82	mE	201	PEB	C2C-C1C-NC	4.07	113.05	107.57
84	CO	1001	CYC	CMA-C3A-C4A	4.07	131.33	125.06
82	jE	201	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
87	AN	819	CLA	C3B-C4B-NB	-4.07	106.74	110.52
82	YG	202	PEB	C2A-C1A-NA	4.07	111.78	108.27
82	hO	201	PEB	C3B-C4B-NB	4.07	115.96	110.05
82	L5	202	PEB	C1C-C2C-C3C	-4.07	102.81	107.62
85	c6	617	BCR	C7-C8-C9	4.07	132.38	126.23
82	TA	201	PEB	C3D-C4D-ND	4.07	115.23	107.26
82	ZG	202	PEB	CHC-C1D-ND	-4.07	108.58	113.72
82	HQ	202	PEB	C2C-C1C-NC	4.06	113.05	107.57
85	A2	804	BCR	C28-C27-C26	-4.06	106.82	114.08
84	EO	1001	CYC	OB-C4B-C3B	-4.06	123.63	128.04
82	HH	1002	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	kH	203	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	QO	201	PEB	C1D-CHC-C4C	-4.06	107.26	113.26
82	dE	204	PEB	C2C-C1C-NC	4.06	113.04	107.57
82	f4	201	PEB	CHB-C1C-C2C	-4.06	117.98	127.15
82	XD	201	PEB	CHC-C1D-ND	-4.06	108.58	113.72
82	NE	202	PEB	C3D-C4D-ND	4.06	115.23	107.26
83	AO	302	PUB	CMA-C2A-C1A	4.06	130.95	121.39
82	H7	201	PEB	C2A-C1A-NA	4.06	111.78	108.27
82	QB	202	PEB	C3D-C4D-ND	4.06	115.23	107.26
82	EJ	202	PEB	CHC-C4C-NC	4.06	126.65	121.15
82	lK	202	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	cO	203	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
83	A4	303	PUB	CMA-C2A-C1A	4.06	130.94	121.39
82	18	202	PEB	C2C-C1C-NC	4.06	113.04	107.57
82	GM	203	PEB	CHC-C1D-ND	-4.06	108.58	113.72
82	fO	201	PEB	CHB-C1C-C2C	-4.06	117.99	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	J7	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
82	GF	202	PEB	C1D-CHC-C4C	-4.06	107.27	113.26
84	N1	1001	CYC	CMD-C2D-C1D	4.06	131.51	125.56
82	cK	202	PEB	C2C-C1C-NC	4.06	113.04	107.57
82	eJ	201	PEB	CMC-C3C-C4C	4.06	131.37	127.06
82	HJ	201	PEB	C4B-C3B-C2B	-4.06	102.29	106.78
96	vL	201	HEM	CHD-C1D-ND	4.06	128.83	124.42
82	b4	201	PEB	CHB-C4B-C3B	-4.06	115.92	125.32
84	IE	1001	CYC	C2D-C1D-ND	4.06	113.11	107.40
82	d1	202	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	GD	201	PEB	CHC-C1D-ND	-4.06	108.59	113.72
82	WQ	201	PEB	CHC-C1D-ND	-4.06	108.59	113.72
83	M5	303	PUB	CHA-C4A-NA	-4.06	108.59	113.72
85	B2	839	BCR	C34-C9-C10	-4.06	117.24	122.92
82	CJ	202	PEB	OA-C1A-C2A	-4.06	122.94	126.17
82	YJ	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
82	BK	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
82	lK	203	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	gO	202	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	GK	201	PEB	OD-C4D-ND	-4.06	119.92	125.93
82	aF	201	PEB	C1B-C2B-C3B	-4.06	101.85	106.51
82	UK	201	PEB	CAC-C2C-C3C	4.06	136.37	127.07
82	GK	201	PEB	C2A-C1A-NA	4.06	111.77	108.27
82	HF	201	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	18	203	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
82	TJ	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
82	O4	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
82	KP	201	PEB	OA-C1A-C2A	-4.06	122.95	126.17
82	FK	201	PEB	CHC-C4C-NC	4.06	126.64	121.15
95	BN	844	DGD	O2G-C1B-C2B	4.06	120.25	111.50
82	W1	203	PEB	CHB-C1C-C2C	-4.06	118.00	127.15
82	DH	1002	PEB	CMB-C2B-C1B	4.06	131.31	125.06
82	Y1	202	PEB	C1C-C2C-C3C	-4.06	102.82	107.62
83	xF	305	PUB	C3B-C4B-NB	4.06	113.03	107.57
82	lF	202	PEB	OA-C1A-C2A	-4.06	122.95	126.17
82	GF	203	PEB	C1C-CHB-C4B	4.06	137.38	128.28
84	J1	1001	CYC	C4D-C3D-C2D	-4.06	102.83	107.62
82	KP	202	PEB	C3B-C4B-NB	4.06	115.95	110.05
82	RQ	201	PEB	C1C-C2C-C3C	-4.06	102.83	107.62
82	PJ	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
82	BQ	201	PEB	OA-C1A-C2A	-4.06	122.95	126.17
82	aH	202	PEB	CMB-C2B-C1B	4.06	131.31	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eM	201	PEB	CMB-C2B-C1B	4.06	131.31	125.06
82	SH	203	PEB	CHB-C1C-C2C	-4.06	118.00	127.15
85	hL	102	BCR	C16-C17-C18	-4.06	121.52	127.31
82	eA	301	PEB	CHC-C4C-NC	4.06	126.64	121.15
82	gM	201	PEB	C1C-C2C-C3C	-4.06	102.83	107.62
82	HD	202	PEB	C2C-C1C-NC	4.06	113.03	107.57
82	dG	204	PEB	C2C-C1C-NC	4.06	113.03	107.57
84	IE	1001	CYC	CMD-C2D-C1D	4.06	131.50	125.56
92	B6	622	LMG	O7-C10-C11	4.05	120.24	111.50
82	PH	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	GM	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	S9	203	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	CF	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	UB	302	PEB	CHC-C4C-NC	4.05	126.64	121.15
82	H9	203	PEB	CHA-C1B-NB	-4.05	116.45	124.93
82	d1	201	PEB	C1C-C2C-C3C	-4.05	102.83	107.62
85	aL	604	BCR	C20-C21-C22	-4.05	121.53	127.31
82	UK	201	PEB	C1D-CHC-C4C	-4.05	107.28	113.26
95	cL	502	DGD	O2G-C1B-C2B	4.05	120.24	111.50
85	cL	518	BCR	C16-C17-C18	-4.05	121.53	127.31
82	ZK	201	PEB	C1C-C2C-C3C	-4.05	102.83	107.62
84	JH	1001	CYC	C4D-C3D-C2D	-4.05	102.83	107.62
85	BN	839	BCR	C34-C9-C10	-4.05	117.25	122.92
82	M9	304	PEB	CMB-C2B-C1B	4.05	131.31	125.06
82	a4	203	PEB	CAC-CBC-CGC	-4.05	104.88	113.60
82	CJ	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	wF	303	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	CM	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	gE	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	EQ	202	PEB	C1C-C2C-C3C	-4.05	102.83	107.62
82	DF	202	PEB	CHA-C1B-NB	-4.05	116.46	124.93
82	CM	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	U4	201	PEB	C4B-NB-C1B	-4.05	98.88	106.51
82	jG	201	PEB	C1C-C2C-C3C	-4.05	102.83	107.62
82	IQ	201	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	cF	203	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	fH	203	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	eJ	201	PEB	OA-C1A-C2A	-4.05	122.95	126.17
83	AG	303	PUB	CMA-C2A-C1A	4.05	130.92	121.39
82	LQ	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
84	E4	1001	CYC	C2B-C1B-NB	4.05	112.92	106.99
82	M9	302	PEB	C4B-C3B-C2B	-4.05	102.30	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jF	202	PEB	CHB-C4B-C3B	-4.05	115.95	125.32
82	1C	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	jM	203	PEB	C3D-C4D-ND	4.05	115.21	107.26
82	F5	201	PEB	C3B-C4B-NB	4.05	115.94	110.05
82	PG	202	PEB	CHA-C1B-NB	-4.05	116.46	124.93
82	ED	202	PEB	C1C-C2C-C3C	-4.05	102.83	107.62
82	QE	202	PEB	C2C-C1C-NC	4.05	113.03	107.57
82	GK	202	PEB	C1D-CHC-C4C	-4.05	107.28	113.26
84	FE	1001	CYC	OB-C4B-C3B	-4.05	123.64	128.04
82	SJ	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	GQ	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	Q5	201	PEB	CMB-C2B-C1B	4.05	131.30	125.06
82	1C	202	PEB	C2C-C1C-NC	4.05	113.02	107.57
82	dE	203	PEB	C2C-C1C-NC	4.05	113.02	107.57
82	dG	203	PEB	C2C-C1C-NC	4.05	113.02	107.57
82	dK	201	PEB	C1C-C2C-C3C	-4.05	102.83	107.62
82	GB	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
82	MB	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
82	Y7	304	PEB	C1C-CHB-C4B	-4.05	119.20	128.28
82	UA	201	PEB	OD-C4D-ND	-4.05	119.93	125.93
82	X5	201	PEB	CHC-C1D-ND	-4.05	108.60	113.72
82	ZF	201	PEB	C1C-C2C-C3C	-4.05	102.84	107.62
82	QO	201	PEB	C4B-NB-C1B	-4.05	98.88	106.51
82	RO	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
82	lE	201	PEB	C2A-C1A-NA	4.05	111.76	108.27
82	Z9	301	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
82	D4	1002	PEB	C2C-C1C-NC	4.05	113.02	107.57
82	HI	202	PEB	CAC-C2C-C1C	4.05	132.21	125.76
82	bO	201	PEB	CHB-C4B-C3B	-4.05	115.96	125.32
84	H1	1001	CYC	C4D-C3D-C2D	-4.05	102.84	107.62
82	VD	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
82	VO	202	PEB	C1C-C2C-C3C	-4.05	102.84	107.62
82	gF	201	PEB	C3B-C4B-NB	4.04	115.93	110.05
82	d1	203	PEB	C2C-C1C-NC	4.04	113.02	107.57
82	MK	203	PEB	C3D-C4D-ND	4.04	115.19	107.26
82	1C	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
82	fG	201	PEB	OA-C1A-C2A	-4.04	122.96	126.17
82	PP	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	EF	201	PEB	CHC-C4C-NC	4.04	126.62	121.15
82	jO	201	PEB	CHB-C4B-C3B	-4.04	115.96	125.32
84	D4	1001	CYC	C1B-C2B-C3B	-4.04	103.65	107.87
82	OO	202	PEB	C3D-C4D-ND	4.04	115.19	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OH	203	PEB	C2A-C1A-NA	4.04	111.76	108.27
82	PA	202	PEB	C1C-C2C-C3C	-4.04	102.84	107.62
82	WD	202	PEB	C1C-C2C-C3C	-4.04	102.84	107.62
82	l1	201	PEB	C1C-C2C-C3C	-4.04	102.84	107.62
82	hG	201	PEB	C2C-C1C-NC	4.04	113.02	107.57
82	OP	203	PEB	CHB-C1C-C2C	-4.04	118.03	127.15
82	N7	201	PEB	CHA-C1B-NB	-4.04	116.47	124.93
85	bL	601	BCR	C16-C17-C18	-4.04	121.54	127.31
82	18	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
84	H4	1001	CYC	OC-C1C-C2C	-4.04	122.96	126.17
82	R4	202	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	X7	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	iK	203	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	XK	202	PEB	C1C-CHB-C4B	4.04	137.35	128.28
82	Q1	201	PEB	C3C-C4C-NC	4.04	111.97	108.33
84	HO	1001	CYC	C1B-NB-C4B	-4.04	105.52	110.67
82	NG	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
82	W1	202	PEB	CMB-C2B-C1B	4.04	131.29	125.06
82	UE	202	PEB	C2A-C1A-NA	4.04	111.76	108.27
82	fG	201	PEB	CHC-C4C-NC	4.04	126.62	121.15
82	ED	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	W1	203	PEB	C1C-CHB-C4B	4.04	137.34	128.28
82	sK	203	PEB	C1B-C2B-C3B	-4.04	101.87	106.51
84	C4	1001	CYC	CMA-C3A-C4A	4.04	131.29	125.06
82	UG	201	PEB	C1C-C2C-C3C	-4.04	102.84	107.62
103	82	309	ZEX	C7-C8-C9	-4.04	120.13	126.23
82	BQ	203	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
82	MP	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
82	P7	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
82	y8	203	PEB	C2C-C1C-NC	4.04	113.01	107.57
82	a1	202	PEB	CMB-C2B-C1B	4.04	131.29	125.06
82	NJ	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
83	xK	305	PUB	C4B-C3B-C2B	-4.04	102.84	107.62
82	G5	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	K5	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
87	82	308	CLA	CMC-C2C-C1C	-4.04	118.89	125.04
84	E3	1001	CYC	C3D-C4D-ND	4.04	113.01	107.57
82	UO	201	PEB	C4B-NB-C1B	-4.04	98.90	106.51
82	OI	201	PEB	C3B-C4B-NB	4.04	115.92	110.05
82	E5	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	jF	201	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
82	S9	203	PEB	CHA-C1B-NB	-4.04	116.48	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O9	202	PEB	C3B-C4B-NB	4.04	115.92	110.05
82	KK	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
82	GB	202	PEB	CHC-C4C-NC	4.04	126.61	121.15
82	k4	201	PEB	OA-C1A-C2A	-4.04	122.96	126.17
82	BD	201	PEB	CHB-C1C-C2C	-4.04	118.04	127.15
82	fJ	203	PEB	C1C-C2C-C3C	-4.04	102.85	107.62
82	YD	201	PEB	CHC-C1D-ND	-4.04	108.61	113.72
82	R1	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
82	fF	201	PEB	C2C-C1C-NC	4.04	113.01	107.57
82	dH	203	PEB	C2C-C1C-NC	4.04	113.01	107.57
82	aO	203	PEB	C2C-C1C-NC	4.04	113.01	107.57
83	AJ	303	PUB	OD-C4D-C3D	-4.04	123.66	128.04
83	AO	303	PUB	CMA-C2A-C1A	4.04	130.89	121.39
82	TF	201	PEB	OA-C1A-NA	4.04	129.83	124.94
82	HP	202	PEB	CHC-C4C-NC	4.04	126.61	121.15
82	VF	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
83	M9	303	PUB	CBA-CAA-C3A	-4.04	106.86	112.98
84	i3	1001	CYC	C3D-C4D-ND	4.04	113.01	107.57
82	P7	202	PEB	C1C-C2C-C3C	-4.04	102.85	107.62
82	Y4	203	PEB	C2C-C1C-NC	4.04	113.01	107.57
82	VD	203	PEB	CHC-C1D-ND	-4.04	108.62	113.72
82	U5	202	PEB	CHC-C1D-ND	-4.04	108.62	113.72
82	U5	202	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
84	DG	1001	CYC	C2D-C1D-ND	4.04	113.07	107.40
95	BL	613	DGD	C1E-O6E-C5E	4.04	121.61	113.69
82	WP	201	PEB	OA-C1A-C2A	-4.04	122.96	126.17
82	HA	202	PEB	C1C-C2C-C3C	-4.04	102.85	107.62
82	1C	203	PEB	C1C-C2C-C3C	-4.04	102.85	107.62
82	V5	201	PEB	CHC-C1D-ND	-4.04	108.62	113.72
82	HF	201	PEB	CMB-C2B-C1B	4.04	131.28	125.06
82	aM	204	PEB	CMB-C2B-C1B	4.04	131.28	125.06
82	b4	201	PEB	C3B-C4B-NB	4.04	115.92	110.05
83	A4	302	PUB	CMA-C2A-C1A	4.04	130.88	121.39
82	GP	202	PEB	C1D-CHC-C4C	-4.04	107.31	113.26
82	WQ	202	PEB	C1C-C2C-C3C	-4.04	102.85	107.62
82	Z9	301	PEB	C1C-C2C-C3C	-4.04	102.85	107.62
83	Z9	305	PUB	CHB-C4B-NB	4.03	134.56	125.32
82	YD	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	QP	202	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	b4	202	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	VQ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	dB	202	PEB	C3D-C4D-ND	4.03	115.17	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	D7	201	PEB	C4B-C3B-C2B	-4.03	102.32	106.78
82	Y9	202	PEB	C1C-C2C-C3C	-4.03	102.85	107.62
82	wC	202	PEB	C1C-C2C-C3C	-4.03	102.85	107.62
82	OI	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	AQ	303	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	pC	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	j4	201	PEB	CHB-C4B-C3B	-4.03	115.99	125.32
82	QM	204	PEB	CHC-C4C-NC	4.03	126.61	121.15
82	D1	1002	PEB	CMB-C2B-C1B	4.03	131.28	125.06
82	OE	201	PEB	C1D-CHC-C4C	-4.03	107.31	113.26
82	GF	201	PEB	OD-C4D-ND	-4.03	119.95	125.93
82	m4	203	PEB	C2C-C1C-NC	4.03	113.00	107.57
82	iO	203	PEB	C2C-C1C-NC	4.03	113.00	107.57
82	eK	203	PEB	CMC-C3C-C4C	4.03	131.34	127.06
83	AJ	303	PUB	C4B-CHB-C1C	-4.03	119.24	128.28
82	Y5	201	PEB	C2A-C1A-NA	4.03	111.75	108.27
82	FP	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
84	JH	1003	CYC	C1D-C2D-C3D	-4.03	102.66	107.79
84	EO	1001	CYC	CHD-C1D-ND	-4.03	116.08	125.32
82	CK	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	WH	201	PEB	CHB-C1C-C2C	-4.03	118.06	127.15
82	nF	201	PEB	CHC-C4C-NC	4.03	126.61	121.15
82	KI	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	18	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	OH	203	PEB	CHB-C1C-C2C	-4.03	118.06	127.15
84	K4	1001	CYC	C1D-C2D-C3D	-4.03	102.66	107.79
82	UB	303	PEB	CHC-C4C-NC	4.03	126.60	121.15
82	H4	1002	PEB	CHC-C4C-NC	4.03	126.60	121.15
82	A4	304	PEB	CHC-C4C-NC	4.03	126.60	121.15
83	Z5	303	PUB	CHA-C4A-NA	-4.03	108.62	113.72
85	CL	502	BCR	C37-C22-C23	4.03	124.43	118.08
82	HB	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	XB	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	cE	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
91	DL	405	PHO	CMB-C2B-C3B	4.03	132.22	124.68
82	Q4	201	PEB	C4B-NB-C1B	-4.03	98.92	106.51
82	LB	201	PEB	C2A-C1A-NA	4.03	111.75	108.27
82	R4	201	PEB	C2A-C1A-NA	4.03	111.75	108.27
82	Q1	203	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
82	iF	202	PEB	C1C-CHB-C4B	4.03	137.32	128.28
82	LG	1002	PEB	C3D-C4D-ND	4.03	115.17	107.26
82	IP	201	PEB	C3D-C4D-ND	4.03	115.17	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Z1	201	PEB	CHA-C4A-NA	4.03	130.00	125.20
82	RK	202	PEB	C3B-C4B-NB	4.03	115.91	110.05
82	BQ	201	PEB	CHB-C1C-C2C	-4.03	118.06	127.15
82	pC	202	PEB	C3D-C4D-ND	4.03	115.16	107.26
82	UJ	202	PEB	OD-C4D-ND	-4.03	119.96	125.93
82	SI	202	PEB	CHC-C4C-NC	4.03	126.60	121.15
82	hE	201	PEB	C2C-C1C-NC	4.03	113.00	107.57
82	SK	202	PEB	C3D-C4D-ND	4.03	115.16	107.26
82	WE	203	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	IJ	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	iF	201	PEB	C1C-C2C-C3C	-4.03	102.86	107.62
87	A2	819	CLA	C3B-C4B-NB	-4.03	106.78	110.52
82	gH	202	PEB	CHC-C4C-NC	4.03	126.60	121.15
82	AO	301	PEB	C2C-C1C-NC	4.03	113.00	107.57
82	SE	201	PEB	C3D-C4D-ND	4.03	115.16	107.26
82	JK	202	PEB	C3D-C4D-ND	4.03	115.16	107.26
82	HI	201	PEB	C1C-C2C-C3C	-4.03	102.86	107.62
83	QM	201	PUB	C1C-C2C-C3C	-4.03	102.33	106.78
82	AP	203	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	k4	201	PEB	C2C-C1C-NC	4.03	112.99	107.57
84	KO	1001	CYC	OB-C4B-C3B	-4.03	123.67	128.04
92	dL	407	LMG	C1-O6-C5	4.03	121.59	113.69
82	jO	201	PEB	CHC-C4C-NC	4.03	126.60	121.15
85	cL	518	BCR	C39-C30-C29	4.03	125.01	108.91
82	JB	202	PEB	C3D-C4D-ND	4.03	115.16	107.26
83	Z9	302	PUB	CBA-CAA-C3A	-4.03	106.87	112.98
82	hO	202	PEB	OA-C1A-C2A	-4.03	122.97	126.17
82	RJ	201	PEB	CHA-C1B-NB	-4.03	116.51	124.93
82	NB	203	PEB	C3D-C4D-ND	4.02	115.16	107.26
82	RO	203	PEB	C3D-C4D-ND	4.02	115.16	107.26
82	SO	201	PEB	C3D-C4D-ND	4.02	115.16	107.26
82	ZB	203	PEB	C1C-C2C-C3C	-4.02	102.86	107.62
82	c4	203	PEB	C1C-C2C-C3C	-4.02	102.86	107.62
82	R1	202	PEB	C2C-C1C-NC	4.02	112.99	107.57
82	E7	201	PEB	C2C-C1C-NC	4.02	112.99	107.57
94	dL	406	PL9	C10-C9-C11	4.02	122.04	115.27
82	f4	201	PEB	C3B-C4B-NB	4.02	115.90	110.05
82	dH	201	PEB	C1C-C2C-C3C	-4.02	102.86	107.62
82	RI	203	PEB	C3D-C4D-ND	4.02	115.15	107.26
82	HO	1002	PEB	CHC-C4C-NC	4.02	126.59	121.15
82	FF	202	PEB	C3B-C4B-NB	4.02	115.90	110.05
82	dB	201	PEB	C3D-C4D-ND	4.02	115.15	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RB	202	PEB	OA-C1A-C2A	-4.02	122.97	126.17
82	mG	202	PEB	C1C-C2C-C3C	-4.02	102.86	107.62
82	PQ	202	PEB	CHC-C4C-NC	4.02	126.59	121.15
82	j1	203	PEB	C1D-CHC-C4C	-4.02	107.32	113.26
82	vC	201	PEB	C2A-C1A-NA	4.02	111.74	108.27
82	EA	201	PEB	C2C-C1C-NC	4.02	112.99	107.57
82	cM	202	PEB	CAB-C3B-C4B	4.02	132.13	125.01
82	CD	202	PEB	C3D-C4D-ND	4.02	115.15	107.26
82	V5	202	PEB	C3D-C4D-ND	4.02	115.15	107.26
82	RJ	202	PEB	CHC-C4C-NC	4.02	126.59	121.15
82	wC	203	PEB	CHC-C4C-NC	4.02	126.59	121.15
82	QB	202	PEB	CMB-C2B-C1B	4.02	131.26	125.06
82	TK	201	PEB	OA-C1A-NA	4.02	129.81	124.94
82	T7	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
82	YA	304	PEB	C1C-CHB-C4B	-4.02	119.26	128.28
82	X7	202	PEB	C3B-C4B-NB	4.02	115.90	110.05
82	O1	201	PEB	C1B-C2B-C3B	-4.02	101.89	106.51
82	VI	203	PEB	C3D-C4D-ND	4.02	115.15	107.26
82	HK	202	PEB	C3D-C4D-ND	4.02	115.15	107.26
82	XD	201	PEB	OA-C1A-C2A	-4.02	122.98	126.17
82	SJ	201	PEB	OA-C1A-C2A	-4.02	122.98	126.17
82	RK	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
82	T4	203	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	YD	202	PEB	C3D-C4D-ND	4.02	115.15	107.26
94	dL	406	PL9	C15-C14-C16	4.02	122.03	115.27
82	S5	201	PEB	CHA-C1B-NB	-4.02	116.52	124.93
82	UE	201	PEB	C1C-CHB-C4B	4.02	137.30	128.28
82	L7	203	PEB	CHC-C1D-ND	-4.02	108.64	113.72
82	UG	201	PEB	C1C-CHB-C4B	4.02	137.30	128.28
82	RD	202	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	VQ	203	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	A4	301	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	wC	201	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
83	xF	305	PUB	C4B-C3B-C2B	-4.02	102.87	107.62
92	bL	623	LMG	O7-C10-C11	4.02	120.16	111.50
82	TB	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
82	LI	202	PEB	CMB-C2B-C1B	4.02	131.25	125.06
84	CG	1001	CYC	C1D-C2D-C3D	-4.02	102.67	107.79
82	d1	203	PEB	C2A-C1A-NA	4.02	111.74	108.27
82	CP	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
82	Y9	201	PEB	CAB-C3B-C4B	4.02	132.12	125.01
82	FK	202	PEB	C3B-C4B-NB	4.02	115.89	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	E4	1001	CYC	CHD-C1D-ND	-4.02	116.11	125.32
82	I5	201	PEB	CHC-C1D-ND	-4.02	108.64	113.72
82	J7	201	PEB	CHC-C1D-ND	-4.02	108.64	113.72
82	cM	201	PEB	C3D-C4D-ND	4.02	115.14	107.26
82	CQ	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
82	K7	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
84	HO	1001	CYC	OC-C1C-C2C	-4.02	122.98	126.17
82	kO	201	PEB	C2C-C1C-NC	4.02	112.98	107.57
87	72	607	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
82	W9	201	PEB	C3D-C4D-ND	4.02	115.14	107.26
82	lJ	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
82	c4	201	PEB	CHC-C4C-NC	4.02	126.59	121.15
87	7N	607	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
84	MO	1001	CYC	C1B-NB-C4B	-4.02	105.55	110.67
82	bO	201	PEB	C3B-C4B-NB	4.02	115.89	110.05
82	QG	202	PEB	C2C-C1C-NC	4.02	112.98	107.57
82	H7	202	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	kF	201	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	W5	202	PEB	CHB-C1C-C2C	-4.02	118.09	127.15
82	jF	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
83	AO	303	PUB	CHA-C1B-NB	4.02	126.59	121.15
84	y3	1001	CYC	CHB-C4A-C3A	4.02	135.23	124.90
84	EE	1001	CYC	C2D-C1D-ND	4.02	113.05	107.40
82	ZG	203	PEB	C1D-CHC-C4C	-4.02	107.33	113.26
82	RH	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
82	hM	201	PEB	CHB-C1C-C2C	-4.02	118.09	127.15
82	aO	203	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	YI	201	PEB	CAC-C2C-C1C	4.02	132.16	125.76
82	uC	203	PEB	CHC-C4C-NC	4.02	126.58	121.15
82	UO	201	PEB	C1D-CHC-C4C	-4.02	107.33	113.26
82	SH	202	PEB	CHC-C1D-ND	-4.02	108.64	113.72
82	P5	201	PEB	CHC-C1D-ND	-4.02	108.64	113.72
82	MD	201	PEB	C3D-C4D-ND	4.02	115.14	107.26
82	UD	201	PEB	C1C-C2C-C3C	-4.02	102.87	107.62
82	RO	202	PEB	CHC-C1D-ND	-4.02	108.64	113.72
82	MK	202	PEB	C2C-C1C-NC	4.02	112.98	107.57
85	CL	516	BCR	C30-C25-C26	-4.02	116.96	122.61
82	QK	203	PEB	C1B-C2B-C3B	-4.01	101.90	106.51
82	P7	201	PEB	CHC-C4C-NC	4.01	126.58	121.15
82	E5	202	PEB	C3D-C4D-ND	4.01	115.14	107.26
82	gK	201	PEB	C3B-C4B-NB	4.01	115.89	110.05
82	EK	201	PEB	C3D-C4D-ND	4.01	115.14	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PA	201	PEB	OD-C4D-ND	-4.01	119.98	125.93
84	IE	1001	CYC	OB-C4B-C3B	-4.01	123.68	128.04
82	T7	203	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
82	T5	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
82	WD	201	PEB	CHC-C1D-ND	-4.01	108.65	113.72
82	JF	202	PEB	C1C-CHB-C4B	4.01	137.28	128.28
82	UM	201	PEB	C1C-CHB-C4B	4.01	137.28	128.28
87	32	307	CLA	CHB-C1B-C2B	-4.01	115.90	127.24
82	aJ	201	PEB	CHC-C4C-NC	4.01	126.58	121.15
82	R5	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
84	JO	1001	CYC	C2B-C1B-NB	4.01	112.86	106.99
82	DA	202	PEB	C3C-C4C-NC	4.01	111.94	108.33
82	JF	201	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
82	wK	303	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
82	WH	203	PEB	CHB-C1C-C2C	-4.01	118.10	127.15
82	XA	202	PEB	C3B-C4B-NB	4.01	115.89	110.05
82	WF	201	PEB	C1B-C2B-C3B	-4.01	101.90	106.51
82	hJ	201	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
82	O5	202	PEB	C4B-C3B-C2B	-4.01	102.34	106.78
82	gB	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
84	G4	1001	CYC	C3D-C4D-ND	4.01	112.97	107.57
82	qC	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
82	LE	1002	PEB	OA-C1A-C2A	-4.01	122.98	126.17
82	TM	201	PEB	C1D-CHC-C4C	4.01	119.17	113.26
84	N3	1001	CYC	C3D-C4D-ND	4.01	112.97	107.57
84	t3	1001	CYC	C3D-C4D-ND	4.01	112.97	107.57
82	q8	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
82	TO	203	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
85	AN	804	BCR	C24-C23-C22	-4.01	120.17	126.23
82	SM	201	PEB	CHC-C4C-NC	4.01	126.58	121.15
82	nK	201	PEB	CHC-C4C-NC	4.01	126.58	121.15
85	C6	508	BCR	C15-C16-C17	-4.01	115.26	123.47
82	R4	203	PEB	C3D-C4D-ND	4.01	115.13	107.26
82	SH	203	PEB	C1D-CHC-C4C	4.01	119.17	113.26
84	FE	1001	CYC	C1D-C2D-C3D	-4.01	102.68	107.79
82	dF	201	PEB	C2C-C1C-NC	4.01	112.97	107.57
84	C3	1001	CYC	C3D-C4D-ND	4.01	112.97	107.57
84	G3	1001	CYC	C3D-C4D-ND	4.01	112.97	107.57
82	JI	201	PEB	C3B-C4B-NB	4.01	115.88	110.05
85	A2	804	BCR	C24-C23-C22	-4.01	120.18	126.23
82	lE	203	PEB	C3D-C4D-ND	4.01	115.13	107.26
82	nK	202	PEB	C3D-C4D-ND	4.01	115.13	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cO	202	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
84	KO	1001	CYC	C1D-C2D-C3D	-4.01	102.68	107.79
87	42	605	CLA	CHB-C4A-NA	4.01	130.06	124.51
84	HO	1001	CYC	CHA-C4D-C3D	-4.01	118.11	127.15
82	PG	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	SI	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
83	AM	303	PUB	C4B-CHB-C1C	-4.01	119.29	128.28
82	NJ	201	PEB	C2A-C1A-NA	4.01	111.73	108.27
82	RD	201	PEB	C1C-C2C-C3C	-4.01	102.88	107.62
82	RA	201	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	JM	201	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	gO	202	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	XD	203	PEB	CHC-C1D-ND	-4.01	108.65	113.72
82	A5	201	PEB	CHC-C1D-ND	-4.01	108.65	113.72
82	R5	201	PEB	CHC-C1D-ND	-4.01	108.65	113.72
82	NJ	202	PEB	CHC-C4C-NC	4.01	126.57	121.15
82	GJ	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	GB	203	PEB	C2A-C1A-NA	4.01	111.73	108.27
82	WD	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	EF	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	gJ	201	PEB	C4B-C3B-C2B	-4.01	102.35	106.78
82	HJ	201	PEB	CMC-C3C-C4C	4.01	131.31	127.06
84	BE	1001	CYC	CMA-C3A-C4A	4.01	131.24	125.06
82	NI	202	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	WM	203	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	h4	202	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	FB	201	PEB	C2C-C1C-NC	4.01	112.97	107.57
82	VM	201	PEB	C2C-C1C-NC	4.01	112.97	107.57
87	32	304	CLA	C16-C17-C18	4.01	134.86	115.98
82	JQ	201	PEB	CHC-C4C-NC	4.01	126.57	121.15
83	YA	302	PUB	CBA-CAA-C3A	-4.01	106.90	112.98
82	O1	203	PEB	C2A-C1A-NA	4.01	111.73	108.27
85	hL	102	BCR	C11-C10-C9	-4.01	121.59	127.31
85	B6	602	BCR	C3-C4-C5	-4.01	106.92	114.08
82	jK	201	PEB	C4B-C3B-C2B	-4.01	102.35	106.78
82	S1	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	lF	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	eM	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	LD	203	PEB	OA-C1A-C2A	-4.01	122.99	126.17
82	VD	202	PEB	C1C-C2C-C3C	-4.01	102.89	107.62
82	UQ	201	PEB	C1C-C2C-C3C	-4.01	102.89	107.62
84	GO	1001	CYC	CMD-C2D-C1D	4.01	131.43	125.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WB	402	PEB	CAC-C2C-C3C	4.01	136.24	127.07
82	LM	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	bO	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
82	CQ	201	PEB	CHC-C1D-ND	-4.01	108.66	113.72
82	HA	202	PEB	C1C-CHB-C4B	4.00	137.26	128.28
82	SP	201	PEB	C1C-C2C-C3C	-4.00	102.89	107.62
82	RQ	203	PEB	C1C-C2C-C3C	-4.00	102.89	107.62
82	K5	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	X5	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
84	K3	1001	CYC	C3D-C4D-ND	4.00	112.96	107.57
82	X7	201	PEB	CMB-C2B-C1B	4.00	131.23	125.06
95	AL	416	DGD	C1E-O6E-C5E	4.00	121.55	113.69
82	QM	202	PEB	CHB-C1C-C2C	-4.00	118.12	127.15
82	ZE	201	PEB	C4B-C3B-C2B	-4.00	102.35	106.78
85	BN	841	BCR	C15-C14-C13	-4.00	121.60	127.31
82	V4	202	PEB	C1C-C2C-C3C	-4.00	102.89	107.62
82	Y5	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	gJ	201	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	JB	201	PEB	OD-C4D-ND	-4.00	120.00	125.93
82	g1	201	PEB	C2C-C1C-NC	4.00	112.96	107.57
82	RB	201	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	N5	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	EQ	201	PEB	C3B-C4B-NB	4.00	115.87	110.05
87	3N	305	CLA	C16-C17-C18	4.00	134.84	115.98
82	OG	201	PEB	OD-C4D-ND	-4.00	120.00	125.93
82	gH	203	PEB	CHC-C1D-ND	-4.00	108.66	113.72
84	W3	1001	CYC	CHB-C4A-C3A	4.00	135.19	124.90
82	RH	202	PEB	C2C-C1C-NC	4.00	112.96	107.57
82	RF	202	PEB	C3B-C4B-NB	4.00	115.87	110.05
84	M4	1001	CYC	C2D-C1D-ND	4.00	113.03	107.40
82	SG	201	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	v8	201	PEB	C2A-C1A-NA	4.00	111.72	108.27
82	ZB	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
82	LG	1002	PEB	OA-C1A-C2A	-4.00	122.99	126.17
82	CP	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
82	hM	202	PEB	OA-C1A-C2A	-4.00	122.99	126.17
82	ZJ	202	PEB	C4B-C3B-C2B	-4.00	102.35	106.78
82	DD	203	PEB	C1B-C2B-C3B	-4.00	101.91	106.51
82	h4	201	PEB	C3B-C4B-NB	4.00	115.87	110.05
82	pC	202	PEB	CAB-C3B-C4B	4.00	132.09	125.01
82	C5	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	L9	201	PEB	C3D-C4D-ND	4.00	115.11	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	kK	201	PEB	C1C-C2C-C3C	-4.00	102.89	107.62
92	D6	407	LMG	O7-C10-C11	4.00	120.12	111.50
82	a4	203	PEB	C2C-C1C-NC	4.00	112.96	107.57
84	P3	1001	CYC	C3D-C4D-ND	4.00	112.96	107.57
84	e3	1001	CYC	C3D-C4D-ND	4.00	112.96	107.57
82	IJ	203	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	QF	203	PEB	C1B-C2B-C3B	-4.00	101.91	106.51
82	DF	202	PEB	C3C-C4C-NC	4.00	111.93	108.33
82	QJ	202	PEB	CHB-C1C-C2C	-4.00	118.12	127.15
82	AJ	302	PEB	CMB-C2B-C1B	4.00	131.22	125.06
82	JA	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
84	J4	1001	CYC	OC-C1C-C2C	-4.00	122.99	126.17
82	Q9	202	PEB	CHB-C1C-C2C	-4.00	118.12	127.15
85	B2	841	BCR	C15-C14-C13	-4.00	121.60	127.31
84	J4	1001	CYC	C2B-C1B-NB	4.00	112.84	106.99
88	CL	521	LHG	O7-C7-C8	4.00	120.12	111.50
82	A4	305	PEB	CHC-C4C-NC	4.00	126.56	121.15
82	iF	202	PEB	CHC-C4C-NC	4.00	126.56	121.15
84	p3	1001	CYC	C3D-C4D-ND	4.00	112.96	107.57
84	HH	1001	CYC	C4D-C3D-C2D	-4.00	102.89	107.62
82	FA	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	F7	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
82	UK	201	PEB	OA-C1A-C2A	4.00	129.35	126.17
82	YQ	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
82	jM	201	PEB	CHC-C4C-NC	4.00	126.56	121.15
84	BG	1001	CYC	CMD-C2D-C1D	4.00	131.42	125.56
87	7N	604	CLA	CAA-C2A-C3A	-4.00	104.27	114.26
82	eB	202	PEB	CMB-C2B-C1B	4.00	131.22	125.06
92	JL	103	LMG	O7-C10-C11	4.00	120.12	111.50
82	C5	201	PEB	CHC-C1D-ND	-4.00	108.67	113.72
85	KN	101	BCR	C12-C13-C14	4.00	125.08	118.94
82	Z5	305	PEB	C1B-C2B-C3B	-4.00	101.92	106.51
95	lL	101	DGD	O2G-C1B-C2B	4.00	120.12	111.50
82	WF	203	PEB	C2C-C1C-NC	4.00	112.95	107.57
82	PE	201	PEB	C3D-C4D-ND	4.00	115.10	107.26
82	JK	201	PEB	C3D-C4D-ND	4.00	115.10	107.26
82	hO	201	PEB	C3D-C4D-ND	4.00	115.10	107.26
84	EG	1001	CYC	C2D-C1D-ND	4.00	113.02	107.40
82	FJ	202	PEB	C3D-C4D-ND	4.00	115.10	107.26
84	NH	1001	CYC	CMD-C2D-C1D	4.00	131.41	125.56
82	u8	203	PEB	CHC-C4C-NC	4.00	126.56	121.15
82	iK	202	PEB	C1C-CHB-C4B	4.00	137.25	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SJ	203	PEB	C1C-C2C-C3C	-4.00	102.90	107.62
82	XA	201	PEB	CMB-C2B-C1B	4.00	131.22	125.06
82	RE	202	PEB	C3D-C4D-ND	4.00	115.10	107.26
82	RF	201	PEB	CHA-C1B-NB	-4.00	116.57	124.93
82	YM	201	PEB	C1C-CHB-C4B	4.00	137.24	128.28
82	VB	201	PEB	CMB-C2B-C1B	4.00	131.22	125.06
82	Z1	201	PEB	C1C-C2C-C3C	-4.00	102.90	107.62
82	JF	202	PEB	C3D-C4D-ND	4.00	115.10	107.26
82	ZE	203	PEB	C1D-CHC-C4C	-4.00	107.36	113.26
87	3N	308	CLA	CHB-C1B-C2B	-4.00	115.95	127.24
82	RA	202	PEB	C3B-C4B-NB	4.00	115.86	110.05
82	GK	202	PEB	C3D-C4D-ND	4.00	115.10	107.26
82	YA	301	PEB	C2A-C1A-NA	4.00	111.72	108.27
82	cG	202	PEB	CHC-C4C-NC	3.99	126.56	121.15
85	LN	201	BCR	C16-C17-C18	-3.99	121.61	127.31
85	L2	201	BCR	C16-C17-C18	-3.99	121.61	127.31
82	CM	202	PEB	C3D-C4D-ND	3.99	115.10	107.26
82	PD	202	PEB	CHC-C4C-NC	3.99	126.56	121.15
82	J4	1002	PEB	C2A-C1A-NA	3.99	111.72	108.27
82	ZJ	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	I5	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	SO	201	PEB	CMA-C2A-C1A	-3.99	103.79	112.40
82	OG	201	PEB	C1D-CHC-C4C	-3.99	107.37	113.26
82	KM	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	Y4	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	w8	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	BP	202	PEB	CHA-C1B-NB	-3.99	116.58	124.93
82	mJ	202	PEB	C4B-C3B-C2B	-3.99	102.36	106.78
82	Q5	201	PEB	C2C-C1C-NC	3.99	112.95	107.57
84	g3	1001	CYC	C3D-C4D-ND	3.99	112.95	107.57
82	CQ	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	DK	201	PEB	C1C-C2C-C3C	-3.99	102.90	107.62
88	aL	607	LHG	O7-C7-C8	3.99	120.11	111.50
82	QE	201	PEB	C1D-CHC-C4C	-3.99	107.37	113.26
82	gM	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	M5	305	PEB	C1B-C2B-C3B	-3.99	101.92	106.51
84	T3	1001	CYC	C3D-C4D-ND	3.99	112.95	107.57
82	DA	201	PEB	C4B-C3B-C2B	-3.99	102.36	106.78
82	L5	202	PEB	C4B-C3B-C2B	-3.99	102.36	106.78
83	AM	304	PUB	C1C-C2C-C3C	-3.99	102.36	106.78
85	aL	604	BCR	C7-C8-C9	-3.99	120.20	126.23
82	NB	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YH	202	PEB	C1C-C2C-C3C	-3.99	102.90	107.62
82	H1	1002	PEB	C1C-C2C-C3C	-3.99	102.90	107.62
82	LI	201	PEB	CAC-C2C-C1C	3.99	132.12	125.76
82	JJ	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	YJ	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	GP	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	E7	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
87	4N	605	CLA	CHB-C4A-NA	3.99	130.03	124.51
82	GK	203	PEB	C1C-CHB-C4B	3.99	137.23	128.28
84	NE	201	CYC	C2D-C1D-ND	3.99	113.01	107.40
82	D7	201	PEB	C2C-C1C-NC	3.99	112.95	107.57
82	Y5	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
85	CL	501	BCR	C7-C8-C9	-3.99	120.20	126.23
82	Y7	301	PEB	C1C-C2C-C3C	-3.99	102.90	107.62
82	GB	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	T4	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
84	v3	1001	CYC	C3D-C4D-ND	3.99	112.94	107.57
82	UH	202	PEB	OD-C4D-ND	-3.99	120.02	125.93
82	B9	201	PEB	CHC-C4C-NC	3.99	126.55	121.15
82	cO	201	PEB	CHC-C4C-NC	3.99	126.55	121.15
82	UB	302	PEB	C2A-C1A-NA	3.99	111.71	108.27
82	D4	1002	PEB	C2A-C1A-NA	3.99	111.71	108.27
82	ZB	203	PEB	CHA-C1B-NB	-3.99	116.59	124.93
82	U7	201	PEB	OD-C4D-ND	-3.99	120.02	125.93
82	j4	201	PEB	CHC-C4C-NC	3.99	126.55	121.15
82	eM	201	PEB	CMC-C3C-C4C	3.99	131.29	127.06
82	PH	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	NJ	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	R7	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	aM	204	PEB	C1C-C2C-C3C	-3.99	102.91	107.62
83	yK	303	PUB	C1C-C2C-C3C	-3.99	102.37	106.78
82	P5	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	F7	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
82	h1	201	PEB	CHC-C1D-ND	-3.99	108.68	113.72
83	YA	302	PUB	C3B-C4B-NB	3.99	112.94	107.57
84	A3	1001	CYC	C3D-C4D-ND	3.99	112.94	107.57
84	J3	1001	CYC	C3D-C4D-ND	3.99	112.94	107.57
84	R3	1001	CYC	C3D-C4D-ND	3.99	112.94	107.57
82	AO	304	PEB	CHC-C4C-NC	3.99	126.55	121.15
82	cE	202	PEB	CHC-C4C-NC	3.99	126.55	121.15
82	i4	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	J7	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iO	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	EA	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
82	aB	201	PEB	CHC-C1D-ND	-3.99	108.68	113.72
82	NK	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
87	72	604	CLA	CAA-C2A-C3A	-3.99	104.30	114.26
82	zF	501	PEB	C3B-C4B-NB	3.99	115.85	110.05
84	H4	1001	CYC	CHA-C4D-C3D	-3.99	118.16	127.15
83	Y7	302	PUB	C3B-C4B-NB	3.99	112.94	107.57
84	m3	1001	CYC	C3D-C4D-ND	3.99	112.94	107.57
82	EI	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	HM	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	mM	201	PEB	CHC-C1D-ND	3.99	118.77	113.72
82	oK	201	PEB	CHC-C4C-NC	3.99	126.55	121.15
82	S4	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
95	L6	102	DGD	O2G-C1B-C2B	3.99	120.09	111.50
82	qF	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
82	OP	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	F9	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
82	eK	203	PEB	OA-C1A-C2A	-3.99	123.00	126.17
84	JO	1001	CYC	OC-C1C-C2C	-3.99	123.00	126.17
82	GF	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
82	KF	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
82	FF	201	PEB	C1C-C2C-C3C	-3.99	102.91	107.62
82	G7	202	PEB	C1C-C2C-C3C	-3.99	102.91	107.62
85	Z6	101	BCR	C33-C5-C6	-3.99	120.05	124.53
85	c6	603	BCR	C38-C26-C25	-3.99	120.05	124.53
82	M9	305	PEB	C1C-CHB-C4B	-3.99	119.34	128.28
82	gF	203	PEB	CHB-C1C-C2C	-3.98	118.16	127.15
82	QB	204	PEB	C3D-C4D-ND	3.98	115.08	107.26
82	AD	304	PEB	CHB-C1C-NC	-3.98	116.19	125.32
82	FA	202	PEB	C2A-C1A-NA	3.98	111.71	108.27
82	sK	201	PEB	OA-C1A-C2A	-3.98	123.00	126.17
82	LD	201	PEB	C1C-C2C-C3C	-3.98	102.91	107.62
83	Y7	302	PUB	CBA-CAA-C3A	-3.98	106.94	112.98
82	dK	201	PEB	C2C-C1C-NC	3.98	112.94	107.57
82	g1	202	PEB	CHC-C4C-NC	3.98	126.54	121.15
83	yF	303	PUB	CMA-C2A-C1A	3.98	130.76	121.39
82	VA	201	PEB	C1B-C2B-C3B	-3.98	101.93	106.51
82	VD	203	PEB	C1C-C2C-C3C	-3.98	102.91	107.62
82	g4	202	PEB	C1C-C2C-C3C	-3.98	102.91	107.62
84	GO	1001	CYC	C3D-C4D-ND	3.98	112.94	107.57
84	l3	1001	CYC	C3D-C4D-ND	3.98	112.94	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	A5	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	lM	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	TF	202	PEB	C3B-C4B-NB	3.98	115.84	110.05
82	hB	301	PEB	C4B-C3B-C2B	-3.98	102.37	106.78
82	ZE	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	WQ	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	wF	303	PEB	C1C-C2C-C3C	-3.98	102.91	107.62
82	SB	203	PEB	OD-C4D-ND	-3.98	120.03	125.93
84	KG	202	CYC	C2D-C1D-ND	3.98	113.00	107.40
85	c6	602	BCR	C24-C23-C22	-3.98	120.22	126.23
85	fL	101	BCR	C15-C14-C13	-3.98	121.63	127.31
82	cK	203	PEB	OA-C1A-C2A	-3.98	123.01	126.17
84	LG	1001	CYC	C2D-C1D-ND	3.98	113.00	107.40
82	YP	503	PEB	CHC-C4C-NC	3.98	126.54	121.15
82	yC	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
85	BL	617	BCR	C11-C10-C9	-3.98	121.63	127.31
82	NQ	202	PEB	OA-C1A-C2A	-3.98	123.01	126.17
82	TQ	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
82	fO	201	PEB	C3B-C4B-NB	3.98	115.84	110.05
82	YO	203	PEB	C2C-C1C-NC	3.98	112.93	107.57
82	gB	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	H7	202	PEB	C1C-CHB-C4B	3.98	137.21	128.28
82	TB	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
83	xK	306	PUB	C3B-C4B-NB	3.98	112.93	107.57
83	yF	303	PUB	C1C-C2C-C3C	-3.98	102.38	106.78
82	wC	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
82	aG	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
84	BG	1001	CYC	CMA-C3A-C4A	3.98	131.19	125.06
82	hH	201	PEB	C1B-C2B-C3B	-3.98	101.94	106.51
82	BA	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	IB	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	QB	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	U9	204	PEB	C3D-C4D-ND	3.98	115.07	107.26
82	JQ	203	PEB	CHB-C1C-C2C	-3.98	118.17	127.15
82	GD	202	PEB	CAC-CBC-CGC	-3.98	105.04	113.60
82	w8	203	PEB	CHC-C4C-NC	3.98	126.53	121.15
82	h4	201	PEB	C3D-C4D-ND	3.98	115.06	107.26
85	BN	842	BCR	C12-C13-C14	-3.98	112.84	118.94
82	O9	201	PEB	CAB-C3B-C4B	3.98	132.05	125.01
82	AO	301	PEB	C1C-C2C-C3C	-3.98	102.92	107.62
88	D6	401	LHG	O7-C7-C8	3.98	120.08	111.50
87	BN	827	CLA	CMB-C2B-C1B	-3.98	119.31	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aH	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
82	HD	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	nF	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
83	Z9	305	PUB	C2C-C1C-NC	3.98	115.83	110.05
82	jJ	203	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	qC	201	PEB	C2C-C1C-NC	3.98	112.93	107.57
85	LN	201	BCR	C15-C14-C13	-3.98	121.63	127.31
82	HQ	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	Y9	203	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	XQ	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
83	QJ	201	PUB	CHA-C4A-NA	-3.98	108.69	113.72
82	Y9	201	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	vF	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	UG	202	PEB	CHC-C4C-NC	3.98	126.53	121.15
82	TB	201	PEB	OD-C4D-ND	-3.98	120.04	125.93
82	cF	203	PEB	OD-C4D-ND	-3.98	120.04	125.93
82	KA	201	PEB	C3B-C4B-NB	3.98	115.83	110.05
82	VO	202	PEB	C3B-C4B-NB	3.98	115.83	110.05
82	ZE	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
85	BN	803	BCR	C20-C19-C18	3.98	137.59	126.42
82	JD	201	PEB	CHC-C4C-NC	3.98	126.53	121.15
82	b1	202	PEB	OA-C1A-C2A	-3.98	123.01	126.17
82	SE	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
84	H4	1001	CYC	C1B-NB-C4B	-3.98	105.61	110.67
82	FP	201	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	hJ	201	PEB	C3D-C4D-ND	3.98	115.06	107.26
82	N5	201	PEB	CHC-C1D-ND	-3.97	108.69	113.72
82	DI	202	PEB	C1C-C2C-C3C	-3.97	102.92	107.62
82	QP	203	PEB	C1C-C2C-C3C	-3.97	102.92	107.62
84	G4	1001	CYC	CMD-C2D-C1D	3.97	131.38	125.56
82	SP	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
82	vK	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
82	AO	305	PEB	OA-C1A-C2A	-3.97	123.01	126.17
82	TK	202	PEB	C3B-C4B-NB	3.97	115.83	110.05
82	R7	202	PEB	C3B-C4B-NB	3.97	115.83	110.05
82	mE	202	PEB	C1C-C2C-C3C	-3.97	102.92	107.62
82	aM	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
82	AO	305	PEB	C3D-C4D-ND	3.97	115.06	107.26
84	K1	1001	CYC	C4D-CHA-C1A	3.97	137.19	128.28
82	W9	201	PEB	CAB-C3B-C4B	3.97	132.04	125.01
83	yK	303	PUB	CMA-C2A-C1A	3.97	130.74	121.39
82	DP	202	PEB	OA-C1A-C2A	-3.97	123.01	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	P1	201	PEB	OA-C1A-C2A	-3.97	123.01	126.17
82	XD	201	PEB	CHB-C1C-C2C	-3.97	118.19	127.15
82	TJ	201	PEB	C1D-CHC-C4C	3.97	119.11	113.26
82	SQ	201	PEB	C3B-C4B-NB	3.97	115.83	110.05
82	K7	201	PEB	C3B-C4B-NB	3.97	115.83	110.05
82	LA	203	PEB	CHC-C1D-ND	-3.97	108.70	113.72
82	O4	201	PEB	CMA-C2A-C1A	-3.97	103.84	112.40
92	ML	101	LMG	O1-C1-C2	3.97	114.50	108.30
82	LD	201	PEB	CHB-C1C-C2C	-3.97	118.19	127.15
84	K4	1001	CYC	C2D-C1D-ND	3.97	112.98	107.40
84	GG	1001	CYC	C2B-C1B-NB	3.97	112.80	106.99
82	D7	202	PEB	C3C-C4C-NC	3.97	111.91	108.33
82	T7	203	PEB	OA-C1A-C2A	-3.97	123.02	126.17
82	JK	202	PEB	C1C-CHB-C4B	3.97	137.19	128.28
82	hM	201	PEB	C1C-C2C-C3C	-3.97	102.93	107.62
82	cE	201	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	cG	201	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	lK	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
85	HL	103	BCR	C3-C4-C5	-3.97	106.99	114.08
84	NO	1001	CYC	CHD-C1D-ND	-3.97	116.22	125.32
82	OO	201	PEB	CMA-C2A-C1A	-3.97	103.84	112.40
82	JA	201	PEB	CHC-C1D-ND	-3.97	108.70	113.72
82	RG	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	fE	201	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	Y7	301	PEB	C2A-C1A-NA	3.97	111.70	108.27
82	jJ	201	PEB	CHA-C1B-NB	-3.97	116.63	124.93
82	MP	201	PEB	CHC-C4C-NC	3.97	126.52	121.15
82	OJ	201	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	XD	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	rF	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	a4	203	PEB	C1C-C2C-C3C	-3.97	102.93	107.62
84	FE	1001	CYC	CHD-C1D-ND	-3.97	116.23	125.32
84	CG	1001	CYC	CHD-C1D-ND	-3.97	116.23	125.32
82	BP	201	PEB	CHC-C1D-ND	-3.97	108.70	113.72
82	EQ	201	PEB	CHC-C1D-ND	-3.97	108.70	113.72
82	aH	202	PEB	OA-C1A-C2A	-3.97	123.02	126.17
82	TA	203	PEB	C1C-C2C-C3C	-3.97	102.93	107.62
84	DE	1001	CYC	CMA-C3A-C4A	3.97	131.18	125.06
82	DK	203	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	DQ	203	PEB	C1B-C2B-C3B	-3.97	101.95	106.51
85	B2	842	BCR	C12-C13-C14	-3.97	112.85	118.94
85	K2	102	BCR	C12-C13-C14	3.97	125.03	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QH	201	PEB	C3C-C4C-NC	3.97	111.91	108.33
82	RF	201	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	G5	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
82	UG	202	PEB	C2C-C1C-NC	3.97	112.92	107.57
82	GJ	203	PEB	OA-C1A-C2A	-3.97	123.02	126.17
82	LI	202	PEB	CHC-C1D-ND	-3.97	108.70	113.72
82	SG	203	PEB	C3D-C4D-ND	3.97	115.04	107.26
82	VP	202	PEB	CHA-C1B-NB	-3.97	116.63	124.93
84	c3	1001	CYC	C3D-C4D-ND	3.97	112.91	107.57
82	DF	203	PEB	C3D-C4D-ND	3.97	115.04	107.26
82	RK	201	PEB	CHA-C1B-NB	-3.97	116.63	124.93
82	M7	201	PEB	CHA-C1B-NB	-3.97	116.63	124.93
82	HM	201	PEB	C1C-CHB-C4B	-3.97	119.39	128.28
84	MO	1001	CYC	C2C-C1C-NC	3.97	111.69	108.27
82	KP	201	PEB	C2C-C1C-NC	3.97	112.91	107.57
82	wF	303	PEB	C2C-C1C-NC	3.97	112.91	107.57
82	fG	201	PEB	C3D-C4D-ND	3.97	115.04	107.26
82	FM	201	PEB	C1D-CHC-C4C	3.97	119.11	113.26
82	TB	202	PEB	C1C-C2C-C3C	-3.97	102.93	107.62
82	a4	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
82	Z9	304	PEB	C1C-CHB-C4B	-3.97	119.39	128.28
85	B2	802	BCR	C20-C19-C18	3.97	137.56	126.42
82	OH	201	PEB	C1B-C2B-C3B	-3.97	101.95	106.51
82	oF	201	PEB	CHC-C4C-NC	3.97	126.52	121.15
82	iK	202	PEB	CHC-C4C-NC	3.97	126.52	121.15
82	GI	201	PEB	C2A-C1A-NA	3.97	111.69	108.27
84	DG	1001	CYC	CMA-C3A-C4A	3.97	131.17	125.06
82	EM	202	PEB	OA-C1A-C2A	-3.97	123.02	126.17
82	qF	202	PEB	C2C-C1C-NC	3.97	112.91	107.57
82	cG	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
82	ZG	201	PEB	C4B-C3B-C2B	-3.96	102.39	106.78
84	M4	1001	CYC	C2C-C1C-NC	3.96	111.69	108.27
82	PJ	201	PEB	CMC-C3C-C4C	3.96	131.26	127.06
82	ZG	201	PEB	C3D-C4D-ND	3.96	115.04	107.26
82	iM	202	PEB	CHC-C4C-NC	3.96	126.52	121.15
83	AH	304	PUB	CHB-C1C-NC	-3.96	116.33	124.58
82	jM	203	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	FO	1002	PEB	C3D-C4D-ND	3.96	115.04	107.26
82	b4	202	PEB	C3D-C4D-ND	3.96	115.04	107.26
82	cJ	202	PEB	C3D-C4D-ND	3.96	115.04	107.26
82	T4	201	PEB	C2A-C1A-NA	3.96	111.69	108.27
82	xF	304	PEB	C2A-C1A-NA	3.96	111.69	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jM	203	PEB	CHB-C1C-C2C	-3.96	118.21	127.15
87	B2	827	CLA	CMB-C2B-C1B	-3.96	119.33	125.37
82	RJ	201	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	HK	201	PEB	CMB-C2B-C1B	3.96	131.17	125.06
82	SF	203	PEB	OA-C1A-C2A	-3.96	123.02	126.17
82	cB	401	PEB	OA-C1A-C2A	-3.96	123.02	126.17
82	HP	202	PEB	CHA-C1B-NB	-3.96	116.64	124.93
82	Y4	203	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	BB	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	SF	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	xK	304	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	U1	202	PEB	OD-C4D-ND	-3.96	120.06	125.93
82	gK	203	PEB	CHB-C1C-C2C	-3.96	118.21	127.15
82	M5	304	PEB	C3C-C4C-NC	3.96	111.90	108.33
82	p8	202	PEB	CAB-C3B-C4B	3.96	132.02	125.01
82	RB	201	PEB	OA-C1A-C2A	-3.96	123.02	126.17
82	ZE	201	PEB	OA-C1A-C2A	-3.96	123.02	126.17
82	XI	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
82	WK	203	PEB	C2C-C1C-NC	3.96	112.91	107.57
82	OP	201	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	VI	203	PEB	C1D-CHC-C4C	-3.96	107.42	113.26
103	82	309	ZEX	C18-C5-C6	-3.96	120.08	124.53
82	BJ	301	PEB	C2C-C1C-NC	3.96	112.91	107.57
82	kJ	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	PF	201	PEB	CHA-C1B-NB	-3.96	116.65	124.93
82	dB	201	PEB	OA-C1A-C2A	-3.96	123.02	126.17
82	aE	201	PEB	OA-C1A-C2A	-3.96	123.02	126.17
84	M4	1001	CYC	C1D-C2D-C3D	-3.96	102.75	107.79
85	b6	601	BCR	C11-C10-C9	-3.96	121.66	127.31
82	JF	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	aO	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
103	8N	309	ZEX	C18-C5-C6	-3.96	120.08	124.53
82	XF	203	PEB	C1C-CHB-C4B	3.96	137.16	128.28
82	JD	203	PEB	CHB-C1C-C2C	-3.96	118.22	127.15
82	QB	203	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	RD	203	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
85	BL	617	BCR	C20-C21-C22	-3.96	121.66	127.31
82	uC	202	PEB	C2C-C1C-NC	3.96	112.90	107.57
82	TA	203	PEB	OA-C1A-C2A	-3.96	123.03	126.17
82	PI	202	PEB	OA-C1A-C2A	-3.96	123.03	126.17
82	GP	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
82	hM	203	PEB	OA-C1A-C2A	-3.96	123.03	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lO	201	PEB	C1B-C2B-C3B	-3.96	101.96	106.51
82	MA	201	PEB	CHA-C1B-NB	-3.96	116.65	124.93
82	WI	202	PEB	C2A-C1A-NA	3.96	111.69	108.27
84	LE	1001	CYC	C2C-C1C-NC	3.96	111.69	108.27
82	D9	202	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	GQ	202	PEB	CAC-CBC-CGC	-3.96	105.08	113.60
82	YA	304	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	qK	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
85	CL	516	BCR	C39-C30-C29	3.96	124.74	108.91
82	XJ	202	PEB	CHC-C1D-ND	-3.96	108.72	113.72
85	A2	848	BCR	C16-C17-C18	-3.96	121.66	127.31
82	M5	305	PEB	C3D-C4D-ND	3.96	115.03	107.26
82	RK	201	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
84	73	1002	CYC	C4D-C3D-C2D	-3.96	102.94	107.62
84	73	1002	CYC	CAB-C3B-C4B	3.96	127.63	121.38
82	VA	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
82	FQ	203	PEB	C4B-C3B-C2B	-3.96	102.40	106.78
82	N7	202	PEB	C3B-C4B-NB	3.96	115.81	110.05
82	S1	202	PEB	CHC-C1D-ND	-3.96	108.72	113.72
82	DQ	201	PEB	C3C-C4C-NC	3.96	111.89	108.33
82	HQ	201	PEB	C1C-C2C-C3C	-3.96	102.94	107.62
82	LE	1002	PEB	C3D-C4D-ND	3.96	115.02	107.26
82	PJ	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
83	M5	303	PUB	OD-C4D-C3D	-3.96	123.75	128.04
82	sK	203	PEB	CBA-CAA-C3A	-3.96	104.66	113.47
82	GI	203	PEB	OA-C1A-C2A	-3.96	123.03	126.17
82	qK	202	PEB	C2C-C1C-NC	3.96	112.90	107.57
82	kM	201	PEB	C2C-C1C-NC	3.96	112.90	107.57
83	Z5	303	PUB	CAC-C2C-C1C	3.96	132.01	125.01
82	S4	201	PEB	CMA-C2A-C1A	-3.96	103.88	112.40
82	YG	201	PEB	C3D-C4D-ND	3.96	115.02	107.26
82	fK	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
92	bL	624	LMG	O7-C10-C11	3.96	120.03	111.50
83	Z5	303	PUB	OD-C4D-C3D	-3.96	123.75	128.04
82	XF	202	PEB	C1C-CHB-C4B	3.96	137.15	128.28
82	DD	203	PEB	CHB-C1C-C2C	-3.96	118.22	127.15
82	XJ	201	PEB	C2C-C1C-NC	3.96	112.90	107.57
82	q8	201	PEB	C2C-C1C-NC	3.96	112.90	107.57
82	ZM	201	PEB	C3D-C4D-ND	3.96	115.02	107.26
82	rK	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
82	QH	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
85	AN	846	BCR	C11-C10-C9	-3.96	121.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KK	202	PEB	CHC-C4C-NC	3.95	126.50	121.15
82	DA	201	PEB	C2C-C1C-NC	3.95	112.90	107.57
82	JB	202	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	w8	202	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	DB	203	PEB	C3D-C4D-ND	3.95	115.02	107.26
84	M4	1001	CYC	C1B-NB-C4B	-3.95	105.63	110.67
82	Q5	202	PEB	CMC-C3C-C4C	3.95	131.25	127.06
82	MA	201	PEB	C2A-C1A-NA	3.95	111.68	108.27
82	RE	202	PEB	CHC-C4C-NC	3.95	126.50	121.15
82	k1	201	PEB	CBA-CAA-C3A	3.95	122.27	113.47
82	OF	203	PEB	OA-C1A-C2A	-3.95	123.03	126.17
82	QB	204	PEB	CMB-C2B-C1B	3.95	131.15	125.06
92	DL	402	LMG	C1-O6-C5	3.95	121.45	113.69
82	WK	201	PEB	C1B-C2B-C3B	-3.95	101.97	106.51
82	HD	201	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	cM	201	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	ZG	202	PEB	C3D-C4D-ND	3.95	115.02	107.26
82	UE	202	PEB	CHC-C4C-NC	3.95	126.50	121.15
82	QJ	204	PEB	CHC-C4C-NC	3.95	126.50	121.15
82	d4	201	PEB	CHC-C4C-NC	3.95	126.50	121.15
84	CG	1001	CYC	OB-C4B-C3B	-3.95	123.75	128.04
87	4N	610	CLA	CAA-C2A-C3A	-3.95	104.38	114.26
82	F5	202	PEB	C3C-C4C-NC	3.95	111.89	108.33
82	HF	201	PEB	C1B-C2B-C3B	-3.95	101.97	106.51
82	Y5	201	PEB	C1B-C2B-C3B	-3.95	101.97	106.51
82	pK	202	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	KA	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
82	AA	202	PEB	CHA-C1B-NB	-3.95	116.66	124.93
82	iJ	201	PEB	C2C-C1C-NC	3.95	112.89	107.57
82	SH	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	KQ	202	PEB	CHA-C1B-NB	-3.95	116.67	124.93
82	JO	1002	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
82	WP	201	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	q8	202	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	fE	203	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	RI	203	PEB	C2A-C1A-NA	3.95	111.68	108.27
82	RK	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	XQ	201	PEB	CHB-C1C-C2C	-3.95	118.23	127.15
87	42	610	CLA	CAA-C2A-C3A	-3.95	104.39	114.26
85	KN	104	BCR	C11-C10-C9	-3.95	121.67	127.31
82	sF	203	PEB	CBA-CAA-C3A	-3.95	104.67	113.47
82	AQ	304	PEB	CHB-C1C-NC	-3.95	116.27	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	M5	303	PUB	CAC-C2C-C1C	3.95	132.00	125.01
85	K2	105	BCR	C11-C10-C9	-3.95	121.67	127.31
85	b6	602	BCR	C11-C10-C9	-3.95	121.67	127.31
82	PM	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	gH	203	PEB	C2A-C1A-NA	3.95	111.68	108.27
82	SM	203	PEB	CHB-C1C-C2C	-3.95	118.24	127.15
82	ZB	203	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	YF	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	A7	202	PEB	CHA-C1B-NB	-3.95	116.67	124.93
82	P7	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
82	BM	301	PEB	CMB-C2B-C1B	3.95	131.15	125.06
82	HI	201	PEB	C3B-C4B-NB	3.95	115.80	110.05
82	K7	201	PEB	CBC-CAC-C2C	3.95	123.60	112.63
82	MQ	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	lG	203	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	FP	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
82	U1	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
82	Y1	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
82	w8	203	PEB	C3D-C4D-ND	3.95	115.01	107.26
82	RQ	202	PEB	C1C-C2C-C3C	-3.95	102.95	107.62
82	GI	201	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
82	T1	201	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
82	AO	305	PEB	CHC-C4C-NC	3.95	126.49	121.15
82	wK	303	PEB	C2C-C1C-NC	3.95	112.89	107.57
82	KB	301	PEB	CMB-C2B-C1B	3.95	131.14	125.06
82	EP	203	PEB	CHC-C1D-ND	-3.95	108.73	113.72
82	FQ	203	PEB	OD-C4D-ND	-3.95	120.08	125.93
82	KD	202	PEB	CHA-C1B-NB	-3.95	116.67	124.93
82	U1	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	b4	201	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	B7	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	KB	304	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	QH	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	UP	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
84	HG	1001	CYC	C2D-C1D-ND	3.95	112.95	107.40
82	X7	201	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	RM	202	PEB	C1C-CHB-C4B	-3.95	119.43	128.28
82	tK	202	PEB	CBC-CAC-C2C	3.95	123.59	112.63
82	DO	1002	PEB	C2C-C1C-NC	3.95	112.89	107.57
82	H7	201	PEB	C2C-C1C-NC	3.95	112.89	107.57
82	HG	1002	PEB	C3D-C4D-ND	3.95	115.00	107.26
82	dM	201	PEB	C3D-C4D-ND	3.95	115.00	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QH	201	PEB	CHC-C1D-ND	-3.95	108.73	113.72
82	V1	202	PEB	CHC-C1D-ND	-3.95	108.73	113.72
82	TA	202	PEB	CHA-C1B-NB	-3.95	116.68	124.93
82	GM	202	PEB	C1D-CHC-C4C	-3.95	107.44	113.26
82	JM	201	PEB	CMB-C2B-C1B	3.95	131.14	125.06
82	TF	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
88	DL	407	LHG	O7-C7-C8	3.95	120.00	111.50
82	AI	202	PEB	OA-C1A-C2A	-3.95	123.04	126.17
82	kO	202	PEB	C1C-C2C-C3C	-3.95	102.96	107.62
82	gH	201	PEB	C2C-C1C-NC	3.95	112.88	107.57
82	TI	201	PEB	C2A-C1A-NA	3.95	111.67	108.27
85	b6	601	BCR	C7-C8-C9	-3.94	120.27	126.23
82	W5	201	PEB	C3D-C4D-ND	3.94	115.00	107.26
85	bL	603	BCR	C16-C17-C18	-3.94	121.68	127.31
87	52	607	CLA	CAA-C2A-C3A	-3.94	101.98	112.78
82	P7	201	PEB	OD-C4D-ND	-3.94	120.09	125.93
82	s8	202	PEB	C1C-C2C-C3C	-3.94	102.96	107.62
82	fG	203	PEB	C1C-C2C-C3C	-3.94	102.96	107.62
82	QM	203	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	F4	1002	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	xC	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
82	TH	202	PEB	CMC-C3C-C4C	3.94	131.24	127.06
82	T1	202	PEB	CMC-C3C-C4C	3.94	131.24	127.06
82	HI	202	PEB	CHA-C1B-C2B	3.94	135.04	124.90
82	YK	201	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	dQ	401	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	UE	202	PEB	C2C-C1C-NC	3.94	112.88	107.57
84	LO	1001	CYC	C2B-C1B-NB	3.94	112.76	106.99
85	AN	848	BCR	C16-C17-C18	-3.94	121.68	127.31
82	TO	202	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	B5	201	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	dD	401	PEB	C3D-C4D-ND	3.94	115.00	107.26
82	VQ	203	PEB	CHC-C1D-ND	-3.94	108.73	113.72
82	XQ	203	PEB	CHC-C1D-ND	-3.94	108.73	113.72
82	FF	201	PEB	CHC-C4C-NC	3.94	126.49	121.15
84	EO	1001	CYC	C2D-C1D-ND	3.94	112.94	107.40
82	T7	202	PEB	CHA-C1B-NB	-3.94	116.69	124.93
82	jM	201	PEB	OA-C1A-C2A	-3.94	123.04	126.17
82	U7	202	PEB	C2A-C1A-NA	3.94	111.67	108.27
82	18	202	PEB	C1C-C2C-C3C	-3.94	102.96	107.62
82	PJ	201	PEB	OD-C4D-ND	-3.94	120.09	125.93
82	d1	202	PEB	C2C-C1C-NC	3.94	112.88	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OE	201	PEB	OD-C4D-ND	-3.94	120.09	125.93
87	5N	607	CLA	CAA-C2A-C3A	-3.94	101.98	112.78
85	FL	101	BCR	C7-C8-C9	-3.94	120.28	126.23
85	CL	501	BCR	C3-C4-C5	-3.94	107.04	114.08
82	Z5	305	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	XK	203	PEB	C1C-CHB-C4B	3.94	137.12	128.28
82	J4	1002	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	X7	202	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	FH	1002	PEB	C3D-C4D-ND	3.94	114.99	107.26
84	KO	1001	CYC	C2D-C1D-ND	3.94	112.94	107.40
82	SK	202	PEB	CHA-C1B-C2B	3.94	135.03	124.90
82	YQ	202	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	W1	201	PEB	CAC-CBC-CGC	3.94	122.08	113.60
82	hH	201	PEB	CHB-C1C-C2C	-3.94	118.26	127.15
84	HE	1001	CYC	C2D-C1D-ND	3.94	112.94	107.40
83	A4	303	PUB	CHA-C1B-NB	3.94	126.48	121.15
82	W9	202	PEB	C1C-C2C-C3C	-3.94	102.96	107.62
82	A4	305	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	fF	202	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	QB	201	PEB	OA-C1A-C2A	-3.94	123.04	126.17
82	EP	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
82	GM	201	PEB	CMB-C2B-C1B	3.94	131.13	125.06
82	M5	301	PEB	CMB-C2B-C1B	3.94	131.13	125.06
82	FA	203	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	gG	201	PEB	CHC-C4C-NC	3.94	126.48	121.15
82	cK	203	PEB	OD-C4D-ND	-3.94	120.09	125.93
88	D6	406	LHG	O7-C7-C8	3.94	119.99	111.50
82	ED	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
82	h1	202	PEB	CHB-C1C-C2C	-3.94	118.27	127.15
82	iJ	201	PEB	CHA-C1B-NB	-3.94	116.69	124.93
82	Q1	201	PEB	CHC-C1D-ND	-3.94	108.74	113.72
82	fM	203	PEB	C1C-CHB-C4B	3.94	137.11	128.28
84	IE	1001	CYC	C4D-C3D-C2D	-3.94	102.97	107.62
82	N7	203	PEB	C3D-C4D-ND	3.94	114.98	107.26
82	fB	301	PEB	C3D-C4D-ND	3.94	114.98	107.26
82	TO	201	PEB	C2A-C1A-NA	3.94	111.67	108.27
82	ZM	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
82	fH	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
82	DQ	203	PEB	CHB-C1C-C2C	-3.94	118.27	127.15
82	KA	201	PEB	CBC-CAC-C2C	3.94	123.56	112.63
82	TP	202	PEB	CMB-C2B-C1B	3.94	131.13	125.06
82	JM	201	PEB	C2C-C1C-NC	3.94	112.87	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	L7	201	PEB	C2C-C1C-NC	3.94	112.87	107.57
82	SD	201	PEB	C3B-C4B-NB	3.94	115.78	110.05
84	W3	1001	CYC	CMB-C2B-C1B	3.94	129.08	124.17
82	LQ	201	PEB	CHB-C1C-C2C	-3.94	118.27	127.15
83	AM	303	PUB	C1C-C2C-C3C	-3.94	102.43	106.78
84	LE	1001	CYC	C2D-C1D-ND	3.94	112.93	107.40
82	F7	202	PEB	C2A-C1A-NA	3.94	111.67	108.27
84	N4	1001	CYC	CHD-C1D-ND	-3.94	116.30	125.32
83	A1	304	PUB	CHB-C1C-NC	-3.94	116.39	124.58
82	MM	203	PEB	C3C-C4C-NC	3.94	111.88	108.33
82	TD	201	PEB	OA-C1A-C2A	-3.94	123.04	126.17
82	TI	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
82	w8	201	PEB	C1C-C2C-C3C	-3.94	102.97	107.62
82	zK	501	PEB	C3B-C4B-NB	3.93	115.77	110.05
82	DO	1002	PEB	C3D-C4D-ND	3.93	114.98	107.26
82	XQ	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
82	dG	201	PEB	C3D-C4D-ND	3.93	114.98	107.26
82	YA	304	PEB	C2A-C1A-NA	3.93	111.67	108.27
84	E4	1001	CYC	C2D-C1D-ND	3.93	112.93	107.40
82	rC	201	PEB	CHC-C4C-NC	3.93	126.47	121.15
82	fO	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
84	KH	1001	CYC	C4D-CHA-C1A	3.93	137.10	128.28
82	aB	201	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
82	MF	202	PEB	C2C-C1C-NC	3.93	112.87	107.57
82	kH	201	PEB	CBA-CAA-C3A	3.93	122.23	113.47
82	JB	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
82	B7	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
84	DH	1001	CYC	OB-C4B-C3B	-3.93	123.77	128.04
82	yK	301	PEB	C3D-C4D-ND	3.93	114.98	107.26
82	fH	201	PEB	C1C-C2C-C3C	-3.93	102.97	107.62
82	U4	201	PEB	C1D-CHC-C4C	-3.93	107.46	113.26
82	OM	201	PEB	C3D-C4D-ND	3.93	114.98	107.26
82	Y7	304	PEB	C3D-C4D-ND	3.93	114.98	107.26
82	qC	201	PEB	OD-C4D-ND	-3.93	120.10	125.93
82	Z5	304	PEB	C3C-C4C-NC	3.93	111.87	108.33
82	AE	301	PEB	CHC-C1D-ND	-3.93	108.75	113.72
82	SK	203	PEB	OA-C1A-C2A	-3.93	123.05	126.17
82	vC	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
82	SM	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	UI	201	PEB	C1C-C2C-C3C	-3.93	102.97	107.62
82	J7	201	PEB	C1C-CHB-C4B	-3.93	119.46	128.28
88	d6	402	LHG	O7-C7-C8	3.93	119.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	DH	1001	CYC	C2D-C1D-ND	3.93	112.93	107.40
82	V4	202	PEB	C3B-C4B-NB	3.93	115.77	110.05
82	ID	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	HK	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	V7	201	PEB	C1B-C2B-C3B	-3.93	101.99	106.51
82	UP	203	PEB	OA-C1A-C2A	-3.93	123.05	126.17
83	AJ	303	PUB	C1C-C2C-C3C	-3.93	102.43	106.78
82	tK	201	PEB	C2C-C1C-NC	3.93	112.86	107.57
83	A1	303	PUB	C1D-CHC-C4C	-3.93	104.81	113.37
92	XL	601	LMG	O7-C10-C11	3.93	119.97	111.50
82	SH	203	PEB	CHC-C1D-ND	-3.93	108.75	113.72
82	YE	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
85	FL	101	BCR	C28-C27-C26	-3.93	107.06	114.08
82	qK	202	PEB	C1C-CHB-C4B	3.93	137.10	128.28
82	XJ	201	PEB	C1C-C2C-C3C	-3.93	102.97	107.62
84	HO	1001	CYC	CHB-C1B-NB	-3.93	117.62	126.06
82	WI	201	PEB	C1C-C2C-C3C	-3.93	102.98	107.62
88	l6	101	LHG	O7-C7-C8	3.93	119.97	111.50
82	HE	1002	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	QP	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	JJ	201	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
82	UM	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	yF	301	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	CK	202	PEB	C3B-C4B-NB	3.93	115.76	110.05
82	QP	201	PEB	CHA-C1B-NB	-3.93	116.72	124.93
82	lM	202	PEB	CMB-C2B-C1B	3.93	131.11	125.06
82	VF	201	PEB	OA-C1A-NA	3.93	129.70	124.94
82	qC	202	PEB	C1C-C2C-C3C	-3.93	102.98	107.62
82	C7	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
82	Y5	203	PEB	CAC-CBC-CGC	-3.93	105.15	113.60
82	EJ	203	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	xF	304	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	PP	202	PEB	CHA-C1B-NB	-3.93	116.72	124.93
82	eM	202	PEB	CHC-C4C-NC	3.93	126.46	121.15
82	LQ	201	PEB	C1C-C2C-C3C	-3.93	102.98	107.62
84	E4	1001	CYC	C1D-C2D-C3D	-3.93	102.79	107.79
85	L2	201	BCR	C15-C14-C13	-3.93	121.71	127.31
82	M7	201	PEB	C2A-C1A-NA	3.93	111.66	108.27
82	UE	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	TK	202	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	k4	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	KI	203	PEB	OA-C1A-C2A	-3.93	123.05	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EP	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
82	KF	201	PEB	C3C-C4C-NC	3.93	111.87	108.33
82	QO	201	PEB	C3C-C4C-NC	3.93	111.87	108.33
82	YI	202	PEB	CHC-C4C-NC	3.93	126.46	121.15
82	AA	201	PEB	CAB-CBB-CGB	-3.93	105.15	113.60
82	DP	201	PEB	CHC-C1D-ND	-3.93	108.76	113.72
82	f1	201	PEB	C1C-C2C-C3C	-3.93	102.98	107.62
82	D9	203	PEB	C2A-C1A-NA	3.93	111.66	108.27
82	z8	201	PEB	C2C-C1C-NC	3.93	112.86	107.57
82	KP	201	PEB	CHC-C1D-ND	-3.93	108.76	113.72
82	mF	201	PEB	C4B-C3B-C2B	-3.93	102.44	106.78
82	GA	202	PEB	C1C-C2C-C3C	-3.93	102.98	107.62
82	NF	202	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	xC	202	PEB	C3D-C4D-ND	3.93	114.96	107.26
82	O9	201	PEB	CAA-C3A-C4A	-3.92	102.59	112.67
82	WB	401	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	F1	1002	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	iH	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	DB	201	PEB	C2A-C1A-NA	3.92	111.66	108.27
82	NI	203	PEB	C2A-C1A-NA	3.92	111.66	108.27
82	RI	203	PEB	C3C-C4C-NC	3.92	111.86	108.33
84	y3	1001	CYC	CMB-C2B-C1B	3.92	129.07	124.17
82	XA	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	ZB	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	ZB	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	VM	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	Q1	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	dH	202	PEB	C2C-C1C-NC	3.92	112.86	107.57
82	R7	202	PEB	OD-C4D-ND	-3.92	120.12	125.93
82	OB	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	f4	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	Z5	301	PEB	CMB-C2B-C1B	3.92	131.11	125.06
82	ZH	201	PEB	C1C-C2C-C3C	-3.92	102.98	107.62
82	V1	202	PEB	C1C-C2C-C3C	-3.92	102.98	107.62
82	eB	201	PEB	CHA-C1B-NB	-3.92	116.73	124.93
82	GE	1002	PEB	C3B-C4B-NB	3.92	115.76	110.05
82	UH	202	PEB	CHC-C4C-NC	3.92	126.46	121.15
82	L5	201	PEB	C2C-C1C-NC	3.92	112.85	107.57
82	IM	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
82	m4	203	PEB	C3D-C4D-ND	3.92	114.96	107.26
84	MO	1001	CYC	C1D-C2D-C3D	-3.92	102.79	107.79
82	Y7	303	PEB	OA-C1A-C2A	-3.92	123.05	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	sC	202	PEB	C1C-C2C-C3C	-3.92	102.98	107.62
82	JO	1002	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	dB	201	PEB	CHC-C4C-NC	3.92	126.46	121.15
82	FD	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
85	KN	101	BCR	C35-C13-C12	3.92	124.26	118.08
82	uC	203	PEB	C2C-C1C-NC	3.92	112.85	107.57
82	XM	202	PEB	C1C-CHB-C4B	-3.92	119.49	128.28
82	RD	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	GM	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	H5	203	PEB	CHC-C4C-NC	3.92	126.46	121.15
85	A2	846	BCR	C11-C10-C9	-3.92	121.71	127.31
82	SP	202	PEB	C1B-C2B-C3B	-3.92	102.00	106.51
82	AJ	302	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	bB	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	RP	201	PEB	OA-C1A-C2A	-3.92	123.06	126.17
82	gG	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
82	V1	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	N4	1002	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	T7	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	T4	203	PEB	C2C-C1C-NC	3.92	112.85	107.57
82	TA	203	PEB	C2A-C1A-NA	3.92	111.65	108.27
82	YD	202	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
82	NA	202	PEB	C3B-C4B-NB	3.92	115.75	110.05
82	WM	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	lG	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	RA	202	PEB	OD-C4D-ND	-3.92	120.12	125.93
82	LQ	203	PEB	OA-C1A-C2A	-3.92	123.06	126.17
85	A6	401	BCR	C38-C26-C25	-3.92	120.13	124.53
82	fB	301	PEB	C1C-C2C-C3C	-3.92	102.99	107.62
82	P4	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	H9	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
84	CO	1001	CYC	CHB-C4A-NA	-3.92	116.73	124.93
82	VK	201	PEB	OA-C1A-NA	3.92	129.69	124.94
82	LI	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	hF	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	mO	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
84	BE	1001	CYC	CMD-C2D-C1D	3.92	131.30	125.56
82	EM	201	PEB	OA-C1A-C2A	-3.92	123.06	126.17
82	L9	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	hK	201	PEB	CMB-C2B-C1B	3.92	131.10	125.06
82	GF	202	PEB	CHC-C1D-ND	-3.92	108.77	113.72
82	UG	201	PEB	C3D-C4D-ND	3.92	114.95	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NM	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	D5	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	pK	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
82	FM	201	PEB	C1C-CHB-C4B	-3.92	119.50	128.28
91	DL	405	PHO	C4A-C3A-C2A	-3.92	99.11	102.84
82	KJ	203	PEB	OA-C1A-C2A	-3.92	123.06	126.17
84	C4	1001	CYC	CHB-C4A-NA	-3.92	116.74	124.93
82	FK	201	PEB	C1C-C2C-C3C	-3.92	102.99	107.62
82	TK	201	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	kO	202	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	Q5	201	PEB	C1B-C2B-C3B	-3.92	102.01	106.51
82	aH	201	PEB	CHC-C4C-NC	3.92	126.45	121.15
82	DO	1002	PEB	C2A-C1A-NA	3.92	111.65	108.27
82	AG	301	PEB	CHC-C1D-ND	-3.92	108.77	113.72
82	u8	202	PEB	C2C-C1C-NC	3.92	112.85	107.57
82	CF	202	PEB	C3B-C4B-NB	3.92	115.75	110.05
82	NQ	204	PEB	CHB-C1C-C2C	-3.92	118.31	127.15
82	TA	203	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	YB	201	PEB	CHC-C4C-NC	3.92	126.45	121.15
82	XJ	202	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	DM	201	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	AO	304	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	xF	303	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	aJ	202	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	BB	201	PEB	C2A-C1A-NA	3.92	111.65	108.27
82	YO	203	PEB	C3D-C4D-ND	3.92	114.94	107.26
82	FJ	201	PEB	C1C-C2C-C3C	-3.92	102.99	107.62
82	1C	202	PEB	C1C-C2C-C3C	-3.92	102.99	107.62
82	t8	202	PEB	CHB-C1C-NC	-3.92	116.35	125.32
82	QI	201	PEB	CMB-C2B-C1B	3.92	131.09	125.06
82	eG	201	PEB	C2C-C1C-NC	3.92	112.84	107.57
84	H4	1001	CYC	CHB-C1B-NB	-3.92	117.65	126.06
84	KO	1001	CYC	C2C-C1C-NC	3.91	111.65	108.27
82	J9	202	PEB	C1C-C2C-C3C	-3.91	102.99	107.62
82	dB	201	PEB	C1C-C2C-C3C	-3.91	102.99	107.62
82	tF	201	PEB	C2C-C1C-NC	3.91	112.84	107.57
82	RP	202	PEB	C3D-C4D-ND	3.91	114.94	107.26
82	dE	201	PEB	C3D-C4D-ND	3.91	114.94	107.26
85	b6	601	BCR	C24-C23-C22	-3.91	120.32	126.23
82	J9	202	PEB	CHB-C1C-C2C	-3.91	118.32	127.15
82	HB	201	PEB	C1C-C2C-C3C	-3.91	102.99	107.62
82	RF	201	PEB	C1C-C2C-C3C	-3.91	102.99	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	pF	202	PEB	C1C-C2C-C3C	-3.91	102.99	107.62
85	FN	202	BCR	C34-C9-C8	3.91	124.24	118.08
82	lM	203	PEB	C2A-C1A-NA	3.91	111.65	108.27
82	M9	302	PEB	CHA-C1B-NB	-3.91	116.75	124.93
85	c6	603	BCR	C1-C6-C5	-3.91	117.10	122.61
85	F2	203	BCR	C34-C9-C8	3.91	124.24	118.08
82	WM	203	PEB	CHC-C1D-ND	-3.91	108.77	113.72
82	J9	203	PEB	CHC-C1D-ND	-3.91	108.77	113.72
82	r8	201	PEB	CHC-C4C-NC	3.91	126.44	121.15
82	NB	202	PEB	C3D-C4D-ND	3.91	114.94	107.26
82	JK	202	PEB	CHB-C4B-C3B	-3.91	116.27	125.32
84	LG	1001	CYC	C2B-C1B-NB	3.91	112.72	106.99
82	HD	201	PEB	CHA-C1B-NB	-3.91	116.75	124.93
82	dB	202	PEB	C2A-C1A-NA	3.91	111.65	108.27
82	CI	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
92	jL	101	LMG	O7-C10-C11	3.91	119.93	111.50
82	zC	201	PEB	C1C-CHB-C4B	3.91	137.06	128.28
82	HE	1002	PEB	C2C-C1C-NC	3.91	112.84	107.57
82	EP	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	WH	202	PEB	C1D-CHC-C4C	-3.91	107.49	113.26
84	HO	1001	CYC	C1B-C2B-C3B	-3.91	103.79	107.87
82	XB	202	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	HI	202	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	RI	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
82	UJ	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
82	SP	203	PEB	OA-C1A-C2A	-3.91	123.06	126.17
82	QH	203	PEB	C1B-C2B-C3B	-3.91	102.02	106.51
82	h1	202	PEB	C1B-C2B-C3B	-3.91	102.02	106.51
82	bO	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	VQ	202	PEB	C1C-C2C-C3C	-3.91	103.00	107.62
82	aK	203	PEB	C1C-C2C-C3C	-3.91	103.00	107.62
82	HB	202	PEB	CHC-C4C-NC	3.91	126.44	121.15
82	S9	201	PEB	CMB-C2B-C1B	3.91	131.09	125.06
82	FO	1002	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	UA	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
82	GF	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
82	JA	201	PEB	C1C-CHB-C4B	-3.91	119.51	128.28
84	GE	1001	CYC	C2B-C1B-NB	3.91	112.71	106.99
82	bK	202	PEB	C1C-C2C-C3C	-3.91	103.00	107.62
82	MQ	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	UD	201	PEB	C2C-C1C-NC	3.91	112.84	107.57
82	wC	201	PEB	C2C-C1C-NC	3.91	112.84	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	tF	202	PEB	CBC-CAC-C2C	3.91	123.49	112.63
82	VI	203	PEB	CHA-C1B-C2B	3.91	134.95	124.90
82	x8	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	lM	203	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	YP	503	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	gJ	201	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	WH	201	PEB	CAC-CBC-CGC	3.91	122.02	113.60
82	EJ	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
82	hG	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	J7	202	PEB	C1B-C2B-C3B	-3.91	102.02	106.51
82	GM	201	PEB	CHA-C1B-NB	-3.91	116.76	124.93
82	VQ	203	PEB	CMC-C3C-C4C	3.91	131.20	127.06
82	hE	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	FD	203	PEB	C4B-C3B-C2B	-3.91	102.46	106.78
84	NE	201	CYC	C2B-C1B-NB	3.91	112.71	106.99
82	eF	201	PEB	C1B-C2B-C3B	-3.91	102.02	106.51
82	UB	303	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	EQ	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
82	BD	201	PEB	OA-C1A-C2A	-3.91	123.07	126.17
82	lJ	203	PEB	OA-C1A-C2A	-3.91	123.07	126.17
82	G9	202	PEB	CHA-C4A-NA	-3.91	120.56	125.20
82	H4	1002	PEB	C3D-C4D-ND	3.91	114.92	107.26
82	YO	202	PEB	C4B-C3B-C2B	-3.91	102.46	106.78
82	cJ	201	PEB	C4B-C3B-C2B	-3.91	102.46	106.78
82	HK	202	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	UM	203	PEB	C2A-C1A-NA	3.91	111.64	108.27
85	c6	617	BCR	C28-C27-C26	-3.91	107.10	114.08
82	gG	202	PEB	C3D-C4D-ND	3.91	114.92	107.26
82	u8	203	PEB	C2C-C1C-NC	3.91	112.83	107.57
84	L4	1001	CYC	C2B-C1B-NB	3.91	112.71	106.99
82	VI	203	PEB	C4B-C3B-C2B	-3.91	102.46	106.78
84	HO	1001	CYC	C1A-C2A-C3A	-3.91	102.46	106.78
82	GK	201	PEB	CAC-CBC-CGC	-3.91	105.20	113.60
82	N5	201	PEB	C3D-C4D-ND	3.91	114.92	107.26
82	W9	202	PEB	C1C-CHB-C4B	3.91	137.04	128.28
92	J6	102	LMG	C7-O1-C1	-3.91	106.11	113.74
82	OP	203	PEB	C1B-C2B-C3B	-3.91	102.02	106.51
82	HA	201	PEB	C2A-C1A-NA	3.91	111.64	108.27
82	MJ	203	PEB	C2A-C1A-NA	3.91	111.64	108.27
84	D1	1001	CYC	C4D-CHA-C1A	3.91	137.04	128.28
82	VH	201	PEB	C3D-C4D-ND	3.91	114.92	107.26
82	RQ	201	PEB	C3D-C4D-ND	3.91	114.92	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	a1	201	PEB	C1C-C2C-C3C	-3.91	103.00	107.62
82	uC	203	PEB	C1C-C2C-C3C	-3.91	103.00	107.62
82	CJ	203	PEB	CHA-C1B-NB	-3.91	116.76	124.93
84	GG	1001	CYC	C2D-C1D-ND	3.91	112.89	107.40
82	wK	302	PEB	CMB-C2B-C1B	3.91	131.08	125.06
82	TO	201	PEB	C3D-C4D-ND	3.91	114.92	107.26
82	M5	301	PEB	C3D-C4D-ND	3.91	114.92	107.26
82	iM	202	PEB	C3D-C4D-ND	3.91	114.92	107.26
88	L6	101	LHG	O7-C7-C8	3.91	119.92	111.50
82	LA	201	PEB	C1C-C2C-C3C	-3.90	103.00	107.62
82	XD	202	PEB	C1C-C2C-C3C	-3.90	103.00	107.62
82	ID	201	PEB	CHC-C4C-NC	3.90	126.43	121.15
82	hB	301	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	kG	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	dH	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	IQ	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	SB	201	PEB	CMB-C2B-C1B	3.90	131.08	125.06
85	K2	102	BCR	C35-C13-C12	3.90	124.23	118.08
82	aH	201	PEB	C1C-CHB-C4B	3.90	137.04	128.28
82	dH	203	PEB	CHC-C1D-ND	-3.90	108.78	113.72
82	FJ	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	OQ	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	F5	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	LM	201	PEB	C2C-C1C-NC	3.90	112.83	107.57
82	GJ	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	FF	201	PEB	OD-C4D-ND	-3.90	120.15	125.93
82	HD	201	PEB	C2A-C1A-NA	3.90	111.64	108.27
82	SI	202	PEB	CMB-C2B-C1B	3.90	131.07	125.06
84	JH	1001	CYC	C2B-C1B-NB	3.90	112.70	106.99
82	UH	201	PEB	C1C-C2C-C3C	-3.90	103.01	107.62
82	z8	201	PEB	C1C-CHB-C4B	3.90	137.03	128.28
82	ZM	202	PEB	CMB-C2B-C1B	3.90	131.07	125.06
82	KJ	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	y8	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
82	rF	201	PEB	CHA-C4A-NA	3.90	129.84	125.20
82	fJ	203	PEB	CHB-C1C-C2C	-3.90	118.35	127.15
82	UE	201	PEB	C1C-C2C-C3C	-3.90	103.01	107.62
82	XA	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
84	KH	1001	CYC	C1B-C2B-C3B	-3.90	103.80	107.87
82	A4	304	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	wC	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	q8	201	PEB	OD-C4D-ND	-3.90	120.15	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	BN	843	BCR	C16-C17-C18	-3.90	121.74	127.31
82	HI	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	mF	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	jM	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	Z5	305	PEB	CHB-C4B-NB	-3.90	116.46	124.58
82	II	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	ND	204	PEB	CHB-C1C-C2C	-3.90	118.35	127.15
82	WP	202	PEB	OD-C4D-ND	-3.90	120.15	125.93
82	GP	202	PEB	C1B-C2B-C3B	-3.90	102.03	106.51
84	EO	1001	CYC	C1D-C2D-C3D	-3.90	102.82	107.79
85	C6	508	BCR	C11-C10-C9	-3.90	121.74	127.31
82	SB	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	a1	201	PEB	CHC-C4C-NC	3.90	126.43	121.15
94	DL	401	PL9	C20-C19-C21	3.90	121.83	115.27
82	H9	203	PEB	OA-C1A-C2A	-3.90	123.07	126.17
82	HF	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	j4	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
84	FG	1001	CYC	CHD-C1D-ND	-3.90	116.39	125.32
92	j6	101	LMG	C7-O1-C1	-3.90	106.12	113.74
82	CJ	203	PEB	CHC-C1D-ND	-3.90	108.79	113.72
82	d1	203	PEB	CHC-C1D-ND	-3.90	108.79	113.72
82	UA	202	PEB	C2A-C1A-NA	3.90	111.64	108.27
82	YB	202	PEB	C2A-C1A-NA	3.90	111.64	108.27
82	JJ	201	PEB	C2A-C1A-NA	3.90	111.64	108.27
82	xC	202	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
82	K9	202	PEB	CHA-C4A-NA	-3.90	120.57	125.20
82	UP	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	hK	202	PEB	C3D-C4D-ND	3.90	114.91	107.26
87	aL	606	CLA	CMD-C2D-C3D	-3.90	118.64	127.61
82	Z5	301	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	kO	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	PK	201	PEB	CHA-C1B-NB	-3.90	116.78	124.93
82	Z9	301	PEB	CHA-C1B-NB	-3.90	116.78	124.93
84	D1	1001	CYC	C2D-C1D-ND	3.90	112.88	107.40
82	eG	203	PEB	CMB-C2B-C1B	3.90	131.07	125.06
82	R4	202	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
82	PH	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	eO	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	aH	201	PEB	C1C-C2C-C3C	-3.90	103.01	107.62
84	NH	1001	CYC	CHA-C4D-C3D	-3.90	118.36	127.15
82	tC	202	PEB	CHB-C1C-NC	-3.90	116.39	125.32
82	g1	202	PEB	C2C-C1C-NC	3.90	112.82	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	852	CLA	CHD-C1D-C2D	3.90	133.66	125.48
82	aE	202	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	dH	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	BA	202	PEB	CHA-C1B-NB	-3.90	116.78	124.93
84	D1	1001	CYC	C1B-C2B-C3B	-3.90	103.80	107.87
82	MJ	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	NP	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
82	R5	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
103	82	310	ZEX	C8-C9-C10	3.90	124.92	118.94
82	JO	1002	PEB	CAC-CBC-CGC	-3.90	105.22	113.60
85	kL	100	BCR	C10-C11-C12	3.90	135.38	123.22
83	AH	303	PUB	C1D-CHC-C4C	-3.90	104.89	113.37
82	D4	1002	PEB	C3D-C4D-ND	3.90	114.90	107.26
82	UF	201	PEB	OA-C1A-C2A	3.90	129.27	126.17
82	TJ	201	PEB	CHA-C1B-NB	-3.90	116.78	124.93
82	LD	202	PEB	C3D-C4D-ND	3.90	114.90	107.26
82	K5	201	PEB	C3D-C4D-ND	3.90	114.90	107.26
87	6N	608	CLA	C5-C3-C2	-3.90	111.39	122.65
82	PM	202	PEB	CMB-C2B-C1B	3.90	131.06	125.06
82	CA	201	PEB	C3D-C4D-ND	3.90	114.90	107.26
82	aG	202	PEB	C3D-C4D-ND	3.90	114.90	107.26
82	PA	202	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
82	Q4	201	PEB	C3C-C4C-NC	3.90	111.84	108.33
82	Y4	201	PEB	C2A-C1A-NA	3.90	111.63	108.27
82	II	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
82	OH	201	PEB	C2C-C1C-NC	3.89	112.82	107.57
82	zC	201	PEB	C2C-C1C-NC	3.89	112.82	107.57
82	kM	201	PEB	C1D-CHC-C4C	3.89	119.00	113.26
82	YG	201	PEB	CHB-C4B-C3B	-3.89	116.31	125.32
84	IG	1001	CYC	C4D-C3D-C2D	-3.89	103.02	107.62
82	TF	201	PEB	C3D-C4D-ND	3.89	114.90	107.26
83	AM	304	PUB	CHA-C1B-NB	3.89	126.42	121.15
82	VA	201	PEB	CMB-C2B-C1B	3.89	131.06	125.06
82	V9	202	PEB	CHA-C4A-NA	-3.89	120.58	125.20
85	J2	102	BCR	C28-C27-C26	-3.89	107.12	114.08
82	AD	303	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	VE	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	cB	403	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	T7	202	PEB	C1C-NC-C4C	-3.89	102.67	109.60
82	aJ	202	PEB	CMB-C2B-C1B	3.89	131.06	125.06
82	mK	201	PEB	C4B-C3B-C2B	-3.89	102.47	106.78
82	UD	202	PEB	C3D-C4D-ND	3.89	114.90	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	T4	201	PEB	C3D-C4D-ND	3.89	114.90	107.26
85	JN	102	BCR	C28-C27-C26	-3.89	107.12	114.08
84	DH	1003	CYC	C1B-CHB-C4A	-3.89	118.57	128.08
87	A2	852	CLA	CHD-C1D-C2D	3.89	133.65	125.48
82	FJ	201	PEB	C2C-C1C-NC	3.89	112.81	107.57
95	aL	603	DGD	O2G-C1B-C2B	3.89	119.89	111.50
82	DF	201	PEB	C1C-C2C-C3C	-3.89	103.02	107.62
82	L7	201	PEB	C1C-C2C-C3C	-3.89	103.02	107.62
82	WJ	203	PEB	CHC-C1D-ND	-3.89	108.80	113.72
82	QH	203	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	YH	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	VI	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	O9	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	bO	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	AD	301	PEB	C3D-C4D-ND	3.89	114.90	107.26
82	DB	202	PEB	CMB-C2B-C1B	3.89	131.06	125.06
82	qC	201	PEB	CHC-C4C-NC	3.89	126.42	121.15
82	B7	202	PEB	CHA-C1B-NB	-3.89	116.79	124.93
82	HM	201	PEB	CHC-C1D-ND	3.89	118.65	113.72
82	AM	302	PEB	CHC-C1D-ND	-3.89	108.80	113.72
82	eE	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	GJ	203	PEB	C2A-C1A-NA	3.89	111.63	108.27
82	iJ	202	PEB	CMB-C2B-C1B	3.89	131.06	125.06
82	GG	1002	PEB	C3B-C4B-NB	3.89	115.71	110.05
82	LF	201	PEB	OA-C1A-NA	3.89	129.66	124.94
84	J1	1001	CYC	C2B-C1B-NB	3.89	112.69	106.99
82	SF	202	PEB	CHA-C1B-C2B	3.89	134.91	124.90
82	WD	201	PEB	OD-C4D-ND	-3.89	120.17	125.93
82	KJ	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	JQ	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
84	DO	1001	CYC	CHD-C1D-ND	-3.89	116.41	125.32
82	u8	203	PEB	C1C-C2C-C3C	-3.89	103.02	107.62
82	DM	201	PEB	CHA-C1B-NB	-3.89	116.79	124.93
82	JI	201	PEB	C2C-C1C-NC	3.89	112.81	107.57
82	F7	201	PEB	C2A-C1A-NA	3.89	111.63	108.27
82	s8	203	PEB	C1C-C2C-C3C	-3.89	103.02	107.62
82	XK	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	XM	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	l4	201	PEB	C1B-C2B-C3B	-3.89	102.04	106.51
85	B2	843	BCR	C16-C17-C18	-3.89	121.76	127.31
82	x8	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	NH	1002	PEB	C3D-C4D-ND	3.89	114.89	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TD	202	PEB	CMB-C2B-C1B	3.89	131.05	125.06
82	VI	203	PEB	CMB-C2B-C1B	3.89	131.05	125.06
82	RK	201	PEB	C2C-C1C-NC	3.89	112.81	107.57
82	NP	201	PEB	C1C-C2C-C3C	-3.89	103.02	107.62
82	UO	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	eG	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	iO	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	aK	202	PEB	CHA-C1B-NB	-3.89	116.80	124.93
82	aK	202	PEB	CHC-C4C-NC	3.89	126.41	121.15
82	N1	1002	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	kE	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	kK	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
95	C6	523	DGD	O2G-C1B-C2B	3.89	119.88	111.50
82	KM	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	V7	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	pF	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
84	LG	1001	CYC	C2C-C1C-NC	3.89	111.62	108.27
82	xK	302	PEB	CHB-C1C-NC	-3.89	116.41	125.32
84	KG	202	CYC	C2B-C1B-NB	3.89	112.68	106.99
82	XI	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	EJ	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	HO	1002	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	i1	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	RG	202	PEB	CHC-C4C-NC	3.89	126.41	121.15
82	mH	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	f1	201	PEB	C2C-C1C-NC	3.89	112.81	107.57
82	LQ	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	cH	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	lJ	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
82	aB	202	PEB	C2A-C1A-NA	3.89	111.62	108.27
82	U5	203	PEB	CMB-C2B-C1B	3.89	131.05	125.06
82	XM	201	PEB	C1C-C2C-C3C	-3.89	103.03	107.62
87	32	310	CLA	O2D-CGD-CBD	3.89	118.17	111.27
84	EH	1001	CYC	C2D-C1D-ND	3.89	112.86	107.40
82	YE	201	PEB	CHB-C4B-C3B	-3.89	116.33	125.32
82	I9	202	PEB	CHA-C4A-NA	-3.89	120.58	125.20
82	V7	201	PEB	CMB-C2B-C1B	3.89	131.05	125.06
87	3N	310	CLA	O2D-CGD-CBD	3.89	118.17	111.27
82	UI	201	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
82	FM	202	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
82	JM	201	PEB	C3D-C4D-ND	3.89	114.88	107.26
82	YM	201	PEB	C3D-C4D-ND	3.89	114.88	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	E5	201	PEB	C3D-C4D-ND	3.89	114.88	107.26
82	X5	201	PEB	C3D-C4D-ND	3.89	114.88	107.26
82	YB	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
82	O5	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
84	DE	1001	CYC	C2D-C1D-ND	3.89	112.86	107.40
84	H4	1001	CYC	CAB-C3B-C4B	3.89	127.52	121.38
82	PI	201	PEB	C3D-C4D-ND	3.89	114.88	107.26
82	oK	201	PEB	C3D-C4D-ND	3.89	114.88	107.26
82	b4	201	PEB	CMB-C2B-C1B	3.89	131.05	125.06
82	sF	202	PEB	CMB-C2B-C1B	3.89	131.05	125.06
82	bH	202	PEB	C1C-CHB-C4B	-3.89	119.57	128.28
82	UH	202	PEB	C3D-C4D-ND	3.89	114.88	107.26
82	NO	1002	PEB	C3D-C4D-ND	3.89	114.88	107.26
96	fL	102	HEM	C1B-NB-C4B	3.89	109.09	105.07
82	IQ	201	PEB	CHC-C4C-NC	3.88	126.41	121.15
95	c6	620	DGD	O2G-C1B-C2B	3.88	119.87	111.50
87	d6	406	CLA	O2D-CGD-O1D	-3.88	116.24	123.84
82	TQ	202	PEB	CMB-C2B-C1B	3.88	131.05	125.06
82	CI	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	T5	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	lO	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
84	EE	1001	CYC	C1D-C2D-C3D	-3.88	102.84	107.79
84	EG	1001	CYC	C1D-C2D-C3D	-3.88	102.84	107.79
84	D1	1003	CYC	C1B-CHB-C4A	-3.88	118.59	128.08
82	NI	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	uK	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	eO	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
84	LH	1001	CYC	C2B-C1B-NB	3.88	112.67	106.99
82	KD	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	A5	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	WI	202	PEB	C3C-C4C-NC	3.88	111.83	108.33
82	fJ	203	PEB	C1C-CHB-C4B	3.88	136.99	128.28
87	62	309	CLA	C5-C3-C2	-3.88	111.42	122.65
82	QH	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	iO	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
85	BN	838	BCR	C4-C5-C6	-3.88	117.09	122.73
82	MB	202	PEB	CHC-C1D-ND	-3.88	108.81	113.72
82	lK	202	PEB	C2A-C1A-NA	3.88	111.62	108.27
82	YA	303	PEB	OA-C1A-C2A	-3.88	123.09	126.17
82	Q1	203	PEB	OA-C1A-C2A	-3.88	123.09	126.17
82	j4	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
82	jO	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EJ	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	PO	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	P1	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	e4	203	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	L5	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	UP	201	PEB	C2C-C1C-NC	3.88	112.80	107.57
82	MJ	201	PEB	C3B-C4B-NB	3.88	115.70	110.05
82	KF	202	PEB	CHC-C4C-NC	3.88	126.40	121.15
82	LK	201	PEB	CHC-C4C-NC	3.88	126.40	121.15
82	eM	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	lM	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
82	HM	202	PEB	C1C-CHB-C4B	-3.88	119.58	128.28
88	AL	407	LHG	O7-C7-C8	3.88	119.87	111.50
82	V5	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	A7	201	PEB	CAB-CBB-CGB	-3.88	105.25	113.60
82	TH	201	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
85	KL	100	BCR	C10-C11-C12	3.88	135.33	123.22
82	HK	201	PEB	C1B-C2B-C3B	-3.88	102.05	106.51
103	8N	310	ZEX	C8-C9-C10	3.88	124.90	118.94
85	KN	104	BCR	C34-C9-C10	-3.88	117.49	122.92
82	GF	201	PEB	CAC-CBC-CGC	-3.88	105.25	113.60
82	L5	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
85	bL	601	BCR	C15-C14-C13	-3.88	121.77	127.31
82	b4	201	PEB	CHC-C4C-NC	3.88	126.40	121.15
84	C1	1001	CYC	C1D-C2D-C3D	-3.88	102.85	107.79
82	qF	202	PEB	C1C-CHB-C4B	3.88	136.98	128.28
82	XF	202	PEB	C1C-C2C-C3C	-3.88	103.03	107.62
82	sC	203	PEB	C1C-C2C-C3C	-3.88	103.03	107.62
82	T7	203	PEB	C2A-C1A-NA	3.88	111.62	108.27
82	NA	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	KE	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	I5	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	wF	301	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	tC	202	PEB	CHB-C4B-NB	-3.88	116.50	124.58
82	WB	402	PEB	OA-C1A-C2A	-3.88	123.09	126.17
84	G4	1001	CYC	C1B-NB-C4B	-3.88	105.73	110.67
82	VD	203	PEB	CMC-C3C-C4C	3.88	131.17	127.06
82	ZH	201	PEB	CHA-C4A-NA	3.88	129.82	125.20
82	DP	202	PEB	CHA-C1B-NB	-3.88	116.82	124.93
82	aJ	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	hB	301	PEB	C1C-C2C-C3C	-3.88	103.03	107.62
82	wF	302	PEB	CMB-C2B-C1B	3.88	131.04	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	K2	105	BCR	C34-C9-C10	-3.88	117.49	122.92
82	UF	201	PEB	OD-C4D-ND	-3.88	120.18	125.93
82	AB	501	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	JI	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	RM	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
84	EH	1001	CYC	C2C-C1C-NC	3.88	111.62	108.27
82	NI	203	PEB	C1B-C2B-C3B	-3.88	102.05	106.51
82	h4	201	PEB	C1B-C2B-C3B	-3.88	102.05	106.51
82	hO	201	PEB	C1B-C2B-C3B	-3.88	102.05	106.51
82	kM	201	PEB	CHA-C1B-NB	-3.88	116.82	124.93
82	IM	203	PEB	OA-C1A-C2A	-3.88	123.09	126.17
82	gB	203	PEB	OA-C1A-C2A	-3.88	123.09	126.17
82	rK	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
82	YE	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	JJ	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	L7	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	xC	201	PEB	CMB-C2B-C1B	3.88	131.04	125.06
82	SG	203	PEB	C3C-C4C-NC	3.88	111.82	108.33
82	HQ	201	PEB	C3C-C4C-NC	3.88	111.82	108.33
82	BK	202	PEB	CHB-C4B-C3B	-3.88	116.35	125.32
82	R9	202	PEB	CHA-C4A-NA	-3.88	120.59	125.20
82	M5	305	PEB	CHB-C4B-NB	-3.88	116.51	124.58
82	SM	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
84	K1	1001	CYC	C1B-C2B-C3B	-3.88	103.83	107.87
82	YA	301	PEB	C3D-C4D-ND	3.88	114.87	107.26
82	RH	202	PEB	C1C-C2C-C3C	-3.88	103.04	107.62
82	R1	202	PEB	C1C-C2C-C3C	-3.88	103.04	107.62
88	dL	405	LHG	O7-C7-C8	3.88	119.86	111.50
82	DI	201	PEB	C2A-C1A-NA	3.88	111.61	108.27
82	NJ	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	KQ	201	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	G5	201	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	dE	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
84	FH	1001	CYC	C2B-C1B-NB	3.88	112.66	106.99
82	RO	202	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
82	xF	304	PEB	C2C-C1C-NC	3.88	112.79	107.57
82	GK	202	PEB	CHC-C1D-ND	-3.88	108.82	113.72
82	GI	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	e4	202	PEB	C1C-C2C-C3C	-3.88	103.04	107.62
82	uC	201	PEB	CAC-C2C-C1C	3.88	131.94	125.76
82	SB	201	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	EI	201	PEB	C3D-C4D-ND	3.88	114.86	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RI	201	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	mO	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	CF	201	PEB	CHC-C1D-ND	-3.88	108.82	113.72
92	qL	301	LMG	O7-C10-C11	3.88	119.85	111.50
82	UQ	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
82	F5	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
88	mL	102	LHG	O7-C7-C8	3.87	119.85	111.50
82	IA	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	HJ	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	FK	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	SK	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	uF	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	aK	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
84	DH	1001	CYC	C4D-CHA-C1A	3.87	136.97	128.28
82	QI	201	PEB	C1C-C2C-C3C	-3.87	103.04	107.62
82	XQ	202	PEB	C1C-C2C-C3C	-3.87	103.04	107.62
82	Y4	203	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	E9	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	aM	204	PEB	C3D-C4D-ND	3.87	114.86	107.26
92	JL	102	LMG	O7-C10-C11	3.87	119.85	111.50
85	CL	502	BCR	C23-C24-C25	3.87	138.08	127.20
82	ZM	202	PEB	CHC-C1D-ND	-3.87	108.82	113.72
84	LE	1001	CYC	C2B-C1B-NB	3.87	112.66	106.99
84	D4	1001	CYC	CHD-C1D-ND	-3.87	116.45	125.32
82	DB	202	PEB	CHC-C4C-NC	3.87	126.39	121.15
82	dO	201	PEB	CHC-C4C-NC	3.87	126.39	121.15
82	eM	202	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
82	LP	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
82	AQ	304	PEB	OA-C1A-C2A	-3.87	123.09	126.17
82	TI	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	jO	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	MD	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	TO	203	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	bO	201	PEB	CHC-C4C-NC	3.87	126.39	121.15
82	WI	202	PEB	OD-C4D-C3D	-3.87	120.68	129.46
82	O9	203	PEB	CMB-C2B-C1B	3.87	131.03	125.06
82	U9	202	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
83	AQ	302	PUB	C1C-C2C-C3C	-3.87	102.50	106.78
82	U9	202	PEB	CAB-C3B-C4B	3.87	131.86	125.01
82	C5	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	P5	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
82	U9	203	PEB	C3D-C4D-ND	3.87	114.86	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VO	202	PEB	CMC-C3C-C4C	3.87	131.16	127.06
82	GI	201	PEB	CHA-C1B-C2B	3.87	134.86	124.90
82	D7	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
85	cL	503	BCR	C11-C10-C9	-3.87	121.78	127.31
82	CM	203	PEB	C3C-C4C-NC	3.87	111.82	108.33
82	u8	201	PEB	CAC-C2C-C1C	3.87	131.93	125.76
82	SH	203	PEB	C1C-C2C-C3C	-3.87	103.04	107.62
82	NO	1002	PEB	CHC-C4C-NC	3.87	126.39	121.15
82	EM	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
84	D1	1001	CYC	OB-C4B-C3B	-3.87	123.84	128.04
85	b6	602	BCR	C16-C17-C18	-3.87	121.78	127.31
82	HJ	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
82	U7	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
82	IM	201	PEB	C1C-CHB-C4B	3.87	136.96	128.28
82	q8	201	PEB	CHC-C4C-NC	3.87	126.39	121.15
82	E9	202	PEB	CHA-C4A-NA	-3.87	120.60	125.20
82	JA	202	PEB	C1B-C2B-C3B	-3.87	102.06	106.51
82	GI	203	PEB	C1B-C2B-C3B	-3.87	102.06	106.51
82	MK	203	PEB	C1B-C2B-C3B	-3.87	102.06	106.51
82	LA	201	PEB	C2C-C1C-NC	3.87	112.78	107.57
82	OD	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	NF	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	WJ	203	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	R9	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
84	FE	1002	CYC	CHD-C1D-ND	-3.87	116.45	125.32
82	PJ	201	PEB	C2A-C1A-NA	3.87	111.61	108.27
82	U4	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	G9	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	R9	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	X9	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	aF	202	PEB	CHC-C4C-NC	3.87	126.39	121.15
85	A6	401	BCR	C11-C10-C9	-3.87	121.79	127.31
82	J4	1002	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
82	BF	202	PEB	CHB-C4B-C3B	-3.87	116.37	125.32
82	W1	202	PEB	C1D-CHC-C4C	-3.87	107.55	113.26
82	TA	202	PEB	C1C-NC-C4C	-3.87	102.71	109.60
82	P7	203	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	K9	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	gB	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
82	LF	201	PEB	CHC-C4C-NC	3.87	126.39	121.15
82	KM	203	PEB	C3D-C4D-ND	3.87	114.85	107.26
94	AL	413	PL9	C40-C39-C41	3.87	121.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	X9	202	PEB	CHA-C4A-NA	-3.87	120.61	125.20
84	NE	201	CYC	OB-C4B-C3B	-3.87	123.84	128.04
82	x8	201	PEB	CMB-C2B-C1B	3.87	131.02	125.06
82	TP	201	PEB	CHC-C1D-ND	-3.87	108.83	113.72
82	H9	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	qC	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	Y7	304	PEB	C2A-C1A-NA	3.87	111.61	108.27
85	B2	838	BCR	C4-C5-C6	-3.87	117.12	122.73
82	SP	201	PEB	OA-C1A-C2A	-3.87	123.10	126.17
82	bO	201	PEB	CMB-C2B-C1B	3.87	131.02	125.06
82	YG	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	A9	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	eB	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	eH	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	iO	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
82	LJ	201	PEB	C1C-CHB-C4B	-3.87	119.61	128.28
82	eK	201	PEB	C1B-C2B-C3B	-3.87	102.07	106.51
82	GP	201	PEB	C1C-C2C-C3C	-3.87	103.05	107.62
82	UF	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
82	jK	202	PEB	C3D-C4D-ND	3.87	114.84	107.26
82	wK	301	PEB	C3D-C4D-ND	3.87	114.84	107.26
82	fM	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
82	hM	202	PEB	C3D-C4D-ND	3.87	114.84	107.26
82	a4	202	PEB	C3C-C4C-NC	3.87	111.81	108.33
82	ZK	202	PEB	C2A-C1A-NA	3.87	111.61	108.27
84	KH	1001	CYC	C1D-C2D-C3D	-3.87	102.87	107.79
82	NK	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
94	a6	601	PL9	C7-C3-C4	3.87	120.02	116.88
82	LJ	201	PEB	OD-C4D-ND	-3.87	120.20	125.93
82	bF	202	PEB	C1C-C2C-C3C	-3.87	103.05	107.62
82	V9	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	kM	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	gE	201	PEB	CHC-C4C-NC	3.86	126.38	121.15
82	D9	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	a1	201	PEB	C1C-CHB-C4B	3.86	136.95	128.28
82	rK	201	PEB	CHA-C4A-NA	3.86	129.80	125.20
82	WQ	201	PEB	OD-C4D-ND	-3.86	120.20	125.93
82	AJ	301	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	RJ	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	JQ	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	C9	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	eJ	202	PEB	C3D-C4D-ND	3.86	114.84	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	T9	202	PEB	CHA-C4A-NA	-3.86	120.61	125.20
82	WE	203	PEB	CHB-C1C-C2C	-3.86	118.43	127.15
82	ZG	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	UH	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
84	I1	1001	CYC	C2B-C1B-NB	3.86	112.64	106.99
82	TH	202	PEB	C1D-CHC-C4C	3.86	118.95	113.26
82	b1	202	PEB	CHC-C1D-ND	-3.86	108.84	113.72
82	BA	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	VO	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	B7	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	dG	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	f4	201	PEB	C1C-CHB-C4B	3.86	136.95	128.28
87	B2	811	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
82	V4	202	PEB	CMC-C3C-C4C	3.86	131.16	127.06
82	DM	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	A9	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
84	HH	1001	CYC	CHB-C1B-NB	-3.86	117.77	126.06
82	JF	202	PEB	CHB-C4B-C3B	-3.86	116.38	125.32
82	l1	203	PEB	C1B-C2B-C3B	-3.86	102.07	106.51
82	CP	203	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	g4	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	s8	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	sF	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	tK	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	KJ	203	PEB	C1C-CHB-C4B	3.86	136.94	128.28
84	ME	1001	CYC	C2D-C1D-ND	3.86	112.83	107.40
82	JD	203	PEB	C4B-C3B-C2B	-3.86	102.51	106.78
82	YQ	202	PEB	C4B-C3B-C2B	-3.86	102.51	106.78
96	V6	201	HEM	C1B-NB-C4B	3.86	109.06	105.07
82	VI	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	C9	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
82	jJ	201	PEB	CMB-C2B-C1B	3.86	131.01	125.06
84	E4	1001	CYC	C2C-C1C-NC	3.86	111.60	108.27
82	s8	202	PEB	CHA-C1B-NB	-3.86	116.86	124.93
82	JQ	202	PEB	C1B-C2B-C3B	-3.86	102.07	106.51
84	BE	1002	CYC	C1D-C2D-C3D	-3.86	102.87	107.79
82	w8	201	PEB	C2C-C1C-NC	3.86	112.77	107.57
82	T4	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	N9	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	aF	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	aO	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	kE	201	PEB	CMB-C2B-C1B	3.86	131.01	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bH	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
92	mL	101	LMG	C7-O1-C1	3.86	121.28	113.74
82	F7	202	PEB	C3C-C4C-NC	3.86	111.81	108.33
82	AI	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	LM	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	YP	502	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	eO	202	PEB	C1C-C2C-C3C	-3.86	103.06	107.62
82	CD	201	PEB	CHC-C1D-ND	-3.86	108.84	113.72
82	DB	201	PEB	C1C-C2C-C3C	-3.86	103.06	107.62
82	SB	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	MP	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
82	OJ	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
84	H4	1001	CYC	C1A-C2A-C3A	-3.86	102.51	106.78
95	c6	601	DGD	O2G-C1B-C2B	3.86	119.82	111.50
82	KA	201	PEB	CHC-C4C-NC	3.86	126.37	121.15
82	1C	201	PEB	CHC-C1D-ND	-3.86	108.84	113.72
82	YB	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	PG	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	KI	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	UJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	DH	1002	PEB	OA-C1A-C2A	-3.86	123.11	126.17
82	GD	201	PEB	OD-C4D-ND	-3.86	120.21	125.93
82	AQ	301	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	O9	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	DQ	203	PEB	C1C-C2C-C3C	-3.86	103.06	107.62
82	jF	201	PEB	C1C-C2C-C3C	-3.86	103.06	107.62
82	aM	202	PEB	CHC-C4C-NC	3.86	126.37	121.15
82	OM	203	PEB	CHB-C1C-C2C	-3.86	118.45	127.15
82	DJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	IJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	KM	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	aE	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	mH	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	fM	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
84	BG	1002	CYC	C1D-C2D-C3D	-3.86	102.88	107.79
84	DH	1001	CYC	C1D-C2D-C3D	-3.86	102.88	107.79
82	eK	203	PEB	C1C-C2C-C3C	-3.86	103.06	107.62
82	c1	202	PEB	CAC-CBC-CGC	-3.86	105.30	113.60
85	JN	103	BCR	C20-C19-C18	-3.86	115.58	126.42
82	DA	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	m4	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	j4	201	PEB	C1B-C2B-C3B	-3.86	102.08	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hF	201	PEB	CMB-C2B-C1B	3.86	131.00	125.06
82	OJ	202	PEB	C2A-C1A-NA	3.86	111.60	108.27
82	HG	1002	PEB	C2C-C1C-NC	3.86	112.77	107.57
82	BP	202	PEB	CHC-C4C-NC	3.86	126.37	121.15
82	g4	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	N9	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
84	E1	1001	CYC	C2D-C1D-ND	3.86	112.82	107.40
82	OQ	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
82	sC	201	PEB	OA-C1A-C2A	-3.86	123.11	126.17
82	h1	201	PEB	C2A-C1A-NA	3.86	111.60	108.27
82	WJ	203	PEB	C1C-CHB-C4B	3.86	136.93	128.28
82	WQ	202	PEB	C3D-C4D-ND	3.86	114.82	107.26
82	t8	202	PEB	CHB-C4B-NB	-3.86	116.55	124.58
82	WO	201	PEB	CMA-C2A-C1A	-3.86	104.09	112.40
82	W4	201	PEB	CMA-C2A-C1A	-3.86	104.09	112.40
85	B2	841	BCR	C15-C16-C17	-3.86	115.58	123.47
82	DK	202	PEB	C3C-C4C-NC	3.86	111.80	108.33
82	j1	203	PEB	C3D-C4D-ND	3.86	114.82	107.26
84	CH	1001	CYC	C1D-C2D-C3D	-3.86	102.88	107.79
82	TO	202	PEB	C1C-CHB-C4B	3.85	136.93	128.28
82	kM	201	PEB	OA-C1A-C2A	-3.85	123.11	126.17
82	BB	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
87	32	309	CLA	C2A-C1A-CHA	3.85	130.60	123.86
84	J1	1001	CYC	CMB-C2B-C1B	3.85	128.98	124.17
82	aM	203	PEB	CAC-C2C-C1C	3.85	131.90	125.76
96	v6	201	HEM	C1B-NB-C4B	3.85	109.05	105.07
82	WE	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	Y4	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
96	f6	101	HEM	CBD-CAD-C3D	-3.85	101.92	112.63
82	fK	202	PEB	C2C-C1C-NC	3.85	112.76	107.57
82	YG	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
82	f1	202	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
82	fB	301	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
82	iF	202	PEB	C3B-C4B-NB	3.85	115.66	110.05
82	I9	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	AM	301	PEB	OA-C1A-C2A	-3.85	123.11	126.17
82	YO	201	PEB	C2A-C1A-NA	3.85	111.59	108.27
82	W7	201	PEB	C2A-C1A-NA	3.85	111.59	108.27
87	BN	812	CLA	O2D-CGD-O1D	-3.85	116.30	123.84
82	KQ	201	PEB	CHC-C1D-ND	-3.85	108.85	113.72
82	FD	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	G9	202	PEB	C3D-C4D-ND	3.85	114.82	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	kF	203	PEB	C3C-C4C-NC	3.85	111.80	108.33
87	AL	405	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
84	D1	1001	CYC	C1D-C2D-C3D	-3.85	102.88	107.79
82	WG	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	IM	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	bP	502	PEB	C3D-C4D-ND	3.85	114.82	107.26
85	BN	841	BCR	C15-C16-C17	-3.85	115.58	123.47
82	NP	201	PEB	CHC-C1D-ND	-3.85	108.85	113.72
82	HF	202	PEB	C2A-C1A-NA	3.85	111.59	108.27
84	HO	1001	CYC	CAB-C3B-C4B	3.85	127.46	121.38
82	JJ	201	PEB	C1C-C2C-C3C	-3.85	103.07	107.62
82	GJ	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	DJ	202	PEB	CMB-C2B-C1B	3.85	131.00	125.06
82	TA	202	PEB	C1B-C2B-C3B	-3.85	102.08	106.51
82	XD	201	PEB	C1B-C2B-C3B	-3.85	102.08	106.51
82	T4	202	PEB	C1C-CHB-C4B	3.85	136.92	128.28
82	AG	304	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	II	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	PO	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	J5	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	K9	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	P9	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	oF	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
82	MF	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	i4	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	E9	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	iG	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	eK	202	PEB	C3B-C4B-NB	3.85	115.65	110.05
82	SI	201	PEB	C2C-C1C-NC	3.85	112.76	107.57
82	HF	201	PEB	C3C-C4C-NC	3.85	111.80	108.33
82	dG	204	PEB	CHA-C1B-NB	-3.85	116.88	124.93
85	H6	101	BCR	C24-C23-C22	-3.85	120.42	126.23
82	II	202	PEB	C1B-C2B-C3B	-3.85	102.09	106.51
82	aF	202	PEB	CHA-C1B-NB	-3.85	116.88	124.93
82	SM	203	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	D7	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	hJ	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	aB	201	PEB	C2A-C1A-NA	3.85	111.59	108.27
82	eE	203	PEB	C2A-C1A-NA	3.85	111.59	108.27
82	eG	203	PEB	C1C-CHB-C4B	-3.85	119.65	128.28
82	DD	203	PEB	C1C-C2C-C3C	-3.85	103.07	107.62
82	v8	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	JH	1001	CYC	CMB-C2B-C1B	3.85	128.97	124.17
82	QG	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	N9	202	PEB	CHA-C4A-NA	-3.85	120.63	125.20
82	LK	201	PEB	OA-C1A-NA	3.85	129.60	124.94
82	VI	202	PEB	C1B-C2B-C3B	-3.85	102.09	106.51
83	BJ	302	PUB	CHA-C1B-NB	3.85	126.36	121.15
82	L5	203	PEB	CHC-C1D-ND	-3.85	108.85	113.72
82	YA	301	PEB	C1D-CHC-C4C	3.85	118.93	113.26
82	gB	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
85	J2	103	BCR	C20-C19-C18	-3.85	115.60	126.42
82	B9	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	W9	203	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	iJ	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
83	AM	303	PUB	CBA-CAA-C3A	-3.85	107.14	112.98
82	GE	1002	PEB	CHC-C4C-NC	3.85	126.36	121.15
82	K7	201	PEB	CHC-C4C-NC	3.85	126.36	121.15
82	KK	201	PEB	C3C-C4C-NC	3.85	111.80	108.33
82	eK	203	PEB	C1B-C2B-C3B	-3.85	102.09	106.51
82	vF	202	PEB	OD-C4D-ND	-3.85	120.23	125.93
82	ND	204	PEB	C1C-C2C-C3C	-3.85	103.07	107.62
82	DA	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	P9	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	V9	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	GM	202	PEB	CHC-C4C-NC	3.85	126.36	121.15
82	c4	202	PEB	CHA-C1B-NB	-3.85	116.88	124.93
82	dH	203	PEB	C2A-C1A-NA	3.85	111.59	108.27
82	TQ	203	PEB	CHB-C1C-NC	-3.85	116.51	125.32
82	VA	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	QD	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	EM	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
82	1C	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
82	UQ	201	PEB	C2C-C1C-NC	3.85	112.75	107.57
82	Y7	301	PEB	C3D-C4D-ND	3.85	114.81	107.26
84	F1	1001	CYC	C2D-C1D-ND	3.85	112.81	107.40
103	82	310	ZEX	C27-C26-C25	3.85	129.07	122.84
82	NK	202	PEB	CMB-C2B-C1B	3.85	130.99	125.06
85	fL	101	BCR	C11-C10-C9	-3.85	121.82	127.31
82	WB	401	PEB	C4B-C3B-C2B	-3.85	102.53	106.78
82	VP	201	PEB	C4B-C3B-C2B	-3.85	102.53	106.78
82	UJ	202	PEB	CMA-C2A-C1A	-3.85	104.11	112.40
82	QM	202	PEB	CHC-C1D-ND	-3.85	108.86	113.72
82	VM	202	PEB	CHC-C1D-ND	-3.85	108.86	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	B6	602	BCR	C20-C21-C22	-3.85	121.82	127.31
82	MA	201	PEB	CHB-C1C-C2C	-3.85	118.47	127.15
82	kM	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
84	DO	1001	CYC	OC-C1C-C2C	-3.85	123.11	126.17
82	gH	202	PEB	C2C-C1C-NC	3.85	112.75	107.57
85	B6	602	BCR	C24-C23-C22	-3.85	120.42	126.23
82	YO	203	PEB	C1C-C2C-C3C	-3.85	103.08	107.62
82	T9	201	PEB	C3D-C4D-ND	3.85	114.80	107.26
84	BG	1001	CYC	CHD-C1D-ND	-3.85	116.51	125.32
82	AD	304	PEB	CHC-C1D-ND	-3.85	108.86	113.72
82	UA	202	PEB	C1B-C2B-C3B	-3.85	102.09	106.51
82	IB	202	PEB	C3D-C4D-ND	3.85	114.80	107.26
82	i4	202	PEB	C3D-C4D-ND	3.85	114.80	107.26
82	jF	202	PEB	C3D-C4D-ND	3.85	114.80	107.26
82	gG	201	PEB	C3D-C4D-ND	3.85	114.80	107.26
82	ZI	401	PEB	C2C-C1C-NC	3.85	112.75	107.57
82	NF	202	PEB	CMB-C2B-C1B	3.84	130.99	125.06
82	m1	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
83	xK	306	PUB	CMA-C2A-C1A	3.84	130.43	121.39
82	I9	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	mO	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	jE	201	PEB	C2C-C1C-NC	3.84	112.75	107.57
82	NF	202	PEB	C3B-C4B-NB	3.84	115.64	110.05
82	HK	201	PEB	C3C-C4C-NC	3.84	111.79	108.33
82	KI	203	PEB	C1B-C2B-C3B	-3.84	102.09	106.51
82	XF	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	MM	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	QQ	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	W5	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
85	a6	605	BCR	C16-C17-C18	-3.84	121.82	127.31
82	BK	202	PEB	CMB-C2B-C1B	3.84	130.98	125.06
82	kF	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	hM	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	l1	202	PEB	C1C-C2C-C3C	-3.84	103.08	107.62
82	hJ	201	PEB	CHC-C1D-ND	-3.84	108.86	113.72
82	x8	202	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
82	rC	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	dG	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	TM	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	l4	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	a4	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	bH	201	PEB	C3D-C4D-ND	3.84	114.80	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aM	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	WI	201	PEB	C2A-C1A-NA	3.84	111.58	108.27
82	NA	202	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
87	5N	608	CLA	C2D-C1D-ND	-3.84	107.27	110.10
82	TM	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	c1	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	X9	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	gE	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
87	3N	309	CLA	C2A-C1A-CHA	3.84	130.58	123.86
82	O1	201	PEB	C2C-C1C-NC	3.84	112.74	107.57
82	eE	201	PEB	C2C-C1C-NC	3.84	112.74	107.57
82	WG	203	PEB	CHB-C1C-C2C	-3.84	118.48	127.15
82	XJ	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
82	JD	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	SF	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
82	Y5	201	PEB	C3B-C4B-NB	3.84	115.64	110.05
82	HP	201	PEB	C2C-C1C-NC	3.84	112.74	107.57
82	PE	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	H5	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	JJ	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
82	YE	201	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
82	WF	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	BM	301	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	Q1	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	NP	202	PEB	CHC-C1D-ND	-3.84	108.87	113.72
82	Y5	201	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	lE	203	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	RF	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	M7	201	PEB	CHB-C1C-C2C	-3.84	118.49	127.15
82	iK	202	PEB	C3B-C4B-NB	3.84	115.63	110.05
82	sK	202	PEB	CMB-C2B-C1B	3.84	130.98	125.06
82	CI	202	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
82	cB	403	PEB	CAC-C2C-C3C	3.84	135.86	127.07
82	RK	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	gB	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	lG	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
83	xF	306	PUB	CMA-C2A-C1A	3.84	130.42	121.39
82	PA	203	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	Q1	201	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	XD	203	PEB	C2A-C1A-NA	3.84	111.58	108.27
82	MJ	201	PEB	C1C-CHB-C4B	3.84	136.89	128.28
82	fH	201	PEB	C2C-C1C-NC	3.84	112.74	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gB	201	PEB	CHC-C4C-NC	3.84	126.34	121.15
82	HF	201	PEB	CHC-C1D-ND	-3.84	108.87	113.72
82	XI	202	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
82	eE	203	PEB	C1C-CHB-C4B	-3.84	119.67	128.28
82	fO	201	PEB	C1C-CHB-C4B	3.84	136.89	128.28
82	FF	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	w8	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	O9	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
84	C1	1001	CYC	C2D-C1D-ND	3.84	112.79	107.40
82	J9	203	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
82	hM	202	PEB	CHC-C4C-NC	3.84	126.34	121.15
84	GO	1001	CYC	C1B-NB-C4B	-3.84	105.78	110.67
82	VF	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	XF	203	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	JP	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	w8	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	L9	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
82	uC	201	PEB	OA-C1A-C2A	-3.84	123.12	126.17
84	L1	1001	CYC	C2D-C1D-ND	3.84	112.79	107.40
85	cL	518	BCR	C15-C14-C13	-3.84	121.83	127.31
82	AE	304	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	MK	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	vC	201	PEB	C2C-C1C-NC	3.84	112.74	107.57
82	QG	201	PEB	C3B-C4B-NB	3.84	115.63	110.05
82	i4	201	PEB	C1D-CHC-C4C	-3.84	107.60	113.26
84	K1	1001	CYC	C2D-C1D-ND	3.84	112.79	107.40
82	YO	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	J9	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
82	jO	201	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
82	GK	201	PEB	CHB-C4B-NB	-3.84	116.59	124.58
82	OJ	203	PEB	CHC-C1D-ND	-3.84	108.87	113.72
83	AJ	304	PUB	CHA-C4A-NA	-3.84	108.87	113.72
82	RO	202	PEB	C3D-C4D-ND	3.84	114.78	107.26
82	PQ	202	PEB	C3D-C4D-ND	3.84	114.78	107.26
82	A4	301	PEB	C3D-C4D-ND	3.84	114.78	107.26
82	wC	202	PEB	C3D-C4D-ND	3.84	114.78	107.26
84	KG	202	CYC	CHB-C4A-NA	-3.84	116.91	124.93
82	W4	201	PEB	C4B-NB-C1B	-3.84	99.28	106.51
84	F1	1001	CYC	C2B-C1B-NB	3.84	112.60	106.99
82	WI	201	PEB	CAB-CBB-CGB	3.84	121.86	113.60
82	cH	202	PEB	CAC-CBC-CGC	-3.84	105.35	113.60
84	K1	1001	CYC	C1D-C2D-C3D	-3.84	102.91	107.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EI	202	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
82	XP	201	PEB	C3D-C4D-ND	3.84	114.78	107.26
82	Y1	202	PEB	C3D-C4D-ND	3.84	114.78	107.26
85	cL	503	BCR	C7-C8-C9	-3.84	120.44	126.23
82	PD	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	AM	302	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	fJ	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	IM	201	PEB	OA-C1A-C2A	-3.83	123.12	126.17
95	C6	502	DGD	O2G-C1B-C2B	3.83	119.77	111.50
82	FQ	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	q8	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	eE	203	PEB	C3D-C4D-ND	3.83	114.78	107.26
91	D6	404	PHO	C1-C2-C3	-3.83	119.41	126.04
82	F5	202	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
82	F7	203	PEB	C2C-C1C-NC	3.83	112.73	107.57
82	BI	203	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	UH	201	PEB	CHB-C1C-C2C	-3.83	118.50	127.15
82	BB	201	PEB	OA-C1A-C2A	-3.83	123.12	126.17
82	B5	202	PEB	OD-C4D-ND	-3.83	120.25	125.93
82	DE	1002	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	BP	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	PJ	201	PEB	C2C-C1C-NC	3.83	112.73	107.57
82	CQ	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
82	LA	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	xK	303	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	cO	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	QE	201	PEB	C3B-C4B-NB	3.83	115.62	110.05
82	PP	202	PEB	CHC-C4C-NC	3.83	126.34	121.15
82	d4	201	PEB	CHB-C4B-C3B	-3.83	116.45	125.32
82	J4	1002	PEB	CAC-CBC-CGC	-3.83	105.36	113.60
82	CD	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
85	AL	401	BCR	C20-C21-C22	-3.83	121.84	127.31
84	HG	1001	CYC	CHB-C4A-NA	-3.83	116.92	124.93
82	YM	201	PEB	C3C-C4C-NC	3.83	111.78	108.33
82	KD	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	VJ	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	RP	201	PEB	CHC-C4C-NC	3.83	126.33	121.15
82	VJ	201	PEB	OD-C4D-ND	-3.83	120.25	125.93
82	RE	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	X7	203	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	WF	201	PEB	CMB-C2B-C1B	3.83	130.96	125.06
82	SK	201	PEB	C1C-C2C-C3C	-3.83	103.09	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aF	203	PEB	C1C-C2C-C3C	-3.83	103.09	107.62
82	TD	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
82	b1	202	PEB	C1C-CHB-C4B	-3.83	119.69	128.28
82	uC	202	PEB	C1C-CHB-C4B	3.83	136.87	128.28
82	QJ	204	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	m1	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
82	qC	203	PEB	C3D-C4D-ND	3.83	114.78	107.26
85	B6	601	BCR	C16-C17-C18	-3.83	121.84	127.31
82	GF	201	PEB	CHB-C4B-NB	-3.83	116.61	124.58
82	RF	202	PEB	CMB-C2B-C1B	3.83	130.96	125.06
82	bH	202	PEB	CHC-C1D-ND	-3.83	108.88	113.72
84	E1	1001	CYC	C2C-C1C-NC	3.83	111.58	108.27
82	HI	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	V4	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	eG	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	HD	201	PEB	C3C-C4C-NC	3.83	111.78	108.33
82	DB	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	CJ	203	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	j4	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	c4	203	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	T9	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	zC	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	N7	202	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
82	A9	202	PEB	CHA-C4A-NA	-3.83	120.65	125.20
82	C9	202	PEB	CHA-C4A-NA	-3.83	120.65	125.20
82	P9	202	PEB	CHA-C4A-NA	-3.83	120.65	125.20
82	QM	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	kJ	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	U9	204	PEB	C2A-C1A-NA	3.83	111.57	108.27
82	BI	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	NP	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	U1	201	PEB	C1C-C2C-C3C	-3.83	103.09	107.62
82	UK	201	PEB	OD-C4D-ND	-3.83	120.26	125.93
82	NI	202	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
82	WD	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
82	wC	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
87	5N	608	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
82	ZF	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
92	D6	407	LMG	O6-C1-C2	-3.83	102.25	110.35
82	i4	201	PEB	CHC-C4C-NC	3.83	126.33	121.15
82	jM	202	PEB	C1D-CHC-C4C	3.83	118.90	113.26
82	XQ	201	PEB	C1B-C2B-C3B	-3.83	102.11	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	d1	202	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
82	U7	202	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
82	kO	201	PEB	CHC-C4C-NC	3.83	126.33	121.15
82	sC	202	PEB	CHA-C1B-NB	-3.83	116.93	124.93
82	eH	201	PEB	C3B-C4B-NB	3.83	115.62	110.05
82	VG	202	PEB	C2A-C1A-NA	3.83	111.57	108.27
82	PA	203	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	L9	202	PEB	CHB-C1C-C2C	-3.83	118.52	127.15
82	MB	201	PEB	CHC-C4C-NC	3.83	126.33	121.15
82	gB	202	PEB	CHA-C1B-NB	-3.83	116.93	124.93
82	FQ	202	PEB	C1C-C2C-C3C	-3.83	103.10	107.62
82	RI	202	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
82	cJ	201	PEB	OA-C1A-C2A	-3.83	123.13	126.17
82	kM	201	PEB	C4B-C3B-C2B	-3.83	102.55	106.78
84	HE	1001	CYC	CHB-C4A-NA	-3.83	116.93	124.93
82	mG	201	PEB	CHC-C4C-NC	3.83	126.33	121.15
82	FD	203	PEB	C3D-C4D-ND	3.83	114.77	107.26
82	WO	201	PEB	C4B-NB-C1B	-3.83	99.30	106.51
82	TA	202	PEB	OD-C4D-ND	-3.83	120.26	125.93
82	e1	201	PEB	C3B-C4B-NB	3.82	115.61	110.05
82	AO	304	PEB	OA-C1A-C2A	-3.82	123.13	126.17
82	bB	201	PEB	OA-C1A-C2A	-3.82	123.13	126.17
82	AO	301	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	KQ	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	d1	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	H7	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	gE	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
84	63	901	CYC	C4D-C3D-C2D	-3.82	103.10	107.62
82	fF	202	PEB	C2C-C1C-NC	3.82	112.72	107.57
82	W4	201	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
82	LJ	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	UH	203	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
83	AD	302	PUB	C1C-C2C-C3C	-3.82	102.55	106.78
82	FK	201	PEB	OD-C4D-ND	-3.82	120.27	125.93
82	RM	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	Q9	203	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	wC	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	SK	202	PEB	CHC-C4C-NC	3.82	126.32	121.15
82	NE	202	PEB	C2C-C1C-NC	3.82	112.72	107.57
82	BF	202	PEB	CMB-C2B-C1B	3.82	130.95	125.06
82	sK	202	PEB	OA-C1A-C2A	-3.82	123.13	126.17
82	WA	201	PEB	C2A-C1A-NA	3.82	111.57	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RP	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	gO	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
84	GE	1001	CYC	C2D-C1D-ND	3.82	112.77	107.40
82	FH	1002	PEB	CHC-C4C-NC	3.82	126.32	121.15
82	u8	202	PEB	C1C-CHB-C4B	3.82	136.85	128.28
82	uC	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	tF	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	AD	304	PEB	OA-C1A-C2A	-3.82	123.13	126.17
82	UK	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	r8	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	U1	202	PEB	CHC-C4C-NC	3.82	126.32	121.15
82	xF	302	PEB	CHB-C1C-NC	-3.82	116.56	125.32
84	DH	1001	CYC	C1B-C2B-C3B	-3.82	103.88	107.87
82	KG	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	XK	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	IM	203	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	m4	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
82	BA	201	PEB	OA-C1A-C2A	-3.82	123.14	126.17
82	PI	202	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
82	TI	203	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
82	AM	301	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	i4	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	D9	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
84	E1	1001	CYC	C4D-C3D-C2D	-3.82	103.11	107.62
83	A1	303	PUB	CHB-C4B-NB	-3.82	116.57	125.32
82	a1	201	PEB	OA-C1A-C2A	-3.82	123.14	126.17
82	DP	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	sK	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	gO	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	XK	202	PEB	C1C-C2C-C3C	-3.82	103.11	107.62
82	NQ	204	PEB	C1C-C2C-C3C	-3.82	103.11	107.62
82	ID	201	PEB	CHC-C1D-ND	-3.82	108.89	113.72
82	KD	201	PEB	CHC-C1D-ND	-3.82	108.89	113.72
82	HP	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
85	C6	508	BCR	C3-C4-C5	-3.82	107.26	114.08
82	NB	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	d1	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	jM	202	PEB	CHB-C1C-NC	-3.82	116.57	125.32
88	C6	505	LHG	O7-C7-C8	3.82	119.73	111.50
82	VK	201	PEB	C2C-C1C-NC	3.82	112.71	107.57
82	A1	302	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	F5	201	PEB	C3D-C4D-ND	3.82	114.75	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CJ	201	PEB	CMB-C2B-C1B	3.82	130.94	125.06
82	TB	202	PEB	C2A-C1A-NA	3.82	111.56	108.27
82	EI	202	PEB	C2A-C1A-NA	3.82	111.56	108.27
82	kH	203	PEB	C2A-C1A-NA	3.82	111.56	108.27
82	UH	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	e1	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	hJ	201	PEB	CHB-C1C-C2C	-3.82	118.54	127.15
84	MG	1001	CYC	CHB-C4A-NA	-3.82	116.95	124.93
82	DG	1002	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	Y4	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	CK	201	PEB	CHC-C1D-ND	-3.82	108.89	113.72
82	NM	202	PEB	CHC-C4C-NC	3.82	126.31	121.15
82	xK	302	PEB	C4B-C3B-C2B	-3.82	102.56	106.78
82	gJ	202	PEB	C1C-CHB-C4B	-3.82	119.72	128.28
82	AH	302	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	FQ	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	lE	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	aO	202	PEB	C3C-C4C-NC	3.82	111.77	108.33
84	H1	1001	CYC	CHB-C1B-NB	-3.82	117.86	126.06
82	PO	201	PEB	CHC-C1D-ND	-3.82	108.90	113.72
82	U1	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
82	OE	203	PEB	C4B-C3B-C2B	-3.82	102.56	106.78
83	BM	302	PUB	C1C-C2C-C3C	-3.82	102.56	106.78
84	I4	1001	CYC	C1B-C2B-C3B	-3.82	103.89	107.87
82	X7	201	PEB	OD-C4D-ND	-3.82	120.28	125.93
82	dO	201	PEB	CHB-C4B-C3B	-3.82	116.49	125.32
82	YH	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
85	c6	603	BCR	C24-C23-C22	-3.82	120.47	126.23
82	ID	202	PEB	C2A-C1A-NA	3.82	111.56	108.27
82	PI	202	PEB	C2A-C1A-NA	3.82	111.56	108.27
82	ID	202	PEB	C1C-C2C-C3C	-3.82	103.11	107.62
84	J4	1001	CYC	C2D-C1D-ND	3.82	112.76	107.40
82	PK	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
82	Q9	202	PEB	C1C-CHB-C4B	3.81	136.84	128.28
82	ZG	201	PEB	C3B-C4B-NB	3.81	115.60	110.05
82	LF	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
85	bL	603	BCR	C28-C27-C26	-3.81	107.27	114.08
82	D7	201	PEB	CMB-C2B-C1B	3.81	130.94	125.06
82	pK	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
82	G7	201	PEB	C1D-CHC-C4C	3.81	118.88	113.26
82	L9	201	PEB	C3B-C4B-NB	3.81	115.60	110.05
82	VP	201	PEB	C3D-C4D-ND	3.81	114.74	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	H7	202	PEB	C1B-C2B-C3B	-3.81	102.13	106.51
82	F7	202	PEB	CAC-C2C-C1C	3.81	131.84	125.76
82	PM	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
82	R4	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
82	cO	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
82	HH	1002	PEB	OD-C4D-ND	-3.81	120.28	125.93
82	J5	201	PEB	CHC-C1D-ND	-3.81	108.90	113.72
82	PP	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
82	U1	201	PEB	CHB-C1C-C2C	-3.81	118.55	127.15
82	PF	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
82	BP	201	PEB	OA-C1A-C2A	-3.81	123.14	126.17
84	J1	1001	CYC	C1B-C2B-C3B	-3.81	103.89	107.87
82	SK	202	PEB	CMA-C2A-C1A	-3.81	104.19	112.40
84	N1	1001	CYC	CHA-C4D-C3D	-3.81	118.55	127.15
82	fF	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
84	BE	1001	CYC	CHD-C1D-ND	-3.81	116.59	125.32
82	VJ	201	PEB	CMB-C2B-C1B	3.81	130.93	125.06
82	FD	202	PEB	C1C-C2C-C3C	-3.81	103.11	107.62
82	j4	203	PEB	C1C-C2C-C3C	-3.81	103.11	107.62
85	fL	101	BCR	C4-C5-C6	-3.81	117.20	122.73
82	HQ	201	PEB	CHA-C1B-NB	-3.81	116.96	124.93
82	AK	202	PEB	C1C-C2C-C3C	-3.81	103.12	107.62
82	cE	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
82	eF	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
84	HE	1001	CYC	C2C-C1C-NC	3.81	111.56	108.27
82	P4	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
82	H1	1002	PEB	OD-C4D-ND	-3.81	120.28	125.93
82	V1	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	F4	1002	PEB	CHC-C4C-NC	3.81	126.31	121.15
82	AI	202	PEB	C1B-C2B-C3B	-3.81	102.13	106.51
82	aK	201	PEB	C1C-C2C-C3C	-3.81	103.12	107.62
84	NE	201	CYC	C4D-C3D-C2D	-3.81	103.12	107.62
82	T1	202	PEB	C1D-CHC-C4C	3.81	118.87	113.26
82	KK	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
83	xK	306	PUB	CHA-C4A-NA	-3.81	108.90	113.72
82	DA	201	PEB	CMB-C2B-C1B	3.81	130.93	125.06
82	kG	201	PEB	CMB-C2B-C1B	3.81	130.93	125.06
82	ND	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
82	AF	201	PEB	OA-C1A-C2A	-3.81	123.14	126.17
82	eF	203	PEB	OA-C1A-C2A	-3.81	123.14	126.17
82	JD	202	PEB	C1B-C2B-C3B	-3.81	102.13	106.51
84	LH	1002	CYC	C2D-C1D-ND	3.81	112.75	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	EH	1001	CYC	C4D-C3D-C2D	-3.81	103.12	107.62
84	H1	1001	CYC	CMA-C3A-C4A	3.81	130.93	125.06
82	BI	201	PEB	CAB-CBB-CGB	3.81	121.80	113.60
82	IB	203	PEB	OD-C4D-ND	-3.81	120.29	125.93
87	52	608	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
82	g4	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	XP	202	PEB	CHC-C4C-NC	3.81	126.30	121.15
84	NE	201	CYC	CHB-C4A-NA	-3.81	116.97	124.93
82	IQ	202	PEB	C1C-C2C-C3C	-3.81	103.12	107.62
82	SB	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	VK	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	UM	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	sF	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	M9	301	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	HB	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
82	GM	201	PEB	OA-C1A-C2A	-3.81	123.14	126.17
83	AD	302	PUB	CHC-C1D-ND	-3.81	108.91	113.72
82	RK	202	PEB	CMB-C2B-C1B	3.81	130.93	125.06
82	Y4	202	PEB	C4B-C3B-C2B	-3.81	102.57	106.78
82	PG	201	PEB	C3B-C4B-NB	3.81	115.59	110.05
82	PB	201	PEB	C1C-C2C-C3C	-3.81	103.12	107.62
82	lH	201	PEB	C1C-C2C-C3C	-3.81	103.12	107.62
82	ZJ	202	PEB	CHC-C1D-ND	-3.81	108.91	113.72
82	KF	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	J5	203	PEB	CMB-C2B-C1B	3.81	130.93	125.06
82	VE	202	PEB	C2A-C1A-NA	3.81	111.56	108.27
82	l1	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
82	b4	201	PEB	OA-C1A-C2A	-3.81	123.15	126.17
82	RH	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	BP	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	I7	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	Q1	202	PEB	C1C-C2C-C3C	-3.81	103.12	107.62
82	FP	201	PEB	CHA-C1B-NB	-3.81	116.97	124.93
82	SF	202	PEB	CHC-C4C-NC	3.81	126.30	121.15
82	aG	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	XM	201	PEB	C2A-C1A-NA	3.81	111.55	108.27
82	q8	202	PEB	C2A-C1A-NA	3.81	111.55	108.27
84	CH	1001	CYC	C2D-C1D-ND	3.81	112.75	107.40
82	JM	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	NM	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
82	MM	201	PEB	OA-C1A-C2A	-3.81	123.15	126.17
82	JK	202	PEB	C3B-C4B-NB	3.81	115.58	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U9	201	PEB	C3B-C4B-NB	3.81	115.58	110.05
84	G4	1001	CYC	C1D-C2D-C3D	-3.81	102.94	107.79
82	hB	301	PEB	C2C-C1C-NC	3.81	112.70	107.57
85	H6	101	BCR	C4-C5-C6	-3.81	117.21	122.73
82	YI	201	PEB	C3D-C4D-ND	3.81	114.72	107.26
82	w8	201	PEB	C3D-C4D-ND	3.81	114.72	107.26
82	HK	201	PEB	CHC-C1D-ND	-3.81	108.91	113.72
82	YP	501	PEB	C4B-C3B-C2B	-3.81	102.57	106.78
82	CD	202	PEB	CHC-C4C-NC	3.81	126.30	121.15
82	GG	1002	PEB	CHC-C4C-NC	3.81	126.30	121.15
82	AF	202	PEB	C1C-C2C-C3C	-3.80	103.12	107.62
82	k1	202	PEB	C1C-C2C-C3C	-3.80	103.12	107.62
82	AP	201	PEB	OD-C4D-ND	-3.80	120.29	125.93
82	RE	201	PEB	CAB-C3B-C4B	3.80	131.74	125.01
96	E6	101	HEM	C4B-C3B-C2B	-3.80	104.09	107.11
92	AL	411	LMG	O7-C10-C11	3.80	119.70	111.50
82	TJ	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	u8	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	eK	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	DK	203	PEB	CHB-C4B-C3B	-3.80	116.52	125.32
82	YA	304	PEB	OA-C1A-C2A	-3.80	123.15	126.17
82	HB	202	PEB	CHC-C1D-ND	-3.80	108.91	113.72
82	XF	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	e4	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	z8	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
85	hL	102	BCR	C28-C27-C26	-3.80	107.28	114.08
82	uF	201	PEB	CHA-C1B-NB	-3.80	116.98	124.93
82	HF	202	PEB	C3B-C4B-NB	3.80	115.58	110.05
82	eF	202	PEB	C3B-C4B-NB	3.80	115.58	110.05
82	QE	201	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	BI	202	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	VD	202	PEB	C2C-C1C-NC	3.80	112.69	107.57
84	FG	1001	CYC	C1B-C2B-C3B	-3.80	103.90	107.87
82	D5	201	PEB	CMB-C2B-C1B	3.80	130.92	125.06
82	lH	202	PEB	C1B-C2B-C3B	-3.80	102.14	106.51
82	oK	201	PEB	C1B-C2B-C3B	-3.80	102.14	106.51
82	NJ	201	PEB	C1D-CHC-C4C	3.80	118.86	113.26
82	SJ	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	H9	202	PEB	C3B-C4B-NB	3.80	115.58	110.05
84	KH	1001	CYC	C2D-C1D-ND	3.80	112.75	107.40
85	J2	102	BCR	C30-C25-C26	-3.80	117.26	122.61
82	SD	202	PEB	C3D-C4D-ND	3.80	114.72	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GI	203	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	HA	202	PEB	C1B-C2B-C3B	-3.80	102.14	106.51
82	TD	203	PEB	CHB-C1C-NC	-3.80	116.61	125.32
82	XA	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	RF	201	PEB	C2C-C1C-NC	3.80	112.69	107.57
82	QJ	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	DF	203	PEB	CHB-C4B-C3B	-3.80	116.52	125.32
82	XK	203	PEB	C3B-C4B-NB	3.80	115.58	110.05
84	H4	1001	CYC	C1B-C2B-C3B	-3.80	103.90	107.87
82	V7	202	PEB	C2A-C1A-NA	3.80	111.55	108.27
84	LH	1002	CYC	C2C-C1C-NC	3.80	111.55	108.27
82	UI	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	c4	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	eE	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	FA	203	PEB	C2C-C1C-NC	3.80	112.69	107.57
82	U9	203	PEB	CHA-C1B-NB	-3.80	116.98	124.93
82	EJ	201	PEB	C3C-C4C-NC	3.80	111.75	108.33
82	FD	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
82	SI	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
87	B2	818	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
82	TE	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
82	k4	201	PEB	CHC-C4C-NC	3.80	126.29	121.15
82	kH	202	PEB	C1D-CHC-C4C	3.80	118.86	113.26
82	bP	502	PEB	CHC-C1D-ND	-3.80	108.92	113.72
82	FA	201	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	QP	202	PEB	C1C-C2C-C3C	-3.80	103.13	107.62
82	b1	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	r8	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	HJ	202	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
82	e4	201	PEB	CHC-C1D-ND	-3.80	108.92	113.72
82	18	201	PEB	CHC-C1D-ND	-3.80	108.92	113.72
87	52	608	CLA	C2D-C1D-ND	-3.80	107.30	110.10
82	dE	204	PEB	CHA-C1B-NB	-3.80	116.98	124.93
82	XF	202	PEB	CMB-C2B-C1B	3.80	130.91	125.06
82	AI	202	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	GQ	201	PEB	OD-C4D-ND	-3.80	120.30	125.93
82	ZM	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	GP	203	PEB	C3D-C4D-ND	3.80	114.71	107.26
84	IO	1001	CYC	C1B-C2B-C3B	-3.80	103.91	107.87
82	18	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
82	Q9	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
82	mK	201	PEB	OA-C1A-C2A	-3.80	123.15	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QG	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
84	IG	1001	CYC	C1D-C2D-C3D	-3.80	102.95	107.79
82	CF	202	PEB	CHC-C4C-NC	3.80	126.29	121.15
82	F1	1002	PEB	CHC-C4C-NC	3.80	126.29	121.15
82	eJ	202	PEB	CHC-C4C-NC	3.80	126.29	121.15
82	WD	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	q8	203	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	U5	201	PEB	C1C-C2C-C3C	-3.80	103.13	107.62
82	AF	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	D1	1002	PEB	C3D-C4D-ND	3.80	114.71	107.26
103	8N	310	ZEX	C27-C26-C25	3.80	128.99	122.84
82	eE	203	PEB	CMB-C2B-C1B	3.80	130.91	125.06
82	JO	1002	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	PO	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
82	YA	304	PEB	CHB-C1C-NC	-3.80	116.62	125.32
82	LP	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	d4	201	PEB	C3B-C4B-NB	3.80	115.57	110.05
84	FH	1001	CYC	C2D-C1D-ND	3.80	112.73	107.40
82	AH	305	PEB	OA-C1A-C2A	-3.80	123.16	126.17
82	JH	1002	PEB	OA-C1A-C2A	-3.80	123.16	126.17
82	XQ	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
82	KQ	201	PEB	C2A-C1A-NA	3.80	111.55	108.27
82	PE	201	PEB	C3B-C4B-NB	3.80	115.57	110.05
82	m4	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
82	fJ	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
82	Q5	201	PEB	C3D-C4D-ND	3.80	114.70	107.26
82	jJ	201	PEB	C3D-C4D-ND	3.80	114.70	107.26
82	MP	201	PEB	CHB-C4B-C3B	-3.79	116.54	125.32
82	fH	201	PEB	CHC-C4C-NC	3.79	126.28	121.15
82	HA	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	RO	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	Q9	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	AK	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
82	YO	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
84	MG	1001	CYC	C2C-C1C-NC	3.79	111.54	108.27
82	OK	202	PEB	C4B-C3B-C2B	-3.79	102.58	106.78
82	mG	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	gM	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	lM	203	PEB	CHC-C4C-NC	3.79	126.28	121.15
82	JD	203	PEB	C1C-CHB-C4B	3.79	136.79	128.28
82	TO	203	PEB	C2C-C1C-NC	3.79	112.68	107.57
82	m4	201	PEB	CMB-C2B-C1B	3.79	130.91	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	L5	201	PEB	CMB-C2B-C1B	3.79	130.91	125.06
82	LB	201	PEB	OD-C4D-ND	-3.79	120.31	125.93
95	lL	101	DGD	C1E-O6E-C5E	3.79	121.13	113.69
82	EA	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
82	S1	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
82	nK	201	PEB	C2C-C1C-NC	3.79	112.68	107.57
82	WM	202	PEB	CMB-C2B-C1B	3.79	130.91	125.06
82	UF	201	PEB	CMB-C2B-C3B	-3.79	115.82	126.12
82	NJ	202	PEB	CAB-C3B-C4B	3.79	131.72	125.01
82	TA	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	SI	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	TQ	201	PEB	C1C-C2C-C3C	-3.79	103.14	107.62
82	L9	202	PEB	C1C-C2C-C3C	-3.79	103.14	107.62
82	XA	201	PEB	C2A-C1A-NA	3.79	111.54	108.27
82	c4	201	PEB	C2A-C1A-NA	3.79	111.54	108.27
82	eG	203	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	OO	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
82	lM	203	PEB	CHA-C1B-NB	-3.79	117.00	124.93
82	mO	202	PEB	CHA-C1B-NB	-3.79	117.00	124.93
82	WH	202	PEB	C1C-CHB-C4B	-3.79	119.78	128.28
82	HM	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
91	d6	404	PHO	C4A-C3A-C2A	-3.79	99.23	102.84
92	XL	601	LMG	O1-C1-C2	3.79	114.22	108.30
82	dK	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	eK	203	PEB	CMB-C2B-C1B	3.79	130.90	125.06
82	gB	201	PEB	C2A-C1A-NA	3.79	111.54	108.27
82	TO	202	PEB	CHA-C1B-NB	-3.79	117.00	124.93
84	MG	1001	CYC	C2D-C1D-ND	3.79	112.73	107.40
82	dM	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
82	cK	202	PEB	C1C-C2C-C3C	-3.79	103.14	107.62
84	BE	1002	CYC	CBB-CAB-C3B	-3.79	101.98	112.43
82	YO	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	O9	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
82	S5	203	PEB	CMB-C2B-C1B	3.79	130.90	125.06
82	LI	202	PEB	CHC-C4C-NC	3.79	126.28	121.15
85	JN	102	BCR	C30-C25-C26	-3.79	117.28	122.61
87	ON	203	CLA	C3B-C4B-NB	-3.79	107.00	110.52
82	kH	202	PEB	C1C-C2C-C3C	-3.79	103.14	107.62
82	RO	202	PEB	CMB-C2B-C1B	3.79	130.90	125.06
82	SQ	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	T4	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
82	sF	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FA	202	PEB	CAC-C2C-C1C	3.79	131.80	125.76
82	cO	203	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	WP	202	PEB	C3B-C4B-NB	3.79	115.56	110.05
82	ZK	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	OM	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	Y7	301	PEB	C1D-CHC-C4C	3.79	118.84	113.26
84	FE	1002	CYC	C1B-C2B-C3B	-3.79	103.92	107.87
82	N4	1002	PEB	CHC-C4C-NC	3.79	126.28	121.15
82	mE	201	PEB	CHC-C4C-NC	3.79	126.28	121.15
82	O5	203	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	mF	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	RJ	202	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
82	v8	201	PEB	C2C-C1C-NC	3.79	112.67	107.57
82	P4	201	PEB	CHC-C1D-ND	-3.79	108.93	113.72
83	xF	306	PUB	CHA-C4A-NA	-3.79	108.93	113.72
84	E1	1001	CYC	C4D-CHA-C1A	3.79	136.78	128.28
82	T4	203	PEB	CAB-C3B-C4B	3.79	131.71	125.01
82	WH	203	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	XJ	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	cE	201	PEB	CHC-C4C-NC	3.79	126.28	121.15
82	AH	301	PEB	CHA-C1B-NB	-3.79	117.01	124.93
82	JQ	203	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
82	MF	203	PEB	C1B-C2B-C3B	-3.79	102.16	106.51
87	4N	609	CLA	CAA-C2A-C3A	-3.79	107.26	116.10
82	SF	202	PEB	CMA-C2A-C1A	-3.79	104.24	112.40
82	DI	202	PEB	CMB-C2B-C1B	3.79	130.90	125.06
84	HH	1001	CYC	C2B-C1B-NB	3.79	112.53	106.99
82	IB	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	GI	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	UM	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	iE	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	LM	202	PEB	CAB-C3B-C4B	3.79	131.71	125.01
82	uF	201	PEB	C2A-C1A-NA	3.79	111.54	108.27
84	73	1002	CYC	C2C-C1C-NC	3.79	111.54	108.27
82	OD	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
87	B2	815	CLA	O2D-CGD-O1D	-3.79	116.44	123.84
82	QE	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	TP	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	m1	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	rC	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	iM	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
82	QG	201	PEB	C3C-C4C-NC	3.79	111.74	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LM	202	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
82	U9	204	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
82	eJ	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
82	eF	203	PEB	CMB-C2B-C1B	3.79	130.89	125.06
82	TP	202	PEB	CHC-C4C-NC	3.79	126.27	121.15
82	Z9	304	PEB	C2A-C1A-NA	3.79	111.54	108.27
87	BN	816	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
82	nF	201	PEB	C2C-C1C-NC	3.78	112.67	107.57
82	PM	201	PEB	C1C-C2C-C3C	-3.78	103.15	107.62
87	BN	824	CLA	CMB-C2B-C1B	-3.78	119.61	125.37
82	NM	201	PEB	CMB-C2B-C1B	3.78	130.89	125.06
82	JF	202	PEB	C3B-C4B-NB	3.78	115.55	110.05
82	QP	203	PEB	OA-C1A-C2A	-3.78	123.16	126.17
82	jJ	201	PEB	OA-C1A-C2A	-3.78	123.16	126.17
82	PF	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	DJ	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	dG	204	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	dJ	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	xF	302	PEB	C4B-C3B-C2B	-3.78	102.59	106.78
82	AE	304	PEB	C1D-CHC-C4C	-3.78	107.68	113.26
82	VI	203	PEB	C1C-NC-C4C	-3.78	102.86	109.60
82	XM	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	S4	201	PEB	C1C-CHB-C4B	3.78	136.77	128.28
82	R7	203	PEB	CAC-C2C-C1C	3.78	131.79	125.76
82	OF	202	PEB	C4B-C3B-C2B	-3.78	102.59	106.78
82	kM	202	PEB	C4B-C3B-C2B	-3.78	102.59	106.78
82	F7	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	SE	202	PEB	C3C-C4C-NC	3.78	111.74	108.33
82	j1	203	PEB	C1C-C2C-C3C	-3.78	103.15	107.62
82	eF	203	PEB	C1C-C2C-C3C	-3.78	103.15	107.62
82	fJ	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	WO	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
82	pK	202	PEB	OD-C4D-ND	-3.78	120.33	125.93
82	XF	201	PEB	C2C-C1C-NC	3.78	112.67	107.57
82	JJ	202	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
82	RG	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	W1	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	dK	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	Y7	304	PEB	CHB-C1C-NC	-3.78	116.66	125.32
82	RG	201	PEB	CAB-C3B-C4B	3.78	131.70	125.01
82	KJ	203	PEB	C1B-C2B-C3B	-3.78	102.17	106.51
82	YP	503	PEB	C3D-C4D-ND	3.78	114.68	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mE	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	A1	301	PEB	CHA-C1B-NB	-3.78	117.02	124.93
82	JO	1002	PEB	C2C-C1C-NC	3.78	112.66	107.57
82	mM	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
87	A2	809	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
82	XA	201	PEB	OD-C4D-ND	-3.78	120.33	125.93
82	tF	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
82	VH	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
82	U5	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
84	ME	1001	CYC	CHB-C4A-NA	-3.78	117.03	124.93
82	xC	202	PEB	CHC-C1D-ND	-3.78	108.94	113.72
82	QD	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	hE	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	NG	201	PEB	C2C-C1C-NC	3.78	112.66	107.57
82	F5	203	PEB	C3D-C4D-ND	3.78	114.67	107.26
85	AN	846	BCR	C28-C27-C26	-3.78	107.33	114.08
84	GO	1001	CYC	C1D-C2D-C3D	-3.78	102.98	107.79
82	OD	201	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
82	NQ	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	J9	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
87	L2	206	CLA	CMB-C2B-C1B	-3.78	119.61	125.37
82	WM	203	PEB	C3C-C4C-NC	3.78	111.73	108.33
85	cL	503	BCR	C3-C4-C5	-3.78	107.33	114.08
82	cB	403	PEB	CHC-C1D-ND	-3.78	108.94	113.72
82	B9	201	PEB	C3B-C4B-NB	3.78	115.55	110.05
82	iO	201	PEB	C1D-CHC-C4C	-3.78	107.69	113.26
82	CD	202	PEB	C2A-C1A-NA	3.78	111.53	108.27
82	YE	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
82	QM	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
82	HI	202	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
85	FL	101	BCR	C20-C19-C18	3.78	137.03	126.42
82	rC	202	PEB	C2C-C1C-NC	3.78	112.66	107.57
82	j4	201	PEB	CMB-C2B-C1B	3.78	130.88	125.06
82	BB	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	VE	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	PO	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	W5	201	PEB	C1B-C2B-C3B	-3.78	102.17	106.51
82	X7	202	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
82	W4	201	PEB	CHA-C1B-NB	-3.78	117.03	124.93
82	AM	302	PEB	OA-C1A-C2A	-3.78	123.17	126.17
82	c4	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
82	SO	201	PEB	C1C-CHB-C4B	3.78	136.75	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WK	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	a1	201	PEB	CMB-C2B-C1B	3.78	130.88	125.06
82	mO	202	PEB	CMB-C2B-C1B	3.78	130.88	125.06
84	JO	1001	CYC	C2D-C1D-ND	3.78	112.71	107.40
92	j6	102	LMG	O7-C10-C11	3.78	119.64	111.50
85	c6	617	BCR	C37-C22-C21	-3.78	117.63	122.92
82	IB	201	PEB	CHC-C4C-NC	3.78	126.26	121.15
82	AM	301	PEB	CHC-C4C-NC	3.78	126.26	121.15
82	FO	1002	PEB	CHC-C4C-NC	3.78	126.26	121.15
82	M9	305	PEB	C2A-C1A-NA	3.78	111.53	108.27
84	K4	1001	CYC	C2C-C1C-NC	3.78	111.53	108.27
82	PQ	203	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	F9	203	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	aF	201	PEB	C1C-C2C-C3C	-3.78	103.16	107.62
82	kK	202	PEB	C1C-C2C-C3C	-3.78	103.16	107.62
82	SM	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	PP	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
82	tC	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
84	BE	1002	CYC	CAD-CBD-CGD	-3.78	105.48	113.60
82	TB	202	PEB	CHA-C1B-NB	-3.78	117.04	124.93
82	U5	202	PEB	C3D-C4D-ND	3.77	114.67	107.26
82	jH	203	PEB	C3D-C4D-ND	3.77	114.67	107.26
82	NB	201	PEB	C2A-C1A-NA	3.77	111.53	108.27
82	Y9	203	PEB	C2A-C1A-NA	3.77	111.53	108.27
84	N1	1001	CYC	C2D-C1D-ND	3.77	112.70	107.40
82	VF	201	PEB	C2C-C1C-NC	3.77	112.65	107.57
82	hE	203	PEB	OA-C1A-C2A	-3.77	123.17	126.17
84	BG	1002	CYC	CAD-CBD-CGD	-3.77	105.48	113.60
82	dF	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	iG	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	OH	203	PEB	C1C-CHB-C4B	3.77	136.75	128.28
82	JQ	203	PEB	C1C-CHB-C4B	3.77	136.75	128.28
82	AD	303	PEB	CHA-C1B-NB	-3.77	117.04	124.93
82	XK	202	PEB	CMB-C2B-C1B	3.77	130.88	125.06
82	aH	201	PEB	CMB-C2B-C1B	3.77	130.88	125.06
82	ZE	201	PEB	C3B-C4B-NB	3.77	115.54	110.05
82	SA	202	PEB	OD-C4D-ND	-3.77	120.34	125.93
84	BG	1002	CYC	CBB-CAB-C3B	-3.77	102.03	112.43
84	JH	1001	CYC	C1B-C2B-C3B	-3.77	103.93	107.87
82	mH	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
85	A2	846	BCR	C28-C27-C26	-3.77	107.34	114.08
82	cO	201	PEB	C2A-C1A-NA	3.77	111.53	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	EO	1001	CYC	C2C-C1C-NC	3.77	111.53	108.27
82	HK	202	PEB	C3B-C4B-NB	3.77	115.54	110.05
82	W1	202	PEB	C1C-CHB-C4B	-3.77	119.82	128.28
82	EJ	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
82	HB	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	vK	202	PEB	OD-C4D-ND	-3.77	120.34	125.93
82	cK	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
82	YI	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	GM	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	f1	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	T7	202	PEB	C1B-C2B-C3B	-3.77	102.18	106.51
84	D4	1001	CYC	OC-C1C-C2C	-3.77	123.17	126.17
82	QM	203	PEB	CHA-C1B-NB	-3.77	117.04	124.93
82	QE	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	jM	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
84	EH	1001	CYC	C4D-CHA-C1A	3.77	136.74	128.28
82	T7	203	PEB	C3B-C4B-NB	3.77	115.53	110.05
92	J6	102	LMG	O8-C28-C29	3.77	123.74	111.91
83	AQ	302	PUB	CHC-C1D-ND	-3.77	108.95	113.72
82	GI	203	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	UJ	203	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	CQ	202	PEB	CHC-C4C-NC	3.77	126.25	121.15
82	MJ	203	PEB	C3C-C4C-NC	3.77	111.73	108.33
82	IJ	201	PEB	C1C-CHB-C4B	3.77	136.74	128.28
82	dJ	201	PEB	C1C-CHB-C4B	3.77	136.74	128.28
87	AN	809	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
82	TQ	203	PEB	OA-C1A-C2A	-3.77	123.17	126.17
82	G7	202	PEB	OA-C1A-C2A	-3.77	123.17	126.17
82	PE	202	PEB	CHC-C4C-NC	3.77	126.25	121.15
82	dG	202	PEB	C1C-C2C-C3C	-3.77	103.16	107.62
82	dO	201	PEB	C3B-C4B-NB	3.77	115.53	110.05
84	MG	1001	CYC	C1B-C2B-C3B	-3.77	103.94	107.87
82	QM	202	PEB	C1C-CHB-C4B	3.77	136.74	128.28
85	AL	401	BCR	C7-C8-C9	-3.77	120.54	126.23
82	NI	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	MJ	203	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	a1	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
82	DK	201	PEB	OA-C1A-NA	3.77	129.51	124.94
82	UK	201	PEB	CMB-C2B-C3B	-3.77	115.89	126.12
82	FI	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
84	HG	1001	CYC	C2C-C1C-NC	3.77	111.52	108.27
82	GA	201	PEB	C1D-CHC-C4C	3.77	118.81	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XI	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	aB	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	hG	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	lJ	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	jG	201	PEB	C2C-C1C-NC	3.77	112.65	107.57
82	VA	202	PEB	C1B-C2B-C3B	-3.77	102.18	106.51
82	IB	203	PEB	CHA-C1B-NB	-3.77	117.05	124.93
87	6N	610	CLA	CAA-C2A-C3A	-3.77	104.84	114.26
82	D9	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	BD	201	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
82	J5	202	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
82	QK	203	PEB	C1C-C2C-C3C	-3.77	103.17	107.62
87	42	609	CLA	CAA-C2A-C3A	-3.77	107.31	116.10
84	DO	1001	CYC	C1B-NB-C4B	-3.77	105.87	110.67
82	BP	202	PEB	CMB-C2B-C1B	3.77	130.87	125.06
85	FN	204	BCR	C16-C17-C18	-3.77	121.93	127.31
82	fH	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	WI	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	sK	203	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	QH	202	PEB	C1C-C2C-C3C	-3.77	103.17	107.62
82	GD	201	PEB	OA-C1A-C2A	-3.77	123.18	126.17
82	JM	202	PEB	CHC-C4C-NC	3.77	126.25	121.15
82	iO	201	PEB	CHC-C4C-NC	3.77	126.25	121.15
82	LD	202	PEB	CHA-C1B-C2B	3.77	134.59	124.90
82	W1	203	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	RI	202	PEB	C2A-C1A-NA	3.77	111.52	108.27
82	bP	502	PEB	C2A-C1A-NA	3.77	111.52	108.27
85	BL	617	BCR	C3-C4-C5	-3.77	107.35	114.08
82	XA	202	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
82	PK	201	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
82	UM	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
82	F5	201	PEB	C1C-C2C-C3C	-3.77	103.17	107.62
82	WH	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
82	jJ	203	PEB	CHB-C1C-C2C	-3.77	118.65	127.15
82	XP	201	PEB	CHC-C1D-ND	-3.77	108.96	113.72
84	M1	201	CYC	CMD-C2D-C1D	3.77	131.07	125.56
82	JB	202	PEB	C2A-C1A-NA	3.77	111.52	108.27
82	NI	202	PEB	C2A-C1A-NA	3.77	111.52	108.27
82	L5	203	PEB	C2A-C1A-NA	3.77	111.52	108.27
82	jM	203	PEB	C2A-C1A-NA	3.77	111.52	108.27
82	RI	202	PEB	C3D-C4D-ND	3.76	114.65	107.26
82	B5	203	PEB	C3D-C4D-ND	3.76	114.65	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	819	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
82	v8	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
82	TA	203	PEB	C3B-C4B-NB	3.76	115.53	110.05
82	FP	201	PEB	CHC-C4C-NC	3.76	126.24	121.15
82	J4	1002	PEB	C2C-C1C-NC	3.76	112.64	107.57
82	BP	201	PEB	C1C-C2C-C3C	-3.76	103.17	107.62
82	O9	202	PEB	CMA-C2A-C1A	-3.76	104.29	112.40
84	JH	1003	CYC	C2B-C1B-NB	3.76	112.50	106.99
82	aJ	201	PEB	CHA-C1B-NB	-3.76	117.06	124.93
82	VA	202	PEB	C2A-C1A-NA	3.76	111.52	108.27
82	IQ	202	PEB	C2A-C1A-NA	3.76	111.52	108.27
82	WH	201	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	R9	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	aM	204	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	KM	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	OQ	201	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	H5	201	PEB	C1C-CHB-C4B	3.76	136.72	128.28
82	r8	202	PEB	C2C-C1C-NC	3.76	112.64	107.57
82	mG	203	PEB	C3D-C4D-ND	3.76	114.64	107.26
82	R4	202	PEB	CMB-C2B-C1B	3.76	130.86	125.06
82	JD	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	GK	201	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	XF	201	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	ZK	201	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	DD	201	PEB	C3B-C4B-NB	3.76	115.52	110.05
82	SB	202	PEB	CHC-C1D-ND	-3.76	108.97	113.72
82	W1	203	PEB	C1C-C2C-C3C	-3.76	103.17	107.62
82	cK	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
82	P4	201	PEB	C2A-C1A-NA	3.76	111.52	108.27
82	O5	201	PEB	C2A-C1A-NA	3.76	111.52	108.27
82	QF	201	PEB	CHB-C4B-C3B	-3.76	116.62	125.32
82	eF	203	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
82	u8	201	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	T7	202	PEB	C3D-C4D-ND	3.76	114.64	107.26
83	AJ	303	PUB	CHA-C1B-NB	3.76	126.24	121.15
83	BJ	302	PUB	C1C-C2C-C3C	-3.76	102.62	106.78
82	PD	203	PEB	C3D-C4D-ND	3.76	114.64	107.26
82	D5	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
84	KG	202	CYC	OB-C4B-C3B	-3.76	123.96	128.04
92	j6	101	LMG	O8-C28-C29	3.76	123.71	111.91
82	PH	201	PEB	CMB-C2B-C1B	3.76	130.85	125.06
82	TQ	203	PEB	OD-C4D-ND	-3.76	120.36	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DF	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
87	F2	205	CLA	C2C-C1C-NC	3.76	113.49	109.97
82	JB	202	PEB	CHA-C1B-NB	-3.76	117.07	124.93
82	1C	201	PEB	CHC-C4C-NC	3.76	126.24	121.15
82	cG	201	PEB	CHC-C4C-NC	3.76	126.24	121.15
82	t8	201	PEB	OA-C1A-C2A	-3.76	123.18	126.17
82	AG	304	PEB	C1D-CHC-C4C	-3.76	107.71	113.26
87	LN	206	CLA	CMB-C2B-C1B	-3.76	119.64	125.37
82	LA	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	LK	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
85	cL	504	BCR	C19-C18-C17	3.76	124.71	118.94
82	WO	201	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
82	PF	202	PEB	C2A-C1A-NA	3.76	111.51	108.27
82	WF	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	T9	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
82	cK	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
82	OH	202	PEB	CHC-C4C-NC	3.76	126.23	121.15
82	eO	201	PEB	CHC-C1D-ND	-3.76	108.97	113.72
82	IK	203	PEB	C3C-C4C-NC	3.76	111.72	108.33
82	LK	201	PEB	CHA-C1B-NB	-3.76	117.07	124.93
82	TG	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	L7	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	NM	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
82	lF	202	PEB	C2A-C1A-NA	3.76	111.51	108.27
82	WK	201	PEB	CMB-C2B-C1B	3.76	130.85	125.06
82	MM	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	gF	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	GA	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
82	A9	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
82	rF	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
82	DJ	201	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	RO	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	R4	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
82	VI	202	PEB	C2A-C1A-NA	3.76	111.51	108.27
82	qC	202	PEB	C2A-C1A-NA	3.76	111.51	108.27
82	mE	202	PEB	C2A-C1A-NA	3.76	111.51	108.27
84	I1	1001	CYC	C2C-C1C-NC	3.76	111.51	108.27
82	OM	203	PEB	CHA-C1B-NB	-3.76	117.08	124.93
82	YM	203	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	WM	202	PEB	CAC-C2C-C1C	3.76	131.74	125.76
82	KF	202	PEB	CHA-C1B-C2B	3.76	134.56	124.90
87	62	311	CLA	CAA-C2A-C3A	-3.76	104.88	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cF	203	PEB	C4B-C3B-C2B	-3.76	102.63	106.78
82	XD	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	bP	501	PEB	C3D-C4D-ND	3.76	114.63	107.26
82	k1	202	PEB	C1D-CHC-C4C	3.76	118.79	113.26
82	AQ	303	PEB	CHA-C1B-NB	-3.76	117.08	124.93
82	eF	203	PEB	CHA-C1B-NB	-3.76	117.08	124.93
82	f1	201	PEB	CHC-C4C-NC	3.75	126.23	121.15
82	PO	201	PEB	CHA-C1B-NB	-3.75	117.08	124.93
82	eK	203	PEB	CHA-C1B-NB	-3.75	117.08	124.93
83	yF	302	PUB	C1C-C2C-C3C	-3.75	102.63	106.78
84	M1	201	CYC	C2B-C1B-NB	3.75	112.48	106.99
82	vC	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	mF	201	PEB	OA-C1A-C2A	-3.75	123.19	126.17
85	cL	518	BCR	C3-C4-C5	-3.75	107.37	114.08
82	OG	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	J7	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	HD	201	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
82	kM	201	PEB	C1C-C2C-C3C	-3.75	103.18	107.62
82	S7	202	PEB	CHC-C4C-NC	3.75	126.23	121.15
82	FM	202	PEB	CMB-C2B-C1B	3.75	130.84	125.06
92	ML	101	LMG	C8-O7-C10	-3.75	108.55	117.79
82	B9	201	PEB	CAA-C3A-C4A	-3.75	103.04	112.67
82	iG	202	PEB	CHC-C1D-ND	-3.75	108.98	113.72
85	AL	401	BCR	C11-C10-C9	-3.75	121.95	127.31
82	TI	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	IP	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	S5	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	U5	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	t8	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	aH	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	V7	202	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
84	DE	1001	CYC	C4A-C3A-C2A	-3.75	102.20	106.51
82	XM	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
82	DH	1002	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	xC	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	kG	201	PEB	C2C-C1C-NC	3.75	112.62	107.57
82	O5	201	PEB	C3B-C4B-NB	3.75	115.51	110.05
82	L9	202	PEB	C1C-CHB-C4B	3.75	136.70	128.28
82	AI	203	PEB	OD-C4D-C3D	-3.75	120.96	129.46
82	LQ	202	PEB	CHA-C1B-C2B	3.75	134.55	124.90
82	jJ	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
82	AP	201	PEB	C3B-C4B-NB	3.75	115.51	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	R4	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	U4	202	PEB	CHC-C4C-NC	3.75	126.23	121.15
82	gM	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
82	DI	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	cG	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	RH	201	PEB	C3B-C4B-NB	3.75	115.50	110.05
82	PO	202	PEB	C1C-C2C-C3C	-3.75	103.19	107.62
82	ZF	201	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
82	U1	203	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
82	TM	202	PEB	CHC-C1D-ND	-3.75	108.98	113.72
82	GM	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	QM	204	PEB	C3D-C4D-ND	3.75	114.62	107.26
82	y8	203	PEB	C1D-CHC-C4C	3.75	118.78	113.26
82	tK	203	PEB	CHA-C1B-NB	-3.75	117.09	124.93
82	B9	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	dE	204	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	jF	202	PEB	C1C-CHB-C4B	3.75	136.69	128.28
82	E9	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	XK	201	PEB	C2C-C1C-NC	3.75	112.62	107.57
82	EP	203	PEB	C1C-C2C-C3C	-3.75	103.19	107.62
82	KE	201	PEB	C2A-C1A-NA	3.75	111.50	108.27
82	PG	202	PEB	CHC-C4C-NC	3.75	126.22	121.15
82	sC	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	jK	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	OJ	203	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
82	kF	202	PEB	C1C-C2C-C3C	-3.75	103.19	107.62
82	QB	201	PEB	CHC-C1D-ND	-3.75	108.98	113.72
82	AK	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	c4	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	L5	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	iE	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	KA	201	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
82	WF	203	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
82	PP	201	PEB	C3B-C4B-NB	3.75	115.50	110.05
82	XI	202	PEB	C2A-C1A-NA	3.75	111.50	108.27
82	V7	201	PEB	C2A-C1A-NA	3.75	111.50	108.27
84	GO	1001	CYC	C2C-C1C-NC	3.75	111.50	108.27
82	KM	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	DD	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	IP	202	PEB	CHB-C1C-C2C	-3.75	118.69	127.15
82	rF	201	PEB	OD-C4D-ND	-3.75	120.38	125.93
82	wK	301	PEB	OD-C4D-ND	-3.75	120.38	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LA	202	PEB	C3C-C4C-NC	3.75	111.71	108.33
82	QE	202	PEB	CHC-C1D-ND	-3.75	108.98	113.72
83	AH	303	PUB	CHB-C4B-NB	-3.75	116.74	125.32
82	WB	402	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	AH	305	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	KJ	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	gK	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	RA	203	PEB	CAC-C2C-C1C	3.75	131.73	125.76
82	GJ	201	PEB	OD-C4D-ND	-3.75	120.38	125.93
82	GM	201	PEB	CHC-C4C-NC	3.75	126.22	121.15
82	K9	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	V9	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	tC	201	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	Z4	201	PEB	C1B-C2B-C3B	-3.75	102.21	106.51
82	VG	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	R1	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	x8	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	dE	202	PEB	C1C-C2C-C3C	-3.75	103.19	107.62
84	KG	202	CYC	C4D-C3D-C2D	-3.75	103.19	107.62
82	NK	202	PEB	C3B-C4B-NB	3.75	115.50	110.05
82	HA	201	PEB	OD-C4D-ND	-3.75	120.38	125.93
82	RA	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	ZK	201	PEB	CHC-C4C-NC	3.75	126.22	121.15
85	F2	204	BCR	C16-C17-C18	-3.75	121.96	127.31
87	FN	205	CLA	C2C-C1C-NC	3.75	113.48	109.97
82	XQ	201	PEB	C2A-C1A-NA	3.75	111.50	108.27
82	GA	201	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	W9	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	lO	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
82	XF	203	PEB	C3B-C4B-NB	3.75	115.50	110.05
82	DB	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	OE	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
82	jK	201	PEB	C1C-C2C-C3C	-3.74	103.19	107.62
84	IE	1001	CYC	C2B-C1B-NB	3.74	112.47	106.99
82	OG	203	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
82	H5	201	PEB	CHB-C1C-C2C	-3.74	118.70	127.15
82	GB	201	PEB	C3D-C4D-ND	3.74	114.61	107.26
82	MP	202	PEB	C3D-C4D-ND	3.74	114.61	107.26
82	mK	202	PEB	C3D-C4D-ND	3.74	114.61	107.26
82	Z1	201	PEB	CHC-C4C-NC	3.74	126.22	121.15
82	SD	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	jH	201	PEB	C3D-C4D-ND	3.74	114.60	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QK	201	PEB	CHB-C4B-C3B	-3.74	116.66	125.32
82	YG	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
82	lG	201	PEB	CHB-C1C-C2C	-3.74	118.70	127.15
82	GP	202	PEB	C3B-C4B-NB	3.74	115.49	110.05
82	XB	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	QQ	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	kJ	201	PEB	C2C-C1C-NC	3.74	112.61	107.57
82	mE	203	PEB	C2A-C1A-NA	3.74	111.50	108.27
82	OH	202	PEB	CHA-C1B-NB	-3.74	117.11	124.93
87	B2	823	CLA	CMB-C2B-C1B	-3.74	119.67	125.37
82	x8	202	PEB	CHC-C1D-ND	-3.74	108.99	113.72
82	LF	201	PEB	CHA-C1B-NB	-3.74	117.11	124.93
82	CI	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	VI	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	S7	202	PEB	OD-C4D-ND	-3.74	120.39	125.93
84	IG	1001	CYC	C2B-C1B-NB	3.74	112.47	106.99
82	BD	203	PEB	C3B-C4B-NB	3.74	115.49	110.05
82	PI	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	EP	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	mE	203	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	U5	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
82	lJ	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
82	pF	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
82	KJ	201	PEB	OD-C4D-ND	-3.74	120.39	125.93
82	CF	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	VG	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	SQ	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	R7	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
83	M5	302	PUB	CMB-C2B-C1B	-3.74	123.10	127.06
82	fO	201	PEB	CHB-C4B-C3B	-3.74	116.67	125.32
85	BN	842	BCR	C20-C21-C22	-3.74	121.97	127.31
82	kE	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	Z9	303	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	TD	201	PEB	C1C-C2C-C3C	-3.74	103.20	107.62
82	TD	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
85	Z6	101	BCR	C29-C30-C25	3.74	116.24	110.48
82	PA	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	EI	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	II	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	P7	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
82	H7	201	PEB	OD-C4D-ND	-3.74	120.39	125.93
82	O4	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	G9	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
87	AN	834	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
82	L9	203	PEB	C2A-C1A-NA	3.74	111.50	108.27
82	P4	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
87	BL	622	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
82	RB	201	PEB	CAB-C3B-C4B	3.74	131.62	125.01
82	RJ	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
82	GK	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
82	fB	301	PEB	C2C-C1C-NC	3.74	112.61	107.57
82	rF	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
82	GQ	201	PEB	OA-C1A-C2A	-3.74	123.20	126.17
82	CK	202	PEB	CHC-C4C-NC	3.74	126.21	121.15
82	OJ	203	PEB	CHA-C1B-NB	-3.74	117.11	124.93
88	d6	407	LHG	O7-C7-C8	3.74	119.56	111.50
82	X7	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
84	NO	1001	CYC	C2D-C1D-ND	3.74	112.65	107.40
82	S9	201	PEB	OD-C4D-ND	-3.74	120.39	125.93
82	AI	202	PEB	C3D-C4D-ND	3.74	114.59	107.26
82	FD	203	PEB	C1C-C2C-C3C	-3.74	103.20	107.62
84	KO	1001	CYC	C1B-C2B-C3B	-3.74	103.97	107.87
82	LQ	201	PEB	C1C-CHB-C4B	3.74	136.66	128.28
82	zF	501	PEB	CHC-C4C-NC	3.74	126.21	121.15
82	oF	201	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
84	ME	1001	CYC	C1B-NB-C4B	-3.74	105.91	110.67
82	WK	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
82	B9	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
82	MB	201	PEB	OD-C4D-ND	-3.74	120.39	125.93
82	ND	203	PEB	C3D-C4D-ND	3.74	114.59	107.26
82	CI	202	PEB	C2A-C1A-NA	3.74	111.49	108.27
82	S4	202	PEB	CHC-C4C-NC	3.74	126.21	121.15
82	WP	201	PEB	C2C-C1C-NC	3.74	112.60	107.57
84	W3	1001	CYC	CAD-C3D-C4D	3.74	131.71	125.76
82	CB	202	PEB	CAB-CBB-CGB	-3.74	105.56	113.60
82	BQ	201	PEB	C4B-C3B-C2B	-3.74	102.65	106.78
82	KK	202	PEB	CHA-C1B-C2B	3.74	134.51	124.90
82	MJ	203	PEB	CMD-C2D-C3D	-3.74	124.80	130.06
82	t8	202	PEB	C3D-C4D-ND	3.74	114.59	107.26
92	dL	407	LMG	C4-C3-C2	3.74	117.34	110.82
82	D1	1002	PEB	OA-C1A-C2A	-3.74	123.20	126.17
82	W1	201	PEB	OA-C1A-C2A	-3.74	123.20	126.17
82	eA	301	PEB	OA-C1A-C2A	-3.74	123.20	126.17
82	jJ	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QE	201	PEB	C3C-C4C-NC	3.74	111.69	108.33
82	MM	203	PEB	C2A-C1A-NA	3.74	111.49	108.27
82	l4	202	PEB	C2A-C1A-NA	3.74	111.49	108.27
82	mG	202	PEB	C2A-C1A-NA	3.74	111.49	108.27
82	mO	201	PEB	CMB-C2B-C1B	3.74	130.82	125.06
82	f4	201	PEB	CHB-C4B-C3B	-3.74	116.68	125.32
85	bL	602	BCR	C34-C9-C8	3.74	123.96	118.08
82	FQ	203	PEB	C1C-C2C-C3C	-3.73	103.21	107.62
82	K7	201	PEB	C4B-C3B-C2B	-3.73	102.65	106.78
82	dH	202	PEB	C1B-C2B-C3B	-3.73	102.22	106.51
82	s8	203	PEB	C3D-C4D-ND	3.73	114.59	107.26
82	iK	202	PEB	C3D-C4D-ND	3.73	114.59	107.26
82	DG	1002	PEB	CAB-C3B-C4B	3.73	131.62	125.01
85	fL	101	BCR	C20-C19-C18	3.73	136.91	126.42
82	AK	202	PEB	OA-C1A-C2A	-3.73	123.20	126.17
82	N9	202	PEB	OA-C1A-C2A	-3.73	123.20	126.17
82	KI	203	PEB	C2A-C1A-NA	3.73	111.49	108.27
82	TM	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
84	L1	1001	CYC	C2C-C1C-NC	3.73	111.49	108.27
82	VP	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	j1	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
85	h6	102	BCR	C24-C23-C22	-3.73	120.59	126.23
87	A2	834	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
83	Z5	302	PUB	CMB-C2B-C1B	-3.73	123.10	127.06
82	jK	202	PEB	C1C-CHB-C4B	3.73	136.66	128.28
82	W9	202	PEB	CHB-C1C-C2C	-3.73	118.73	127.15
87	A6	402	CLA	C1-C2-C3	-3.73	119.59	126.04
82	BQ	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	A1	305	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	fK	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	EF	201	PEB	C1C-CHB-C4B	3.73	136.65	128.28
82	B7	202	PEB	C1C-C2C-C3C	-3.73	103.21	107.62
82	eK	201	PEB	C1C-C2C-C3C	-3.73	103.21	107.62
82	lE	201	PEB	CHB-C1C-C2C	-3.73	118.73	127.15
82	XK	203	PEB	CHB-C4B-C3B	-3.73	116.68	125.32
82	SB	203	PEB	C2A-C1A-NA	3.73	111.49	108.27
82	SH	202	PEB	OA-C1A-C2A	-3.73	123.20	126.17
82	jO	201	PEB	CMB-C2B-C1B	3.73	130.81	125.06
82	OH	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	H1	1002	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	eF	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
87	BN	827	CLA	C2D-C1D-ND	-3.73	107.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lG	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	CM	203	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	U9	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
87	A2	852	CLA	CHC-C1C-NC	3.73	129.86	124.20
82	KM	203	PEB	C3B-C4B-NB	3.73	115.48	110.05
82	BQ	203	PEB	C3B-C4B-NB	3.73	115.48	110.05
82	m4	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
82	RA	202	PEB	C1C-CHB-C4B	3.73	136.65	128.28
82	T1	201	PEB	C3B-C4B-NB	3.73	115.47	110.05
82	gF	201	PEB	CHC-C1D-ND	-3.73	109.00	113.72
82	BJ	301	PEB	C1D-CHC-C4C	3.73	118.76	113.26
82	KI	203	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	JP	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	QB	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
84	LH	1001	CYC	C2C-C1C-NC	3.73	111.49	108.27
82	sF	203	PEB	C3D-C4D-ND	3.73	114.58	107.26
82	S1	202	PEB	CMB-C2B-C1B	3.73	130.81	125.06
82	YO	203	PEB	CAB-C3B-C4B	3.73	131.61	125.01
82	ZJ	201	PEB	CHC-C1D-ND	3.73	118.44	113.72
82	HQ	201	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
82	hJ	201	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
82	rK	202	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
82	kJ	201	PEB	CMC-C3C-C4C	3.73	131.01	127.06
82	AQ	304	PEB	CHC-C1D-ND	-3.73	109.01	113.72
82	VE	202	PEB	C3D-C4D-ND	3.73	114.57	107.26
82	LO	1002	PEB	C3D-C4D-ND	3.73	114.57	107.26
84	D1	1003	CYC	CHB-C1B-NB	-3.73	118.05	126.06
82	aE	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	FA	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
85	B6	602	BCR	C38-C26-C25	-3.73	120.34	124.53
82	bP	501	PEB	CHC-C1D-ND	-3.73	109.01	113.72
82	zK	501	PEB	CHC-C4C-NC	3.73	126.19	121.15
87	O2	203	CLA	C3B-C4B-NB	-3.73	107.06	110.52
82	DF	201	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
82	NM	202	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
82	J9	202	PEB	C1C-CHB-C4B	3.73	136.64	128.28
82	P4	201	PEB	CHA-C1B-NB	-3.73	117.14	124.93
82	AE	301	PEB	C3D-C4D-ND	3.73	114.57	107.26
82	sF	203	PEB	C1C-C2C-C3C	-3.73	103.22	107.62
82	1C	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
82	VQ	202	PEB	C2C-C1C-NC	3.73	112.59	107.57
82	rK	201	PEB	OD-C4D-ND	-3.73	120.41	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ND	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	DP	201	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	FQ	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	l4	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	Y7	304	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	TO	203	PEB	CAB-C3B-C4B	3.73	131.60	125.01
82	eF	201	PEB	C1C-C2C-C3C	-3.73	103.22	107.62
82	WM	203	PEB	C3D-C4D-ND	3.73	114.57	107.26
82	DQ	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
82	B9	202	PEB	C3B-C4B-NB	3.73	115.47	110.05
82	LP	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
82	J9	201	PEB	CBB-CAB-C3B	3.73	122.98	112.63
82	NP	202	PEB	CMB-C2B-C1B	3.73	130.80	125.06
82	iE	201	PEB	CHA-C1B-NB	-3.73	117.14	124.93
82	KK	203	PEB	OD-C4D-ND	-3.73	120.41	125.93
82	X9	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	dE	204	PEB	OA-C1A-C2A	-3.73	123.21	126.17
82	H9	201	PEB	C3B-C4B-NB	3.73	115.47	110.05
82	DP	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
82	H9	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
85	B2	838	BCR	C16-C15-C14	-3.73	115.84	123.47
85	FL	101	BCR	C21-C20-C19	3.73	134.84	123.22
82	kO	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
82	Q9	201	PEB	C2C-C1C-NC	3.72	112.59	107.57
82	SF	201	PEB	C1C-C2C-C3C	-3.72	103.22	107.62
84	H1	1001	CYC	C2B-C1B-NB	3.72	112.44	106.99
85	BL	618	BCR	C16-C17-C18	-3.72	122.00	127.31
82	NA	202	PEB	C3C-C4C-NC	3.72	111.69	108.33
82	AP	201	PEB	C1B-C2B-C3B	-3.72	102.23	106.51
82	EM	203	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	J5	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	LM	201	PEB	CHB-C1C-NC	-3.72	116.79	125.32
82	O1	202	PEB	CHA-C1B-NB	-3.72	117.14	124.93
82	qF	203	PEB	C1C-C2C-C3C	-3.72	103.22	107.62
84	D4	1001	CYC	C1B-NB-C4B	-3.72	105.93	110.67
82	DK	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	M9	304	PEB	C3D-C4D-ND	3.72	114.56	107.26
87	B2	805	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
82	PK	202	PEB	C2A-C1A-NA	3.72	111.48	108.27
82	R7	202	PEB	C1C-CHB-C4B	3.72	136.63	128.28
82	SA	202	PEB	CHC-C4C-NC	3.72	126.19	121.15
82	DA	203	PEB	C3D-C4D-ND	3.72	114.56	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QB	203	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	VP	202	PEB	CMB-C2B-C1B	3.72	130.80	125.06
82	E7	201	PEB	C1C-C2C-C3C	-3.72	103.22	107.62
82	kJ	201	PEB	C1C-C2C-C3C	-3.72	103.22	107.62
84	FH	1001	CYC	C4D-CHA-C1A	3.72	136.63	128.28
82	T7	202	PEB	OD-C4D-ND	-3.72	120.42	125.93
82	xC	201	PEB	C2C-C1C-NC	3.72	112.58	107.57
84	DO	1001	CYC	CMB-C2B-C1B	3.72	128.81	124.17
96	FL	102	HEM	C1B-NB-C4B	3.72	108.92	105.07
82	u8	203	PEB	CHA-C1B-NB	-3.72	117.15	124.93
82	BP	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
82	VE	201	PEB	CAC-C2C-C1C	3.72	131.69	125.76
82	lJ	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
82	dF	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
84	NH	1001	CYC	C2D-C1D-ND	3.72	112.63	107.40
82	18	202	PEB	C1C-CHB-C4B	3.72	136.63	128.28
82	q8	203	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
82	JI	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	l1	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	gJ	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	hM	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	FH	1002	PEB	CHC-C1D-ND	-3.72	109.02	113.72
82	aG	202	PEB	OA-C1A-C2A	-3.72	123.22	126.17
82	kF	202	PEB	C2A-C1A-NA	3.72	111.48	108.27
85	CL	516	BCR	C24-C23-C22	-3.72	120.61	126.23
82	iE	202	PEB	CHC-C1D-ND	-3.72	109.02	113.72
82	EK	201	PEB	C1C-CHB-C4B	3.72	136.62	128.28
82	IF	203	PEB	C3C-C4C-NC	3.72	111.68	108.33
82	DE	1002	PEB	CAB-C3B-C4B	3.72	131.59	125.01
82	s8	201	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
82	iF	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	BA	202	PEB	C1C-C2C-C3C	-3.72	103.22	107.62
87	BN	806	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
84	y3	1001	CYC	CAD-C3D-C4D	3.72	131.69	125.76
82	d1	203	PEB	CHC-C4C-NC	3.72	126.18	121.15
85	BL	618	BCR	C24-C23-C22	-3.72	120.61	126.23
82	bH	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
82	Y4	203	PEB	CAB-C3B-C4B	3.72	131.59	125.01
84	K4	1001	CYC	C1B-C2B-C3B	-3.72	103.99	107.87
82	J1	1002	PEB	OA-C1A-C2A	-3.72	123.22	126.17
82	VF	201	PEB	C1C-C2C-C3C	-3.72	103.22	107.62
82	cM	202	PEB	C3D-C4D-ND	3.72	114.56	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FA	202	PEB	C3C-C4C-NC	3.72	111.68	108.33
85	aL	604	BCR	C16-C17-C18	-3.72	122.00	127.31
82	BJ	301	PEB	CMB-C2B-C1B	3.72	130.79	125.06
82	qF	202	PEB	C3D-C4D-ND	3.72	114.55	107.26
82	fH	203	PEB	C1C-CHB-C4B	3.72	136.62	128.28
84	ME	1001	CYC	C2C-C1C-NC	3.72	111.48	108.27
82	xF	302	PEB	CHA-C1B-NB	-3.72	117.16	124.93
82	m4	202	PEB	CMB-C2B-C1B	3.72	130.79	125.06
82	NA	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
87	AN	852	CLA	CHC-C1C-NC	3.72	129.84	124.20
82	H7	202	PEB	CHA-C4A-NA	3.72	129.62	125.20
82	aG	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
82	B5	202	PEB	C3D-C4D-ND	3.72	114.55	107.26
87	CL	513	CLA	CAA-C2A-C3A	-3.72	102.60	112.78
82	O1	203	PEB	C1C-CHB-C4B	3.72	136.62	128.28
82	IQ	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
82	cO	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
82	RM	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
84	H1	1001	CYC	C2C-C1C-NC	3.72	111.48	108.27
82	A1	305	PEB	OA-C1A-C2A	-3.72	123.22	126.17
82	L4	1002	PEB	C3D-C4D-ND	3.72	114.55	107.26
82	z8	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
82	XD	202	PEB	C2C-C1C-NC	3.71	112.57	107.57
82	VA	203	PEB	CHC-C4C-NC	3.71	126.18	121.15
82	pK	202	PEB	CAB-C3B-C4B	3.71	131.58	125.01
82	TD	203	PEB	OD-C4D-ND	-3.71	120.43	125.93
82	GD	201	PEB	C3D-C4D-ND	3.71	114.55	107.26
82	HB	202	PEB	CMB-C2B-C1B	3.71	130.78	125.06
82	jF	201	PEB	OA-C1A-NA	3.71	129.44	124.94
82	ID	201	PEB	C3D-C4D-ND	3.71	114.55	107.26
82	kG	201	PEB	C3D-C4D-ND	3.71	114.55	107.26
82	dE	203	PEB	CHA-C1B-NB	-3.71	117.16	124.93
82	cJ	201	PEB	CMC-C3C-C4C	3.71	131.00	127.06
84	DH	1003	CYC	CHB-C1B-NB	-3.71	118.08	126.06
82	mG	202	PEB	C3D-C4D-ND	3.71	114.55	107.26
82	e4	203	PEB	CAB-C3B-C4B	3.71	131.58	125.01
82	pF	202	PEB	CAB-C3B-C4B	3.71	131.58	125.01
87	BL	623	CLA	CHB-C4A-NA	3.71	129.65	124.51
82	DO	1002	PEB	CAC-CBC-CGC	-3.71	105.61	113.60
83	AJ	303	PUB	CBA-CAA-C3A	-3.71	107.35	112.98
91	a6	613	PHO	C1-C2-C3	-3.71	119.62	126.04
82	KD	201	PEB	C2A-C1A-NA	3.71	111.47	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NJ	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
82	Y9	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
87	AN	852	CLA	CHD-C1D-ND	-3.71	121.04	124.45
87	7N	603	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
84	N4	1001	CYC	C2D-C1D-ND	3.71	112.62	107.40
82	KK	201	PEB	C1C-CHB-C4B	3.71	136.61	128.28
85	BN	838	BCR	C16-C15-C14	-3.71	115.87	123.47
95	B6	620	DGD	O2G-C1B-C2B	3.71	119.50	111.50
82	FB	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	SJ	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	SJ	203	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	fO	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	P1	201	PEB	CMB-C2B-C1B	3.71	130.78	125.06
82	lO	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
82	PM	201	PEB	CHA-C1B-NB	-3.71	117.17	124.93
84	C1	1001	CYC	C2B-C1B-NB	3.71	112.42	106.99
83	AH	304	PUB	OA-C1A-NA	-3.71	120.43	125.93
82	g4	203	PEB	C3B-C4B-NB	3.71	115.45	110.05
82	gO	203	PEB	C3B-C4B-NB	3.71	115.45	110.05
82	p8	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
85	FL	101	BCR	C35-C13-C14	-3.71	117.72	122.92
82	BM	301	PEB	OA-C1A-C2A	-3.71	123.22	126.17
82	BD	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	fJ	203	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	CP	203	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	f1	203	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	aJ	203	PEB	C3D-C4D-ND	3.71	114.54	107.26
83	xK	301	PUB	CMA-C2A-C1A	3.71	130.12	121.39
82	FQ	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
84	g3	1001	CYC	CHD-C1D-C2D	3.71	136.60	127.49
82	C9	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
92	DL	402	LMG	C4-C3-C2	3.71	117.30	110.82
82	TH	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
84	c3	1001	CYC	CHD-C1D-C2D	3.71	136.60	127.49
82	eJ	201	PEB	C2A-C1A-NA	3.71	111.47	108.27
82	TB	201	PEB	C1D-CHC-C4C	-3.71	107.79	113.26
82	pF	201	PEB	C1C-CHB-C4B	-3.71	119.96	128.28
83	xF	301	PUB	CMA-C2A-C1A	3.71	130.12	121.39
82	x8	201	PEB	C2C-C1C-NC	3.71	112.57	107.57
82	kE	201	PEB	C2C-C1C-NC	3.71	112.57	107.57
82	V7	203	PEB	CHC-C4C-NC	3.71	126.17	121.15
82	e1	202	PEB	C1D-CHC-C4C	3.71	118.72	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KQ	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
82	jH	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
82	sC	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
82	D4	1002	PEB	CAC-CBC-CGC	-3.71	105.62	113.60
82	M5	301	PEB	C1C-CHB-C4B	-3.71	119.97	128.28
82	MK	202	PEB	C1C-C2C-C3C	-3.71	103.24	107.62
82	1C	202	PEB	C1C-CHB-C4B	3.71	136.60	128.28
84	D4	1001	CYC	CMB-C2B-C1B	3.71	128.80	124.17
82	JA	203	PEB	C3D-C4D-ND	3.71	114.53	107.26
82	mF	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
87	2N	311	CLA	CAA-C2A-C3A	-3.71	105.00	114.26
82	sK	203	PEB	C1C-C2C-C3C	-3.71	103.24	107.62
82	j1	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
84	H1	1001	CYC	CMD-C2D-C1D	3.71	130.99	125.56
82	AP	202	PEB	C3D-C4D-ND	3.71	114.53	107.26
82	GQ	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
82	Q5	203	PEB	C3D-C4D-ND	3.71	114.53	107.26
82	mK	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
82	f1	203	PEB	C1C-CHB-C4B	3.71	136.59	128.28
82	ZH	201	PEB	CHC-C4C-NC	3.71	126.17	121.15
82	DK	203	PEB	C3B-C4B-NB	3.71	115.44	110.05
82	M7	201	PEB	OD-C4D-C3D	-3.71	121.06	129.46
82	ZE	203	PEB	OA-C1A-C2A	-3.71	123.23	126.17
82	TI	203	PEB	C2A-C1A-NA	3.71	111.47	108.27
82	18	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
82	pC	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
82	XJ	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
85	k6	102	BCR	C23-C22-C21	3.71	124.63	118.94
82	L7	202	PEB	C3C-C4C-NC	3.71	111.67	108.33
82	ND	202	PEB	C3D-C4D-ND	3.70	114.53	107.26
82	XP	202	PEB	C3D-C4D-ND	3.70	114.53	107.26
82	O5	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
82	aE	202	PEB	C4B-C3B-C2B	-3.70	102.68	106.78
87	bL	613	CLA	CHB-C4A-NA	3.70	129.63	124.51
82	cF	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
82	CF	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	mO	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	BA	201	PEB	CHC-C4C-NC	3.70	126.16	121.15
82	jF	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
82	LD	201	PEB	C1C-CHB-C4B	3.70	136.59	128.28
82	qK	203	PEB	C1C-C2C-C3C	-3.70	103.24	107.62
82	N7	201	PEB	C3D-C4D-ND	3.70	114.53	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	J3	1001	CYC	CHD-C1D-C2D	3.70	136.58	127.49
82	UE	201	PEB	CHC-C1D-ND	-3.70	109.04	113.72
82	O1	202	PEB	CHC-C4C-NC	3.70	126.16	121.15
82	ZJ	201	PEB	C4B-C3B-C2B	-3.70	102.68	106.78
82	HH	1002	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	U5	202	PEB	C1C-CHB-C4B	3.70	136.59	128.28
82	PO	201	PEB	C2A-C1A-NA	3.70	111.47	108.27
82	P7	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	qF	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	W5	203	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	gO	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	NQ	202	PEB	C1C-C2C-C3C	-3.70	103.25	107.62
82	P4	202	PEB	C1C-C2C-C3C	-3.70	103.25	107.62
85	cL	504	BCR	C11-C10-C9	-3.70	122.03	127.31
82	SE	201	PEB	CHC-C4C-NC	3.70	126.16	121.15
82	A4	301	PEB	CHC-C4C-NC	3.70	126.16	121.15
82	BI	203	PEB	C2C-C1C-NC	3.70	112.56	107.57
82	j1	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
84	DG	1001	CYC	C4A-C3A-C2A	-3.70	102.26	106.51
82	JH	1002	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	kK	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	jG	201	PEB	CHC-C4C-NC	3.70	126.16	121.15
82	GB	203	PEB	CHC-C1D-ND	-3.70	109.04	113.72
82	IQ	201	PEB	CHC-C1D-ND	-3.70	109.04	113.72
82	WD	201	PEB	C3B-C4B-NB	3.70	115.43	110.05
82	WQ	201	PEB	C3B-C4B-NB	3.70	115.43	110.05
82	gK	202	PEB	C1B-C2B-C3B	-3.70	102.26	106.51
84	C3	1001	CYC	CHD-C1D-C2D	3.70	136.57	127.49
84	IE	1001	CYC	C1D-C2D-C3D	-3.70	103.08	107.79
82	tK	203	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	kH	202	PEB	CHB-C1C-C2C	-3.70	118.80	127.15
82	d4	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	I9	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	jH	203	PEB	C1C-C2C-C3C	-3.70	103.25	107.62
82	DF	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	Y9	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	mE	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
84	F1	1001	CYC	C4D-CHA-C1A	3.70	136.58	128.28
82	UK	202	PEB	C1B-C2B-C3B	-3.70	102.26	106.51
82	fG	201	PEB	C1B-C2B-C3B	-3.70	102.26	106.51
82	JP	202	PEB	CMB-C2B-C1B	3.70	130.76	125.06
82	cM	202	PEB	CMB-C2B-C1B	3.70	130.76	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YB	202	PEB	CHC-C4C-NC	3.70	126.16	121.15
82	HQ	201	PEB	C2A-C1A-NA	3.70	111.46	108.27
82	i4	202	PEB	C1C-CHB-C4B	3.70	136.58	128.28
85	A2	804	BCR	C16-C17-C18	-3.70	122.03	127.31
84	MG	1001	CYC	C1D-C2D-C3D	-3.70	103.08	107.79
82	b1	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	tC	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
82	VA	201	PEB	C2C-C1C-NC	3.70	112.55	107.57
84	m3	1001	CYC	CHD-C1D-C2D	3.70	136.57	127.49
84	v3	1001	CYC	CHD-C1D-C2D	3.70	136.57	127.49
82	F1	1002	PEB	CHC-C1D-ND	-3.70	109.05	113.72
91	DL	405	PHO	C4D-CHA-CBD	-3.70	106.84	108.52
85	LN	205	BCR	C19-C18-C17	-3.70	113.27	118.94
82	MA	201	PEB	OD-C4D-C3D	-3.70	121.08	129.46
82	RP	201	PEB	CHA-C1B-NB	-3.70	117.20	124.93
82	ZB	202	PEB	CHC-C4C-NC	3.70	126.15	121.15
82	rF	202	PEB	C1B-C2B-C3B	-3.70	102.26	106.51
82	J5	203	PEB	C3D-C4D-ND	3.70	114.51	107.26
82	HM	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	TK	201	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
84	L4	1001	CYC	C4D-C3D-C2D	-3.70	103.25	107.62
82	RA	202	PEB	C3C-C4C-NC	3.70	111.66	108.33
82	jM	202	PEB	CAC-C2C-C1C	3.70	131.65	125.76
82	B7	201	PEB	CHC-C4C-NC	3.70	126.15	121.15
82	CJ	202	PEB	C3D-C4D-ND	3.70	114.51	107.26
82	II	202	PEB	C2A-C1A-NA	3.70	111.46	108.27
82	mG	203	PEB	C2A-C1A-NA	3.70	111.46	108.27
82	HH	1002	PEB	C2C-C1C-NC	3.70	112.55	107.57
82	NM	201	PEB	CHA-C1B-NB	-3.70	117.20	124.93
82	gK	202	PEB	C3D-C4D-ND	3.70	114.51	107.26
82	DK	202	PEB	C1B-C2B-C3B	-3.70	102.26	106.51
87	72	603	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
82	ND	202	PEB	C1C-C2C-C3C	-3.70	103.25	107.62
82	N7	203	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
82	gF	202	PEB	C2A-C1A-NA	3.70	111.46	108.27
82	DE	1002	PEB	C2C-C1C-NC	3.70	112.55	107.57
82	NQ	203	PEB	C3D-C4D-ND	3.70	114.51	107.26
82	bK	201	PEB	C3D-C4D-ND	3.70	114.51	107.26
82	WM	203	PEB	C1C-CHB-C4B	3.70	136.57	128.28
84	FE	1002	CYC	C1D-C2D-C3D	-3.70	103.08	107.79
84	y3	1001	CYC	CHD-C1D-C2D	3.70	136.56	127.49
85	IN	101	BCR	C33-C5-C4	3.70	120.72	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B5	201	PEB	CHC-C1D-ND	-3.70	109.05	113.72
82	H5	203	PEB	C3D-C4D-ND	3.70	114.51	107.26
82	DA	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
82	N7	202	PEB	OD-C4D-ND	-3.69	120.46	125.93
82	pF	202	PEB	OD-C4D-ND	-3.69	120.46	125.93
87	22	611	CLA	CAA-C2A-C3A	-3.69	105.03	114.26
82	OH	202	PEB	C2A-C1A-NA	3.69	111.46	108.27
85	I2	101	BCR	C33-C5-C4	3.69	120.71	113.62
82	XP	201	PEB	C3B-C4B-NB	3.69	115.42	110.05
84	G3	1001	CYC	CHD-C1D-C2D	3.69	136.56	127.49
84	CH	1001	CYC	C2B-C1B-NB	3.69	112.40	106.99
84	A3	1001	CYC	CHD-C1D-C2D	3.69	136.56	127.49
82	B5	202	PEB	C1C-CHB-C4B	3.69	136.57	128.28
82	QM	204	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	A4	304	PEB	OA-C1A-C2A	-3.69	123.24	126.17
92	ML	101	LMG	C7-O1-C1	3.69	120.95	113.74
82	QG	202	PEB	CHC-C1D-ND	-3.69	109.05	113.72
82	KG	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
84	K1	1001	CYC	CHA-C4D-C3D	-3.69	118.82	127.15
82	aM	201	PEB	CHC-C4C-NC	3.69	126.15	121.15
82	pK	201	PEB	C1C-CHB-C4B	-3.69	120.00	128.28
82	ZF	202	PEB	C2A-C1A-NA	3.69	111.46	108.27
82	CQ	202	PEB	C2A-C1A-NA	3.69	111.46	108.27
82	mO	201	PEB	C2A-C1A-NA	3.69	111.46	108.27
82	D7	203	PEB	C3D-C4D-ND	3.69	114.50	107.26
84	I4	1001	CYC	C1B-NB-C4B	-3.69	105.97	110.67
82	W5	201	PEB	OD-C4D-ND	-3.69	120.46	125.93
82	UB	303	PEB	CHC-C1D-ND	-3.69	109.05	113.72
82	CK	203	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	g4	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	P9	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	TA	203	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
85	BN	803	BCR	C38-C26-C25	-3.69	120.38	124.53
82	RG	201	PEB	CHC-C1D-ND	-3.69	109.05	113.72
82	g4	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	lK	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	VB	201	PEB	OD-C4D-ND	-3.69	120.46	125.93
87	cL	512	CLA	CMB-C2B-C1B	-3.69	119.75	125.37
82	WJ	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	AP	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	T7	201	PEB	C2C-C1C-NC	3.69	112.54	107.57
82	GQ	202	PEB	C2A-C1A-NA	3.69	111.45	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	HH	1001	CYC	C2C-C1C-NC	3.69	111.45	108.27
82	s8	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	zC	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	fG	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
84	HH	1001	CYC	CMD-C2D-C1D	3.69	130.97	125.56
82	PO	202	PEB	CMB-C2B-C1B	3.69	130.75	125.06
84	HH	1001	CYC	CMA-C3A-C4A	3.69	130.75	125.06
82	WA	201	PEB	CHB-C1C-C2C	-3.69	118.82	127.15
82	jF	202	PEB	C3B-C4B-NB	3.69	115.42	110.05
84	l3	1001	CYC	CHD-C1D-C2D	3.69	136.55	127.49
82	TP	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	NQ	204	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	eB	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	fH	203	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	xK	302	PEB	CHA-C1B-NB	-3.69	117.21	124.93
82	KG	201	PEB	C2A-C1A-NA	3.69	111.45	108.27
84	W3	1001	CYC	CHD-C1D-C2D	3.69	136.55	127.49
82	W7	201	PEB	CHB-C1C-C2C	-3.69	118.83	127.15
82	HP	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
88	m6	102	LHG	O7-C7-C8	3.69	119.45	111.50
82	mM	201	PEB	C1D-CHC-C4C	3.69	118.70	113.26
82	W5	202	PEB	C1C-C2C-C3C	-3.69	103.26	107.62
82	ZF	201	PEB	CHC-C4C-NC	3.69	126.14	121.15
82	JM	202	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
82	oF	203	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
82	KF	201	PEB	C1C-CHB-C4B	3.69	136.55	128.28
82	bF	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
85	b6	603	BCR	C3-C4-C5	-3.69	107.49	114.08
82	BB	201	PEB	CMB-C2B-C1B	3.69	130.74	125.06
82	KI	201	PEB	CHC-C1D-ND	3.69	118.39	113.72
82	f4	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	uF	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
82	GI	201	PEB	C1D-CHC-C4C	-3.69	107.82	113.26
82	jM	201	PEB	CMB-C2B-C1B	3.69	130.74	125.06
82	qC	203	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
82	eH	201	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
82	m4	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	dE	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	OI	203	PEB	C3D-C4D-ND	3.69	114.49	107.26
82	TQ	203	PEB	C3D-C4D-ND	3.69	114.49	107.26
82	Z9	304	PEB	C3D-C4D-ND	3.69	114.49	107.26
84	R3	1001	CYC	CHD-C1D-C2D	3.69	136.54	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	KH	1001	CYC	CHA-C4D-C3D	-3.69	118.83	127.15
84	i3	1001	CYC	CHD-C1D-C2D	3.69	136.54	127.49
82	HI	203	PEB	C3D-C4D-ND	3.69	114.49	107.26
82	BQ	203	PEB	C3D-C4D-ND	3.69	114.49	107.26
85	J2	102	BCR	C27-C26-C25	-3.69	117.38	122.73
82	QM	203	PEB	CHC-C4C-NC	3.69	126.14	121.15
82	V7	201	PEB	C2C-C1C-NC	3.69	112.54	107.57
82	IP	201	PEB	C1B-C2B-C3B	-3.69	102.28	106.51
82	fE	201	PEB	C1B-C2B-C3B	-3.69	102.28	106.51
82	YD	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
82	XQ	203	PEB	C2A-C1A-NA	3.69	111.45	108.27
82	aJ	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
82	f1	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	hG	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	aG	202	PEB	CHC-C4C-NC	3.69	126.14	121.15
82	Z5	301	PEB	C1C-CHB-C4B	-3.69	120.02	128.28
83	A1	304	PUB	OA-C1A-NA	-3.69	120.47	125.93
82	YJ	202	PEB	CHC-C4C-NC	3.69	126.14	121.15
82	QQ	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
82	aO	201	PEB	C2A-C1A-NA	3.69	111.45	108.27
82	TA	201	PEB	C2C-C1C-NC	3.69	112.53	107.57
82	k1	202	PEB	CHB-C1C-C2C	-3.69	118.84	127.15
82	KD	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
82	iO	202	PEB	C1C-CHB-C4B	3.68	136.55	128.28
82	lH	201	PEB	C3D-C4D-ND	3.68	114.49	107.26
82	XF	203	PEB	CHB-C4B-C3B	-3.68	116.79	125.32
82	d1	203	PEB	C4B-C3B-C2B	-3.68	102.70	106.78
87	B2	834	CLA	CHB-C1B-NB	3.68	128.16	124.26
84	t3	1001	CYC	CHD-C1D-C2D	3.68	136.53	127.49
82	RI	203	PEB	CMB-C2B-C1B	3.68	130.74	125.06
82	Q9	202	PEB	C3D-C4D-ND	3.68	114.49	107.26
82	GK	203	PEB	OD-C4D-ND	-3.68	120.47	125.93
84	P3	1001	CYC	CHD-C1D-C2D	3.68	136.53	127.49
84	e3	1001	CYC	CHD-C1D-C2D	3.68	136.53	127.49
84	p3	1001	CYC	CHD-C1D-C2D	3.68	136.53	127.49
82	T7	203	PEB	C4B-C3B-C2B	-3.68	102.70	106.78
82	SI	201	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	aB	202	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	HA	203	PEB	C3D-C4D-ND	3.68	114.49	107.26
82	lH	202	PEB	C3D-C4D-ND	3.68	114.49	107.26
82	SK	201	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
84	K4	1001	CYC	CHD-C1D-ND	-3.68	116.88	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LP	201	PEB	OA-C1A-C2A	-3.68	123.24	126.17
82	c4	202	PEB	OA-C1A-C2A	-3.68	123.24	126.17
82	mE	201	PEB	OA-C1A-C2A	-3.68	123.24	126.17
82	wF	301	PEB	OD-C4D-ND	-3.68	120.47	125.93
82	CK	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	rK	201	PEB	C3D-C4D-ND	3.68	114.48	107.26
85	AN	804	BCR	C16-C17-C18	-3.68	122.05	127.31
82	ZM	201	PEB	CMC-C3C-C4C	3.68	130.96	127.06
82	Z9	304	PEB	C3B-C4B-NB	3.68	115.41	110.05
82	OG	202	PEB	C1D-CHC-C4C	-3.68	107.83	113.26
82	OJ	201	PEB	CHC-C4C-NC	3.68	126.13	121.15
82	TD	203	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	FM	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	IA	201	PEB	CHA-C1B-NB	-3.68	117.23	124.93
82	VK	201	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	RO	203	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	cM	201	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
82	OG	202	PEB	CMB-C2B-C1B	3.68	130.73	125.06
82	UD	201	PEB	C2A-C1A-NA	3.68	111.45	108.27
82	yC	203	PEB	C1D-CHC-C4C	3.68	118.69	113.26
82	DA	203	PEB	CHC-C1D-ND	-3.68	109.07	113.72
82	t8	202	PEB	C2C-C1C-NC	3.68	112.53	107.57
82	Z1	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	fJ	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
82	VM	202	PEB	CMB-C2B-C1B	3.68	130.73	125.06
82	JB	201	PEB	C1D-CHC-C4C	-3.68	107.83	113.26
85	c6	617	BCR	C34-C9-C8	3.68	123.88	118.08
82	s8	201	PEB	C1C-CHB-C4B	3.68	136.54	128.28
82	aE	202	PEB	CHC-C4C-NC	3.68	126.13	121.15
82	bP	501	PEB	CHC-C4C-NC	3.68	126.13	121.15
82	UI	201	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	QJ	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	PH	202	PEB	CAC-CBC-CGC	-3.68	105.68	113.60
82	GK	201	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	EM	201	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
82	UG	201	PEB	CHC-C1D-ND	-3.68	109.07	113.72
82	p8	202	PEB	OD-C4D-ND	-3.68	120.48	125.93
85	B2	842	BCR	C20-C21-C22	-3.68	122.06	127.31
82	dG	204	PEB	OA-C1A-C2A	-3.68	123.25	126.17
82	jK	202	PEB	C3B-C4B-NB	3.68	115.40	110.05
82	D5	203	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	nK	201	PEB	C3D-C4D-ND	3.68	114.48	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	zK	501	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	UB	302	PEB	CAC-C2C-C1C	-3.68	119.90	125.76
82	mJ	201	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	lJ	201	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
82	XK	201	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
82	XD	201	PEB	C2A-C1A-NA	3.68	111.44	108.27
82	eA	301	PEB	CMB-C2B-C1B	3.68	130.73	125.06
82	ZH	201	PEB	C3B-C4B-NB	3.68	115.40	110.05
82	dE	203	PEB	C3D-C4D-ND	3.68	114.48	107.26
82	IJ	203	PEB	OA-C1A-C2A	-3.68	123.25	126.17
82	bG	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
82	p8	201	PEB	CHC-C1D-ND	-3.68	109.07	113.72
82	OJ	203	PEB	C3C-C4C-NC	3.68	111.64	108.33
82	QG	201	PEB	C2A-C1A-NA	3.68	111.44	108.27
82	XJ	201	PEB	C2A-C1A-NA	3.68	111.44	108.27
82	L4	1002	PEB	C2A-C1A-NA	3.68	111.44	108.27
84	G4	1001	CYC	C2C-C1C-NC	3.68	111.44	108.27
85	K6	102	BCR	C23-C22-C21	3.68	124.58	118.94
82	HA	202	PEB	CHA-C4A-NA	3.68	129.58	125.20
82	WJ	203	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
84	E3	1001	CYC	CHD-C1D-C2D	3.68	136.52	127.49
84	N3	1001	CYC	CHD-C1D-C2D	3.68	136.52	127.49
82	g4	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
87	B2	827	CLA	C2D-C1D-ND	-3.68	107.39	110.10
87	3N	305	CLA	CHB-C1B-NB	3.68	128.15	124.26
82	Q5	202	PEB	C1C-C2C-C3C	-3.68	103.27	107.62
82	DQ	201	PEB	C3B-C4B-NB	3.68	115.40	110.05
82	LP	202	PEB	CHA-C1B-NB	-3.68	117.24	124.93
85	B2	802	BCR	C38-C26-C25	-3.68	120.40	124.53
82	wC	202	PEB	CAB-C3B-C4B	3.68	131.51	125.01
82	HI	203	PEB	CHC-C4C-NC	3.68	126.12	121.15
82	bO	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
82	J7	203	PEB	CAB-C3B-C4B	3.68	131.51	125.01
82	EM	201	PEB	C1C-CHB-C4B	3.68	136.53	128.28
84	NE	201	CYC	CHD-C1D-ND	-3.68	116.90	125.32
82	yC	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
82	dM	203	PEB	C3D-C4D-ND	3.68	114.47	107.26
82	CA	201	PEB	CHA-C1B-C2B	3.68	134.35	124.90
84	T3	1001	CYC	CHD-C1D-C2D	3.68	136.51	127.49
87	32	304	CLA	CHB-C1B-NB	3.68	128.15	124.26
82	O1	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
82	OK	201	PEB	C1B-C2B-C3B	-3.68	102.29	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YK	203	PEB	C1B-C2B-C3B	-3.68	102.29	106.51
82	ZI	401	PEB	CMC-C3C-C4C	-3.68	123.17	127.06
83	yK	303	PUB	CMB-C2B-C1B	3.68	130.96	127.06
82	UK	201	PEB	C1C-CHB-C4B	3.68	136.52	128.28
82	sC	201	PEB	C1C-CHB-C4B	3.68	136.52	128.28
82	DF	203	PEB	C3B-C4B-NB	3.68	115.39	110.05
82	M9	305	PEB	C3B-C4B-NB	3.68	115.39	110.05
82	oK	203	PEB	C4B-C3B-C2B	-3.68	102.72	106.78
85	BN	843	BCR	C1-C6-C5	-3.67	117.44	122.61
82	cM	202	PEB	OA-C1A-C2A	-3.67	123.25	126.17
82	VA	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
82	TM	201	PEB	C1C-C2C-C3C	-3.67	103.28	107.62
82	TJ	201	PEB	OD-C4D-ND	-3.67	120.49	125.93
82	R1	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
82	MA	202	PEB	C3D-C4D-ND	3.67	114.47	107.26
82	b1	203	PEB	C3D-C4D-ND	3.67	114.47	107.26
82	lF	201	PEB	C3D-C4D-ND	3.67	114.47	107.26
84	MG	1001	CYC	C1B-NB-C4B	-3.67	105.99	110.67
82	AK	201	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	HD	203	PEB	OD-C4D-ND	-3.67	120.49	125.93
84	K3	1001	CYC	CHD-C1D-C2D	3.67	136.51	127.49
84	JH	1003	CYC	CMD-C2D-C1D	3.67	130.94	125.56
82	Z1	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
82	EK	202	PEB	OA-C1A-C2A	-3.67	123.25	126.17
82	GF	203	PEB	OD-C4D-ND	-3.67	120.49	125.93
82	uC	203	PEB	CHA-C1B-NB	-3.67	117.25	124.93
82	WE	202	PEB	C3D-C4D-ND	3.67	114.47	107.26
82	e4	203	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
84	HH	1001	CYC	C1B-CHB-C4A	-3.67	119.11	128.08
82	XF	202	PEB	C3C-C4C-NC	3.67	111.64	108.33
82	S9	202	PEB	C3D-C4D-ND	3.67	114.47	107.26
82	fM	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
82	jE	202	PEB	OA-C1A-C2A	-3.67	123.25	126.17
82	kO	202	PEB	OA-C1A-C2A	-3.67	123.25	126.17
82	vK	201	PEB	CHC-C1D-ND	-3.67	109.08	113.72
82	WH	203	PEB	C1C-C2C-C3C	-3.67	103.28	107.62
84	LO	1001	CYC	C4D-C3D-C2D	-3.67	103.28	107.62
82	NA	202	PEB	CMB-C2B-C1B	3.67	130.72	125.06
82	h1	201	PEB	C1C-CHB-C4B	3.67	136.52	128.28
94	a6	601	PL9	C7-C8-C9	-3.67	120.68	126.79
82	iG	201	PEB	CHA-C1B-NB	-3.67	117.25	124.93
83	yF	303	PUB	CMB-C2B-C1B	3.67	130.95	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VO	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
82	GF	201	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
84	KO	1001	CYC	CHB-C4A-NA	-3.67	117.25	124.93
82	QE	202	PEB	CHC-C4C-NC	3.67	126.12	121.15
82	SO	202	PEB	CHC-C4C-NC	3.67	126.12	121.15
84	M3	1001	CYC	CMD-C2D-C1D	3.67	130.94	125.56
82	SA	202	PEB	C1B-C2B-C3B	-3.67	102.29	106.51
82	XK	201	PEB	CHC-C1D-ND	-3.67	109.08	113.72
87	AN	802	CLA	CHB-C4A-NA	3.67	129.59	124.51
82	VJ	201	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	c1	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
84	EE	1001	CYC	C2C-C1C-NC	3.67	111.44	108.27
82	jE	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
82	zF	501	PEB	C3D-C4D-ND	3.67	114.46	107.26
84	FG	1001	CYC	C1D-C2D-C3D	-3.67	103.12	107.79
82	UO	201	PEB	C3C-C4C-NC	3.67	111.64	108.33
82	QF	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
82	NA	203	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	SA	201	PEB	OD-C4D-C3D	-3.67	121.14	129.46
82	MM	201	PEB	C1C-CHB-C4B	3.67	136.51	128.28
84	L3	1001	CYC	CMD-C2D-C1D	3.67	130.93	125.56
82	ZH	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
85	L2	205	BCR	C19-C18-C17	-3.67	113.31	118.94
82	MK	202	PEB	OA-C1A-C2A	-3.67	123.26	126.17
82	O1	201	PEB	OA-C1A-C2A	-3.67	123.26	126.17
87	2N	310	CLA	CAA-C2A-C3A	-3.67	107.54	116.10
82	VG	201	PEB	CAC-C2C-C1C	3.67	131.60	125.76
84	73	1001	CYC	CMD-C2D-C1D	3.67	130.93	125.56
82	DD	203	PEB	C3B-C4B-NB	3.67	115.39	110.05
82	J1	1002	PEB	C3D-C4D-ND	3.67	114.46	107.26
82	M7	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
82	L9	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
82	H5	202	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	FO	1002	PEB	CHC-C1D-ND	-3.67	109.08	113.72
82	NF	201	PEB	CHA-C1B-NB	-3.67	117.26	124.93
82	U4	201	PEB	C3C-C4C-NC	3.67	111.63	108.33
82	U5	201	PEB	OA-C1A-C2A	-3.67	123.26	126.17
82	VA	203	PEB	C1C-C2C-C3C	-3.67	103.29	107.62
82	YF	201	PEB	C1C-C2C-C3C	-3.67	103.29	107.62
82	UO	202	PEB	CHC-C4C-NC	3.67	126.11	121.15
82	EQ	202	PEB	C2A-C1A-NA	3.67	111.43	108.27
82	M9	305	PEB	C3D-C4D-ND	3.67	114.45	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	QM	201	PUB	CHB-C4B-NB	-3.67	116.92	125.32
82	jK	201	PEB	OA-C1A-NA	3.67	129.38	124.94
82	fO	201	PEB	CHC-C4C-NC	3.67	126.11	121.15
82	PH	201	PEB	C3B-C4B-NB	3.67	115.38	110.05
82	kJ	201	PEB	CHA-C1B-NB	-3.67	117.26	124.93
82	VB	202	PEB	CHC-C1D-ND	-3.67	109.09	113.72
82	UD	202	PEB	CHC-C1D-ND	-3.67	109.09	113.72
85	BN	843	BCR	C15-C14-C13	-3.67	122.08	127.31
82	WK	203	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	yC	203	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	jH	202	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
82	g1	201	PEB	C2A-C1A-NA	3.67	111.43	108.27
82	aH	201	PEB	C3D-C4D-ND	3.67	114.45	107.26
82	FD	202	PEB	C4B-C3B-C2B	-3.67	102.73	106.78
82	RP	201	PEB	C4B-C3B-C2B	-3.67	102.73	106.78
82	KP	201	PEB	CMB-C2B-C1B	3.67	130.71	125.06
82	d1	202	PEB	CMB-C2B-C1B	3.67	130.71	125.06
84	C1	1001	CYC	OC-C1C-C2C	-3.66	123.26	126.17
82	UH	203	PEB	C1D-CHC-C4C	-3.66	107.85	113.26
82	dH	203	PEB	CHC-C4C-NC	3.66	126.11	121.15
82	SP	203	PEB	OD-C4D-ND	-3.66	120.50	125.93
82	YJ	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
85	AN	847	BCR	C21-C20-C19	-3.66	111.78	123.22
82	UF	201	PEB	C1C-CHB-C4B	3.66	136.50	128.28
82	kJ	201	PEB	C2A-C1A-NA	3.66	111.43	108.27
82	fG	201	PEB	CMB-C2B-C1B	3.66	130.71	125.06
82	S7	201	PEB	OD-C4D-C3D	-3.66	121.16	129.46
82	JD	202	PEB	CHA-C1B-NB	-3.66	117.27	124.93
82	18	201	PEB	CHC-C4C-NC	3.66	126.11	121.15
85	fL	101	BCR	C21-C20-C19	3.66	134.65	123.22
82	DQ	202	PEB	C1B-C2B-C3B	-3.66	102.30	106.51
82	MF	202	PEB	OA-C1A-C2A	-3.66	123.26	126.17
82	J9	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
82	jJ	202	PEB	C3D-C4D-ND	3.66	114.45	107.26
84	GG	1001	CYC	CHD-C1D-ND	-3.66	116.93	125.32
84	EG	1001	CYC	C2C-C1C-NC	3.66	111.43	108.27
85	B2	840	BCR	C11-C10-C9	-3.66	122.08	127.31
87	BN	834	CLA	CHB-C1B-NB	3.66	128.13	124.26
87	4N	605	CLA	CAA-C2A-C1A	3.66	123.98	111.97
82	M9	302	PEB	C3D-C4D-ND	3.66	114.45	107.26
82	FA	202	PEB	C1B-C2B-C3B	-3.66	102.30	106.51
84	n3	1001	CYC	CMD-C2D-C1D	3.66	130.93	125.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PJ	201	PEB	C1C-C2C-C3C	-3.66	103.29	107.62
82	OF	201	PEB	CHC-C1D-ND	-3.66	109.09	113.72
82	kM	202	PEB	CHC-C1D-ND	-3.66	109.09	113.72
82	GI	201	PEB	C3B-C4B-NB	3.66	115.38	110.05
82	HQ	203	PEB	OD-C4D-ND	-3.66	120.50	125.93
82	c4	201	PEB	OA-C1A-C2A	-3.66	123.26	126.17
87	22	610	CLA	CAA-C2A-C3A	-3.66	107.55	116.10
82	jG	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	KF	203	PEB	OD-C4D-ND	-3.66	120.50	125.93
82	FD	202	PEB	CHA-C1B-NB	-3.66	117.27	124.93
82	SP	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	fE	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	eH	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	iF	203	PEB	OA-C1A-C2A	-3.66	123.26	126.17
82	w8	202	PEB	C2A-C1A-NA	3.66	111.43	108.27
84	63	901	CYC	CMB-C2B-C1B	3.66	128.74	124.17
87	42	605	CLA	CAA-C2A-C1A	3.66	123.97	111.97
82	dJ	201	PEB	C1C-C2C-C3C	-3.66	103.29	107.62
82	CF	201	PEB	CHC-C4C-NC	3.66	126.10	121.15
85	B2	843	BCR	C1-C6-C5	-3.66	117.46	122.61
82	VA	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	fE	203	PEB	CHC-C1D-ND	-3.66	109.09	113.72
87	b6	608	CLA	CAA-C2A-C3A	-3.66	102.76	112.78
82	sC	201	PEB	C1B-C2B-C3B	-3.66	102.31	106.51
82	V7	203	PEB	C1C-C2C-C3C	-3.66	103.30	107.62
82	vK	201	PEB	C1D-CHC-C4C	3.66	118.65	113.26
87	8N	301	CLA	CMB-C2B-C1B	-3.66	119.80	125.37
95	cL	520	DGD	O2G-C1B-C2B	3.66	119.39	111.50
82	l1	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	S5	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	OE	202	PEB	C1D-CHC-C4C	-3.66	107.86	113.26
82	eH	202	PEB	C1D-CHC-C4C	3.66	118.65	113.26
85	JN	102	BCR	C27-C26-C25	-3.66	117.42	122.73
82	TB	202	PEB	C1B-C2B-C3B	-3.66	102.31	106.51
82	HA	203	PEB	C2A-C1A-NA	3.66	111.43	108.27
82	EJ	203	PEB	C2A-C1A-NA	3.66	111.43	108.27
82	XP	201	PEB	OA-C1A-C2A	-3.66	123.26	126.17
82	Y5	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
87	A2	829	CLA	CHB-C4A-NA	3.66	129.57	124.51
82	HP	201	PEB	CHC-C1D-ND	-3.66	109.10	113.72
82	w8	202	PEB	CAB-C3B-C4B	3.66	131.48	125.01
82	AP	202	PEB	CHC-C4C-NC	3.66	126.10	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FQ	202	PEB	CHA-C1B-NB	-3.66	117.28	124.93
82	gH	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
95	CL	523	DGD	O2G-C1B-C2B	3.66	119.38	111.50
85	B2	843	BCR	C15-C14-C13	-3.66	122.09	127.31
82	D9	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
82	YJ	203	PEB	OA-C1A-C2A	-3.66	123.27	126.17
82	OM	202	PEB	OA-C1A-C2A	-3.66	123.27	126.17
82	U9	203	PEB	OA-C1A-C2A	-3.66	123.27	126.17
82	N7	201	PEB	CHC-C1D-ND	-3.66	109.10	113.72
84	KO	1001	CYC	CHD-C1D-ND	-3.66	116.94	125.32
82	JK	201	PEB	C2C-C1C-NC	3.66	112.50	107.57
82	tC	202	PEB	C2C-C1C-NC	3.66	112.50	107.57
84	K4	1001	CYC	CHB-C4A-NA	-3.66	117.28	124.93
82	TB	201	PEB	C3D-C4D-ND	3.66	114.43	107.26
82	U9	204	PEB	C1C-CHB-C4B	-3.66	120.08	128.28
82	aM	204	PEB	CHB-C1C-C2C	-3.66	118.90	127.15
82	DM	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
82	g1	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
84	ME	1001	CYC	C1D-C2D-C3D	-3.66	103.13	107.79
82	cB	402	PEB	C2A-C1A-NA	3.66	111.42	108.27
84	u3	1001	CYC	CMD-C2D-C1D	3.66	130.91	125.56
84	w3	1001	CYC	CMD-C2D-C1D	3.66	130.91	125.56
82	C7	201	PEB	CHA-C1B-C2B	3.66	134.30	124.90
82	MF	202	PEB	C1C-C2C-C3C	-3.66	103.30	107.62
82	DD	202	PEB	CHA-C4A-NA	3.66	129.55	125.20
82	jE	201	PEB	C3D-C4D-ND	3.66	114.43	107.26
82	UI	201	PEB	C3B-C4B-NB	3.66	115.37	110.05
82	OK	203	PEB	C3B-C4B-NB	3.66	115.37	110.05
83	wK	304	PUB	OD-C4D-ND	-3.66	120.51	125.93
85	k6	102	BCR	C37-C22-C21	-3.66	117.80	122.92
82	mJ	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
82	VG	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
82	P4	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
82	H7	203	PEB	C2A-C1A-NA	3.66	111.42	108.27
82	CK	201	PEB	CHC-C4C-NC	3.66	126.10	121.15
82	SH	202	PEB	C1C-CHB-C4B	-3.66	120.08	128.28
82	S1	202	PEB	C1C-CHB-C4B	-3.66	120.08	128.28
82	bE	201	PEB	OA-C1A-C2A	-3.65	123.27	126.17
92	aL	611	LMG	O7-C10-C11	3.65	119.38	111.50
84	K1	1001	CYC	C2A-C1A-NA	3.65	115.36	110.05
82	dG	203	PEB	C3D-C4D-ND	3.65	114.43	107.26
82	JB	202	PEB	C1B-C2B-C3B	-3.65	102.31	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	801	CLA	CAA-C2A-C1A	-3.65	100.00	111.97
82	kM	202	PEB	C1C-CHB-C4B	-3.65	120.09	128.28
82	JQ	202	PEB	CHA-C1B-NB	-3.65	117.29	124.93
82	i4	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
82	WG	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
82	GB	201	PEB	CHC-C4C-NC	3.65	126.09	121.15
83	yF	303	PUB	CHA-C1B-NB	3.65	126.09	121.15
82	PD	203	PEB	OA-C1A-C2A	-3.65	123.27	126.17
84	H1	1001	CYC	C1B-CHB-C4A	-3.65	119.16	128.08
82	SF	201	PEB	C1B-C2B-C3B	-3.65	102.31	106.51
82	S7	202	PEB	C1B-C2B-C3B	-3.65	102.31	106.51
82	AG	301	PEB	C3D-C4D-ND	3.65	114.43	107.26
83	NQ	201	PUB	CHB-C4B-NB	-3.65	116.95	125.32
82	Y9	203	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
82	c4	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
82	TJ	201	PEB	C3B-C4B-NB	3.65	115.36	110.05
87	A2	802	CLA	CAA-C2A-C1A	-3.65	100.00	111.97
82	EJ	201	PEB	C1C-CHB-C4B	3.65	136.47	128.28
82	F4	1002	PEB	CHC-C1D-ND	-3.65	109.10	113.72
82	fG	203	PEB	CHC-C1D-ND	-3.65	109.10	113.72
82	BK	201	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
82	YA	303	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	ND	204	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	ZM	202	PEB	CHC-C4C-NC	3.65	126.09	121.15
82	E7	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
87	AN	829	CLA	CHB-C4A-NA	3.65	129.56	124.51
82	QF	203	PEB	C1C-C2C-C3C	-3.65	103.30	107.62
82	CF	203	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	WI	203	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	vF	201	PEB	CHC-C1D-ND	-3.65	109.10	113.72
82	F5	203	PEB	C2A-C1A-NA	3.65	111.42	108.27
87	cL	515	CLA	CAA-C2A-C3A	-3.65	102.78	112.78
82	mO	202	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
82	OQ	201	PEB	C3D-C4D-ND	3.65	114.42	107.26
84	J4	1001	CYC	CMB-C2B-C1B	3.65	128.73	124.17
82	H1	1002	PEB	C2C-C1C-NC	3.65	112.49	107.57
82	aK	203	PEB	C1C-CHB-C4B	3.65	136.47	128.28
82	T1	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	JA	203	PEB	CAB-C3B-C4B	3.65	131.47	125.01
82	eE	202	PEB	C2A-C1A-NA	3.65	111.42	108.27
82	dH	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
82	LM	202	PEB	CHC-C1D-ND	-3.65	109.11	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aJ	204	PEB	C1C-CHB-C4B	3.65	136.47	128.28
82	u8	202	PEB	CHB-C1C-C2C	-3.65	118.92	127.15
84	ME	1001	CYC	C1B-C2B-C3B	-3.65	104.06	107.87
87	42	604	CLA	C3D-C2D-C1D	3.65	110.81	105.83
82	OI	203	PEB	CHC-C4C-NC	3.65	126.09	121.15
82	eK	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
82	AD	304	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	d1	203	PEB	C3D-C4D-ND	3.65	114.42	107.26
82	QB	201	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
82	RE	201	PEB	CAB-CBB-CGB	-3.65	105.75	113.60
82	f4	201	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
82	F4	1002	PEB	OD-C4D-ND	-3.65	120.52	125.93
83	BM	302	PUB	OD-C4D-ND	-3.65	120.52	125.93
82	cM	202	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
82	uC	202	PEB	CHB-C1C-C2C	-3.65	118.92	127.15
82	YP	501	PEB	C3D-C4D-ND	3.65	114.42	107.26
84	k3	1001	CYC	CMD-C2D-C1D	3.65	130.90	125.56
82	OM	203	PEB	CHC-C1D-ND	-3.65	109.11	113.72
82	SA	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
82	oF	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
83	Z9	302	PUB	CHB-C1C-NC	-3.65	116.98	124.58
82	V1	201	PEB	CHA-C4A-NA	3.65	129.54	125.20
85	B6	601	BCR	C33-C5-C6	-3.65	120.43	124.53
91	aL	610	PHO	CMA-C3A-C4A	-3.65	106.39	114.38
82	OF	203	PEB	C3B-C4B-NB	3.65	115.36	110.05
82	RQ	203	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
84	IO	1001	CYC	C1B-NB-C4B	-3.65	106.02	110.67
82	HB	203	PEB	C2A-C1A-NA	3.65	111.42	108.27
82	N4	1002	PEB	C2A-C1A-NA	3.65	111.42	108.27
82	gK	202	PEB	C2A-C1A-NA	3.65	111.42	108.27
84	CO	1001	CYC	C1B-C2B-C3B	-3.65	104.06	107.87
82	ZM	202	PEB	CAB-C3B-C4B	3.65	131.46	125.01
82	SG	201	PEB	CHC-C4C-NC	3.65	126.09	121.15
84	GE	1001	CYC	CHD-C1D-ND	-3.65	116.96	125.32
82	SP	202	PEB	CHA-C1B-NB	-3.65	117.30	124.93
82	CA	201	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
82	UF	202	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
82	GK	202	PEB	CAC-C2C-C3C	3.65	135.42	127.07
82	L7	201	PEB	OA-C1A-C2A	-3.65	123.27	126.17
82	SE	202	PEB	C4B-C3B-C2B	-3.65	102.75	106.78
82	JH	1002	PEB	C4B-C3B-C2B	-3.65	102.75	106.78
82	Z5	305	PEB	C4B-C3B-C2B	-3.65	102.75	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	f1	202	PEB	CMD-C2D-C3D	3.65	135.21	130.06
82	SH	202	PEB	CMB-C2B-C1B	3.65	130.68	125.06
82	JB	201	PEB	C3D-C4D-ND	3.65	114.41	107.26
82	NP	201	PEB	C2C-C1C-NC	3.65	112.48	107.57
82	Q1	202	PEB	CHB-C1C-C2C	-3.65	118.92	127.15
82	F7	202	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
82	iM	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
82	IJ	203	PEB	C2A-C1A-NA	3.65	111.42	108.27
82	OG	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
82	TH	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
85	A2	848	BCR	C16-C15-C14	-3.65	116.01	123.47
82	DD	202	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
82	DP	202	PEB	CMB-C2B-C1B	3.65	130.68	125.06
82	SJ	202	PEB	CHC-C4C-NC	3.65	126.08	121.15
87	B2	805	CLA	CMB-C2B-C1B	-3.65	119.82	125.37
82	U1	203	PEB	C1D-CHC-C4C	-3.65	107.88	113.26
82	XM	201	PEB	C2C-C1C-NC	3.65	112.48	107.57
82	R4	203	PEB	C1C-C2C-C3C	-3.65	103.31	107.62
85	K6	102	BCR	C37-C22-C21	-3.65	117.82	122.92
82	G7	201	PEB	CMB-C2B-C1B	3.64	130.68	125.06
82	Y9	202	PEB	C1C-CHB-C4B	3.64	136.46	128.28
82	VQ	203	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	a4	202	PEB	C2A-C1A-NA	3.64	111.42	108.27
82	dJ	201	PEB	C2A-C1A-NA	3.64	111.42	108.27
82	kM	201	PEB	C2A-C1A-NA	3.64	111.42	108.27
82	R7	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
82	y8	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
94	dL	406	PL9	C20-C19-C21	3.64	121.40	115.27
84	F3	1001	CYC	CMD-C2D-C1D	3.64	130.90	125.56
85	BN	803	BCR	C24-C23-C22	3.64	131.74	126.23
82	P4	202	PEB	CMB-C2B-C1B	3.64	130.68	125.06
82	AG	301	PEB	CHC-C4C-NC	3.64	126.08	121.15
82	OK	201	PEB	CHC-C1D-ND	-3.64	109.11	113.72
82	UP	202	PEB	CHC-C1D-ND	-3.64	109.11	113.72
82	UJ	201	PEB	C1B-C2B-C3B	-3.64	102.32	106.51
85	bL	602	BCR	C11-C10-C9	-3.64	122.11	127.31
82	UF	201	PEB	C2A-C1A-NA	-3.64	105.13	108.27
82	DB	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	QK	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	hJ	203	PEB	OA-C1A-C2A	-3.64	123.28	126.17
84	W3	1001	CYC	CAB-C3B-C4B	3.64	127.13	121.38
88	AL	406	LHG	O7-C7-C8	3.64	119.35	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gJ	201	PEB	CHB-C1C-NC	-3.64	116.97	125.32
87	A2	801	CLA	CHB-C4A-NA	3.64	129.55	124.51
82	P1	201	PEB	CHA-C1B-NB	-3.64	117.31	124.93
82	NA	201	PEB	CHC-C1D-ND	-3.64	109.11	113.72
82	OM	201	PEB	CHA-C1B-C2B	3.64	134.27	124.90
94	D6	408	PL9	C37-C38-C39	-3.64	118.89	127.66
82	AH	302	PEB	CHC-C4C-NC	3.64	126.08	121.15
82	IQ	202	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
82	HJ	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	aM	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	hM	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	GM	203	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	HP	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	aF	203	PEB	CHB-C1C-C2C	-3.64	118.93	127.15
82	YB	201	PEB	C3D-C4D-ND	3.64	114.41	107.26
82	JD	203	PEB	C3D-C4D-ND	3.64	114.41	107.26
82	OE	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
82	fM	203	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
82	P4	202	PEB	C1C-CHB-C4B	3.64	136.45	128.28
82	VE	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	IJ	201	PEB	CHC-C1D-ND	-3.64	109.12	113.72
82	DG	1002	PEB	C2C-C1C-NC	3.64	112.47	107.57
82	VB	202	PEB	C3B-C4B-NB	3.64	115.35	110.05
82	GD	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
84	h3	1001	CYC	CMD-C2D-C1D	3.64	130.89	125.56
82	YM	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	KI	201	PEB	CHA-C1B-C2B	3.64	134.26	124.90
82	WG	203	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	i1	202	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	CF	203	PEB	C1C-C2C-C3C	-3.64	103.32	107.62
82	lM	201	PEB	CHC-C1D-ND	-3.64	109.12	113.72
82	XQ	202	PEB	C2C-C1C-NC	3.64	112.47	107.57
82	iF	201	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
82	ZO	201	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
82	hJ	202	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	NK	201	PEB	CHA-C1B-NB	-3.64	117.32	124.93
82	dG	203	PEB	CHA-C1B-NB	-3.64	117.32	124.93
82	TE	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	QB	203	PEB	CHC-C1D-ND	-3.64	109.12	113.72
85	b6	602	BCR	C34-C9-C8	3.64	123.81	118.08
95	lL	101	DGD	O6E-C5E-C4E	3.64	116.30	109.69
82	ID	202	PEB	C4B-C3B-C2B	-3.64	102.75	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JM	201	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
84	H3	1001	CYC	CMD-C2D-C1D	3.64	130.89	125.56
84	o3	1001	CYC	CMD-C2D-C1D	3.64	130.89	125.56
82	fM	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	XK	202	PEB	C3C-C4C-NC	3.64	111.61	108.33
82	OM	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
82	jE	201	PEB	CHC-C4C-NC	3.64	126.08	121.15
82	m1	202	PEB	CAA-C3A-C4A	3.64	122.02	112.67
82	WQ	202	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	P4	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	bF	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
83	yK	302	PUB	C1C-C2C-C3C	-3.64	102.75	106.78
95	BL	614	DGD	O2G-C1B-C2B	3.64	119.34	111.50
85	A2	847	BCR	C21-C20-C19	-3.64	111.86	123.22
82	AI	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
82	fH	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	qK	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	iH	202	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	WI	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
82	u8	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
82	BA	201	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
82	SA	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	QH	203	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	iO	202	PEB	CMB-C2B-C1B	3.64	130.67	125.06
82	fH	202	PEB	CMD-C2D-C3D	3.64	135.19	130.06
82	N7	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
83	M9	303	PUB	CHB-C1C-NC	-3.64	117.01	124.58
87	4N	604	CLA	C3D-C2D-C1D	3.64	110.80	105.83
82	KQ	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	G7	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
84	MO	1001	CYC	CMA-C3A-C4A	3.64	130.66	125.06
82	SF	201	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
82	B7	201	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
82	jM	202	PEB	C3D-C4D-ND	3.64	114.39	107.26
82	C7	201	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
85	AN	848	BCR	C16-C15-C14	-3.64	116.02	123.47
83	QJ	201	PUB	C4B-CHB-C1C	-3.64	120.13	128.28
82	tK	203	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	MM	201	PEB	C1D-CHC-C4C	-3.64	107.89	113.26
82	HI	201	PEB	C2C-C1C-NC	3.64	112.47	107.57
82	RB	201	PEB	C4C-C3C-C2C	-3.64	104.14	107.50
82	M5	305	PEB	C4B-C3B-C2B	-3.64	102.76	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W9	202	PEB	C3D-C4D-ND	3.64	114.39	107.26
82	oF	203	PEB	C3D-C4D-ND	3.64	114.39	107.26
84	H4	1001	CYC	CMB-C2B-C1B	3.64	128.71	124.17
83	xK	305	PUB	CHC-C1D-ND	-3.64	109.12	113.72
82	OH	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	Q9	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
82	EA	201	PEB	C1C-C2C-C3C	-3.64	103.32	107.62
84	q3	1001	CYC	CMD-C2D-C1D	3.64	130.88	125.56
87	A2	852	CLA	CHD-C1D-ND	-3.64	121.11	124.45
82	f1	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
82	IB	202	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
82	AF	201	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
82	pC	201	PEB	CHC-C1D-ND	-3.64	109.12	113.72
82	mH	202	PEB	CAA-C3A-C4A	3.64	122.01	112.67
82	RA	202	PEB	C3D-C4D-ND	3.64	114.39	107.26
84	I3	1001	CYC	CMD-C2D-C1D	3.63	130.88	125.56
82	J9	202	PEB	OA-C1A-C2A	-3.63	123.28	126.17
82	nF	201	PEB	C3D-C4D-ND	3.63	114.39	107.26
82	HB	201	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	B9	202	PEB	C1B-C2B-C3B	-3.63	102.33	106.51
82	WB	401	PEB	C2A-C1A-NA	3.63	111.41	108.27
82	AI	203	PEB	C2A-C1A-NA	3.63	111.41	108.27
82	Z5	304	PEB	C2A-C1A-NA	3.63	111.41	108.27
87	BN	806	CLA	CMB-C2B-C1B	-3.63	119.83	125.37
84	EG	1001	CYC	C2B-C1B-NB	3.63	112.31	106.99
82	JQ	203	PEB	C3D-C4D-ND	3.63	114.39	107.26
82	V7	202	PEB	C3D-C4D-ND	3.63	114.39	107.26
83	AH	304	PUB	CHB-C4B-NB	-3.63	117.00	125.32
82	b4	202	PEB	CHC-C4C-NC	3.63	126.07	121.15
82	D7	203	PEB	CHC-C1D-ND	-3.63	109.13	113.72
82	GJ	201	PEB	OA-C1A-C2A	-3.63	123.28	126.17
82	XK	203	PEB	OA-C1A-C2A	-3.63	123.28	126.17
82	dH	203	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	lK	202	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	b1	203	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
82	W5	202	PEB	C2C-C1C-NC	3.63	112.46	107.57
82	d1	201	PEB	C2A-C1A-NA	3.63	111.41	108.27
94	D6	408	PL9	C22-C23-C24	-3.63	118.91	127.66
84	H3	1001	CYC	CAB-C3B-C4B	3.63	127.12	121.38
82	WA	201	PEB	CHA-C1B-NB	-3.63	117.33	124.93
82	iK	201	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	OD	201	PEB	C3D-C4D-ND	3.63	114.39	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	B3	1001	CYC	CMD-C2D-C1D	3.63	130.88	125.56
82	CK	203	PEB	OA-C1A-C2A	-3.63	123.28	126.17
82	cO	202	PEB	OA-C1A-C2A	-3.63	123.28	126.17
82	FO	1002	PEB	OD-C4D-ND	-3.63	120.55	125.93
82	kJ	201	PEB	OD-C4D-ND	-3.63	120.55	125.93
82	QD	202	PEB	C2A-C1A-NA	3.63	111.40	108.27
95	b6	621	DGD	C1E-O6E-C5E	3.63	120.82	113.69
82	hO	202	PEB	C3D-C4D-ND	3.63	114.39	107.26
84	MO	1001	CYC	C1B-C2B-C3B	-3.63	104.08	107.87
82	XP	201	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	D5	203	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	CM	201	PEB	CHC-C4C-NC	3.63	126.06	121.15
82	MK	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
84	y3	1001	CYC	CAB-C3B-C4B	3.63	127.11	121.38
85	B6	601	BCR	C3-C4-C5	-3.63	107.59	114.08
82	I7	201	PEB	CHA-C1B-NB	-3.63	117.34	124.93
82	P1	201	PEB	C3B-C4B-NB	3.63	115.33	110.05
82	sC	203	PEB	OA-C1A-C2A	-3.63	123.29	126.17
82	H7	203	PEB	C3D-C4D-ND	3.63	114.38	107.26
84	O3	1001	CYC	CMD-C2D-C1D	3.63	130.88	125.56
82	CF	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
82	LE	1002	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	LJ	201	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
82	eB	202	PEB	CHC-C4C-NC	3.63	126.06	121.15
82	Y9	203	PEB	CMB-C2B-C1B	3.63	130.66	125.06
82	cF	201	PEB	CMB-C2B-C1B	3.63	130.66	125.06
82	U9	201	PEB	CAB-C3B-C4B	3.63	131.43	125.01
85	CL	516	BCR	C15-C14-C13	-3.63	122.13	127.31
84	Q3	1001	CYC	CMD-C2D-C1D	3.63	130.88	125.56
82	QH	202	PEB	C1C-CHB-C4B	3.63	136.42	128.28
82	VE	202	PEB	CHC-C4C-NC	3.63	126.06	121.15
82	kM	201	PEB	CMB-C2B-C1B	3.63	130.65	125.06
82	kF	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
83	xK	301	PUB	CMB-C2B-C1B	3.63	130.91	127.06
82	BF	201	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
82	JD	201	PEB	OA-C1A-C2A	-3.63	123.29	126.17
82	kO	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
82	Z9	301	PEB	C3D-C4D-ND	3.63	114.38	107.26
82	dH	202	PEB	CMB-C2B-C1B	3.63	130.65	125.06
82	LH	1003	PEB	C3B-C4B-NB	3.63	115.33	110.05
94	d6	408	PL9	C37-C38-C39	-3.63	118.92	127.66
82	SP	203	PEB	C3D-C4D-ND	3.63	114.38	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PO	202	PEB	C1C-CHB-C4B	3.63	136.42	128.28
82	GA	201	PEB	CMB-C2B-C1B	3.63	130.65	125.06
82	QP	202	PEB	CHB-C1C-C2C	-3.63	118.96	127.15
82	QK	201	PEB	C3D-C4D-ND	3.63	114.38	107.26
84	U3	1001	CYC	CMD-C2D-C1D	3.63	130.87	125.56
82	mJ	201	PEB	OD-C4D-ND	-3.63	120.56	125.93
85	L2	205	BCR	C21-C20-C19	-3.63	111.90	123.22
82	DA	203	PEB	C1D-CHC-C4C	-3.63	107.91	113.26
84	S3	1001	CYC	CMD-C2D-C1D	3.63	130.87	125.56
85	fL	101	BCR	C28-C27-C26	-3.63	107.60	114.08
82	O1	201	PEB	C3D-C4D-ND	3.63	114.38	107.26
82	eG	202	PEB	C2A-C1A-NA	3.63	111.40	108.27
84	KG	202	CYC	C1D-C2D-C3D	-3.63	103.17	107.79
82	JQ	201	PEB	OA-C1A-C2A	-3.63	123.29	126.17
82	cH	201	PEB	C3B-C4B-NB	3.63	115.33	110.05
82	W1	201	PEB	CHA-C1B-NB	-3.63	117.35	124.93
82	KK	203	PEB	C1D-CHC-C4C	-3.63	107.91	113.26
82	cK	202	PEB	C1D-CHC-C4C	-3.63	107.91	113.26
82	jG	201	PEB	C3D-C4D-ND	3.63	114.38	107.26
82	DI	202	PEB	CHC-C1D-ND	-3.63	109.14	113.72
82	P1	202	PEB	CAC-CBC-CGC	-3.63	105.80	113.60
82	eO	203	PEB	CAB-C3B-C4B	3.63	131.43	125.01
82	aB	202	PEB	C3D-C4D-ND	3.63	114.37	107.26
82	1C	203	PEB	C3D-C4D-ND	3.63	114.37	107.26
82	oK	203	PEB	C3D-C4D-ND	3.63	114.37	107.26
82	L1	1002	PEB	C3B-C4B-NB	3.63	115.32	110.05
82	e1	201	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
87	5N	608	CLA	CAA-C2A-C3A	-3.63	107.64	116.10
82	mM	201	PEB	OA-C1A-C2A	-3.63	123.29	126.17
84	G4	1001	CYC	C2D-C1D-ND	3.63	112.50	107.40
82	fH	203	PEB	C2C-C1C-NC	3.63	112.45	107.57
87	A2	852	CLA	C4A-NA-C1A	3.63	108.34	106.71
82	EJ	201	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
82	iG	201	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
82	vF	201	PEB	C1D-CHC-C4C	3.63	118.60	113.26
84	d3	1001	CYC	CMD-C2D-C1D	3.63	130.87	125.56
82	B9	203	PEB	CMB-C2B-C1B	3.63	130.65	125.06
82	CM	202	PEB	C2A-C1A-NA	3.62	111.40	108.27
82	QF	201	PEB	C3D-C4D-ND	3.62	114.37	107.26
82	AJ	301	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	v8	202	PEB	CHA-C1B-NB	-3.62	117.35	124.93
82	dF	201	PEB	CHA-C1B-NB	-3.62	117.35	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QH	202	PEB	CHB-C1C-C2C	-3.62	118.97	127.15
82	NI	203	PEB	C4B-C3B-C2B	-3.62	102.77	106.78
87	BN	805	CLA	CMB-C2B-C1B	-3.62	119.85	125.37
82	HM	201	PEB	C3B-C4B-NB	3.62	115.32	110.05
82	aM	203	PEB	CHB-C1C-NC	-3.62	117.02	125.32
83	A1	304	PUB	CHB-C4B-NB	-3.62	117.02	125.32
87	2N	309	CLA	CAC-C3C-C4C	3.62	129.51	124.81
82	NO	1002	PEB	C2A-C1A-NA	3.62	111.40	108.27
82	kJ	201	PEB	C4B-C3B-C2B	-3.62	102.77	106.78
82	QF	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	E7	201	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	QG	202	PEB	CHC-C4C-NC	3.62	126.05	121.15
84	k3	1001	CYC	CAB-C3B-C4B	3.62	127.10	121.38
82	PH	201	PEB	CHA-C1B-NB	-3.62	117.35	124.93
82	LJ	201	PEB	CHA-C1B-NB	-3.62	117.35	124.93
84	LH	1001	CYC	C1B-NB-C4B	-3.62	106.06	110.67
88	B6	617	LHG	O7-C7-C8	3.62	119.31	111.50
83	AJ	304	PUB	CBA-CAA-C3A	-3.62	107.48	112.98
82	gF	202	PEB	C3D-C4D-ND	3.62	114.37	107.26
82	Q9	203	PEB	OD-C4D-ND	-3.62	120.56	125.93
82	fJ	202	PEB	C2A-C1A-NA	3.62	111.40	108.27
84	IE	1001	CYC	CHB-C4A-NA	-3.62	117.36	124.93
82	OI	201	PEB	CHC-C4C-NC	3.62	126.05	121.15
82	BD	203	PEB	C3D-C4D-ND	3.62	114.37	107.26
82	Y1	201	PEB	C3D-C4D-ND	3.62	114.37	107.26
82	Y7	303	PEB	C3D-C4D-ND	3.62	114.37	107.26
82	hE	203	PEB	C3D-C4D-ND	3.62	114.37	107.26
82	AF	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	wF	302	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	tK	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	M9	302	PEB	C1B-C2B-C3B	-3.62	102.35	106.51
84	d3	1001	CYC	CAB-C3B-C4B	3.62	127.10	121.38
83	ND	201	PUB	CHB-C4B-NB	-3.62	117.02	125.32
82	YA	303	PEB	C4B-C3B-C2B	-3.62	102.77	106.78
82	VK	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	wC	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	mO	203	PEB	C3B-C4B-NB	3.62	115.32	110.05
84	D3	1001	CYC	CMD-C2D-C1D	3.62	130.86	125.56
82	ZG	203	PEB	C3D-C4D-ND	3.62	114.36	107.26
85	A2	847	BCR	C15-C14-C13	-3.62	122.14	127.31
82	AE	301	PEB	OA-C1A-C2A	-3.62	123.29	126.17
82	LG	1002	PEB	C4B-C3B-C2B	-3.62	102.78	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	m4	202	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
85	FN	204	BCR	C7-C8-C9	-3.62	120.76	126.23
85	BN	840	BCR	C11-C10-C9	-3.62	122.14	127.31
85	I2	101	BCR	C20-C21-C22	-3.62	122.14	127.31
82	PD	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	WK	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	YF	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
84	y3	1001	CYC	C1D-C2D-C3D	-3.62	103.18	107.79
82	AG	304	PEB	CMB-C2B-C1B	3.62	130.64	125.06
88	ML	102	LHG	O7-C7-C8	3.62	119.30	111.50
83	QJ	201	PUB	CHB-C4B-NB	-3.62	117.03	125.32
85	LN	205	BCR	C21-C20-C19	-3.62	111.92	123.22
82	DF	201	PEB	OA-C1A-NA	3.62	129.33	124.94
82	j4	203	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
91	a6	613	PHO	CBC-CAC-C3C	-3.62	107.58	112.88
82	dM	201	PEB	C3C-C4C-NC	3.62	111.59	108.33
82	EA	201	PEB	CMB-C2B-C1B	3.62	130.64	125.06
82	OE	202	PEB	CMB-C2B-C1B	3.62	130.64	125.06
84	C4	1001	CYC	C1B-C2B-C3B	-3.62	104.09	107.87
82	VP	201	PEB	C3B-C4B-NB	3.62	115.31	110.05
82	IK	203	PEB	OD-C4D-ND	-3.62	120.57	125.93
82	NA	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	iO	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
84	D1	1001	CYC	C2C-C1C-NC	3.62	111.39	108.27
87	52	608	CLA	CAA-C2A-C3A	-3.62	107.65	116.10
82	KE	201	PEB	CMB-C2B-C1B	3.62	130.64	125.06
82	mE	203	PEB	CHC-C4C-NC	3.62	126.05	121.15
82	Z1	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
82	ZJ	201	PEB	OD-C4D-ND	-3.62	120.57	125.93
82	P1	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	qK	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	KJ	202	PEB	C3C-C4C-NC	3.62	111.59	108.33
83	Z9	305	PUB	C2B-C1B-NB	3.62	111.59	108.33
82	BI	202	PEB	CHA-C1B-C2B	3.62	134.21	124.90
84	KG	202	CYC	CHD-C1D-ND	-3.62	117.03	125.32
85	AN	847	BCR	C15-C14-C13	-3.62	122.15	127.31
82	LQ	201	PEB	CHA-C1B-NB	-3.62	117.36	124.93
82	a1	201	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	wC	204	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	eH	201	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	Y7	304	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
82	PA	203	PEB	CAB-CBB-CGB	-3.62	105.82	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O1	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	JP	202	PEB	CHA-C1B-NB	-3.62	117.36	124.93
85	B2	802	BCR	C24-C23-C22	3.62	131.70	126.23
82	gH	203	PEB	C1C-CHB-C4B	3.62	136.39	128.28
82	NF	202	PEB	CHB-C4B-C3B	-3.62	116.95	125.32
82	YF	203	PEB	CHA-C1B-C2B	3.62	134.20	124.90
82	PO	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	cK	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	J1	1002	PEB	C1D-CHC-C4C	-3.62	107.92	113.26
82	ZE	203	PEB	CHC-C4C-NC	3.62	126.04	121.15
82	LI	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
82	GQ	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
84	FG	1001	CYC	C2D-C1D-ND	3.62	112.48	107.40
82	iE	201	PEB	CMB-C2B-C1B	3.62	130.63	125.06
85	K2	105	BCR	C27-C26-C25	-3.62	117.48	122.73
84	HO	1001	CYC	CMB-C2B-C1B	3.62	128.68	124.17
82	S5	203	PEB	CHC-C4C-NC	3.62	126.04	121.15
82	mG	201	PEB	OA-C1A-C2A	-3.62	123.30	126.17
82	hM	201	PEB	OA-C1A-C2A	-3.62	123.30	126.17
85	AN	847	BCR	C37-C22-C23	3.62	123.77	118.08
82	DM	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
82	WE	203	PEB	CMB-C2B-C1B	3.62	130.63	125.06
82	sF	202	PEB	C1C-C2C-C3C	-3.62	103.35	107.62
82	eG	202	PEB	C1C-C2C-C3C	-3.62	103.35	107.62
82	ZK	202	PEB	OD-C4D-ND	-3.62	120.57	125.93
87	B2	804	CLA	CMB-C2B-C1B	-3.62	119.86	125.37
82	UD	201	PEB	C3D-C4D-ND	3.62	114.35	107.26
85	cL	518	BCR	C28-C27-C26	-3.62	107.62	114.08
82	GB	201	PEB	CMB-C2B-C1B	3.62	130.63	125.06
82	RG	201	PEB	CAB-CBB-CGB	-3.61	105.82	113.60
82	iH	202	PEB	C1D-CHC-C4C	3.61	118.59	113.26
82	VB	202	PEB	C3D-C4D-ND	3.61	114.35	107.26
82	L5	202	PEB	C3D-C4D-ND	3.61	114.35	107.26
82	QJ	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
82	hG	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
82	CK	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	DK	201	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
82	nF	201	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
82	ZJ	202	PEB	CMB-C2B-C1B	3.61	130.63	125.06
82	cK	202	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
82	aF	203	PEB	C1C-CHB-C4B	3.61	136.39	128.28
82	bO	202	PEB	CHC-C4C-NC	3.61	126.04	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	L3	1001	CYC	CAB-C3B-C4B	3.61	127.09	121.38
84	n3	1001	CYC	CAB-C3B-C4B	3.61	127.09	121.38
82	WF	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	AJ	301	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	bK	202	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	AK	202	PEB	C2C-C1C-NC	3.61	112.44	107.57
82	DQ	202	PEB	CHA-C4A-NA	3.61	129.50	125.20
84	j3	1001	CYC	CMD-C2D-C1D	3.61	130.85	125.56
82	AE	304	PEB	CMB-C2B-C1B	3.61	130.63	125.06
82	WE	203	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
82	l1	201	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
82	PO	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
82	N7	202	PEB	CMB-C2B-C1B	3.61	130.63	125.06
82	RE	201	PEB	CHC-C1D-ND	-3.61	109.15	113.72
82	pC	202	PEB	CHC-C1D-ND	-3.61	109.15	113.72
82	FJ	202	PEB	CHC-C4C-NC	3.61	126.04	121.15
82	f4	201	PEB	CHC-C4C-NC	3.61	126.04	121.15
82	YK	201	PEB	C1C-C2C-C3C	-3.61	103.35	107.62
82	fJ	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
82	ED	202	PEB	C3D-C4D-ND	3.61	114.35	107.26
82	uC	203	PEB	C3D-C4D-ND	3.61	114.35	107.26
82	TK	202	PEB	C1D-CHC-C4C	3.61	118.58	113.26
96	v6	201	HEM	CHA-C4D-ND	3.61	128.83	124.37
82	R7	202	PEB	C3C-C4C-NC	3.61	111.58	108.33
84	D3	1001	CYC	CAB-C3B-C4B	3.61	127.08	121.38
82	YO	203	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
84	M4	1001	CYC	C1B-C2B-C3B	-3.61	104.10	107.87
82	YI	201	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
82	gF	202	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
84	EE	1001	CYC	C2B-C1B-NB	3.61	112.28	106.99
82	y8	203	PEB	C1C-CHB-C4B	-3.61	120.18	128.28
84	K4	1001	CYC	C1B-NB-C4B	-3.61	106.07	110.67
84	h3	1001	CYC	CAB-C3B-C4B	3.61	127.08	121.38
82	J5	201	PEB	C3B-C4B-NB	3.61	115.30	110.05
82	DF	202	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	TQ	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	oF	203	PEB	CHC-C4C-NC	3.61	126.04	121.15
82	gO	201	PEB	CHC-C4C-NC	3.61	126.04	121.15
84	q3	1001	CYC	CAB-C3B-C4B	3.61	127.08	121.38
82	RD	202	PEB	CHA-C1B-NB	-3.61	117.38	124.93
82	W7	201	PEB	CHA-C1B-NB	-3.61	117.38	124.93
85	B6	601	BCR	C24-C23-C22	-3.61	120.78	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A2	847	BCR	C37-C22-C23	3.61	123.77	118.08
92	d6	409	LMG	O7-C10-C11	3.61	119.28	111.50
82	D7	203	PEB	C1D-CHC-C4C	-3.61	107.93	113.26
82	YQ	202	PEB	C2A-C1A-NA	3.61	111.39	108.27
82	OI	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
82	WQ	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
82	V5	201	PEB	OA-C1A-C2A	-3.61	123.30	126.17
82	U9	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
82	DF	201	PEB	CHC-C1D-ND	-3.61	109.16	113.72
82	gG	201	PEB	C3B-C4B-NB	3.61	115.30	110.05
84	f3	1001	CYC	CMD-C2D-C1D	3.61	130.85	125.56
82	FP	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
84	H1	1001	CYC	C1B-C2B-C3B	-3.61	104.11	107.87
84	GO	1001	CYC	C2D-C1D-ND	3.61	112.47	107.40
82	QE	203	PEB	C3D-C4D-ND	3.61	114.34	107.26
85	bL	602	BCR	C3-C4-C5	-3.61	107.63	114.08
82	CA	201	PEB	OA-C1A-C2A	-3.61	123.30	126.17
83	M5	303	PUB	CMD-C2D-C3D	3.61	133.18	127.77
82	lF	202	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
82	cF	201	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
84	C4	1001	CYC	C1B-NB-C4B	-3.61	106.08	110.67
82	lF	202	PEB	CHB-C1C-C2C	-3.61	119.01	127.15
84	I3	1001	CYC	CAB-C3B-C4B	3.61	127.08	121.38
82	KB	302	PEB	CHA-C1B-NB	-3.61	117.39	124.93
82	AQ	304	PEB	C3D-C4D-ND	3.61	114.34	107.26
82	LQ	203	PEB	C3D-C4D-ND	3.61	114.34	107.26
84	Q3	1001	CYC	CAB-C3B-C4B	3.61	127.08	121.38
82	V9	202	PEB	CHA-C1B-NB	-3.61	117.39	124.93
83	xF	301	PUB	CMB-C2B-C1B	3.61	130.88	127.06
85	C6	508	BCR	C28-C27-C26	-3.61	107.64	114.08
85	KN	104	BCR	C27-C26-C25	-3.61	117.49	122.73
82	OH	201	PEB	C3D-C4D-ND	3.61	114.34	107.26
84	DG	1001	CYC	C1D-C2D-C3D	-3.61	103.20	107.79
82	FM	202	PEB	CHC-C1D-ND	-3.61	109.16	113.72
82	YI	202	PEB	C2A-C1A-NA	3.61	111.38	108.27
82	WP	202	PEB	C1B-C2B-C3B	-3.61	102.37	106.51
82	b4	201	PEB	CHB-C1C-C2C	-3.61	119.01	127.15
84	w3	1001	CYC	CAB-C3B-C4B	3.61	127.07	121.38
84	LE	1001	CYC	C1D-C2D-C3D	-3.61	103.20	107.79
84	LG	1001	CYC	C1D-C2D-C3D	-3.61	103.20	107.79
82	TH	201	PEB	C3D-C4D-ND	3.61	114.33	107.26
82	h4	202	PEB	C3D-C4D-ND	3.61	114.33	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	F9	202	PEB	C3D-C4D-ND	3.61	114.33	107.26
82	YM	202	PEB	OA-C1A-C2A	-3.61	123.31	126.17
83	yK	303	PUB	CHA-C1B-NB	3.61	126.03	121.15
82	Z9	301	PEB	C1B-C2B-C3B	-3.61	102.37	106.51
82	EK	201	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
82	vC	202	PEB	CHA-C1B-NB	-3.61	117.39	124.93
82	V1	203	PEB	C2A-C1A-NA	3.61	111.38	108.27
82	mJ	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
84	L4	1001	CYC	C2D-C1D-ND	3.61	112.47	107.40
82	i1	202	PEB	C1D-CHC-C4C	3.61	118.57	113.26
82	U5	203	PEB	CAC-CBC-CGC	-3.61	105.84	113.60
87	A2	801	CLA	CHD-C1D-ND	-3.61	121.14	124.45
82	UQ	201	PEB	C3D-C4D-ND	3.60	114.33	107.26
84	LG	1001	CYC	CHA-C4D-C3D	-3.60	119.02	127.15
85	B2	839	BCR	C33-C5-C6	-3.60	120.48	124.53
84	E4	1001	CYC	C4D-CHA-C1A	3.60	136.37	128.28
82	i4	202	PEB	CMB-C2B-C1B	3.60	130.62	125.06
82	jG	202	PEB	OA-C1A-C2A	-3.60	123.31	126.17
82	w8	204	PEB	C3D-C4D-ND	3.60	114.33	107.26
82	Y5	201	PEB	CHC-C1D-ND	-3.60	109.16	113.72
82	V1	201	PEB	C1C-CHB-C4B	3.60	136.37	128.28
84	EO	1001	CYC	C4D-CHA-C1A	3.60	136.37	128.28
85	F2	204	BCR	C7-C8-C9	-3.60	120.79	126.23
82	AO	301	PEB	CHC-C4C-NC	3.60	126.03	121.15
82	eG	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
87	82	306	CLA	CMB-C2B-C1B	-3.60	119.88	125.37
82	LP	202	PEB	CMB-C2B-C1B	3.60	130.61	125.06
85	BN	839	BCR	C33-C5-C6	-3.60	120.48	124.53
82	QG	203	PEB	C3D-C4D-ND	3.60	114.33	107.26
82	YA	304	PEB	C4B-C3B-C2B	-3.60	102.79	106.78
82	B9	203	PEB	C4B-C3B-C2B	-3.60	102.79	106.78
82	DK	201	PEB	CHC-C1D-ND	-3.60	109.17	113.72
82	dK	201	PEB	CHA-C1B-NB	-3.60	117.39	124.93
82	C5	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
82	C7	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
82	NA	202	PEB	OD-C4D-ND	-3.60	120.59	125.93
82	TD	202	PEB	C1D-CHC-C4C	3.60	118.57	113.26
82	R4	201	PEB	C3B-C4B-NB	3.60	115.29	110.05
82	cB	403	PEB	C3D-C4D-ND	3.60	114.33	107.26
82	hG	203	PEB	C3D-C4D-ND	3.60	114.33	107.26
82	bP	501	PEB	CMB-C2B-C1B	3.60	130.61	125.06
84	M3	1001	CYC	CAB-C3B-C4B	3.60	127.07	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	sF	201	PEB	C3B-C4B-NB	3.60	115.29	110.05
84	GO	1001	CYC	C1B-C2B-C3B	-3.60	104.11	107.87
82	WH	201	PEB	C1B-C2B-C3B	-3.60	102.37	106.51
82	O1	202	PEB	C1B-C2B-C3B	-3.60	102.37	106.51
82	XB	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
82	GF	201	PEB	C1C-C2C-C3C	-3.60	103.36	107.62
82	GF	202	PEB	CAC-C2C-C3C	3.60	135.32	127.07
82	iO	203	PEB	CHC-C4C-NC	3.60	126.02	121.15
82	cB	402	PEB	C3D-C4D-ND	3.60	114.33	107.26
82	RJ	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
82	V4	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
82	W9	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
82	LF	202	PEB	C3B-C4B-NB	3.60	115.29	110.05
82	DB	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
82	YH	201	PEB	C3D-C4D-ND	3.60	114.33	107.26
82	ZM	201	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	MF	202	PEB	C3D-C4D-ND	3.60	114.32	107.26
84	W3	1001	CYC	C1D-C2D-C3D	-3.60	103.20	107.79
82	TQ	202	PEB	C1D-CHC-C4C	3.60	118.56	113.26
82	ZH	203	PEB	C3D-C4D-ND	3.60	114.32	107.26
82	OK	202	PEB	CHA-C1B-NB	-3.60	117.40	124.93
82	OJ	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
82	J1	1002	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	Q5	203	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	y8	203	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	nK	201	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	JF	201	PEB	C2C-C1C-NC	3.60	112.42	107.57
82	pC	202	PEB	OD-C4D-ND	-3.60	120.60	125.93
82	SM	203	PEB	C1C-CHB-C4B	3.60	136.35	128.28
84	IG	1001	CYC	CHB-C4A-NA	-3.60	117.40	124.93
82	RJ	201	PEB	CHC-C1D-ND	3.60	118.28	113.72
82	YI	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
82	QJ	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
82	Q1	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
82	RQ	202	PEB	CHA-C1B-NB	-3.60	117.40	124.93
82	Q5	201	PEB	CHA-C1B-NB	-3.60	117.40	124.93
84	u3	1001	CYC	CAB-C3B-C4B	3.60	127.06	121.38
82	VD	203	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	UI	201	PEB	C2C-C1C-NC	3.60	112.42	107.57
82	HA	203	PEB	C1C-CHB-C4B	3.60	136.35	128.28
82	GK	201	PEB	CHC-C1D-ND	-3.60	109.17	113.72
82	F5	202	PEB	CHC-C1D-ND	-3.60	109.17	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	K6	102	BCR	C28-C27-C26	-3.60	107.65	114.08
82	QK	201	PEB	C3B-C4B-NB	3.60	115.28	110.05
84	EH	1001	CYC	C2A-C1A-NA	3.60	115.28	110.05
85	IN	101	BCR	C20-C21-C22	-3.60	122.17	127.31
82	OF	201	PEB	C1B-C2B-C3B	-3.60	102.38	106.51
82	ND	204	PEB	C1C-CHB-C4B	3.60	136.35	128.28
82	LO	1002	PEB	C2A-C1A-NA	3.60	111.38	108.27
82	XK	202	PEB	OA-C1A-C2A	-3.60	123.31	126.17
84	F4	1001	CYC	CMA-C3A-C4A	3.60	130.60	125.06
82	a4	201	PEB	C3B-C4B-NB	3.60	115.28	110.05
82	Z5	301	PEB	C3B-C4B-NB	3.60	115.28	110.05
82	QJ	202	PEB	CHC-C1D-ND	-3.60	109.17	113.72
85	B2	841	BCR	C21-C20-C19	-3.60	111.99	123.22
82	IF	203	PEB	C1C-NC-C4C	-3.60	103.20	109.60
85	J2	102	BCR	C24-C23-C22	3.60	131.67	126.23
82	oK	203	PEB	CHC-C4C-NC	3.60	126.02	121.15
82	jM	201	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	eK	201	PEB	C3D-C4D-ND	3.60	114.32	107.26
84	U3	1001	CYC	CAB-C3B-C4B	3.60	127.06	121.38
82	eK	203	PEB	C2A-C1A-NA	3.60	111.37	108.27
82	cJ	202	PEB	CHB-C4B-NB	-3.60	117.09	124.58
82	RA	203	PEB	C1D-CHC-C4C	-3.60	107.95	113.26
83	Z5	303	PUB	CMD-C2D-C3D	3.60	133.17	127.77
82	gB	202	PEB	CMB-C2B-C1B	3.60	130.60	125.06
84	B3	1001	CYC	CAB-C3B-C4B	3.60	127.06	121.38
84	LE	1001	CYC	CHA-C4D-C3D	-3.60	119.04	127.15
82	PJ	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
84	CO	1001	CYC	C1B-NB-C4B	-3.60	106.09	110.67
82	dH	203	PEB	C3D-C4D-ND	3.60	114.31	107.26
82	QI	201	PEB	C2A-C1A-NA	3.60	111.37	108.27
82	gH	201	PEB	C2A-C1A-NA	3.60	111.37	108.27
82	A1	302	PEB	CHC-C4C-NC	3.60	126.02	121.15
82	a4	203	PEB	CHC-C4C-NC	3.60	126.02	121.15
82	fO	201	PEB	C1B-C2B-C3B	-3.60	102.38	106.51
82	Q1	202	PEB	C1C-CHB-C4B	3.60	136.35	128.28
82	H7	203	PEB	C1C-CHB-C4B	3.60	136.35	128.28
82	KF	203	PEB	C1D-CHC-C4C	-3.60	107.95	113.26
82	P4	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	aJ	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
82	M5	301	PEB	C3B-C4B-NB	3.60	115.28	110.05
82	Z5	301	PEB	C1B-C2B-C3B	-3.60	102.38	106.51
82	L7	202	PEB	C1B-C2B-C3B	-3.60	102.38	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	kH	203	PEB	C1B-C2B-C3B	-3.60	102.38	106.51
82	YK	201	PEB	C1D-CHC-C4C	3.60	118.56	113.26
82	N9	202	PEB	CHA-C1B-NB	-3.59	117.41	124.93
82	R9	202	PEB	CHA-C1B-NB	-3.59	117.41	124.93
85	d6	405	BCR	C7-C8-C9	-3.59	120.80	126.23
82	KI	201	PEB	C2A-C1A-NA	3.59	111.37	108.27
82	R7	203	PEB	C3D-C4D-ND	3.59	114.31	107.26
84	F3	1001	CYC	CAB-C3B-C4B	3.59	127.06	121.38
82	m4	203	PEB	C3B-C4B-NB	3.59	115.28	110.05
82	oF	201	PEB	C4B-C3B-C2B	-3.59	102.80	106.78
82	NQ	203	PEB	OA-C1A-C2A	-3.59	123.31	126.17
82	xF	302	PEB	OA-C1A-C2A	-3.59	123.31	126.17
82	sK	202	PEB	C1C-C2C-C3C	-3.59	103.37	107.62
84	g3	1001	CYC	CMA-C3A-C4A	3.59	130.60	125.06
84	l3	1001	CYC	CMA-C3A-C4A	3.59	130.60	125.06
84	O3	1001	CYC	CAB-C3B-C4B	3.59	127.06	121.38
82	T4	201	PEB	C3B-C4B-NB	3.59	115.28	110.05
82	M9	305	PEB	CHC-C4C-NC	3.59	126.01	121.15
82	OJ	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
82	EJ	203	PEB	C1D-CHC-C4C	-3.59	107.96	113.26
82	eE	202	PEB	C1C-C2C-C3C	-3.59	103.37	107.62
82	gK	201	PEB	CHC-C1D-ND	-3.59	109.18	113.72
87	AN	802	CLA	CHD-C1D-ND	-3.59	121.15	124.45
87	DL	406	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
82	pF	202	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
85	BN	841	BCR	C21-C20-C19	-3.59	112.00	123.22
82	GD	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
82	aM	203	PEB	C3D-C4D-ND	3.59	114.31	107.26
82	KB	301	PEB	C2A-C1A-NA	3.59	111.37	108.27
82	aJ	204	PEB	C1B-C2B-C3B	-3.59	102.38	106.51
82	eG	201	PEB	CMB-C2B-C1B	3.59	130.60	125.06
87	4N	608	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
96	E6	101	HEM	CBA-CAA-C2A	-3.59	102.65	112.63
84	GG	1001	CYC	C1D-C2D-C3D	-3.59	103.22	107.79
82	RK	202	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
82	O5	203	PEB	C3B-C4B-NB	3.59	115.27	110.05
82	BD	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
84	o3	1001	CYC	CAB-C3B-C4B	3.59	127.05	121.38
82	PM	201	PEB	C2A-C1A-NA	3.59	111.37	108.27
82	M5	304	PEB	C2A-C1A-NA	3.59	111.37	108.27
82	OI	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
82	B7	203	PEB	C3D-C4D-ND	3.59	114.31	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NK	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
82	MP	201	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
82	aM	203	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
82	NP	201	PEB	OA-C1A-C2A	-3.59	123.32	126.17
82	fJ	203	PEB	OA-C1A-C2A	-3.59	123.32	126.17
84	j3	1001	CYC	CAB-C3B-C4B	3.59	127.05	121.38
82	EK	202	PEB	C2A-C1A-NA	3.59	111.37	108.27
82	XF	201	PEB	CHC-C1D-ND	-3.59	109.18	113.72
82	RF	202	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
82	YJ	203	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
82	WH	201	PEB	CHA-C1B-NB	-3.59	117.42	124.93
82	JP	201	PEB	CHC-C4C-NC	3.59	126.01	121.15
83	QM	201	PUB	C4B-CHB-C1C	-3.59	120.23	128.28
82	cK	201	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
82	WD	202	PEB	CMB-C2B-C1B	3.59	130.59	125.06
82	KB	301	PEB	C3D-C4D-ND	3.59	114.30	107.26
82	T1	201	PEB	C3D-C4D-ND	3.59	114.30	107.26
82	j1	202	PEB	C3D-C4D-ND	3.59	114.30	107.26
85	B6	601	BCR	C11-C10-C9	-3.59	122.19	127.31
82	VH	201	PEB	C1C-CHB-C4B	3.59	136.33	128.28
82	cO	203	PEB	OA-C1A-C2A	-3.59	123.32	126.17
83	A1	303	PUB	C3B-C4B-NB	3.59	112.41	107.57
82	OH	201	PEB	C1C-C2C-C3C	-3.59	103.38	107.62
82	fE	201	PEB	CMB-C2B-C1B	3.59	130.59	125.06
82	aK	203	PEB	CHB-C1C-C2C	-3.59	119.05	127.15
82	FI	201	PEB	CHC-C1D-ND	-3.59	109.18	113.72
82	aO	201	PEB	C3B-C4B-NB	3.59	115.27	110.05
82	XB	202	PEB	CMB-C2B-C1B	3.59	130.59	125.06
82	TP	202	PEB	OA-C1A-C2A	-3.59	123.32	126.17
82	Z9	304	PEB	CHC-C4C-NC	3.59	126.00	121.15
82	p8	202	PEB	CHC-C1D-ND	-3.59	109.19	113.72
82	eM	202	PEB	C1C-CHB-C4B	-3.59	120.24	128.28
84	73	1001	CYC	CAB-C3B-C4B	3.59	127.05	121.38
85	k6	102	BCR	C28-C27-C26	-3.59	107.67	114.08
87	22	602	CLA	O2D-CGD-CBD	3.59	117.64	111.27
82	SG	203	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
82	SF	201	PEB	C1C-CHB-C4B	3.59	136.33	128.28
82	18	203	PEB	C3D-C4D-ND	3.59	114.30	107.26
82	ED	202	PEB	C2A-C1A-NA	3.59	111.36	108.27
82	oK	203	PEB	C2A-C1A-NA	3.59	111.36	108.27
82	XM	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
84	S3	1001	CYC	CAB-C3B-C4B	3.59	127.04	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BF	202	PEB	C3B-C4B-NB	3.59	115.27	110.05
82	i4	203	PEB	CHC-C4C-NC	3.59	126.00	121.15
84	JO	1001	CYC	CMB-C2B-C1B	3.59	128.65	124.17
84	L4	1001	CYC	CHA-C4D-C3D	-3.59	119.06	127.15
82	BA	201	PEB	C1D-CHC-C4C	-3.59	107.97	113.26
95	b6	622	DGD	C1E-O6E-C5E	3.59	120.73	113.69
82	cH	201	PEB	C3D-C4D-ND	3.59	114.30	107.26
84	f3	1001	CYC	CAB-C3B-C4B	3.59	127.04	121.38
85	B2	842	BCR	C11-C12-C13	3.59	136.49	126.42
82	TP	201	PEB	OA-C1A-C2A	-3.59	123.32	126.17
82	YK	202	PEB	C3D-C4D-ND	3.59	114.29	107.26
82	ZH	202	PEB	C2A-C1A-NA	3.59	111.36	108.27
82	RD	203	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
82	M5	301	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
82	D7	202	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
87	2N	303	CLA	O2D-CGD-CBD	3.59	117.64	111.27
91	dL	403	PHO	CMA-C3A-C4A	-3.59	106.53	114.38
82	HG	1002	PEB	CAB-C3B-C4B	3.59	131.35	125.01
82	AF	202	PEB	C4B-C3B-C2B	-3.58	102.81	106.78
82	OH	202	PEB	C1B-C2B-C3B	-3.58	102.39	106.51
82	JP	201	PEB	C3D-C4D-ND	3.58	114.29	107.26
82	EF	202	PEB	OA-C1A-C2A	-3.58	123.32	126.17
82	OF	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	ZJ	201	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	AM	301	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	HB	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
82	OE	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
82	A1	302	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	aH	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	NK	202	PEB	CHB-C4B-C3B	-3.58	117.03	125.32
82	PO	202	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
82	aK	201	PEB	C3D-C4D-ND	3.58	114.29	107.26
82	i1	201	PEB	CHC-C4C-NC	3.58	126.00	121.15
82	RB	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
82	P7	203	PEB	CAB-CBB-CGB	-3.58	105.89	113.60
82	EQ	202	PEB	C3D-C4D-ND	3.58	114.29	107.26
82	gE	201	PEB	C3B-C4B-NB	3.58	115.26	110.05
82	UJ	201	PEB	C1C-CHB-C4B	3.58	136.32	128.28
87	42	608	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
84	p3	1001	CYC	CMA-C3A-C4A	3.58	130.58	125.06
88	M6	101	LHG	C5-O7-C7	-3.58	108.97	117.79
82	K9	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	D7	201	PEB	CAB-C3B-C4B	3.58	131.35	125.01
82	SB	201	PEB	OD-C4D-ND	-3.58	120.62	125.93
82	B9	201	PEB	CHC-C1D-ND	-3.58	109.19	113.72
82	TQ	201	PEB	OD-C4D-C3D	-3.58	121.34	129.46
82	jM	202	PEB	C2A-C1A-NA	3.58	111.36	108.27
82	C9	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	ZO	202	PEB	CHC-C4C-NC	3.58	126.00	121.15
82	OH	203	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	Z4	202	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	cO	202	PEB	CMB-C2B-C1B	3.58	130.58	125.06
84	M4	1001	CYC	CMA-C3A-C4A	3.58	130.58	125.06
82	f1	203	PEB	C2C-C1C-NC	3.58	112.39	107.57
82	AE	301	PEB	CHC-C4C-NC	3.58	126.00	121.15
82	yC	203	PEB	C1C-CHB-C4B	-3.58	120.25	128.28
82	VQ	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
82	ZE	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
82	VQ	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
82	FP	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
82	L7	202	PEB	C3B-C4B-NB	3.58	115.26	110.05
82	mF	201	PEB	C1C-C2C-C3C	-3.58	103.39	107.62
84	D1	1001	CYC	C1B-NB-C4B	-3.58	106.11	110.67
82	AG	301	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	LI	201	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	LM	202	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	dG	202	PEB	C1C-CHB-C4B	3.58	136.31	128.28
82	LB	201	PEB	CMB-C2B-C1B	3.58	130.58	125.06
84	N3	1001	CYC	CMA-C3A-C4A	3.58	130.58	125.06
82	PH	202	PEB	C3D-C4D-ND	3.58	114.28	107.26
82	W1	201	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
96	V6	201	HEM	CHA-C4D-ND	3.58	128.79	124.37
82	Z5	305	PEB	C3B-C4B-NB	3.58	115.26	110.05
82	X9	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
87	22	609	CLA	CAC-C3C-C4C	3.58	129.46	124.81
82	fE	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
84	I1	1001	CYC	C1B-NB-C4B	-3.58	106.11	110.67
82	QB	204	PEB	C2A-C1A-NA	3.58	111.36	108.27
82	IM	201	PEB	C3C-C4C-NC	3.58	111.56	108.33
82	oF	201	PEB	C3B-C4B-NB	3.58	115.26	110.05
82	eH	203	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
82	gE	201	PEB	CMB-C2B-C1B	3.58	130.58	125.06
82	IJ	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
82	UP	203	PEB	C4B-C3B-C2B	-3.58	102.82	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	k1	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
84	W3	1001	CYC	C4D-C3D-C2D	-3.58	103.39	107.62
83	AH	303	PUB	C3B-C4B-NB	3.58	112.39	107.57
82	e1	201	PEB	C3D-C4D-ND	3.58	114.28	107.26
84	F4	1001	CYC	C2D-C1D-ND	3.58	112.43	107.40
83	QJ	201	PUB	C1B-C2B-C3B	-3.58	104.20	107.50
82	O7	201	PEB	CBA-CAA-C3A	-3.58	105.50	113.47
95	lL	101	DGD	O6D-C5D-C4D	3.58	116.19	109.69
82	cH	201	PEB	CMB-C2B-C1B	3.58	130.57	125.06
85	BN	842	BCR	C11-C12-C13	3.58	136.47	126.42
82	VQ	203	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
82	pK	202	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
82	S5	201	PEB	C2C-C1C-NC	3.58	112.39	107.57
82	hJ	201	PEB	CHA-C1B-NB	-3.58	117.45	124.93
82	KD	202	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	RA	201	PEB	CAB-CBB-CGB	-3.58	105.90	113.60
82	c1	201	PEB	CMB-C2B-C1B	3.58	130.57	125.06
88	I6	101	LHG	C5-O7-C7	-3.58	108.98	117.79
82	O1	201	PEB	C1C-C2C-C3C	-3.58	103.39	107.62
82	mK	201	PEB	C1C-C2C-C3C	-3.58	103.39	107.62
82	HI	202	PEB	C3B-C4B-NB	3.58	115.25	110.05
82	OK	203	PEB	C2A-C1A-NA	3.58	111.36	108.27
82	GQ	201	PEB	CMB-C2B-C1B	3.58	130.57	125.06
84	G4	1001	CYC	C1B-C2B-C3B	-3.58	104.14	107.87
82	SB	203	PEB	CHA-C1B-NB	-3.58	117.45	124.93
82	LD	201	PEB	CHA-C1B-NB	-3.58	117.45	124.93
82	OF	202	PEB	C3D-C4D-ND	3.58	114.28	107.26
82	OH	202	PEB	OD-C4D-ND	-3.58	120.63	125.93
82	gO	203	PEB	CHC-C4C-NC	3.58	125.99	121.15
82	NM	202	PEB	C1C-CHB-C4B	-3.58	120.26	128.28
82	W5	203	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
83	A1	303	PUB	C1C-C2C-C3C	-3.58	102.82	106.78
82	SQ	201	PEB	CHB-C4B-C3B	-3.58	117.05	125.32
88	C6	505	LHG	O8-C23-C24	3.58	123.13	111.91
82	bK	201	PEB	CHA-C1B-NB	-3.58	117.45	124.93
82	DQ	203	PEB	C3B-C4B-NB	3.58	115.25	110.05
82	iG	201	PEB	CHC-C4C-NC	3.58	125.99	121.15
82	GB	202	PEB	CMB-C2B-C1B	3.58	130.57	125.06
84	E3	1001	CYC	CMA-C3A-C4A	3.58	130.57	125.06
84	m3	1001	CYC	CMA-C3A-C4A	3.58	130.57	125.06
82	QJ	203	PEB	CHA-C1B-NB	-3.58	117.45	124.93
83	AG	302	PUB	C1D-CHC-C4C	-3.58	105.59	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IB	201	PEB	C4B-C3B-C2B	-3.58	102.83	106.78
82	iK	203	PEB	OA-C1A-C2A	-3.58	123.33	126.17
82	gG	201	PEB	CMB-C2B-C1B	3.58	130.57	125.06
83	AE	302	PUB	C1D-CHC-C4C	-3.58	105.59	113.37
82	FJ	201	PEB	CMC-C3C-C4C	3.58	130.85	127.06
82	bB	201	PEB	CMC-C3C-C4C	3.58	130.85	127.06
82	aE	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
82	fH	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
84	F4	1001	CYC	C2C-C1C-NC	3.58	111.36	108.27
82	R7	201	PEB	CAB-CBB-CGB	-3.57	105.91	113.60
84	DE	1001	CYC	CHB-C4A-NA	-3.57	117.45	124.93
82	eE	201	PEB	CMB-C2B-C1B	3.57	130.57	125.06
82	U9	203	PEB	CHC-C4C-NC	3.57	125.99	121.15
82	VJ	201	PEB	OA-C1A-C2A	-3.57	123.33	126.17
82	ZO	202	PEB	OA-C1A-C2A	-3.57	123.33	126.17
82	fM	202	PEB	C3D-C4D-ND	3.57	114.27	107.26
82	R7	202	PEB	C1B-C2B-C3B	-3.57	102.40	106.51
84	63	901	CYC	CMD-C2D-C1D	3.57	130.79	125.56
82	dJ	201	PEB	OD-C4D-ND	-3.57	120.64	125.93
87	42	608	CLA	CAA-C2A-C3A	-3.57	102.99	112.78
84	R3	1001	CYC	CMA-C3A-C4A	3.57	130.57	125.06
84	v3	1001	CYC	CMA-C3A-C4A	3.57	130.57	125.06
84	N1	1001	CYC	C1D-C2D-C3D	-3.57	103.24	107.79
82	SB	201	PEB	CHC-C1D-ND	-3.57	109.20	113.72
85	h6	102	BCR	C15-C14-C13	-3.57	122.21	127.31
84	LO	1001	CYC	CHA-C4D-C3D	-3.57	119.09	127.15
84	i3	1001	CYC	CMA-C3A-C4A	3.57	130.57	125.06
82	G9	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
84	DG	1001	CYC	CHB-C4A-NA	-3.57	117.46	124.93
82	t8	201	PEB	CAB-CBB-CGB	-3.57	105.91	113.60
82	Y4	203	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	J5	203	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	GM	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
82	a4	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
87	aL	606	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
82	OF	202	PEB	CHB-C1C-C2C	-3.57	119.09	127.15
82	aK	202	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
82	E9	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
82	bF	201	PEB	CHA-C1B-NB	-3.57	117.46	124.93
82	NQ	202	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	JM	202	PEB	OA-C1A-C2A	-3.57	123.33	126.17
82	Z1	203	PEB	C3D-C4D-ND	3.57	114.27	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	b1	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
82	fJ	203	PEB	C2A-C1A-NA	3.57	111.35	108.27
84	LO	1001	CYC	C2C-C1C-NC	3.57	111.35	108.27
85	B6	621	BCR	C38-C26-C27	3.57	120.48	113.62
82	iG	201	PEB	CMB-C2B-C1B	3.57	130.56	125.06
84	GE	1001	CYC	CHB-C4A-NA	-3.57	117.46	124.93
82	R4	201	PEB	OD-C4D-ND	-3.57	120.64	125.93
85	BN	839	BCR	C15-C14-C13	-3.57	122.21	127.31
82	LH	1003	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	Q1	203	PEB	C3D-C4D-ND	3.57	114.27	107.26
82	WG	203	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
82	KK	202	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
82	A9	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
84	J3	1001	CYC	CMA-C3A-C4A	3.57	130.56	125.06
82	sF	201	PEB	CHA-C1B-NB	-3.57	117.47	124.93
82	NK	202	PEB	CHB-C1C-NC	-3.57	117.14	125.32
82	MP	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
82	M5	305	PEB	C3B-C4B-NB	3.57	115.24	110.05
82	OJ	203	PEB	C1C-CHB-C4B	3.57	136.29	128.28
84	FE	1002	CYC	CHA-C4D-C3D	-3.57	119.10	127.15
82	FK	202	PEB	OD-C4D-ND	-3.57	120.64	125.93
82	aJ	202	PEB	CHC-C4C-NC	3.57	125.98	121.15
82	LA	201	PEB	OA-C1A-C2A	-3.57	123.33	126.17
82	iG	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
85	J2	103	BCR	C11-C10-C9	-3.57	122.22	127.31
82	CD	201	PEB	CHB-C4B-C3B	-3.57	117.06	125.32
82	I9	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
84	FE	1002	CYC	C2D-C1D-ND	3.57	112.42	107.40
82	AK	201	PEB	CHC-C4C-NC	3.57	125.98	121.15
84	EH	1001	CYC	C1B-C2B-C3B	-3.57	104.15	107.87
82	QJ	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
82	R1	201	PEB	OA-C1A-C2A	-3.57	123.34	126.17
82	P9	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
84	FO	1001	CYC	CMA-C3A-C4A	3.57	130.56	125.06
82	PM	202	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	a4	202	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	gG	202	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
82	RO	202	PEB	C1C-CHB-C4B	3.57	136.28	128.28
82	aK	201	PEB	CHC-C1D-ND	-3.57	109.21	113.72
82	QI	201	PEB	C3D-C4D-ND	3.57	114.26	107.26
82	fG	203	PEB	C3D-C4D-ND	3.57	114.26	107.26
82	aK	203	PEB	C3D-C4D-ND	3.57	114.26	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	CO	1001	CYC	C2C-C1C-NC	3.57	111.35	108.27
82	pF	202	PEB	CMB-C2B-C1B	3.57	130.56	125.06
82	gM	201	PEB	CMB-C2B-C1B	3.57	130.56	125.06
82	D7	203	PEB	OA-C1A-C2A	-3.57	123.34	126.17
82	kH	201	PEB	OA-C1A-C2A	-3.57	123.34	126.17
82	vC	202	PEB	OD-C4D-ND	-3.57	120.65	125.93
82	SD	201	PEB	CHB-C4B-C3B	-3.57	117.07	125.32
82	tC	201	PEB	CAB-CBB-CGB	-3.57	105.93	113.60
82	CK	203	PEB	C1C-C2C-C3C	-3.57	103.41	107.62
82	WJ	203	PEB	C3B-C4B-NB	3.57	115.24	110.05
85	JN	102	BCR	C24-C23-C22	3.57	131.62	126.23
82	DA	202	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
82	RA	203	PEB	C3D-C4D-ND	3.57	114.26	107.26
82	D9	203	PEB	OD-C4D-ND	-3.57	120.65	125.93
82	RM	202	PEB	CAB-C3B-C4B	3.57	131.32	125.01
82	R9	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
82	QB	204	PEB	C3B-C4B-NB	3.57	115.24	110.05
82	UK	202	PEB	C3B-C4B-NB	3.57	115.24	110.05
82	NP	201	PEB	C4B-C3B-C2B	-3.57	102.84	106.78
82	L1	1002	PEB	C4B-C3B-C2B	-3.57	102.84	106.78
82	m4	203	PEB	CHC-C4C-NC	3.57	125.97	121.15
82	jF	201	PEB	CHC-C4C-NC	3.57	125.97	121.15
82	mG	203	PEB	CHC-C4C-NC	3.57	125.97	121.15
82	dJ	201	PEB	C3D-C4D-ND	3.57	114.25	107.26
82	UQ	202	PEB	CHC-C1D-ND	-3.57	109.21	113.72
82	SJ	203	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
82	bO	201	PEB	CHB-C1C-C2C	-3.57	119.11	127.15
82	TA	202	PEB	C1C-CHB-C4B	3.57	136.28	128.28
82	HE	1002	PEB	CAB-C3B-C4B	3.57	131.32	125.01
82	X7	203	PEB	CHB-C1C-NC	-3.57	117.15	125.32
84	C3	1001	CYC	CMA-C3A-C4A	3.57	130.55	125.06
82	P9	201	PEB	C2A-C1A-NA	3.56	111.35	108.27
85	JN	103	BCR	C11-C10-C9	-3.56	122.22	127.31
84	e3	1001	CYC	CMA-C3A-C4A	3.56	130.55	125.06
82	dJ	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	L7	201	PEB	CHC-C4C-NC	3.56	125.97	121.15
84	KO	1001	CYC	C1B-NB-C4B	-3.56	106.13	110.67
87	AN	849	CLA	CMB-C2B-C3B	3.56	135.22	126.59
82	NQ	204	PEB	C1C-CHB-C4B	3.56	136.28	128.28
82	Y1	202	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
82	VB	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
82	JH	1002	PEB	C3B-C4B-NB	3.56	115.23	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KA	201	PEB	CMB-C2B-C1B	3.56	130.55	125.06
82	TJ	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
82	GJ	201	PEB	CHC-C4C-NC	3.56	125.97	121.15
87	B2	824	CLA	C2A-C1A-CHA	3.56	130.09	123.86
82	jG	201	PEB	C1D-CHC-C4C	-3.56	108.00	113.26
82	Q5	201	PEB	C1C-C2C-C3C	-3.56	103.41	107.62
83	xK	301	PUB	CAB-C3B-C4B	3.56	131.44	125.76
82	ZG	203	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	G5	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	N5	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	S7	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	gM	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	XA	203	PEB	CHB-C1C-NC	-3.56	117.16	125.32
82	CM	202	PEB	C3C-C4C-NC	3.56	111.54	108.33
82	TF	202	PEB	C1C-CHB-C4B	3.56	136.27	128.28
82	CQ	201	PEB	CHB-C4B-C3B	-3.56	117.08	125.32
82	OA	201	PEB	CBA-CAA-C3A	-3.56	105.53	113.47
82	E9	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
82	KJ	203	PEB	C3B-C4B-NB	3.56	115.23	110.05
82	CM	203	PEB	C1C-CHB-C4B	3.56	136.27	128.28
87	BN	825	CLA	C2A-C1A-CHA	3.56	130.09	123.86
82	RK	202	PEB	CHB-C4B-C3B	-3.56	117.08	125.32
82	IK	203	PEB	C1C-NC-C4C	-3.56	103.26	109.60
87	2N	301	CLA	CHB-C1B-NB	3.56	128.03	124.26
82	AF	201	PEB	CHC-C4C-NC	3.56	125.97	121.15
82	UD	202	PEB	OD-C4D-ND	-3.56	120.65	125.93
83	ND	201	PUB	OA-C1A-NA	-3.56	120.65	125.93
82	SK	201	PEB	C1C-CHB-C4B	3.56	136.27	128.28
84	J3	1001	CYC	CAB-C3B-C4B	3.56	127.00	121.38
82	b1	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
85	cL	503	BCR	C20-C21-C22	-3.56	122.23	127.31
82	OM	202	PEB	CMC-C3C-C2C	3.56	133.31	125.61
82	UJ	202	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
92	BL	611	LMG	O1-C1-C2	3.56	113.86	108.30
82	Z1	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
82	T9	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
84	L4	1001	CYC	C2C-C1C-NC	3.56	111.34	108.27
84	c3	1001	CYC	CMA-C3A-C4A	3.56	130.55	125.06
96	VL	201	HEM	C1B-NB-C4B	3.56	108.75	105.07
82	N7	202	PEB	C3C-C4C-NC	3.56	111.54	108.33
82	LD	203	PEB	C3D-C4D-ND	3.56	114.25	107.26
82	UF	202	PEB	CHC-C4C-NC	3.56	125.97	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	K7	201	PEB	CMB-C2B-C1B	3.56	130.55	125.06
82	Y4	202	PEB	CHC-C1D-ND	-3.56	109.22	113.72
82	W5	202	PEB	C1C-CHB-C4B	3.56	136.27	128.28
82	QF	203	PEB	C3D-C4D-ND	3.56	114.24	107.26
82	AJ	301	PEB	CHA-C1B-NB	-3.56	117.49	124.93
82	T9	202	PEB	CHA-C1B-NB	-3.56	117.49	124.93
84	FO	1001	CYC	C2D-C1D-ND	3.56	112.40	107.40
84	LO	1001	CYC	C2D-C1D-ND	3.56	112.40	107.40
87	A2	849	CLA	CMB-C2B-C3B	3.56	135.21	126.59
82	QK	203	PEB	C3D-C4D-ND	3.56	114.24	107.26
82	AJ	301	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
82	jK	201	PEB	CHC-C4C-NC	3.56	125.97	121.15
82	VD	203	PEB	C3D-C4D-ND	3.56	114.24	107.26
84	DE	1001	CYC	C1D-C2D-C3D	-3.56	103.26	107.79
82	RO	201	PEB	OD-C4D-ND	-3.56	120.66	125.93
82	DF	201	PEB	C3D-C4D-ND	3.56	114.24	107.26
82	WH	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
82	KP	202	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
82	NI	203	PEB	C1D-CHC-C4C	-3.56	108.01	113.26
82	SG	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	bG	201	PEB	CHC-C1D-ND	-3.56	109.22	113.72
82	G9	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
82	hE	203	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
82	pK	202	PEB	CMB-C2B-C1B	3.56	130.54	125.06
95	C6	503	DGD	C4E-C3E-C2E	3.56	117.03	110.82
82	nK	201	PEB	C1C-C2C-C3C	-3.56	103.42	107.62
84	CG	1001	CYC	C4D-C3D-C2D	-3.56	103.42	107.62
83	AM	303	PUB	OD-C4D-C3D	-3.56	124.18	128.04
84	HH	1001	CYC	C1B-C2B-C3B	-3.56	104.16	107.87
82	HJ	201	PEB	C3B-C4B-NB	3.56	115.22	110.05
82	Q5	203	PEB	C3B-C4B-NB	3.56	115.22	110.05
82	OJ	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
82	B7	203	PEB	C4B-C3B-C2B	-3.56	102.85	106.78
82	e4	201	PEB	CHA-C1B-NB	-3.56	117.49	124.93
82	EA	201	PEB	OD-C4D-ND	-3.56	120.66	125.93
82	DQ	203	PEB	OD-C4D-ND	-3.56	120.66	125.93
82	jJ	201	PEB	OD-C4D-ND	-3.56	120.66	125.93
82	IM	203	PEB	C2A-C1A-NA	3.56	111.34	108.27
82	BQ	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
84	FG	1001	CYC	CHA-C4D-C3D	-3.56	119.13	127.15
82	AH	302	PEB	CHA-C1B-NB	-3.56	117.49	124.93
84	C4	1001	CYC	CHD-C1D-ND	-3.56	117.17	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WJ	203	PEB	OD-C4D-ND	-3.56	120.66	125.93
82	PP	202	PEB	CMB-C2B-C1B	3.56	130.54	125.06
84	K3	1001	CYC	CMA-C3A-C4A	3.56	130.54	125.06
85	F2	203	BCR	C15-C16-C17	-3.56	116.19	123.47
82	kH	201	PEB	C4B-C3B-C2B	-3.56	102.85	106.78
82	VQ	203	PEB	OD-C4D-C3D	-3.56	121.40	129.46
82	tK	203	PEB	OD-C4D-C3D	-3.56	121.40	129.46
82	TF	202	PEB	C1D-CHC-C4C	3.56	118.50	113.26
82	R4	202	PEB	C1C-CHB-C4B	3.56	136.26	128.28
82	V9	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
82	O7	201	PEB	C1C-NC-C4C	-3.56	103.27	109.60
82	GF	201	PEB	CHC-C1D-ND	-3.56	109.23	113.72
85	K6	102	BCR	C33-C5-C4	3.56	120.45	113.62
82	i1	201	PEB	OD-C4D-ND	-3.56	120.66	125.93
82	TP	201	PEB	C2C-C1C-NC	3.56	112.36	107.57
92	D6	409	LMG	O7-C10-C11	3.56	119.16	111.50
82	g1	202	PEB	C1D-CHC-C4C	3.56	118.50	113.26
84	GE	1001	CYC	C1D-C2D-C3D	-3.55	103.26	107.79
82	ZH	203	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
82	a1	202	PEB	CHA-C1B-NB	-3.55	117.50	124.93
87	CL	518	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
82	SG	203	PEB	C1D-CHC-C4C	-3.55	108.02	113.26
82	sK	201	PEB	CHA-C1B-NB	-3.55	117.50	124.93
84	GG	1001	CYC	CHB-C4A-NA	-3.55	117.50	124.93
84	NE	201	CYC	C1D-C2D-C3D	-3.55	103.26	107.79
82	QP	201	PEB	C3B-C4B-NB	3.55	115.22	110.05
83	NQ	201	PUB	OA-C1A-NA	-3.55	120.67	125.93
82	g4	203	PEB	CHC-C4C-NC	3.55	125.96	121.15
82	VA	201	PEB	C1C-C2C-C3C	-3.55	103.42	107.62
83	wF	304	PUB	CBA-CAA-C3A	-3.55	107.59	112.98
82	bB	201	PEB	C3B-C4B-NB	3.55	115.22	110.05
84	P3	1001	CYC	CMA-C3A-C4A	3.55	130.54	125.06
82	UI	202	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
82	gE	202	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
82	R1	201	PEB	C2A-C1A-NA	3.55	111.34	108.27
82	OJ	203	PEB	OA-C1A-C2A	-3.55	123.35	126.17
82	OM	203	PEB	OA-C1A-C2A	-3.55	123.35	126.17
82	eJ	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
82	nF	201	PEB	C1C-C2C-C3C	-3.55	103.42	107.62
82	WE	203	PEB	C3B-C4B-NB	3.55	115.22	110.05
84	KH	1001	CYC	C2A-C1A-NA	3.55	115.22	110.05
98	BN	837	PQN	C11-C12-C13	-3.55	120.88	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KE	201	PEB	CHC-C4C-NC	3.55	125.96	121.15
85	C6	507	BCR	C33-C5-C6	-3.55	120.54	124.53
92	DL	402	LMG	O1-C7-C8	-3.55	102.33	110.90
82	JA	201	PEB	C3B-C4B-NB	3.55	115.22	110.05
82	ZH	202	PEB	C3B-C4B-NB	3.55	115.22	110.05
82	OH	203	PEB	C3D-C4D-ND	3.55	114.23	107.26
82	iK	203	PEB	C3D-C4D-ND	3.55	114.23	107.26
82	ND	204	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	u8	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	uC	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	aG	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
87	4N	608	CLA	CAA-C2A-C3A	-3.55	103.05	112.78
82	cK	201	PEB	CMB-C2B-C1B	3.55	130.53	125.06
82	JK	201	PEB	CAA-C3A-C2A	-3.55	105.39	114.26
82	AI	203	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
82	TJ	202	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
82	eO	203	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
85	d6	405	BCR	C15-C14-C13	-3.55	122.24	127.31
82	gM	201	PEB	CHA-C1B-NB	-3.55	117.50	124.93
82	E7	202	PEB	C3D-C4D-ND	3.55	114.23	107.26
84	t3	1001	CYC	CMA-C3A-C4A	3.55	130.53	125.06
82	iE	201	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
82	fM	203	PEB	CHC-C1D-ND	-3.55	109.23	113.72
84	BG	1002	CYC	C4D-C3D-C2D	-3.55	103.42	107.62
82	uF	201	PEB	OD-C4D-C3D	-3.55	121.42	129.46
82	IA	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
82	I7	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
82	aF	203	PEB	C3D-C4D-ND	3.55	114.22	107.26
82	BA	203	PEB	C1D-CHC-C4C	-3.55	108.02	113.26
82	GD	201	PEB	CMB-C2B-C1B	3.55	130.53	125.06
82	T7	202	PEB	C1C-CHB-C4B	3.55	136.24	128.28
87	8N	306	CLA	C2A-C1A-CHA	3.55	130.07	123.86
82	sF	202	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	R7	203	PEB	C1D-CHC-C4C	-3.55	108.02	113.26
84	NO	1001	CYC	C1D-C2D-C3D	-3.55	103.27	107.79
82	BA	203	PEB	C3B-C4B-NB	3.55	115.21	110.05
82	IQ	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
82	O5	203	PEB	OA-C1A-C2A	-3.55	123.35	126.17
91	A6	407	PHO	C1-C2-C3	-3.55	119.91	126.04
82	B7	201	PEB	C1D-CHC-C4C	-3.55	108.02	113.26
82	HB	201	PEB	CHC-C4C-NC	-3.55	116.34	121.15
82	AF	202	PEB	C2C-C1C-NC	3.55	112.35	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	C3	1001	CYC	CAB-C3B-C4B	3.55	126.98	121.38
82	LD	203	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	PQ	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	UQ	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
82	P7	203	PEB	CHC-C1D-ND	-3.55	109.23	113.72
82	CM	203	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
83	xF	301	PUB	CAB-C3B-C4B	3.55	131.41	125.76
82	LP	202	PEB	CHC-C4C-NC	3.55	125.95	121.15
82	j4	203	PEB	OA-C1A-C2A	-3.55	123.35	126.17
82	S5	202	PEB	OD-C4D-ND	-3.55	120.67	125.93
82	LE	1002	PEB	C2C-C1C-NC	3.55	112.35	107.57
91	d6	404	PHO	C1-C2-C3	-3.55	119.91	126.04
82	NF	201	PEB	C4B-C3B-C2B	-3.55	102.86	106.78
82	F5	201	PEB	C4B-C3B-C2B	-3.55	102.86	106.78
85	kL	100	BCR	C31-C1-C6	-3.55	104.55	110.30
82	CJ	202	PEB	C2A-C1A-NA	3.55	111.33	108.27
84	T3	1001	CYC	CAB-C3B-C4B	3.55	126.98	121.38
82	W7	201	PEB	C1B-C2B-C3B	-3.55	102.44	106.51
84	D1	1003	CYC	CMB-C2B-C1B	3.55	128.60	124.17
84	N4	1001	CYC	C1D-C2D-C3D	-3.55	103.27	107.79
82	tK	202	PEB	CHB-C4B-C3B	-3.55	117.11	125.32
82	UK	202	PEB	CMB-C2B-C1B	3.55	130.53	125.06
82	T5	201	PEB	OA-C1A-C2A	-3.55	123.35	126.17
85	HL	103	BCR	C24-C23-C22	-3.55	120.88	126.23
82	NH	1002	PEB	C3B-C4B-NB	3.55	115.21	110.05
83	AM	303	PUB	CHA-C1B-NB	3.55	125.95	121.15
82	I7	202	PEB	C1B-C2B-C3B	-3.55	102.44	106.51
82	aF	202	PEB	C1B-C2B-C3B	-3.55	102.44	106.51
82	LG	1002	PEB	C2C-C1C-NC	3.55	112.35	107.57
82	c1	201	PEB	C3D-C4D-ND	3.55	114.22	107.26
82	IB	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
85	cL	518	BCR	C7-C8-C9	-3.55	120.88	126.23
83	xF	305	PUB	CHC-C1D-ND	-3.55	109.24	113.72
82	VA	202	PEB	C1C-CHB-C4B	3.55	136.23	128.28
82	Y9	203	PEB	OD-C4D-ND	-3.55	120.68	125.93
82	lK	202	PEB	CHB-C1C-C2C	-3.55	119.15	127.15
82	hE	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
84	BE	1002	CYC	C4D-C3D-C2D	-3.55	103.43	107.62
82	OA	201	PEB	C1C-NC-C4C	-3.55	103.29	109.60
82	AF	201	PEB	CHB-C1C-C2C	-3.55	119.15	127.15
82	LA	201	PEB	CHC-C4C-NC	3.55	125.95	121.15
82	KB	302	PEB	C2A-C1A-NA	3.54	111.33	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RP	201	PEB	C2C-C1C-NC	3.54	112.34	107.57
82	JH	1002	PEB	C1D-CHC-C4C	-3.54	108.03	113.26
82	VD	202	PEB	CHA-C1B-NB	-3.54	117.52	124.93
82	TD	201	PEB	OD-C4D-C3D	-3.54	121.43	129.46
84	EO	1001	CYC	C1B-NB-C4B	-3.54	106.16	110.67
82	N7	203	PEB	C3B-C4B-NB	3.54	115.20	110.05
96	vL	201	HEM	C1B-NB-C4B	3.54	108.73	105.07
87	a6	608	CLA	C1-C2-C3	-3.54	119.91	126.04
82	jH	202	PEB	C3D-C4D-ND	3.54	114.21	107.26
82	CB	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	MF	203	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	OH	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	g1	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	gH	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
91	D6	404	PHO	C4-C3-C5	3.54	121.23	115.27
82	MP	203	PEB	C2C-C1C-NC	3.54	112.34	107.57
82	aO	202	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
82	ZM	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
82	K9	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
82	lH	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
82	TB	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	RO	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	HB	203	PEB	OD-C4D-ND	-3.54	120.68	125.93
82	yF	301	PEB	OD-C4D-ND	-3.54	120.68	125.93
84	K3	1001	CYC	CAB-C3B-C4B	3.54	126.97	121.38
84	J3	1001	CYC	C1A-C2A-C3A	-3.54	102.86	106.78
82	v8	202	PEB	OD-C4D-ND	-3.54	120.68	125.93
87	12	608	CLA	C2D-C1D-ND	-3.54	107.49	110.10
84	T3	1001	CYC	CMA-C3A-C4A	3.54	130.52	125.06
82	MB	202	PEB	CAA-C3A-C2A	-3.54	105.41	114.26
82	SD	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
84	CH	1001	CYC	OC-C1C-C2C	-3.54	123.36	126.17
82	M9	302	PEB	CHC-C4C-NC	3.54	125.94	121.15
82	JB	201	PEB	CHC-C1D-ND	-3.54	109.24	113.72
83	yF	303	PUB	CHC-C1D-ND	-3.54	109.24	113.72
85	FN	202	BCR	C15-C16-C17	-3.54	116.22	123.47
82	gB	202	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
82	xF	304	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
83	AE	303	PUB	C1C-C2C-C3C	-3.54	102.86	106.78
84	E4	1001	CYC	C1B-NB-C4B	-3.54	106.16	110.67
82	Z9	301	PEB	CHC-C4C-NC	3.54	125.94	121.15
82	KF	202	PEB	C1B-C2B-C3B	-3.54	102.44	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	hL	102	BCR	C7-C8-C9	-3.54	120.88	126.23
85	B2	838	BCR	C24-C23-C22	3.54	131.59	126.23
82	Q5	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	DI	202	PEB	C3D-C4D-ND	3.54	114.21	107.26
82	wK	302	PEB	OA-C1A-C2A	-3.54	123.36	126.17
84	DO	1001	CYC	CHA-C4D-C3D	-3.54	119.16	127.15
82	R7	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
87	12	607	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
84	g3	1001	CYC	C1A-C2A-C3A	-3.54	102.86	106.78
87	22	605	CLA	CHB-C1B-NB	3.54	128.01	124.26
84	FE	1001	CYC	C2B-C1B-NB	3.54	112.17	106.99
84	ME	1001	CYC	C4D-C3D-C2D	-3.54	103.44	107.62
82	KM	203	PEB	C1B-C2B-C3B	-3.54	102.44	106.51
82	WG	203	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	gM	201	PEB	C1C-CHB-C4B	-3.54	120.34	128.28
82	TF	201	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
82	SE	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	UM	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	A4	301	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	eF	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	mM	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	BK	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	A9	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
82	C9	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
82	F5	201	PEB	CAA-C3A-C4A	-3.54	103.58	112.67
82	JF	201	PEB	CAA-C3A-C2A	-3.54	105.42	114.26
82	JQ	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	PA	203	PEB	CHC-C1D-ND	-3.54	109.25	113.72
84	NH	1001	CYC	C1D-C2D-C3D	-3.54	103.28	107.79
82	BA	203	PEB	C3D-C4D-ND	3.54	114.20	107.26
82	aO	202	PEB	C2A-C1A-NA	3.54	111.32	108.27
84	G3	1001	CYC	CMA-C3A-C4A	3.54	130.51	125.06
87	bL	604	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
84	HE	1001	CYC	C4D-CHA-C1A	3.54	136.22	128.28
82	QB	204	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
82	LK	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
82	L7	203	PEB	C3D-C4D-ND	3.54	114.20	107.26
83	QM	201	PUB	CHA-C4A-NA	-3.54	109.25	113.72
85	A2	845	BCR	C7-C8-C9	-3.54	120.89	126.23
82	V4	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	E5	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	X5	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DA	201	PEB	CAB-C3B-C4B	3.54	131.27	125.01
84	A3	1001	CYC	CMA-C3A-C4A	3.54	130.51	125.06
82	lK	203	PEB	C3D-C4D-ND	3.54	114.20	107.26
82	VG	202	PEB	CHC-C4C-NC	3.54	125.94	121.15
82	sK	201	PEB	C3B-C4B-NB	3.54	115.19	110.05
87	KN	105	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
87	82	305	CLA	C2A-C1A-CHA	3.54	130.04	123.86
82	UP	203	PEB	C3B-C4B-NB	3.54	115.19	110.05
82	RP	201	PEB	C2A-C1A-NA	3.54	111.32	108.27
82	EB	501	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
82	U9	204	PEB	C2C-C1C-NC	3.54	112.33	107.57
84	D4	1001	CYC	CHA-C4D-C3D	-3.54	119.17	127.15
82	uK	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
82	gO	203	PEB	OA-C1A-C2A	-3.54	123.36	126.17
87	1N	608	CLA	C2D-C1D-ND	-3.54	107.50	110.10
82	aO	203	PEB	CHC-C4C-NC	3.54	125.94	121.15
82	dJ	202	PEB	CHA-C1B-NB	-3.54	117.54	124.93
83	Z9	305	PUB	CMA-C2A-C1A	3.54	129.71	121.39
82	RB	201	PEB	CMB-C2B-C1B	3.54	130.51	125.06
82	sK	202	PEB	C2A-C1A-NA	3.54	111.32	108.27
82	QH	203	PEB	C3D-C4D-ND	3.54	114.20	107.26
82	TK	202	PEB	C1C-CHB-C4B	3.54	136.21	128.28
87	CL	513	CLA	CHD-C1D-ND	-3.54	121.20	124.45
82	KI	201	PEB	OD-C4D-C3D	-3.54	121.45	129.46
82	RF	202	PEB	CHB-C4B-C3B	-3.54	117.14	125.32
82	dO	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
84	EH	1001	CYC	C1D-C2D-C3D	-3.54	103.29	107.79
83	AJ	304	PUB	C1D-CHC-C4C	-3.54	105.68	113.37
82	tF	202	PEB	CAC-C2C-C3C	3.54	135.17	127.07
84	EG	1001	CYC	OB-C4B-C3B	-3.54	124.20	128.04
82	VM	202	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
82	cF	201	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
82	F7	203	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
87	CL	509	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
82	gH	202	PEB	C1D-CHC-C4C	3.53	118.47	113.26
82	ZH	201	PEB	CMB-C2B-C1B	3.53	130.51	125.06
82	Z1	201	PEB	CMB-C2B-C1B	3.53	130.51	125.06
84	BG	1002	CYC	CHB-C1B-NB	-3.53	118.47	126.06
84	EE	1001	CYC	C4D-C3D-C2D	-3.53	103.44	107.62
85	B2	839	BCR	C15-C14-C13	-3.53	122.27	127.31
82	JQ	202	PEB	C3D-C4D-ND	3.53	114.19	107.26
82	sK	202	PEB	C3D-C4D-ND	3.53	114.19	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	b6	605	CLA	CHB-C1B-C2B	-3.53	117.26	127.24
84	E1	1001	CYC	C1D-C2D-C3D	-3.53	103.29	107.79
82	UQ	202	PEB	OD-C4D-ND	-3.53	120.69	125.93
82	LA	202	PEB	C3B-C4B-NB	3.53	115.19	110.05
82	N9	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
82	cE	202	PEB	C2A-C1A-NA	3.53	111.32	108.27
84	A3	1001	CYC	C1A-C2A-C3A	-3.53	102.87	106.78
82	d1	202	PEB	OD-C4D-ND	-3.53	120.70	125.93
82	O7	201	PEB	OD-C4D-ND	-3.53	120.70	125.93
82	AP	203	PEB	C2C-C1C-NC	3.53	112.33	107.57
82	R4	202	PEB	C3C-C4C-NC	3.53	111.51	108.33
82	oK	202	PEB	OA-C1A-C2A	-3.53	123.36	126.17
83	yK	302	PUB	CBA-CAA-C3A	-3.53	107.62	112.98
82	AF	202	PEB	C3D-C4D-ND	3.53	114.19	107.26
82	I7	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
82	fB	301	PEB	CHC-C1D-ND	-3.53	109.25	113.72
87	AN	852	CLA	C4A-NA-C1A	3.53	108.29	106.71
83	QM	201	PUB	CMA-C2A-C1A	3.53	129.70	121.39
87	K2	106	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
82	f1	202	PEB	C3D-C4D-ND	3.53	114.19	107.26
91	AL	410	PHO	CMA-C3A-C4A	-3.53	106.64	114.38
82	eO	201	PEB	CHA-C1B-NB	-3.53	117.55	124.93
82	MB	201	PEB	OA-C1A-C2A	-3.53	123.36	126.17
82	NP	202	PEB	OA-C1A-C2A	-3.53	123.36	126.17
82	K5	201	PEB	OA-C1A-C2A	-3.53	123.36	126.17
82	cO	201	PEB	OA-C1A-C2A	-3.53	123.36	126.17
82	dH	203	PEB	C1C-CHB-C4B	-3.53	120.36	128.28
82	uF	203	PEB	C3D-C4D-ND	3.53	114.19	107.26
82	WI	202	PEB	C3B-C4B-NB	3.53	115.19	110.05
84	e3	1001	CYC	C1A-C2A-C3A	-3.53	102.87	106.78
84	m3	1001	CYC	C1A-C2A-C3A	-3.53	102.87	106.78
87	82	308	CLA	C3B-C4B-NB	-3.53	107.24	110.52
82	jE	201	PEB	C1D-CHC-C4C	-3.53	108.05	113.26
84	E1	1001	CYC	C1B-C2B-C3B	-3.53	104.19	107.87
82	LJ	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
85	B2	802	BCR	C39-C30-C29	3.53	123.03	108.91
82	tF	202	PEB	CHB-C4B-C3B	-3.53	117.15	125.32
82	FF	202	PEB	OD-C4D-ND	-3.53	120.70	125.93
82	bE	201	PEB	CHC-C1D-ND	-3.53	109.26	113.72
82	kH	203	PEB	CHA-C1B-NB	-3.53	117.55	124.93
84	FG	1001	CYC	CHB-C4A-NA	-3.53	117.55	124.93
85	CL	516	BCR	C16-C17-C18	-3.53	122.27	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FA	203	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
82	eB	201	PEB	OA-C1A-C2A	-3.53	123.37	126.17
82	xK	302	PEB	OA-C1A-C2A	-3.53	123.37	126.17
82	GF	203	PEB	CHC-C4C-NC	3.53	125.93	121.15
84	HO	1001	CYC	C4D-C3D-C2D	-3.53	103.45	107.62
83	A1	303	PUB	CBB-CAB-C3B	3.53	122.44	112.63
82	YB	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
82	I9	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
82	mK	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
82	TM	202	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
91	DL	405	PHO	CMA-C3A-C4A	-3.53	106.65	114.38
82	DK	201	PEB	C3D-C4D-ND	3.53	114.18	107.26
82	V4	201	PEB	CHA-C1B-NB	-3.53	117.55	124.93
82	N1	1002	PEB	C3B-C4B-NB	3.53	115.18	110.05
82	PE	201	PEB	CAB-CBB-CGB	-3.53	106.01	113.60
82	LF	201	PEB	C2C-C1C-NC	3.53	112.32	107.57
84	J4	1001	CYC	CHA-C4D-C3D	-3.53	119.19	127.15
82	gO	201	PEB	OA-C1A-C2A	-3.53	123.37	126.17
82	WJ	201	PEB	CHA-C1B-C2B	3.53	133.97	124.90
82	eF	201	PEB	C3D-C4D-ND	3.53	114.18	107.26
82	DD	203	PEB	OD-C4D-ND	-3.53	120.70	125.93
82	d1	203	PEB	C1C-CHB-C4B	-3.53	120.37	128.28
84	e3	1001	CYC	CAB-C3B-C4B	3.53	126.95	121.38
84	p3	1001	CYC	CAB-C3B-C4B	3.53	126.95	121.38
84	DH	1003	CYC	CMB-C2B-C1B	3.53	128.57	124.17
82	ZE	201	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	OF	203	PEB	C2A-C1A-NA	3.53	111.31	108.27
84	DH	1001	CYC	C2C-C1C-NC	3.53	111.31	108.27
85	CL	501	BCR	C10-C11-C12	-3.53	112.20	123.22
82	U1	203	PEB	C3B-C4B-NB	3.53	115.18	110.05
82	YO	202	PEB	CHC-C1D-ND	-3.53	109.26	113.72
84	FE	1001	CYC	C4D-C3D-C2D	-3.53	103.45	107.62
84	GG	1001	CYC	C1B-C2B-C3B	-3.53	104.19	107.87
82	bK	202	PEB	CMC-C3C-C2C	-3.53	117.97	125.61
82	PG	202	PEB	CAC-C2C-C3C	3.53	135.15	127.07
82	YF	203	PEB	C1B-C2B-C3B	-3.53	102.46	106.51
82	g4	201	PEB	CHC-C4C-NC	3.53	125.92	121.15
82	L9	203	PEB	CHC-C4C-NC	3.53	125.92	121.15
82	aO	201	PEB	CHA-C1B-NB	-3.53	117.55	124.93
82	JD	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
82	PB	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
82	EF	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
94	a6	601	PL9	C7-C3-C2	-3.53	118.66	123.30
82	fJ	203	PEB	CHC-C1D-ND	-3.53	109.26	113.72
82	hM	201	PEB	CHC-C1D-ND	-3.53	109.26	113.72
82	WF	203	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	H4	1002	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	HA	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
92	D6	409	LMG	O1-C7-C8	-3.53	102.39	110.90
85	AN	845	BCR	C7-C8-C9	-3.53	120.91	126.23
85	JN	102	BCR	C11-C10-C9	-3.53	122.28	127.31
82	EA	201	PEB	C1B-C2B-C3B	-3.53	102.46	106.51
82	aF	201	PEB	CHC-C1D-ND	-3.53	109.26	113.72
84	G3	1001	CYC	C1A-C2A-C3A	-3.53	102.88	106.78
82	ED	201	PEB	CHB-C4B-C3B	-3.53	117.16	125.32
82	IA	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
82	W7	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
82	eM	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
85	B2	802	BCR	C30-C25-C26	-3.53	117.65	122.61
82	PP	201	PEB	OA-C1A-C2A	-3.53	123.37	126.17
82	I5	201	PEB	OA-C1A-C2A	-3.53	123.37	126.17
82	LE	1002	PEB	CAC-CBC-CGC	-3.53	106.01	113.60
82	sF	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
82	SJ	201	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	l1	202	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	k4	201	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	FP	202	PEB	CMB-C2B-C1B	3.53	130.49	125.06
82	Q9	201	PEB	C3B-C4B-NB	3.53	115.18	110.05
82	S1	201	PEB	CHA-C1B-C2B	3.53	133.97	124.90
82	hM	202	PEB	CAB-C3B-C4B	3.53	131.25	125.01
82	LG	1002	PEB	CAC-CBC-CGC	-3.53	106.02	113.60
84	KG	202	CYC	C1B-C2B-C3B	-3.53	104.19	107.87
82	XM	202	PEB	CAB-C3B-C4B	3.53	131.25	125.01
82	XM	202	PEB	OA-C1A-C2A	-3.53	123.37	126.17
82	EF	202	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	X9	201	PEB	C2A-C1A-NA	3.53	111.31	108.27
82	JB	202	PEB	C3B-C4B-NB	3.53	115.18	110.05
82	UH	203	PEB	C3B-C4B-NB	3.53	115.18	110.05
82	P5	201	PEB	C3B-C4B-NB	3.53	115.18	110.05
82	aF	203	PEB	CMC-C3C-C4C	3.53	130.80	127.06
82	IF	203	PEB	OD-C4D-ND	-3.52	120.71	125.93
82	O1	202	PEB	OD-C4D-ND	-3.52	120.71	125.93
82	YB	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
82	TP	201	PEB	CAC-CBC-CGC	-3.52	106.02	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	FE	1002	CYC	C4A-C3A-C2A	-3.52	102.46	106.51
82	GA	201	PEB	C3B-C4B-NB	3.52	115.18	110.05
84	G3	1001	CYC	CAB-C3B-C4B	3.52	126.94	121.38
82	XQ	203	PEB	C3D-C4D-ND	3.52	114.17	107.26
82	PO	203	PEB	CHC-C4C-NC	3.52	125.92	121.15
82	eF	203	PEB	OD-C4D-ND	-3.52	120.71	125.93
85	k6	102	BCR	C33-C5-C4	3.52	120.39	113.62
82	W9	203	PEB	CMB-C2B-C1B	3.52	130.49	125.06
82	UD	202	PEB	OA-C1A-C2A	-3.52	123.37	126.17
82	VD	203	PEB	OA-C1A-C2A	-3.52	123.37	126.17
82	OE	202	PEB	OA-C1A-C2A	-3.52	123.37	126.17
92	x6	601	LMG	C8-O7-C10	-3.52	109.11	117.79
83	yF	302	PUB	CBA-CAA-C3A	-3.52	107.63	112.98
82	YF	201	PEB	C1D-CHC-C4C	3.52	118.45	113.26
82	iH	201	PEB	OD-C4D-ND	-3.52	120.71	125.93
82	bF	202	PEB	CMC-C3C-C2C	-3.52	117.98	125.61
82	AK	201	PEB	CHB-C1C-C2C	-3.52	119.20	127.15
82	fH	202	PEB	C3D-C4D-ND	3.52	114.17	107.26
84	C3	1001	CYC	C1A-C2A-C3A	-3.52	102.88	106.78
82	B7	203	PEB	C3B-C4B-NB	3.52	115.17	110.05
82	yF	301	PEB	C2A-C1A-NA	3.52	111.31	108.27
82	Q9	201	PEB	CHC-C4C-NC	3.52	125.92	121.15
87	8N	308	CLA	C3B-C4B-NB	-3.52	107.25	110.52
82	aG	201	PEB	C3B-C4B-NB	3.52	115.17	110.05
82	DF	202	PEB	C4B-C3B-C2B	-3.52	102.88	106.78
82	G7	202	PEB	C3D-C4D-ND	3.52	114.17	107.26
82	GA	202	PEB	C3D-C4D-ND	3.52	114.17	107.26
85	BL	617	BCR	C36-C18-C17	-3.52	117.99	122.92
82	S5	201	PEB	OA-C1A-C2A	-3.52	123.37	126.17
82	WH	201	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
82	iJ	202	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
82	OK	202	PEB	C3D-C4D-ND	3.52	114.17	107.26
82	vF	201	PEB	C3D-C4D-ND	3.52	114.17	107.26
82	wK	302	PEB	CHA-C1B-NB	-3.52	117.57	124.93
85	B6	621	BCR	C27-C26-C25	-3.52	117.62	122.73
85	BN	803	BCR	C30-C25-C26	-3.52	117.65	122.61
82	UG	203	PEB	C3D-C4D-ND	3.52	114.17	107.26
84	y3	1001	CYC	C4D-C3D-C2D	-3.52	103.46	107.62
82	DA	202	PEB	CHB-C1C-C2C	-3.52	119.21	127.15
87	bL	618	CLA	CMB-C2B-C1B	-3.52	120.01	125.37
82	KF	201	PEB	C2A-C1A-NA	3.52	111.31	108.27
82	dK	201	PEB	C2A-C1A-NA	3.52	111.31	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aK	203	PEB	CMC-C3C-C4C	3.52	130.79	127.06
82	fH	202	PEB	C3B-C4B-NB	3.52	115.17	110.05
82	A5	201	PEB	OA-C1A-C2A	-3.52	123.37	126.17
82	GD	201	PEB	CAB-C3B-C4B	3.52	131.24	125.01
82	EJ	203	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
82	QB	203	PEB	OD-C4D-ND	-3.52	120.72	125.93
83	AH	303	PUB	CBB-CAB-C3B	3.52	122.41	112.63
84	HG	1001	CYC	C4D-CHA-C1A	3.52	136.18	128.28
85	BN	803	BCR	C39-C30-C29	3.52	122.98	108.91
85	BL	618	BCR	C15-C14-C13	-3.52	122.29	127.31
82	LA	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
82	GP	201	PEB	CAC-CBC-CGC	-3.52	106.03	113.60
88	BL	610	LHG	O7-C7-C8	3.52	119.08	111.50
82	VO	201	PEB	CHA-C1B-NB	-3.52	117.57	124.93
82	qC	202	PEB	OD-C4D-ND	-3.52	120.72	125.93
85	BN	838	BCR	C24-C23-C22	3.52	131.55	126.23
84	L4	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
87	1N	609	CLA	CAA-C2A-C3A	-3.52	105.47	114.26
85	k6	102	BCR	C33-C5-C6	-3.52	120.58	124.53
82	MF	202	PEB	C2A-C1A-NA	3.52	111.31	108.27
82	A4	305	PEB	C2A-C1A-NA	3.52	111.31	108.27
82	dE	202	PEB	C1C-CHB-C4B	3.52	136.17	128.28
82	rC	202	PEB	OD-C4D-ND	-3.52	120.72	125.93
84	A3	1001	CYC	CAB-C3B-C4B	3.52	126.94	121.38
82	EF	201	PEB	CAB-C3B-C4B	3.52	131.23	125.01
82	SB	201	PEB	CHA-C1B-NB	-3.52	117.57	124.93
82	OA	202	PEB	OA-C1A-C2A	-3.52	123.38	126.17
82	YF	202	PEB	OA-C1A-C2A	-3.52	123.38	126.17
82	d4	202	PEB	OA-C1A-C2A	-3.52	123.38	126.17
84	BE	1002	CYC	CHB-C1B-NB	-3.52	118.51	126.06
82	NE	202	PEB	CHC-C4C-NC	3.52	125.91	121.15
82	TB	201	PEB	CHC-C1D-ND	-3.52	109.27	113.72
82	u8	201	PEB	C3D-C4D-ND	3.52	114.16	107.26
82	OK	202	PEB	CHB-C1C-C2C	-3.52	119.22	127.15
82	NF	202	PEB	CHB-C1C-NC	-3.52	117.26	125.32
82	TM	202	PEB	C2A-C1A-NA	3.52	111.31	108.27
82	j4	203	PEB	CHA-C1B-NB	-3.52	117.58	124.93
82	WB	401	PEB	C3B-C4B-NB	3.52	115.17	110.05
82	kH	202	PEB	CMB-C2B-C1B	3.52	130.48	125.06
82	OQ	201	PEB	CHC-C4C-NC	3.52	125.91	121.15
82	iH	201	PEB	CHC-C4C-NC	3.52	125.91	121.15
82	BA	203	PEB	C4B-C3B-C2B	-3.52	102.89	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VQ	203	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
84	K3	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
84	N3	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
84	i3	1001	CYC	CAB-C3B-C4B	3.52	126.93	121.38
82	lF	203	PEB	C3D-C4D-ND	3.52	114.16	107.26
87	8N	306	CLA	CHB-C4A-NA	3.52	129.38	124.51
84	EE	1001	CYC	OB-C4B-C3B	-3.52	124.22	128.04
82	BP	201	PEB	CHA-C1B-NB	-3.52	117.58	124.93
82	RH	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
82	lG	202	PEB	OA-C1A-C2A	-3.52	123.38	126.17
82	TM	201	PEB	C1C-CHB-C4B	-3.52	120.40	128.28
82	SE	202	PEB	C1D-CHC-C4C	-3.52	108.07	113.26
84	E1	1001	CYC	C2A-C1A-NA	3.52	115.16	110.05
82	v8	202	PEB	C3D-C4D-ND	3.52	114.16	107.26
82	MM	201	PEB	OD-C4D-ND	-3.52	120.72	125.93
82	F9	201	PEB	OD-C4D-ND	-3.52	120.72	125.93
82	DK	202	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
82	Y7	303	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
82	dH	201	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
82	FB	201	PEB	C2A-C1A-NA	3.52	111.30	108.27
82	LK	201	PEB	C2C-C1C-NC	3.52	112.31	107.57
82	UP	203	PEB	C2C-C1C-NC	3.52	112.31	107.57
82	EK	202	PEB	C3D-C4D-ND	3.52	114.16	107.26
82	WK	202	PEB	OD-C4D-ND	-3.52	120.72	125.93
82	IP	202	PEB	OD-C4D-ND	-3.52	120.72	125.93
82	UE	203	PEB	C3D-C4D-ND	3.52	114.16	107.26
82	IA	202	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
84	G4	1001	CYC	CHD-C1D-ND	-3.51	117.27	125.32
84	JH	1003	CYC	C4D-C3D-C2D	-3.51	103.47	107.62
82	t8	202	PEB	CAB-C3B-C4B	3.51	131.23	125.01
87	2N	303	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
82	OF	203	PEB	C4B-C3B-C2B	-3.51	102.89	106.78
84	t3	1001	CYC	C1A-C2A-C3A	-3.51	102.89	106.78
82	aE	201	PEB	C3B-C4B-NB	3.51	115.16	110.05
82	OP	203	PEB	C1C-CHB-C4B	3.51	136.16	128.28
82	S5	202	PEB	C1C-CHB-C4B	3.51	136.16	128.28
82	J9	201	PEB	CAB-C3B-C4B	3.51	131.23	125.01
82	F5	203	PEB	OA-C1A-C2A	-3.51	123.38	126.17
82	T5	202	PEB	OA-C1A-C2A	-3.51	123.38	126.17
82	iM	201	PEB	OA-C1A-C2A	-3.51	123.38	126.17
82	MP	201	PEB	C2C-C1C-NC	3.51	112.30	107.57
82	r8	202	PEB	CHA-C1B-NB	-3.51	117.58	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NI	203	PEB	C3B-C4B-NB	3.51	115.16	110.05
82	I5	201	PEB	C3B-C4B-NB	3.51	115.16	110.05
82	SB	202	PEB	C4B-C3B-C2B	-3.51	102.89	106.78
85	J2	102	BCR	C11-C10-C9	-3.51	122.30	127.31
82	LH	1003	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
84	v3	1001	CYC	CAB-C3B-C4B	3.51	126.93	121.38
82	UP	201	PEB	C1D-CHC-C4C	-3.51	108.08	113.26
82	F9	203	PEB	OA-C1A-C2A	-3.51	123.38	126.17
82	WM	203	PEB	CHA-C1B-NB	-3.51	117.58	124.93
82	kO	202	PEB	CHA-C1B-NB	-3.51	117.58	124.93
82	BD	203	PEB	C1C-CHB-C4B	3.51	136.16	128.28
82	BQ	203	PEB	C1C-CHB-C4B	3.51	136.16	128.28
82	V7	202	PEB	C1C-CHB-C4B	3.51	136.16	128.28
82	Q7	202	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
83	yK	302	PUB	OD-C4D-ND	-3.51	120.73	125.93
82	YK	203	PEB	CHA-C1B-C2B	3.51	133.93	124.90
82	j1	201	PEB	CHC-C4C-NC	3.51	125.90	121.15
82	jH	201	PEB	CHC-C4C-NC	3.51	125.90	121.15
82	M9	301	PEB	CHC-C4C-NC	3.51	125.90	121.15
82	wF	302	PEB	CHA-C1B-NB	-3.51	117.59	124.93
82	W1	201	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
82	oK	201	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
82	C5	202	PEB	OA-C1A-C2A	-3.51	123.38	126.17
82	dH	202	PEB	OD-C4D-ND	-3.51	120.73	125.93
82	EF	202	PEB	C3D-C4D-ND	3.51	114.15	107.26
84	BG	1002	CYC	CHA-C4D-C3D	-3.51	119.23	127.15
82	QM	202	PEB	OD-C4D-ND	-3.51	120.73	125.93
82	CJ	203	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
82	I5	201	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
82	ZB	201	PEB	CMB-C2B-C1B	3.51	130.47	125.06
85	B2	841	BCR	C1-C6-C5	-3.51	117.67	122.61
83	BM	302	PUB	CHA-C1B-NB	3.51	125.90	121.15
94	d6	408	PL9	C10-C9-C11	3.51	121.18	115.27
87	AN	839	CLA	CMB-C2B-C1B	-3.51	120.02	125.37
82	V1	202	PEB	C3D-C4D-ND	3.51	114.15	107.26
85	K2	102	BCR	C27-C26-C25	-3.51	117.64	122.73
82	VH	201	PEB	CHA-C4A-NA	3.51	129.38	125.20
83	AG	303	PUB	C1C-C2C-C3C	-3.51	102.90	106.78
82	kH	203	PEB	C1C-CHB-C4B	3.51	136.15	128.28
82	GQ	201	PEB	CAB-C3B-C4B	3.51	131.22	125.01
82	DB	203	PEB	C3B-C4B-NB	3.51	115.15	110.05
82	LB	201	PEB	C3B-C4B-NB	3.51	115.15	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MJ	202	PEB	C3B-C4B-NB	3.51	115.15	110.05
84	FE	1002	CYC	CHB-C4A-NA	-3.51	117.59	124.93
87	1N	607	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
82	BP	201	PEB	C2C-C1C-NC	3.51	112.30	107.57
82	HQ	203	PEB	OA-C1A-C2A	-3.51	123.38	126.17
82	ZG	203	PEB	CHC-C4C-NC	3.51	125.90	121.15
84	E3	1001	CYC	C1A-C2A-C3A	-3.51	102.90	106.78
84	HO	1001	CYC	C2A-C1A-NA	3.51	115.15	110.05
82	OA	201	PEB	OD-C4D-ND	-3.51	120.73	125.93
84	N3	1001	CYC	CAB-C3B-C4B	3.51	126.92	121.38
82	EA	202	PEB	C3D-C4D-ND	3.51	114.14	107.26
82	TP	201	PEB	CAC-C2C-C1C	3.51	131.35	125.76
82	l1	201	PEB	C1C-CHB-C4B	3.51	136.15	128.28
84	M1	201	CYC	C4D-C3D-C2D	-3.51	103.47	107.62
82	VH	202	PEB	CHA-C4A-NA	3.51	129.38	125.20
82	kH	202	PEB	CHC-C1D-ND	-3.51	109.29	113.72
82	RE	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
83	AQ	302	PUB	CAB-C3B-C4B	3.51	131.35	125.76
82	VP	201	PEB	C2C-C1C-NC	3.51	112.30	107.57
82	VA	203	PEB	C3D-C4D-ND	3.51	114.14	107.26
84	I1	1001	CYC	CHA-C4D-C3D	-3.51	119.24	127.15
82	SF	202	PEB	CHC-C1D-ND	-3.51	109.29	113.72
84	BG	1001	CYC	C2D-C1D-ND	3.51	112.33	107.40
82	xK	304	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
84	i3	1001	CYC	C1A-C2A-C3A	-3.51	102.90	106.78
82	u8	201	PEB	CBA-CAA-C3A	3.51	121.28	113.47
84	t3	1001	CYC	CAB-C3B-C4B	3.51	126.92	121.38
82	GJ	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
82	O5	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
82	NJ	201	PEB	OD-C4D-ND	-3.51	120.73	125.93
82	W9	203	PEB	OD-C4D-ND	-3.51	120.73	125.93
82	eH	203	PEB	CHA-C1B-NB	-3.51	117.60	124.93
82	R5	202	PEB	OA-C1A-C2A	-3.51	123.39	126.17
82	s8	203	PEB	OA-C1A-C2A	-3.51	123.39	126.17
82	iF	201	PEB	OA-C1A-C2A	-3.51	123.39	126.17
82	VG	201	PEB	CHC-C1D-ND	-3.51	109.29	113.72
82	ID	201	PEB	OD-C4D-ND	-3.51	120.74	125.93
82	AA	201	PEB	CHA-C1B-NB	-3.51	117.60	124.93
82	SF	201	PEB	C3B-C4B-NB	3.51	115.15	110.05
82	AK	202	PEB	CHC-C1D-ND	-3.51	109.29	113.72
82	KJ	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
82	cG	202	PEB	C2A-C1A-NA	3.51	111.30	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	kH	201	PEB	C2A-C1A-NA	3.51	111.30	108.27
83	wK	304	PUB	CBA-CAA-C3A	-3.51	107.66	112.98
82	A7	201	PEB	CHA-C1B-NB	-3.51	117.60	124.93
82	UG	202	PEB	OD-C4D-ND	-3.51	120.74	125.93
82	yK	301	PEB	OD-C4D-ND	-3.51	120.74	125.93
82	R5	201	PEB	OA-C1A-C2A	-3.51	123.39	126.17
82	lM	201	PEB	OA-C1A-C2A	-3.51	123.39	126.17
82	D1	1002	PEB	CHC-C4C-NC	3.51	125.89	121.15
87	d6	403	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
82	ZO	201	PEB	C1C-CHB-C4B	3.50	136.14	128.28
82	r8	202	PEB	OD-C4D-ND	-3.50	120.74	125.93
82	RD	203	PEB	C3D-C4D-ND	3.50	114.14	107.26
84	JO	1001	CYC	CHA-C4D-C3D	-3.50	119.24	127.15
82	GF	202	PEB	CAC-CBC-CGC	3.50	121.14	113.60
84	m3	1001	CYC	CAB-C3B-C4B	3.50	126.91	121.38
85	c6	602	BCR	C15-C14-C13	-3.50	122.31	127.31
83	AD	302	PUB	CAB-C3B-C4B	3.50	131.34	125.76
83	yK	303	PUB	CHC-C1D-ND	-3.50	109.29	113.72
82	vC	202	PEB	C3D-C4D-ND	3.50	114.13	107.26
82	E7	201	PEB	OD-C4D-ND	-3.50	120.74	125.93
82	JD	202	PEB	C3B-C4B-NB	3.50	115.15	110.05
82	KG	201	PEB	CHC-C4C-NC	3.50	125.89	121.15
82	NG	201	PEB	CHC-C4C-NC	3.50	125.89	121.15
84	l3	1001	CYC	CAB-C3B-C4B	3.50	126.91	121.38
82	Z4	201	PEB	C1C-CHB-C4B	3.50	136.14	128.28
85	C6	508	BCR	C36-C18-C19	3.50	123.60	118.08
82	II	203	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
82	qK	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
82	EK	201	PEB	CAB-C3B-C4B	3.50	131.21	125.01
82	TO	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	hB	301	PEB	CHC-C1D-ND	-3.50	109.29	113.72
82	S7	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
84	HH	1001	CYC	C1D-C2D-C3D	-3.50	103.33	107.79
82	LA	203	PEB	C3D-C4D-ND	3.50	114.13	107.26
82	OD	201	PEB	CHC-C4C-NC	3.50	125.89	121.15
82	W5	201	PEB	CHC-C4C-NC	3.50	125.89	121.15
82	GF	201	PEB	C3C-C4C-NC	3.50	111.49	108.33
82	dM	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
82	ZE	202	PEB	OD-C4D-ND	-3.50	120.74	125.93
82	UH	203	PEB	OD-C4D-ND	-3.50	120.74	125.93
83	wF	304	PUB	OD-C4D-ND	-3.50	120.74	125.93
82	EQ	201	PEB	CHB-C4B-C3B	-3.50	117.22	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	wK	302	PEB	C3D-C4D-ND	3.50	114.13	107.26
98	B2	837	PQN	C16-C15-C13	-3.50	104.27	113.45
84	E3	1001	CYC	CAB-C3B-C4B	3.50	126.91	121.38
82	N7	202	PEB	CHA-C4A-NA	3.50	129.37	125.20
82	PG	202	PEB	CMB-C2B-C1B	3.50	130.46	125.06
82	iH	201	PEB	CMB-C2B-C1B	3.50	130.46	125.06
82	U4	201	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	N5	201	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	H9	201	PEB	CAB-C3B-C4B	3.50	131.20	125.01
82	P5	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
82	KF	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	CK	203	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	dM	201	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	RA	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	dF	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	PE	202	PEB	CMB-C2B-C1B	3.50	130.46	125.06
82	mO	203	PEB	CHC-C4C-NC	3.50	125.89	121.15
82	SK	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
82	WP	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
85	KN	101	BCR	C27-C26-C25	-3.50	117.65	122.73
82	l1	201	PEB	CHA-C1B-NB	-3.50	117.61	124.93
82	B7	203	PEB	C1D-CHC-C4C	-3.50	108.09	113.26
82	iK	203	PEB	OD-C4D-ND	-3.50	120.75	125.93
84	FE	1002	CYC	CMB-C2B-C1B	3.50	128.54	124.17
82	D7	202	PEB	CHB-C1C-C2C	-3.50	119.25	127.15
82	OG	203	PEB	C3B-C4B-NB	3.50	115.14	110.05
87	12	609	CLA	CAA-C2A-C3A	-3.50	105.52	114.26
84	EG	1001	CYC	C4D-C3D-C2D	-3.50	103.48	107.62
83	Z5	302	PUB	C2B-C1B-NB	3.50	111.48	108.33
82	uK	202	PEB	C3D-C4D-ND	3.50	114.12	107.26
82	R5	201	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	Z4	202	PEB	CHC-C4C-NC	3.50	125.89	121.15
82	M5	305	PEB	CHC-C4C-NC	3.50	125.89	121.15
82	E5	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	R5	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	T5	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	H7	202	PEB	C3D-C4D-ND	3.50	114.12	107.26
82	aF	201	PEB	C3D-C4D-ND	3.50	114.12	107.26
84	P3	1001	CYC	C1A-C2A-C3A	-3.50	102.91	106.78
82	r8	201	PEB	CBA-CAA-C3A	3.50	121.26	113.47
82	a4	201	PEB	CHA-C1B-NB	-3.50	117.61	124.93
84	GO	1001	CYC	CHD-C1D-ND	-3.50	117.31	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HQ	203	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	CK	203	PEB	CHC-C4C-NC	3.50	125.88	121.15
82	V5	201	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	wF	302	PEB	C3D-C4D-ND	3.50	114.12	107.26
82	hJ	203	PEB	C3D-C4D-ND	3.50	114.12	107.26
92	CL	519	LMG	O7-C10-C11	3.50	119.04	111.50
82	i1	201	PEB	CMB-C2B-C1B	3.50	130.45	125.06
82	BI	201	PEB	OD-C4D-ND	-3.50	120.75	125.93
82	X5	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	ED	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
82	dG	203	PEB	OA-C1A-C2A	-3.50	123.39	126.17
87	72	608	CLA	CAA-C2A-C3A	-3.50	107.94	116.10
82	k1	202	PEB	CMB-C2B-C1B	3.50	130.45	125.06
82	KK	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	s8	203	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	kK	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	AK	202	PEB	C3D-C4D-ND	3.50	114.12	107.26
84	P3	1001	CYC	CAB-C3B-C4B	3.50	126.90	121.38
82	iF	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
84	p3	1001	CYC	C1A-C2A-C3A	-3.50	102.91	106.78
82	AE	304	PEB	CHC-C4C-NC	3.50	125.88	121.15
85	KN	104	BCR	C23-C22-C21	3.50	124.31	118.94
82	WH	203	PEB	CMB-C2B-C1B	3.50	130.45	125.06
82	GJ	203	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	gK	203	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
82	MJ	202	PEB	OD-C4D-ND	-3.50	120.75	125.93
82	u8	201	PEB	CHB-C4B-C3B	-3.50	117.23	125.32
82	HB	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
82	iE	201	PEB	CHC-C4C-NC	3.50	125.88	121.15
82	h1	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
82	FF	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
82	qF	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
82	XA	201	PEB	CHA-C1B-NB	-3.50	117.62	124.93
82	AQ	304	PEB	OD-C4D-ND	-3.50	120.75	125.93
82	k1	202	PEB	C3D-C4D-ND	3.50	114.12	107.26
87	82	305	CLA	CHB-C4A-NA	3.50	129.35	124.51
82	KK	201	PEB	C3B-C4B-NB	3.50	115.13	110.05
82	NA	202	PEB	CHA-C4A-NA	3.50	129.36	125.20
87	A6	403	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
82	gH	203	PEB	C3D-C4D-ND	3.50	114.12	107.26
82	k1	202	PEB	CHC-C1D-ND	-3.50	109.30	113.72
82	NB	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	v3	1001	CYC	C1A-C2A-C3A	-3.50	102.91	106.78
82	uC	201	PEB	CBA-CAA-C3A	3.50	121.25	113.47
82	UE	202	PEB	OD-C4D-ND	-3.50	120.75	125.93
82	LJ	202	PEB	OA-C1A-C2A	-3.50	123.39	126.17
82	QJ	204	PEB	C2A-C1A-NA	3.50	111.29	108.27
84	FE	1001	CYC	C2C-C1C-NC	3.50	111.29	108.27
85	KL	100	BCR	C31-C1-C6	-3.50	104.63	110.30
82	PE	202	PEB	CAC-C2C-C3C	3.49	135.07	127.07
82	j1	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
88	I6	101	LHG	O7-C7-C8	3.49	119.03	111.50
82	vK	201	PEB	C3D-C4D-ND	3.49	114.12	107.26
82	UM	202	PEB	CHC-C4C-NC	3.49	125.88	121.15
84	g3	1001	CYC	CAB-C3B-C4B	3.49	126.90	121.38
82	lJ	202	PEB	CHA-C1B-C2B	3.49	133.89	124.90
84	R3	1001	CYC	C1A-C2A-C3A	-3.49	102.92	106.78
82	WG	201	PEB	C3B-C4B-NB	3.49	115.13	110.05
82	lK	203	PEB	CHA-C1B-C2B	3.49	133.88	124.90
83	M5	302	PUB	C2B-C1B-NB	3.49	111.48	108.33
82	kG	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
82	PF	202	PEB	OA-C1A-C2A	-3.49	123.39	126.17
82	MQ	202	PEB	OA-C1A-C2A	-3.49	123.39	126.17
94	a6	601	PL9	C31-C29-C28	3.49	128.19	121.12
82	iF	203	PEB	C3D-C4D-ND	3.49	114.11	107.26
82	QH	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	S4	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	HB	201	PEB	CMC-C3C-C2C	-3.49	118.05	125.61
82	GK	201	PEB	CHA-C1B-C2B	3.49	133.88	124.90
82	YM	203	PEB	C2A-C1A-NA	3.49	111.28	108.27
96	VL	201	HEM	CHB-C1B-NB	3.49	128.68	124.37
82	UO	202	PEB	OA-C1A-C2A	-3.49	123.40	126.17
82	UQ	202	PEB	OA-C1A-C2A	-3.49	123.40	126.17
82	UI	202	PEB	CHC-C4C-NC	3.49	125.88	121.15
82	q8	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
82	ZF	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	XD	203	PEB	C3D-C4D-ND	3.49	114.11	107.26
82	VD	203	PEB	OD-C4D-C3D	-3.49	121.55	129.46
82	TJ	201	PEB	C1C-CHB-C4B	-3.49	120.45	128.28
82	DH	1002	PEB	CHC-C4C-NC	3.49	125.88	121.15
82	KJ	203	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
82	EQ	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
82	VP	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
82	h4	202	PEB	C2A-C1A-NA	3.49	111.28	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eF	203	PEB	C2A-C1A-NA	3.49	111.28	108.27
82	SA	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
87	12	609	CLA	CHB-C4A-NA	3.49	129.34	124.51
82	uF	203	PEB	OA-C1A-C2A	-3.49	123.40	126.17
82	bH	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
87	BL	620	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
82	V1	203	PEB	CHA-C4A-NA	3.49	129.36	125.20
87	B2	825	CLA	CMB-C2B-C1B	-3.49	120.05	125.37
82	WA	201	PEB	CMB-C2B-C1B	3.49	130.44	125.06
82	FQ	201	PEB	CMA-C2A-C1A	-3.49	104.88	112.40
82	W1	202	PEB	C3D-C4D-ND	3.49	114.11	107.26
82	X7	201	PEB	CHA-C1B-NB	-3.49	117.63	124.93
82	dE	204	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
87	BN	801	CLA	CMB-C2B-C1B	-3.49	120.05	125.37
82	aJ	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
82	Z5	305	PEB	CHC-C4C-NC	3.49	125.87	121.15
85	CL	516	BCR	C7-C8-C9	-3.49	120.96	126.23
82	SH	203	PEB	C3D-C4D-ND	3.49	114.11	107.26
82	J7	201	PEB	C3B-C4B-NB	3.49	115.13	110.05
84	LO	1001	CYC	C1A-C2A-C3A	-3.49	102.92	106.78
82	BM	301	PEB	CAC-CBC-CGC	-3.49	106.09	113.60
82	UO	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	OI	203	PEB	CMB-C2B-C1B	3.49	130.44	125.06
84	DH	1001	CYC	C1B-NB-C4B	-3.49	106.23	110.67
84	H4	1001	CYC	C4D-C3D-C2D	-3.49	103.50	107.62
82	AJ	301	PEB	C3B-C4B-NB	3.49	115.12	110.05
87	7N	608	CLA	CAA-C2A-C3A	-3.49	107.96	116.10
87	32	309	CLA	CHB-C4A-NA	3.49	129.34	124.51
82	AD	304	PEB	OD-C4D-ND	-3.49	120.76	125.93
82	IP	203	PEB	C2C-C1C-NC	3.49	112.27	107.57
84	73	1002	CYC	C1B-C2B-C3B	-3.49	104.23	107.87
85	BN	841	BCR	C1-C6-C5	-3.49	117.70	122.61
82	W5	201	PEB	CHC-C1D-ND	-3.49	109.31	113.72
84	c3	1001	CYC	C1A-C2A-C3A	-3.49	102.92	106.78
82	VD	203	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	SQ	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
82	f1	202	PEB	C3B-C4B-NB	3.49	115.12	110.05
82	TM	201	PEB	CHA-C1B-NB	-3.49	117.64	124.93
82	tC	202	PEB	CAB-C3B-C4B	3.49	131.18	125.01
82	II	203	PEB	C1D-CHC-C4C	-3.49	108.11	113.26
82	d1	201	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
82	FQ	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	uC	202	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
98	BN	837	PQN	C16-C15-C13	-3.49	104.31	113.45
96	vL	201	HEM	CHB-C1B-NB	3.49	128.68	124.37
82	BP	201	PEB	OD-C4D-ND	-3.49	120.76	125.93
82	IK	201	PEB	CMB-C2B-C3B	-3.49	116.65	126.12
87	22	605	CLA	CMB-C2B-C3B	3.49	132.63	123.59
82	eF	202	PEB	CHB-C1C-C2C	-3.49	119.28	127.15
96	f6	101	HEM	CBA-CAA-C2A	-3.49	102.94	112.63
82	AK	202	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
82	L1	1002	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	X5	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
82	VK	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
82	hM	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
82	oK	203	PEB	C3B-C4B-NB	3.49	115.12	110.05
82	HJ	202	PEB	CHB-C4B-NB	-3.49	117.32	124.58
82	uC	201	PEB	CHB-C4B-C3B	-3.49	117.25	125.32
82	KK	201	PEB	CMB-C2B-C1B	3.49	130.43	125.06
85	b6	602	BCR	C33-C5-C6	-3.49	120.61	124.53
82	O1	203	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
84	JH	1003	CYC	C1B-C2B-C3B	-3.49	104.23	107.87
87	22	602	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
82	CP	201	PEB	C3D-C4D-ND	3.49	114.10	107.26
82	P7	202	PEB	C3B-C4B-NB	3.49	115.12	110.05
82	IM	203	PEB	CHA-C1B-NB	-3.49	117.64	124.93
82	OK	203	PEB	C3D-C4D-ND	3.49	114.10	107.26
87	3N	309	CLA	CHB-C4A-NA	3.49	129.33	124.51
92	B6	618	LMG	C8-O7-C10	-3.49	109.21	117.79
87	2N	301	CLA	CMB-C2B-C3B	3.49	132.62	123.59
82	G7	201	PEB	C3B-C4B-NB	3.49	115.12	110.05
84	NE	201	CYC	C1B-C2B-C3B	-3.49	104.23	107.87
82	Y9	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
82	NB	202	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	TD	203	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	YF	201	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	g1	201	PEB	C3D-C4D-ND	3.48	114.10	107.26
82	G5	201	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
82	K5	201	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
84	l3	1001	CYC	C1A-C2A-C3A	-3.48	102.93	106.78
82	eG	203	PEB	CHB-C1C-NC	-3.48	117.34	125.32
82	lH	202	PEB	CHC-C1D-ND	-3.48	109.32	113.72
84	c3	1001	CYC	CAB-C3B-C4B	3.48	126.88	121.38
82	ID	202	PEB	OA-C1A-C2A	-3.48	123.40	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JI	201	PEB	OA-C1A-C2A	-3.48	123.40	126.17
82	M5	301	PEB	OD-C4D-ND	-3.48	120.77	125.93
87	BN	811	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
82	lF	203	PEB	CHA-C1B-C2B	3.48	133.86	124.90
84	IO	1001	CYC	C2C-C1C-NC	3.48	111.28	108.27
82	K5	201	PEB	C3B-C4B-NB	3.48	115.12	110.05
82	MP	203	PEB	C3D-C4D-ND	3.48	114.09	107.26
84	BE	1002	CYC	CHA-C4D-C3D	-3.48	119.29	127.15
84	LH	1001	CYC	CHA-C4D-C3D	-3.48	119.29	127.15
82	cB	401	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
82	SP	203	PEB	C2C-C1C-NC	3.48	112.26	107.57
82	UA	202	PEB	OD-C4D-ND	-3.48	120.77	125.93
82	ZF	202	PEB	OD-C4D-ND	-3.48	120.77	125.93
82	T7	201	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	wC	204	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	yK	301	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	hO	202	PEB	C2A-C1A-NA	3.48	111.28	108.27
82	W9	203	PEB	CHC-C4C-NC	3.48	125.86	121.15
98	B2	837	PQN	C11-C12-C13	-3.48	121.00	126.79
82	NA	203	PEB	C3B-C4B-NB	3.48	115.11	110.05
82	bK	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
82	RA	202	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
82	YE	202	PEB	CMC-C3C-C4C	-3.48	123.37	127.06
83	yF	302	PUB	OD-C4D-ND	-3.48	120.77	125.93
82	SH	201	PEB	CHA-C1B-C2B	3.48	133.85	124.90
82	hG	201	PEB	C1C-C2C-C3C	-3.48	103.51	107.62
82	jM	203	PEB	C1C-CHB-C4B	3.48	136.09	128.28
87	dL	404	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
82	AB	501	PEB	C3B-C4B-NB	3.48	115.11	110.05
82	JP	201	PEB	C3B-C4B-NB	3.48	115.11	110.05
82	PG	201	PEB	CAB-CBB-CGB	-3.48	106.11	113.60
82	gF	201	PEB	OD-C4D-ND	-3.48	120.77	125.93
82	KB	302	PEB	OD-C4D-C3D	-3.48	121.57	129.46
82	O1	203	PEB	C3D-C4D-ND	3.48	114.09	107.26
82	dM	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
82	AP	203	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
82	gM	201	PEB	CMC-C3C-C4C	3.48	130.75	127.06
82	VQ	201	PEB	C3B-C4B-NB	3.48	115.11	110.05
82	G5	201	PEB	C3B-C4B-NB	3.48	115.11	110.05
85	A2	846	BCR	C7-C8-C9	-3.48	120.98	126.23
82	kJ	202	PEB	OD-C4D-ND	-3.48	120.78	125.93
85	BL	617	BCR	C20-C19-C18	3.48	136.19	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VO	202	PEB	OD-C4D-C3D	-3.48	121.58	129.46
82	RB	201	PEB	C1C-C2C-C3C	-3.48	103.51	107.62
82	BI	202	PEB	CMB-C2B-C1B	3.48	130.42	125.06
82	F5	201	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
82	KA	201	PEB	C3D-C4D-ND	3.48	114.08	107.26
87	AN	811	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
82	CM	202	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
82	KJ	203	PEB	CMB-C2B-C1B	3.48	130.42	125.06
82	LP	201	PEB	C3B-C4B-NB	3.48	115.11	110.05
82	kM	202	PEB	CAB-C3B-C4B	3.48	131.16	125.01
82	C5	201	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
85	K6	102	BCR	C33-C5-C6	-3.48	120.62	124.53
94	a6	601	PL9	C17-C18-C19	-3.48	119.28	127.66
82	ED	202	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
82	hG	203	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
82	MK	203	PEB	CMB-C2B-C1B	3.48	130.42	125.06
82	LD	203	PEB	CHC-C1D-ND	-3.48	109.32	113.72
82	AF	202	PEB	CHC-C1D-ND	-3.48	109.32	113.72
82	AG	304	PEB	CHC-C4C-NC	3.48	125.86	121.15
92	B6	619	LMG	C8-O7-C10	-3.48	109.23	117.79
82	RH	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
82	eB	202	PEB	C2A-C1A-NA	3.48	111.27	108.27
82	a4	201	PEB	OD-C4D-ND	-3.48	120.78	125.93
84	R3	1001	CYC	CAB-C3B-C4B	3.48	126.87	121.38
82	X5	202	PEB	OA-C1A-C2A	-3.48	123.41	126.17
82	b1	201	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
82	YA	301	PEB	CHC-C1D-ND	-3.48	109.33	113.72
82	iM	201	PEB	C1D-CHC-C4C	3.48	118.38	113.26
82	u8	202	PEB	C1C-C2C-C3C	-3.48	103.51	107.62
82	rC	202	PEB	CHA-C1B-NB	-3.48	117.66	124.93
82	uC	201	PEB	CMB-C2B-C1B	3.48	130.42	125.06
82	WA	201	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
84	M1	201	CYC	C1B-C2B-C3B	-3.48	104.24	107.87
82	O5	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
82	oF	203	PEB	C3B-C4B-NB	3.48	115.11	110.05
82	SP	202	PEB	CHC-C4C-NC	3.48	125.85	121.15
82	U1	203	PEB	OD-C4D-ND	-3.48	120.78	125.93
82	VO	202	PEB	OA-C1A-C2A	-3.48	123.41	126.17
82	Y9	202	PEB	OA-C1A-C2A	-3.48	123.41	126.17
82	eK	202	PEB	CHB-C1C-C2C	-3.48	119.31	127.15
82	PQ	203	PEB	OD-C4D-ND	-3.48	120.78	125.93
82	L9	203	PEB	OD-C4D-ND	-3.48	120.78	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gJ	202	PEB	CHC-C1D-ND	-3.48	109.33	113.72
82	UG	201	PEB	C4B-C3B-C2B	-3.48	102.94	106.78
82	LJ	202	PEB	C4B-C3B-C2B	-3.48	102.94	106.78
82	H5	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
82	T1	201	PEB	CAB-C3B-C4B	3.48	131.16	125.01
82	PK	202	PEB	OA-C1A-C2A	-3.47	123.41	126.17
82	VM	202	PEB	OA-C1A-C2A	-3.47	123.41	126.17
82	O1	203	PEB	OA-C1A-C2A	-3.47	123.41	126.17
87	1N	609	CLA	CHB-C4A-NA	3.47	129.32	124.51
82	rC	201	PEB	CBA-CAA-C3A	3.47	121.20	113.47
87	A2	837	CLA	O2A-CGA-O1A	-3.47	114.82	123.59
82	VM	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
82	OP	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
82	H4	1002	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
82	GP	201	PEB	C3D-C4D-ND	3.47	114.08	107.26
84	CO	1001	CYC	CHD-C1D-ND	-3.47	117.36	125.32
82	SF	203	PEB	C2A-C1A-NA	3.47	111.27	108.27
82	iJ	201	PEB	C2A-C1A-NA	3.47	111.27	108.27
82	FI	202	PEB	CHC-C4C-NC	3.47	125.85	121.15
82	ED	202	PEB	CMB-C2B-C1B	3.47	130.41	125.06
82	kJ	202	PEB	CMB-C2B-C1B	3.47	130.41	125.06
85	B2	839	BCR	C8-C9-C10	3.47	124.27	118.94
84	H1	1001	CYC	C1D-C2D-C3D	-3.47	103.36	107.79
82	U5	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
87	A2	839	CLA	CMB-C2B-C1B	-3.47	120.08	125.37
82	d1	202	PEB	CHA-C1B-NB	-3.47	117.67	124.93
82	kH	202	PEB	C3D-C4D-ND	3.47	114.08	107.26
82	GF	201	PEB	CHA-C1B-C2B	3.47	133.83	124.90
82	xF	302	PEB	C3D-C4D-ND	3.47	114.07	107.26
84	73	1001	CYC	CAD-C3D-C4D	3.47	131.29	125.76
82	SK	201	PEB	CMC-C3C-C4C	3.47	130.74	127.06
82	IF	201	PEB	CMB-C2B-C3B	-3.47	116.69	126.12
82	J1	1002	PEB	C3B-C4B-NB	3.47	115.10	110.05
82	C5	201	PEB	C3B-C4B-NB	3.47	115.10	110.05
84	EO	1001	CYC	C1B-C2B-C3B	-3.47	104.25	107.87
82	zF	501	PEB	CHB-C4B-C3B	-3.47	117.28	125.32
82	tK	202	PEB	CAC-C2C-C3C	3.47	135.02	127.07
82	JP	202	PEB	CHC-C4C-NC	3.47	125.85	121.15
82	FD	201	PEB	CMA-C2A-C1A	-3.47	104.92	112.40
82	dH	201	PEB	CHC-C1D-ND	-3.47	109.33	113.72
82	gH	201	PEB	C3D-C4D-ND	3.47	114.07	107.26
82	I7	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	u8	202	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
82	WE	201	PEB	C1D-CHC-C4C	-3.47	108.14	113.26
82	jJ	203	PEB	C1C-CHB-C4B	3.47	136.07	128.28
82	RG	202	PEB	CMB-C2B-C1B	3.47	130.41	125.06
82	QQ	201	PEB	CMB-C2B-C1B	3.47	130.41	125.06
82	VH	201	PEB	C2A-C1A-NA	3.47	111.27	108.27
82	MK	202	PEB	C2A-C1A-NA	3.47	111.27	108.27
82	PA	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
82	e4	201	PEB	C3B-C4B-NB	3.47	115.10	110.05
82	EP	202	PEB	CHC-C4C-NC	3.47	125.85	121.15
87	1N	608	CLA	CAA-C2A-C3A	-3.47	108.00	116.10
82	SJ	203	PEB	C1C-CHB-C4B	3.47	136.07	128.28
82	MA	202	PEB	C2A-C1A-NA	3.47	111.27	108.27
82	QJ	202	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
82	CF	202	PEB	CHB-C4B-C3B	-3.47	117.29	125.32
82	a1	202	PEB	CHC-C1D-ND	-3.47	109.33	113.72
82	aB	202	PEB	CHC-C1D-ND	-3.47	109.33	113.72
87	cL	515	CLA	CMD-C2D-C1D	3.47	130.83	124.71
82	A5	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
82	JD	202	PEB	CHC-C4C-NC	3.47	125.84	121.15
82	ZG	201	PEB	C2A-C1A-NA	3.47	111.26	108.27
82	JP	201	PEB	C2A-C1A-NA	3.47	111.26	108.27
82	bB	201	PEB	C2A-C1A-NA	3.47	111.26	108.27
82	N4	1002	PEB	OD-C4D-ND	-3.47	120.79	125.93
82	q8	202	PEB	C3C-C4C-NC	3.47	111.46	108.33
82	N5	201	PEB	C3B-C4B-NB	3.47	115.10	110.05
87	12	608	CLA	CAA-C2A-C3A	-3.47	108.00	116.10
87	B2	810	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
82	Y7	301	PEB	CHC-C1D-ND	-3.47	109.33	113.72
85	AN	847	BCR	C16-C17-C18	-3.47	122.36	127.31
82	N7	202	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
84	H4	1001	CYC	C2A-C1A-NA	3.47	115.09	110.05
82	OH	203	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
92	BL	611	LMG	C8-O7-C10	-3.47	109.25	117.79
82	b1	203	PEB	CHA-C1B-NB	-3.47	117.68	124.93
84	FE	1001	CYC	CMB-C2B-C1B	3.47	128.50	124.17
82	TG	201	PEB	C2A-C1A-NA	3.47	111.26	108.27
82	bH	202	PEB	C2A-C1A-NA	3.47	111.26	108.27
84	C4	1001	CYC	C2C-C1C-NC	3.47	111.26	108.27
82	HI	202	PEB	OD-C4D-C3D	-3.47	121.60	129.46
82	OJ	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
82	W1	203	PEB	CMB-C2B-C1B	3.47	130.41	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O5	201	PEB	CMB-C2B-C1B	3.47	130.41	125.06
84	FO	1001	CYC	CHB-C4A-NA	-3.47	117.68	124.93
87	AN	837	CLA	O2A-CGA-O1A	-3.47	114.84	123.59
82	S1	202	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
82	O7	201	PEB	CHA-C4A-NA	3.47	129.33	125.20
82	cG	201	PEB	CMB-C2B-C1B	3.47	130.40	125.06
82	RD	201	PEB	C2C-C1C-NC	3.47	112.24	107.57
82	IQ	201	PEB	OD-C4D-ND	-3.47	120.79	125.93
82	sC	203	PEB	CHC-C4C-NC	3.47	125.84	121.15
82	P5	202	PEB	OA-C1A-C2A	-3.47	123.42	126.17
82	K7	201	PEB	C3D-C4D-ND	3.47	114.06	107.26
82	DD	203	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
84	F4	1001	CYC	CHB-C4A-NA	-3.47	117.68	124.93
82	SK	203	PEB	C2A-C1A-NA	3.47	111.26	108.27
84	H1	1001	CYC	C4A-C3A-C2A	-3.47	102.53	106.51
82	jG	201	PEB	CMB-C2B-C1B	3.47	130.40	125.06
82	PM	202	PEB	CHC-C4C-NC	3.47	125.84	121.15
82	w8	204	PEB	CMC-C3C-C4C	3.47	130.74	127.06
92	C6	501	LMG	O7-C10-C11	3.47	118.97	111.50
82	ZI	401	PEB	CHA-C1B-NB	-3.47	117.68	124.93
87	C6	513	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
82	SI	201	PEB	OA-C1A-C2A	-3.47	123.42	126.17
82	PM	202	PEB	OA-C1A-C2A	-3.47	123.42	126.17
82	G5	202	PEB	OA-C1A-C2A	-3.47	123.42	126.17
83	BM	302	PUB	OA-C1A-NA	-3.47	120.80	125.93
82	V4	201	PEB	C3B-C4B-NB	3.47	115.09	110.05
82	A5	201	PEB	C3B-C4B-NB	3.47	115.09	110.05
82	BI	201	PEB	C2A-C1A-NA	3.47	111.26	108.27
82	TH	201	PEB	CAB-C3B-C4B	3.47	131.14	125.01
82	ZO	201	PEB	CHB-C4B-NB	3.47	131.79	124.58
82	RE	201	PEB	CHA-C1B-NB	-3.47	117.68	124.93
82	bF	202	PEB	OD-C4D-ND	-3.47	120.80	125.93
82	bK	201	PEB	OD-C4D-ND	-3.47	120.80	125.93
84	CG	1001	CYC	C2B-C1B-NB	3.47	112.06	106.99
82	WE	201	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
82	Z5	304	PEB	CHA-C1B-C2B	3.47	133.81	124.90
82	w8	204	PEB	C2A-C1A-NA	3.46	111.26	108.27
82	PD	203	PEB	OD-C4D-ND	-3.46	120.80	125.93
82	BB	203	PEB	CAC-CBC-CGC	-3.46	106.15	113.60
82	ZE	202	PEB	CAC-CBC-CGC	-3.46	106.15	113.60
82	wK	301	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
84	j3	1001	CYC	CAD-C3D-C4D	3.46	131.28	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GP	203	PEB	CHC-C4C-NC	3.46	125.84	121.15
94	A6	410	PL9	C10-C9-C11	3.46	121.10	115.27
82	U1	202	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
82	gO	201	PEB	C1D-CHC-C4C	-3.46	108.15	113.26
82	EJ	201	PEB	C3B-C4B-NB	3.46	115.09	110.05
82	V5	201	PEB	C3B-C4B-NB	3.46	115.09	110.05
82	S9	202	PEB	C3C-C4C-NC	3.46	111.45	108.33
84	o3	1001	CYC	CAD-C3D-C4D	3.46	131.28	125.76
82	AA	202	PEB	CHC-C4C-NC	3.46	125.84	121.15
82	DP	201	PEB	C2A-C1A-NA	3.46	111.26	108.27
85	bL	602	BCR	C36-C18-C17	-3.46	118.07	122.92
82	h1	201	PEB	C3D-C4D-ND	3.46	114.06	107.26
82	CM	201	PEB	OA-C1A-C2A	-3.46	123.42	126.17
82	N5	202	PEB	OA-C1A-C2A	-3.46	123.42	126.17
82	U7	201	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
82	H7	203	PEB	CBB-CAB-C3B	3.46	122.25	112.63
82	MF	203	PEB	CMB-C2B-C1B	3.46	130.40	125.06
82	yF	301	PEB	CMB-C2B-C1B	3.46	130.40	125.06
82	jG	202	PEB	CHC-C4C-NC	3.46	125.84	121.15
85	K2	105	BCR	C23-C22-C21	3.46	124.25	118.94
82	mM	202	PEB	CHC-C1D-ND	-3.46	109.34	113.72
82	M5	304	PEB	CHA-C1B-C2B	3.46	133.81	124.90
82	IK	203	PEB	CMC-C3C-C4C	3.46	130.73	127.06
82	F5	201	PEB	OD-C4D-ND	-3.46	120.80	125.93
82	rC	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
84	KH	1001	CYC	C4A-C3A-C2A	-3.46	102.53	106.51
82	uC	201	PEB	C3D-C4D-ND	3.46	114.05	107.26
84	I3	1001	CYC	CAD-C3D-C4D	3.46	131.28	125.76
84	u3	1001	CYC	CAD-C3D-C4D	3.46	131.28	125.76
84	w3	1001	CYC	CAD-C3D-C4D	3.46	131.28	125.76
82	F5	202	PEB	C2A-C1A-NA	3.46	111.26	108.27
82	iF	203	PEB	OD-C4D-ND	-3.46	120.80	125.93
82	S1	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	cG	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	YH	202	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
82	OA	201	PEB	CHA-C4A-NA	3.46	129.32	125.20
82	HI	201	PEB	C2A-C1A-NA	3.46	111.26	108.27
82	OI	202	PEB	C2A-C1A-NA	3.46	111.26	108.27
82	WK	203	PEB	C2A-C1A-NA	3.46	111.26	108.27
82	EM	203	PEB	C2A-C1A-NA	3.46	111.26	108.27
82	W7	202	PEB	C2A-C1A-NA	3.46	111.26	108.27
85	A2	804	BCR	C15-C14-C13	-3.46	122.37	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KB	301	PEB	CAC-C2C-C3C	3.46	135.00	127.07
82	DB	201	PEB	CHC-C1D-ND	-3.46	109.34	113.72
82	aM	204	PEB	CHC-C1D-ND	-3.46	109.34	113.72
83	QJ	201	PUB	CBA-CAA-C3A	3.46	118.23	112.98
82	NQ	204	PEB	CHA-C1B-NB	-3.46	117.69	124.93
82	QA	202	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
82	FP	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
82	sK	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
82	eO	202	PEB	OD-C4D-ND	-3.46	120.80	125.93
82	S7	201	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
82	SK	202	PEB	OD-C4D-ND	-3.46	120.80	125.93
82	aB	202	PEB	CHC-C4C-NC	3.46	125.83	121.15
82	WG	201	PEB	C1D-CHC-C4C	-3.46	108.15	113.26
82	GA	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
82	YA	301	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
82	L9	202	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
82	dM	203	PEB	OA-C1A-C2A	-3.46	123.42	126.17
84	I4	1001	CYC	CMA-C3A-C4A	3.46	130.39	125.06
87	3N	308	CLA	CMB-C2B-C1B	-3.46	120.10	125.37
82	e4	202	PEB	C3C-C4C-NC	3.46	111.45	108.33
84	D1	1001	CYC	CHB-C1B-NB	-3.46	118.63	126.06
82	ZG	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
82	E7	201	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
84	IO	1001	CYC	CMA-C3A-C4A	3.46	130.39	125.06
82	ED	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
82	DK	202	PEB	C2A-C1A-NA	3.46	111.25	108.27
82	qC	201	PEB	C2A-C1A-NA	3.46	111.25	108.27
82	LK	201	PEB	C1C-C2C-C3C	-3.46	103.53	107.62
82	l1	203	PEB	C1C-CHB-C4B	-3.46	120.53	128.28
82	H5	202	PEB	C1C-CHB-C4B	3.46	136.04	128.28
82	Z5	301	PEB	OD-C4D-ND	-3.46	120.81	125.93
82	RI	203	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	YK	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	aG	201	PEB	CMB-C2B-C1B	3.46	130.39	125.06
85	BN	803	BCR	C29-C30-C25	3.46	115.81	110.48
83	AH	303	PUB	C1C-C2C-C3C	-3.46	102.95	106.78
84	MG	1001	CYC	C4D-C3D-C2D	-3.46	103.53	107.62
82	FM	201	PEB	CAB-C3B-C4B	3.46	131.13	125.01
82	RO	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	V4	202	PEB	OD-C4D-C3D	-3.46	121.62	129.46
82	Y7	301	PEB	C4B-C3B-C2B	-3.46	102.96	106.78
82	vK	201	PEB	C4B-C3B-C2B	-3.46	102.96	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	1C	202	PEB	CHB-C1C-C2C	-3.46	119.35	127.15
82	PJ	201	PEB	CHA-C1B-NB	-3.46	117.70	124.93
82	TG	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	HA	201	PEB	CHA-C1B-NB	-3.46	117.70	124.93
84	LH	1001	CYC	C4D-CHA-C1A	3.46	136.03	128.28
82	KP	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	eG	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	cJ	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	KD	201	PEB	C4B-C3B-C2B	-3.46	102.96	106.78
82	OI	202	PEB	C4B-C3B-C2B	-3.46	102.96	106.78
82	Z1	203	PEB	C4B-C3B-C2B	-3.46	102.96	106.78
82	JQ	202	PEB	CHC-C4C-NC	3.46	125.83	121.15
82	SO	202	PEB	OA-C1A-C2A	-3.46	123.42	126.17
87	A2	811	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
82	ND	204	PEB	CHA-C1B-NB	-3.46	117.70	124.93
82	xC	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
82	IA	201	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
84	LG	1001	CYC	CAD-C3D-C4D	-3.46	120.26	125.76
82	OF	201	PEB	C1C-C2C-C3C	-3.46	103.54	107.62
82	A7	202	PEB	CHC-C4C-NC	3.46	125.83	121.15
82	eE	203	PEB	CHB-C1C-NC	-3.46	117.40	125.32
82	NM	201	PEB	CBC-CAC-C2C	-3.46	103.03	112.63
82	RQ	203	PEB	C3D-C4D-ND	3.46	114.04	107.26
82	xK	302	PEB	C3D-C4D-ND	3.46	114.04	107.26
82	T4	203	PEB	C4B-C3B-C2B	-3.46	102.96	106.78
82	D9	203	PEB	C4B-C3B-C2B	-3.46	102.96	106.78
82	j1	203	PEB	OD-C4D-ND	-3.46	120.81	125.93
85	BN	839	BCR	C8-C9-C10	3.46	124.24	118.94
82	ZG	202	PEB	CAC-CBC-CGC	-3.45	106.17	113.60
82	EJ	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	dO	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
85	B2	802	BCR	C29-C30-C25	3.45	115.80	110.48
84	k3	1001	CYC	CAD-C3D-C4D	3.45	131.26	125.76
82	YM	201	PEB	C3B-C4B-NB	3.45	115.07	110.05
82	d1	201	PEB	C3B-C4B-NB	3.45	115.07	110.05
85	fL	101	BCR	C1-C6-C5	-3.45	117.75	122.61
82	HA	203	PEB	CBB-CAB-C3B	3.45	122.22	112.63
82	GM	201	PEB	OD-C4D-ND	-3.45	120.81	125.93
82	c1	201	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
82	E5	201	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
82	qK	201	PEB	CHB-C1C-C2C	-3.45	119.36	127.15
82	VG	201	PEB	C3B-C4B-NB	3.45	115.07	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VO	201	PEB	C3B-C4B-NB	3.45	115.07	110.05
82	O5	203	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
82	DK	203	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	I5	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	B5	202	PEB	CHC-C1D-ND	-3.45	109.36	113.72
83	xK	301	PUB	CHA-C1B-NB	3.45	125.82	121.15
82	RG	201	PEB	CHA-C1B-NB	-3.45	117.71	124.93
82	dE	201	PEB	CMB-C2B-C1B	3.45	130.38	125.06
82	iE	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
82	V7	201	PEB	C1C-C2C-C3C	-3.45	103.54	107.62
82	UA	201	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
82	DP	201	PEB	C3B-C4B-NB	3.45	115.07	110.05
82	NI	203	PEB	C3D-C4D-ND	3.45	114.03	107.26
82	UE	201	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
84	T3	1001	CYC	C1A-C2A-C3A	-3.45	102.96	106.78
82	cE	201	PEB	CMB-C2B-C1B	3.45	130.38	125.06
85	CL	502	BCR	C3-C4-C5	-3.45	107.91	114.08
82	SK	202	PEB	CHC-C1D-ND	-3.45	109.36	113.72
82	gF	202	PEB	CHC-C1D-ND	-3.45	109.36	113.72
82	VQ	202	PEB	C3D-C4D-ND	3.45	114.03	107.26
82	zK	501	PEB	CHB-C4B-C3B	-3.45	117.33	125.32
87	A2	823	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
87	aL	605	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
82	PO	201	PEB	C3B-C4B-NB	3.45	115.07	110.05
82	M5	305	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	E7	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	OM	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
82	TQ	203	PEB	C2A-C1A-NA	3.45	111.25	108.27
94	AL	413	PL9	C31-C32-C33	-3.45	100.54	111.88
82	dB	202	PEB	CMB-C2B-C1B	3.45	130.38	125.06
82	H5	202	PEB	OD-C4D-ND	-3.45	120.82	125.93
82	WH	203	PEB	CHA-C1B-NB	-3.45	117.71	124.93
82	CK	202	PEB	CHB-C4B-C3B	-3.45	117.33	125.32
82	RF	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
82	RO	203	PEB	C2C-C1C-NC	3.45	112.22	107.57
82	TJ	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	IP	203	PEB	C2A-C1A-NA	3.45	111.25	108.27
82	mM	201	PEB	C1C-CHB-C4B	-3.45	120.54	128.28
84	HE	1001	CYC	CHA-C4D-C3D	-3.45	119.36	127.15
82	P5	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
82	18	202	PEB	CHB-C1C-C2C	-3.45	119.37	127.15
84	q3	1001	CYC	CAD-C3D-C4D	3.45	131.26	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BF	201	PEB	CHA-C1B-NB	-3.45	117.72	124.93
82	gJ	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
84	BG	1002	CYC	C2B-C1B-NB	3.45	112.04	106.99
82	xK	303	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
82	BK	201	PEB	CHA-C1B-NB	-3.45	117.72	124.93
82	DB	201	PEB	CMB-C2B-C1B	3.45	130.38	125.06
82	dQ	401	PEB	CAC-CBC-CGC	-3.45	106.18	113.60
82	sF	201	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
82	g1	202	PEB	OA-C1A-NA	3.45	129.12	124.94
82	ZH	201	PEB	C3D-C4D-ND	3.45	114.03	107.26
84	N4	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
82	CF	203	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
82	Z4	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
82	RP	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	s8	203	PEB	CHC-C4C-NC	3.45	125.82	121.15
82	uC	202	PEB	C1C-C2C-C3C	-3.45	103.55	107.62
82	u8	201	PEB	CAA-C3A-C2A	-3.45	105.64	114.26
82	SE	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
82	qF	201	PEB	CHB-C1C-C2C	-3.45	119.37	127.15
82	MP	203	PEB	C3B-C4B-NB	3.45	115.06	110.05
82	HJ	202	PEB	CMB-C2B-C1B	3.45	130.37	125.06
82	ND	202	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
82	cK	201	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
82	E9	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
82	fO	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
84	D4	1001	CYC	C2D-C1D-ND	3.45	112.25	107.40
85	AN	846	BCR	C7-C8-C9	-3.45	121.03	126.23
82	DJ	202	PEB	C1C-CHB-C4B	-3.45	120.55	128.28
82	LQ	201	PEB	CHC-C1D-ND	-3.45	109.36	113.72
84	FG	1001	CYC	CMB-C2B-C1B	3.45	128.47	124.17
85	d6	405	BCR	C37-C22-C23	3.45	123.51	118.08
82	EP	201	PEB	CHC-C4C-NC	3.45	125.81	121.15
82	rK	201	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
82	CP	202	PEB	C1D-CHC-C4C	-3.45	108.17	113.26
85	bL	602	BCR	C20-C19-C18	3.45	136.10	126.42
82	DD	203	PEB	C2A-C1A-NA	3.45	111.24	108.27
82	FD	202	PEB	C2A-C1A-NA	3.45	111.24	108.27
82	LQ	203	PEB	CHC-C1D-ND	-3.45	109.36	113.72
82	H7	201	PEB	CHA-C1B-NB	-3.45	117.72	124.93
82	L5	203	PEB	CAC-CBC-CGC	-3.45	106.19	113.60
82	YG	202	PEB	CMC-C3C-C4C	-3.45	123.41	127.06
85	fL	101	BCR	C35-C13-C14	-3.45	118.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W1	203	PEB	CHA-C1B-NB	-3.45	117.72	124.93
82	NM	202	PEB	CAB-C3B-C4B	3.45	131.10	125.01
84	H4	1001	CYC	C4D-CHA-C1A	3.45	136.01	128.28
84	N4	1001	CYC	CMB-C2B-C1B	3.45	128.47	124.17
82	SH	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
82	uC	201	PEB	CAA-C3A-C2A	-3.45	105.65	114.26
87	4N	609	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
82	U7	202	PEB	OD-C4D-ND	-3.45	120.83	125.93
82	JM	201	PEB	C2A-C1A-NA	3.45	111.24	108.27
87	AN	823	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
82	EB	501	PEB	C3B-C4B-NB	3.44	115.06	110.05
82	mO	203	PEB	CHC-C1D-ND	-3.44	109.37	113.72
85	B2	840	BCR	C1-C6-C7	3.44	125.52	115.78
82	cH	201	PEB	C1B-C2B-C3B	-3.44	102.55	106.51
88	cL	501	LHG	O8-C23-C24	3.44	120.41	111.38
82	VD	202	PEB	C3D-C4D-ND	3.44	114.02	107.26
82	GF	201	PEB	CHB-C1C-NC	3.44	133.21	125.32
82	HJ	201	PEB	C1C-CHB-C4B	-3.44	120.56	128.28
82	UJ	203	PEB	C2A-C1A-NA	3.44	111.24	108.27
82	CJ	203	PEB	C3C-C4C-NC	3.44	111.43	108.33
82	mM	202	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
82	OG	202	PEB	CBA-CAA-C3A	-3.44	105.80	113.47
82	S5	201	PEB	C3B-C4B-NB	3.44	115.06	110.05
82	J9	203	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	1C	201	PEB	OD-C4D-ND	-3.44	120.83	125.93
84	Q3	1001	CYC	CAD-C3D-C4D	3.44	131.25	125.76
84	E4	1001	CYC	C1B-C2B-C3B	-3.44	104.28	107.87
82	NF	201	PEB	CHC-C4C-NC	3.44	125.81	121.15
82	wC	204	PEB	CMC-C3C-C4C	3.44	130.71	127.06
82	QD	201	PEB	CMB-C2B-C1B	3.44	130.37	125.06
82	uC	201	PEB	CAB-CBB-CGB	-3.44	106.19	113.60
82	QH	203	PEB	CHA-C1B-NB	-3.44	117.73	124.93
82	KM	203	PEB	CHA-C1B-NB	-3.44	117.73	124.93
82	dH	202	PEB	CHA-C1B-NB	-3.44	117.73	124.93
82	V7	203	PEB	C2A-C1A-NA	3.44	111.24	108.27
84	FE	1002	CYC	C2C-C1C-NC	3.44	111.24	108.27
82	eO	202	PEB	C3C-C4C-NC	3.44	111.43	108.33
87	A2	828	CLA	C2B-C1B-NB	3.44	112.54	110.23
82	R4	202	PEB	C3B-C4B-NB	3.44	115.06	110.05
82	Q1	201	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
82	SK	203	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	ZH	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	u8	201	PEB	CMB-C2B-C1B	3.44	130.37	125.06
82	AP	203	PEB	C3B-C4B-NB	3.44	115.06	110.05
82	IJ	202	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
82	qC	203	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	QF	202	PEB	C3D-C4D-ND	3.44	114.01	107.26
82	YQ	201	PEB	C3D-C4D-ND	3.44	114.01	107.26
82	UM	201	PEB	C3C-C4C-NC	3.44	111.43	108.33
84	BE	1001	CYC	C2D-C1D-ND	3.44	112.24	107.40
82	DM	201	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
82	FI	201	PEB	OA-C1A-C2A	-3.44	123.44	126.17
82	AQ	301	PEB	OA-C1A-C2A	-3.44	123.44	126.17
84	d3	1001	CYC	OC-C1C-C2C	-3.44	123.44	126.17
82	OE	202	PEB	CBA-CAA-C3A	-3.44	105.81	113.47
82	P4	202	PEB	CHC-C1D-ND	-3.44	109.37	113.72
84	M3	1001	CYC	CAD-C3D-C4D	3.44	131.24	125.76
82	WF	202	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	MQ	202	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	MM	201	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
82	LK	201	PEB	CBC-CAC-C2C	-3.44	103.07	112.63
82	T5	201	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
85	kL	100	BCR	C35-C13-C12	3.44	123.50	118.08
82	SP	202	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	R7	203	PEB	CHB-C4B-C3B	-3.44	117.36	125.32
82	D5	201	PEB	OA-C1A-C2A	-3.44	123.44	126.17
82	E5	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17
84	j3	1001	CYC	OC-C1C-C2C	-3.44	123.44	126.17
82	AA	202	PEB	C3D-C4D-ND	3.44	114.01	107.26
84	D4	1001	CYC	CHB-C4A-NA	-3.44	117.74	124.93
82	RO	202	PEB	CAB-C3B-C4B	3.44	131.09	125.01
82	L9	202	PEB	CAB-C3B-C4B	3.44	131.09	125.01
84	F3	1001	CYC	CAD-C3D-C4D	3.44	131.24	125.76
82	VF	201	PEB	C2A-C1A-NA	3.44	111.24	108.27
82	XA	201	PEB	CHC-C4C-NC	3.44	125.80	121.15
82	jE	202	PEB	CHC-C4C-NC	3.44	125.80	121.15
82	RI	203	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
82	V7	203	PEB	C3D-C4D-ND	3.44	114.01	107.26
82	VF	202	PEB	OD-C4D-ND	-3.44	120.83	125.93
82	UB	301	PEB	CMB-C2B-C1B	3.44	130.36	125.06
84	U3	1001	CYC	CAD-C3D-C4D	3.44	131.24	125.76
82	LF	201	PEB	C1C-C2C-C3C	-3.44	103.56	107.62
82	OK	201	PEB	C1C-C2C-C3C	-3.44	103.56	107.62
82	OE	203	PEB	OA-C1A-C2A	-3.44	123.44	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RB	202	PEB	OD-C4D-ND	-3.44	120.84	125.93
82	N7	201	PEB	OD-C4D-ND	-3.44	120.84	125.93
82	NJ	202	PEB	CHC-C1D-ND	-3.44	109.37	113.72
82	OJ	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
82	FI	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
82	sC	203	PEB	C2A-C1A-NA	3.44	111.24	108.27
82	GK	203	PEB	CHC-C4C-NC	3.44	125.80	121.15
82	GK	202	PEB	CAC-CBC-CGC	3.44	121.00	113.60
82	BM	301	PEB	CHB-C1C-NC	-3.44	117.44	125.32
84	L3	1001	CYC	CAD-C3D-C4D	3.44	131.24	125.76
82	NA	202	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
82	VD	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
82	hB	301	PEB	CAB-CBB-CGB	3.44	121.00	113.60
82	KJ	203	PEB	C3C-C4C-NC	3.44	111.43	108.33
82	lJ	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17
82	CJ	201	PEB	OD-C4D-ND	-3.44	120.84	125.93
82	KF	201	PEB	CMB-C2B-C1B	3.44	130.36	125.06
82	TO	202	PEB	CMB-C2B-C1B	3.44	130.36	125.06
82	Y5	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
82	GK	201	PEB	CHB-C1C-NC	3.44	133.19	125.32
82	CB	201	PEB	CHA-C1B-NB	-3.44	117.74	124.93
87	32	307	CLA	CMB-C2B-C1B	-3.44	120.14	125.37
87	AN	831	CLA	CHB-C1B-NB	3.44	127.89	124.26
82	aE	201	PEB	CMB-C2B-C1B	3.44	130.36	125.06
84	f3	1001	CYC	CAD-C3D-C4D	3.44	131.24	125.76
84	h3	1001	CYC	CAD-C3D-C4D	3.44	131.24	125.76
82	m1	202	PEB	CHC-C1D-ND	-3.44	109.38	113.72
82	W9	202	PEB	CHC-C1D-ND	-3.44	109.38	113.72
82	VH	202	PEB	C2A-C1A-NA	3.44	111.23	108.27
82	lG	203	PEB	C2A-C1A-NA	3.44	111.23	108.27
82	aM	203	PEB	C2A-C1A-NA	3.44	111.23	108.27
82	J9	203	PEB	CMB-C2B-C1B	3.44	130.35	125.06
82	r8	201	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
95	C6	521	DGD	C2G-O2G-C1B	-3.44	109.33	117.79
84	NO	1001	CYC	C4D-C3D-C2D	-3.44	103.56	107.62
82	iK	202	PEB	OD-C4D-ND	-3.44	120.84	125.93
87	42	609	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
82	RI	203	PEB	CHA-C1B-C2B	3.43	133.73	124.90
82	WG	201	PEB	C1B-C2B-C3B	-3.43	102.56	106.51
85	B6	602	BCR	C16-C17-C18	-3.43	122.41	127.31
82	AE	301	PEB	C2A-C1A-NA	3.43	111.23	108.27
82	OG	202	PEB	OA-C1A-C2A	-3.43	123.44	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	A5	202	PEB	OA-C1A-C2A	-3.43	123.44	126.17
82	V5	202	PEB	OA-C1A-C2A	-3.43	123.44	126.17
82	kM	202	PEB	OA-C1A-C2A	-3.43	123.44	126.17
84	k3	1001	CYC	OC-C1C-C2C	-3.43	123.44	126.17
82	rF	202	PEB	CHB-C4B-C3B	-3.43	117.37	125.32
82	LG	1002	PEB	C3B-C4B-NB	3.43	115.05	110.05
82	m1	201	PEB	C3B-C4B-NB	3.43	115.05	110.05
82	P4	201	PEB	C3B-C4B-NB	3.43	115.05	110.05
82	oK	201	PEB	C3B-C4B-NB	3.43	115.05	110.05
82	ZO	201	PEB	OD-C4D-ND	-3.43	120.84	125.93
82	mJ	201	PEB	CAB-C3B-C4B	3.43	131.09	125.01
82	BK	201	PEB	C1D-CHC-C4C	3.43	118.32	113.26
82	OP	201	PEB	C3D-C4D-ND	3.43	114.00	107.26
95	cL	519	DGD	O2G-C1B-C2B	3.43	118.90	111.50
82	bH	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
82	RQ	203	PEB	CHB-C1C-C2C	-3.43	119.40	127.15
82	YI	201	PEB	OD-C4D-ND	-3.43	120.84	125.93
82	Z1	201	PEB	C3D-C4D-ND	3.43	114.00	107.26
85	BN	840	BCR	C1-C6-C7	3.43	125.49	115.78
82	dD	401	PEB	CAC-CBC-CGC	-3.43	106.21	113.60
82	xC	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
82	uK	201	PEB	OA-C1A-C2A	-3.43	123.44	126.17
84	S3	1001	CYC	OC-C1C-C2C	-3.43	123.44	126.17
87	22	609	CLA	CMB-C2B-C1B	-3.43	120.14	125.37
82	sK	202	PEB	CHA-C1B-NB	-3.43	117.75	124.93
82	YD	201	PEB	C3D-C4D-ND	3.43	114.00	107.26
82	AQ	301	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	RQ	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
84	F4	1001	CYC	C4A-C3A-C2A	-3.43	102.57	106.51
82	rK	202	PEB	CHB-C4B-C3B	-3.43	117.38	125.32
82	hE	203	PEB	CHC-C1D-ND	-3.43	109.38	113.72
82	Q1	203	PEB	CHA-C1B-NB	-3.43	117.75	124.93
82	X7	201	PEB	CHC-C4C-NC	3.43	125.80	121.15
82	u8	201	PEB	CAB-CBB-CGB	-3.43	106.22	113.60
82	XM	201	PEB	CMB-C2B-C1B	3.43	130.35	125.06
82	QF	203	PEB	CMA-C2A-C1A	-3.43	105.00	112.40
82	CP	202	PEB	OD-C4D-ND	-3.43	120.84	125.93
82	aO	201	PEB	OD-C4D-ND	-3.43	120.84	125.93
82	bK	201	PEB	CHC-C1D-ND	-3.43	109.38	113.72
82	GB	203	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
82	Z1	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
82	A1	302	PEB	CMB-C2B-C1B	3.43	130.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DF	202	PEB	C3B-C4B-NB	3.43	115.04	110.05
82	cF	201	PEB	C3B-C4B-NB	3.43	115.04	110.05
82	ZK	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	hG	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	NP	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
82	RQ	201	PEB	C2C-C1C-NC	3.43	112.19	107.57
84	E3	1001	CYC	C4D-C3D-C2D	-3.43	103.56	107.62
82	EJ	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
82	HM	202	PEB	C3B-C4B-NB	3.43	115.04	110.05
82	OG	203	PEB	OA-C1A-C2A	-3.43	123.44	126.17
82	GP	203	PEB	OA-C1A-C2A	-3.43	123.44	126.17
84	NO	1001	CYC	OB-C4B-C3B	-3.43	124.32	128.04
85	BN	838	BCR	C11-C12-C13	3.43	136.05	126.42
84	F1	1001	CYC	C1D-C2D-C3D	-3.43	103.42	107.79
87	8N	303	CLA	CHB-C4A-NA	3.43	129.26	124.51
82	l1	203	PEB	CHC-C1D-ND	-3.43	109.38	113.72
82	QD	201	PEB	C1C-CHB-C4B	3.43	135.97	128.28
82	AJ	301	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
82	V1	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
84	I1	1001	CYC	C1D-C2D-C3D	-3.43	103.42	107.79
82	g4	201	PEB	CMB-C2B-C1B	3.43	130.35	125.06
82	P7	202	PEB	C1C-CHB-C4B	3.43	135.97	128.28
82	qF	202	PEB	CHB-C1C-C2C	3.43	134.89	127.15
82	T9	201	PEB	OA-C1A-C2A	-3.43	123.45	126.17
82	R4	203	PEB	C2C-C1C-NC	3.43	112.19	107.57
82	l4	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	XF	201	PEB	CHA-C1B-NB	-3.43	117.76	124.93
82	PA	202	PEB	C1C-CHB-C4B	3.43	135.97	128.28
82	MP	203	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
82	T4	202	PEB	CMB-C2B-C1B	3.43	130.34	125.06
85	AN	804	BCR	C15-C14-C13	-3.43	122.42	127.31
82	NA	201	PEB	OD-C4D-ND	-3.43	120.85	125.93
82	OP	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
84	d3	1001	CYC	CAD-C3D-C4D	3.43	131.22	125.76
82	FJ	202	PEB	CAB-C3B-C4B	3.43	131.07	125.01
82	QK	202	PEB	C3D-C4D-ND	3.43	113.99	107.26
85	HL	103	BCR	C11-C10-C9	-3.43	122.42	127.31
82	BD	202	PEB	OA-C1A-C2A	-3.43	123.45	126.17
82	PQ	203	PEB	OA-C1A-C2A	-3.43	123.45	126.17
84	S3	1001	CYC	CAD-C3D-C4D	3.43	131.22	125.76
82	QQ	201	PEB	C1C-CHB-C4B	3.43	135.97	128.28
84	DO	1001	CYC	C2D-C1D-ND	3.43	112.22	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	B2	838	BCR	C11-C12-C13	3.43	136.05	126.42
84	K1	1001	CYC	C4A-C3A-C2A	-3.43	102.57	106.51
82	AO	305	PEB	C2A-C1A-NA	3.43	111.23	108.27
85	HL	103	BCR	C16-C17-C18	-3.43	122.42	127.31
82	eK	203	PEB	OD-C4D-ND	-3.43	120.85	125.93
82	gK	201	PEB	CHA-C1B-C2B	3.43	133.71	124.90
87	62	308	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
84	FO	1001	CYC	CHB-C1B-NB	-3.43	118.70	126.06
82	AM	301	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	QK	203	PEB	CMA-C2A-C1A	-3.43	105.02	112.40
87	5N	609	CLA	CAA-C2A-C3A	-3.43	105.70	114.26
82	KP	202	PEB	C1D-CHC-C4C	-3.43	108.20	113.26
82	AA	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
82	KQ	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
87	52	609	CLA	CAA-C2A-C3A	-3.43	105.70	114.26
85	A2	848	BCR	C11-C10-C9	-3.43	122.42	127.31
82	WB	402	PEB	OD-C4D-ND	-3.43	120.85	125.93
82	OI	201	PEB	OD-C4D-ND	-3.43	120.85	125.93
82	BD	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	gH	203	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	oK	203	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
82	II	203	PEB	C1C-NC-C4C	-3.43	103.50	109.60
82	HM	202	PEB	CHC-C4C-NC	3.43	125.79	121.15
82	FD	202	PEB	CMC-C3C-C4C	3.43	130.69	127.06
82	JP	201	PEB	C2C-C1C-NC	3.43	112.19	107.57
84	NH	1001	CYC	CHB-C1B-NB	-3.43	118.70	126.06
84	NO	1001	CYC	C1B-C2B-C3B	-3.43	104.30	107.87
82	U5	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
84	O3	1001	CYC	CAD-C3D-C4D	3.43	131.22	125.76
84	V3	1001	CYC	C1B-CHB-C4A	3.43	136.45	128.08
82	fM	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
82	Q5	201	PEB	CAB-CBB-CGB	-3.43	106.23	113.60
82	FM	202	PEB	CAA-C3A-C4A	3.43	121.47	112.67
82	U9	202	PEB	C3C-C4C-NC	3.43	111.42	108.33
82	a1	201	PEB	OD-C4D-ND	-3.43	120.86	125.93
82	aH	202	PEB	CHC-C1D-ND	-3.42	109.39	113.72
82	x8	202	PEB	C3B-C4B-NB	3.42	115.03	110.05
82	AB	501	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
82	RF	201	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
82	J9	202	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
85	aL	604	BCR	C24-C23-C22	-3.42	121.06	126.23
96	fL	102	HEM	CBD-CAD-C3D	-3.42	103.11	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GI	201	PEB	C1C-NC-C4C	-3.42	103.50	109.60
82	M7	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
87	5N	609	CLA	CHB-C4A-NA	3.42	129.25	124.51
82	Y9	202	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
82	rC	202	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
84	B3	1001	CYC	CAD-C3D-C4D	3.42	131.22	125.76
85	A2	847	BCR	C3-C4-C5	-3.42	107.96	114.08
85	BL	617	BCR	C34-C9-C8	3.42	123.47	118.08
82	HJ	201	PEB	CMB-C2B-C1B	3.42	130.34	125.06
82	bF	202	PEB	CMB-C2B-C1B	3.42	130.34	125.06
82	dJ	202	PEB	CMB-C2B-C1B	3.42	130.34	125.06
82	iK	201	PEB	OA-C1A-C2A	-3.42	123.45	126.17
82	d1	201	PEB	CHC-C1D-ND	-3.42	109.39	113.72
82	GQ	201	PEB	CAB-CBB-CGB	-3.42	106.24	113.60
84	D3	1001	CYC	CAD-C3D-C4D	3.42	131.21	125.76
82	GF	203	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
82	KM	201	PEB	OD-C4D-ND	-3.42	120.86	125.93
82	qK	203	PEB	C3D-C4D-ND	3.42	113.97	107.26
94	d6	408	PL9	C32-C33-C34	-3.42	119.42	127.66
84	I1	1001	CYC	C4D-CHA-C1A	3.42	135.96	128.28
82	Z4	201	PEB	CHB-C4B-NB	3.42	131.70	124.58
84	e3	1001	CYC	C4D-C3D-C2D	-3.42	103.58	107.62
82	UM	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
82	YP	502	PEB	CHC-C4C-NC	3.42	125.78	121.15
82	aH	201	PEB	OD-C4D-ND	-3.42	120.86	125.93
87	A2	831	CLA	CHB-C1B-NB	3.42	127.88	124.26
82	WM	203	PEB	C3B-C4B-NB	3.42	115.03	110.05
84	JH	1001	CYC	CHB-C4A-C3A	3.42	133.70	124.90
82	UI	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
82	fB	301	PEB	CAB-CBB-CGB	3.42	120.97	113.60
84	HO	1001	CYC	C4D-CHA-C1A	3.42	135.96	128.28
82	hE	201	PEB	C1C-C2C-C3C	-3.42	103.58	107.62
82	h1	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
82	jJ	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
84	J1	1001	CYC	CHB-C4A-C3A	3.42	133.70	124.90
84	LH	1001	CYC	C1D-C2D-C3D	-3.42	103.43	107.79
85	d6	405	BCR	C33-C5-C6	-3.42	120.69	124.53
84	LE	1001	CYC	CAD-C3D-C4D	-3.42	120.31	125.76
82	PA	203	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
82	RM	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
82	FP	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
84	IO	1001	CYC	C1A-C2A-C3A	-3.42	103.00	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	f4	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
82	fF	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
82	sC	202	PEB	C3D-C4D-ND	3.42	113.97	107.26
87	2N	309	CLA	CMB-C2B-C1B	-3.42	120.16	125.37
82	WA	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
82	RD	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
82	q8	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
84	DH	1001	CYC	CHB-C1B-NB	-3.42	118.71	126.06
82	vK	202	PEB	C3B-C4B-NB	3.42	115.03	110.05
84	CG	1001	CYC	CMB-C2B-C1B	3.42	128.44	124.17
82	RA	203	PEB	CHB-C4B-C3B	-3.42	117.41	125.32
82	S9	201	PEB	CHB-C4B-C3B	-3.42	117.41	125.32
82	iK	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
82	Q5	202	PEB	CAB-C3B-C4B	3.42	131.06	125.01
82	fE	202	PEB	CHC-C4C-NC	3.42	125.78	121.15
84	J4	1001	CYC	C4D-C3D-C2D	-3.42	103.58	107.62
82	Y5	202	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
82	W5	203	PEB	C3B-C4B-NB	3.42	115.02	110.05
95	JL	101	DGD	O2G-C1B-C2B	3.42	118.87	111.50
82	eK	201	PEB	OA-C1A-C2A	-3.42	123.45	126.17
82	RO	202	PEB	C3C-C4C-NC	3.42	111.41	108.33
82	HO	1002	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
82	gB	203	PEB	C1D-CHC-C4C	3.42	118.30	113.26
84	EG	1001	CYC	C2A-C1A-NA	3.42	115.02	110.05
82	DB	203	PEB	CBB-CAB-C3B	-3.42	103.13	112.63
96	v6	201	HEM	C4C-NC-C1C	3.42	108.70	105.35
84	H3	1001	CYC	CAD-C3D-C4D	3.42	131.21	125.76
82	IJ	201	PEB	C3B-C4B-NB	3.42	115.02	110.05
82	IF	203	PEB	CMA-C2A-C1A	-3.42	105.03	112.40
82	UK	201	PEB	C2A-C1A-NA	-3.42	105.33	108.27
82	wF	301	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
82	YK	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
82	EK	202	PEB	C3B-C4B-NB	3.42	115.02	110.05
87	bL	613	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
87	BL	605	CLA	CHB-C4A-NA	3.42	129.24	124.51
82	BB	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
82	SB	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
84	CG	1001	CYC	C2C-C1C-NC	3.42	111.22	108.27
82	g4	201	PEB	C1D-CHC-C4C	-3.42	108.22	113.26
82	V9	201	PEB	OA-C1A-C2A	-3.42	123.46	126.17
82	yK	301	PEB	CMB-C2B-C1B	3.42	130.33	125.06
82	HD	203	PEB	C3D-C4D-ND	3.42	113.96	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CQ	201	PEB	C3D-C4D-ND	3.42	113.96	107.26
82	BB	202	PEB	CHA-C1B-NB	-3.42	117.79	124.93
82	M5	304	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
83	Z9	302	PUB	CHA-C1B-NB	3.42	125.77	121.15
87	HL	101	CLA	CMB-C2B-C1B	-3.42	120.17	125.37
82	KJ	203	PEB	OD-C4D-ND	-3.42	120.87	125.93
82	cB	401	PEB	C2A-C1A-NA	3.42	111.22	108.27
82	Q7	201	PEB	C3C-C4C-NC	3.42	111.41	108.33
87	52	609	CLA	CHB-C4A-NA	3.42	129.24	124.51
84	x3	1001	CYC	C1B-CHB-C4A	3.42	136.43	128.08
82	SE	202	PEB	C3B-C4B-NB	3.42	115.02	110.05
82	U4	202	PEB	OA-C1A-C2A	-3.42	123.46	126.17
82	K5	202	PEB	OA-C1A-C2A	-3.42	123.46	126.17
82	gE	201	PEB	OA-C1A-C2A	-3.42	123.46	126.17
84	DH	1001	CYC	C4A-C3A-C2A	-3.42	102.59	106.51
82	CJ	203	PEB	CMB-C2B-C1B	3.42	130.32	125.06
82	QB	203	PEB	CAC-CBC-CGC	-3.42	106.25	113.60
82	hH	201	PEB	CAB-CBB-CGB	-3.42	106.25	113.60
84	GE	1001	CYC	C1B-C2B-C3B	-3.42	104.31	107.87
82	LM	201	PEB	C1C-CHB-C4B	-3.42	120.62	128.28
82	RJ	202	PEB	CAB-C3B-C4B	3.42	131.05	125.01
82	qC	202	PEB	C3C-C4C-NC	3.42	111.41	108.33
82	FK	201	PEB	C4B-C3B-C2B	-3.41	103.00	106.78
82	P7	203	PEB	C4B-C3B-C2B	-3.41	103.00	106.78
82	LF	201	PEB	OD-C4D-ND	-3.41	120.87	125.93
82	SF	203	PEB	OD-C4D-ND	-3.41	120.87	125.93
82	O4	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
82	YF	201	PEB	OA-C1A-C2A	-3.41	123.46	126.17
82	X7	203	PEB	C1C-CHB-C4B	3.41	135.94	128.28
84	BE	1002	CYC	C2B-C1B-NB	3.41	111.99	106.99
82	VA	203	PEB	C2C-C1C-NC	3.41	112.17	107.57
85	BL	618	BCR	C28-C27-C26	-3.41	107.98	114.08
82	SJ	203	PEB	C2A-C1A-NA	3.41	111.22	108.27
82	aM	201	PEB	C2A-C1A-NA	3.41	111.22	108.27
85	A2	847	BCR	C16-C17-C18	-3.41	122.44	127.31
82	gJ	202	PEB	CMB-C2B-C1B	3.41	130.32	125.06
87	6N	607	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
82	UK	202	PEB	CHC-C4C-NC	3.41	125.77	121.15
88	CL	522	LHG	O8-C23-C24	3.41	120.33	111.38
82	Q9	201	PEB	CAB-C3B-C4B	3.41	131.05	125.01
84	N3	1001	CYC	C4D-C3D-C2D	-3.41	103.59	107.62
82	hE	203	PEB	C3B-C4B-NB	3.41	115.01	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AD	301	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
83	M9	303	PUB	CHA-C1B-NB	3.41	125.77	121.15
84	n3	1001	CYC	CAD-C3D-C4D	3.41	131.20	125.76
82	LD	201	PEB	CHC-C1D-ND	-3.41	109.41	113.72
82	YF	203	PEB	CHC-C1D-ND	-3.41	109.41	113.72
85	JN	103	BCR	C7-C8-C9	-3.41	121.08	126.23
82	EF	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
82	CF	201	PEB	OD-C4D-ND	-3.41	120.88	125.93
82	WJ	201	PEB	OD-C4D-ND	-3.41	120.88	125.93
85	KL	100	BCR	C35-C13-C12	3.41	123.45	118.08
82	EQ	202	PEB	CMC-C3C-C4C	3.41	130.68	127.06
84	N4	1001	CYC	C4D-C3D-C2D	-3.41	103.59	107.62
87	B2	834	CLA	C3B-C4B-NB	-3.41	107.35	110.52
82	W1	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	KP	201	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
82	EQ	202	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
84	EG	1001	CYC	C1A-C2A-C3A	-3.41	103.01	106.78
82	ND	204	PEB	C1D-CHC-C4C	3.41	118.29	113.26
87	DL	404	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
82	UF	202	PEB	OD-C4D-ND	-3.41	120.88	125.93
82	J7	202	PEB	OD-C4D-ND	-3.41	120.88	125.93
82	gF	203	PEB	CHA-C1B-C2B	3.41	133.67	124.90
82	MM	201	PEB	C3C-C4C-NC	3.41	111.40	108.33
84	LH	1002	CYC	C1B-C2B-C3B	-3.41	104.31	107.87
82	VQ	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
82	SH	202	PEB	C3B-C4B-NB	3.41	115.01	110.05
82	R4	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	jH	201	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
82	XA	203	PEB	C1C-CHB-C4B	3.41	135.93	128.28
84	K3	1001	CYC	C4D-C3D-C2D	-3.41	103.59	107.62
92	dL	407	LMG	O7-C10-C11	3.41	118.85	111.50
82	PO	202	PEB	CHC-C1D-ND	-3.41	109.41	113.72
82	UF	202	PEB	CMB-C2B-C1B	3.41	130.31	125.06
82	dH	201	PEB	C3B-C4B-NB	3.41	115.01	110.05
82	IP	203	PEB	C3D-C4D-ND	3.41	113.95	107.26
82	SO	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
82	SH	201	PEB	OA-C1A-C2A	-3.41	123.46	126.17
82	g4	202	PEB	C1C-CHB-C4B	3.41	135.93	128.28
82	OB	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	RB	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	hH	201	PEB	C3D-C4D-ND	3.41	113.95	107.26
82	z8	201	PEB	CMB-C2B-C1B	3.41	130.31	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	dL	408	LHG	O7-C7-C8	3.41	118.85	111.50
95	BL	614	DGD	C4E-C3E-C2E	3.41	116.77	110.82
82	gM	201	PEB	OD-C4D-ND	-3.41	120.88	125.93
82	s8	202	PEB	C3D-C4D-ND	3.41	113.95	107.26
82	SH	201	PEB	CHB-C1C-C2C	-3.41	119.46	127.15
84	GE	1001	CYC	C4D-C3D-C2D	-3.41	103.59	107.62
82	CD	201	PEB	C3D-C4D-ND	3.41	113.95	107.26
82	gE	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	lE	203	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	zC	201	PEB	CMB-C2B-C1B	3.41	130.31	125.06
82	kG	202	PEB	CMB-C2B-C1B	3.41	130.31	125.06
82	UH	202	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
82	zC	202	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
82	YF	203	PEB	CHA-C4A-NA	3.41	129.26	125.20
82	TF	202	PEB	OD-C4D-C3D	-3.41	121.74	129.46
82	NP	201	PEB	C3B-C4B-NB	3.41	115.00	110.05
82	q8	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
87	D6	405	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
82	fG	202	PEB	CHC-C4C-NC	3.41	125.76	121.15
82	mH	202	PEB	CHC-C1D-ND	-3.41	109.41	113.72
82	iJ	201	PEB	OD-C4D-ND	-3.41	120.88	125.93
82	LF	201	PEB	CBC-CAC-C2C	-3.41	103.16	112.63
82	QO	201	PEB	OD-C4D-ND	-3.41	120.88	125.93
85	AN	848	BCR	C11-C10-C9	-3.41	122.45	127.31
82	RP	202	PEB	CMB-C2B-C1B	3.41	130.31	125.06
82	UK	202	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
82	I9	201	PEB	OA-C1A-C2A	-3.41	123.47	126.17
84	JO	1001	CYC	C4D-C3D-C2D	-3.41	103.59	107.62
84	m3	1001	CYC	C4D-C3D-C2D	-3.41	103.59	107.62
82	LF	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	KM	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
82	Q5	201	PEB	C4C-C3C-C2C	-3.41	104.36	107.50
82	QP	203	PEB	C3D-C4D-ND	3.41	113.94	107.26
84	GE	1001	CYC	C1B-NB-C4B	-3.41	106.33	110.67
84	N1	1001	CYC	CHB-C1B-NB	-3.41	118.75	126.06
82	18	201	PEB	OD-C4D-ND	-3.41	120.89	125.93
82	O9	203	PEB	OD-C4D-ND	-3.41	120.89	125.93
82	lE	203	PEB	CHC-C4C-NC	3.41	125.76	121.15
82	lH	202	PEB	C1C-CHB-C4B	-3.41	120.64	128.28
82	SG	203	PEB	C1B-C2B-C3B	-3.41	102.60	106.51
82	dG	204	PEB	C1B-C2B-C3B	-3.41	102.60	106.51
96	FL	102	HEM	CHA-C4D-ND	3.41	128.57	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	R4	202	PEB	CAB-C3B-C4B	3.40	131.03	125.01
82	j1	201	PEB	C4B-C3B-C2B	-3.40	103.01	106.78
84	HE	1001	CYC	C1D-C2D-C3D	-3.40	103.45	107.79
82	HI	202	PEB	C3D-C4D-ND	3.40	113.94	107.26
84	I4	1001	CYC	C2C-C1C-NC	3.40	111.21	108.27
84	HG	1001	CYC	CHA-C4D-C3D	-3.40	119.47	127.15
84	u3	1001	CYC	OC-C1C-C2C	-3.40	123.47	126.17
85	b6	602	BCR	C7-C8-C9	3.40	131.38	126.23
82	BA	201	PEB	C3B-C4B-NB	3.40	115.00	110.05
82	AI	203	PEB	CHA-C1B-C2B	3.40	133.65	124.90
82	eM	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
84	F4	1001	CYC	CHB-C1B-NB	-3.40	118.75	126.06
82	AH	302	PEB	CMB-C2B-C1B	3.40	130.31	125.06
83	AM	304	PUB	CHA-C4A-NA	-3.40	109.42	113.72
82	gH	202	PEB	OA-C1A-NA	3.40	129.06	124.94
88	C6	505	LHG	O8-C23-O10	-3.40	115.00	123.59
82	b4	201	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
82	h1	202	PEB	CAB-CBB-CGB	-3.40	106.28	113.60
82	F5	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
84	i3	1001	CYC	C4D-C3D-C2D	-3.40	103.60	107.62
82	UH	203	PEB	CHA-C1B-NB	-3.40	117.81	124.93
82	LJ	202	PEB	CHC-C4C-NC	3.40	125.75	121.15
82	XJ	202	PEB	CHC-C4C-NC	3.40	125.75	121.15
82	KB	304	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
84	I1	1001	CYC	C1A-C2A-C3A	-3.40	103.02	106.78
84	C1	1001	CYC	C1B-NB-C4B	-3.40	106.34	110.67
82	i1	201	PEB	C3D-C4D-ND	3.40	113.94	107.26
82	TO	202	PEB	CAC-C2C-C1C	3.40	131.18	125.76
84	KH	1001	CYC	C1B-CHB-C4A	-3.40	119.77	128.08
82	MJ	201	PEB	C3C-C4C-NC	3.40	111.40	108.33
82	kO	202	PEB	C3C-C4C-NC	3.40	111.40	108.33
82	PK	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
94	D6	408	PL9	C15-C14-C16	3.40	121.00	115.27
82	WI	202	PEB	CMB-C2B-C1B	3.40	130.30	125.06
82	kE	202	PEB	CMB-C2B-C1B	3.40	130.30	125.06
82	kM	202	PEB	CMB-C2B-C1B	3.40	130.30	125.06
82	CP	201	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
82	f4	202	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
82	QA	202	PEB	C3D-C4D-ND	3.40	113.94	107.26
84	GG	1001	CYC	C1B-NB-C4B	-3.40	106.34	110.67
82	AH	301	PEB	C2A-C1A-NA	3.40	111.21	108.27
82	UH	202	PEB	C2A-C1A-NA	3.40	111.21	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WH	201	PEB	C2A-C1A-NA	3.40	111.21	108.27
84	M4	1001	CYC	CHB-C4A-NA	-3.40	117.82	124.93
82	VD	201	PEB	C3B-C4B-NB	3.40	115.00	110.05
82	c1	202	PEB	CHC-C1D-ND	-3.40	109.42	113.72
84	D3	1001	CYC	OC-C1C-C2C	-3.40	123.47	126.17
84	n3	1001	CYC	OC-C1C-C2C	-3.40	123.47	126.17
82	SP	203	PEB	CHB-C1C-NC	-3.40	117.53	125.32
82	gO	202	PEB	C1C-CHB-C4B	3.40	135.91	128.28
82	YJ	203	PEB	C3C-C4C-NC	3.40	111.39	108.33
82	TH	201	PEB	OD-C4D-C3D	-3.40	121.75	129.46
82	HJ	202	PEB	CAB-C3B-C4B	3.40	131.03	125.01
82	Q9	201	PEB	O2B-CGB-CBB	3.40	124.96	114.03
82	YA	301	PEB	CMD-C2D-C3D	3.40	134.86	130.06
82	LE	1002	PEB	C3B-C4B-NB	3.40	115.00	110.05
82	SK	201	PEB	C3B-C4B-NB	3.40	115.00	110.05
82	TP	201	PEB	OD-C4D-ND	-3.40	120.89	125.93
82	jE	201	PEB	CMB-C2B-C1B	3.40	130.30	125.06
82	AG	301	PEB	C2A-C1A-NA	3.40	111.20	108.27
82	OF	203	PEB	C3D-C4D-ND	3.40	113.93	107.26
87	AN	828	CLA	C2B-C1B-NB	3.40	112.51	110.23
82	YQ	202	PEB	CHC-C4C-NC	3.40	125.75	121.15
82	iK	202	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
82	mH	201	PEB	C3B-C4B-NB	3.40	115.00	110.05
82	EQ	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
84	U3	1001	CYC	OC-C1C-C2C	-3.40	123.47	126.17
82	aB	201	PEB	CMB-C2B-C1B	3.40	130.30	125.06
82	h4	201	PEB	CMA-C2A-C1A	-3.40	105.07	112.40
82	VE	201	PEB	CHC-C1D-ND	-3.40	109.42	113.72
82	v8	201	PEB	C1C-CHB-C4B	3.40	135.91	128.28
82	VO	202	PEB	CHA-C1B-NB	-3.40	117.82	124.93
82	EP	201	PEB	CHA-C1B-NB	-3.40	117.82	124.93
82	GA	202	PEB	CHC-C4C-NC	3.40	125.75	121.15
82	dB	202	PEB	C3B-C4B-NB	3.40	115.00	110.05
82	GF	203	PEB	CMB-C2B-C1B	3.40	130.30	125.06
82	RQ	203	PEB	C2A-C1A-NA	3.40	111.20	108.27
82	VA	203	PEB	CAC-C2C-C1C	3.40	131.18	125.76
84	p3	1001	CYC	C4D-C3D-C2D	-3.40	103.60	107.62
82	FJ	201	PEB	CBC-CAC-C2C	-3.40	103.18	112.63
82	P9	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
84	I3	1001	CYC	OC-C1C-C2C	-3.40	123.47	126.17
82	DA	203	PEB	C3B-C4B-NB	3.40	114.99	110.05
82	SG	201	PEB	OD-C4D-ND	-3.40	120.89	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	M9	302	PEB	CHB-C1C-C2C	-3.40	119.48	127.15
82	UH	202	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	gG	201	PEB	CHA-C1B-NB	-3.40	117.82	124.93
82	dG	201	PEB	CMB-C2B-C1B	3.40	130.30	125.06
84	MO	1001	CYC	C2A-C1A-NA	3.40	114.99	110.05
85	c6	603	BCR	C33-C5-C4	3.40	120.14	113.62
82	YF	201	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	oF	203	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	B5	202	PEB	C1C-C2C-C3C	-3.40	103.60	107.62
82	D7	203	PEB	C3B-C4B-NB	3.40	114.99	110.05
82	DQ	203	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
82	rF	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
82	jH	201	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	SD	202	PEB	C3B-C4B-NB	3.40	114.99	110.05
82	f1	203	PEB	C1C-C2C-C3C	-3.40	103.61	107.62
82	S5	203	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
87	8N	308	CLA	CHB-C4A-NA	3.40	129.21	124.51
82	jM	203	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	QG	201	PEB	OD-C4D-ND	-3.40	120.90	125.93
82	F4	1002	PEB	C3B-C4B-NB	3.40	114.99	110.05
82	SK	203	PEB	C3D-C4D-ND	3.40	113.92	107.26
82	QJ	203	PEB	OA-C1A-C2A	-3.40	123.47	126.17
82	fK	202	PEB	OA-C1A-C2A	-3.40	123.47	126.17
85	J2	103	BCR	C7-C8-C9	-3.40	121.10	126.23
82	dJ	202	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	jM	202	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
82	EA	201	PEB	C1D-CHC-C4C	-3.40	108.25	113.26
82	QF	201	PEB	C1C-CHB-C4B	3.40	135.90	128.28
82	IB	202	PEB	C2A-C1A-NA	3.40	111.20	108.27
82	Q9	203	PEB	C2A-C1A-NA	3.40	111.20	108.27
82	CK	201	PEB	OD-C4D-ND	-3.40	120.90	125.93
82	RD	203	PEB	CHB-C1C-C2C	-3.40	119.49	127.15
84	GE	1001	CYC	CHA-C4D-C3D	-3.40	119.49	127.15
82	NQ	202	PEB	CHC-C4C-NC	3.40	125.74	121.15
84	HE	1001	CYC	C4D-C3D-C2D	-3.39	103.61	107.62
82	O1	203	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
82	GP	201	PEB	C2C-C1C-NC	3.39	112.14	107.57
82	SM	202	PEB	OA-C1A-C2A	-3.39	123.47	126.17
85	k6	102	BCR	C36-C18-C17	-3.39	118.17	122.92
82	A7	202	PEB	C3D-C4D-ND	3.39	113.92	107.26
85	bL	603	BCR	C24-C23-C22	-3.39	121.11	126.23
82	KM	201	PEB	CMB-C2B-C1B	3.39	130.29	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	LH	1001	CYC	C1B-C2B-C3B	-3.39	104.33	107.87
84	I1	1001	CYC	C1B-C2B-C3B	-3.39	104.33	107.87
82	OK	203	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	r8	202	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	dG	204	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	bF	201	PEB	OD-C4D-ND	-3.39	120.90	125.93
84	J3	1001	CYC	C4D-C3D-C2D	-3.39	103.61	107.62
82	B7	201	PEB	C3B-C4B-NB	3.39	114.99	110.05
82	W9	201	PEB	O2B-CGB-CBB	3.39	124.93	114.03
82	PB	201	PEB	CHC-C4C-NC	3.39	125.74	121.15
82	ZE	201	PEB	CHC-C1D-ND	-3.39	109.43	113.72
82	JI	201	PEB	CHC-C1D-ND	-3.39	109.43	113.72
82	SF	202	PEB	OD-C4D-ND	-3.39	120.90	125.93
82	gG	201	PEB	OA-C1A-C2A	-3.39	123.47	126.17
84	M3	1001	CYC	OC-C1C-C2C	-3.39	123.47	126.17
84	73	1001	CYC	OC-C1C-C2C	-3.39	123.47	126.17
82	II	203	PEB	C3B-C4B-NB	3.39	114.98	110.05
82	AP	202	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	fH	203	PEB	C1C-C2C-C3C	-3.39	103.61	107.62
84	T3	1001	CYC	C4D-C3D-C2D	-3.39	103.61	107.62
82	PP	201	PEB	CMB-C2B-C1B	3.39	130.29	125.06
82	c1	202	PEB	CHA-C1B-C2B	3.39	133.62	124.90
82	W7	201	PEB	C3C-C4C-NC	3.39	111.39	108.33
85	h6	102	BCR	C28-C27-C26	-3.39	108.02	114.08
82	NP	201	PEB	OD-C4D-ND	-3.39	120.90	125.93
82	TA	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
84	R3	1001	CYC	C4D-C3D-C2D	-3.39	103.61	107.62
82	hG	203	PEB	C3B-C4B-NB	3.39	114.98	110.05
82	EP	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
87	BN	808	CLA	CHB-C4A-NA	3.39	129.20	124.51
82	G7	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	kF	202	PEB	CHC-C4C-NC	3.39	125.74	121.15
82	OI	201	PEB	CAB-CBB-CGB	3.39	120.90	113.60
82	dH	201	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
84	HH	1001	CYC	C4A-C3A-C2A	-3.39	102.61	106.51
82	RO	201	PEB	CHA-C1B-NB	-3.39	117.84	124.93
82	EF	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
82	kF	202	PEB	C2C-C1C-NC	3.39	112.14	107.57
85	K6	102	BCR	C36-C18-C17	-3.39	118.17	122.92
82	tK	203	PEB	CHB-C1C-C2C	-3.39	119.50	127.15
82	dE	203	PEB	OA-C1A-C2A	-3.39	123.48	126.17
84	o3	1001	CYC	OC-C1C-C2C	-3.39	123.48	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VA	203	PEB	C2A-C1A-NA	3.39	111.20	108.27
82	YJ	203	PEB	C2A-C1A-NA	3.39	111.20	108.27
82	B5	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
82	hM	201	PEB	C1C-CHB-C4B	3.39	135.89	128.28
87	A2	831	CLA	CMB-C2B-C1B	-3.39	120.20	125.37
82	NK	201	PEB	CHC-C4C-NC	3.39	125.74	121.15
82	BA	202	PEB	OD-C4D-ND	-3.39	120.91	125.93
82	QF	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
82	TM	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
82	b1	202	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
92	bL	623	LMG	C8-O7-C10	-3.39	109.44	117.79
82	R4	201	PEB	CHA-C1B-NB	-3.39	117.84	124.93
82	sF	202	PEB	CHA-C1B-NB	-3.39	117.84	124.93
82	H5	201	PEB	CMB-C2B-C1B	3.39	130.28	125.06
82	iM	202	PEB	CMB-C2B-C1B	3.39	130.28	125.06
82	wK	303	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	FF	201	PEB	C2C-C1C-NC	3.39	112.14	107.57
82	HD	203	PEB	C2A-C1A-NA	3.39	111.19	108.27
82	hO	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
94	D6	408	PL9	C32-C33-C34	-3.39	119.50	127.66
96	V6	201	HEM	C4C-NC-C1C	3.39	108.67	105.35
82	XF	203	PEB	OD-C4D-ND	-3.39	120.91	125.93
82	lG	203	PEB	CHC-C4C-NC	3.39	125.74	121.15
82	FO	1002	PEB	C3B-C4B-NB	3.39	114.98	110.05
83	yF	303	PUB	C4A-CHA-C1B	-3.39	108.26	113.26
82	F9	202	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
84	LO	1001	CYC	CMB-C2B-C1B	3.39	128.40	124.17
82	IB	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
87	b6	609	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
84	G4	1001	CYC	C4D-CHA-C1A	3.39	135.88	128.28
82	VE	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
84	c3	1001	CYC	C4D-C3D-C2D	-3.39	103.62	107.62
87	B2	807	CLA	CHB-C4A-NA	3.39	129.20	124.51
82	IK	203	PEB	CMA-C2A-C1A	-3.39	105.10	112.40
82	qK	202	PEB	CHB-C1C-C2C	3.39	134.79	127.15
82	hO	201	PEB	CMA-C2A-C1A	-3.39	105.10	112.40
82	ZI	401	PEB	CAB-C3B-C4B	3.39	131.00	125.01
84	DO	1001	CYC	CHB-C4A-NA	-3.39	117.85	124.93
82	RK	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
82	PP	202	PEB	OD-C4D-ND	-3.39	120.91	125.93
82	VJ	201	PEB	C2A-C1A-NA	3.39	111.19	108.27
82	k1	201	PEB	C2A-C1A-NA	3.39	111.19	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	x8	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
82	cE	201	PEB	C2A-C1A-NA	3.39	111.19	108.27
82	ZE	201	PEB	C1C-CHB-C4B	3.39	135.88	128.28
82	GA	202	PEB	CHC-C1D-ND	-3.39	109.44	113.72
82	EB	501	PEB	OA-C1A-C2A	-3.39	123.48	126.17
82	Q1	202	PEB	OA-C1A-C2A	-3.39	123.48	126.17
84	JO	1001	CYC	C4A-C3A-C2A	-3.39	102.62	106.51
84	D1	1001	CYC	C4A-C3A-C2A	-3.39	102.62	106.51
82	DK	203	PEB	OD-C4D-ND	-3.39	120.91	125.93
94	a6	601	PL9	C22-C23-C24	-3.39	119.51	127.66
95	a6	602	DGD	O1G-C1A-C2A	3.39	122.53	111.91
82	BJ	301	PEB	C2A-C1A-NA	3.39	111.19	108.27
82	gE	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
82	EQ	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	W5	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
82	eJ	202	PEB	OD-C4D-ND	-3.39	120.91	125.93
84	N4	1001	CYC	OB-C4B-C3B	-3.39	124.37	128.04
84	Q3	1001	CYC	OC-C1C-C2C	-3.39	123.48	126.17
82	AI	203	PEB	C3B-C4B-NB	3.39	114.97	110.05
84	G3	1001	CYC	C4D-C3D-C2D	-3.39	103.62	107.62
82	G7	202	PEB	CHC-C1D-ND	-3.39	109.44	113.72
82	T1	201	PEB	OD-C4D-C3D	-3.39	121.79	129.46
84	F4	1001	CYC	C1D-C2D-C3D	-3.39	103.48	107.79
82	OG	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
82	hE	201	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
82	RJ	201	PEB	CMB-C2B-C1B	3.39	130.28	125.06
85	AN	847	BCR	C3-C4-C5	-3.38	108.03	114.08
83	xF	301	PUB	CHA-C1B-NB	3.38	125.73	121.15
85	B6	621	BCR	C23-C24-C25	-3.38	117.70	127.20
82	1C	203	PEB	OA-C1A-C2A	-3.38	123.48	126.17
82	wF	303	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	DQ	201	PEB	C1C-CHB-C4B	3.38	135.87	128.28
84	v3	1001	CYC	C4D-C3D-C2D	-3.38	103.62	107.62
84	FO	1001	CYC	C2C-C1C-NC	3.38	111.19	108.27
82	PJ	201	PEB	C1D-CHC-C4C	3.38	118.25	113.26
82	RB	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	FJ	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	GA	201	PEB	OD-C4D-C3D	-3.38	121.79	129.46
84	O3	1001	CYC	OC-C1C-C2C	-3.38	123.48	126.17
82	Y7	301	PEB	CHA-C1B-NB	-3.38	117.86	124.93
84	MO	1001	CYC	CHB-C4A-NA	-3.38	117.86	124.93
82	FI	201	PEB	C1C-C2C-C3C	-3.38	103.62	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	t3	1001	CYC	C4D-C3D-C2D	-3.38	103.62	107.62
82	N1	1002	PEB	CAB-C3B-C4B	3.38	130.99	125.01
82	FD	201	PEB	C1B-C2B-C3B	-3.38	102.62	106.51
82	AO	301	PEB	C1B-C2B-C3B	-3.38	102.62	106.51
87	B2	833	CLA	C3B-C4B-NB	-3.38	107.38	110.52
83	xF	301	PUB	OD-C4D-ND	-3.38	120.92	125.93
82	TE	201	PEB	C3B-C4B-NB	3.38	114.97	110.05
82	gB	203	PEB	C3B-C4B-NB	3.38	114.97	110.05
82	ZG	201	PEB	C1C-CHB-C4B	3.38	135.87	128.28
84	w3	1001	CYC	OC-C1C-C2C	-3.38	123.48	126.17
82	GK	202	PEB	CAB-C3B-C4B	3.38	130.99	125.01
82	RK	202	PEB	CAB-C3B-C4B	3.38	130.99	125.01
88	iL	101	LHG	O7-C7-C8	3.38	118.79	111.50
82	B7	201	PEB	CHA-C1B-NB	-3.38	117.86	124.93
82	EF	202	PEB	C3B-C4B-NB	3.38	114.97	110.05
82	JK	201	PEB	CHC-C1D-ND	-3.38	109.45	113.72
82	JK	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	U1	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	F4	1002	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	A1	301	PEB	C2A-C1A-NA	3.38	111.19	108.27
84	C3	1001	CYC	C4D-C3D-C2D	-3.38	103.62	107.62
84	g3	1001	CYC	C4D-C3D-C2D	-3.38	103.62	107.62
82	PJ	202	PEB	CMB-C2B-C1B	3.38	130.27	125.06
82	TM	202	PEB	CMB-C2B-C1B	3.38	130.27	125.06
82	AA	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
82	KM	203	PEB	C3C-C4C-NC	3.38	111.38	108.33
82	PQ	203	PEB	CMB-C2B-C1B	3.38	130.27	125.06
82	fK	202	PEB	C1C-C2C-C3C	-3.38	103.62	107.62
82	BA	201	PEB	CHA-C1B-NB	-3.38	117.86	124.93
82	NQ	204	PEB	C2A-C1A-NA	3.38	111.19	108.27
82	j4	202	PEB	C2A-C1A-NA	3.38	111.19	108.27
82	eO	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
82	AD	303	PEB	C3D-C4D-ND	3.38	113.89	107.26
82	cM	201	PEB	CMC-C3C-C4C	3.38	130.64	127.06
82	k4	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	W9	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	kO	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
82	Q1	203	PEB	CHC-C4C-NC	3.38	125.72	121.15
84	GO	1001	CYC	C4D-CHA-C1A	3.38	135.86	128.28
82	aJ	204	PEB	C3C-C4C-NC	3.38	111.38	108.33
82	YK	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
82	YK	202	PEB	OA-C1A-C2A	-3.38	123.49	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	C9	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
82	V4	202	PEB	CHA-C1B-NB	-3.38	117.86	124.93
82	CM	203	PEB	OD-C4D-ND	-3.38	120.92	125.93
82	UM	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
82	OI	202	PEB	CMB-C2B-C1B	3.38	130.27	125.06
85	a6	605	BCR	C33-C5-C6	-3.38	120.73	124.53
82	L9	202	PEB	OD-C4D-ND	-3.38	120.92	125.93
82	ZJ	202	PEB	CAB-C3B-C4B	3.38	130.99	125.01
82	WA	201	PEB	C3C-C4C-NC	3.38	111.37	108.33
94	A6	410	PL9	C7-C8-C9	-3.38	121.17	126.79
82	f1	203	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
82	gG	201	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
82	HP	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
82	N9	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
82	XB	202	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	mG	201	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	aF	202	PEB	CHB-C1C-C2C	-3.38	119.53	127.15
82	NO	1002	PEB	OD-C4D-ND	-3.38	120.93	125.93
82	oF	201	PEB	CHA-C4A-NA	-3.38	121.19	125.20
87	82	302	CLA	C3C-C4C-NC	-3.38	106.78	110.57
84	K1	1001	CYC	C1B-CHB-C4A	-3.38	119.83	128.08
87	AN	831	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
82	YD	202	PEB	CHC-C4C-NC	3.38	125.72	121.15
84	E1	1001	CYC	CHA-C4D-C3D	-3.38	119.53	127.15
82	S5	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
82	dE	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
82	YK	201	PEB	C2A-C1A-NA	3.38	111.18	108.27
82	QP	203	PEB	C2A-C1A-NA	3.38	111.18	108.27
84	NH	1001	CYC	C2C-C1C-NC	3.38	111.18	108.27
82	WE	201	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	lK	202	PEB	C3B-C4B-NB	3.38	114.96	110.05
83	yK	303	PUB	C4A-CHA-C1B	-3.38	108.28	113.26
94	aL	601	PL9	C40-C39-C41	3.38	120.95	115.27
82	VF	202	PEB	CAC-CBC-CGC	-3.38	106.34	113.60
84	P3	1001	CYC	C4D-C3D-C2D	-3.38	103.63	107.62
82	UJ	201	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	M5	304	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	mE	201	PEB	C3B-C4B-NB	3.38	114.96	110.05
84	CH	1001	CYC	C1B-C2B-C3B	-3.38	104.35	107.87
82	WA	202	PEB	CHA-C1B-NB	-3.38	117.87	124.93
82	Q4	201	PEB	CHA-C1B-NB	-3.38	117.87	124.93
82	kH	202	PEB	C1C-CHB-C4B	3.38	135.85	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HF	202	PEB	OA-C1A-C2A	-3.38	123.49	126.17
82	fH	203	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
84	FG	1001	CYC	C4A-C3A-C2A	-3.38	102.63	106.51
82	W5	202	PEB	C2A-C1A-NA	3.38	111.18	108.27
82	NH	1002	PEB	CAB-C3B-C4B	3.38	130.98	125.01
82	dD	401	PEB	CMB-C2B-C1B	3.38	130.26	125.06
82	bE	201	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	wF	301	PEB	C3B-C4B-NB	3.38	114.96	110.05
82	CJ	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
82	CM	203	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
82	q8	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
82	PF	202	PEB	OD-C4D-ND	-3.38	120.93	125.93
82	dJ	202	PEB	OD-C4D-ND	-3.38	120.93	125.93
84	NO	1001	CYC	CMB-C2B-C1B	3.38	128.38	124.17
82	cO	201	PEB	CMB-C2B-C1B	3.37	130.26	125.06
82	gF	201	PEB	CHB-C4B-C3B	-3.37	117.51	125.32
82	VA	202	PEB	CHA-C1B-NB	-3.37	117.87	124.93
82	KF	202	PEB	CHB-C1C-C2C	-3.37	119.54	127.15
82	MD	202	PEB	OD-C4D-ND	-3.37	120.93	125.93
82	X9	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
82	gM	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
84	F3	1001	CYC	OC-C1C-C2C	-3.37	123.49	126.17
82	P4	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	AD	304	PEB	CHB-C4B-NB	-3.37	117.56	124.58
82	BQ	202	PEB	C1B-C2B-C3B	-3.37	102.63	106.51
82	B7	202	PEB	C1B-C2B-C3B	-3.37	102.63	106.51
82	QF	203	PEB	C1C-NC-C4C	-3.37	103.59	109.60
82	AQ	304	PEB	CHB-C4B-NB	-3.37	117.56	124.58
82	SG	203	PEB	C1C-CHB-C4B	3.37	135.85	128.28
82	aM	204	PEB	OD-C4D-ND	-3.37	120.93	125.93
82	CF	203	PEB	CHC-C4C-NC	3.37	125.72	121.15
82	AE	301	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	PM	201	PEB	CAB-C3B-C4B	3.37	130.98	125.01
82	QB	201	PEB	C3B-C4B-NB	3.37	114.96	110.05
82	SQ	202	PEB	C3B-C4B-NB	3.37	114.96	110.05
82	QB	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	kE	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	WD	201	PEB	C1D-CHC-C4C	-3.37	108.28	113.26
82	sF	202	PEB	C4C-C3C-C2C	-3.37	104.39	107.50
82	kK	202	PEB	C2C-C1C-NC	3.37	112.11	107.57
82	LD	202	PEB	OD-C4D-ND	-3.37	120.93	125.93
82	bK	202	PEB	OD-C4D-ND	-3.37	120.93	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iH	201	PEB	C3D-C4D-ND	3.37	113.88	107.26
82	M9	301	PEB	CAB-C3B-C4B	3.37	130.98	125.01
82	rK	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	YG	202	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
84	DH	1003	CYC	C1A-C2A-C3A	-3.37	103.05	106.78
82	Q4	201	PEB	OD-C4D-ND	-3.37	120.93	125.93
82	T4	202	PEB	CAC-C2C-C1C	3.37	131.13	125.76
82	DM	202	PEB	CHC-C4C-NC	3.37	125.71	121.15
82	XB	201	PEB	CMB-C2B-C1B	3.37	130.26	125.06
82	F7	201	PEB	CMB-C2B-C1B	3.37	130.26	125.06
85	fL	101	BCR	C2-C1-C6	3.37	115.67	110.48
82	YF	201	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	HG	1002	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	S4	202	PEB	OD-C4D-C3D	-3.37	121.82	129.46
82	hM	201	PEB	C3C-C4C-NC	3.37	111.37	108.33
82	V7	203	PEB	CAC-C2C-C1C	3.37	131.13	125.76
82	AQ	304	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	fG	202	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	RB	202	PEB	CMB-C2B-C1B	3.37	130.26	125.06
82	Y5	201	PEB	CMB-C2B-C1B	3.37	130.26	125.06
82	SE	202	PEB	C1C-CHB-C4B	3.37	135.84	128.28
82	G7	202	PEB	CHC-C4C-NC	3.37	125.71	121.15
82	eJ	202	PEB	CAB-C3B-C4B	3.37	130.97	125.01
82	iF	202	PEB	OD-C4D-ND	-3.37	120.94	125.93
82	KA	202	PEB	C3D-C4D-ND	3.37	113.87	107.26
82	dG	202	PEB	CMB-C2B-C1B	3.37	130.25	125.06
82	GK	203	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	z8	202	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	EA	202	PEB	OA-C1A-C2A	-3.37	123.49	126.17
82	BQ	202	PEB	OA-C1A-C2A	-3.37	123.49	126.17
82	IJ	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	EK	201	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	YF	203	PEB	C3D-C4D-ND	3.37	113.87	107.26
82	O4	201	PEB	C4B-NB-C1B	-3.37	100.16	106.51
82	GD	201	PEB	CAB-CBB-CGB	-3.37	106.35	113.60
82	FK	201	PEB	C2C-C1C-NC	3.37	112.11	107.57
82	FA	201	PEB	CMB-C2B-C1B	3.37	130.25	125.06
82	OH	202	PEB	C1C-CHB-C4B	-3.37	120.72	128.28
82	QK	203	PEB	C1C-NC-C4C	-3.37	103.60	109.60
87	82	308	CLA	CHB-C4A-NA	3.37	129.17	124.51
82	TA	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	GG	1002	PEB	C2A-C1A-NA	3.37	111.18	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	KG	202	CYC	C2C-C1C-NC	3.37	111.18	108.27
82	PO	203	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	A1	305	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	XP	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
82	RK	202	PEB	CMC-C3C-C4C	3.37	130.63	127.06
84	V3	1001	CYC	CMB-C2B-C1B	3.37	128.37	124.17
84	H3	1001	CYC	OC-C1C-C2C	-3.37	123.49	126.17
84	JO	1001	CYC	OB-C4B-C3B	-3.37	124.38	128.04
82	wK	301	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	QE	203	PEB	OD-C4D-ND	-3.37	120.94	125.93
82	gK	201	PEB	CHB-C4B-C3B	-3.37	117.53	125.32
82	UA	202	PEB	C3D-C4D-ND	3.37	113.87	107.26
82	WP	201	PEB	CMB-C2B-C1B	3.37	130.25	125.06
82	RD	203	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	B5	203	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	iH	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	gM	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
82	VA	203	PEB	CAB-C3B-C4B	3.37	130.97	125.01
82	W7	202	PEB	CHA-C1B-NB	-3.37	117.89	124.93
82	Q1	202	PEB	CHA-C1B-C2B	3.37	133.56	124.90
82	SE	202	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
82	LQ	203	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
82	SO	202	PEB	OD-C4D-C3D	-3.37	121.83	129.46
82	LQ	203	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	W5	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	qC	203	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	j4	203	PEB	C3C-C4C-NC	3.37	111.36	108.33
84	FE	1001	CYC	CHB-C4A-NA	-3.37	117.89	124.93
82	KK	203	PEB	CHB-C1C-C2C	-3.37	119.55	127.15
85	kL	100	BCR	C15-C14-C13	-3.37	122.50	127.31
94	aL	601	PL9	C35-C34-C36	3.37	120.94	115.27
82	Z1	202	PEB	OA-C1A-C2A	-3.37	123.50	126.17
82	H7	203	PEB	OA-C1A-C2A	-3.37	123.50	126.17
84	f3	1001	CYC	OC-C1C-C2C	-3.37	123.50	126.17
82	OQ	202	PEB	C4B-C3B-C2B	-3.37	103.06	106.78
82	vC	201	PEB	C1C-CHB-C4B	3.37	135.84	128.28
95	D6	410	DGD	O2G-C1B-C2B	3.37	118.76	111.50
87	CL	511	CLA	CMB-C2B-C1B	-3.37	120.24	125.37
83	BJ	302	PUB	OA-C1A-NA	-3.37	120.94	125.93
82	XP	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	gG	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
82	O5	201	PEB	CHC-C1D-ND	-3.37	109.46	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FP	201	PEB	C2C-C1C-NC	3.37	112.11	107.57
82	gF	201	PEB	CHA-C1B-C2B	3.37	133.56	124.90
82	OD	202	PEB	C4B-C3B-C2B	-3.37	103.06	106.78
84	L4	1001	CYC	CMB-C2B-C1B	3.37	128.37	124.17
82	QB	204	PEB	OD-C4D-ND	-3.37	120.94	125.93
82	LI	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
82	Z9	301	PEB	CHB-C1C-C2C	-3.37	119.55	127.15
82	DJ	201	PEB	CHA-C1B-NB	-3.37	117.89	124.93
82	cH	202	PEB	CHA-C1B-C2B	3.37	133.56	124.90
82	UF	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	rF	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
82	AD	304	PEB	CHA-C1B-NB	-3.37	117.89	124.93
82	bO	202	PEB	C2A-C1A-NA	3.37	111.17	108.27
87	82	302	CLA	CHB-C4A-NA	3.37	129.17	124.51
82	BQ	201	PEB	C3C-C4C-NC	3.37	111.36	108.33
82	cK	201	PEB	C3B-C4B-NB	3.37	114.94	110.05
82	YH	202	PEB	CMC-C3C-C4C	3.37	130.63	127.06
84	EH	1001	CYC	CHA-C4D-C3D	-3.37	119.56	127.15
91	dL	403	PHO	C4A-C3A-C2A	-3.37	99.64	102.84
84	HG	1001	CYC	C4D-C3D-C2D	-3.37	103.64	107.62
82	jJ	203	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
82	G7	201	PEB	OD-C4D-C3D	-3.37	121.83	129.46
84	EO	1001	CYC	CHB-C4A-NA	-3.36	117.89	124.93
82	MK	203	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	eO	202	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	SB	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	ZH	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	lK	203	PEB	C1B-C2B-C3B	-3.36	102.64	106.51
82	q8	203	PEB	OD-C4D-ND	-3.36	120.95	125.93
82	kM	202	PEB	CHC-C4C-NC	3.36	125.70	121.15
82	HB	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
82	FQ	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
82	CP	203	PEB	C1D-CHC-C4C	-3.36	108.30	113.26
82	S5	202	PEB	CAB-C3B-C4B	3.36	130.96	125.01
87	22	605	CLA	C3B-C4B-NB	-3.36	107.98	110.23
85	b6	602	BCR	C3-C4-C5	-3.36	108.07	114.08
82	wF	301	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	cB	402	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	WF	202	PEB	CHB-C1C-C2C	-3.36	119.56	127.15
82	U7	202	PEB	C3D-C4D-ND	3.36	113.86	107.26
82	WM	202	PEB	OA-C1A-C2A	-3.36	123.50	126.17
84	NO	1001	CYC	CMA-C3A-C4A	3.36	130.24	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FM	201	PEB	C3B-C4B-NB	3.36	114.94	110.05
84	x3	1001	CYC	CHB-C4A-C3A	3.36	133.55	124.90
83	xK	301	PUB	OD-C4D-ND	-3.36	120.95	125.93
82	SF	201	PEB	CMC-C3C-C4C	3.36	130.62	127.06
87	4N	608	CLA	CHB-C1B-NB	3.36	127.82	124.26
84	A3	1001	CYC	C4D-C3D-C2D	-3.36	103.65	107.62
82	PO	203	PEB	CAB-C3B-C4B	3.36	130.96	125.01
82	RK	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	EM	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	LP	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	mE	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	eG	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
84	FO	1001	CYC	C1D-C2D-C3D	-3.36	103.51	107.79
82	JA	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
82	RF	202	PEB	CMC-C3C-C4C	3.36	130.62	127.06
82	G9	201	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	Q7	202	PEB	C3D-C4D-ND	3.36	113.86	107.26
82	ZG	201	PEB	CHC-C1D-ND	-3.36	109.47	113.72
82	VP	201	PEB	CHC-C1D-ND	-3.36	109.47	113.72
82	L9	201	PEB	CHC-C1D-ND	-3.36	109.47	113.72
82	gE	201	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	JB	202	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	FI	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
82	uF	201	PEB	CHB-C1C-C2C	-3.36	119.57	127.15
82	ED	202	PEB	CAC-CBC-CGC	-3.36	106.37	113.60
82	MM	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
87	B2	818	CLA	C3B-C4B-NB	-3.36	107.40	110.52
82	gK	202	PEB	CHC-C1D-ND	-3.36	109.47	113.72
82	QP	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
82	RF	202	PEB	CAB-C3B-C4B	3.36	130.96	125.01
82	HD	203	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	KK	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
84	E4	1001	CYC	CHB-C4A-NA	-3.36	117.90	124.93
82	EM	203	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	WQ	201	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	S5	202	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	O7	202	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	R9	201	PEB	OA-C1A-C2A	-3.36	123.50	126.17
82	DQ	203	PEB	C2A-C1A-NA	3.36	111.17	108.27
82	SP	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
84	DH	1001	CYC	CMA-C3A-C4A	3.36	130.24	125.06
82	VA	203	PEB	OD-C4D-ND	-3.36	120.95	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	e4	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
87	AL	404	CLA	O2D-CGD-CBD	3.36	117.24	111.27
84	l3	1001	CYC	C4D-C3D-C2D	-3.36	103.65	107.62
82	CI	201	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	TQ	203	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
87	42	608	CLA	CHB-C1B-NB	3.36	127.81	124.26
82	ZB	202	PEB	CMB-C2B-C1B	3.36	130.24	125.06
82	dO	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
82	dB	202	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	fM	202	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
84	I4	1001	CYC	C1A-C2A-C3A	-3.36	103.06	106.78
82	JA	202	PEB	CHA-C1B-NB	-3.36	117.91	124.93
82	YA	301	PEB	CHA-C1B-NB	-3.36	117.91	124.93
82	YK	203	PEB	CHB-C1C-C2C	-3.36	119.57	127.15
82	i4	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
82	xF	302	PEB	C2A-C1A-NA	3.36	111.17	108.27
84	FG	1001	CYC	C2C-C1C-NC	3.36	111.17	108.27
84	FH	1001	CYC	C1D-C2D-C3D	-3.36	103.51	107.79
82	gE	201	PEB	CHA-C1B-NB	-3.36	117.91	124.93
82	OO	201	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
84	J1	1001	CYC	C4A-C3A-C2A	-3.36	102.65	106.51
82	QP	203	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
82	cJ	202	PEB	CHC-C4C-NC	3.36	125.69	121.15
82	DK	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
82	GF	202	PEB	CAB-C3B-C4B	3.36	130.95	125.01
82	m4	203	PEB	CHC-C1D-ND	-3.36	109.47	113.72
82	YO	202	PEB	C3C-C4C-NC	3.36	111.36	108.33
82	R4	202	PEB	CHA-C1B-NB	-3.36	117.91	124.93
82	SJ	201	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	j1	203	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	dG	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
82	UJ	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
82	rC	201	PEB	C3B-C4B-NB	3.36	114.93	110.05
82	cO	203	PEB	C3B-C4B-NB	3.36	114.93	110.05
84	EE	1001	CYC	C2A-C1A-NA	3.36	114.93	110.05
85	A2	845	BCR	C38-C26-C25	-3.36	120.76	124.53
82	FO	1002	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
82	jH	203	PEB	OD-C4D-ND	-3.36	120.96	125.93
82	Z5	304	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	wF	303	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	NB	201	PEB	CHA-C1B-NB	-3.36	117.91	124.93
82	X7	202	PEB	OD-C4D-C3D	-3.36	121.85	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OH	203	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
82	VG	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
82	kO	202	PEB	CAB-C3B-C4B	3.36	130.95	125.01
82	SG	203	PEB	C3B-C4B-NB	3.36	114.93	110.05
82	cE	201	PEB	C3B-C4B-NB	3.36	114.93	110.05
82	QK	201	PEB	C1C-CHB-C4B	3.36	135.81	128.28
82	oK	201	PEB	CHA-C4A-NA	-3.36	121.21	125.20
82	TD	203	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
82	WP	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
82	MJ	201	PEB	OD-C4D-ND	-3.36	120.96	125.93
82	lF	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
82	DI	201	PEB	CAA-C3A-C2A	-3.36	105.87	114.26
84	CG	1001	CYC	CHB-C4A-NA	-3.36	117.91	124.93
82	hO	201	PEB	C1C-CHB-C4B	3.36	135.81	128.28
82	TI	202	PEB	C1B-C2B-C3B	-3.36	102.66	106.51
82	QP	201	PEB	OD-C4D-ND	-3.36	120.96	125.93
82	HB	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
82	mG	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
82	gJ	202	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
84	M1	201	CYC	CHD-C1D-ND	-3.36	117.63	125.32
82	oK	201	PEB	CHB-C1C-C2C	-3.35	119.58	127.15
82	DF	201	PEB	OD-C4D-ND	-3.35	120.96	125.93
82	xK	302	PEB	C2A-C1A-NA	3.35	111.17	108.27
84	NE	201	CYC	C2C-C1C-NC	3.35	111.17	108.27
85	fL	101	BCR	C24-C23-C22	3.35	131.30	126.23
82	VM	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
82	TP	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
82	oF	201	PEB	CHB-C1C-C2C	-3.35	119.58	127.15
82	QH	202	PEB	CHA-C1B-C2B	3.35	133.53	124.90
82	J7	202	PEB	CHA-C1B-NB	-3.35	117.92	124.93
85	AN	845	BCR	C38-C26-C25	-3.35	120.76	124.53
83	Z9	305	PUB	C4B-NB-C1B	-3.35	103.63	109.60
88	dL	408	LHG	O8-C23-C24	3.35	122.43	111.91
82	QG	201	PEB	CAB-C3B-C4B	3.35	130.94	125.01
82	RF	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
82	cG	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
82	XK	201	PEB	CHA-C1B-NB	-3.35	117.92	124.93
82	fE	202	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
82	aF	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
84	LO	1001	CYC	C2A-C1A-NA	3.35	114.93	110.05
82	DD	201	PEB	C1C-CHB-C4B	3.35	135.80	128.28
82	EM	201	PEB	C3B-C4B-NB	3.35	114.93	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XJ	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
82	YJ	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
87	A2	806	CLA	CHB-C4A-NA	3.35	129.15	124.51
82	XA	201	PEB	CAC-CBC-CGC	-3.35	106.39	113.60
82	aK	202	PEB	CHB-C1C-C2C	-3.35	119.59	127.15
82	hG	203	PEB	CHC-C1D-ND	-3.35	109.48	113.72
82	mO	201	PEB	C3B-C4B-NB	3.35	114.92	110.05
82	BQ	203	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	K9	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	S9	203	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	i1	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
82	A7	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
87	aL	606	CLA	O2A-CGA-CBA	3.35	122.43	111.91
82	EK	202	PEB	CHC-C4C-NC	3.35	125.69	121.15
82	Y4	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
82	CJ	203	PEB	C1C-CHB-C4B	3.35	135.80	128.28
82	WK	202	PEB	CHB-C1C-C2C	-3.35	119.59	127.15
82	F5	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
82	DM	201	PEB	C1C-CHB-C4B	-3.35	120.77	128.28
82	Z5	305	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	18	203	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	EI	201	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
84	FO	1001	CYC	C4A-C3A-C2A	-3.35	102.66	106.51
85	kL	100	BCR	C19-C18-C17	3.35	124.08	118.94
84	EG	1001	CYC	CHB-C4A-NA	-3.35	117.92	124.93
82	eF	201	PEB	C1C-CHB-C4B	3.35	135.79	128.28
82	HP	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
87	b6	612	CLA	C1-C2-C3	-3.35	120.25	126.04
82	b1	202	PEB	CHB-C1C-NC	-3.35	117.65	125.32
82	AD	301	PEB	CHC-C1D-ND	-3.35	109.49	113.72
82	JD	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	AH	305	PEB	CHB-C1C-NC	-3.35	117.65	125.32
82	AO	305	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
82	MB	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
84	x3	1001	CYC	CMB-C2B-C1B	3.35	128.35	124.17
82	FF	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	IF	203	PEB	CHA-C1B-NB	-3.35	117.93	124.93
91	A6	407	PHO	CBC-CAC-C3C	-3.35	107.98	112.88
87	BN	818	CLA	C4-C3-C5	3.35	120.91	115.27
84	J1	1001	CYC	CAD-CBD-CGD	-3.35	106.40	113.60
82	BI	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	QJ	203	PEB	C4B-C3B-C2B	-3.35	103.08	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mF	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
82	MB	202	PEB	CMB-C2B-C1B	3.35	130.22	125.06
82	V7	203	PEB	C2C-C1C-NC	3.35	112.08	107.57
82	ZB	203	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
82	GI	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
82	d1	201	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
82	YO	202	PEB	C3B-C4B-NB	3.35	114.92	110.05
82	QH	203	PEB	CHC-C4C-NC	3.35	125.68	121.15
82	GM	203	PEB	C3C-C4C-NC	3.35	111.35	108.33
84	GG	1001	CYC	C4D-C3D-C2D	-3.35	103.66	107.62
84	IG	1001	CYC	C1B-C2B-C3B	-3.35	104.38	107.87
82	YA	304	PEB	CMB-C2B-C1B	3.35	130.22	125.06
82	GB	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	UB	303	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	bB	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	TI	201	PEB	C1C-NC-C4C	-3.35	103.64	109.60
82	A4	301	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
82	F7	203	PEB	CAC-CBC-CGC	-3.35	106.40	113.60
82	wF	301	PEB	CHC-C1D-ND	-3.35	109.49	113.72
82	HQ	203	PEB	C3D-C4D-ND	3.35	113.83	107.26
82	B7	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
82	ZK	202	PEB	C3B-C4B-NB	3.35	114.92	110.05
82	DP	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	HP	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
85	KL	100	BCR	C19-C18-C17	3.35	124.08	118.94
84	J4	1001	CYC	C4A-C3A-C2A	-3.35	102.67	106.51
82	aO	202	PEB	CMB-C2B-C1B	3.35	130.22	125.06
82	RJ	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	y8	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
84	q3	1001	CYC	OC-C1C-C2C	-3.35	123.51	126.17
82	eM	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
84	CH	1001	CYC	C1B-NB-C4B	-3.35	106.41	110.67
82	Q4	201	PEB	C1C-CHB-C4B	3.35	135.79	128.28
82	WD	201	PEB	CAC-C2C-C1C	3.35	131.09	125.76
82	OF	202	PEB	C3B-C4B-NB	3.35	114.92	110.05
82	Y1	201	PEB	CHA-C1B-NB	-3.35	117.93	124.93
82	HB	203	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	TB	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	PD	203	PEB	CMB-C2B-C1B	3.35	130.22	125.06
82	CF	203	PEB	CHB-C1C-C2C	-3.35	119.60	127.15
82	IF	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
82	AI	201	PEB	C1B-C2B-C3B	-3.35	102.67	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	qC	202	PEB	CHA-C1B-NB	-3.35	117.93	124.93
82	U1	203	PEB	C3D-C4D-ND	3.35	113.82	107.26
82	dE	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	uF	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
82	VE	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
82	TG	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
82	hF	201	PEB	CAB-CBB-CGB	-3.35	106.40	113.60
87	52	606	CLA	CMA-C3A-C4A	3.35	120.76	111.77
82	bF	201	PEB	CHC-C1D-ND	-3.35	109.49	113.72
82	LF	202	PEB	CBC-CAC-C2C	3.35	121.92	112.63
82	S7	201	PEB	C3C-C4C-NC	3.35	111.34	108.33
87	bL	606	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
82	TK	202	PEB	OD-C4D-C3D	-3.34	121.88	129.46
82	AI	201	PEB	C1D-CHC-C4C	-3.34	108.32	113.26
82	dE	201	PEB	OD-C4D-ND	-3.34	120.97	125.93
84	V3	1001	CYC	CHB-C4A-C3A	3.34	133.50	124.90
82	PP	201	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
82	yK	301	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
82	hK	201	PEB	CAB-CBB-CGB	-3.34	106.41	113.60
82	YB	201	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	II	201	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	wK	301	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	AH	305	PEB	C2A-C1A-NA	3.34	111.16	108.27
82	oF	203	PEB	C2A-C1A-NA	3.34	111.16	108.27
82	Y7	304	PEB	CMB-C2B-C1B	3.34	130.21	125.06
82	OE	201	PEB	OA-C1A-C2A	-3.34	123.51	126.17
87	5N	606	CLA	CMA-C3A-C4A	3.34	120.76	111.77
82	QB	202	PEB	CHC-C4C-NC	3.34	125.67	121.15
82	Y1	202	PEB	CMC-C3C-C4C	3.34	130.60	127.06
87	A2	834	CLA	O2D-CGD-CBD	3.34	117.21	111.27
82	O1	202	PEB	C1C-CHB-C4B	-3.34	120.78	128.28
87	BN	834	CLA	C3B-C4B-NB	-3.34	107.41	110.52
82	VJ	202	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
82	gK	203	PEB	CHA-C1B-C2B	3.34	133.50	124.90
82	RO	202	PEB	CHA-C1B-NB	-3.34	117.94	124.93
82	wF	302	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	OM	203	PEB	C1C-CHB-C4B	3.34	135.78	128.28
82	E9	202	PEB	C2A-C1A-NA	3.34	111.16	108.27
82	mO	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
82	Q5	203	PEB	CHA-C1B-NB	-3.34	117.94	124.93
82	hJ	201	PEB	OA-C1A-C2A	-3.34	123.52	126.17
82	PD	201	PEB	C3D-C4D-ND	3.34	113.82	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	h1	202	PEB	C3D-C4D-ND	3.34	113.82	107.26
87	8N	303	CLA	C3C-C4C-NC	-3.34	106.82	110.57
82	gK	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
82	QO	201	PEB	C1C-CHB-C4B	3.34	135.78	128.28
87	BN	810	CLA	CHB-C4A-NA	3.34	129.13	124.51
82	K7	202	PEB	C3D-C4D-ND	3.34	113.82	107.26
82	OK	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
82	eE	201	PEB	C3B-C4B-NB	3.34	114.91	110.05
82	G9	202	PEB	CHB-C4B-C3B	3.34	133.05	125.32
82	S1	201	PEB	CHB-C1C-C2C	-3.34	119.61	127.15
84	EE	1001	CYC	CHB-C4A-NA	-3.34	117.94	124.93
87	22	604	CLA	CAA-C2A-C3A	-3.34	105.91	114.26
82	LQ	202	PEB	OD-C4D-ND	-3.34	120.98	125.93
82	gF	203	PEB	OD-C4D-ND	-3.34	120.98	125.93
82	Y7	301	PEB	CMD-C2D-C3D	3.34	134.78	130.06
95	a6	603	DGD	O6E-C5E-C4E	3.34	115.76	109.69
82	kK	201	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
84	h3	1001	CYC	OC-C1C-C2C	-3.34	123.52	126.17
82	DG	1002	PEB	C3B-C4B-NB	3.34	114.91	110.05
82	vF	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
87	BN	833	CLA	C3B-C4B-NB	-3.34	107.42	110.52
84	C1	1001	CYC	C1B-C2B-C3B	-3.34	104.38	107.87
82	m1	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
82	vF	202	PEB	CHC-C1D-ND	-3.34	109.50	113.72
82	RD	202	PEB	CHC-C4C-NC	3.34	125.67	121.15
82	QE	201	PEB	CAB-C3B-C4B	3.34	130.92	125.01
82	HM	202	PEB	CHB-C4B-NB	-3.34	117.62	124.58
82	JQ	202	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
82	O7	201	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
82	M9	301	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
82	AJ	302	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	IJ	201	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	SP	201	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	lO	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
84	KH	1001	CYC	C2C-C1C-NC	3.34	111.15	108.27
88	C6	522	LHG	O8-C23-C24	3.34	120.14	111.38
82	GI	202	PEB	C1D-CHC-C4C	-3.34	108.33	113.26
84	L1	1001	CYC	C1B-C2B-C3B	-3.34	104.39	107.87
82	BD	203	PEB	OA-C1A-C2A	-3.34	123.52	126.17
82	e4	202	PEB	OA-C1A-C2A	-3.34	123.52	126.17
84	L3	1001	CYC	OC-C1C-C2C	-3.34	123.52	126.17
82	TQ	201	PEB	C3D-C4D-ND	3.34	113.81	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KK	203	PEB	C3B-C4B-NB	3.34	114.91	110.05
85	CL	502	BCR	C11-C10-C9	-3.34	122.54	127.31
82	WP	202	PEB	CHA-C1B-NB	-3.34	117.95	124.93
82	gH	202	PEB	CAA-C3A-C2A	-3.34	105.91	114.26
82	AF	202	PEB	OD-C4D-ND	-3.34	120.98	125.93
82	T7	201	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
84	LH	1001	CYC	C1A-C2A-C3A	-3.34	103.09	106.78
82	D5	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	X7	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
87	6N	608	CLA	C4-C3-C2	-3.34	112.99	122.65
82	UB	301	PEB	C2A-C1A-NA	3.34	111.15	108.27
82	gO	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
82	HK	202	PEB	OA-C1A-C2A	-3.34	123.52	126.17
82	RD	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	fO	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	GK	203	PEB	CMB-C2B-C1B	3.34	130.21	125.06
82	a4	202	PEB	CMB-C2B-C1B	3.34	130.21	125.06
82	dK	202	PEB	CHC-C4C-NC	-3.34	116.63	121.15
82	AQ	303	PEB	C3D-C4D-ND	3.34	113.81	107.26
82	PE	201	PEB	CHA-C1B-NB	-3.34	117.95	124.93
82	hJ	203	PEB	C2A-C1A-NA	3.34	111.15	108.27
87	B2	817	CLA	C4-C3-C5	3.34	120.89	115.27
82	VK	202	PEB	CAC-CBC-CGC	-3.34	106.42	113.60
87	AN	834	CLA	O2D-CGD-CBD	3.34	117.20	111.27
82	CF	201	PEB	CHA-C1B-NB	-3.34	117.95	124.93
82	RM	202	PEB	CHC-C4C-NC	3.34	125.67	121.15
82	KI	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	Y5	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	G7	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	bH	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
82	SM	203	PEB	CHC-C1D-ND	-3.34	109.50	113.72
82	R4	202	PEB	OD-C4D-ND	-3.34	120.98	125.93
82	LJ	202	PEB	CAC-C2C-C1C	3.34	131.08	125.76
82	KF	203	PEB	C3B-C4B-NB	3.34	114.90	110.05
82	XJ	202	PEB	C3B-C4B-NB	3.34	114.90	110.05
82	LA	202	PEB	CHA-C4A-NA	3.34	129.17	125.20
82	L7	202	PEB	CHA-C4A-NA	3.34	129.17	125.20
82	XB	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
82	eJ	201	PEB	OD-C4D-ND	-3.34	120.99	125.93
82	LK	202	PEB	CBC-CAC-C2C	3.34	121.90	112.63
87	B2	809	CLA	CHB-C4A-NA	3.34	129.13	124.51
84	M3	1001	CYC	CAA-C2A-C1A	3.34	130.91	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	tK	201	PEB	OD-C4D-ND	-3.34	120.99	125.93
82	EQ	202	PEB	CAC-CBC-CGC	-3.34	106.42	113.60
82	gO	201	PEB	CMB-C2B-C1B	3.34	130.20	125.06
83	xK	306	PUB	C1C-C2C-C3C	-3.34	103.09	106.78
85	a6	605	BCR	C3-C4-C5	-3.34	108.12	114.08
82	QM	202	PEB	C2A-C1A-NA	3.34	111.15	108.27
82	OP	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
82	NQ	204	PEB	C1D-CHC-C4C	3.34	118.17	113.26
82	GJ	203	PEB	OD-C4D-ND	-3.34	120.99	125.93
82	QO	201	PEB	CHA-C1B-NB	-3.34	117.95	124.93
82	YK	203	PEB	CHA-C4A-NA	3.34	129.17	125.20
82	fF	202	PEB	C1C-C2C-C3C	-3.34	103.68	107.62
82	DE	1002	PEB	C3B-C4B-NB	3.34	114.90	110.05
82	U5	202	PEB	CAB-C3B-C4B	3.34	130.91	125.01
82	sK	203	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
82	UB	303	PEB	OA-C1A-C2A	-3.34	123.52	126.17
82	fM	203	PEB	OA-C1A-C2A	-3.34	123.52	126.17
82	q8	202	PEB	CHA-C1B-NB	-3.34	117.96	124.93
84	J4	1001	CYC	OB-C4B-C3B	-3.34	124.42	128.04
82	QA	201	PEB	C3C-C4C-NC	3.34	111.33	108.33
82	MP	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
82	PD	203	PEB	C3B-C4B-NB	3.33	114.90	110.05
82	N9	202	PEB	CHB-C4B-C3B	3.33	133.03	125.32
85	BL	616	BCR	C11-C10-C9	-3.33	122.55	127.31
82	ZH	203	PEB	OD-C4D-ND	-3.33	120.99	125.93
82	IM	203	PEB	OD-C4D-ND	-3.33	120.99	125.93
82	dE	204	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
82	kF	201	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
82	yF	301	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
82	kJ	202	PEB	C1C-CHB-C4B	-3.33	120.80	128.28
95	C6	504	DGD	O1G-C1A-C2A	3.33	122.37	111.91
82	WJ	201	PEB	OA-C1A-C2A	-3.33	123.52	126.17
82	AO	301	PEB	OA-C1A-C2A	-3.33	123.52	126.17
84	L4	1001	CYC	C2A-C1A-NA	3.33	114.90	110.05
82	LE	1002	PEB	CAC-C2C-C1C	3.33	131.07	125.76
82	c4	201	PEB	CMB-C2B-C1B	3.33	130.20	125.06
82	AH	302	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
82	J5	202	PEB	C1C-CHB-C4B	3.33	135.76	128.28
82	HO	1002	PEB	C3B-C4B-NB	3.33	114.90	110.05
82	L1	1002	PEB	OD-C4D-C3D	-3.33	121.91	129.46
82	KP	202	PEB	OD-C4D-ND	-3.33	120.99	125.93
82	B7	203	PEB	OD-C4D-ND	-3.33	120.99	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RJ	202	PEB	C1C-CHB-C4B	-3.33	120.81	128.28
84	x3	1001	CYC	CHB-C1B-C2B	-3.33	120.34	126.95
82	oK	202	PEB	CHC-C4C-NC	3.33	125.66	121.15
87	62	309	CLA	C4-C3-C2	-3.33	113.01	122.65
82	WM	202	PEB	CHA-C1B-NB	-3.33	117.96	124.93
84	B3	1001	CYC	OC-C1C-C2C	-3.33	123.52	126.17
82	RG	202	PEB	CAC-CBC-CGC	-3.33	106.43	113.60
82	H1	1002	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
82	QM	204	PEB	C2A-C1A-NA	3.33	111.15	108.27
84	N1	1001	CYC	C2C-C1C-NC	3.33	111.15	108.27
82	MB	201	PEB	CHC-C1D-ND	-3.33	109.51	113.72
82	qF	203	PEB	C3D-C4D-ND	3.33	113.80	107.26
82	NI	201	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
82	V7	202	PEB	CHA-C1B-NB	-3.33	117.96	124.93
82	DF	203	PEB	OD-C4D-ND	-3.33	120.99	125.93
84	y3	1001	CYC	C4D-CHA-C1A	3.33	135.75	128.28
82	LA	202	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
82	KF	201	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
82	lF	203	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
84	J1	1001	CYC	C1B-NB-C4B	-3.33	106.43	110.67
82	SE	201	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	CJ	201	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	X7	201	PEB	CAC-CBC-CGC	-3.33	106.43	113.60
82	U5	201	PEB	C3B-C4B-NB	3.33	114.89	110.05
82	EA	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
82	QF	201	PEB	C1D-CHC-C4C	-3.33	108.34	113.26
82	FI	201	PEB	C2C-C1C-NC	3.33	112.06	107.57
82	dQ	401	PEB	CHC-C4C-NC	3.33	125.66	121.15
82	ZF	201	PEB	C3B-C4B-NB	3.33	114.89	110.05
82	f4	202	PEB	CMB-C2B-C1B	3.33	130.19	125.06
84	N4	1001	CYC	CMA-C3A-C4A	3.33	130.19	125.06
82	LK	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	HP	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	hO	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	K9	202	PEB	CHB-C4B-C3B	3.33	133.02	125.32
82	PJ	202	PEB	OA-C1A-C2A	-3.33	123.53	126.17
82	AQ	301	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	U1	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	xF	303	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
84	HG	1001	CYC	C1D-C2D-C3D	-3.33	103.55	107.79
87	CL	506	CLA	CHB-C4A-NA	3.33	129.12	124.51
87	AN	806	CLA	CHB-C4A-NA	3.33	129.12	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PG	201	PEB	CHA-C1B-NB	-3.33	117.97	124.93
85	C6	508	BCR	C19-C18-C17	-3.33	113.83	118.94
82	DJ	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
82	HM	201	PEB	CMB-C2B-C1B	3.33	130.19	125.06
82	E7	201	PEB	C1D-CHC-C4C	-3.33	108.35	113.26
82	QH	201	PEB	C1C-CHB-C4B	3.33	135.75	128.28
82	gJ	202	PEB	CHB-C4B-NB	-3.33	117.65	124.58
82	IM	203	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
82	IB	202	PEB	CHC-C1D-ND	-3.33	109.51	113.72
82	YK	203	PEB	CHC-C1D-ND	-3.33	109.51	113.72
95	AL	414	DGD	C3G-O3G-C1D	-3.33	107.23	113.74
82	LM	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	mH	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
87	A2	830	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
82	PQ	201	PEB	C3D-C4D-ND	3.33	113.79	107.26
82	S4	202	PEB	OA-C1A-C2A	-3.33	123.53	126.17
82	SB	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
84	C1	1001	CYC	CHD-C4C-NC	3.33	129.16	125.20
85	CL	502	BCR	C36-C18-C19	-3.33	112.83	118.08
82	YK	203	PEB	C3D-C4D-ND	3.33	113.79	107.26
82	AD	301	PEB	C3B-C4B-NB	3.33	114.89	110.05
82	PI	201	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
82	BF	201	PEB	C1D-CHC-C4C	3.33	118.16	113.26
82	UJ	203	PEB	CAC-C2C-C1C	3.33	131.06	125.76
82	F5	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
82	Q9	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
82	g1	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	gG	201	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	UB	302	PEB	CMC-C3C-C2C	3.33	132.81	125.61
82	m4	201	PEB	C3B-C4B-NB	3.33	114.89	110.05
82	aK	201	PEB	OA-C1A-C2A	-3.33	123.53	126.17
82	ND	203	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	lK	202	PEB	C1C-CHB-C4B	3.33	135.75	128.28
84	GG	1001	CYC	C4D-CHA-C1A	3.33	135.75	128.28
82	dG	202	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
84	D3	1001	CYC	CAA-C2A-C1A	3.33	130.90	125.01
82	SO	201	PEB	C4B-NB-C1B	-3.33	100.24	106.51
82	TQ	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
84	EE	1001	CYC	C1A-C2A-C3A	-3.33	103.10	106.78
82	SA	202	PEB	C3B-C4B-NB	3.33	114.89	110.05
84	I1	1001	CYC	C2A-C1A-NA	3.33	114.89	110.05
87	2N	305	CLA	CAA-C2A-C3A	-3.33	105.95	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UH	203	PEB	C3D-C4D-ND	3.33	113.79	107.26
82	V7	203	PEB	CAB-C3B-C4B	3.33	130.90	125.01
85	C6	508	BCR	C33-C5-C6	-3.33	120.79	124.53
82	j4	201	PEB	C1C-CHB-C4B	3.33	135.74	128.28
82	f4	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
85	J2	102	BCR	C38-C26-C27	3.33	120.01	113.62
82	aE	202	PEB	CHA-C1B-NB	-3.33	117.97	124.93
82	OP	203	PEB	CMB-C2B-C1B	3.33	130.19	125.06
82	KK	202	PEB	CHB-C1C-C2C	-3.33	119.64	127.15
82	LK	202	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	VI	201	PEB	C1D-CHC-C4C	-3.33	108.35	113.26
82	DA	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
84	DO	1001	CYC	C1D-C2D-C3D	-3.33	103.55	107.79
82	s8	201	PEB	CAB-CBB-CGB	-3.33	106.44	113.60
84	JH	1001	CYC	CAD-CBD-CGD	-3.33	106.44	113.60
84	V3	1001	CYC	CHB-C1B-C2B	-3.33	120.36	126.95
82	HI	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	GP	202	PEB	CHA-C1B-NB	-3.33	117.98	124.93
82	LK	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	fG	203	PEB	C2A-C1A-NA	3.33	111.14	108.27
82	JF	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
84	NO	1001	CYC	C1A-C2A-C3A	-3.33	103.10	106.78
82	cH	202	PEB	CHC-C1D-ND	-3.33	109.52	113.72
82	A9	201	PEB	OA-C1A-C2A	-3.33	123.53	126.17
82	Z5	304	PEB	C3B-C4B-NB	3.33	114.89	110.05
82	h4	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
82	X7	202	PEB	C3C-C4C-NC	3.33	111.33	108.33
82	I9	202	PEB	CHB-C4B-C3B	3.32	133.01	125.32
82	PQ	201	PEB	CHB-C1C-C2C	-3.32	119.65	127.15
82	D7	203	PEB	C4B-C3B-C2B	-3.32	103.10	106.78
82	RO	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	eA	301	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	jO	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	cO	202	PEB	OD-C4D-C3D	-3.32	121.93	129.46
82	bG	201	PEB	C3B-C4B-NB	3.32	114.89	110.05
82	XI	201	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
82	YJ	202	PEB	C3B-C4B-NB	3.32	114.88	110.05
82	eJ	201	PEB	C3B-C4B-NB	3.32	114.88	110.05
82	BK	202	PEB	OD-C4D-ND	-3.32	121.01	125.93
82	TO	203	PEB	C4B-C3B-C2B	-3.32	103.10	106.78
82	S1	202	PEB	C4B-C3B-C2B	-3.32	103.10	106.78
82	L9	203	PEB	C4B-C3B-C2B	-3.32	103.10	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SF	203	PEB	C3D-C4D-ND	3.32	113.78	107.26
82	lM	201	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	VI	201	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
82	A7	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
83	M5	303	PUB	CMA-C2A-C1A	3.32	129.21	121.39
87	BN	826	CLA	C3B-C4B-NB	-3.32	107.43	110.52
82	eO	201	PEB	C3B-C4B-NB	3.32	114.88	110.05
84	d3	1001	CYC	CAA-C2A-C1A	3.32	130.89	125.01
82	WA	202	PEB	C3D-C4D-ND	3.32	113.78	107.26
82	V1	203	PEB	CHC-C1D-ND	-3.32	109.52	113.72
82	L9	203	PEB	CMB-C2B-C1B	3.32	130.18	125.06
82	D5	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
84	D1	1003	CYC	C1A-C2A-C3A	-3.32	103.11	106.78
82	EF	202	PEB	CHC-C4C-NC	3.32	125.65	121.15
82	KJ	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
82	r8	201	PEB	C3B-C4B-NB	3.32	114.88	110.05
82	oF	202	PEB	CHA-C1B-NB	-3.32	117.98	124.93
84	u3	1001	CYC	CAA-C2A-C1A	3.32	130.89	125.01
82	KI	202	PEB	C1D-CHC-C4C	-3.32	108.36	113.26
85	bL	602	BCR	C21-C20-C19	3.32	133.58	123.22
82	OE	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
82	RI	201	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
82	h4	201	PEB	OA-C1A-C2A	-3.32	123.53	126.17
82	yC	202	PEB	OA-C1A-C2A	-3.32	123.53	126.17
85	CL	501	BCR	C20-C21-C22	-3.32	122.57	127.31
82	DA	201	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	OA	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	QD	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
82	AH	305	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
87	2N	311	CLA	CHB-C4A-NA	3.32	129.10	124.51
82	WG	203	PEB	CHC-C1D-ND	-3.32	109.52	113.72
84	F1	1001	CYC	CHA-C4D-C3D	-3.32	119.66	127.15
82	CI	201	PEB	C1D-CHC-C4C	-3.32	108.36	113.26
84	F3	1001	CYC	CAA-C2A-C1A	3.32	130.88	125.01
82	DB	203	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
82	UB	301	PEB	CHA-C1B-NB	-3.32	117.99	124.93
85	BN	840	BCR	C29-C30-C25	3.32	115.59	110.48
82	jM	201	PEB	C2A-C1A-NA	3.32	111.14	108.27
82	QE	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
85	KL	100	BCR	C15-C14-C13	-3.32	122.57	127.31
84	DH	1003	CYC	C2A-C1A-NA	3.32	114.88	110.05
84	U3	1001	CYC	CAA-C2A-C1A	3.32	130.88	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	V9	202	PEB	CHB-C4B-C3B	3.32	133.00	125.32
84	S3	1001	CYC	CAA-C2A-C1A	3.32	130.88	125.01
82	QE	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
82	NQ	203	PEB	OD-C4D-ND	-3.32	121.01	125.93
82	jF	202	PEB	OD-C4D-ND	-3.32	121.01	125.93
82	WJ	203	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
84	JH	1001	CYC	C4A-C3A-C2A	-3.32	102.70	106.51
82	d1	203	PEB	CHA-C1B-C2B	3.32	133.44	124.90
87	BN	819	CLA	C3B-C4B-NB	-3.32	107.44	110.52
82	BF	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
82	gH	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
84	73	1001	CYC	CAA-C2A-C1A	3.32	130.88	125.01
82	FD	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
82	IM	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
82	lH	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
94	D6	408	PL9	C7-C8-C9	-3.32	121.27	126.79
82	QH	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
82	oF	202	PEB	C3D-C4D-ND	3.32	113.77	107.26
82	S1	201	PEB	OA-C1A-C2A	-3.32	123.53	126.17
82	Y5	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
82	XI	201	PEB	C1D-CHC-C4C	-3.32	108.36	113.26
82	LG	1002	PEB	CAC-C2C-C1C	3.32	131.05	125.76
82	g1	202	PEB	CAA-C3A-C2A	-3.32	105.97	114.26
84	h3	1001	CYC	CAA-C2A-C1A	3.32	130.88	125.01
82	vF	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
82	WM	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
82	O5	202	PEB	C3C-C4C-NC	3.32	111.32	108.33
84	BE	1001	CYC	C2B-C1B-NB	3.32	111.84	106.99
84	JH	1003	CYC	CHD-C1D-ND	-3.32	117.72	125.32
82	U1	203	PEB	CHA-C1B-NB	-3.32	117.99	124.93
87	62	311	CLA	CHB-C4A-NA	3.32	129.10	124.51
87	F2	205	CLA	CHB-C4A-NA	3.32	129.10	124.51
82	SE	202	PEB	OD-C4D-ND	-3.32	121.02	125.93
82	JJ	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
82	OQ	201	PEB	C1D-CHC-C4C	-3.32	108.36	113.26
87	c6	606	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
82	VM	201	PEB	CMC-C3C-C4C	3.32	130.58	127.06
82	hJ	202	PEB	OA-C1A-C2A	-3.32	123.54	126.17
82	JP	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
82	VP	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
82	fF	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
82	GK	203	PEB	C3D-C4D-ND	3.32	113.77	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	GG	1001	CYC	CHA-C4D-C3D	-3.32	119.67	127.15
82	FQ	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
82	QK	201	PEB	C1D-CHC-C4C	-3.32	108.37	113.26
84	I3	1001	CYC	CAA-C2A-C1A	3.32	130.88	125.01
82	QQ	201	PEB	C3B-C4B-NB	3.32	114.87	110.05
82	P9	202	PEB	CHB-C4B-C3B	3.32	132.99	125.32
82	RI	201	PEB	C1D-CHC-C4C	-3.32	108.37	113.26
82	HH	1002	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
82	HI	203	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
82	A4	305	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
82	lG	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
85	B2	840	BCR	C29-C30-C25	3.32	115.58	110.48
82	VP	202	PEB	CHC-C4C-NC	3.32	125.64	121.15
82	b4	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
82	hH	201	PEB	C2A-C1A-NA	3.32	111.13	108.27
82	S9	201	PEB	OA-C1A-C2A	-3.32	123.54	126.17
82	vK	202	PEB	OA-C1A-C2A	-3.32	123.54	126.17
82	ZB	202	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	V7	203	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	hE	203	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	qF	202	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	T9	202	PEB	CHB-C4B-C3B	3.31	132.99	125.32
82	YD	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
83	Z5	303	PUB	CMA-C2A-C1A	3.31	129.19	121.39
82	IF	203	PEB	CMC-C3C-C4C	3.31	130.57	127.06
84	IE	1001	CYC	C1B-C2B-C3B	-3.31	104.41	107.87
82	i1	201	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
82	gO	202	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
82	dG	201	PEB	C4B-C3B-C2B	-3.31	103.11	106.78
87	AL	404	CLA	C3B-C4B-NB	-3.31	107.44	110.52
82	QD	201	PEB	CHC-C4C-NC	3.31	125.64	121.15
82	UO	201	PEB	OD-C4D-C3D	-3.31	121.95	129.46
82	UK	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	c4	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	E9	202	PEB	CHB-C4B-C3B	3.31	132.98	125.32
82	YP	502	PEB	OA-C1A-C2A	-3.31	123.54	126.17
82	S9	202	PEB	OA-C1A-C2A	-3.31	123.54	126.17
82	AP	203	PEB	C3D-C4D-ND	3.31	113.76	107.26
82	oK	202	PEB	CHA-C1B-NB	-3.31	118.00	124.93
82	AM	301	PEB	C4B-C3B-C2B	-3.31	103.11	106.78
82	PD	201	PEB	CHB-C1C-C2C	-3.31	119.67	127.15
84	FH	1001	CYC	CHA-C4D-C3D	-3.31	119.67	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IJ	202	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	YJ	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	d1	201	PEB	C1C-CHB-C4B	3.31	135.71	128.28
82	d4	201	PEB	CMB-C2B-C1B	3.31	130.17	125.06
87	32	303	CLA	C2A-C1A-CHA	3.31	129.65	123.86
84	D4	1001	CYC	C1D-C2D-C3D	-3.31	103.57	107.79
82	PP	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	D7	201	PEB	C2A-C1A-NA	3.31	111.13	108.27
84	C1	1001	CYC	C4A-C3A-C2A	-3.31	102.70	106.51
82	ZB	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
83	wF	304	PUB	C1C-C2C-C3C	-3.31	103.12	106.78
82	RA	203	PEB	CAC-CBC-CGC	-3.31	106.47	113.60
82	MD	201	PEB	CAB-CBB-CGB	-3.31	106.47	113.60
82	R7	203	PEB	CAC-CBC-CGC	-3.31	106.47	113.60
84	M1	201	CYC	C1B-NB-C4B	-3.31	106.45	110.67
82	QI	201	PEB	CHC-C1D-ND	-3.31	109.53	113.72
82	dH	201	PEB	C1C-CHB-C4B	3.31	135.71	128.28
84	73	1002	CYC	CMB-C2B-C1B	3.31	128.30	124.17
87	32	310	CLA	C2A-C1A-CHA	3.31	129.64	123.85
82	sC	201	PEB	CAB-CBB-CGB	-3.31	106.47	113.60
82	BF	202	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	AQ	301	PEB	C3B-C4B-NB	3.31	114.87	110.05
82	IM	201	PEB	CHC-C1D-ND	-3.31	109.53	113.72
82	Y5	201	PEB	CHA-C1B-NB	-3.31	118.00	124.93
82	FQ	202	PEB	CMC-C3C-C4C	3.31	130.57	127.06
82	N7	203	PEB	CHB-C4B-C3B	-3.31	117.66	125.32
82	NA	203	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	pC	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
88	c6	619	LHG	O8-C23-C24	3.31	120.06	111.38
82	ZF	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	hF	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
82	WQ	201	PEB	C1D-CHC-C4C	-3.31	108.37	113.26
82	A1	305	PEB	CHB-C1C-NC	-3.31	117.73	125.32
82	HD	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
82	WK	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
82	DK	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
87	22	611	CLA	CHB-C4A-NA	3.31	129.09	124.51
87	6N	610	CLA	CHB-C4A-NA	3.31	129.09	124.51
82	RH	202	PEB	OD-C4D-C3D	-3.31	121.96	129.46
84	j3	1001	CYC	CAA-C2A-C1A	3.31	130.87	125.01
82	z8	202	PEB	CHC-C1D-ND	-3.31	109.53	113.72
82	O5	203	PEB	CMB-C2B-C1B	3.31	130.16	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IB	203	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	pC	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	kJ	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	hM	203	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	HK	201	PEB	CMA-C2A-C1A	-3.31	105.27	112.40
85	C6	507	BCR	C38-C26-C25	-3.31	120.81	124.53
82	UK	202	PEB	OD-C4D-ND	-3.31	121.03	125.93
82	S9	203	PEB	OD-C4D-ND	-3.31	121.03	125.93
82	aK	202	PEB	OD-C4D-ND	-3.31	121.03	125.93
84	IE	1001	CYC	C2A-C1A-NA	3.31	114.86	110.05
84	B3	1001	CYC	CAA-C2A-C1A	3.31	130.87	125.01
82	GB	201	PEB	CHA-C1B-NB	-3.31	118.01	124.93
82	gF	203	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
82	bO	201	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
87	72	608	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
82	PI	201	PEB	C1D-CHC-C4C	-3.31	108.38	113.26
82	PD	202	PEB	CHA-C1B-C2B	3.31	133.41	124.90
84	O3	1001	CYC	CAA-C2A-C1A	3.31	130.87	125.01
82	ZH	203	PEB	C3B-C4B-NB	3.31	114.86	110.05
85	aL	604	BCR	C11-C10-C9	-3.31	122.59	127.31
82	gO	202	PEB	CMB-C2B-C1B	3.31	130.16	125.06
82	SA	202	PEB	C3D-C4D-ND	3.31	113.75	107.26
82	A9	202	PEB	CHB-C4B-C3B	3.31	132.97	125.32
82	AQ	301	PEB	CHC-C1D-ND	-3.31	109.54	113.72
83	QM	201	PUB	CHC-C1D-ND	-3.31	109.54	113.72
82	Q1	201	PEB	C1C-CHB-C4B	3.31	135.70	128.28
82	AM	301	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	C9	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	P9	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
82	wK	303	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
84	BE	1002	CYC	C4A-C3A-C2A	-3.31	102.71	106.51
82	m4	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	VA	202	PEB	OD-C4D-ND	-3.31	121.03	125.93
82	lE	203	PEB	OD-C4D-ND	-3.31	121.03	125.93
82	R9	202	PEB	CHB-C4B-C3B	3.31	132.97	125.32
82	HQ	203	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
84	D1	1001	CYC	CMA-C3A-C4A	3.31	130.16	125.06
82	CK	203	PEB	CHB-C1C-C2C	-3.31	119.69	127.15
84	DG	1001	CYC	CHA-C4D-C3D	-3.31	119.69	127.15
84	n3	1001	CYC	CAA-C2A-C1A	3.31	130.86	125.01
82	KI	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	b4	201	PEB	CAB-CBB-CGB	-3.31	106.48	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PQ	202	PEB	CHA-C1B-C2B	3.31	133.41	124.90
82	ZK	201	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	S7	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	UG	203	PEB	CHC-C4C-NC	3.31	125.63	121.15
84	L3	1001	CYC	CAA-C2A-C1A	3.31	130.86	125.01
82	AD	301	PEB	OA-C1A-C2A	-3.31	123.54	126.17
82	KM	201	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
82	lF	203	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
82	IK	203	PEB	CHA-C1B-NB	-3.31	118.01	124.93
82	WQ	201	PEB	CAC-C2C-C1C	3.31	131.03	125.76
82	QJ	204	PEB	OD-C4D-ND	-3.31	121.03	125.93
82	QM	203	PEB	OD-C4D-ND	-3.31	121.03	125.93
83	yK	303	PUB	OA-C1A-NA	-3.31	121.03	125.93
82	HQ	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
84	N4	1001	CYC	C1A-C2A-C3A	-3.31	103.12	106.78
82	O7	201	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	nK	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	TI	201	PEB	CMB-C2B-C1B	3.31	130.16	125.06
82	BB	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
82	HO	1002	PEB	C2A-C1A-NA	3.31	111.12	108.27
96	fL	102	HEM	CHB-C1B-NB	3.31	128.45	124.37
87	cL	515	CLA	CHD-C1D-ND	-3.31	121.42	124.45
82	dF	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
82	O4	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
85	b6	602	BCR	C34-C9-C10	-3.31	118.29	122.92
82	HD	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	GJ	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	OM	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	kE	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	L5	201	PEB	CHA-C1B-NB	-3.31	118.02	124.93
82	YO	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
82	EP	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	fE	202	PEB	CMB-C2B-C1B	3.31	130.16	125.06
82	TD	201	PEB	C3D-C4D-ND	3.31	113.75	107.26
82	HA	203	PEB	CHC-C4C-NC	3.31	125.62	121.15
82	HK	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
82	BI	201	PEB	C2C-C1C-NC	3.31	112.02	107.57
84	k3	1001	CYC	CAA-C2A-C1A	3.31	130.86	125.01
82	NM	201	PEB	C3B-C4B-NB	3.31	114.86	110.05
82	HA	203	PEB	OA-C1A-C2A	-3.31	123.55	126.17
82	TF	202	PEB	OA-C1A-C2A	-3.31	123.55	126.17
82	EK	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	W3	1001	CYC	C4D-CHA-C1A	3.31	135.69	128.28
84	JH	1003	CYC	C1B-NB-C4B	-3.30	106.46	110.67
82	MQ	201	PEB	CAB-CBB-CGB	-3.30	106.49	113.60
82	WE	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
82	YE	202	PEB	C4B-C3B-C2B	-3.30	103.12	106.78
82	MP	202	PEB	C4B-C3B-C2B	-3.30	103.12	106.78
82	dH	203	PEB	CHA-C1B-C2B	3.30	133.40	124.90
84	D1	1003	CYC	CMA-C3A-C4A	3.30	130.15	125.06
82	p8	202	PEB	CHB-C4B-C3B	3.30	132.96	125.32
85	BN	803	BCR	C33-C5-C4	3.30	119.96	113.62
82	MJ	203	PEB	CAC-C2C-C1C	3.30	131.03	125.76
84	o3	1001	CYC	CAA-C2A-C1A	3.30	130.85	125.01
83	M5	302	PUB	CBA-CAA-C3A	-3.30	107.97	112.98
82	QG	202	PEB	C1B-C2B-C3B	-3.30	102.71	106.51
87	b6	613	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
82	U9	201	PEB	O2B-CGB-CBB	3.30	124.64	114.03
82	WB	402	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	AD	304	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	LO	1002	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	aE	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	J5	201	PEB	C2A-C1A-NA	3.30	111.12	108.27
82	OO	201	PEB	C4B-NB-C1B	-3.30	100.29	106.51
82	Q7	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	tF	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	mO	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	ED	202	PEB	CMC-C3C-C4C	3.30	130.56	127.06
82	hM	201	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
87	CL	507	CLA	CMB-C2B-C1B	-3.30	120.34	125.37
82	dQ	401	PEB	CMB-C2B-C1B	3.30	130.15	125.06
92	bL	611	LMG	O7-C10-C11	3.30	118.62	111.50
82	LD	203	PEB	C3B-C4B-NB	3.30	114.85	110.05
82	J7	203	PEB	C3B-C4B-NB	3.30	114.85	110.05
82	IP	203	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	LM	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	ZM	201	PEB	C1C-CHB-C4B	-3.30	120.88	128.28
84	63	901	CYC	C1B-CHB-C4A	3.30	136.15	128.08
84	Q3	1001	CYC	CAA-C2A-C1A	3.30	130.85	125.01
82	RD	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
82	O1	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
82	fO	202	PEB	CMB-C2B-C1B	3.30	130.15	125.06
87	A6	404	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
82	N9	202	PEB	C2A-C1A-NA	3.30	111.12	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A2	846	BCR	C15-C16-C17	3.30	130.24	123.47
82	NM	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	yC	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	hK	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	LQ	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	RQ	203	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	qC	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	FD	202	PEB	CHC-C4C-NC	3.30	125.62	121.15
82	O5	202	PEB	C3B-C4B-NB	3.30	114.85	110.05
82	GK	201	PEB	C3C-C4C-NC	3.30	111.31	108.33
82	FA	203	PEB	CAC-CBC-CGC	-3.30	106.50	113.60
82	dJ	201	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
84	q3	1001	CYC	CAA-C2A-C1A	3.30	130.85	125.01
87	JN	101	CLA	CAA-C2A-C3A	-3.30	106.01	114.26
82	QA	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	WJ	203	PEB	CHA-C1B-NB	-3.30	118.03	124.93
82	AQ	304	PEB	CHA-C1B-NB	-3.30	118.03	124.93
82	A9	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
82	AD	304	PEB	CHC-C4C-NC	3.30	125.62	121.15
82	oF	202	PEB	CHC-C4C-NC	3.30	125.62	121.15
82	KF	202	PEB	CMA-C2A-C1A	-3.30	105.29	112.40
84	N4	1001	CYC	C2A-C1A-NA	3.30	114.85	110.05
82	mG	203	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	OP	203	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	Z5	305	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	tC	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	SO	202	PEB	CMB-C2B-C1B	3.30	130.15	125.06
82	EI	201	PEB	C1D-CHC-C4C	-3.30	108.39	113.26
82	II	201	PEB	C1D-CHC-C4C	-3.30	108.39	113.26
82	NI	201	PEB	C1D-CHC-C4C	-3.30	108.39	113.26
82	FQ	203	PEB	C3C-C4C-NC	3.30	111.30	108.33
84	CH	1001	CYC	CMB-C2B-C1B	3.30	128.29	124.17
82	G9	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
82	T9	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
84	K1	1001	CYC	C2C-C1C-NC	3.30	111.12	108.27
82	KJ	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	SJ	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	RA	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
82	UM	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	y8	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	DI	201	PEB	CBC-CAC-C2C	-3.30	103.46	112.63
82	YH	201	PEB	CHA-C1B-NB	-3.30	118.03	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	310	CLA	C2A-C1A-CHA	3.30	129.61	123.85
82	LI	201	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
82	Q1	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
82	S4	201	PEB	C4B-NB-C1B	-3.30	100.29	106.51
82	HF	201	PEB	CMA-C2A-C1A	-3.30	105.29	112.40
82	O4	201	PEB	CHA-C1B-NB	-3.30	118.03	124.93
82	AD	303	PEB	CMB-C2B-C1B	3.30	130.15	125.06
96	E6	101	HEM	CBD-CAD-C3D	-3.30	103.46	112.63
82	KK	202	PEB	CMA-C2A-C1A	-3.30	105.29	112.40
84	CG	1001	CYC	C1B-C2B-C3B	-3.30	104.43	107.87
82	wF	302	PEB	CHC-C1D-ND	-3.30	109.55	113.72
82	NG	201	PEB	CAC-CBC-CGC	-3.30	106.50	113.60
94	D6	408	PL9	C27-C28-C29	-3.30	119.72	127.66
82	lJ	201	PEB	C3B-C4B-NB	3.30	114.85	110.05
82	OI	203	PEB	C2A-C1A-NA	3.30	111.12	108.27
82	KP	201	PEB	OD-C4D-C3D	-3.30	121.98	129.46
82	C9	202	PEB	CHB-C4B-C3B	3.30	132.95	125.32
82	sC	203	PEB	OD-C4D-ND	-3.30	121.04	125.93
82	b1	203	PEB	CMB-C2B-C1B	3.30	130.14	125.06
82	LH	1003	PEB	OD-C4D-C3D	-3.30	121.99	129.46
82	HF	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	tC	201	PEB	C2C-C1C-NC	3.30	112.01	107.57
82	TO	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
84	BG	1001	CYC	C2B-C1B-NB	3.30	111.82	106.99
82	J5	203	PEB	CAC-CBC-CGC	-3.30	106.51	113.60
82	aJ	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
82	OG	201	PEB	CHA-C1B-NB	-3.30	118.03	124.93
82	RQ	202	PEB	CHC-C4C-NC	3.30	125.61	121.15
82	JI	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	LF	202	PEB	OD-C4D-ND	-3.30	121.05	125.93
82	xK	304	PEB	OD-C4D-ND	-3.30	121.05	125.93
82	lJ	203	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
84	CH	1001	CYC	CHD-C4C-NC	3.30	129.12	125.20
82	HM	201	PEB	OD-C4D-ND	-3.30	121.05	125.93
82	t8	201	PEB	OD-C4D-ND	-3.30	121.05	125.93
85	FL	101	BCR	C11-C10-C9	-3.30	122.61	127.31
82	i4	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
82	hM	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
84	f3	1001	CYC	CAA-C2A-C1A	3.30	130.84	125.01
87	3N	304	CLA	C2A-C1A-CHA	3.30	129.62	123.86
82	U9	203	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
82	HE	1002	PEB	C3B-C4B-NB	3.30	114.84	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	s8	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
82	dE	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
82	JF	201	PEB	CHC-C1D-ND	-3.30	109.55	113.72
82	W5	203	PEB	CHC-C1D-ND	-3.30	109.55	113.72
82	KP	201	PEB	CHA-C1B-NB	-3.30	118.04	124.93
85	JN	102	BCR	C38-C26-C27	3.30	119.95	113.62
82	eJ	201	PEB	C1C-CHB-C4B	-3.30	120.89	128.28
82	k1	202	PEB	C1C-CHB-C4B	3.30	135.67	128.28
82	QK	201	PEB	OD-C4D-ND	-3.30	121.05	125.93
85	fL	101	BCR	C16-C17-C18	-3.30	122.61	127.31
87	c6	610	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
85	c6	602	BCR	C38-C26-C25	-3.30	120.83	124.53
82	QP	202	PEB	C4B-C3B-C2B	-3.30	103.14	106.78
82	dK	201	PEB	C4B-C3B-C2B	-3.30	103.14	106.78
82	bO	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
84	H3	1001	CYC	CAA-C2A-C1A	3.30	130.84	125.01
82	UE	203	PEB	CHC-C4C-NC	3.30	125.61	121.15
82	eF	201	PEB	CHA-C1B-NB	-3.30	118.04	124.93
82	J5	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
82	OJ	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
82	HD	203	PEB	CMB-C2B-C1B	3.29	130.14	125.06
82	W5	201	PEB	CMB-C2B-C1B	3.29	130.14	125.06
82	P1	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
83	xF	306	PUB	C1C-C2C-C3C	-3.29	103.14	106.78
82	XK	203	PEB	OD-C4D-ND	-3.29	121.05	125.93
82	KM	202	PEB	C1B-C2B-C3B	-3.29	102.72	106.51
82	hJ	202	PEB	C1B-C2B-C3B	-3.29	102.72	106.51
82	X9	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	jJ	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	eK	201	PEB	C1C-CHB-C4B	3.29	135.67	128.28
82	eG	201	PEB	CHA-C1B-NB	-3.29	118.04	124.93
82	S4	202	PEB	CMB-C2B-C1B	3.29	130.14	125.06
82	cB	403	PEB	OD-C4D-ND	-3.29	121.05	125.93
87	FN	205	CLA	CHB-C4A-NA	3.29	129.07	124.51
94	d6	408	PL9	C15-C14-C16	3.29	120.81	115.27
82	XA	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
87	2N	301	CLA	C3B-C4B-NB	-3.29	108.02	110.23
82	X9	202	PEB	CHB-C4B-C3B	3.29	132.94	125.32
82	SG	201	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	ND	202	PEB	CHC-C4C-NC	3.29	125.61	121.15
82	Q5	202	PEB	CHC-C4C-NC	3.29	125.61	121.15
82	j4	203	PEB	CAB-C3B-C4B	3.29	130.84	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	D5	202	PEB	C1C-CHB-C4B	3.29	135.67	128.28
82	gJ	201	PEB	CHC-C1D-ND	3.29	117.89	113.72
82	NB	203	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	18	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	SG	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
82	LQ	203	PEB	C3B-C4B-NB	3.29	114.84	110.05
82	YQ	202	PEB	C3B-C4B-NB	3.29	114.84	110.05
82	OM	202	PEB	OD-C4D-ND	-3.29	121.05	125.93
82	DJ	201	PEB	CHB-C1C-NC	-3.29	117.78	125.32
82	z8	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
82	F5	201	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	p8	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	EP	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	BA	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	iH	201	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
87	BN	824	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
84	D1	1003	CYC	C2A-C1A-NA	3.29	114.84	110.05
82	M7	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	oK	202	PEB	C3D-C4D-ND	3.29	113.72	107.26
82	VB	202	PEB	CHC-C4C-NC	3.29	125.60	121.15
82	OA	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
84	FH	1001	CYC	C4D-C3D-C2D	-3.29	103.73	107.62
82	HB	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
82	MD	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
82	dO	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
82	XA	202	PEB	OD-C4D-C3D	-3.29	122.00	129.46
82	zC	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
82	SO	201	PEB	CHC-C4C-NC	3.29	125.60	121.15
82	YO	201	PEB	C3B-C4B-NB	3.29	114.83	110.05
82	ZB	203	PEB	OA-C1A-C2A	-3.29	123.56	126.17
84	63	901	CYC	C1B-NB-C4B	-3.29	106.48	110.67
82	OD	201	PEB	C1D-CHC-C4C	-3.29	108.41	113.26
82	mJ	202	PEB	C1D-CHC-C4C	-3.29	108.41	113.26
82	FK	202	PEB	CAB-C3B-C4B	3.29	130.83	125.01
82	XA	203	PEB	CMB-C2B-C1B	3.29	130.13	125.06
82	HQ	203	PEB	CMB-C2B-C1B	3.29	130.13	125.06
87	12	601	CLA	CHB-C4A-NA	3.29	129.06	124.51
82	f1	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
82	aG	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
82	IP	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	A1	302	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	eE	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	wK	302	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	AA	201	PEB	C3D-C4D-ND	3.29	113.71	107.26
82	AF	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
82	VB	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	LD	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
85	B2	838	BCR	C10-C11-C12	3.29	133.48	123.22
84	J4	1001	CYC	CHD-C1D-ND	-3.29	117.78	125.32
82	S5	201	PEB	C1C-C2C-C3C	-3.29	103.73	107.62
82	R1	202	PEB	OD-C4D-C3D	-3.29	122.01	129.46
87	B2	823	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
82	FF	202	PEB	CAB-C3B-C4B	3.29	130.83	125.01
84	w3	1001	CYC	CAA-C2A-C1A	3.29	130.83	125.01
82	PF	202	PEB	CHB-C4B-C3B	-3.29	117.71	125.32
82	WK	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
85	fL	101	BCR	C19-C18-C17	-3.29	113.89	118.94
87	CL	510	CLA	CHB-C1B-NB	3.29	127.74	124.26
87	A2	837	CLA	C1-O2A-CGA	3.29	125.07	116.44
82	LJ	202	PEB	CAB-C3B-C4B	3.29	130.83	125.01
82	kK	203	PEB	CHB-C1C-C2C	-3.29	119.73	127.15
82	nF	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	jH	203	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	h4	201	PEB	C1C-CHB-C4B	3.29	135.66	128.28
82	DF	203	PEB	OA-C1A-C2A	-3.29	123.56	126.17
82	FQ	201	PEB	OA-C1A-C2A	-3.29	123.56	126.17
82	aG	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	WG	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	hE	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	CB	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
82	U5	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
84	J4	1001	CYC	C1D-C2D-C3D	-3.29	103.60	107.79
82	QM	203	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	Z9	303	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	jO	201	PEB	C1C-CHB-C4B	3.29	135.65	128.28
84	NH	1001	CYC	CAD-CBD-CGD	-3.29	106.53	113.60
82	BI	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
82	RO	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
83	yF	303	PUB	OA-C1A-NA	-3.29	121.06	125.93
82	PO	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
82	eK	201	PEB	CHA-C1B-NB	-3.29	118.06	124.93
82	SJ	201	PEB	CMB-C2B-C1B	3.29	130.12	125.06
82	XF	202	PEB	OA-C1A-C2A	-3.29	123.56	126.17
82	RD	202	PEB	C3D-C4D-ND	3.29	113.71	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	DE	1001	CYC	CHA-C4D-C3D	-3.29	119.74	127.15
85	bL	603	BCR	C15-C14-C13	-3.29	122.62	127.31
82	FD	203	PEB	C1C-NC-C4C	-3.29	103.75	109.60
84	C1	1001	CYC	CMB-C2B-C1B	3.29	128.27	124.17
82	FD	203	PEB	C3C-C4C-NC	3.29	111.29	108.33
82	c4	203	PEB	C3B-C4B-NB	3.29	114.83	110.05
82	hG	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
82	NA	203	PEB	CHB-C4B-C3B	-3.29	117.72	125.32
82	iF	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
82	bE	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
82	N7	203	PEB	C2A-C1A-NA	3.29	111.11	108.27
82	JD	201	PEB	C1B-C2B-C3B	-3.29	102.74	106.51
82	LD	203	PEB	C1B-C2B-C3B	-3.29	102.74	106.51
82	F9	202	PEB	C1B-C2B-C3B	-3.29	102.74	106.51
94	a6	601	PL9	C10-C9-C11	3.28	120.80	115.27
82	bH	202	PEB	CHB-C1C-NC	-3.28	117.80	125.32
82	M5	305	PEB	OD-C4D-ND	-3.28	121.06	125.93
92	bL	623	LMG	O1-C1-C2	3.28	113.43	108.30
82	CK	201	PEB	CHA-C1B-NB	-3.28	118.06	124.93
87	AN	830	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
82	VQ	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	cO	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	BI	202	PEB	C1C-NC-C4C	-3.28	103.75	109.60
82	GP	203	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
82	S9	203	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
82	hE	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
82	bH	202	PEB	CHB-C4B-NB	-3.28	117.74	124.58
87	A2	824	CLA	CHB-C4A-NA	3.28	129.05	124.51
82	YK	201	PEB	CMB-C2B-C1B	3.28	130.12	125.06
82	OP	202	PEB	OA-C1A-C2A	-3.28	123.56	126.17
82	i1	202	PEB	OA-C1A-C2A	-3.28	123.56	126.17
82	xC	202	PEB	CHA-C4A-NA	-3.28	121.30	125.20
82	M5	304	PEB	C4C-C3C-C2C	-3.28	104.47	107.50
85	C6	508	BCR	C27-C26-C25	-3.28	117.96	122.73
82	dE	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
82	WI	201	PEB	C2C-C1C-NC	3.28	111.99	107.57
82	AK	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
82	zC	201	PEB	C3B-C4B-NB	3.28	114.83	110.05
84	DO	1001	CYC	C2A-C1A-NA	3.28	114.83	110.05
82	eK	202	PEB	CHA-C1B-NB	-3.28	118.06	124.93
84	MG	1001	CYC	C4D-CHA-C1A	3.28	135.65	128.28
82	RE	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PH	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
82	H5	203	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
85	BN	838	BCR	C10-C11-C12	3.28	133.46	123.22
82	R9	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
84	JO	1001	CYC	C2C-C1C-NC	3.28	111.10	108.27
82	TJ	202	PEB	CHC-C4C-NC	3.28	125.59	121.15
82	jK	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
82	fO	201	PEB	OA-C1A-C2A	-3.28	123.56	126.17
82	D5	203	PEB	CMB-C2B-C1B	3.28	130.12	125.06
82	fG	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06
82	OF	202	PEB	CHB-C4B-C3B	-3.28	117.72	125.32
82	LJ	201	PEB	C1D-CHC-C4C	3.28	118.10	113.26
82	gJ	202	PEB	CAB-C3B-C4B	3.28	130.82	125.01
88	BL	610	LHG	O8-C23-C24	3.28	122.21	111.91
82	dF	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
82	sF	203	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
82	NE	202	PEB	CAC-CBC-CGC	-3.28	106.54	113.60
82	QD	201	PEB	C3B-C4B-NB	3.28	114.82	110.05
82	H4	1002	PEB	C3B-C4B-NB	3.28	114.82	110.05
82	eE	201	PEB	CHA-C1B-NB	-3.28	118.07	124.93
87	JN	101	CLA	CHB-C4A-NA	3.28	129.05	124.51
82	II	203	PEB	C3C-C4C-NC	3.28	111.29	108.33
82	P4	202	PEB	C3C-C4C-NC	3.28	111.29	108.33
82	TD	201	PEB	CAC-CBC-CGC	-3.28	106.54	113.60
82	OQ	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	dB	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	bP	501	PEB	C2A-C1A-NA	3.28	111.10	108.27
84	JH	1001	CYC	C1B-NB-C4B	-3.28	106.49	110.67
82	MD	202	PEB	OA-C1A-C2A	-3.28	123.56	126.17
82	A7	201	PEB	C3D-C4D-ND	3.28	113.70	107.26
82	WK	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
82	TI	202	PEB	C1D-CHC-C4C	-3.28	108.42	113.26
95	c6	601	DGD	O1G-C1A-C2A	3.28	122.20	111.91
82	bH	201	PEB	CHB-C1C-C2C	-3.28	119.75	127.15
82	bO	201	PEB	CAB-CBB-CGB	-3.28	106.54	113.60
82	eE	201	PEB	CHC-C4C-NC	3.28	125.59	121.15
82	FQ	203	PEB	C1C-NC-C4C	-3.28	103.76	109.60
82	PQ	203	PEB	C3B-C4B-NB	3.28	114.82	110.05
82	SB	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	tK	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	S9	203	PEB	CAC-CBC-CGC	-3.28	106.54	113.60
87	AN	824	CLA	CHB-C4A-NA	3.28	129.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	qK	203	PEB	OA-C1A-C2A	-3.28	123.56	126.17
85	AN	846	BCR	C15-C16-C17	3.28	130.19	123.47
85	B2	802	BCR	C33-C5-C4	3.28	119.92	113.62
82	aF	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
82	OO	201	PEB	CHA-C1B-NB	-3.28	118.07	124.93
87	J2	101	CLA	CAA-C2A-C3A	-3.28	106.06	114.26
82	OK	202	PEB	CHB-C4B-C3B	-3.28	117.73	125.32
84	NO	1001	CYC	CAD-CBD-CGD	-3.28	106.55	113.60
82	GI	201	PEB	CMB-C2B-C1B	3.28	130.11	125.06
82	MP	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
82	Y4	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
82	AI	203	PEB	CMB-C2B-C1B	3.28	130.11	125.06
82	iM	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
85	K2	102	BCR	C16-C17-C18	-3.28	122.63	127.31
82	KF	203	PEB	CHB-C1C-C2C	-3.28	119.75	127.15
82	D4	1002	PEB	CAC-C2C-C1C	3.28	130.98	125.76
84	F3	1001	CYC	C4D-CHA-C1A	3.28	135.63	128.28
82	MF	202	PEB	C1B-C2B-C3B	-3.28	102.75	106.51
82	QG	203	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	PP	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	Z1	202	PEB	CHC-C1D-ND	-3.28	109.58	113.72
82	aB	202	PEB	CHB-C1C-C2C	-3.28	119.76	127.15
82	vF	201	PEB	CHC-C4C-NC	3.28	125.58	121.15
82	TE	201	PEB	C4B-C3B-C2B	-3.28	103.16	106.78
87	CL	515	CLA	CHB-C4A-NA	3.28	129.04	124.51
82	JP	202	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	Z1	203	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	Y4	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	CB	202	PEB	C1C-CHB-C4B	-3.28	120.93	128.28
85	F2	203	BCR	C16-C17-C18	-3.28	122.63	127.31
82	zC	202	PEB	CHC-C1D-ND	-3.28	109.58	113.72
82	IP	201	PEB	C3B-C4B-NB	3.28	114.81	110.05
87	AN	837	CLA	C1-O2A-CGA	3.28	125.04	116.44
82	TI	203	PEB	CHC-C4C-NC	3.28	125.58	121.15
82	FQ	202	PEB	CHC-C4C-NC	3.28	125.58	121.15
82	F9	202	PEB	C3C-C4C-NC	3.28	111.28	108.33
82	BB	202	PEB	CMB-C2B-C1B	3.28	130.11	125.06
87	b6	616	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
87	BL	622	CLA	CHB-C4A-NA	3.28	129.04	124.51
82	f1	202	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	d4	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
82	S5	201	PEB	C2A-C1A-NA	3.28	111.10	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cJ	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
82	YM	201	PEB	C4B-C3B-C2B	-3.28	103.16	106.78
84	C3	1001	CYC	C1B-CHB-C4A	3.28	136.08	128.08
82	VH	202	PEB	CHC-C1D-ND	-3.28	109.58	113.72
82	HJ	202	PEB	CHC-C1D-ND	-3.28	109.58	113.72
82	D5	201	PEB	C1B-C2B-C3B	-3.28	102.75	106.51
84	BG	1002	CYC	C4A-C3A-C2A	-3.28	102.75	106.51
82	TJ	201	PEB	CMB-C2B-C1B	3.28	130.11	125.06
82	cB	402	PEB	C3B-C4B-NB	3.27	114.81	110.05
82	AI	203	PEB	C1D-CHC-C4C	-3.27	108.43	113.26
82	L7	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	U4	201	PEB	OD-C4D-C3D	-3.27	122.04	129.46
82	aJ	203	PEB	C2A-C1A-NA	3.27	111.10	108.27
82	S1	202	PEB	CHA-C1B-NB	-3.27	118.08	124.93
82	GA	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	j4	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	M9	304	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	ZM	201	PEB	CHB-C1C-NC	-3.27	117.82	125.32
85	AN	804	BCR	C33-C5-C4	3.27	119.91	113.62
82	RE	202	PEB	CAC-CBC-CGC	-3.27	106.56	113.60
82	X7	203	PEB	CMB-C2B-C1B	3.27	130.11	125.06
82	WF	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	EM	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	B5	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	mK	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	XA	202	PEB	C3C-C4C-NC	3.27	111.28	108.33
82	SM	203	PEB	OA-C1A-C2A	-3.27	123.57	126.17
82	aJ	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	PB	201	PEB	C4C-C3C-C2C	-3.27	104.48	107.50
83	NQ	201	PUB	C3B-C4B-NB	3.27	111.98	107.57
82	O9	202	PEB	CAC-C2C-C3C	3.27	134.57	127.07
82	FI	201	PEB	C2A-C1A-NA	3.27	111.09	108.27
82	I9	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
84	NE	201	CYC	C1B-NB-C4B	-3.27	106.50	110.67
82	mO	202	PEB	C1C-CHB-C4B	3.27	135.62	128.28
82	b1	202	PEB	CHB-C4B-NB	-3.27	117.77	124.58
82	kE	202	PEB	CHC-C1D-ND	-3.27	109.58	113.72
82	fH	202	PEB	CHA-C1B-NB	-3.27	118.09	124.93
92	DL	402	LMG	O7-C10-C11	3.27	118.56	111.50
84	h3	1001	CYC	C4D-CHA-C1A	3.27	135.62	128.28
82	AP	203	PEB	OD-C4D-C3D	-3.27	122.04	129.46
82	cO	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hM	202	PEB	CAB-CBB-CGB	-3.27	106.56	113.60
82	DJ	202	PEB	OA-C1A-C2A	-3.27	123.57	126.17
82	Q9	202	PEB	OA-C1A-C2A	-3.27	123.57	126.17
82	iE	201	PEB	OA-C1A-C2A	-3.27	123.57	126.17
82	BA	203	PEB	OD-C4D-ND	-3.27	121.08	125.93
82	DJ	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
87	42	603	CLA	CMB-C2B-C1B	-3.27	120.39	125.37
82	XF	202	PEB	CHC-C1D-ND	-3.27	109.58	113.72
82	DB	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
82	CP	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
82	P4	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
82	aO	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	S7	202	PEB	C3D-C4D-ND	3.27	113.68	107.26
82	aM	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	aM	204	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
84	N4	1001	CYC	CAD-CBD-CGD	-3.27	106.56	113.60
82	gJ	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
83	AD	302	PUB	OA-C1A-NA	-3.27	121.08	125.93
82	Q9	202	PEB	C3C-C4C-NC	3.27	111.28	108.33
82	J7	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
84	D4	1001	CYC	C2A-C1A-NA	3.27	114.81	110.05
83	Z5	302	PUB	CBA-CAA-C3A	-3.27	108.02	112.98
82	XB	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	CJ	203	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
84	H4	1001	CYC	C2C-C1C-NC	3.27	111.09	108.27
87	BN	825	CLA	CHB-C1B-NB	3.27	127.72	124.26
82	WF	203	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	PQ	203	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	kK	202	PEB	CHC-C4C-NC	3.27	125.58	121.15
82	EM	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
84	w3	1001	CYC	C4D-CHA-C1A	3.27	135.62	128.28
82	ZM	202	PEB	CHB-C4B-NB	-3.27	117.77	124.58
82	RM	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
82	KK	203	PEB	CMB-C2B-C1B	3.27	130.10	125.06
82	i4	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
82	hE	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
85	FN	202	BCR	C16-C17-C18	-3.27	122.64	127.31
82	K9	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
82	fE	203	PEB	C2A-C1A-NA	3.27	111.09	108.27
82	fK	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
82	aF	201	PEB	OA-C1A-C2A	-3.27	123.57	126.17
84	J3	1001	CYC	C1B-CHB-C4A	3.27	136.07	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	N3	1001	CYC	C1B-CHB-C4A	3.27	136.07	128.08
84	v3	1001	CYC	C1B-CHB-C4A	3.27	136.07	128.08
82	OE	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
82	iJ	202	PEB	C1C-CHB-C4B	-3.27	120.95	128.28
95	C6	502	DGD	O1G-C1A-C2A	3.27	122.17	111.91
84	FH	1001	CYC	C1B-NB-C4B	-3.27	106.51	110.67
82	NP	202	PEB	CAC-CBC-CGC	-3.27	106.57	113.60
82	YJ	203	PEB	C3B-C4B-NB	3.27	114.81	110.05
82	w8	204	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
85	FN	204	BCR	C11-C10-C9	-3.27	122.64	127.31
87	A2	812	CLA	CHB-C4A-NA	3.27	129.03	124.51
82	JQ	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
82	H7	203	PEB	CHC-C1D-ND	-3.27	109.59	113.72
84	73	1001	CYC	C4D-CHA-C1A	3.27	135.61	128.28
82	d1	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
84	DH	1003	CYC	CMA-C3A-C4A	3.27	130.10	125.06
82	mJ	201	PEB	C3B-C4B-NB	3.27	114.80	110.05
87	O2	201	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
84	FO	1001	CYC	CHD-C1D-ND	-3.27	117.83	125.32
82	OG	201	PEB	OA-C1A-C2A	-3.27	123.57	126.17
82	LI	201	PEB	CAC-CBC-CGC	-3.27	106.57	113.60
82	YF	203	PEB	CHB-C1C-C2C	-3.27	119.78	127.15
82	xK	302	PEB	OD-C4D-ND	-3.27	121.09	125.93
87	A2	837	CLA	C2A-C1A-CHA	3.27	129.57	123.86
84	IO	1001	CYC	C2A-C1A-NA	3.27	114.80	110.05
84	Q3	1001	CYC	C4D-CHA-C1A	3.27	135.61	128.28
85	b6	603	BCR	C20-C21-C22	-3.27	122.65	127.31
87	7N	608	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
82	P1	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
82	T4	201	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
82	fM	201	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
82	SA	201	PEB	C3C-C4C-NC	3.27	111.27	108.33
84	JH	1003	CYC	CMA-C3A-C4A	3.27	130.09	125.06
84	LG	1001	CYC	OB-C4B-C3B	-3.27	124.50	128.04
82	WF	203	PEB	C3B-C4B-NB	3.27	114.80	110.05
82	V9	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
84	c3	1001	CYC	C1B-CHB-C4A	3.27	136.06	128.08
82	jO	202	PEB	OD-C4D-C3D	-3.27	122.06	129.46
82	l1	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
82	yC	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
82	WG	203	PEB	C1C-CHB-C4B	3.27	135.61	128.28
84	O3	1001	CYC	C4D-CHA-C1A	3.27	135.61	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Z9	303	PEB	CHC-C4C-NC	3.27	125.57	121.15
82	W1	203	PEB	OD-C4D-ND	-3.27	121.09	125.93
84	KG	202	CYC	C1B-NB-C4B	-3.27	106.51	110.67
85	A2	804	BCR	C33-C5-C4	3.27	119.89	113.62
82	dM	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
82	gM	202	PEB	C1C-CHB-C4B	-3.27	120.96	128.28
82	GB	203	PEB	CHC-C4C-NC	3.27	125.57	121.15
82	YM	201	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
84	J1	1001	CYC	C1D-C2D-C3D	-3.27	103.63	107.79
82	KF	203	PEB	CMB-C2B-C1B	3.26	130.09	125.06
82	LM	201	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
84	u3	1001	CYC	C4D-CHA-C1A	3.26	135.60	128.28
82	HM	202	PEB	CBB-CAB-C3B	3.26	121.70	112.63
84	63	901	CYC	C2D-C1D-ND	3.26	111.99	107.40
82	hG	201	PEB	OD-C4D-C3D	-3.26	122.06	129.46
82	B7	202	PEB	CMB-C2B-C1B	3.26	130.09	125.06
87	1N	601	CLA	CHB-C4A-NA	3.26	129.03	124.51
84	g3	1001	CYC	C1B-CHB-C4A	3.26	136.06	128.08
82	WM	201	PEB	CHA-C1B-C2B	3.26	133.29	124.90
82	EP	203	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
82	Q7	202	PEB	C3B-C4B-NB	3.26	114.80	110.05
82	c4	202	PEB	OD-C4D-C3D	-3.26	122.07	129.46
82	B5	201	PEB	OD-C4D-C3D	-3.26	122.07	129.46
82	eE	201	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
82	CF	203	PEB	C2A-C1A-NA	3.26	111.09	108.27
84	T3	1001	CYC	C1B-CHB-C4A	3.26	136.05	128.08
82	SP	203	PEB	CAC-C2C-C1C	3.26	130.96	125.76
82	LM	202	PEB	CHC-C4C-NC	3.26	125.56	121.15
82	mF	201	PEB	CHC-C4C-NC	3.26	125.56	121.15
82	hG	202	PEB	CHC-C4C-NC	3.26	125.56	121.15
82	TF	202	PEB	CHB-C4B-C3B	-3.26	117.77	125.32
82	eG	202	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
82	JK	202	PEB	OD-C4D-ND	-3.26	121.10	125.93
84	GE	1001	CYC	C4D-CHA-C1A	3.26	135.60	128.28
87	cL	515	CLA	CHB-C4A-NA	3.26	129.02	124.51
82	hE	202	PEB	CHC-C4C-NC	3.26	125.56	121.15
84	FE	1001	CYC	C1B-C2B-C3B	-3.26	104.47	107.87
84	LE	1001	CYC	CBD-CAD-C3D	3.26	121.69	112.63
82	W1	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
82	iO	202	PEB	C3B-C4B-NB	3.26	114.79	110.05
82	EP	203	PEB	C2A-C1A-NA	3.26	111.08	108.27
85	BL	618	BCR	C11-C10-C9	-3.26	122.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OM	203	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
82	AG	301	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
82	mF	202	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
84	JO	1001	CYC	CHD-C1D-ND	-3.26	117.85	125.32
82	IP	201	PEB	CHA-C1B-NB	-3.26	118.11	124.93
82	Z1	203	PEB	C3B-C4B-NB	3.26	114.79	110.05
82	nF	202	PEB	C3B-C4B-NB	3.26	114.79	110.05
82	RE	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	AO	304	PEB	C1D-CHC-C4C	-3.26	108.45	113.26
82	XF	202	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
82	fG	203	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
87	ON	201	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
82	LA	201	PEB	CHC-C1D-ND	-3.26	109.60	113.72
94	a6	601	PL9	C37-C38-C39	-3.26	119.81	127.66
82	RP	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
84	LH	1001	CYC	C2A-C1A-NA	3.26	114.79	110.05
84	BG	1002	CYC	CMB-C2B-C1B	3.26	128.24	124.17
82	iM	202	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
82	P4	202	PEB	OD-C4D-ND	-3.26	121.10	125.93
82	jH	201	PEB	CHB-C1C-C2C	-3.26	119.80	127.15
84	ME	1001	CYC	C4D-CHA-C1A	3.26	135.59	128.28
82	ZF	201	PEB	OA-C1A-C2A	-3.26	123.58	126.17
82	gK	202	PEB	C3B-C4B-NB	3.26	114.79	110.05
84	NO	1001	CYC	C2A-C1A-NA	3.26	114.79	110.05
82	WJ	202	PEB	C3D-C4D-ND	3.26	113.66	107.26
82	W7	202	PEB	C3D-C4D-ND	3.26	113.66	107.26
82	EP	201	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
82	DQ	201	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	hG	201	PEB	C2A-C1A-NA	3.26	111.08	108.27
84	LE	1001	CYC	OB-C4B-C3B	-3.26	124.50	128.04
84	M3	1001	CYC	C4D-CHA-C1A	3.26	135.59	128.28
84	R3	1001	CYC	C1B-CHB-C4A	3.26	136.04	128.08
82	L5	203	PEB	CAC-C2C-C1C	3.26	130.95	125.76
87	dL	401	CLA	CHB-C4A-NA	3.26	129.02	124.51
82	mF	202	PEB	C3B-C4B-NB	3.26	114.79	110.05
84	M4	1001	CYC	C2A-C1A-NA	3.26	114.79	110.05
82	IQ	202	PEB	CMB-C2B-C1B	3.26	130.08	125.06
82	EI	202	PEB	CHC-C4C-NC	3.26	125.56	121.15
84	f3	1001	CYC	C4D-CHA-C1A	3.26	135.59	128.28
82	SM	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
82	AO	301	PEB	OD-C4D-ND	-3.26	121.10	125.93
82	eM	202	PEB	OD-C4D-ND	-3.26	121.10	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	4N	603	CLA	CMB-C2B-C1B	-3.26	120.41	125.37
82	dO	201	PEB	C1C-CHB-C4B	3.26	135.59	128.28
84	t3	1001	CYC	C1B-CHB-C4A	3.26	136.04	128.08
82	XK	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	YK	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	cF	203	PEB	C2A-C1A-NA	3.26	111.08	108.27
85	C6	508	BCR	C38-C26-C27	3.26	119.88	113.62
82	WH	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
82	c4	201	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
82	F5	202	PEB	C1D-CHC-C4C	-3.26	108.45	113.26
82	QM	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
87	AN	812	CLA	CHB-C4A-NA	3.26	129.02	124.51
82	QF	203	PEB	CHB-C4B-NB	-3.26	117.80	124.58
82	AH	302	PEB	OA-C1A-C2A	-3.26	123.58	126.17
84	p3	1001	CYC	C1B-CHB-C4A	3.26	136.04	128.08
82	EK	202	PEB	C1D-CHC-C4C	-3.26	108.45	113.26
82	MM	201	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	H1	1002	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	cF	203	PEB	C3C-C4C-NC	3.26	111.27	108.33
82	aO	203	PEB	C3B-C4B-NB	3.26	114.79	110.05
82	fH	202	PEB	OD-C4D-ND	-3.26	121.11	125.93
82	KI	203	PEB	CHC-C4C-NC	3.26	125.56	121.15
82	dD	401	PEB	CHC-C4C-NC	3.26	125.56	121.15
82	mJ	202	PEB	CHC-C1D-ND	-3.26	109.60	113.72
84	H4	1001	CYC	O2A-CGA-CBA	3.26	124.49	114.03
82	O1	202	PEB	CHB-C4B-NB	-3.26	117.80	124.58
82	RG	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
82	SJ	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
85	BL	618	BCR	C16-C15-C14	-3.26	116.80	123.47
87	B2	818	CLA	CHB-C1B-NB	3.26	127.70	124.26
87	B6	613	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
82	lF	202	PEB	C1C-CHB-C4B	3.26	135.58	128.28
82	JI	201	PEB	CAA-C3A-C2A	-3.26	106.12	114.26
82	A4	304	PEB	C1D-CHC-C4C	-3.26	108.45	113.26
83	Z9	305	PUB	CBB-CAB-C3B	3.26	121.67	112.63
82	UG	201	PEB	C3B-C4B-NB	3.26	114.78	110.05
82	L5	201	PEB	C3B-C4B-NB	3.26	114.78	110.05
84	H3	1001	CYC	C4D-CHA-C1A	3.26	135.58	128.28
82	lM	203	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
87	BN	805	CLA	C3B-C4B-NB	-3.26	107.50	110.52
87	B2	826	CLA	C3B-C4B-NB	-3.26	107.50	110.52
82	AA	202	PEB	CMB-C2B-C1B	3.26	130.08	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	I3	1001	CYC	C4D-CHA-C1A	3.26	135.58	128.28
82	wK	301	PEB	CHC-C1D-ND	-3.26	109.61	113.72
82	QQ	201	PEB	C4B-C3B-C2B	-3.26	103.18	106.78
82	WP	201	PEB	C2A-C1A-NA	3.25	111.08	108.27
82	AQ	304	PEB	CHC-C4C-NC	3.25	125.55	121.15
84	j3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
82	U9	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
87	B2	804	CLA	C3B-C4B-NB	-3.25	107.50	110.52
82	WK	203	PEB	C3D-C4D-ND	3.25	113.64	107.26
82	F7	202	PEB	C1C-CHB-C4B	3.25	135.58	128.28
84	DH	1003	CYC	C4D-CHA-C1A	3.25	135.58	128.28
84	L3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
84	U3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
84	o3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
82	Z5	304	PEB	C4C-C3C-C2C	-3.25	104.50	107.50
82	MA	201	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
82	JF	202	PEB	CHA-C1B-NB	-3.25	118.13	124.93
84	i3	1001	CYC	C1B-CHB-C4A	3.25	136.03	128.08
85	KN	101	BCR	C16-C17-C18	-3.25	122.67	127.31
82	KQ	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
82	j4	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
82	JH	1002	PEB	C2A-C1A-NA	3.25	111.08	108.27
84	S3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
84	k3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
82	RB	201	PEB	CAB-CBB-CGB	-3.25	106.60	113.60
82	UM	202	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
82	ZF	202	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	SH	202	PEB	CHA-C1B-NB	-3.25	118.13	124.93
82	DP	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
83	K7	203	PUB	OD-C4D-ND	-3.25	121.11	125.93
84	B3	1001	CYC	C4D-CHA-C1A	3.25	135.58	128.28
82	UB	301	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
82	JP	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
82	lM	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
82	u8	202	PEB	C1D-CHC-C4C	3.25	118.05	113.26
82	hM	202	PEB	CHA-C1B-NB	-3.25	118.13	124.93
82	MK	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
82	dM	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
91	AL	410	PHO	CMB-C2B-C3B	3.25	130.76	124.68
84	F1	1001	CYC	C4D-C3D-C2D	-3.25	103.78	107.62
82	WE	203	PEB	CHC-C1D-ND	-3.25	109.61	113.72
82	eF	202	PEB	CHA-C1B-NB	-3.25	118.13	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	e4	201	PEB	C2A-C1A-NA	3.25	111.08	108.27
82	SB	201	PEB	CHC-C4C-NC	3.25	125.55	121.15
82	II	202	PEB	CHC-C4C-NC	3.25	125.55	121.15
84	E3	1001	CYC	C1B-CHB-C4A	3.25	136.03	128.08
84	P3	1001	CYC	C1B-CHB-C4A	3.25	136.03	128.08
82	YD	202	PEB	OA-C1A-C2A	-3.25	123.59	126.17
82	CB	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
82	VP	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
82	kM	201	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	IK	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
82	hG	203	PEB	OD-C4D-ND	-3.25	121.11	125.93
85	bL	601	BCR	C11-C10-C9	-3.25	122.67	127.31
82	mJ	201	PEB	C1D-CHC-C4C	3.25	118.05	113.26
82	DO	1002	PEB	CAC-C2C-C1C	3.25	130.94	125.76
82	BD	201	PEB	C3C-C4C-NC	3.25	111.26	108.33
82	mK	202	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	MF	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
82	Q7	201	PEB	CHA-C4A-NA	3.25	129.07	125.20
87	82	302	CLA	CHC-C4B-NB	3.25	127.70	124.26
82	XK	202	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
82	GP	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
82	VP	202	PEB	CAC-CBC-CGC	-3.25	106.61	113.60
82	lJ	202	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	h4	201	PEB	CHB-C4B-C3B	-3.25	117.80	125.32
82	sC	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
82	mJ	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
82	gB	201	PEB	CAA-C3A-C2A	-3.25	106.14	114.26
82	UD	201	PEB	CMB-C2B-C1B	3.25	130.07	125.06
82	M5	301	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	mM	201	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	WK	203	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
82	d4	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
82	dO	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
82	AO	304	PEB	OD-C4D-ND	-3.25	121.11	125.93
82	V7	202	PEB	C1C-NC-C4C	-3.25	103.81	109.60
82	PJ	201	PEB	CMB-C2B-C1B	3.25	130.07	125.06
85	F2	204	BCR	C11-C10-C9	-3.25	122.67	127.31
82	m4	202	PEB	C1C-CHB-C4B	3.25	135.57	128.28
82	RA	202	PEB	C1C-NC-C4C	-3.25	103.81	109.60
82	KP	202	PEB	CHB-C4B-C3B	-3.25	117.80	125.32
82	OA	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	FH	1002	PEB	C4B-C3B-C2B	-3.25	103.19	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	wK	304	PUB	C1C-C2C-C3C	-3.25	103.19	106.78
82	UQ	201	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	vK	201	PEB	CHC-C4C-NC	3.25	125.55	121.15
82	M9	304	PEB	CHC-C4C-NC	3.25	125.55	121.15
82	UI	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
82	AG	304	PEB	CHA-C1B-NB	-3.25	118.14	124.93
87	72	609	CLA	CAA-C2A-C3A	-3.25	106.14	114.26
82	F5	202	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	J5	203	PEB	C3B-C4B-NB	3.25	114.78	110.05
82	H7	203	PEB	CHC-C4C-NC	3.25	125.55	121.15
82	EM	203	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
87	62	310	CLA	CAA-C2A-C3A	-3.25	108.52	116.10
84	CH	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
84	G3	1001	CYC	C1B-CHB-C4A	3.25	136.02	128.08
82	LI	201	PEB	C2A-C1A-NA	3.25	111.07	108.27
82	H9	203	PEB	C2A-C1A-NA	3.25	111.07	108.27
84	D3	1001	CYC	C4D-CHA-C1A	3.25	135.57	128.28
82	vK	202	PEB	CHC-C1D-ND	-3.25	109.61	113.72
84	FE	1002	CYC	CAD-CBD-CGD	-3.25	106.61	113.60
84	DO	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
82	WH	203	PEB	OD-C4D-ND	-3.25	121.12	125.93
82	ZK	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
82	a4	203	PEB	C3B-C4B-NB	3.25	114.77	110.05
82	GI	203	PEB	CHC-C4C-NC	3.25	125.54	121.15
82	kF	203	PEB	CHB-C1C-C2C	-3.25	119.82	127.15
87	b6	608	CLA	CHB-C4A-NA	3.25	129.00	124.51
82	e4	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	D5	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
84	HO	1001	CYC	O2A-CGA-CBA	3.25	124.46	114.03
83	K7	203	PUB	OA-C1A-NA	-3.25	121.12	125.93
82	DF	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
82	mF	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
82	RD	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
84	D4	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
84	D1	1003	CYC	C4D-CHA-C1A	3.25	135.56	128.28
82	JP	202	PEB	CAC-CBC-CGC	-3.25	106.62	113.60
82	t8	201	PEB	C2C-C1C-NC	3.25	111.94	107.57
87	AN	828	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
82	1C	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	dQ	401	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	TM	202	PEB	CHC-C4C-NC	3.25	125.54	121.15
87	A2	828	CLA	CAA-C2A-C3A	-3.25	103.89	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CP	201	PEB	CHC-C1D-ND	-3.25	109.62	113.72
83	KA	203	PUB	OD-C4D-ND	-3.25	121.12	125.93
82	PE	202	PEB	CAC-CBC-CGC	-3.25	106.62	113.60
84	L1	1001	CYC	C1D-C2D-C3D	-3.25	103.66	107.79
82	TK	202	PEB	CHB-C4B-C3B	-3.25	117.81	125.32
82	1C	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	kE	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	cG	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	kG	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
82	aJ	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
84	NE	201	CYC	C1A-C2A-C3A	-3.25	103.19	106.78
82	QA	201	PEB	CBB-CAB-C3B	-3.25	103.61	112.63
82	g4	202	PEB	C3C-C4C-NC	3.24	111.25	108.33
84	q3	1001	CYC	C4D-CHA-C1A	3.24	135.56	128.28
82	FK	202	PEB	OA-C1A-C2A	-3.24	123.59	126.17
82	gE	201	PEB	CAC-C2C-C1C	3.24	130.93	125.76
82	PO	202	PEB	OD-C4D-ND	-3.24	121.12	125.93
82	HA	202	PEB	CHC-C1D-ND	-3.24	109.62	113.72
82	XK	202	PEB	CHC-C1D-ND	-3.24	109.62	113.72
84	73	1002	CYC	CMD-C2D-C1D	3.24	130.31	125.56
82	aM	204	PEB	C2A-C1A-NA	3.24	111.07	108.27
82	Y5	202	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
82	U1	203	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
82	E7	202	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
82	ZJ	202	PEB	C3B-C4B-NB	3.24	114.77	110.05
82	FM	202	PEB	C3B-C4B-NB	3.24	114.77	110.05
82	wF	303	PEB	C3B-C4B-NB	3.24	114.77	110.05
82	pC	202	PEB	CHB-C4B-C3B	3.24	132.82	125.32
84	JO	1001	CYC	C1D-C2D-C3D	-3.24	103.66	107.79
92	b6	624	LMG	O8-C28-C29	3.24	122.09	111.91
82	VI	202	PEB	CHC-C4C-NC	3.24	125.54	121.15
82	KP	202	PEB	CHA-C1B-NB	-3.24	118.15	124.93
85	BL	616	BCR	C16-C17-C18	-3.24	122.68	127.31
84	73	1002	CYC	C2B-C1B-NB	3.24	111.74	106.99
82	NJ	202	PEB	C3B-C4B-NB	3.24	114.77	110.05
82	PP	202	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
82	aK	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
82	MK	202	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
82	T4	202	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
82	W7	202	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
82	jG	201	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
84	A3	1001	CYC	C1B-CHB-C4A	3.24	136.00	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	e3	1001	CYC	C1B-CHB-C4A	3.24	136.00	128.08
82	FA	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
82	HP	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
82	PH	201	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
85	bL	602	BCR	C33-C5-C6	-3.24	120.89	124.53
87	7N	609	CLA	CAA-C2A-C3A	-3.24	106.16	114.26
82	NJ	201	PEB	CHA-C4A-NA	3.24	129.06	125.20
82	LA	201	PEB	C2A-C1A-NA	3.24	111.07	108.27
82	BK	202	PEB	C2A-C1A-NA	3.24	111.07	108.27
84	K3	1001	CYC	C1B-CHB-C4A	3.24	136.00	128.08
82	VO	201	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	IP	203	PEB	C3B-C4B-NB	3.24	114.77	110.05
84	I4	1001	CYC	C2A-C1A-NA	3.24	114.77	110.05
82	ZG	202	PEB	C1D-CHC-C4C	-3.24	108.48	113.26
82	ID	202	PEB	CMB-C2B-C1B	3.24	130.06	125.06
84	HE	1001	CYC	C4A-C3A-C2A	-3.24	102.79	106.51
84	E4	1001	CYC	C4A-C3A-C2A	-3.24	102.79	106.51
82	S1	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
82	j1	201	PEB	CHB-C1C-C2C	-3.24	119.84	127.15
82	OP	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	W4	201	PEB	CHA-C4A-NA	3.24	129.06	125.20
82	PI	202	PEB	CHC-C4C-NC	3.24	125.54	121.15
82	PK	202	PEB	CHB-C4B-C3B	-3.24	117.82	125.32
84	NO	1001	CYC	C2B-C1B-NB	3.24	111.73	106.99
82	J5	203	PEB	OA-C1A-C2A	-3.24	123.60	126.17
82	lH	202	PEB	OA-C1A-C2A	-3.24	123.60	126.17
82	AP	203	PEB	C2A-C1A-NA	3.24	111.07	108.27
82	e1	202	PEB	CMB-C2B-C1B	3.24	130.06	125.06
82	YP	503	PEB	CHC-C1D-ND	-3.24	109.62	113.72
82	OE	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	V7	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	eG	201	PEB	CHC-C4C-NC	3.24	125.53	121.15
82	AG	304	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
82	BJ	301	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
83	xK	301	PUB	CMD-C2D-C3D	3.24	132.63	127.77
82	OP	201	PEB	C3B-C4B-NB	3.24	114.76	110.05
83	Z5	302	PUB	C1C-C2C-C3C	-3.24	103.20	106.78
85	AN	846	BCR	C3-C4-C5	-3.24	108.29	114.08
87	AN	806	CLA	CMB-C2B-C1B	-3.24	120.43	125.37
87	2N	306	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
87	6N	609	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
84	l3	1001	CYC	C1B-CHB-C4A	3.24	136.00	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PA	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	F9	202	PEB	CHC-C1D-ND	-3.24	109.62	113.72
82	RI	202	PEB	CHC-C4C-NC	3.24	125.53	121.15
82	PB	201	PEB	C3B-C4B-NB	3.24	114.76	110.05
82	HP	202	PEB	C2A-C1A-NA	3.24	111.07	108.27
82	KP	201	PEB	C2A-C1A-NA	3.24	111.07	108.27
87	AN	837	CLA	C2A-C1A-CHA	3.24	129.52	123.86
82	XB	201	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
82	IM	201	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
82	EK	201	PEB	CHA-C1B-NB	-3.24	118.16	124.93
87	J2	101	CLA	CHB-C4A-NA	3.24	128.99	124.51
82	UQ	201	PEB	CMB-C2B-C1B	3.24	130.05	125.06
82	j1	201	PEB	C1C-CHB-C4B	3.24	135.55	128.28
82	RD	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
84	m3	1001	CYC	C1B-CHB-C4A	3.24	136.00	128.08
82	XI	202	PEB	CHC-C4C-NC	3.24	125.53	121.15
82	EM	202	PEB	CHC-C4C-NC	3.24	125.53	121.15
82	Z5	301	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
82	J7	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	A4	304	PEB	C2A-C1A-NA	3.24	111.06	108.27
82	RG	201	PEB	C3B-C4B-NB	3.24	114.76	110.05
91	aL	610	PHO	C4D-CHA-CBD	-3.24	107.05	108.52
82	KP	201	PEB	C3D-C4D-ND	3.24	113.61	107.26
82	eH	203	PEB	CMB-C2B-C1B	3.24	130.05	125.06
82	dG	202	PEB	CHA-C1B-NB	-3.24	118.16	124.93
82	bG	201	PEB	OD-C4D-ND	-3.24	121.13	125.93
82	lG	201	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
82	Y7	301	PEB	C4C-C3C-C2C	-3.24	104.51	107.50
85	Z6	101	BCR	C38-C26-C25	-3.24	120.89	124.53
82	AP	202	PEB	C3B-C4B-NB	3.24	114.76	110.05
82	gB	202	PEB	C3B-C4B-NB	3.24	114.76	110.05
82	tK	203	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
82	iO	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
84	F4	1001	CYC	CHD-C1D-ND	-3.24	117.90	125.32
82	N4	1002	PEB	CMB-C2B-C1B	3.24	130.05	125.06
82	aE	202	PEB	C2A-C1A-NA	3.24	111.06	108.27
82	AI	203	PEB	CAC-C2C-C1C	3.24	130.92	125.76
82	WD	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
82	QK	203	PEB	CHB-C4B-NB	-3.24	117.84	124.58
82	QA	202	PEB	C3B-C4B-NB	3.24	114.76	110.05
82	uC	202	PEB	OD-C4D-C3D	-3.24	122.12	129.46
87	BN	834	CLA	CMB-C2B-C1B	-3.24	120.44	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Z1	203	PEB	CHC-C4C-NC	3.24	125.53	121.15
82	TD	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
84	MO	1001	CYC	C1A-C2A-C3A	-3.24	103.20	106.78
82	wK	302	PEB	CHC-C1D-ND	-3.24	109.63	113.72
84	LG	1001	CYC	CBD-CAD-C3D	3.24	121.62	112.63
82	GG	1002	PEB	OD-C4D-C3D	-3.24	122.13	129.46
82	j4	202	PEB	OD-C4D-C3D	-3.24	122.13	129.46
82	ED	202	PEB	OD-C4D-ND	-3.24	121.14	125.93
82	EQ	202	PEB	OD-C4D-ND	-3.24	121.14	125.93
82	eE	203	PEB	CHA-C1B-C2B	3.24	133.22	124.90
82	WO	201	PEB	CHA-C4A-NA	3.24	129.05	125.20
82	GF	203	PEB	C3D-C4D-ND	3.24	113.61	107.26
82	GM	203	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
82	sF	202	PEB	CHC-C4C-NC	3.24	125.53	121.15
82	z8	202	PEB	CHA-C1B-NB	-3.24	118.16	124.93
82	VA	202	PEB	C1C-NC-C4C	-3.24	103.84	109.60
85	C6	508	BCR	C21-C20-C19	3.24	133.31	123.22
82	SF	201	PEB	OD-C4D-ND	-3.24	121.14	125.93
82	qK	202	PEB	OD-C4D-ND	-3.24	121.14	125.93
85	Z6	101	BCR	C39-C30-C29	3.24	121.85	108.91
82	mH	201	PEB	CHC-C1D-ND	-3.24	109.63	113.72
82	DD	201	PEB	C2A-C1A-NA	3.24	111.06	108.27
82	ID	201	PEB	C2A-C1A-NA	3.24	111.06	108.27
82	PG	202	PEB	CAC-CBC-CGC	-3.24	106.64	113.60
82	SH	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
82	LM	201	PEB	CMB-C2B-C1B	3.24	130.05	125.06
82	MM	201	PEB	C3B-C4B-NB	3.24	114.75	110.05
85	KL	100	BCR	C11-C12-C13	3.24	135.50	126.42
87	A2	832	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
82	WE	203	PEB	C1C-CHB-C4B	3.24	135.54	128.28
82	AP	201	PEB	CHA-C1B-NB	-3.23	118.17	124.93
84	I1	1001	CYC	C4D-C3D-C2D	-3.23	103.80	107.62
82	eJ	201	PEB	C1D-CHC-C4C	3.23	118.03	113.26
85	I2	101	BCR	C7-C8-C9	-3.23	121.35	126.23
82	TK	202	PEB	OA-C1A-C2A	-3.23	123.60	126.17
82	BK	202	PEB	C1B-C2B-C3B	-3.23	102.79	106.51
82	S5	201	PEB	CMB-C2B-C1B	3.23	130.04	125.06
82	WH	201	PEB	C3B-C4B-NB	3.23	114.75	110.05
82	OJ	203	PEB	C3B-C4B-NB	3.23	114.75	110.05
82	uC	202	PEB	C1D-CHC-C4C	3.23	118.03	113.26
82	BI	203	PEB	C1C-C2C-C3C	-3.23	103.80	107.62
82	s8	201	PEB	OD-C4D-ND	-3.23	121.14	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AE	304	PEB	CHA-C1B-NB	-3.23	118.17	124.93
82	QM	202	PEB	C3C-C4C-NC	3.23	111.24	108.33
87	A2	805	CLA	C3B-C4B-NB	-3.23	107.52	110.52
82	PK	202	PEB	C3B-C4B-NB	3.23	114.75	110.05
82	d4	201	PEB	C1C-CHB-C4B	3.23	135.53	128.28
84	n3	1001	CYC	C4D-CHA-C1A	3.23	135.53	128.28
82	NI	203	PEB	OD-C4D-C3D	-3.23	122.13	129.46
85	H6	101	BCR	C16-C15-C14	-3.23	116.85	123.47
87	CL	513	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
82	a4	201	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
82	w8	202	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
82	L5	202	PEB	OD-C4D-ND	-3.23	121.14	125.93
82	QQ	201	PEB	CHC-C4C-NC	3.23	125.53	121.15
82	sC	202	PEB	CMB-C2B-C1B	3.23	130.04	125.06
85	c6	617	BCR	C33-C5-C4	3.23	119.83	113.62
82	LM	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
82	QE	201	PEB	CAC-C2C-C1C	3.23	130.91	125.76
82	RQ	202	PEB	C3D-C4D-ND	3.23	113.60	107.26
84	JH	1001	CYC	C1D-C2D-C3D	-3.23	103.67	107.79
84	M4	1001	CYC	C4A-C3A-C2A	-3.23	102.80	106.51
82	YF	201	PEB	CHA-C1B-NB	-3.23	118.17	124.93
82	N5	201	PEB	CMA-C2A-C1A	-3.23	105.44	112.40
82	KD	202	PEB	CMB-C2B-C1B	3.23	130.04	125.06
82	AQ	303	PEB	CMB-C2B-C1B	3.23	130.04	125.06
87	22	606	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
82	SH	202	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
82	gG	201	PEB	CAC-C2C-C1C	3.23	130.91	125.76
82	Q9	202	PEB	C1D-CHC-C4C	3.23	118.02	113.26
82	FJ	201	PEB	CHA-C4A-NA	3.23	129.05	125.20
82	AH	301	PEB	OD-C4D-ND	-3.23	121.14	125.93
82	P1	201	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	CI	202	PEB	CHC-C4C-NC	3.23	125.52	121.15
82	NI	202	PEB	CHC-C4C-NC	3.23	125.52	121.15
87	A2	851	CLA	CHB-C4A-NA	3.23	128.98	124.51
82	CQ	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
82	R1	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
82	O5	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
82	FA	202	PEB	C1C-CHB-C4B	3.23	135.53	128.28
82	ZB	203	PEB	CBB-CAB-C3B	-3.23	103.65	112.63
82	CP	201	PEB	C2C-C1C-NC	3.23	111.92	107.57
82	gB	203	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	qC	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HG	1002	PEB	OA-C1A-C2A	-3.23	123.60	126.17
82	CD	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
82	YK	203	PEB	OD-C4D-ND	-3.23	121.14	125.93
82	gK	203	PEB	OD-C4D-ND	-3.23	121.14	125.93
82	g4	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
82	dH	201	PEB	CMB-C2B-C1B	3.23	130.04	125.06
82	m1	201	PEB	CHC-C1D-ND	-3.23	109.64	113.72
84	d3	1001	CYC	C4D-CHA-C1A	3.23	135.53	128.28
82	eJ	202	PEB	CHB-C4B-NB	-3.23	117.86	124.58
82	TQ	201	PEB	CAC-CBC-CGC	-3.23	106.65	113.60
82	Z9	304	PEB	CHA-C1B-C2B	3.23	133.21	124.90
84	CH	1001	CYC	C4D-C3D-C2D	-3.23	103.80	107.62
84	K1	1001	CYC	C4D-C3D-C2D	-3.23	103.80	107.62
82	QP	201	PEB	CHC-C1D-ND	-3.23	109.64	113.72
82	gO	202	PEB	CHC-C1D-ND	-3.23	109.64	113.72
82	hG	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
82	k4	201	PEB	C3B-C4B-NB	3.23	114.75	110.05
82	Y1	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
82	M7	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	WG	202	PEB	OD-C4D-ND	-3.23	121.15	125.93
87	6N	609	CLA	CAA-C2A-C3A	-3.23	108.56	116.10
82	D5	203	PEB	C3B-C4B-NB	3.23	114.75	110.05
87	5N	601	CLA	CHB-C4A-NA	3.23	128.98	124.51
82	M9	305	PEB	CHA-C1B-C2B	3.23	133.20	124.90
82	UJ	203	PEB	CMB-C2B-C1B	3.23	130.04	125.06
82	m4	201	PEB	OD-C4D-ND	-3.23	121.15	125.93
82	PB	201	PEB	CHB-C1C-C2C	-3.23	119.87	127.15
82	dG	201	PEB	OA-C1A-C2A	-3.23	123.61	126.17
82	OO	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	O1	203	PEB	C3C-C4C-NC	3.23	111.24	108.33
82	EF	201	PEB	CHA-C1B-NB	-3.23	118.18	124.93
85	A6	401	BCR	C7-C8-C9	-3.23	121.36	126.23
82	ZH	202	PEB	CHC-C1D-ND	-3.23	109.64	113.72
82	AD	303	PEB	C1D-CHC-C4C	-3.23	108.50	113.26
82	F5	203	PEB	CHC-C4C-NC	3.23	125.52	121.15
82	A4	301	PEB	OD-C4D-ND	-3.23	121.15	125.93
84	IG	1001	CYC	C1A-C2A-C3A	-3.23	103.21	106.78
87	62	310	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
82	YA	301	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	W5	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	fJ	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	JA	202	PEB	C3B-C4B-NB	3.23	114.74	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WK	203	PEB	C3B-C4B-NB	3.23	114.74	110.05
82	B5	203	PEB	C3B-C4B-NB	3.23	114.74	110.05
82	iJ	202	PEB	CHC-C4C-NC	3.23	125.52	121.15
82	LP	201	PEB	OD-C4D-ND	-3.23	121.15	125.93
82	WF	201	PEB	OA-C1A-C2A	-3.23	123.61	126.17
82	J1	1002	PEB	C2A-C1A-NA	3.23	111.06	108.27
83	YA	302	PUB	C1C-C2C-C3C	-3.23	103.21	106.78
83	M5	302	PUB	C1C-C2C-C3C	-3.23	103.21	106.78
82	G5	201	PEB	CMA-C2A-C1A	-3.23	105.45	112.40
84	D1	1001	CYC	CMB-C2B-C1B	3.23	128.20	124.17
85	BL	617	BCR	C21-C20-C19	3.23	133.29	123.22
82	aK	201	PEB	C1D-CHC-C4C	3.23	118.01	113.26
82	d1	203	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	K7	201	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	ZH	203	PEB	CHC-C4C-NC	3.23	125.52	121.15
82	NJ	202	PEB	C1C-CHB-C4B	-3.23	121.05	128.28
82	P5	201	PEB	CMA-C2A-C1A	-3.23	105.45	112.40
84	LH	1001	CYC	C4D-C3D-C2D	-3.23	103.81	107.62
82	EM	201	PEB	C2A-C1A-NA	3.23	111.05	108.27
82	A1	305	PEB	C2A-C1A-NA	3.23	111.05	108.27
82	dF	202	PEB	CHC-C4C-NC	-3.23	116.78	121.15
82	wC	204	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
82	BI	202	PEB	OD-C4D-C3D	-3.23	122.15	129.46
82	lJ	203	PEB	C1C-CHB-C4B	-3.23	121.05	128.28
82	Y4	201	PEB	C3B-C4B-NB	3.23	114.74	110.05
82	mK	201	PEB	C3B-C4B-NB	3.23	114.74	110.05
82	DB	201	PEB	CHA-C1B-NB	-3.23	118.19	124.93
82	NO	1002	PEB	CMB-C2B-C1B	3.23	130.03	125.06
83	AJ	303	PUB	OA-C1A-NA	-3.23	121.15	125.93
82	F9	203	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
87	A2	806	CLA	CMB-C2B-C1B	-3.23	120.46	125.37
85	AN	848	BCR	C20-C19-C18	3.23	135.48	126.42
82	UF	201	PEB	CHA-C1B-NB	-3.22	118.19	124.93
85	H6	101	BCR	C38-C26-C27	3.22	119.81	113.62
82	w8	204	PEB	C3B-C4B-NB	3.22	114.74	110.05
84	IG	1001	CYC	C2A-C1A-NA	3.22	114.74	110.05
82	J5	201	PEB	CMB-C2B-C1B	3.22	130.03	125.06
82	wK	303	PEB	CMB-C2B-C1B	3.22	130.03	125.06
82	R7	203	PEB	OA-C1A-C2A	-3.22	123.61	126.17
82	R5	201	PEB	CMA-C2A-C1A	-3.22	105.45	112.40
82	WF	203	PEB	C3D-C4D-ND	3.22	113.59	107.26
82	xF	304	PEB	OD-C4D-ND	-3.22	121.15	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	B2	834	CLA	CMB-C2B-C1B	-3.22	120.46	125.37
87	bL	614	CLA	CMB-C2B-C1B	-3.22	120.46	125.37
82	VB	201	PEB	C4B-C3B-C2B	-3.22	103.21	106.78
82	b1	201	PEB	CHB-C1C-C2C	-3.22	119.88	127.15
82	SM	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	g4	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
87	BN	806	CLA	CMB-C2B-C3B	3.22	134.40	126.59
82	OP	201	PEB	C2C-C1C-NC	3.22	111.91	107.57
82	r8	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	IJ	203	PEB	C1C-CHB-C4B	-3.22	121.05	128.28
82	jH	201	PEB	C1C-CHB-C4B	3.22	135.51	128.28
82	t8	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	OG	202	PEB	OD-C4D-ND	-3.22	121.16	125.93
87	8N	303	CLA	CHC-C4B-NB	3.22	127.67	124.26
82	K7	202	PEB	CHC-C4C-NC	3.22	125.51	121.15
84	K1	1001	CYC	CMA-C3A-C4A	3.22	130.03	125.06
84	IE	1001	CYC	C1A-C2A-C3A	-3.22	103.22	106.78
84	KG	202	CYC	C1A-C2A-C3A	-3.22	103.22	106.78
82	YF	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	VM	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	yC	203	PEB	CHB-C4B-NB	-3.22	117.87	124.58
82	KK	203	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	YM	201	PEB	CMB-C2B-C1B	3.22	130.03	125.06
82	UD	201	PEB	C3B-C4B-NB	3.22	114.74	110.05
85	A2	848	BCR	C20-C19-C18	3.22	135.47	126.42
82	j1	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
83	ND	201	PUB	C3B-C4B-NB	3.22	111.91	107.57
94	a6	601	PL9	C42-C43-C44	-3.22	119.90	127.66
84	M1	201	CYC	CMA-C3A-C4A	3.22	130.03	125.06
82	dH	203	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	XM	202	PEB	CHC-C4C-NC	3.22	125.51	121.15
84	BE	1002	CYC	CMB-C2B-C1B	3.22	128.19	124.17
82	iK	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
82	r8	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
85	kL	100	BCR	C11-C12-C13	3.22	135.46	126.42
82	AP	203	PEB	CAC-CBC-CGC	-3.22	106.67	113.60
84	FG	1001	CYC	CAD-CBD-CGD	-3.22	106.67	113.60
82	QP	201	PEB	CHC-C4C-NC	3.22	125.51	121.15
82	Y4	202	PEB	C3C-C4C-NC	3.22	111.23	108.33
82	V5	201	PEB	CMA-C2A-C1A	-3.22	105.46	112.40
82	R7	202	PEB	C1C-NC-C4C	-3.22	103.87	109.60
82	L7	201	PEB	CHC-C1D-ND	-3.22	109.65	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	V1	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	oF	203	PEB	CHA-C1B-NB	-3.22	118.20	124.93
84	F1	1001	CYC	C1B-NB-C4B	-3.22	106.57	110.67
82	A5	201	PEB	CMA-C2A-C1A	-3.22	105.46	112.40
82	eM	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
82	aB	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
82	mE	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
82	Y7	301	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	jO	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
84	MO	1001	CYC	C4A-C3A-C2A	-3.22	102.81	106.51
82	UP	201	PEB	CMA-C2A-C1A	-3.22	105.46	112.40
82	gO	202	PEB	C3C-C4C-NC	3.22	111.23	108.33
82	RE	201	PEB	C3B-C4B-NB	3.22	114.73	110.05
82	BI	201	PEB	CHC-C4C-NC	3.22	125.51	121.15
82	I5	201	PEB	CMA-C2A-C1A	-3.22	105.46	112.40
82	VD	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	GP	202	PEB	CHB-C4B-C3B	-3.22	117.87	125.32
84	BG	1001	CYC	C1B-C2B-C3B	-3.22	104.51	107.87
82	eG	203	PEB	CHA-C1B-C2B	3.22	133.18	124.90
85	B2	840	BCR	C1-C6-C5	-3.22	118.08	122.61
82	NA	203	PEB	C1C-CHB-C4B	3.22	135.50	128.28
82	YA	301	PEB	C4C-C3C-C2C	-3.22	104.53	107.50
82	SG	203	PEB	OD-C4D-ND	-3.22	121.16	125.93
82	dK	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
84	N1	1001	CYC	CAD-CBD-CGD	-3.22	106.68	113.60
82	RQ	203	PEB	OA-C1A-C2A	-3.22	123.61	126.17
87	O2	201	CLA	CAA-C2A-C3A	-3.22	108.59	116.10
82	y8	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
82	WA	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	AE	304	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	WE	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	g4	202	PEB	CHC-C1D-ND	-3.22	109.65	113.72
84	LH	1002	CYC	C1D-C2D-C3D	-3.22	103.69	107.79
82	GP	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	MP	203	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	YF	203	PEB	OD-C4D-ND	-3.22	121.16	125.93
87	B2	805	CLA	CMB-C2B-C3B	3.22	134.38	126.59
94	aL	601	PL9	C25-C24-C26	3.22	120.68	115.27
82	AI	202	PEB	CHC-C4C-NC	3.22	125.50	121.15
82	dE	202	PEB	CHA-C1B-NB	-3.22	118.20	124.93
82	T5	201	PEB	CMA-C2A-C1A	-3.22	105.47	112.40
82	hO	201	PEB	CMB-C2B-C1B	3.22	130.02	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	22	606	CLA	CHB-C4A-NA	3.22	128.96	124.51
82	UE	201	PEB	C3B-C4B-NB	3.22	114.73	110.05
82	b4	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	FJ	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
82	aJ	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
82	LQ	203	PEB	CHB-C1C-C2C	-3.22	119.89	127.15
85	IN	101	BCR	C7-C8-C9	-3.22	121.37	126.23
82	XF	203	PEB	CHB-C1C-NC	-3.22	117.95	125.32
83	AJ	304	PUB	C4B-CHB-C1C	-3.22	121.07	128.28
82	gH	202	PEB	CAA-C3A-C4A	3.22	120.93	112.67
84	E1	1001	CYC	CHB-C4A-C3A	3.22	133.17	124.90
82	K5	201	PEB	CMA-C2A-C1A	-3.22	105.47	112.40
82	fH	201	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	hJ	203	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
82	QG	201	PEB	CAC-C2C-C1C	3.22	130.88	125.76
82	NA	201	PEB	CHC-C4C-NC	3.22	125.50	121.15
82	mM	202	PEB	CHC-C4C-NC	3.22	125.50	121.15
82	W9	203	PEB	CHC-C1D-ND	-3.22	109.66	113.72
82	BD	203	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	UG	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
82	hO	201	PEB	CHB-C4B-C3B	-3.22	117.88	125.32
82	RQ	201	PEB	C1B-C2B-C3B	-3.22	102.82	106.51
82	WJ	202	PEB	CHA-C1B-NB	-3.22	118.21	124.93
82	QA	201	PEB	CHA-C4A-NA	3.22	129.03	125.20
82	wC	204	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
82	eA	301	PEB	OD-C4D-C3D	-3.22	122.17	129.46
82	HM	202	PEB	OD-C4D-ND	-3.22	121.17	125.93
82	d1	201	PEB	CMB-C2B-C1B	3.21	130.01	125.06
82	H7	202	PEB	CHB-C1C-C2C	-3.21	119.90	127.15
82	eM	201	PEB	CHC-C1D-ND	3.21	117.79	113.72
87	BL	623	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
82	BF	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	IK	203	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	tC	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	fE	203	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	AG	304	PEB	C3B-C4B-NB	3.21	114.72	110.05
87	BN	819	CLA	CHB-C1B-NB	3.21	127.66	124.26
82	SB	202	PEB	OD-C4D-ND	-3.21	121.17	125.93
82	LD	201	PEB	OD-C4D-ND	-3.21	121.17	125.93
82	NE	202	PEB	C4B-C3B-C2B	-3.21	103.22	106.78
82	AP	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
84	DO	1001	CYC	C2C-C1C-NC	3.21	111.04	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	S4	201	PEB	CHC-C4C-NC	3.21	125.50	121.15
82	ZM	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	lF	202	PEB	CMC-C3C-C4C	3.21	130.47	127.06
82	U9	203	PEB	OD-C4D-ND	-3.21	121.17	125.93
82	x8	202	PEB	CHA-C4A-NA	-3.21	121.38	125.20
82	HB	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	wC	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	RK	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	L7	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	dM	203	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	GF	203	PEB	CHB-C1C-C2C	-3.21	119.90	127.15
82	Y9	202	PEB	OD-C4D-ND	-3.21	121.17	125.93
82	hJ	202	PEB	OD-C4D-ND	-3.21	121.17	125.93
87	B6	611	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
82	P1	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
82	KF	203	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	QQ	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	UG	203	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	OJ	203	PEB	OD-C4D-ND	-3.21	121.17	125.93
84	H4	1001	CYC	CMA-C3A-C4A	3.21	130.01	125.06
82	ZG	203	PEB	C2A-C1A-NA	3.21	111.04	108.27
87	AL	404	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
87	C6	515	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
82	VP	201	PEB	CHA-C1B-NB	-3.21	118.21	124.93
82	QP	202	PEB	C3D-C4D-ND	3.21	113.56	107.26
82	RH	201	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	lK	202	PEB	CMC-C3C-C4C	3.21	130.47	127.06
82	AE	304	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	EP	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	WG	201	PEB	OD-C4D-C3D	-3.21	122.18	129.46
82	ZE	202	PEB	C1D-CHC-C4C	-3.21	108.52	113.26
82	XI	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	GJ	203	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	SP	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	yF	301	PEB	C3B-C4B-NB	3.21	114.72	110.05
87	3N	301	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
82	AM	302	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	D9	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
84	BG	1002	CYC	C2C-C1C-NC	3.21	111.04	108.27
87	52	604	CLA	CHB-C4A-NA	3.21	128.95	124.51
82	u8	202	PEB	OD-C4D-C3D	-3.21	122.19	129.46
82	JK	202	PEB	CHA-C1B-NB	-3.21	118.22	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XQ	202	PEB	CHA-C1B-NB	-3.21	118.22	124.93
82	HB	201	PEB	CMB-C2B-C1B	3.21	130.01	125.06
82	h4	201	PEB	CMB-C2B-C1B	3.21	130.01	125.06
82	O4	201	PEB	OD-C4D-ND	-3.21	121.17	125.93
82	CM	203	PEB	C3B-C4B-NB	3.21	114.72	110.05
85	B6	621	BCR	C24-C23-C22	-3.21	121.38	126.23
85	fL	101	BCR	C7-C8-C9	-3.21	121.38	126.23
82	nK	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	YK	201	PEB	CHA-C1B-NB	-3.21	118.22	124.93
82	lG	201	PEB	C1C-CHB-C4B	3.21	135.48	128.28
82	YF	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	NG	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	DO	1002	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	YQ	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
84	GG	1001	CYC	C1A-C2A-C3A	-3.21	103.23	106.78
82	XK	203	PEB	CHB-C1C-NC	-3.21	117.97	125.32
82	JJ	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
82	Y4	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
82	MF	203	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	yK	301	PEB	C3B-C4B-NB	3.21	114.72	110.05
87	12	610	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
87	bL	620	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
82	KK	203	PEB	C3D-C4D-ND	3.21	113.56	107.26
82	C5	201	PEB	CMA-C2A-C1A	-3.21	105.48	112.40
82	SG	201	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	P9	201	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
87	AN	805	CLA	C3B-C4B-NB	-3.21	107.54	110.52
82	RG	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	hE	201	PEB	OD-C4D-C3D	-3.21	122.19	129.46
82	ZJ	202	PEB	CHC-C4C-NC	3.21	125.49	121.15
82	HA	203	PEB	CHC-C1D-ND	-3.21	109.67	113.72
82	SH	201	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
82	s8	203	PEB	OD-C4D-ND	-3.21	121.18	125.93
82	iF	201	PEB	OD-C4D-ND	-3.21	121.18	125.93
82	QH	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
82	VI	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	T5	202	PEB	CHC-C4C-NC	3.21	125.49	121.15
82	Z5	304	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
88	AL	406	LHG	O8-C23-C24	3.21	121.97	111.91
84	V3	1001	CYC	CAA-C2A-C1A	3.21	130.68	125.01
87	A2	811	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
82	RQ	202	PEB	OD-C4D-ND	-3.21	121.18	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JA	203	PEB	C3B-C4B-NB	3.21	114.72	110.05
82	G7	201	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
82	YJ	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	BA	202	PEB	CMB-C2B-C1B	3.21	130.00	125.06
82	UJ	201	PEB	CMB-C2B-C1B	3.21	130.00	125.06
82	ZO	202	PEB	CMB-C2B-C1B	3.21	130.00	125.06
82	A7	202	PEB	CMB-C2B-C1B	3.21	130.00	125.06
87	A2	820	CLA	O2A-C1-C2	-3.21	100.21	108.64
82	f4	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
84	C1	1001	CYC	C4D-C3D-C2D	-3.21	103.83	107.62
82	KI	203	PEB	C3B-C4B-NB	3.21	114.71	110.05
82	OI	202	PEB	OD-C4D-C3D	-3.21	122.19	129.46
82	BI	203	PEB	CMB-C2B-C1B	3.21	130.00	125.06
87	AN	832	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
82	RH	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	SQ	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	WF	202	PEB	C3B-C4B-NB	3.21	114.71	110.05
82	kH	202	PEB	CMC-C3C-C4C	3.21	130.46	127.06
82	VF	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
82	KK	203	PEB	C2A-C1A-NA	3.21	111.04	108.27
87	ON	201	CLA	CAA-C2A-C3A	-3.21	108.62	116.10
82	T1	201	PEB	C3C-C4C-NC	3.21	111.22	108.33
82	SP	201	PEB	C2C-C1C-NC	3.21	111.89	107.57
82	sK	201	PEB	CHC-C4C-NC	3.21	125.49	121.15
82	FB	201	PEB	CMB-C2B-C1B	3.21	130.00	125.06
92	J6	102	LMG	O6-C1-C2	-3.21	103.56	110.35
82	k1	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
95	lL	101	DGD	O1G-C1A-C2A	3.21	121.97	111.91
82	KJ	202	PEB	C3B-C4B-NB	3.21	114.71	110.05
82	dQ	401	PEB	C3B-C4B-NB	3.21	114.71	110.05
82	YP	503	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
82	k1	202	PEB	CMC-C3C-C4C	3.21	130.46	127.06
82	CM	203	PEB	CMB-C2B-C1B	3.21	130.00	125.06
82	m4	201	PEB	CHC-C4C-NC	3.21	125.49	121.15
82	JJ	202	PEB	CMA-C2A-C1A	-3.21	105.49	112.40
82	E7	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
85	BN	840	BCR	C1-C6-C5	-3.21	118.10	122.61
82	Z4	202	PEB	OD-C4D-ND	-3.20	121.18	125.93
87	AN	811	CLA	CAA-C2A-C3A	-3.20	104.00	112.78
92	mL	101	LMG	C8-O7-C10	-3.20	109.90	117.79
82	ZB	201	PEB	CAA-C3A-C2A	-3.20	106.25	114.26
82	MB	202	PEB	CMA-C2A-C1A	-3.20	105.50	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jO	202	PEB	CMB-C2B-C1B	3.20	130.00	125.06
82	rC	201	PEB	OA-C1A-C2A	-3.20	123.62	126.17
82	OI	201	PEB	CAC-CBC-CGC	-3.20	106.71	113.60
82	F1	1002	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	dM	201	PEB	OD-C4D-ND	-3.20	121.18	125.93
82	NQ	202	PEB	C3B-C4B-NB	3.20	114.71	110.05
87	AN	820	CLA	O2A-C1-C2	-3.20	100.21	108.64
87	2N	303	CLA	C2B-C1B-NB	3.20	112.38	110.23
85	CL	502	BCR	C21-C20-C19	-3.20	113.22	123.22
82	YF	201	PEB	CMB-C2B-C1B	3.20	130.00	125.06
82	wF	303	PEB	CMB-C2B-C1B	3.20	130.00	125.06
82	WM	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	UK	201	PEB	CHA-C1B-NB	-3.20	118.23	124.93
82	UP	201	PEB	CHA-C1B-NB	-3.20	118.23	124.93
82	P5	202	PEB	CHC-C4C-NC	3.20	125.48	121.15
82	LO	1002	PEB	OD-C4D-C3D	-3.20	122.20	129.46
82	WM	201	PEB	OD-C4D-ND	-3.20	121.18	125.93
82	18	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	UM	203	PEB	CMC-C3C-C4C	-3.20	123.67	127.06
85	c6	603	BCR	C8-C7-C6	3.20	136.20	127.20
82	I5	202	PEB	CHC-C4C-NC	3.20	125.48	121.15
82	V5	202	PEB	CHC-C4C-NC	3.20	125.48	121.15
82	PJ	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	HJ	202	PEB	C1C-CHB-C4B	-3.20	121.10	128.28
87	B2	829	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
82	W9	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	hG	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
87	BL	605	CLA	C3B-C4B-NB	-3.20	107.54	110.52
82	N7	203	PEB	C1C-CHB-C4B	3.20	135.46	128.28
82	QE	203	PEB	CBA-CAA-C3A	-3.20	106.34	113.47
84	KO	1001	CYC	CBC-CAC-C3C	-3.20	106.34	113.47
82	TM	202	PEB	C1D-CHC-C4C	-3.20	108.53	113.26
82	KA	201	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	QA	201	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	OK	203	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	A4	304	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	SE	201	PEB	C3B-C4B-NB	3.20	114.71	110.05
82	KJ	201	PEB	C3B-C4B-NB	3.20	114.71	110.05
82	PO	202	PEB	C3B-C4B-NB	3.20	114.71	110.05
82	N1	1002	PEB	OA-C1A-C2A	-3.20	123.63	126.17
82	O4	201	PEB	C1C-CHB-C4B	3.20	135.46	128.28
82	R7	203	PEB	CMB-C2B-C1B	3.20	130.00	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	H9	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	JF	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	KK	201	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	TD	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	UP	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
84	K4	1001	CYC	CBC-CAC-C3C	-3.20	106.34	113.47
82	PG	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	MP	201	PEB	C1C-CHB-C4B	3.20	135.46	128.28
82	OM	202	PEB	C1D-CHC-C4C	-3.20	108.54	113.26
82	Z9	303	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	M5	304	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	gB	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	UH	203	PEB	OA-C1A-C2A	-3.20	123.63	126.17
82	iG	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
82	OJ	202	PEB	C1C-CHB-C4B	-3.20	121.10	128.28
87	cL	507	CLA	CHB-C4A-NA	3.20	128.94	124.51
85	A2	846	BCR	C3-C4-C5	-3.20	108.36	114.08
82	f1	201	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	w8	204	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	hG	203	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	iO	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
82	kG	202	PEB	CHC-C1D-ND	-3.20	109.67	113.72
84	HO	1001	CYC	C2C-C1C-NC	3.20	111.03	108.27
82	T9	202	PEB	CBA-CAA-C3A	-3.20	106.34	113.47
84	KH	1001	CYC	CMA-C3A-C4A	3.20	129.99	125.06
82	YI	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	BP	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	cE	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	U4	201	PEB	CHB-C4B-NB	3.20	131.24	124.58
87	BN	829	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
82	IP	202	PEB	CHC-C1D-ND	-3.20	109.68	113.72
82	q8	202	PEB	CHC-C1D-ND	-3.20	109.68	113.72
82	kH	203	PEB	CHC-C1D-ND	-3.20	109.68	113.72
82	CJ	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
84	EO	1001	CYC	C4A-C3A-C2A	-3.20	102.83	106.51
82	MB	202	PEB	C1D-CHC-C4C	-3.20	108.54	113.26
87	42	608	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
82	DJ	202	PEB	CHB-C4B-NB	-3.20	117.92	124.58
85	c6	602	BCR	C4-C5-C6	-3.20	118.09	122.73
82	AF	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	fM	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	YO	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	x3	1001	CYC	CAA-C2A-C1A	3.20	130.67	125.01
82	X5	201	PEB	CMA-C2A-C1A	-3.20	105.51	112.40
82	dH	201	PEB	CHA-C1B-NB	-3.20	118.24	124.93
87	AN	851	CLA	CHB-C4A-NA	3.20	128.94	124.51
82	cM	201	PEB	C1C-CHB-C4B	-3.20	121.11	128.28
82	GE	1002	PEB	CAC-CBC-CGC	-3.20	106.72	113.60
84	N4	1001	CYC	C2B-C1B-NB	3.20	111.67	106.99
82	U1	203	PEB	OA-C1A-C2A	-3.20	123.63	126.17
82	NM	201	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	VP	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	H5	202	PEB	CHC-C1D-ND	-3.20	109.68	113.72
95	C6	503	DGD	O2G-C1B-O1B	-3.20	115.97	123.70
82	SD	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	YK	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	TO	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	dB	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
82	aM	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
84	HO	1001	CYC	CMA-C3A-C4A	3.20	129.99	125.06
82	D7	201	PEB	CHA-C1B-C2B	3.20	133.12	124.90
84	MG	1001	CYC	C2A-C1A-NA	3.20	114.70	110.05
82	R5	202	PEB	CHC-C4C-NC	3.20	125.48	121.15
92	j6	101	LMG	O6-C1-C2	-3.20	103.58	110.35
82	YB	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
82	g4	203	PEB	CAB-C3B-C2B	3.20	133.83	127.88
82	V4	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
82	lK	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
84	MG	1001	CYC	C1A-C2A-C3A	-3.20	103.24	106.78
82	H9	203	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
82	GE	1002	PEB	OD-C4D-C3D	-3.20	122.22	129.46
82	SO	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	U9	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
82	v8	201	PEB	CMB-C2B-C1B	3.20	129.99	125.06
82	dK	202	PEB	CHB-C1C-NC	-3.20	118.00	125.32
83	xF	301	PUB	CMD-C2D-C3D	3.20	132.57	127.77
82	NI	202	PEB	C3B-C4B-NB	3.20	114.70	110.05
82	N9	202	PEB	CBA-CAA-C3A	-3.20	106.35	113.47
82	H5	201	PEB	C2C-C1C-NC	3.20	111.88	107.57
82	CF	201	PEB	C4B-C3B-C2B	-3.20	103.25	106.78
82	MJ	203	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
82	SM	203	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
82	D9	201	PEB	CAB-C3B-C4B	3.20	130.66	125.01
82	JJ	201	PEB	C3B-C4B-NB	3.20	114.70	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	k1	201	PEB	C3B-C4B-NB	3.20	114.70	110.05
84	J4	1001	CYC	C2C-C1C-NC	3.20	111.03	108.27
82	lO	201	PEB	C4B-NB-C1B	-3.20	100.49	106.51
82	OM	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
82	wC	202	PEB	CAB-CBB-CGB	-3.20	106.73	113.60
82	KF	203	PEB	C3D-C4D-ND	3.20	113.53	107.26
82	TF	202	PEB	C4B-C3B-C2B	-3.20	103.25	106.78
82	W1	202	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
84	NH	1001	CYC	C4A-C3A-C2A	-3.20	102.84	106.51
82	DA	201	PEB	CHA-C1B-C2B	3.20	133.12	124.90
82	oK	203	PEB	CHA-C1B-NB	-3.20	118.25	124.93
84	W3	1001	CYC	C1B-CHB-C4A	3.20	135.89	128.08
82	F9	202	PEB	C1C-CHB-C4B	3.19	135.45	128.28
82	A1	301	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	mF	201	PEB	CMB-C2B-C1B	3.19	129.98	125.06
82	SH	203	PEB	C2A-C1A-NA	3.19	111.03	108.27
82	SP	201	PEB	C2A-C1A-NA	3.19	111.03	108.27
82	dE	204	PEB	C2A-C1A-NA	3.19	111.03	108.27
82	RI	202	PEB	C3B-C4B-NB	3.19	114.70	110.05
82	UF	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	fH	202	PEB	CHB-C4B-NB	-3.19	117.93	124.58
82	w8	202	PEB	CAB-CBB-CGB	-3.19	106.73	113.60
82	g4	202	PEB	CMB-C2B-C1B	3.19	129.98	125.06
82	mJ	202	PEB	CMB-C2B-C1B	3.19	129.98	125.06
82	TE	201	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	YO	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	lG	203	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	M9	304	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	c4	203	PEB	CHC-C4C-NC	3.19	125.47	121.15
82	GK	203	PEB	CHB-C1C-C2C	-3.19	119.94	127.15
82	oK	203	PEB	OD-C4D-C3D	-3.19	122.22	129.46
82	GI	203	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	AE	304	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	QH	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	J5	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	E9	201	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
82	lE	201	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
84	N1	1001	CYC	C4A-C3A-C2A	-3.19	102.84	106.51
82	kH	203	PEB	C3D-C4D-ND	3.19	113.53	107.26
82	OH	202	PEB	CHB-C4B-NB	-3.19	117.93	124.58
84	MO	1001	CYC	C4D-C3D-C2D	-3.19	103.85	107.62
82	VB	201	PEB	C2A-C1A-NA	3.19	111.03	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bF	201	PEB	C2A-C1A-NA	3.19	111.03	108.27
82	H7	202	PEB	CHC-C1D-ND	-3.19	109.68	113.72
85	BN	840	BCR	C33-C5-C6	-3.19	120.94	124.53
82	RJ	202	PEB	CHA-C1B-NB	-3.19	118.25	124.93
82	Q7	201	PEB	CBB-CAB-C3B	-3.19	103.75	112.63
82	OG	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	RM	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	iO	203	PEB	C3B-C4B-NB	3.19	114.69	110.05
95	hL	101	DGD	O1G-C1A-C2A	3.19	121.93	111.91
82	QH	201	PEB	CHA-C1B-NB	-3.19	118.25	124.93
82	AK	201	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	U5	203	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	fM	202	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
95	lL	101	DGD	C1D-C2D-C3D	3.19	116.64	110.00
82	II	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	HH	1002	PEB	C2A-C1A-NA	3.19	111.03	108.27
82	QG	203	PEB	CBA-CAA-C3A	-3.19	106.36	113.47
82	A9	202	PEB	CBA-CAA-C3A	-3.19	106.36	113.47
82	q8	202	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
82	rC	202	PEB	CHA-C4A-NA	-3.19	121.41	125.20
82	w8	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	UA	201	PEB	C3C-C4C-NC	3.19	111.21	108.33
82	OH	203	PEB	C3C-C4C-NC	3.19	111.21	108.33
82	C9	202	PEB	CBA-CAA-C3A	-3.19	106.36	113.47
82	I9	202	PEB	CBA-CAA-C3A	-3.19	106.36	113.47
82	F5	201	PEB	CAB-CBB-CGB	-3.19	106.73	113.60
82	SM	202	PEB	C2A-C1A-NA	3.19	111.02	108.27
82	aB	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	HM	202	PEB	CHC-C1D-ND	-3.19	109.69	113.72
87	b6	615	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
84	E1	1001	CYC	C4A-C3A-C2A	-3.19	102.84	106.51
82	F7	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
91	aL	610	PHO	CMB-C2B-C3B	3.19	130.65	124.68
82	EF	202	PEB	C1D-CHC-C4C	-3.19	108.55	113.26
82	SJ	202	PEB	C1D-CHC-C4C	-3.19	108.55	113.26
82	IJ	202	PEB	CMA-C2A-C1A	-3.19	105.53	112.40
82	WH	202	PEB	CHB-C1C-NC	-3.19	118.01	125.32
82	UI	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
87	4N	608	CLA	CMB-C2B-C1B	-3.19	120.51	125.37
82	L5	202	PEB	CAB-C3B-C4B	3.19	130.65	125.01
82	E9	202	PEB	CBA-CAA-C3A	-3.19	106.36	113.47
85	B2	838	BCR	C30-C25-C26	-3.19	118.12	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WE	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	R9	201	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
84	KH	1001	CYC	C4D-C3D-C2D	-3.19	103.85	107.62
82	UE	203	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	V4	202	PEB	C2A-C1A-NA	3.19	111.02	108.27
82	QB	201	PEB	OD-C4D-C3D	-3.19	122.23	129.46
82	E5	201	PEB	CMA-C2A-C1A	-3.19	105.53	112.40
82	DK	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	TO	201	PEB	CHC-C4C-NC	3.19	125.47	121.15
82	YO	202	PEB	CMB-C2B-C1B	3.19	129.98	125.06
82	W5	203	PEB	CAC-CBC-CGC	-3.19	106.74	113.60
85	K2	102	BCR	C8-C7-C6	3.19	136.16	127.20
87	B6	604	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
82	EM	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	MQ	201	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	gM	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
82	V9	202	PEB	CBA-CAA-C3A	-3.19	106.37	113.47
82	D9	201	PEB	O2B-CGB-CBB	3.19	124.28	114.03
87	82	306	CLA	CAC-C3C-C2C	3.19	132.98	127.53
82	G9	201	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
82	GD	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
82	HJ	202	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	UM	203	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	eF	203	PEB	C3D-C4D-ND	3.19	113.52	107.26
95	C6	502	DGD	O6D-C1D-C2D	-3.19	103.60	110.35
82	MP	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	mJ	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	KA	202	PEB	CHC-C4C-NC	3.19	125.46	121.15
82	ZB	203	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	qK	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	MJ	202	PEB	CMA-C2A-C1A	-3.19	105.53	112.40
87	aL	605	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
85	B6	621	BCR	C3-C4-C5	-3.19	108.39	114.08
84	DH	1001	CYC	CMB-C2B-C1B	3.19	128.15	124.17
82	PI	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	RJ	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
82	ZE	203	PEB	C2A-C1A-NA	3.19	111.02	108.27
82	PD	203	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
84	EH	1001	CYC	C4A-C3A-C2A	-3.19	102.85	106.51
82	PM	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	jH	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	HA	202	PEB	CHB-C1C-C2C	-3.19	119.96	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OO	201	PEB	C1C-CHB-C4B	3.19	135.43	128.28
82	aJ	204	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	XF	201	PEB	C1C-C2C-C3C	-3.19	103.85	107.62
82	UO	202	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
85	h6	102	BCR	C3-C4-C5	-3.19	108.39	114.08
82	MQ	202	PEB	C2A-C1A-NA	3.19	111.02	108.27
82	rC	202	PEB	C2A-C1A-NA	3.19	111.02	108.27
84	y3	1001	CYC	C1B-CHB-C4A	3.19	135.87	128.08
82	AM	301	PEB	C3B-C4B-NB	3.19	114.68	110.05
82	JF	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	A1	305	PEB	OD-C4D-ND	-3.19	121.21	125.93
82	j1	203	PEB	C3C-C4C-NC	3.19	111.20	108.33
82	S5	201	PEB	C3C-C4C-NC	3.19	111.20	108.33
82	NP	201	PEB	CHC-C4C-NC	3.19	125.46	121.15
87	1N	610	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
82	AH	301	PEB	CMB-C2B-C1B	3.19	129.97	125.06
82	P9	202	PEB	CBA-CAA-C3A	-3.19	106.37	113.47
82	AJ	302	PEB	OA-C1A-C2A	-3.19	123.64	126.17
82	TB	202	PEB	CMC-C3C-C2C	-3.19	118.71	125.61
84	EH	1001	CYC	CHB-C4A-C3A	3.19	133.09	124.90
82	qC	202	PEB	CHC-C1D-ND	-3.19	109.69	113.72
85	B6	602	BCR	C28-C27-C26	-3.19	108.39	114.08
82	L5	203	PEB	C4B-C3B-C2B	-3.19	103.26	106.78
82	WI	203	PEB	OD-C4D-ND	-3.19	121.21	125.93
84	63	901	CYC	C2B-C1B-NB	3.19	111.65	106.99
82	TP	201	PEB	C2A-C1A-NA	3.19	111.02	108.27
85	BN	838	BCR	C30-C25-C26	-3.19	118.13	122.61
82	AD	301	PEB	OD-C4D-C3D	-3.19	122.24	129.46
88	bL	612	LHG	O8-C23-C24	3.19	121.90	111.91
82	KM	202	PEB	C3C-C4C-NC	3.18	111.20	108.33
82	hJ	201	PEB	C3C-C4C-NC	3.18	111.20	108.33
82	lJ	201	PEB	C3C-C4C-NC	3.18	111.20	108.33
82	W1	202	PEB	CHB-C1C-NC	-3.18	118.02	125.32
82	jM	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	y8	203	PEB	CHB-C4B-NB	-3.18	117.95	124.58
82	OG	203	PEB	C1B-C2B-C3B	-3.18	102.85	106.51
82	X9	202	PEB	CBA-CAA-C3A	-3.18	106.38	113.47
82	A4	304	PEB	CHA-C1B-NB	-3.18	118.27	124.93
82	CJ	203	PEB	OD-C4D-ND	-3.18	121.21	125.93
82	J7	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	wC	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
83	Y7	302	PUB	C1C-C2C-C3C	-3.18	103.26	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	B6	601	BCR	C7-C8-C9	-3.18	121.42	126.23
82	mE	202	PEB	CMC-C3C-C4C	3.18	130.44	127.06
82	VO	202	PEB	CMB-C2B-C1B	3.18	129.97	125.06
82	M5	301	PEB	OA-C1A-C2A	-3.18	123.64	126.17
82	EI	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	EP	203	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	OI	201	PEB	C2A-C1A-NA	3.18	111.02	108.27
82	IQ	201	PEB	C2A-C1A-NA	3.18	111.02	108.27
83	KA	203	PUB	OA-C1A-NA	-3.18	121.21	125.93
82	V9	201	PEB	C1B-C2B-C3B	-3.18	102.85	106.51
82	R9	202	PEB	CBA-CAA-C3A	-3.18	106.38	113.47
82	PE	201	PEB	CHC-C1D-ND	-3.18	109.70	113.72
82	FP	202	PEB	CHA-C1B-NB	-3.18	118.27	124.93
82	UB	301	PEB	OD-C4D-C3D	-3.18	122.25	129.46
82	MM	203	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
84	d3	1001	CYC	C1A-C2A-C3A	-3.18	103.26	106.78
85	c6	617	BCR	C21-C20-C19	3.18	133.15	123.22
82	WG	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	kO	201	PEB	C3B-C4B-NB	3.18	114.68	110.05
87	8N	301	CLA	CAC-C3C-C2C	3.18	132.97	127.53
82	YO	201	PEB	OD-C4D-ND	-3.18	121.21	125.93
82	Y5	203	PEB	OD-C4D-ND	-3.18	121.21	125.93
82	W9	202	PEB	OD-C4D-ND	-3.18	121.21	125.93
82	LD	203	PEB	CHB-C1C-C2C	-3.18	119.97	127.15
82	CI	202	PEB	CHA-C1B-NB	-3.18	118.27	124.93
82	JB	202	PEB	CMC-C3C-C2C	-3.18	118.72	125.61
82	Z5	301	PEB	OA-C1A-C2A	-3.18	123.64	126.17
82	BD	201	PEB	CMB-C2B-C1B	3.18	129.97	125.06
82	O7	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
82	LO	1002	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	LP	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	m4	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	kG	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	BJ	301	PEB	CHB-C1C-NC	-3.18	118.03	125.32
82	AH	305	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	EK	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
87	52	601	CLA	CHB-C4A-NA	3.18	128.91	124.51
82	CB	201	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	cM	201	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	qF	203	PEB	OA-C1A-C2A	-3.18	123.64	126.17
82	DB	202	PEB	CHA-C1B-NB	-3.18	118.28	124.93
82	MM	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O9	203	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
84	GE	1001	CYC	C1A-C2A-C3A	-3.18	103.26	106.78
82	JB	201	PEB	C3C-C4C-NC	3.18	111.20	108.33
82	IA	201	PEB	OD-C4D-C3D	-3.18	122.25	129.46
82	iH	201	PEB	CHC-C1D-ND	-3.18	109.70	113.72
82	TI	203	PEB	C3B-C4B-NB	3.18	114.68	110.05
82	IF	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
85	BN	838	BCR	C27-C26-C25	-3.18	118.11	122.73
87	CL	510	CLA	CMB-C2B-C3B	3.18	134.29	126.59
82	VG	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	GM	203	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	GQ	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
84	F3	1001	CYC	C1A-C2A-C3A	-3.18	103.26	106.78
87	22	609	CLA	C3B-C4B-NB	-3.18	107.56	110.52
87	1N	610	CLA	C3B-C4B-NB	-3.18	107.56	110.52
82	EM	202	PEB	CHA-C1B-NB	-3.18	118.28	124.93
82	G5	202	PEB	CHC-C4C-NC	3.18	125.45	121.15
82	N5	202	PEB	CHC-C4C-NC	3.18	125.45	121.15
82	PP	202	PEB	CHC-C1D-ND	-3.18	109.70	113.72
82	tF	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
82	dO	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
82	WI	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	UM	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	W1	203	PEB	OA-C1A-C2A	-3.18	123.64	126.17
82	X9	201	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
82	IP	202	PEB	C1C-CHB-C4B	3.18	135.41	128.28
84	BG	1001	CYC	C4D-CHA-C1A	3.18	135.41	128.28
82	EM	203	PEB	C3B-C4B-NB	3.18	114.67	110.05
82	VE	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	D4	1002	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	XD	202	PEB	CHA-C1B-NB	-3.18	118.28	124.93
82	bH	201	PEB	OD-C4D-C3D	-3.18	122.25	129.46
87	AN	821	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
87	A2	821	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
82	l1	201	PEB	C3D-C4D-ND	3.18	113.50	107.26
82	CK	203	PEB	C2A-C1A-NA	3.18	111.01	108.27
82	BD	203	PEB	CHA-C1B-NB	-3.18	118.28	124.93
82	R4	203	PEB	CAB-CBB-CGB	3.18	120.44	113.60
82	mM	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	SM	203	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
82	gJ	201	PEB	CHB-C4B-NB	-3.18	117.96	124.58
87	AN	814	CLA	CHB-C4A-NA	3.18	128.91	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	2N	309	CLA	C3B-C4B-NB	-3.18	107.57	110.52
82	MP	201	PEB	CMA-C2A-C1A	-3.18	105.55	112.40
82	lM	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	G9	202	PEB	CBA-CAA-C3A	-3.18	106.39	113.47
82	h4	202	PEB	CHC-C1D-ND	-3.18	109.70	113.72
82	AK	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
82	FQ	201	PEB	C3C-C4C-NC	3.18	111.19	108.33
87	2N	306	CLA	CHB-C4A-NA	3.18	128.91	124.51
82	AB	501	PEB	OA-C1A-C2A	-3.18	123.65	126.17
82	cK	202	PEB	CHA-C1B-NB	-3.18	118.28	124.93
82	XK	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	g4	201	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
82	E5	202	PEB	CHC-C4C-NC	3.18	125.45	121.15
82	WE	201	PEB	OD-C4D-C3D	-3.18	122.26	129.46
87	bL	621	CLA	CHB-C4A-NA	3.18	128.91	124.51
85	B2	840	BCR	C37-C22-C21	-3.18	118.47	122.92
84	LH	1002	CYC	CHA-C1A-C2A	-3.18	117.97	125.32
84	I3	1001	CYC	C1A-C2A-C3A	-3.18	103.27	106.78
82	ZE	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	Y4	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	hE	201	PEB	C2A-C1A-NA	3.18	111.01	108.27
82	WP	201	PEB	CHA-C1B-NB	-3.18	118.29	124.93
82	h1	201	PEB	CHA-C1B-NB	-3.18	118.29	124.93
82	mO	201	PEB	CHA-C1B-NB	-3.18	118.29	124.93
87	CL	506	CLA	C3C-C4C-NC	-3.18	107.01	110.57
82	U9	202	PEB	OA-C1A-C2A	-3.18	123.65	126.17
82	lJ	202	PEB	CMA-C2A-C1A	-3.18	105.56	112.40
82	PG	201	PEB	CHC-C1D-ND	-3.18	109.70	113.72
87	5N	604	CLA	CHB-C4A-NA	3.18	128.91	124.51
87	R2	202	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
82	kK	201	PEB	C3B-C4B-NB	3.18	114.67	110.05
82	cJ	201	PEB	CMB-C2B-C1B	3.18	129.96	125.06
82	JK	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	cB	402	PEB	OD-C4D-ND	-3.18	121.22	125.93
87	B2	828	CLA	C3B-C4B-NB	-3.18	107.57	110.52
85	B2	840	BCR	C33-C5-C6	-3.18	120.96	124.53
82	SF	203	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
82	YM	203	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
84	H3	1001	CYC	C1A-C2A-C3A	-3.18	103.27	106.78
82	C5	202	PEB	CHC-C4C-NC	3.18	125.45	121.15
82	mO	201	PEB	CHC-C4C-NC	3.18	125.45	121.15
82	Z9	304	PEB	CHB-C4B-NB	-3.18	117.97	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	sC	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
87	4N	610	CLA	CHB-C4A-NA	3.18	128.90	124.51
82	VO	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
82	iO	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
82	JD	201	PEB	CMB-C2B-C1B	3.18	129.96	125.06
82	IM	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	LQ	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
82	aF	201	PEB	C1D-CHC-C4C	3.18	117.94	113.26
87	BN	802	CLA	CHC-C4B-NB	3.18	127.62	124.26
82	iM	202	PEB	C1C-CHB-C4B	-3.18	121.16	128.28
84	BG	1001	CYC	OB-C4B-C3B	-3.18	124.59	128.04
82	NH	1002	PEB	OA-C1A-C2A	-3.18	123.65	126.17
82	AO	304	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
82	Q1	201	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
82	eO	202	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
82	K9	202	PEB	CBA-CAA-C3A	-3.18	106.40	113.47
87	A2	819	CLA	CHB-C4A-NA	3.18	128.90	124.51
82	UH	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
82	I9	201	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
82	T9	201	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
82	BD	201	PEB	C3B-C4B-NB	3.18	114.67	110.05
82	oF	201	PEB	OD-C4D-ND	-3.18	121.23	125.93
82	UO	201	PEB	CHB-C4B-NB	3.18	131.19	124.58
82	QE	203	PEB	CHC-C1D-ND	-3.18	109.71	113.72
82	pK	201	PEB	CHC-C4C-NC	3.17	125.45	121.15
82	AD	301	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	EM	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	dK	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
84	ME	1001	CYC	C1A-C2A-C3A	-3.17	103.27	106.78
82	AI	202	PEB	C3B-C4B-NB	3.17	114.67	110.05
83	Z9	302	PUB	C2C-C1C-NC	3.17	114.67	110.05
82	SK	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	P7	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	L9	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	bB	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	gO	203	PEB	CAB-C3B-C2B	3.17	133.79	127.88
82	M9	305	PEB	CHB-C4B-NB	-3.17	117.97	124.58
82	FI	201	PEB	OD-C4D-C3D	-3.17	122.27	129.46
84	ME	1001	CYC	CHA-C4D-C3D	-3.17	119.99	127.15
82	II	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	dE	201	PEB	C3B-C4B-NB	3.17	114.67	110.05
82	YA	303	PEB	C2A-C1A-NA	3.17	111.01	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iK	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	PD	203	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
82	SK	203	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
82	IM	202	PEB	CHA-C1B-C2B	3.17	133.06	124.90
87	82	306	CLA	CMC-C2C-C1C	-3.17	120.21	125.04
82	Q4	201	PEB	CHA-C4A-NA	3.17	128.98	125.20
82	NB	202	PEB	C3B-C4B-NB	3.17	114.67	110.05
82	WA	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
82	fJ	203	PEB	C3C-C4C-NC	3.17	111.19	108.33
82	PE	202	PEB	C1B-C2B-C3B	-3.17	102.86	106.51
82	WP	201	PEB	C1B-C2B-C3B	-3.17	102.86	106.51
82	OA	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	WB	402	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	OE	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	d4	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	P7	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	dE	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	kF	201	PEB	C3B-C4B-NB	3.17	114.66	110.05
82	KI	203	PEB	CHA-C1B-NB	-3.17	118.30	124.93
82	O9	201	PEB	O2B-CGB-CBB	3.17	124.22	114.03
82	OA	202	PEB	C3D-C4D-ND	3.17	113.48	107.26
82	YA	303	PEB	CMB-C2B-C1B	3.17	129.95	125.06
82	Y4	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
87	B2	824	CLA	CHB-C1B-NB	3.17	127.61	124.26
82	dD	401	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
84	EH	1001	CYC	C1A-C2A-C3A	-3.17	103.27	106.78
82	f1	202	PEB	CHB-C4B-NB	-3.17	117.98	124.58
82	RE	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	QJ	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	wK	303	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	GD	202	PEB	CAC-C2C-C3C	3.17	134.33	127.07
87	KN	103	CLA	CHB-C4A-NA	3.17	128.90	124.51
82	EA	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	aG	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
82	IB	203	PEB	C3B-C4B-NB	3.17	114.66	110.05
84	u3	1001	CYC	C1A-C2A-C3A	-3.17	103.27	106.78
87	KN	105	CLA	CHB-C1B-NB	3.17	127.61	124.26
87	B2	816	CLA	CHB-C1B-NB	3.17	127.61	124.26
95	c6	601	DGD	O6D-C1D-C2D	-3.17	103.64	110.35
82	OJ	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
82	S5	203	PEB	OA-C1A-C2A	-3.17	123.65	126.17
82	KF	201	PEB	OD-C4D-ND	-3.17	121.23	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	xF	305	PUB	OA-C1A-NA	-3.17	121.23	125.93
82	SJ	203	PEB	C3C-C4C-NC	3.17	111.19	108.33
83	M9	303	PUB	C2C-C1C-NC	3.17	114.66	110.05
84	KG	202	CYC	C2A-C1A-NA	3.17	114.66	110.05
82	NI	202	PEB	CHA-C1B-NB	-3.17	118.30	124.93
82	OI	201	PEB	C2C-C1C-NC	3.17	111.84	107.57
82	mG	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
82	GI	203	PEB	CHA-C1B-NB	-3.17	118.30	124.93
82	EF	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	gH	203	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	sK	202	PEB	C4C-C3C-C2C	-3.17	104.57	107.50
82	N7	201	PEB	CHC-C4C-NC	3.17	125.44	121.15
82	sK	202	PEB	CHC-C4C-NC	3.17	125.44	121.15
82	O7	202	PEB	C3D-C4D-ND	3.17	113.48	107.26
82	JM	202	PEB	CMB-C2B-C1B	3.17	129.94	125.06
82	jO	201	PEB	C4B-NB-C1B	-3.17	100.54	106.51
82	OH	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
82	UP	201	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
84	G4	1001	CYC	C1A-C2A-C3A	-3.17	103.28	106.78
82	MA	202	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
82	AD	303	PEB	OD-C4D-ND	-3.17	121.23	125.93
82	hF	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
82	wC	201	PEB	C2A-C1A-NA	3.17	111.00	108.27
82	cJ	202	PEB	C2A-C1A-NA	3.17	111.00	108.27
87	BN	828	CLA	C3B-C4B-NB	-3.17	107.58	110.52
85	KL	100	BCR	C27-C26-C25	-3.17	118.13	122.73
82	S5	201	PEB	CHC-C1D-ND	-3.17	109.72	113.72
83	AJ	304	PUB	CMA-C2A-C1A	3.17	128.84	121.39
84	BE	1001	CYC	OB-C4B-C3B	-3.17	124.60	128.04
82	L4	1002	PEB	OD-C4D-C3D	-3.17	122.28	129.46
82	bF	202	PEB	CHB-C4B-C3B	-3.17	117.99	125.32
85	C6	507	BCR	C10-C11-C12	-3.17	113.33	123.22
87	B2	801	CLA	CHC-C4B-NB	3.17	127.61	124.26
84	NO	1001	CYC	C4D-CHA-C1A	3.17	135.39	128.28
82	XI	202	PEB	CHA-C1B-NB	-3.17	118.31	124.93
82	kE	201	PEB	CHA-C1B-NB	-3.17	118.31	124.93
82	EB	501	PEB	C2A-C1A-NA	3.17	111.00	108.27
82	z8	202	PEB	C2A-C1A-NA	3.17	111.00	108.27
92	B6	618	LMG	O1-C1-C2	3.17	113.25	108.30
82	J7	201	PEB	OD-C4D-ND	-3.17	121.24	125.93
82	PG	201	PEB	CAC-C2C-C1C	3.17	130.81	125.76
82	RI	202	PEB	CHA-C1B-NB	-3.17	118.31	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mG	202	PEB	CMC-C3C-C4C	3.17	130.42	127.06
82	AP	203	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
82	PJ	201	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
82	PH	202	PEB	CMB-C2B-C1B	3.17	129.94	125.06
82	YI	201	PEB	CMB-C2B-C1B	3.17	129.94	125.06
82	hK	201	PEB	CHC-C4C-NC	3.17	125.44	121.15
82	IB	203	PEB	C2A-C1A-NA	3.17	111.00	108.27
82	E7	202	PEB	C2A-C1A-NA	3.17	111.00	108.27
82	w8	201	PEB	C2A-C1A-NA	3.17	111.00	108.27
82	nK	202	PEB	CHB-C4B-C3B	-3.17	117.99	125.32
82	TO	201	PEB	CHA-C1B-NB	-3.17	118.31	124.93
82	VP	202	PEB	CHC-C1D-ND	-3.17	109.72	113.72
82	X5	202	PEB	CHC-C1D-ND	-3.17	109.72	113.72
82	BI	202	PEB	C3D-C4D-ND	3.17	113.47	107.26
87	RN	202	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
82	YI	201	PEB	CAC-CBC-CGC	-3.17	106.79	113.60
82	QM	204	PEB	OD-C4D-C3D	-3.17	122.29	129.46
82	A5	202	PEB	CHC-C4C-NC	3.17	125.43	121.15
82	OO	201	PEB	OD-C4D-ND	-3.17	121.24	125.93
82	lM	201	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
82	L5	203	PEB	C3B-C4B-NB	3.17	114.65	110.05
82	wC	204	PEB	C3B-C4B-NB	3.17	114.65	110.05
82	aF	203	PEB	C3B-C4B-NB	3.17	114.65	110.05
82	II	202	PEB	CHA-C1B-NB	-3.17	118.31	124.93
82	JO	1002	PEB	CMB-C2B-C1B	3.17	129.94	125.06
82	Y7	303	PEB	CMB-C2B-C1B	3.17	129.94	125.06
82	vK	202	PEB	CMB-C2B-C1B	3.17	129.94	125.06
82	AO	304	PEB	C2A-C1A-NA	3.17	111.00	108.27
82	jM	203	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
82	XK	201	PEB	C1C-C2C-C3C	-3.17	103.88	107.62
82	Q1	201	PEB	CHA-C1B-NB	-3.17	118.31	124.93
82	TM	201	PEB	OD-C4D-ND	-3.17	121.24	125.93
82	PF	202	PEB	C3B-C4B-NB	3.17	114.65	110.05
82	FQ	202	PEB	C3B-C4B-NB	3.17	114.65	110.05
82	oF	203	PEB	OD-C4D-C3D	-3.16	122.29	129.46
82	DB	201	PEB	CMA-C2A-C1A	-3.16	105.58	112.40
87	12	610	CLA	C3B-C4B-NB	-3.16	107.58	110.52
82	AG	304	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
82	GM	202	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
82	dM	202	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
84	h3	1001	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
85	BN	840	BCR	C7-C8-C9	-3.16	121.45	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YK	202	PEB	CHC-C4C-NC	3.16	125.43	121.15
82	L7	201	PEB	CAB-CBB-CGB	-3.16	106.79	113.60
82	Y5	202	PEB	OD-C4D-ND	-3.16	121.24	125.93
82	ZO	202	PEB	C2A-C1A-NA	3.16	111.00	108.27
87	K2	106	CLA	CHB-C1B-NB	3.16	127.61	124.26
82	AO	304	PEB	CHA-C1B-NB	-3.16	118.31	124.93
96	f6	101	HEM	CHD-C1D-ND	3.16	127.86	124.42
92	b6	620	LMG	C8-O7-C10	-3.16	110.00	117.79
82	QP	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	N9	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	dF	202	PEB	CHB-C1C-NC	-3.16	118.07	125.32
82	YH	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
82	fJ	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
84	D4	1001	CYC	C2C-C1C-NC	3.16	111.00	108.27
82	QG	201	PEB	C1C-CHB-C4B	3.16	135.38	128.28
82	Q7	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	KQ	201	PEB	C3B-C4B-NB	3.16	114.65	110.05
84	JH	1001	CYC	C2A-C1A-NA	3.16	114.65	110.05
82	UB	302	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
84	73	1001	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
82	jH	203	PEB	C3C-C4C-NC	3.16	111.18	108.33
82	fF	202	PEB	CHC-C1D-ND	3.16	117.73	113.72
82	vC	202	PEB	CAB-C3B-C4B	3.16	130.60	125.01
82	WF	202	PEB	CHC-C4C-NC	3.16	125.43	121.15
84	EE	1001	CYC	C4D-CHA-C1A	3.16	135.37	128.28
87	CL	508	CLA	CHB-C4A-NA	3.16	128.88	124.51
83	AQ	302	PUB	C4A-CHA-C1B	3.16	117.92	113.26
82	AO	304	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	EP	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	h4	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	jE	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
84	HG	1001	CYC	C4A-C3A-C2A	-3.16	102.88	106.51
82	gF	202	PEB	C3B-C4B-NB	3.16	114.65	110.05
82	g1	202	PEB	CAA-C3A-C4A	3.16	120.79	112.67
87	aL	606	CLA	C6-C5-C3	-3.16	105.16	113.45
85	C6	507	BCR	C16-C17-C18	-3.16	122.80	127.31
82	GA	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
82	m4	201	PEB	CHA-C1B-NB	-3.16	118.32	124.93
82	JA	203	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	UG	203	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	GG	1002	PEB	CAC-CBC-CGC	-3.16	106.80	113.60
82	BQ	201	PEB	CMB-C2B-C1B	3.16	129.93	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mM	202	PEB	CAB-C3B-C4B	3.16	130.60	125.01
82	OM	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	S1	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	RP	202	PEB	CHA-C1B-NB	-3.16	118.32	124.93
85	b6	601	BCR	C38-C26-C25	-3.16	120.98	124.53
82	mE	201	PEB	CMB-C2B-C1B	3.16	129.93	125.06
82	lK	203	PEB	CMB-C2B-C1B	3.16	129.93	125.06
82	BI	203	PEB	C2A-C1A-NA	3.16	111.00	108.27
82	kM	202	PEB	CHB-C4B-NB	-3.16	118.00	124.58
82	VI	202	PEB	CHA-C1B-NB	-3.16	118.32	124.93
82	aJ	202	PEB	C3B-C4B-NB	3.16	114.65	110.05
83	xK	301	PUB	CAB-CBB-CGB	-3.16	106.80	113.60
82	QE	201	PEB	C1C-CHB-C4B	3.16	135.37	128.28
82	GQ	202	PEB	CAC-C2C-C3C	3.16	134.31	127.07
82	WG	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	A4	304	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	TH	201	PEB	C3C-C4C-NC	3.16	111.18	108.33
82	RI	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	DI	201	PEB	CMB-C2B-C1B	3.16	129.93	125.06
87	8N	301	CLA	CMC-C2C-C1C	-3.16	120.23	125.04
82	YA	301	PEB	OD-C4D-C3D	-3.16	122.30	129.46
82	LA	201	PEB	CAB-CBB-CGB	-3.16	106.80	113.60
82	fK	202	PEB	CHC-C1D-ND	3.16	117.72	113.72
82	l1	201	PEB	CHC-C1D-ND	-3.16	109.73	113.72
82	UQ	201	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
82	jJ	203	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
82	sC	201	PEB	CHC-C4C-NC	3.16	125.43	121.15
82	H5	201	PEB	OD-C4D-C3D	-3.16	122.30	129.46
82	r8	202	PEB	CHA-C4A-NA	-3.16	121.45	125.20
82	iM	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
82	eH	202	PEB	CMB-C2B-C1B	3.16	129.93	125.06
82	CI	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	qF	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	V1	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
82	VH	201	PEB	CHC-C4C-NC	3.16	125.42	121.15
87	dL	409	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
85	KN	101	BCR	C8-C7-C6	3.16	136.07	127.20
84	j3	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
84	MG	1001	CYC	CHA-C4D-C3D	-3.16	120.02	127.15
82	W7	201	PEB	C1D-CHC-C4C	3.16	117.91	113.26
85	AL	401	BCR	C36-C18-C17	-3.16	118.50	122.92
84	NE	201	CYC	C2A-C1A-NA	3.16	114.64	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	42	610	CLA	CHB-C4A-NA	3.16	128.88	124.51
82	LG	1002	PEB	C2A-C1A-NA	3.16	111.00	108.27
82	cK	203	PEB	C2A-C1A-NA	3.16	111.00	108.27
82	D4	1002	PEB	CMB-C2B-C1B	3.16	129.93	125.06
84	L1	1001	CYC	CHA-C1A-C2A	-3.16	118.01	125.32
84	M3	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
84	BE	1001	CYC	C4D-CHA-C1A	3.16	135.37	128.28
82	UH	202	PEB	C3B-C4B-NB	3.16	114.64	110.05
82	RB	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	KK	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	s8	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
84	CO	1001	CYC	C4D-CHA-C1A	3.16	135.36	128.28
82	EI	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	kG	201	PEB	CHA-C1B-NB	-3.16	118.33	124.93
82	MJ	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
82	O1	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
84	q3	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
82	MM	202	PEB	C3B-C4B-NB	3.16	114.64	110.05
82	BP	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
82	i4	203	PEB	C3B-C4B-NB	3.16	114.64	110.05
85	bL	603	BCR	C11-C10-C9	-3.16	122.80	127.31
82	X5	202	PEB	CHC-C4C-NC	3.16	125.42	121.15
82	TB	201	PEB	C3C-C4C-NC	3.16	111.17	108.33
82	JI	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	TP	202	PEB	OD-C4D-ND	-3.16	121.25	125.93
82	VB	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	YK	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	H9	202	PEB	C1C-NC-C4C	-3.16	103.98	109.60
87	BN	817	CLA	CHB-C1B-NB	3.16	127.60	124.26
87	C6	519	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
82	bK	202	PEB	CHB-C4B-C3B	-3.16	118.02	125.32
82	KM	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
82	AQ	301	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
87	cL	505	CLA	CHB-C4A-NA	3.16	128.88	124.51
82	W5	202	PEB	CHA-C4A-NA	-3.16	121.45	125.20
82	UF	202	PEB	C2A-C1A-NA	3.16	110.99	108.27
82	MK	203	PEB	C2A-C1A-NA	3.16	110.99	108.27
82	UF	202	PEB	C3D-C4D-ND	3.16	113.45	107.26
82	AQ	303	PEB	C1D-CHC-C4C	-3.16	108.60	113.26
83	AD	302	PUB	C4A-CHA-C1B	3.16	117.91	113.26
82	AD	303	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
82	K9	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eM	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
82	vC	201	PEB	CMB-C2B-C1B	3.16	129.92	125.06
84	D3	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
84	S3	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
84	D4	1001	CYC	C4D-C3D-C2D	-3.16	103.89	107.62
82	KD	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
82	KF	201	PEB	C1B-C2B-C3B	-3.16	102.89	106.51
82	GM	201	PEB	C1B-C2B-C3B	-3.16	102.89	106.51
82	T4	201	PEB	CHC-C4C-NC	3.15	125.42	121.15
82	uF	203	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
82	VQ	201	PEB	OD-C4D-C3D	-3.15	122.31	129.46
85	BN	840	BCR	C37-C22-C21	-3.15	118.50	122.92
82	uK	201	PEB	CHA-C1B-C2B	3.15	133.01	124.90
82	O1	203	PEB	OD-C4D-ND	-3.15	121.26	125.93
82	S1	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
82	K7	202	PEB	OD-C4D-C3D	-3.15	122.31	129.46
82	fF	202	PEB	CMC-C3C-C2C	-3.15	118.78	125.61
82	U5	202	PEB	C3B-C4B-NB	3.15	114.64	110.05
82	XF	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
82	dJ	201	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
84	U3	1001	CYC	C1A-C2A-C3A	-3.15	103.29	106.78
82	lO	202	PEB	OD-C4D-C3D	-3.15	122.31	129.46
84	J1	1001	CYC	CAD-C3D-C4D	3.15	130.78	125.76
82	CI	202	PEB	C3B-C4B-NB	3.15	114.64	110.05
82	dG	201	PEB	C3B-C4B-NB	3.15	114.64	110.05
84	LG	1001	CYC	CMB-C2B-C1B	3.15	128.10	124.17
85	c6	603	BCR	C34-C9-C10	-3.15	118.51	122.92
85	B2	838	BCR	C27-C26-C25	-3.15	118.15	122.73
82	HD	201	PEB	C1C-CHB-C4B	3.15	135.35	128.28
84	EG	1001	CYC	C4D-CHA-C1A	3.15	135.35	128.28
82	KA	202	PEB	OD-C4D-C3D	-3.15	122.32	129.46
82	MD	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
82	gO	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
82	fK	202	PEB	CMC-C3C-C2C	-3.15	118.78	125.61
82	hF	201	PEB	CHC-C4C-NC	3.15	125.42	121.15
82	PO	202	PEB	C3C-C4C-NC	3.15	111.17	108.33
82	U4	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
82	mG	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
82	ZK	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
82	II	203	PEB	OD-C4D-C3D	-3.15	122.32	129.46
82	CP	201	PEB	C3B-C4B-NB	3.15	114.63	110.05
82	kH	201	PEB	C3B-C4B-NB	3.15	114.63	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	fJ	201	PEB	C3B-C4B-NB	3.15	114.63	110.05
84	BE	1002	CYC	C2C-C1C-NC	3.15	110.99	108.27
82	IQ	202	PEB	C1C-CHB-C4B	3.15	135.35	128.28
82	WF	203	PEB	CHC-C1D-ND	-3.15	109.74	113.72
82	fJ	202	PEB	CHB-C1C-NC	-3.15	118.10	125.32
82	BB	203	PEB	CHC-C4C-NC	3.15	125.41	121.15
82	XJ	201	PEB	C3B-C4B-NB	3.15	114.63	110.05
82	IM	203	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
82	A4	304	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
82	PI	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
92	aL	611	LMG	O8-C28-C29	3.15	121.80	111.91
82	PI	202	PEB	CHA-C1B-NB	-3.15	118.34	124.93
87	CL	503	CLA	CHB-C4A-NA	3.15	128.87	124.51
87	bL	614	CLA	CHB-C4A-NA	3.15	128.87	124.51
87	AN	820	CLA	C3B-C4B-NB	-3.15	107.59	110.52
82	AB	501	PEB	CHC-C1D-ND	-3.15	109.74	113.72
82	RA	203	PEB	CMB-C2B-C1B	3.15	129.92	125.06
85	b6	602	BCR	C36-C18-C19	3.15	123.04	118.08
82	YM	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
82	iF	203	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
85	cL	504	BCR	C21-C20-C19	-3.15	113.39	123.22
82	EM	203	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
82	EA	202	PEB	CMB-C2B-C1B	3.15	129.91	125.06
82	EI	202	PEB	CHA-C1B-NB	-3.15	118.34	124.93
82	BQ	203	PEB	CHA-C1B-NB	-3.15	118.34	124.93
82	IM	201	PEB	C3B-C4B-NB	3.15	114.63	110.05
82	DK	203	PEB	C1C-CHB-C4B	3.15	135.35	128.28
82	FB	201	PEB	OD-C4D-C3D	-3.15	122.32	129.46
82	SO	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
82	JF	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
82	FI	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
82	jE	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
82	eK	203	PEB	C3D-C4D-ND	3.15	113.44	107.26
82	GA	201	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
87	32	308	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
82	jH	203	PEB	C1C-CHB-C4B	3.15	135.34	128.28
82	TI	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	gH	203	PEB	CHA-C1B-NB	-3.15	118.35	124.93
85	c6	602	BCR	C33-C5-C4	3.15	119.67	113.62
87	cL	515	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
84	N4	1001	CYC	C4D-CHA-C1A	3.15	135.34	128.28
82	ZJ	201	PEB	C3B-C4B-NB	3.15	114.63	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	f1	201	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
84	k3	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
84	n3	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
82	A9	201	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
82	aF	203	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
82	NF	201	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	ZG	201	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	AI	201	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	XJ	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
84	F1	1001	CYC	CHD-C1D-ND	-3.15	118.11	125.32
85	cL	503	BCR	C16-C17-C18	-3.15	122.82	127.31
82	AO	305	PEB	CMB-C2B-C1B	3.15	129.91	125.06
82	A1	301	PEB	CMB-C2B-C1B	3.15	129.91	125.06
87	C6	512	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
82	GP	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
83	AQ	302	PUB	OA-C1A-NA	-3.15	121.27	125.93
83	xK	305	PUB	OA-C1A-NA	-3.15	121.27	125.93
82	XK	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
85	J2	103	BCR	C15-C14-C13	-3.15	122.82	127.31
82	s8	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
87	22	602	CLA	C2B-C1B-NB	3.15	112.34	110.23
84	63	901	CYC	CHD-C1D-C2D	-3.15	119.77	127.49
84	M1	201	CYC	C2A-C1A-NA	3.15	114.63	110.05
92	D6	407	LMG	C8-O7-C10	-3.15	110.04	117.79
82	U9	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	H1	1002	PEB	CMC-C3C-C4C	3.15	130.40	127.06
82	ID	202	PEB	C1C-CHB-C4B	3.15	135.34	128.28
82	YD	201	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
82	AM	302	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
82	p8	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
84	O3	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
82	AG	301	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
87	12	604	CLA	CHB-C4A-NA	3.15	128.86	124.51
87	42	608	CLA	CHB-C4A-NA	3.15	128.86	124.51
84	JH	1003	CYC	C2A-C1A-NA	3.15	114.63	110.05
82	l4	201	PEB	C4B-NB-C1B	-3.15	100.58	106.51
82	XI	201	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	xF	302	PEB	OD-C4D-ND	-3.15	121.27	125.93
82	FQ	202	PEB	C3D-C4D-ND	3.15	113.43	107.26
85	cL	518	BCR	C11-C10-C9	-3.15	122.82	127.31
85	B2	838	BCR	C35-C13-C14	-3.15	118.52	122.92
82	hO	202	PEB	CHC-C1D-ND	-3.15	109.74	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	h3	1001	CYC	CAA-CBA-CGA	3.15	120.37	113.60
82	OG	202	PEB	C2A-C1A-NA	3.15	110.98	108.27
84	C4	1001	CYC	C4D-CHA-C1A	3.15	135.34	128.28
82	CJ	203	PEB	C3B-C4B-NB	3.15	114.62	110.05
82	JA	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
84	GO	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
87	bL	617	CLA	CMB-C2B-C1B	-3.15	120.58	125.37
82	ND	203	PEB	C1B-C2B-C3B	-3.15	102.90	106.51
82	WI	202	PEB	CHA-C1B-C2B	3.15	132.99	124.90
87	C6	515	CLA	C3B-C4B-NB	-3.15	107.60	110.52
82	cO	203	PEB	CHC-C4C-NC	3.15	125.41	121.15
84	DO	1001	CYC	C4D-C3D-C2D	-3.15	103.90	107.62
82	GI	202	PEB	C3B-C4B-NB	3.15	114.62	110.05
82	j4	201	PEB	C4B-NB-C1B	-3.14	100.58	106.51
82	s8	201	PEB	CHC-C4C-NC	3.14	125.41	121.15
82	cJ	201	PEB	OD-C4D-ND	-3.14	121.27	125.93
92	A6	408	LMG	O8-C28-C29	3.14	121.78	111.91
82	CP	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
84	IO	1001	CYC	CHB-C4A-NA	-3.14	118.36	124.93
87	BL	619	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
82	NQ	203	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
82	jM	202	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
82	MF	202	PEB	CHC-C4C-NC	3.14	125.40	121.15
82	MB	201	PEB	CAB-CBB-CGB	-3.14	106.84	113.60
82	O7	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	RG	201	PEB	OD-C4D-ND	-3.14	121.27	125.93
82	YO	201	PEB	CMB-C2B-C1B	3.14	129.91	125.06
87	AN	819	CLA	CHB-C4A-NA	3.14	128.86	124.51
87	bL	607	CLA	CHB-C4A-NA	3.14	128.86	124.51
85	BN	838	BCR	C35-C13-C14	-3.14	118.52	122.92
82	AI	202	PEB	CHA-C1B-NB	-3.14	118.36	124.93
82	TI	203	PEB	CHA-C1B-NB	-3.14	118.36	124.93
82	X7	202	PEB	C1C-CHB-C4B	3.14	135.33	128.28
82	OF	201	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
82	hK	201	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
82	Y7	301	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	JQ	201	PEB	CMB-C2B-C1B	3.14	129.90	125.06
82	IB	201	PEB	CHA-C1B-NB	-3.14	118.36	124.93
82	OE	202	PEB	CHA-C1B-NB	-3.14	118.36	124.93
82	dG	201	PEB	CHB-C1C-NC	-3.14	118.12	125.32
82	GE	1002	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	D5	202	PEB	C2A-C1A-NA	3.14	110.98	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cK	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	K5	202	PEB	CHC-C4C-NC	3.14	125.40	121.15
82	GJ	201	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	JO	1002	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	JO	1002	PEB	CAB-C3B-C4B	3.14	130.57	125.01
82	YP	502	PEB	CHA-C1B-NB	-3.14	118.36	124.93
84	73	1001	CYC	CAA-CBA-CGA	3.14	120.36	113.60
82	JJ	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	AQ	303	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
84	BE	1001	CYC	C1B-C2B-C3B	-3.14	104.59	107.87
84	EE	1001	CYC	C1B-C2B-C3B	-3.14	104.59	107.87
82	TK	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
87	1N	602	CLA	CMC-C2C-C1C	-3.14	120.25	125.04
82	lE	201	PEB	C1C-CHB-C4B	3.14	135.33	128.28
82	fM	202	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	aM	203	PEB	CMB-C2B-C1B	3.14	129.90	125.06
83	QJ	201	PUB	C2B-C1B-NB	3.14	111.16	108.33
85	BN	842	BCR	C10-C11-C12	3.14	133.02	123.22
82	J5	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	sF	201	PEB	CHC-C4C-NC	3.14	125.40	121.15
82	WE	202	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	dD	401	PEB	OD-C4D-ND	-3.14	121.28	125.93
85	kL	100	BCR	C27-C26-C25	-3.14	118.17	122.73
82	mK	201	PEB	C4C-C3C-C2C	-3.14	104.60	107.50
82	ED	201	PEB	OD-C4D-C3D	-3.14	122.34	129.46
82	HD	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
82	QD	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
82	O5	203	PEB	CHC-C1D-ND	-3.14	109.75	113.72
82	l1	203	PEB	OA-C1A-C2A	-3.14	123.68	126.17
82	CK	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
82	DP	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
82	A4	305	PEB	CMB-C2B-C1B	3.14	129.90	125.06
85	B2	842	BCR	C10-C11-C12	3.14	133.02	123.22
82	D5	202	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	S9	203	PEB	C2A-C1A-NA	3.14	110.98	108.27
87	4N	608	CLA	CHB-C4A-NA	3.14	128.85	124.51
84	U3	1001	CYC	CAA-CBA-CGA	3.14	120.36	113.60
87	A2	835	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
82	ZO	201	PEB	CHA-C1B-NB	-3.14	118.36	124.93
82	SG	202	PEB	CHC-C1D-ND	-3.14	109.75	113.72
82	K5	202	PEB	CHC-C1D-ND	-3.14	109.75	113.72
87	b6	606	CLA	C1-C2-C3	-3.14	120.61	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DB	202	PEB	C3B-C4B-NB	3.14	114.62	110.05
82	QE	203	PEB	C3B-C4B-NB	3.14	114.62	110.05
83	Y7	302	PUB	OD-C4D-ND	-3.14	121.28	125.93
82	AD	301	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
82	W5	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
87	1N	604	CLA	CHB-C4A-NA	3.14	128.85	124.51
82	zC	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	fO	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	ZG	202	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	XF	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	ZO	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
82	lJ	202	PEB	CHB-C1C-C2C	-3.14	120.07	127.15
94	A6	410	PL9	O1-C4-C3	3.14	124.18	120.72
85	J2	103	BCR	C31-C1-C2	3.14	121.46	108.91
82	PI	201	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	EJ	202	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	xK	302	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	gH	203	PEB	CHB-C1C-C2C	-3.14	120.07	127.15
82	VB	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	YJ	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	lK	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	RO	203	PEB	CAB-CBB-CGB	3.14	120.36	113.60
82	Y4	203	PEB	CAB-CBB-CGB	3.14	120.36	113.60
84	Q3	1001	CYC	CAA-CBA-CGA	3.14	120.36	113.60
84	d3	1001	CYC	CAA-CBA-CGA	3.14	120.36	113.60
82	EP	203	PEB	C3D-C4D-ND	3.14	113.42	107.26
82	O9	201	PEB	CHC-C4C-NC	3.14	125.40	121.15
82	FD	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
82	U9	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
82	HF	201	PEB	CAA-C3A-C2A	3.14	122.10	114.26
82	YO	202	PEB	C1C-CHB-C4B	3.14	135.32	128.28
82	DO	1002	PEB	CMB-C2B-C1B	3.14	129.90	125.06
82	lG	202	PEB	CMB-C2B-C1B	3.14	129.90	125.06
84	M4	1001	CYC	C4D-C3D-C2D	-3.14	103.91	107.62
82	mO	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
85	cL	504	BCR	C23-C24-C25	3.14	136.01	127.20
82	XI	201	PEB	C3B-C4B-NB	3.14	114.61	110.05
84	GE	1001	CYC	C2A-C1A-NA	3.14	114.61	110.05
82	TQ	201	PEB	C1C-CHB-C4B	3.14	135.32	128.28
82	CP	202	PEB	CHC-C4C-NC	3.14	125.39	121.15
82	cJ	202	PEB	CMB-C2B-C1B	3.14	129.90	125.06
82	yK	301	PEB	CHA-C1B-NB	-3.14	118.37	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	CL	507	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
82	KI	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	Z4	202	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	KG	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
82	OP	203	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
82	WK	202	PEB	CAA-C3A-C2A	-3.14	106.42	114.26
84	S3	1001	CYC	CAA-CBA-CGA	3.14	120.35	113.60
82	HB	201	PEB	OD-C4D-C3D	-3.14	122.35	129.46
82	wF	303	PEB	CHA-C1B-C2B	3.14	132.97	124.90
84	I3	1001	CYC	CAA-CBA-CGA	3.14	120.35	113.60
82	F9	203	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	cH	202	PEB	OD-C4D-C3D	-3.14	122.35	129.46
82	WJ	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
82	gG	202	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	W4	201	PEB	C2B-C1B-NB	3.14	117.22	110.53
82	OB	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
82	D9	201	PEB	CHC-C4C-NC	3.14	125.39	121.15
82	N5	202	PEB	CHC-C1D-ND	-3.14	109.76	113.72
82	dG	201	PEB	CHC-C1D-ND	-3.14	109.76	113.72
84	LE	1001	CYC	CMB-C2B-C1B	3.14	128.08	124.17
82	HQ	201	PEB	C1C-CHB-C4B	3.14	135.31	128.28
87	B2	815	CLA	CHB-C4A-NA	3.14	128.85	124.51
85	a6	605	BCR	C24-C23-C22	-3.14	121.50	126.23
82	B5	203	PEB	CHA-C1B-NB	-3.14	118.37	124.93
82	HK	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	qF	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
82	H5	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
82	YA	301	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	kG	201	PEB	C3B-C4B-NB	3.14	114.61	110.05
82	DB	203	PEB	OD-C4D-C3D	-3.14	122.36	129.46
82	RQ	202	PEB	CMB-C2B-C1B	3.14	129.89	125.06
82	L4	1002	PEB	C4B-C3B-C2B	-3.13	103.31	106.78
82	N7	201	PEB	C4B-C3B-C2B	-3.13	103.31	106.78
84	w3	1001	CYC	C1A-C2A-C3A	-3.13	103.31	106.78
82	EQ	201	PEB	OD-C4D-C3D	-3.13	122.36	129.46
87	CL	510	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
82	V1	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
84	D3	1001	CYC	CAA-CBA-CGA	3.13	120.35	113.60
84	L4	1001	CYC	C1D-C2D-C3D	-3.13	103.80	107.79
87	A2	809	CLA	O2D-CGD-CBD	3.13	116.84	111.27
82	YJ	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
82	a1	201	PEB	CHB-C1C-C2C	-3.13	120.08	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	cL	512	CLA	CHB-C1B-NB	3.13	127.58	124.26
87	3N	311	CLA	CHB-C4A-NA	3.13	128.85	124.51
82	CM	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
82	dD	401	PEB	C3B-C4B-NB	3.13	114.61	110.05
82	HK	201	PEB	CAA-C3A-C2A	3.13	122.09	114.26
84	u3	1001	CYC	CAA-CBA-CGA	3.13	120.35	113.60
82	lF	203	PEB	CMB-C2B-C1B	3.13	129.89	125.06
82	EJ	203	PEB	CHA-C1B-NB	-3.13	118.38	124.93
82	yF	301	PEB	CHA-C1B-NB	-3.13	118.38	124.93
84	HH	1001	CYC	CHB-C4A-NA	-3.13	118.38	124.93
85	AN	846	BCR	C20-C19-C18	3.13	135.22	126.42
82	f4	202	PEB	CHC-C4C-NC	3.13	125.39	121.15
87	b6	609	CLA	C3B-C4B-NB	-3.13	107.61	110.52
87	A2	814	CLA	CHB-C4A-NA	3.13	128.84	124.51
82	YJ	201	PEB	C3B-C4B-NB	3.13	114.61	110.05
82	LP	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
82	L5	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
85	J2	103	BCR	C32-C1-C31	-3.13	98.91	108.53
84	o3	1001	CYC	C1A-C2A-C3A	-3.13	103.31	106.78
82	PK	202	PEB	CHC-C4C-NC	-3.13	116.91	121.15
87	D6	402	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
82	i1	201	PEB	CHC-C1D-ND	-3.13	109.76	113.72
82	V5	202	PEB	CHC-C1D-ND	-3.13	109.76	113.72
82	HI	203	PEB	CMB-C2B-C1B	3.13	129.89	125.06
82	QP	203	PEB	C2C-C1C-NC	3.13	111.79	107.57
84	f3	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
82	NI	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
82	j1	203	PEB	C1C-CHB-C4B	3.13	135.31	128.28
82	OD	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
82	SM	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
82	UP	203	PEB	CMB-C2B-C1B	3.13	129.89	125.06
82	UI	201	PEB	C1D-CHC-C4C	-3.13	108.64	113.26
82	SM	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
82	C9	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
82	uC	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
82	NM	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
82	iO	202	PEB	C3C-C4C-NC	3.13	111.15	108.33
82	dE	202	PEB	OD-C4D-ND	-3.13	121.29	125.93
82	mF	202	PEB	CHC-C4C-NC	3.13	125.39	121.15
82	ZE	202	PEB	C3B-C4B-NB	3.13	114.60	110.05
82	aJ	201	PEB	C3B-C4B-NB	3.13	114.60	110.05
82	wK	303	PEB	C3B-C4B-NB	3.13	114.60	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	I7	201	PEB	OD-C4D-C3D	-3.13	122.36	129.46
84	L3	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
82	iJ	201	PEB	CHB-C1C-NC	-3.13	118.15	125.32
87	B6	615	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
82	eM	202	PEB	CAB-C3B-C4B	3.13	130.55	125.01
82	WJ	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
82	zF	501	PEB	CAC-C2C-C3C	3.13	134.24	127.07
82	NB	203	PEB	OD-C4D-C3D	-3.13	122.37	129.46
82	MB	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
82	PH	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
87	CL	507	CLA	CBC-CAC-C3C	3.13	121.06	112.43
84	LO	1001	CYC	CHB-C1B-NB	-3.13	119.34	126.06
84	JH	1001	CYC	CAD-C3D-C4D	3.13	130.75	125.76
82	iH	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
82	T4	201	PEB	CHA-C1B-NB	-3.13	118.39	124.93
82	gG	202	PEB	OD-C4D-ND	-3.13	121.29	125.93
82	SK	203	PEB	C3B-C4B-NB	3.13	114.60	110.05
82	II	203	PEB	CMB-C2B-C1B	3.13	129.88	125.06
82	YI	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
84	DG	1001	CYC	CHD-C1D-ND	-3.13	118.15	125.32
84	FH	1001	CYC	CHD-C1D-ND	-3.13	118.15	125.32
82	jG	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
85	JN	103	BCR	C32-C1-C31	-3.13	98.92	108.53
82	WG	201	PEB	CHC-C1D-ND	-3.13	109.77	113.72
82	PH	202	PEB	CHC-C1D-ND	-3.13	109.77	113.72
82	II	201	PEB	C3B-C4B-NB	3.13	114.60	110.05
87	bL	607	CLA	C4-C3-C5	3.13	120.53	115.27
82	SE	201	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
82	R7	202	PEB	C1D-CHC-C4C	-3.13	108.64	113.26
84	I4	1001	CYC	CHB-C4A-NA	-3.13	118.39	124.93
82	IM	202	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	dF	201	PEB	CMB-C2B-C1B	3.13	129.88	125.06
84	Q3	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
82	nF	202	PEB	CHB-C4B-C3B	-3.13	118.08	125.32
85	bL	602	BCR	C16-C17-C18	-3.13	122.84	127.31
82	DE	1002	PEB	C1D-CHC-C4C	3.13	117.87	113.26
84	n3	1001	CYC	CAA-CBA-CGA	3.13	120.33	113.60
82	qK	201	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
82	fM	203	PEB	C3C-C4C-NC	3.13	111.15	108.33
82	SD	201	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	Y4	202	PEB	C1C-CHB-C4B	3.13	135.30	128.28
82	Q9	202	PEB	CHA-C4A-NA	-3.13	121.49	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TI	202	PEB	C3B-C4B-NB	3.13	114.60	110.05
82	G5	202	PEB	CHC-C1D-ND	-3.13	109.77	113.72
82	T5	202	PEB	CHC-C1D-ND	-3.13	109.77	113.72
82	AQ	301	PEB	OD-C4D-C3D	-3.13	122.37	129.46
82	DG	1002	PEB	C1D-CHC-C4C	3.13	117.87	113.26
82	mO	203	PEB	CBB-CAB-C3B	3.13	121.32	112.63
82	CP	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
82	uF	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
82	QF	201	PEB	CAB-C3B-C4B	3.13	130.54	125.01
82	CK	202	PEB	CAC-C2C-C3C	3.13	134.23	127.07
82	EF	201	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	OF	201	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	UP	202	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	AQ	303	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	FH	1002	PEB	C3B-C4B-NB	3.13	114.60	110.05
82	XM	201	PEB	C3B-C4B-NB	3.13	114.60	110.05
85	F6	101	BCR	C37-C22-C23	3.13	123.00	118.08
85	B2	840	BCR	C7-C8-C9	-3.13	121.51	126.23
82	b1	201	PEB	OD-C4D-C3D	-3.13	122.38	129.46
87	CL	507	CLA	CAC-C3C-C2C	3.13	132.88	127.53
82	UE	203	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	oF	202	PEB	OD-C4D-ND	-3.13	121.30	125.93
82	DP	201	PEB	CMB-C2B-C1B	3.13	129.88	125.06
82	UO	201	PEB	CHB-C1C-C2C	-3.13	120.10	127.15
82	DH	1002	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
82	fK	202	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
82	F5	203	PEB	C3B-C4B-NB	3.13	114.60	110.05
83	K7	203	PUB	CHA-C4A-NA	-3.13	109.77	113.72
82	U7	202	PEB	CHC-C4C-NC	3.13	125.38	121.15
87	A6	402	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
82	R7	202	PEB	CHA-C1B-NB	-3.13	118.39	124.93
87	B6	613	CLA	C3B-C4B-NB	-3.13	107.61	110.52
82	LQ	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
84	HH	1001	CYC	C1B-NB-C4B	-3.13	106.69	110.67
82	DF	203	PEB	C1C-CHB-C4B	3.13	135.29	128.28
82	YF	202	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
82	mE	202	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
82	vF	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
82	Y4	202	PEB	CHA-C1B-NB	-3.13	118.40	124.93
91	A6	407	PHO	CMA-C3A-C4A	-3.12	107.53	114.38
82	U7	201	PEB	C3C-C4C-NC	3.12	111.15	108.33
87	5N	605	CLA	CAA-CBA-CGA	-3.12	104.21	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	K2	104	CLA	CHB-C4A-NA	3.12	128.83	124.51
82	RB	202	PEB	CMC-C3C-C4C	3.12	130.37	127.06
82	Z4	201	PEB	C2B-C1B-NB	3.12	117.20	110.53
85	L2	205	BCR	C30-C25-C26	-3.12	118.21	122.61
87	CL	503	CLA	CMB-C2B-C1B	-3.12	120.61	125.37
82	LB	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
82	XD	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
82	CM	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
85	A2	846	BCR	C20-C19-C18	3.12	135.19	126.42
82	PJ	201	PEB	CHC-C1D-ND	3.12	117.68	113.72
82	kE	201	PEB	C3B-C4B-NB	3.12	114.59	110.05
84	ME	1001	CYC	C2A-C1A-NA	3.12	114.59	110.05
84	L3	1001	CYC	CAA-CBA-CGA	3.12	120.32	113.60
82	NF	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
82	II	202	PEB	C1C-CHB-C4B	-3.12	121.28	128.28
82	KI	203	PEB	C1C-CHB-C4B	-3.12	121.28	128.28
82	OG	202	PEB	CHA-C1B-NB	-3.12	118.40	124.93
82	Z4	201	PEB	CHA-C1B-NB	-3.12	118.40	124.93
82	l4	202	PEB	OD-C4D-C3D	-3.12	122.38	129.46
82	sF	201	PEB	OD-C4D-C3D	-3.12	122.38	129.46
82	QP	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
82	g4	202	PEB	C2A-C1A-NA	3.12	110.97	108.27
82	cB	401	PEB	OD-C4D-ND	-3.12	121.30	125.93
87	B2	811	CLA	CHB-C4A-NA	3.12	128.83	124.51
82	SD	202	PEB	OD-C4D-C3D	-3.12	122.39	129.46
82	SJ	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
84	B3	1001	CYC	CAA-CBA-CGA	3.12	120.32	113.60
82	P7	201	PEB	CHA-C1B-NB	-3.12	118.40	124.93
82	zK	501	PEB	CAC-C2C-C3C	3.12	134.22	127.07
82	PF	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
84	w3	1001	CYC	CAA-CBA-CGA	3.12	120.32	113.60
82	YH	201	PEB	C1C-CHB-C4B	3.12	135.28	128.28
82	HI	203	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	SF	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
82	A1	302	PEB	OA-C1A-C2A	-3.12	123.69	126.17
82	YP	502	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	TQ	202	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	G7	201	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	GB	202	PEB	CHC-C1D-ND	-3.12	109.78	113.72
82	v8	202	PEB	CAB-C3B-C4B	3.12	130.53	125.01
82	RD	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
82	uK	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hO	202	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
82	y8	202	PEB	CMC-C3C-C4C	3.12	130.37	127.06
82	IP	203	PEB	OD-C4D-C3D	-3.12	122.39	129.46
82	UP	203	PEB	OD-C4D-C3D	-3.12	122.39	129.46
82	pF	201	PEB	CHC-C4C-NC	3.12	125.37	121.15
82	RI	201	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	hK	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
87	B6	614	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
84	F3	1001	CYC	CAA-CBA-CGA	3.12	120.32	113.60
82	YG	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
85	JN	103	BCR	C31-C1-C2	3.12	121.39	108.91
82	H5	202	PEB	C3C-C4C-NC	3.12	111.14	108.33
82	LQ	201	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
82	XA	202	PEB	C1C-CHB-C4B	3.12	135.28	128.28
87	BN	812	CLA	CHB-C4A-NA	3.12	128.83	124.51
82	QK	202	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	hK	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
82	F9	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	VD	201	PEB	OD-C4D-C3D	-3.12	122.39	129.46
82	V1	201	PEB	CHC-C4C-NC	3.12	125.37	121.15
82	OK	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	hK	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	PA	201	PEB	CHA-C1B-NB	-3.12	118.41	124.93
82	NJ	201	PEB	CBC-CAC-C2C	-3.12	103.96	112.63
82	CI	201	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	BQ	201	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	gB	201	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	CP	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
82	lJ	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
82	TB	201	PEB	CHC-C4C-NC	3.12	125.37	121.15
87	B6	605	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
84	L4	1001	CYC	CHB-C1B-NB	-3.12	119.36	126.06
82	HF	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
83	AQ	302	PUB	OD-C4D-ND	-3.12	121.31	125.93
82	jE	201	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	AK	201	PEB	CHA-C1B-C2B	3.12	132.92	124.90
87	CL	507	CLA	CAC-C3C-C4C	-3.12	120.76	124.81
82	ZB	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
82	E7	202	PEB	CMB-C2B-C1B	3.12	129.87	125.06
82	x8	202	PEB	CHA-C1B-NB	-3.12	118.41	124.93
82	NB	201	PEB	CHC-C4C-NC	3.12	125.37	121.15
82	S9	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JM	202	PEB	C1C-CHB-C4B	-3.12	121.29	128.28
82	h1	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
84	O3	1001	CYC	CAA-CBA-CGA	3.12	120.31	113.60
82	xC	202	PEB	CHA-C1B-NB	-3.12	118.41	124.93
82	OE	201	PEB	C3B-C4B-NB	3.12	114.58	110.05
82	aK	203	PEB	C3B-C4B-NB	3.12	114.58	110.05
103	8N	309	ZEX	C18-C5-C4	3.12	120.13	114.36
84	k3	1001	CYC	CAA-CBA-CGA	3.12	120.31	113.60
82	OG	203	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	wK	303	PEB	CHA-C1B-C2B	3.12	132.92	124.90
82	QG	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
87	c6	611	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
87	12	602	CLA	CMC-C2C-C1C	-3.12	120.29	125.04
82	UJ	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
87	52	605	CLA	CAA-CBA-CGA	-3.12	104.23	112.51
82	ZO	201	PEB	C2B-C1B-NB	3.12	117.18	110.53
82	SE	201	PEB	CHC-C1D-ND	-3.12	109.78	113.72
82	h1	203	PEB	CHC-C1D-ND	-3.12	109.78	113.72
82	A5	202	PEB	CHC-C1D-ND	-3.12	109.78	113.72
82	C5	202	PEB	CHC-C1D-ND	-3.12	109.78	113.72
82	z8	201	PEB	CBA-CAA-C3A	3.12	120.41	113.47
84	V3	1001	CYC	C4D-C3D-C2D	-3.12	103.94	107.62
84	H1	1001	CYC	CHB-C4A-NA	-3.12	118.41	124.93
82	HP	202	PEB	CMB-C2B-C1B	3.12	129.86	125.06
82	RD	202	PEB	C3B-C4B-NB	3.12	114.58	110.05
82	gO	201	PEB	C3B-C4B-NB	3.12	114.58	110.05
83	xF	301	PUB	CAB-CBB-CGB	-3.12	106.90	113.60
82	wF	301	PEB	CHC-C4C-NC	3.12	125.37	121.15
82	H1	1002	PEB	OA-C1A-C2A	-3.12	123.69	126.17
87	F2	202	CLA	CMC-C2C-C1C	-3.12	120.29	125.04
82	UJ	202	PEB	CHA-C1B-C2B	3.12	132.91	124.90
87	AN	835	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
87	MN	101	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
82	WB	402	PEB	C3B-C4B-NB	3.12	114.58	110.05
82	VI	201	PEB	C3B-C4B-NB	3.12	114.58	110.05
82	GM	203	PEB	C3B-C4B-NB	3.12	114.58	110.05
84	DG	1001	CYC	CAB-C3B-C4B	3.12	126.30	121.38
82	OF	203	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
82	SJ	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
82	MP	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
82	GJ	203	PEB	C3C-C4C-NC	3.12	111.14	108.33
82	m1	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GI	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	PK	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	NP	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	CD	201	PEB	CHC-C4C-NC	3.12	125.37	121.15
82	UO	202	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	dG	204	PEB	C2A-C1A-NA	3.12	110.96	108.27
82	BI	203	PEB	C4C-C3C-C2C	-3.12	104.62	107.50
87	cL	515	CLA	C2D-C1D-ND	-3.12	107.81	110.10
84	D1	1001	CYC	CHD-C1D-ND	-3.12	118.18	125.32
82	AF	201	PEB	CHA-C1B-C2B	3.12	132.91	124.90
82	SH	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	PM	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
82	AE	301	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
82	I5	202	PEB	CHC-C1D-ND	-3.12	109.78	113.72
82	DI	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
82	B9	203	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	SM	203	PEB	C2A-C1A-NA	3.11	110.96	108.27
82	ZO	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	gJ	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
103	82	309	ZEX	C18-C5-C4	3.11	120.12	114.36
82	R5	202	PEB	CHC-C1D-ND	-3.11	109.78	113.72
82	h1	201	PEB	CHB-C1C-C2C	-3.11	120.12	127.15
82	AI	202	PEB	C1C-CHB-C4B	-3.11	121.30	128.28
82	nF	202	PEB	C1C-CHB-C4B	3.11	135.27	128.28
82	EJ	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	OK	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	vK	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	UM	202	PEB	C3B-C4B-NB	3.11	114.58	110.05
87	BN	817	CLA	C3B-C4B-NB	-3.11	107.63	110.52
87	CL	505	CLA	CHB-C4A-NA	3.11	128.82	124.51
82	kO	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
87	b6	608	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
82	e4	202	PEB	C1C-CHB-C4B	3.11	135.26	128.28
82	kH	202	PEB	CHC-C4C-NC	3.11	125.36	121.15
87	A2	809	CLA	CAA-C2A-C3A	-3.11	104.25	112.78
82	AI	201	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	F9	203	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	gB	202	PEB	C2A-C1A-NA	3.11	110.96	108.27
82	Y7	304	PEB	CHA-C1B-C2B	3.11	132.91	124.90
82	JA	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	V4	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	hF	201	PEB	OA-C1A-NA	3.11	128.71	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JB	201	PEB	CHC-C4C-NC	3.11	125.36	121.15
82	B9	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
82	JI	202	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	OE	203	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
82	fF	202	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
82	TG	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
87	FN	201	CLA	CMC-C2C-C1C	-3.11	120.30	125.04
87	32	311	CLA	CHB-C4A-NA	3.11	128.82	124.51
82	Z4	202	PEB	CMB-C2B-C1B	3.11	129.86	125.06
82	vF	202	PEB	CMB-C2B-C1B	3.11	129.86	125.06
82	MK	202	PEB	CHC-C4C-NC	3.11	125.36	121.15
84	M3	1001	CYC	CAA-CBA-CGA	3.11	120.30	113.60
82	VI	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	lF	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
87	cL	509	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
84	I1	1001	CYC	C2D-C1D-ND	3.11	111.77	107.40
82	RA	202	PEB	C1D-CHC-C4C	-3.11	108.67	113.26
85	KL	100	BCR	C21-C20-C19	3.11	132.93	123.22
82	XK	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	FD	202	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	HP	201	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	V9	201	PEB	C3B-C4B-NB	3.11	114.58	110.05
82	FF	201	PEB	CAB-C3B-C4B	3.11	130.51	125.01
82	BD	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
82	Y7	303	PEB	C2A-C1A-NA	3.11	110.95	108.27
85	JN	103	BCR	C15-C14-C13	-3.11	122.87	127.31
84	DH	1001	CYC	CHD-C1D-ND	-3.11	118.19	125.32
82	U4	201	PEB	CHB-C1C-C2C	-3.11	120.13	127.15
82	BP	201	PEB	CHC-C4C-NC	3.11	125.36	121.15
82	kJ	202	PEB	CHC-C4C-NC	3.11	125.36	121.15
83	A1	304	PUB	CHA-C1B-NB	3.11	125.36	121.15
85	LN	205	BCR	C30-C25-C26	-3.11	118.23	122.61
82	VA	203	PEB	CAC-CBC-CGC	-3.11	106.91	113.60
84	E1	1001	CYC	C1A-C2A-C3A	-3.11	103.34	106.78
82	wF	303	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	dG	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	FD	202	PEB	C3D-C4D-ND	3.11	113.36	107.26
82	UK	202	PEB	C3D-C4D-ND	3.11	113.36	107.26
82	EM	202	PEB	CHC-C1D-ND	-3.11	109.79	113.72
82	CP	201	PEB	CMB-C2B-C1B	3.11	129.85	125.06
82	VG	202	PEB	CHA-C1B-NB	-3.11	118.43	124.93
82	TI	203	PEB	C1C-CHB-C4B	-3.11	121.31	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AJ	302	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	EM	202	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	X9	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	AQ	303	PEB	CHC-C4C-NC	3.11	125.36	121.15
83	AG	302	PUB	CHB-C4B-C3B	-3.11	120.13	127.15
84	NH	1001	CYC	CHB-C4A-NA	-3.11	118.43	124.93
82	YO	203	PEB	CAB-CBB-CGB	3.11	120.30	113.60
82	V7	203	PEB	CAC-CBC-CGC	-3.11	106.91	113.60
84	B3	1001	CYC	C1A-C2A-C3A	-3.11	103.34	106.78
87	bL	604	CLA	CHB-C4A-NA	3.11	128.81	124.51
82	i4	202	PEB	C3C-C4C-NC	3.11	111.13	108.33
82	YD	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	VH	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	VE	202	PEB	CHA-C1B-NB	-3.11	118.43	124.93
82	YO	202	PEB	CHA-C1B-NB	-3.11	118.43	124.93
84	q3	1001	CYC	CAA-CBA-CGA	3.11	120.29	113.60
87	b6	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
82	OH	203	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	wC	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
82	W5	203	PEB	C2A-C1A-NA	3.11	110.95	108.27
82	t8	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
82	aM	201	PEB	CHA-C1B-NB	-3.11	118.43	124.93
87	AN	827	CLA	C3B-C4B-NB	-3.11	107.63	110.52
82	WO	201	PEB	C2B-C1B-NB	3.11	117.17	110.53
84	LO	1001	CYC	C1D-C2D-C3D	-3.11	103.83	107.79
82	fG	202	PEB	C3B-C4B-NB	3.11	114.57	110.05
85	H6	101	BCR	C1-C6-C5	-3.11	118.23	122.61
84	o3	1001	CYC	CAA-CBA-CGA	3.11	120.29	113.60
87	BN	816	CLA	CHB-C4A-NA	3.11	128.81	124.51
82	PI	202	PEB	C1C-CHB-C4B	-3.11	121.31	128.28
82	ND	202	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	GI	201	PEB	OD-C4D-C3D	-3.11	122.42	129.46
82	F9	201	PEB	CMB-C2B-C1B	3.11	129.85	125.06
82	VH	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
82	QI	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
82	WI	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	kK	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	U9	201	PEB	CHC-C4C-NC	3.11	125.36	121.15
82	EQ	201	PEB	CHB-C1C-NC	-3.11	118.20	125.32
82	WM	203	PEB	C2A-C1A-NA	3.11	110.95	108.27
85	A6	401	BCR	C2-C1-C6	3.11	115.27	110.48
87	32	312	CLA	CHB-C4A-NA	3.11	128.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	LH	1001	CYC	C2D-C1D-ND	3.11	111.77	107.40
82	Y1	202	PEB	CHC-C1D-ND	-3.11	109.79	113.72
82	gE	202	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	GP	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
82	cF	203	PEB	C1C-CHB-C4B	3.11	135.25	128.28
82	WQ	202	PEB	CHC-C4C-NC	3.11	125.35	121.15
83	ND	201	PUB	C1C-C2C-C3C	-3.11	103.34	106.78
87	A2	820	CLA	C3B-C4B-NB	-3.11	107.63	110.52
82	QP	203	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
82	DM	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
82	hJ	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
82	pK	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
82	S4	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
87	AN	809	CLA	O2D-CGD-CBD	3.11	116.79	111.27
82	lM	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
82	CB	201	PEB	C3D-C4D-ND	3.11	113.35	107.26
82	Y7	304	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	jK	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
82	NJ	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
82	MP	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
82	d4	202	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
84	f3	1001	CYC	CAA-CBA-CGA	3.11	120.29	113.60
82	cF	203	PEB	CAC-C2C-C1C	3.11	130.71	125.76
82	aH	201	PEB	CHB-C1C-C2C	-3.11	120.14	127.15
82	JI	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
82	GI	203	PEB	C1C-CHB-C4B	-3.11	121.32	128.28
82	RP	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
82	XI	202	PEB	C4B-C3B-C2B	-3.11	103.35	106.78
82	T7	201	PEB	CHC-C1D-ND	-3.10	109.80	113.72
87	8N	301	CLA	CHB-C1B-NB	3.10	127.54	124.26
82	QB	203	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	YF	202	PEB	CHC-C4C-NC	3.10	125.35	121.15
82	BB	203	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	IP	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	TM	202	PEB	OD-C4D-ND	-3.10	121.33	125.93
87	B6	610	CLA	C1-C2-C3	-3.10	120.67	126.04
82	mH	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
84	M4	1001	CYC	C1A-C2A-C3A	-3.10	103.35	106.78
82	UF	201	PEB	CHB-C4B-NB	3.10	131.04	124.58
82	D5	201	PEB	C2A-C1A-NA	3.10	110.95	108.27
84	j3	1001	CYC	CAA-CBA-CGA	3.10	120.28	113.60
82	OK	203	PEB	CHC-C1D-ND	-3.10	109.80	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	fO	202	PEB	CHC-C4C-NC	3.10	125.35	121.15
82	XI	202	PEB	C1C-CHB-C4B	-3.10	121.32	128.28
82	eO	202	PEB	C1C-CHB-C4B	3.10	135.24	128.28
82	HH	1002	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	f1	202	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	cB	402	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	dD	401	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	KI	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
83	AO	303	PUB	OD-C4D-ND	-3.10	121.33	125.93
82	jM	201	PEB	CHB-C4B-NB	-3.10	118.12	124.58
82	nK	202	PEB	C1C-CHB-C4B	3.10	135.24	128.28
87	A2	838	CLA	C3B-C4B-NB	-3.10	107.64	110.52
82	WA	201	PEB	C1D-CHC-C4C	3.10	117.83	113.26
87	AN	809	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
84	HG	1001	CYC	CHD-C1D-ND	-3.10	118.21	125.32
82	Y4	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
85	AN	845	BCR	C3-C4-C5	-3.10	108.54	114.08
82	RB	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	aF	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	eF	203	PEB	C3B-C4B-NB	3.10	114.56	110.05
87	ON	202	CLA	C2A-C1A-CHA	3.10	129.28	123.86
82	E9	202	PEB	OD-C4D-ND	-3.10	121.33	125.93
82	GM	202	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	D1	1002	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
82	EA	202	PEB	C2A-C1A-NA	3.10	110.95	108.27
82	QQ	201	PEB	CAC-C2C-C1C	3.10	130.70	125.76
84	H3	1001	CYC	CAA-CBA-CGA	3.10	120.28	113.60
82	J4	1002	PEB	CAB-C3B-C4B	3.10	130.50	125.01
82	GD	202	PEB	C1D-CHC-C4C	-3.10	108.68	113.26
82	NI	202	PEB	C1C-CHB-C4B	-3.10	121.32	128.28
82	YI	202	PEB	CHC-C1D-ND	-3.10	109.80	113.72
82	YP	502	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	R9	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
82	uC	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
82	LM	202	PEB	CHB-C4B-NB	-3.10	118.12	124.58
84	DE	1001	CYC	CAB-C3B-C4B	3.10	126.28	121.38
82	c1	202	PEB	OD-C4D-C3D	-3.10	122.43	129.46
82	aK	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
82	OO	202	PEB	CMB-C2B-C1B	3.10	129.84	125.06
82	U4	202	PEB	C1D-CHC-C4C	3.10	117.83	113.26
82	kH	202	PEB	CAA-C3A-C4A	3.10	120.64	112.67
82	QO	201	PEB	CHA-C4A-NA	3.10	128.89	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	m4	203	PEB	CBB-CAB-C3B	3.10	121.25	112.63
82	P5	202	PEB	CHC-C1D-ND	-3.10	109.80	113.72
82	cF	202	PEB	CHC-C1D-ND	-3.10	109.80	113.72
82	iO	202	PEB	OD-C4D-C3D	-3.10	122.43	129.46
82	ZM	202	PEB	OD-C4D-ND	-3.10	121.33	125.93
82	TO	201	PEB	OD-C4D-ND	-3.10	121.33	125.93
82	VI	203	PEB	CAC-C2C-C1C	3.10	130.70	125.76
82	FB	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
82	fH	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
84	K1	1001	CYC	C1A-C2A-C3A	-3.10	103.35	106.78
87	B6	615	CLA	C3B-C4B-NB	-3.10	107.64	110.52
82	R7	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
82	QG	203	PEB	CHC-C1D-ND	-3.10	109.80	113.72
82	hH	202	PEB	CHC-C1D-ND	-3.10	109.80	113.72
82	CI	202	PEB	C1C-CHB-C4B	-3.10	121.33	128.28
84	N1	1001	CYC	CHB-C4A-NA	-3.10	118.45	124.93
82	wF	302	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
82	XD	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
82	IP	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
82	GB	203	PEB	CAC-CBC-CGC	-3.10	106.93	113.60
82	i4	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	VI	202	PEB	C1C-CHB-C4B	-3.10	121.33	128.28
83	xF	305	PUB	CHA-C1B-NB	3.10	125.34	121.15
82	HE	1002	PEB	OA-C1A-C2A	-3.10	123.71	126.17
82	PQ	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
82	w8	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
82	VJ	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	R9	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
83	NQ	201	PUB	C1C-C2C-C3C	-3.10	103.35	106.78
84	x3	1001	CYC	C4D-C3D-C2D	-3.10	103.96	107.62
82	HQ	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
82	MQ	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
82	S4	202	PEB	C2A-C1A-NA	3.10	110.94	108.27
82	nK	202	PEB	C2A-C1A-NA	3.10	110.94	108.27
87	B6	609	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
85	A2	847	BCR	C11-C12-C13	-3.10	117.71	126.42
82	bE	202	PEB	CHC-C1D-ND	-3.10	109.80	113.72
82	O4	201	PEB	C3C-C4C-NC	3.10	111.12	108.33
84	H1	1001	CYC	C4D-CHA-C1A	3.10	135.23	128.28
82	LJ	202	PEB	OD-C4D-ND	-3.10	121.34	125.93
84	63	901	CYC	OC-C1C-C2C	-3.10	123.71	126.17
82	OG	202	PEB	CHC-C4C-NC	3.10	125.34	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PF	202	PEB	CHC-C4C-NC	-3.10	116.95	121.15
84	E4	1001	CYC	C4D-C3D-C2D	-3.10	103.96	107.62
82	mM	202	PEB	CHA-C1B-NB	-3.10	118.45	124.93
87	M2	101	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
82	F1	1002	PEB	OD-C4D-ND	-3.10	121.34	125.93
82	UE	201	PEB	C2A-C1A-NA	3.10	110.94	108.27
82	VK	202	PEB	C2A-C1A-NA	3.10	110.94	108.27
82	FP	202	PEB	C2A-C1A-NA	3.10	110.94	108.27
82	N9	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
84	HH	1001	CYC	C4D-CHA-C1A	3.10	135.23	128.28
85	F6	101	BCR	C33-C5-C6	-3.10	121.05	124.53
82	KQ	201	PEB	CMB-C2B-C1B	3.10	129.84	125.06
84	63	901	CYC	C1B-C2B-C3B	-3.10	104.64	107.87
82	CP	203	PEB	CHC-C4C-NC	3.10	125.34	121.15
82	k1	202	PEB	CAA-C3A-C4A	3.10	120.63	112.67
82	WJ	203	PEB	C1C-NC-C4C	-3.10	104.08	109.60
82	UD	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
82	xC	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
82	ZK	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
82	wF	301	PEB	OA-C1A-C2A	-3.10	123.71	126.17
82	FK	201	PEB	CAB-C3B-C4B	3.10	130.49	125.01
82	QG	203	PEB	C3B-C4B-NB	3.10	114.56	110.05
82	J4	1002	PEB	CMB-C2B-C1B	3.10	129.83	125.06
82	xK	304	PEB	CHC-C4C-NC	3.10	125.34	121.15
82	YA	304	PEB	CHA-C1B-C2B	3.10	132.87	124.90
82	QJ	204	PEB	C3C-C4C-NC	3.10	111.12	108.33
82	E5	202	PEB	CHC-C1D-ND	-3.10	109.81	113.72
82	TD	202	PEB	OD-C4D-ND	-3.10	121.34	125.93
82	UD	202	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
82	EI	202	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
82	sK	201	PEB	CHB-C1C-C2C	-3.10	120.16	127.15
95	C6	502	DGD	O2E-C2E-C1E	3.10	117.57	110.05
84	IE	1001	CYC	C1B-NB-C4B	-3.10	106.73	110.67
85	BN	838	BCR	C20-C19-C18	-3.10	117.72	126.42
87	AN	819	CLA	CMB-C2B-C1B	-3.10	120.65	125.37
82	ZJ	202	PEB	C1C-CHB-C4B	-3.10	121.34	128.28
82	VJ	202	PEB	OD-C4D-ND	-3.10	121.34	125.93
82	GP	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
83	Z9	302	PUB	OA-C1A-NA	-3.10	121.34	125.93
82	HJ	201	PEB	CHC-C1D-ND	3.10	117.64	113.72
82	UP	203	PEB	C3D-C4D-ND	3.10	113.33	107.26
82	WK	202	PEB	CHA-C1B-C2B	3.10	132.86	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cK	203	PEB	C3C-C4C-NC	3.10	111.12	108.33
82	SQ	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
85	b6	601	BCR	C28-C27-C26	-3.10	108.55	114.08
82	lG	201	PEB	CHA-C1B-NB	-3.10	118.46	124.93
82	CP	202	PEB	C3B-C4B-NB	3.10	114.55	110.05
82	WE	201	PEB	CHC-C1D-ND	-3.10	109.81	113.72
82	OG	203	PEB	CHC-C1D-ND	-3.10	109.81	113.72
82	L5	201	PEB	CHC-C1D-ND	-3.10	109.81	113.72
82	TI	201	PEB	CHA-C1B-C2B	3.10	132.86	124.90
84	63	901	CYC	CHA-C4D-C3D	-3.10	120.17	127.15
82	WM	203	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
82	W7	202	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
82	kK	203	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
82	xF	304	PEB	CHC-C4C-NC	3.10	125.34	121.15
82	eJ	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
83	AE	302	PUB	CHB-C4B-C3B	-3.09	120.17	127.15
87	B2	816	CLA	C3B-C4B-NB	-3.09	107.64	110.52
82	C7	202	PEB	CHC-C1D-ND	-3.09	109.81	113.72
82	hF	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	KI	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	DM	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	KJ	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
82	jG	202	PEB	CMB-C2B-C1B	3.09	129.83	125.06
82	rK	202	PEB	CHA-C1B-NB	-3.09	118.46	124.93
82	YJ	202	PEB	OA-C1A-C2A	-3.09	123.71	126.17
82	CP	202	PEB	CHC-C1D-ND	-3.09	109.81	113.72
84	V3	1001	CYC	CMC-C2C-C1C	3.09	119.07	112.40
82	IP	202	PEB	C2A-C1A-NA	3.09	110.94	108.27
82	jG	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
82	YE	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	KM	203	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	hM	203	PEB	OD-C4D-ND	-3.09	121.35	125.93
83	AD	302	PUB	OD-C4D-ND	-3.09	121.35	125.93
82	Y7	304	PEB	CHB-C4B-NB	-3.09	118.14	124.58
82	MK	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	U1	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	aE	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	gJ	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	RA	202	PEB	CHA-C1B-NB	-3.09	118.46	124.93
82	lH	202	PEB	CHA-C1B-C2B	3.09	132.85	124.90
82	BK	201	PEB	CHB-C1C-C2C	-3.09	120.17	127.15
82	i4	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GK	201	PEB	C1C-CHB-C4B	3.09	135.22	128.28
82	YO	203	PEB	CHC-C1D-ND	-3.09	109.81	113.72
82	VM	201	PEB	CHA-C1B-NB	-3.09	118.46	124.93
82	lH	201	PEB	CMB-C2B-C1B	3.09	129.83	125.06
82	AD	301	PEB	CAC-C2C-C1C	3.09	130.69	125.76
96	v6	201	HEM	CHB-C1B-NB	3.09	128.19	124.37
87	B2	827	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
82	T9	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
87	LN	206	CLA	CMB-C2B-C3B	3.09	134.08	126.59
82	i4	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	LI	202	PEB	CHA-C1B-NB	-3.09	118.46	124.93
82	OJ	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	EK	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	w8	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	V9	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	wC	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	VJ	202	PEB	C1C-CHB-C4B	-3.09	121.35	128.28
82	NK	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	SG	201	PEB	CHC-C1D-ND	-3.09	109.81	113.72
82	AO	301	PEB	CMB-C2B-C1B	3.09	129.83	125.06
82	mK	202	PEB	CHC-C4C-NC	3.09	125.33	121.15
82	u8	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	A9	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
96	G2	201	HEM	C4A-NA-C1A	3.09	108.38	105.35
82	HA	203	PEB	CHA-C4A-NA	-3.09	121.53	125.20
82	Z4	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	R9	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	DD	203	PEB	C3D-C4D-ND	3.09	113.33	107.26
82	LM	201	PEB	CHA-C1B-NB	-3.09	118.47	124.93
82	NK	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	RB	202	PEB	CHC-C1D-ND	-3.09	109.81	113.72
87	dL	404	CLA	CHB-C4A-NA	3.09	128.79	124.51
87	4N	604	CLA	CHB-C4A-NA	3.09	128.79	124.51
82	RI	202	PEB	C1C-CHB-C4B	-3.09	121.35	128.28
82	YO	203	PEB	OA-C1A-C2A	-3.09	123.72	126.17
82	wC	204	PEB	OA-C1A-C2A	-3.09	123.72	126.17
82	PA	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
82	UI	202	PEB	C2A-C1A-NA	3.09	110.94	108.27
82	O5	201	PEB	CHB-C1C-NC	-3.09	118.24	125.32
82	SQ	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	G9	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	lF	201	PEB	OD-C4D-ND	-3.09	121.35	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	oK	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	LI	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	gO	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
87	22	605	CLA	CAB-C3B-C2B	3.09	131.60	123.59
82	YF	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	LI	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	d1	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	C9	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
82	aB	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
85	BL	617	BCR	C16-C17-C18	-3.09	122.90	127.31
83	AH	304	PUB	CHA-C1B-NB	3.09	125.33	121.15
82	HI	203	PEB	CHC-C1D-ND	-3.09	109.81	113.72
83	AH	304	PUB	CMA-C2A-C3A	3.09	136.02	129.67
82	MA	201	PEB	CMB-C2B-C1B	3.09	129.82	125.06
82	Q7	201	PEB	OD-C4D-C3D	-3.09	122.46	129.46
82	WF	203	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	PO	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	J5	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
87	L2	206	CLA	CMB-C2B-C3B	3.09	134.07	126.59
82	QQ	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
82	Y4	203	PEB	OA-C1A-C2A	-3.09	123.72	126.17
84	x3	1001	CYC	CMC-C2C-C1C	3.09	119.06	112.40
87	3N	312	CLA	CHB-C4A-NA	3.09	128.78	124.51
85	kL	100	BCR	C21-C20-C19	3.09	132.86	123.22
82	DB	201	PEB	CHC-C4C-NC	3.09	125.33	121.15
82	HO	1002	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	fH	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
87	1N	602	CLA	C2A-C1A-CHA	3.09	129.26	123.86
85	hL	102	BCR	C24-C23-C22	-3.09	121.57	126.23
82	U1	202	PEB	CHC-C1D-ND	-3.09	109.81	113.72
82	y8	201	PEB	CHC-C1D-ND	-3.09	109.81	113.72
82	RB	202	PEB	CHB-C1C-C2C	-3.09	120.18	127.15
82	RK	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
82	dM	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	QE	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	l1	203	PEB	CHA-C1B-C2B	3.09	132.84	124.90
82	sK	201	PEB	OD-C4D-C3D	-3.09	122.46	129.46
87	1N	603	CLA	CMB-C2B-C1B	-3.09	120.66	125.37
82	OE	201	PEB	CHB-C4B-C3B	-3.09	118.17	125.32
85	c6	617	BCR	C33-C5-C6	-3.09	121.06	124.53
82	QM	204	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	r8	201	PEB	CMB-C2B-C1B	3.09	129.82	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EP	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
82	II	203	PEB	CHB-C4B-NB	-3.09	118.15	124.58
84	e3	1001	CYC	C4D-CHA-C1A	3.09	135.21	128.28
82	F1	1002	PEB	C3B-C4B-NB	3.09	114.54	110.05
85	BN	841	BCR	C8-C9-C10	-3.09	114.20	118.94
82	j4	203	PEB	OD-C4D-ND	-3.09	121.36	125.93
82	OO	201	PEB	C3C-C4C-NC	3.09	111.11	108.33
82	H5	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	hK	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	eO	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
84	EG	1001	CYC	C1B-NB-C4B	-3.09	106.74	110.67
82	xF	303	PEB	OD-C4D-C3D	-3.09	122.46	129.46
82	LF	202	PEB	CAB-C3B-C4B	3.09	130.47	125.01
82	EI	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
82	YQ	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
82	E9	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
82	uC	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
82	PG	201	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
82	QD	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
82	EI	202	PEB	C1C-CHB-C4B	-3.09	121.36	128.28
87	AN	835	CLA	CHB-C4A-NA	3.09	128.78	124.51
87	BN	829	CLA	CHB-C4A-NA	3.09	128.78	124.51
84	EO	1001	CYC	C4D-C3D-C2D	-3.09	103.97	107.62
82	ED	201	PEB	CHB-C1C-NC	-3.09	118.25	125.32
82	ZJ	202	PEB	OD-C4D-ND	-3.09	121.36	125.93
82	aG	201	PEB	CHC-C1D-ND	-3.09	109.82	113.72
82	aJ	203	PEB	CHC-C1D-ND	-3.09	109.82	113.72
82	CQ	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
85	AN	847	BCR	C11-C12-C13	-3.09	117.74	126.42
85	d6	405	BCR	C24-C23-C22	3.09	130.90	126.23
82	SM	201	PEB	CHA-C1B-NB	-3.09	118.47	124.93
87	BN	801	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
87	6N	604	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
87	AN	821	CLA	CHB-C4A-NA	3.09	128.78	124.51
82	mK	201	PEB	CMB-C2B-C1B	3.09	129.82	125.06
82	PE	201	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
84	MO	1001	CYC	C4D-CHA-C1A	3.09	135.21	128.28
84	DG	1001	CYC	C4D-C3D-C2D	-3.09	103.97	107.62
82	RJ	201	PEB	OD-C4D-ND	-3.09	121.36	125.93
82	TQ	201	PEB	CHA-C1B-NB	-3.09	118.48	124.93
82	mF	201	PEB	CHA-C1B-NB	-3.09	118.48	124.93
82	qF	201	PEB	C2A-C1A-NA	3.09	110.93	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y7	301	PEB	OD-C4D-C3D	-3.09	122.47	129.46
87	12	603	CLA	CMB-C2B-C1B	-3.09	120.67	125.37
82	UM	203	PEB	C3B-C4B-NB	3.09	114.54	110.05
82	lJ	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
82	QD	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
82	mK	201	PEB	CHC-C4C-NC	3.09	125.33	121.15
87	c6	615	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
82	TH	202	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
83	xF	301	PUB	CAC-CBC-CGC	-3.09	106.96	113.60
82	fE	202	PEB	C3B-C4B-NB	3.09	114.54	110.05
82	UH	201	PEB	OD-C4D-C3D	-3.09	122.47	129.46
82	VG	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
82	bE	201	PEB	C1D-CHC-C4C	-3.09	108.71	113.26
82	S4	202	PEB	C1B-C2B-C3B	-3.09	102.97	106.51
82	D9	202	PEB	C1B-C2B-C3B	-3.09	102.97	106.51
82	sC	202	PEB	C1B-C2B-C3B	-3.09	102.97	106.51
82	dM	203	PEB	C1B-C2B-C3B	-3.09	102.97	106.51
82	u8	202	PEB	C2A-C1A-NA	3.09	110.93	108.27
82	JO	1002	PEB	CMC-C3C-C4C	3.09	130.33	127.06
82	HP	201	PEB	CAC-C2C-C1C	3.09	130.68	125.76
82	X9	202	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
87	c6	608	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
85	B2	841	BCR	C8-C9-C10	-3.09	114.21	118.94
82	PM	201	PEB	CHB-C4B-NB	-3.08	118.16	124.58
82	O9	201	PEB	CHA-C1B-C2B	-3.08	116.97	124.90
82	ZM	201	PEB	CHA-C1B-C2B	3.08	132.83	124.90
83	A1	303	PUB	OA-C1A-NA	-3.08	121.36	125.93
82	dO	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
85	AL	401	BCR	C24-C23-C22	-3.08	121.57	126.23
82	NI	201	PEB	C3B-C4B-NB	3.08	114.54	110.05
82	J4	1002	PEB	C3B-C4B-NB	3.08	114.54	110.05
84	LO	1001	CYC	OB-C4B-C3B	-3.08	124.69	128.04
82	OG	201	PEB	CHB-C4B-C3B	-3.08	118.18	125.32
85	FL	101	BCR	C16-C17-C18	-3.08	122.91	127.31
82	UF	202	PEB	CHC-C1D-ND	-3.08	109.82	113.72
82	e4	201	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	u8	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
95	h6	101	DGD	O1G-C1A-C2A	3.08	121.59	111.91
82	EM	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	dG	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	dE	201	PEB	CHB-C1C-NC	-3.08	118.25	125.32
82	qC	203	PEB	CHC-C4C-NC	3.08	125.32	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TD	201	PEB	CHA-C1B-NB	-3.08	118.48	124.93
82	BI	203	PEB	CHA-C1B-NB	-3.08	118.48	124.93
82	u8	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	l1	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
82	EK	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	aB	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	vF	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	oK	202	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	dQ	401	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	GF	201	PEB	C1C-CHB-C4B	3.08	135.20	128.28
82	RD	201	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	XQ	203	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	j4	201	PEB	C2B-C1B-NB	3.08	117.11	110.53
82	uF	202	PEB	CHA-C1B-C2B	3.08	132.83	124.90
82	PP	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
85	AN	848	BCR	C37-C22-C23	3.08	122.94	118.08
82	U9	204	PEB	CHB-C1C-NC	-3.08	118.26	125.32
82	UO	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
85	A2	845	BCR	C3-C4-C5	-3.08	108.57	114.08
82	MP	203	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	cB	403	PEB	CHA-C1B-NB	-3.08	118.48	124.93
87	A2	852	CLA	CHB-C4A-NA	3.08	128.78	124.51
82	FI	202	PEB	CHC-C1D-ND	-3.08	109.82	113.72
87	BN	827	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
82	UA	202	PEB	CHC-C4C-NC	3.08	125.32	121.15
82	jE	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
82	g4	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	ZO	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
87	B2	809	CLA	CBA-CAA-C2A	3.08	122.96	113.86
82	OM	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
82	WM	203	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	LE	1002	PEB	C2A-C1A-NA	3.08	110.93	108.27
84	R3	1001	CYC	C4D-CHA-C1A	3.08	135.19	128.28
84	l3	1001	CYC	C4D-CHA-C1A	3.08	135.19	128.28
82	dE	201	PEB	CHC-C1D-ND	-3.08	109.83	113.72
82	jO	201	PEB	C2B-C1B-NB	3.08	117.11	110.53
82	CF	202	PEB	CAC-C2C-C3C	3.08	134.13	127.07
85	BN	803	BCR	C23-C24-C25	3.08	135.86	127.20
82	cK	203	PEB	C1C-CHB-C4B	3.08	135.19	128.28
82	PI	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	N4	1002	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
84	C4	1001	CYC	C1A-C2A-C3A	-3.08	103.37	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QG	203	PEB	OA-C1A-C2A	-3.08	123.72	126.17
82	VO	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	uF	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	T1	201	PEB	CMB-C2B-C1B	3.08	129.81	125.06
82	E9	201	PEB	CMB-C2B-C1B	3.08	129.81	125.06
82	GB	203	PEB	C3B-C4B-NB	3.08	114.53	110.05
82	TA	203	PEB	CHB-C4B-C3B	-3.08	118.19	125.32
82	GD	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
82	qK	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
82	iM	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
85	Z6	101	BCR	C3-C4-C5	-3.08	108.58	114.08
82	BB	203	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	PQ	203	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	E9	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	P9	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	gO	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
87	bL	605	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
82	NI	203	PEB	CMB-C2B-C1B	3.08	129.81	125.06
82	d4	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
82	ZE	201	PEB	C1C-NC-C4C	-3.08	104.12	109.60
82	SJ	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
84	W3	1001	CYC	C2D-C1D-ND	3.08	111.73	107.40
82	WF	202	PEB	CAA-C3A-C2A	-3.08	106.56	114.26
87	I2	102	CLA	CHB-C4A-NA	3.08	128.77	124.51
85	B2	838	BCR	C20-C19-C18	-3.08	117.76	126.42
82	QM	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	QO	201	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	T9	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
82	eG	203	PEB	CMC-C3C-C4C	-3.08	123.80	127.06
82	PE	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
82	Z4	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
82	WK	201	PEB	C3B-C4B-NB	3.08	114.53	110.05
82	aM	201	PEB	C3B-C4B-NB	3.08	114.53	110.05
84	GG	1001	CYC	C2A-C1A-NA	3.08	114.53	110.05
82	QD	201	PEB	CAC-C2C-C1C	3.08	130.67	125.76
82	cK	203	PEB	CAC-C2C-C1C	3.08	130.67	125.76
82	WK	202	PEB	CHC-C4C-NC	3.08	125.32	121.15
82	IB	203	PEB	CHC-C1D-ND	-3.08	109.83	113.72
82	QB	202	PEB	CHA-C1B-NB	-3.08	118.49	124.93
82	OA	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	RA	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
82	MF	203	PEB	OD-C4D-ND	-3.08	121.37	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QK	203	PEB	OD-C4D-ND	-3.08	121.37	125.93
82	Y1	201	PEB	C1C-CHB-C4B	3.08	135.19	128.28
84	E3	1001	CYC	C4D-CHA-C1A	3.08	135.19	128.28
84	p3	1001	CYC	C4D-CHA-C1A	3.08	135.19	128.28
82	zC	201	PEB	CBA-CAA-C3A	3.08	120.32	113.47
84	DH	1001	CYC	CHA-C4D-C3D	-3.08	120.20	127.15
87	72	601	CLA	CHB-C4A-NA	3.08	128.77	124.51
87	AN	828	CLA	CHB-C1B-C2B	-3.08	118.54	127.24
87	A2	828	CLA	CHB-C1B-C2B	-3.08	118.54	127.24
82	OJ	201	PEB	CHA-C1B-NB	-3.08	118.49	124.93
82	QH	203	PEB	C3B-C4B-NB	3.08	114.53	110.05
82	b1	203	PEB	C3B-C4B-NB	3.08	114.53	110.05
82	FM	202	PEB	CAB-C3B-C4B	3.08	130.46	125.01
82	fG	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
82	k1	202	PEB	CHC-C4C-NC	3.08	125.32	121.15
82	k1	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
82	A9	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
82	fJ	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
82	IM	201	PEB	CHA-C1B-NB	-3.08	118.49	124.93
82	QJ	203	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	QP	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	yF	301	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	SI	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
82	rF	202	PEB	C1C-CHB-C4B	3.08	135.19	128.28
82	nK	201	PEB	C1C-CHB-C4B	3.08	135.19	128.28
82	PE	201	PEB	CAC-C2C-C1C	3.08	130.66	125.76
87	BN	824	CLA	CMB-C2B-C3B	3.08	134.04	126.59
82	M7	202	PEB	CHC-C4C-NC	3.08	125.31	121.15
82	CF	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
84	K3	1001	CYC	C4D-CHA-C1A	3.08	135.19	128.28
83	KA	203	PUB	CHA-C4A-NA	-3.08	109.83	113.72
82	R7	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
82	LP	201	PEB	CMB-C2B-C1B	3.08	129.80	125.06
82	OM	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
82	O7	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
87	BN	810	CLA	CBA-CAA-C2A	3.08	122.95	113.86
98	B2	837	PQN	C16-C17-C18	-3.08	105.97	115.92
82	w8	204	PEB	OA-C1A-C2A	-3.08	123.73	126.17
82	DA	203	PEB	C2A-C1A-NA	3.08	110.93	108.27
83	xK	305	PUB	CHA-C1B-NB	3.08	125.31	121.15
84	BG	1001	CYC	CAD-C3D-C4D	3.08	130.66	125.76
95	BL	614	DGD	C3E-C4E-C5E	3.08	115.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YK	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
82	dJ	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
85	B2	802	BCR	C23-C24-C25	3.08	135.84	127.20
82	WA	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
85	B2	841	BCR	C33-C5-C4	3.08	119.53	113.62
82	OF	203	PEB	C1D-CHC-C4C	-3.08	108.72	113.26
82	UO	202	PEB	C1D-CHC-C4C	3.08	117.79	113.26
87	A2	819	CLA	CMB-C2B-C1B	-3.08	120.68	125.37
87	12	602	CLA	C2A-C1A-CHA	3.08	129.24	123.86
82	aE	201	PEB	CHC-C1D-ND	-3.08	109.83	113.72
82	eO	203	PEB	CHC-C1D-ND	-3.08	109.83	113.72
87	bL	622	CLA	CHB-C4A-NA	3.08	128.77	124.51
84	G3	1001	CYC	C4D-CHA-C1A	3.08	135.18	128.28
82	GQ	202	PEB	C1D-CHC-C4C	-3.08	108.72	113.26
87	O2	202	CLA	C2A-C1A-CHA	3.08	129.24	123.86
82	A9	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
82	lE	201	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
82	QK	201	PEB	CAB-C3B-C4B	3.08	130.45	125.01
82	eE	201	PEB	C1B-C2B-C3B	-3.08	102.98	106.51
82	RD	202	PEB	CMB-C2B-C1B	3.08	129.80	125.06
84	m3	1001	CYC	C4D-CHA-C1A	3.08	135.18	128.28
82	SF	203	PEB	C3B-C4B-NB	3.08	114.52	110.05
82	UO	202	PEB	C3B-C4B-NB	3.08	114.52	110.05
82	VJ	202	PEB	CAB-C3B-C4B	3.08	130.45	125.01
84	c3	1001	CYC	C4D-CHA-C1A	3.08	135.18	128.28
82	NA	201	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
82	CD	201	PEB	C1B-C2B-C3B	-3.08	102.98	106.51
82	j1	202	PEB	C1B-C2B-C3B	-3.08	102.98	106.51
82	H7	203	PEB	CHA-C4A-NA	-3.07	121.55	125.20
84	JH	1003	CYC	CMB-C2B-C1B	3.07	128.01	124.17
84	C4	1001	CYC	CHA-C4D-C3D	-3.07	120.21	127.15
88	c6	619	LHG	C5-O7-C7	-3.07	110.22	117.79
82	kH	202	PEB	OD-C4D-ND	-3.07	121.38	125.93
82	d1	203	PEB	CMB-C2B-C1B	3.07	129.80	125.06
87	2N	301	CLA	CAB-C3B-C2B	3.07	131.56	123.59
82	MD	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
87	72	606	CLA	CHB-C4A-NA	3.07	128.76	124.51
82	UI	202	PEB	CMB-C2B-C1B	3.07	129.80	125.06
83	YA	302	PUB	OD-C4D-ND	-3.07	121.38	125.93
82	OO	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	O5	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	uC	202	PEB	C2A-C1A-NA	3.07	110.92	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gF	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	AK	201	PEB	CAB-C3B-C4B	3.07	130.45	125.01
82	K9	201	PEB	C3B-C4B-NB	3.07	114.52	110.05
82	JK	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	BP	202	PEB	CAC-CBC-CGC	-3.07	106.99	113.60
95	c6	601	DGD	O2E-C2E-C1E	3.07	117.51	110.05
82	Q9	203	PEB	CHA-C1B-NB	-3.07	118.50	124.93
82	eG	202	PEB	OD-C4D-ND	-3.07	121.38	125.93
82	aK	203	PEB	CHC-C1D-ND	-3.07	109.84	113.72
87	AN	838	CLA	C3B-C4B-NB	-3.07	107.66	110.52
82	VM	201	PEB	C3B-C4B-NB	3.07	114.52	110.05
82	Q5	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
82	tC	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	UP	202	PEB	CAC-C2C-C1C	3.07	130.66	125.76
82	P9	201	PEB	CMB-C2B-C1B	3.07	129.80	125.06
84	C3	1001	CYC	C4D-CHA-C1A	3.07	135.17	128.28
87	BL	609	CLA	CHB-C4A-NA	3.07	128.76	124.51
87	7N	601	CLA	CHB-C4A-NA	3.07	128.76	124.51
82	ZG	201	PEB	C1C-NC-C4C	-3.07	104.13	109.60
82	vC	202	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
82	UH	202	PEB	CHC-C1D-ND	-3.07	109.84	113.72
82	P4	202	PEB	CMC-C3C-C4C	3.07	130.32	127.06
82	P9	201	PEB	C3B-C4B-NB	3.07	114.52	110.05
87	F2	202	CLA	CHB-C4A-NA	3.07	128.76	124.51
87	7N	606	CLA	CHB-C4A-NA	3.07	128.76	124.51
87	82	306	CLA	CHB-C1B-NB	3.07	127.51	124.26
82	Y4	203	PEB	CHC-C1D-ND	-3.07	109.84	113.72
82	WF	202	PEB	CHA-C1B-C2B	3.07	132.80	124.90
82	LD	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	RQ	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	I7	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	lJ	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	hE	203	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
82	kG	201	PEB	CHC-C4C-NC	3.07	125.31	121.15
82	I9	201	PEB	C3B-C4B-NB	3.07	114.52	110.05
84	P3	1001	CYC	C4D-CHA-C1A	3.07	135.17	128.28
84	i3	1001	CYC	C4D-CHA-C1A	3.07	135.17	128.28
82	QD	201	PEB	OD-C4D-ND	-3.07	121.38	125.93
82	lO	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
84	v3	1001	CYC	C4D-CHA-C1A	3.07	135.17	128.28
82	e4	203	PEB	CHC-C1D-ND	-3.07	109.84	113.72
82	BP	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O1	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	C9	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
82	WK	203	PEB	CHC-C4C-NC	3.07	125.31	121.15
82	fJ	201	PEB	OD-C4D-ND	-3.07	121.38	125.93
87	FN	201	CLA	CHB-C4A-NA	3.07	128.76	124.51
82	rK	202	PEB	C1C-CHB-C4B	3.07	135.17	128.28
82	lG	202	PEB	OD-C4D-C3D	-3.07	122.50	129.46
82	aM	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
83	Z5	302	PUB	C2C-C1C-NC	3.07	114.52	110.05
82	YA	304	PEB	CHB-C4B-NB	-3.07	118.19	124.58
82	FB	201	PEB	CHA-C1B-NB	-3.07	118.51	124.93
84	g3	1001	CYC	C4D-CHA-C1A	3.07	135.17	128.28
82	FH	1002	PEB	OD-C4D-ND	-3.07	121.38	125.93
82	K9	202	PEB	OD-C4D-ND	-3.07	121.38	125.93
82	gE	202	PEB	OD-C4D-ND	-3.07	121.38	125.93
82	VA	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	NI	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
87	IN	102	CLA	CHB-C4A-NA	3.07	128.76	124.51
82	uF	201	PEB	C1C-CHB-C4B	3.07	135.17	128.28
84	J3	1001	CYC	C4D-CHA-C1A	3.07	135.17	128.28
82	dH	203	PEB	CMB-C2B-C1B	3.07	129.79	125.06
82	aG	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
84	J1	1001	CYC	C2A-C1A-NA	3.07	114.51	110.05
82	eE	203	PEB	CMC-C3C-C4C	-3.07	123.81	127.06
82	QF	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	P7	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	mG	203	PEB	OD-C4D-ND	-3.07	121.38	125.93
95	C6	504	DGD	O6D-C1D-C2D	-3.07	103.85	110.35
82	RA	203	PEB	CHB-C1C-NC	-3.07	118.29	125.32
82	aG	202	PEB	C1C-CHB-C4B	-3.07	121.40	128.28
82	eF	202	PEB	C4C-C3C-C2C	-3.07	104.67	107.50
82	YH	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
87	A2	835	CLA	CHB-C4A-NA	3.07	128.76	124.51
82	DB	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	TP	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	NQ	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	SG	201	PEB	CMB-C2B-C1B	3.07	129.79	125.06
87	b6	618	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
82	N4	1002	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	J5	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	I7	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	U1	201	PEB	OD-C4D-C3D	-3.07	122.51	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OE	203	PEB	CHC-C1D-ND	-3.07	109.84	113.72
82	aE	201	PEB	CHC-C4C-NC	3.07	125.30	121.15
87	62	306	CLA	CHB-C4A-NA	3.07	128.75	124.51
87	62	305	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
82	rC	201	PEB	CMB-C2B-C1B	3.07	129.79	125.06
82	P7	203	PEB	OD-C4D-C3D	-3.07	122.51	129.46
82	KA	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	UJ	201	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	S5	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	UG	203	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	dH	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
84	DE	1001	CYC	C2A-C1A-NA	3.07	114.51	110.05
82	GB	201	PEB	OD-C4D-ND	-3.07	121.39	125.93
82	tK	203	PEB	C1C-CHB-C4B	3.07	135.16	128.28
82	WK	203	PEB	CHC-C1D-ND	-3.07	109.84	113.72
84	H1	1001	CYC	CHA-C4D-C3D	-3.07	120.23	127.15
87	B2	829	CLA	CHB-C4A-NA	3.07	128.75	124.51
84	EG	1001	CYC	C1B-C2B-C3B	-3.07	104.67	107.87
82	WK	201	PEB	CMA-C2A-C1A	-3.07	105.79	112.40
82	g4	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
84	T3	1001	CYC	C4D-CHA-C1A	3.07	135.16	128.28
82	X9	202	PEB	OD-C4D-ND	-3.07	121.39	125.93
82	PP	201	PEB	CHA-C1B-NB	-3.07	118.52	124.93
82	AI	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	SP	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	hM	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	TA	201	PEB	CHC-C1D-ND	-3.07	109.84	113.72
84	H1	1001	CYC	C1B-NB-C4B	-3.07	106.76	110.67
82	AO	304	PEB	C3B-C4B-NB	3.07	114.51	110.05
84	HG	1001	CYC	C2A-C1A-NA	3.07	114.51	110.05
82	V9	202	PEB	OD-C4D-ND	-3.07	121.39	125.93
82	nF	201	PEB	C1C-CHB-C4B	3.07	135.16	128.28
82	AB	501	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
82	SO	202	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
82	W7	201	PEB	OD-C4D-C3D	-3.07	122.51	129.46
82	gM	202	PEB	CHC-C4C-NC	3.07	125.30	121.15
95	c6	618	DGD	C2G-O2G-C1B	-3.07	110.24	117.79
82	K9	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	fE	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	hK	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	XJ	202	PEB	OA-C1A-C2A	-3.07	123.73	126.17
82	YH	202	PEB	CHC-C1D-ND	-3.07	109.84	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aF	203	PEB	CHC-C1D-ND	-3.07	109.84	113.72
84	A3	1001	CYC	C4D-CHA-C1A	3.07	135.16	128.28
82	aE	201	PEB	OD-C4D-ND	-3.07	121.39	125.93
83	AE	303	PUB	OA-C1A-NA	-3.07	121.39	125.93
82	N7	203	PEB	C4C-C3C-C2C	-3.07	104.67	107.50
82	IM	201	PEB	C2A-C1A-NA	3.07	110.92	108.27
82	U4	202	PEB	CMB-C2B-C1B	3.07	129.78	125.06
82	fJ	203	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
82	P1	202	PEB	CHC-C1D-ND	-3.07	109.85	113.72
82	KQ	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
82	WF	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	QJ	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	c4	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	jF	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
82	KK	201	PEB	C1C-NC-C4C	-3.07	104.14	109.60
82	WB	401	PEB	OD-C4D-ND	-3.07	121.39	125.93
82	T4	201	PEB	OD-C4D-ND	-3.07	121.39	125.93
82	q8	203	PEB	CHC-C4C-NC	3.06	125.30	121.15
82	DI	202	PEB	CHA-C1B-NB	-3.06	118.52	124.93
82	UP	203	PEB	CHA-C1B-NB	-3.06	118.52	124.93
87	6N	605	CLA	CHB-C4A-NA	3.06	128.75	124.51
82	AP	202	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	eA	301	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	eH	202	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	PA	203	PEB	C2A-C1A-NA	3.06	110.92	108.27
82	ED	202	PEB	C3B-C4B-NB	3.06	114.51	110.05
82	pC	201	PEB	C3B-C4B-NB	3.06	114.51	110.05
82	T9	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
87	A2	827	CLA	C3B-C4B-NB	-3.06	107.67	110.52
82	JQ	201	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
82	V7	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
82	kF	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
82	BJ	301	PEB	CHA-C1B-NB	-3.06	118.52	124.93
96	vL	201	HEM	CHA-C4D-C3D	-3.06	119.58	125.33
82	LK	202	PEB	CAB-C3B-C4B	3.06	130.43	125.01
82	NB	202	PEB	OD-C4D-C3D	-3.06	122.52	129.46
82	lO	201	PEB	C2B-C1B-NB	3.06	117.07	110.53
82	FD	202	PEB	CHB-C1C-C2C	-3.06	120.24	127.15
82	YQ	201	PEB	CHC-C4C-NC	3.06	125.30	121.15
84	F4	1001	CYC	C4D-C3D-C2D	-3.06	104.00	107.62
87	BN	826	CLA	CHB-C4A-NA	3.06	128.75	124.51
87	cL	508	CLA	CHB-C4A-NA	3.06	128.75	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RQ	202	PEB	C3B-C4B-NB	3.06	114.51	110.05
82	SB	203	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	xK	302	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
84	HE	1001	CYC	CHD-C1D-ND	-3.06	118.30	125.32
82	KF	203	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	cF	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	bK	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
87	52	610	CLA	CHB-C4A-NA	3.06	128.75	124.51
87	cL	510	CLA	CHB-C4A-NA	3.06	128.75	124.51
82	C7	201	PEB	OD-C4D-ND	-3.06	121.39	125.93
82	C9	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
83	xF	306	PUB	CHB-C4B-NB	-3.06	118.30	125.32
82	VE	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
82	S5	201	PEB	CBB-CAB-C3B	3.06	121.14	112.63
87	ON	203	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
82	FD	201	PEB	C3C-C4C-NC	3.06	111.09	108.33
82	M9	304	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
82	GB	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
82	N9	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
82	aB	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
82	BB	203	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	TF	201	PEB	OD-C4D-ND	-3.06	121.39	125.93
82	CQ	201	PEB	CHC-C4C-NC	3.06	125.29	121.15
82	HH	1002	PEB	CMC-C3C-C4C	3.06	130.31	127.06
87	AN	834	CLA	CHB-C4A-NA	3.06	128.75	124.51
87	42	604	CLA	CHB-C4A-NA	3.06	128.75	124.51
82	VI	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
87	O2	203	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
87	B2	825	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
87	C6	514	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
82	dJ	201	PEB	C3C-C4C-NC	3.06	111.09	108.33
82	P1	202	PEB	CAC-C2C-C1C	3.06	130.64	125.76
96	GN	201	HEM	C4A-NA-C1A	3.06	108.35	105.35
85	K2	102	BCR	C15-C14-C13	3.06	131.68	127.31
82	XM	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
82	IB	203	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	UP	203	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	zC	201	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
82	dG	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	xF	302	PEB	C3B-C4B-NB	3.06	114.50	110.05
82	WD	202	PEB	CHC-C4C-NC	3.06	125.29	121.15
82	QK	201	PEB	CHC-C4C-NC	3.06	125.29	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GI	201	PEB	CMC-C3C-C4C	3.06	130.31	127.06
82	PF	201	PEB	CHC-C1D-ND	-3.06	109.85	113.72
82	gH	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
83	M9	303	PUB	OA-C1A-NA	-3.06	121.40	125.93
83	yF	302	PUB	CAC-CBC-CGC	-3.06	107.02	113.60
82	SA	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
82	XD	201	PEB	C3C-C4C-NC	3.06	111.09	108.33
82	LO	1002	PEB	C3C-C4C-NC	3.06	111.09	108.33
82	SM	201	PEB	OD-C4D-C3D	-3.06	122.53	129.46
84	DE	1001	CYC	CHD-C1D-ND	-3.06	118.31	125.32
82	AQ	304	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	BB	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	dE	203	PEB	OD-C4D-ND	-3.06	121.40	125.93
83	AG	303	PUB	OA-C1A-NA	-3.06	121.40	125.93
82	A9	201	PEB	CMB-C2B-C1B	3.06	129.78	125.06
82	R7	202	PEB	CHA-C4A-NA	3.06	128.84	125.20
82	EJ	202	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	W1	203	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	dG	204	PEB	OD-C4D-C3D	-3.06	122.53	129.46
82	H7	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	eK	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
87	cL	505	CLA	CAA-C2A-C3A	-3.06	104.40	112.78
82	RI	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
82	PQ	201	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
82	bP	502	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
84	IG	1001	CYC	C1B-NB-C4B	-3.06	106.77	110.67
85	aL	604	BCR	C36-C18-C17	-3.06	118.64	122.92
82	K7	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	jJ	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	OA	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
82	YQ	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
82	TJ	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
96	fL	102	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
82	BF	201	PEB	CHB-C1C-C2C	-3.06	120.25	127.15
82	mF	202	PEB	CAA-C3A-C4A	3.06	120.53	112.67
82	ID	202	PEB	CHC-C4C-NC	3.06	125.29	121.15
82	KE	201	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
82	E7	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
84	G4	1001	CYC	CHB-C4A-NA	-3.06	118.54	124.93
87	b6	612	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
87	AN	803	CLA	C3B-C4B-NB	-3.06	107.68	110.52
84	M4	1001	CYC	C4D-CHA-C1A	3.06	135.14	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A2	848	BCR	C37-C22-C23	3.06	122.89	118.08
92	mL	101	LMG	O8-C28-C29	3.06	121.50	111.91
82	XB	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	jM	203	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	fK	201	PEB	CMB-C2B-C1B	3.06	129.77	125.06
82	CJ	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
82	IK	203	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	GM	203	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	BP	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	Q4	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	eG	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	OM	202	PEB	CHA-C1B-NB	-3.06	118.54	124.93
82	DE	1002	PEB	OD-C4D-C3D	-3.06	122.53	129.46
82	VE	202	PEB	CHB-C1C-NC	-3.06	118.32	125.32
82	QA	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
82	OI	202	PEB	C1C-NC-C4C	-3.06	104.16	109.60
92	A6	408	LMG	C8-O7-C10	-3.06	110.26	117.79
82	DA	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
82	UD	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
82	R9	201	PEB	CMB-C2B-C1B	3.06	129.77	125.06
85	BN	841	BCR	C33-C5-C4	3.06	119.49	113.62
82	DP	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	KQ	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	IA	201	PEB	C3B-C4B-NB	3.06	114.50	110.05
82	eH	203	PEB	C3B-C4B-NB	3.06	114.50	110.05
82	Z9	303	PEB	C3B-C4B-NB	3.06	114.50	110.05
82	R7	203	PEB	CHB-C1C-NC	-3.06	118.32	125.32
82	E5	202	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	I9	201	PEB	CMB-C2B-C1B	3.06	129.77	125.06
83	AE	302	PUB	OD-C4D-ND	-3.06	121.40	125.93
82	L4	1002	PEB	C3B-C4B-NB	3.06	114.50	110.05
82	TD	201	PEB	C1C-CHB-C4B	3.06	135.14	128.28
84	D1	1003	CYC	CHA-C4D-C3D	-3.06	120.25	127.15
82	iM	202	PEB	CHB-C4B-NB	-3.06	118.22	124.58
87	A2	821	CLA	CHB-C4A-NA	3.06	128.74	124.51
87	b6	606	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
82	OA	202	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	OP	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
98	BN	837	PQN	C16-C17-C18	-3.06	106.04	115.92
82	F5	201	PEB	C3C-C4C-NC	3.06	111.08	108.33
82	QO	202	PEB	CHC-C1D-ND	-3.06	109.86	113.72
82	tK	202	PEB	OD-C4D-C3D	-3.06	122.54	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FP	201	PEB	C3B-C4B-NB	3.06	114.49	110.05
82	kE	202	PEB	C3B-C4B-NB	3.06	114.49	110.05
82	UP	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
82	S9	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
83	A1	304	PUB	CMA-C2A-C3A	3.06	135.95	129.67
82	WP	201	PEB	CAC-CBC-CGC	-3.06	107.03	113.60
82	1C	203	PEB	CHC-C4C-NC	3.06	125.28	121.15
82	HA	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
82	QO	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
82	PA	203	PEB	C3B-C4B-NB	3.06	114.49	110.05
82	hM	203	PEB	C3B-C4B-NB	3.06	114.49	110.05
82	PD	201	PEB	OA-C1A-C2A	-3.05	123.74	126.17
87	c6	613	CLA	C3B-C4B-NB	-3.05	107.68	110.52
82	CJ	202	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
82	V4	201	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
82	fE	201	PEB	CAB-CBB-CGB	-3.05	107.03	113.60
87	AN	807	CLA	CAA-C2A-C3A	-3.05	104.41	112.78
82	UE	203	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	ZB	202	PEB	C2A-C1A-NA	3.05	110.91	108.27
82	RD	201	PEB	C2A-C1A-NA	3.05	110.91	108.27
82	KM	203	PEB	C2A-C1A-NA	3.05	110.91	108.27
82	iF	202	PEB	C2A-C1A-NA	3.05	110.91	108.27
82	TF	202	PEB	CAB-C3B-C4B	3.05	130.41	125.01
85	LN	205	BCR	C36-C18-C19	3.05	122.89	118.08
82	EB	501	PEB	CMB-C2B-C1B	3.05	129.77	125.06
82	AE	301	PEB	C3B-C4B-NB	3.05	114.49	110.05
84	J4	1001	CYC	C2A-C1A-NA	3.05	114.49	110.05
82	WA	202	PEB	CHB-C1C-C2C	-3.05	120.26	127.15
82	W7	202	PEB	CHB-C1C-C2C	-3.05	120.26	127.15
82	pC	202	PEB	CHB-C1C-C2C	3.05	134.04	127.15
82	rF	202	PEB	CHA-C1B-NB	-3.05	118.55	124.93
82	A4	301	PEB	CMB-C2B-C1B	3.05	129.77	125.06
82	QP	203	PEB	OD-C4D-C3D	-3.05	122.54	129.46
96	VL	201	HEM	CHA-C4D-C3D	-3.05	119.60	125.33
82	DI	202	PEB	C2A-C1A-NA	3.05	110.91	108.27
84	I4	1001	CYC	C4D-C3D-C2D	-3.05	104.01	107.62
82	TA	202	PEB	C2B-C1B-NB	3.05	117.05	110.53
82	GP	201	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
82	hF	202	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
82	GJ	203	PEB	CMB-C2B-C1B	3.05	129.76	125.06
82	LO	1002	PEB	CMB-C2B-C1B	3.05	129.76	125.06
82	dO	202	PEB	CMB-C2B-C1B	3.05	129.76	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	R4	201	PEB	CHB-C4B-C3B	-3.05	118.26	125.32
82	GM	203	PEB	OD-C4D-ND	-3.05	121.41	125.93
87	aL	606	CLA	CHB-C4A-NA	3.05	128.73	124.51
84	N3	1001	CYC	C4D-CHA-C1A	3.05	135.13	128.28
85	L2	205	BCR	C36-C18-C19	3.05	122.89	118.08
82	HI	202	PEB	CMB-C2B-C1B	3.05	129.76	125.06
82	Z9	303	PEB	C2A-C1A-NA	3.05	110.90	108.27
87	c6	605	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
82	NE	202	PEB	CHA-C1B-NB	-3.05	118.55	124.93
87	B2	823	CLA	CMB-C2B-C3B	3.05	133.98	126.59
82	eK	202	PEB	C4C-C3C-C2C	-3.05	104.68	107.50
87	A2	807	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
82	GJ	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	HK	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	G9	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	WK	203	PEB	OD-C4D-ND	-3.05	121.41	125.93
87	5N	610	CLA	CHB-C4A-NA	3.05	128.73	124.51
82	jM	201	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	jO	202	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	p8	202	PEB	CHB-C1C-C2C	3.05	134.03	127.15
82	CA	202	PEB	CHC-C1D-ND	-3.05	109.86	113.72
84	y3	1001	CYC	C2D-C1D-ND	3.05	111.69	107.40
82	fF	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
82	lJ	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
82	H5	201	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	G9	201	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	eK	203	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	t8	201	PEB	CHC-C4C-NC	3.05	125.28	121.15
82	A7	202	PEB	C2A-C1A-NA	3.05	110.90	108.27
82	R1	201	PEB	C1B-C2B-C3B	-3.05	103.00	106.51
82	T7	203	PEB	CHB-C4B-C3B	-3.05	118.26	125.32
82	hM	202	PEB	CMB-C2B-C1B	3.05	129.76	125.06
87	B6	611	CLA	C3B-C4B-NB	-3.05	107.69	110.52
87	b6	611	CLA	C3B-C4B-NB	-3.05	107.69	110.52
82	KE	201	PEB	CHA-C1B-NB	-3.05	118.55	124.93
82	P4	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
84	t3	1001	CYC	C4D-CHA-C1A	3.05	135.12	128.28
87	AL	404	CLA	CHB-C4A-NA	3.05	128.73	124.51
82	MF	203	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	O1	202	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	fE	201	PEB	C3B-C4B-NB	3.05	114.49	110.05
82	mJ	202	PEB	CAB-C3B-C4B	3.05	130.41	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aO	202	PEB	CAB-C3B-C4B	3.05	130.41	125.01
82	UB	302	PEB	CMB-C2B-C1B	3.05	129.76	125.06
82	FF	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	CP	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	NF	202	PEB	OA-C1A-C2A	-3.05	123.75	126.17
82	P9	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
82	lK	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
84	HO	1001	CYC	C2D-C1D-ND	3.05	111.69	107.40
82	HQ	201	PEB	OD-C4D-C3D	-3.05	122.55	129.46
82	SO	201	PEB	CHA-C4A-NA	3.05	128.83	125.20
82	O5	202	PEB	CAB-C3B-C4B	3.05	130.40	125.01
82	sF	201	PEB	CHB-C1C-C2C	-3.05	120.27	127.15
82	CM	201	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	U9	202	PEB	C3B-C4B-NB	3.05	114.48	110.05
85	BN	839	BCR	C38-C26-C27	3.05	119.47	113.62
84	DH	1001	CYC	C1B-CHB-C4A	-3.05	120.63	128.08
82	Q5	203	PEB	CHC-C4C-NC	3.05	125.28	121.15
82	kE	201	PEB	CHC-C4C-NC	3.05	125.28	121.15
82	WG	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	wK	302	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	MK	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
82	W7	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
82	jJ	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
84	D1	1001	CYC	CHA-C4D-C3D	-3.05	120.27	127.15
82	YH	201	PEB	C1D-CHC-C4C	3.05	117.75	113.26
82	G5	202	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
85	AN	848	BCR	C3-C4-C5	-3.05	108.63	114.08
82	aJ	203	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	M9	304	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	kO	203	PEB	CHC-C1D-ND	-3.05	109.87	113.72
84	CO	1001	CYC	CHA-C4D-C3D	-3.05	120.27	127.15
82	SK	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
82	EP	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
82	U5	203	PEB	CHC-C4C-NC	3.05	125.28	121.15
82	mH	202	PEB	CHC-C4C-NC	3.05	125.28	121.15
87	BN	805	CLA	CMB-C2B-C3B	3.05	133.97	126.59
82	WH	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
82	OP	202	PEB	C1D-CHC-C4C	-3.05	108.76	113.26
83	yK	302	PUB	CAC-CBC-CGC	-3.05	107.04	113.60
82	FQ	202	PEB	CHB-C1C-C2C	-3.05	120.27	127.15
82	PH	201	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	II	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	k6	101	LMG	O7-C10-C11	3.05	118.07	111.50
82	T9	201	PEB	CMB-C2B-C1B	3.05	129.76	125.06
84	DE	1001	CYC	C4D-C3D-C2D	-3.05	104.02	107.62
82	SJ	201	PEB	CHB-C4B-NB	-3.05	118.23	124.58
85	A2	848	BCR	C3-C4-C5	-3.05	108.64	114.08
82	IB	202	PEB	OD-C4D-C3D	-3.05	122.56	129.46
82	IM	203	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	d1	202	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	TO	202	PEB	OA-C1A-C2A	-3.05	123.75	126.17
82	T4	202	PEB	OA-C1A-C2A	-3.05	123.75	126.17
82	TI	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
82	aO	202	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
82	lJ	202	PEB	OD-C4D-ND	-3.05	121.42	125.93
82	RF	202	PEB	OD-C4D-C3D	-3.05	122.56	129.46
82	UB	303	PEB	CMB-C2B-C1B	3.05	129.76	125.06
84	GO	1001	CYC	CMA-C3A-C4A	3.05	129.76	125.06
82	OD	202	PEB	C3B-C4B-NB	3.05	114.48	110.05
87	B2	826	CLA	CHB-C4A-NA	3.05	128.72	124.51
82	k4	202	PEB	CHC-C1D-ND	-3.05	109.87	113.72
82	EM	202	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
82	e4	202	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
82	x8	201	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
82	DM	202	PEB	C1C-CHB-C4B	-3.05	121.45	128.28
82	GD	202	PEB	OD-C4D-ND	-3.05	121.42	125.93
82	I9	202	PEB	OD-C4D-ND	-3.05	121.42	125.93
82	DB	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
87	A2	811	CLA	C2D-C1D-ND	-3.05	107.86	110.10
82	eJ	202	PEB	CHA-C4A-NA	-3.05	121.58	125.20
82	mK	202	PEB	CAA-C3A-C4A	3.05	120.50	112.67
87	8N	308	CLA	CMC-C2C-C3C	3.05	134.39	126.12
82	DD	202	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	EJ	203	PEB	C3B-C4B-NB	3.05	114.48	110.05
82	RH	202	PEB	CMC-C3C-C4C	3.05	130.29	127.06
82	PO	202	PEB	CMC-C3C-C4C	3.05	130.29	127.06
82	KG	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
82	AF	201	PEB	CAB-C3B-C4B	3.05	130.40	125.01
82	LF	201	PEB	CAB-C3B-C4B	3.05	130.40	125.01
82	S9	202	PEB	CHC-C1D-ND	-3.05	109.87	113.72
82	KF	201	PEB	C1C-NC-C4C	-3.05	104.18	109.60
82	V1	201	PEB	CAB-CBB-CGB	-3.05	107.05	113.60
82	bP	501	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
82	K9	201	PEB	CMB-C2B-C1B	3.05	129.75	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	V9	201	PEB	CMB-C2B-C1B	3.05	129.75	125.06
82	X9	201	PEB	CMB-C2B-C1B	3.05	129.75	125.06
82	FK	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
92	XL	601	LMG	O8-C28-C29	3.05	121.47	111.91
82	d4	202	PEB	C3B-C4B-NB	3.05	114.48	110.05
85	c6	603	BCR	C11-C10-C9	-3.05	122.96	127.31
82	RA	201	PEB	CMA-C2A-C1A	-3.05	105.84	112.40
82	F7	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
82	u8	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
82	HM	201	PEB	C2A-C1A-NA	3.04	110.90	108.27
82	S9	201	PEB	CMC-C3C-C4C	3.04	130.29	127.06
82	Z4	201	PEB	C3C-C4C-NC	3.04	111.07	108.33
82	l4	201	PEB	OA-C1A-C2A	-3.04	123.75	126.17
82	HE	1002	PEB	OD-C4D-C3D	-3.04	122.56	129.46
82	GD	201	PEB	C3B-C4B-NB	3.04	114.48	110.05
82	SJ	201	PEB	C3B-C4B-NB	3.04	114.48	110.05
82	Y9	203	PEB	C3B-C4B-NB	3.04	114.48	110.05
82	kO	202	PEB	C3B-C4B-NB	3.04	114.48	110.05
82	F5	203	PEB	CAC-CBC-CGC	-3.04	107.05	113.60
82	Y5	201	PEB	CAB-CBB-CGB	-3.04	107.05	113.60
82	OH	201	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
82	DJ	202	PEB	CAB-C3B-C4B	3.04	130.40	125.01
94	dL	406	PL9	C20-C19-C18	-3.04	115.87	123.68
82	eE	203	PEB	CHB-C4B-NB	-3.04	118.24	124.58
87	cL	511	CLA	C3B-C4B-NB	-3.04	107.69	110.52
82	DQ	202	PEB	C3B-C4B-NB	3.04	114.48	110.05
82	R7	203	PEB	C3B-C4B-NB	3.04	114.48	110.05
82	HM	201	PEB	CAB-C3B-C4B	3.04	130.39	125.01
85	fL	101	BCR	C37-C22-C23	3.04	122.87	118.08
82	AD	304	PEB	C2A-C1A-NA	3.04	110.90	108.27
82	O4	202	PEB	C2A-C1A-NA	3.04	110.90	108.27
82	U4	202	PEB	C2A-C1A-NA	3.04	110.90	108.27
82	eF	202	PEB	C2A-C1A-NA	3.04	110.90	108.27
87	bL	618	CLA	CHB-C4A-NA	3.04	128.72	124.51
82	Y4	203	PEB	OD-C4D-ND	-3.04	121.42	125.93
82	Q7	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
82	ND	203	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
82	YF	201	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
82	I9	202	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
82	SP	202	PEB	C1D-CHC-C4C	-3.04	108.77	113.26
82	N9	201	PEB	CMB-C2B-C1B	3.04	129.75	125.06
96	E6	101	HEM	CMD-C2D-C1D	3.04	129.67	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
96	V6	201	HEM	CHB-C1B-NB	3.04	128.13	124.37
82	Y1	202	PEB	CHB-C4B-C3B	-3.04	118.28	125.32
82	MI	401	PEB	CHC-C1D-ND	-3.04	109.87	113.72
87	C6	520	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
87	3N	313	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
92	bL	611	LMG	O8-C28-C29	3.04	121.46	111.91
85	B2	839	BCR	C38-C26-C27	3.04	119.46	113.62
82	H9	202	PEB	OD-C4D-ND	-3.04	121.42	125.93
82	z8	201	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
82	iK	203	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
82	MP	203	PEB	CHA-C1B-NB	-3.04	118.57	124.93
82	TD	203	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	NP	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
84	DO	1001	CYC	C1A-C2A-C3A	-3.04	103.42	106.78
84	D4	1001	CYC	C1A-C2A-C3A	-3.04	103.42	106.78
82	AQ	301	PEB	CAC-C2C-C1C	3.04	130.61	125.76
82	L4	1002	PEB	C3C-C4C-NC	3.04	111.07	108.33
82	QA	201	PEB	OD-C4D-C3D	-3.04	122.57	129.46
82	QA	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
82	VM	202	PEB	OD-C4D-ND	-3.04	121.42	125.93
82	g1	202	PEB	OD-C4D-ND	-3.04	121.42	125.93
82	DQ	203	PEB	C3D-C4D-ND	3.04	113.23	107.26
82	PP	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	dB	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	MA	202	PEB	CHC-C4C-NC	3.04	125.27	121.15
82	aE	202	PEB	C1C-CHB-C4B	-3.04	121.46	128.28
82	XF	203	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	LI	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	V7	203	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	cG	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	T7	203	PEB	CAB-C3B-C2B	3.04	133.54	127.88
82	TI	202	PEB	CHC-C1D-ND	-3.04	109.88	113.72
82	AJ	301	PEB	OD-C4D-ND	-3.04	121.42	125.93
83	AG	302	PUB	OD-C4D-ND	-3.04	121.42	125.93
82	IB	203	PEB	CMB-C2B-C1B	3.04	129.75	125.06
82	KD	201	PEB	CMB-C2B-C1B	3.04	129.75	125.06
82	C9	201	PEB	CMB-C2B-C1B	3.04	129.75	125.06
82	L9	202	PEB	C2A-C1A-NA	3.04	110.89	108.27
82	S4	201	PEB	CHA-C4A-NA	3.04	128.82	125.20
82	RA	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
82	SB	201	PEB	C3B-C4B-NB	3.04	114.47	110.05
82	ZG	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EP	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	N5	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
87	42	604	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
87	B2	804	CLA	CMB-C2B-C3B	3.04	133.95	126.59
85	LN	201	BCR	C34-C9-C10	-3.04	118.66	122.92
82	Z9	303	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
84	KO	1001	CYC	C1A-C2A-C3A	-3.04	103.42	106.78
82	dB	201	PEB	CMB-C2B-C1B	3.04	129.75	125.06
82	BA	202	PEB	C1D-CHC-C4C	-3.04	108.77	113.26
83	AJ	303	PUB	CHA-C4A-NA	-3.04	109.88	113.72
82	XB	201	PEB	CHA-C1B-NB	-3.04	118.57	124.93
82	r8	201	PEB	CHA-C1B-NB	-3.04	118.57	124.93
82	kF	201	PEB	CHB-C1C-C2C	-3.04	120.29	127.15
82	IQ	202	PEB	CHC-C4C-NC	3.04	125.26	121.15
82	VH	201	PEB	CAB-CBB-CGB	-3.04	107.06	113.60
82	BQ	203	PEB	C2A-C1A-NA	3.04	110.89	108.27
82	LI	201	PEB	C2C-C1C-NC	3.04	111.67	107.57
82	O7	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
83	ND	201	PUB	OD-C4D-ND	-3.04	121.43	125.93
83	AM	304	PUB	OD-C4D-ND	-3.04	121.43	125.93
82	Q4	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
84	D1	1001	CYC	C1B-CHB-C4A	-3.04	120.65	128.08
82	OE	202	PEB	CHC-C4C-NC	3.04	125.26	121.15
82	WA	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
82	TK	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
82	ZM	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
82	bG	201	PEB	C1D-CHC-C4C	-3.04	108.77	113.26
82	XQ	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	Y1	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	OF	203	PEB	CHC-C1D-ND	-3.04	109.88	113.72
82	GP	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
87	A2	852	CLA	C1D-ND-C4D	3.04	108.49	106.33
82	VK	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	hF	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	Q4	201	PEB	CHC-C4C-NC	3.04	125.26	121.15
82	CA	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
82	RA	202	PEB	CHA-C4A-NA	3.04	128.82	125.20
82	g4	201	PEB	C3B-C4B-NB	3.04	114.47	110.05
83	M5	302	PUB	C2C-C1C-NC	3.04	114.47	110.05
85	BL	617	BCR	C33-C5-C6	-3.04	121.12	124.53
96	FL	102	HEM	CBD-CAD-C3D	-3.04	104.19	112.63
82	QP	202	PEB	CMB-C2B-C1B	3.04	129.74	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LP	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
82	h4	202	PEB	CHC-C4C-NC	3.04	125.26	121.15
82	KD	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	WA	201	PEB	OD-C4D-C3D	-3.04	122.58	129.46
82	R7	201	PEB	CMA-C2A-C1A	-3.04	105.85	112.40
87	CL	505	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
82	DI	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
82	cB	403	PEB	C2A-C1A-NA	3.04	110.89	108.27
84	HH	1001	CYC	CHA-C4D-C3D	-3.04	120.30	127.15
84	FO	1001	CYC	C4D-C3D-C2D	-3.04	104.03	107.62
82	xK	303	PEB	OD-C4D-C3D	-3.04	122.58	129.46
82	Q4	202	PEB	CHC-C1D-ND	-3.04	109.88	113.72
82	pC	201	PEB	CMB-C2B-C1B	3.04	129.74	125.06
82	LD	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	OH	201	PEB	CHB-C1C-C2C	-3.04	120.30	127.15
82	IA	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	VB	202	PEB	OA-C1A-C2A	-3.04	123.76	126.17
82	Q7	202	PEB	OA-C1A-C2A	-3.04	123.76	126.17
87	AN	810	CLA	CHB-C4A-NA	3.04	128.71	124.51
82	KB	302	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	1C	203	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	dQ	401	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	VD	201	PEB	CHB-C1C-C2C	-3.04	120.30	127.15
82	d4	201	PEB	CHB-C1C-C2C	-3.04	120.30	127.15
82	AD	303	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	RQ	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	iM	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
82	LJ	201	PEB	C3B-C4B-NB	3.04	114.47	110.05
83	AH	303	PUB	OA-C1A-NA	-3.04	121.43	125.93
82	SA	201	PEB	CBB-CAB-C3B	-3.04	104.19	112.63
87	BL	603	CLA	CMB-C2B-C1B	-3.04	120.75	125.37
82	D5	202	PEB	OA-C1A-C2A	-3.04	123.76	126.17
87	AN	809	CLA	CHB-C4A-NA	3.04	128.71	124.51
82	DA	203	PEB	CMB-C2B-C1B	3.04	129.74	125.06
82	XM	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
82	dO	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
82	l4	201	PEB	C1C-CHB-C4B	3.04	135.09	128.28
82	J5	203	PEB	C2A-C1A-NA	3.04	110.89	108.27
82	eH	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
82	ED	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
82	lM	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
83	M5	302	PUB	CHB-C1C-NC	3.04	130.90	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	a6	603	DGD	C1E-O6E-C5E	3.04	119.65	113.69
82	iF	201	PEB	C1C-CHB-C4B	3.04	135.09	128.28
82	jJ	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
82	aK	202	PEB	C3B-C4B-NB	3.04	114.46	110.05
84	L4	1001	CYC	OB-C4B-C3B	-3.03	124.75	128.04
82	l4	201	PEB	C2B-C1B-NB	3.03	117.01	110.53
82	GB	202	PEB	C4B-C3B-C2B	-3.03	103.42	106.78
82	D7	202	PEB	C4B-C3B-C2B	-3.03	103.42	106.78
82	KB	303	PEB	CHC-C1D-ND	-3.03	109.89	113.72
87	a6	609	CLA	C1-C2-C3	-3.03	121.84	126.75
84	BG	1002	CYC	CAB-C3B-C4B	3.03	126.17	121.38
96	FL	102	HEM	CHB-C1B-NB	3.03	128.12	124.37
82	HH	1002	PEB	CMB-C2B-C1B	3.03	129.74	125.06
82	GM	203	PEB	CMB-C2B-C1B	3.03	129.74	125.06
82	fG	201	PEB	CAB-CBB-CGB	-3.03	107.07	113.60
82	fG	201	PEB	C3B-C4B-NB	3.03	114.46	110.05
82	T4	203	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	KB	301	PEB	OD-C4D-C3D	-3.03	122.58	129.46
82	JD	202	PEB	OD-C4D-C3D	-3.03	122.58	129.46
82	V5	202	PEB	C1B-C2B-C3B	-3.03	103.02	106.51
82	MK	203	PEB	C1C-CHB-C4B	3.03	135.09	128.28
82	LB	201	PEB	CHB-C4B-C3B	-3.03	118.30	125.32
82	JD	203	PEB	CAC-C2C-C1C	3.03	130.59	125.76
84	BE	1001	CYC	CAD-C3D-C4D	3.03	130.59	125.76
94	a6	601	PL9	C30-C29-C28	-3.03	115.89	123.68
82	A4	304	PEB	CMB-C2B-C1B	3.03	129.74	125.06
82	dE	204	PEB	OD-C4D-C3D	-3.03	122.59	129.46
82	TO	201	PEB	CHC-C1D-ND	-3.03	109.89	113.72
82	XJ	201	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	RO	203	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	s8	201	PEB	CHB-C4B-C3B	-3.03	118.30	125.32
82	18	203	PEB	C2A-C1A-NA	3.03	110.89	108.27
82	CF	201	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	H1	1002	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	e1	202	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
87	C6	517	CLA	C3B-C4B-NB	-3.03	107.70	110.52
82	mK	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
82	TA	203	PEB	CAB-C3B-C2B	3.03	133.53	127.88
82	NI	201	PEB	CHC-C1D-ND	-3.03	109.89	113.72
82	mM	202	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	QE	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	GI	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jH	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
87	BL	620	CLA	C2D-C1D-ND	-3.03	107.87	110.10
82	U9	203	PEB	CMB-C2B-C1B	3.03	129.73	125.06
92	ML	101	LMG	O1-C7-C8	-3.03	103.58	110.90
82	lK	202	PEB	CHC-C4C-NC	3.03	125.25	121.15
82	VQ	201	PEB	CHB-C1C-C2C	-3.03	120.31	127.15
82	IF	203	PEB	C2A-C1A-NA	3.03	110.89	108.27
82	1C	203	PEB	C2A-C1A-NA	3.03	110.89	108.27
83	A4	303	PUB	OD-C4D-ND	-3.03	121.44	125.93
82	Q5	203	PEB	CHC-C1D-ND	-3.03	109.89	113.72
87	B2	832	CLA	CHB-C4A-NA	3.03	128.71	124.51
82	S7	201	PEB	CMA-C2A-C1A	-3.03	105.87	112.40
87	82	308	CLA	CMC-C2C-C3C	3.03	134.35	126.12
87	AL	403	CLA	CMB-C2B-C3B	3.03	133.93	126.59
82	BQ	203	PEB	CAC-C2C-C1C	3.03	130.59	125.76
82	KF	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	UK	201	PEB	CHB-C4B-NB	3.03	130.89	124.58
82	Y7	304	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
87	H6	102	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
84	DH	1003	CYC	CHA-C4D-C3D	-3.03	120.31	127.15
82	JK	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
82	GP	201	PEB	CMB-C2B-C1B	3.03	129.73	125.06
82	WF	201	PEB	CMA-C2A-C1A	-3.03	105.87	112.40
82	Q5	202	PEB	CHA-C4A-NA	-3.03	121.60	125.20
82	YJ	203	PEB	OD-C4D-C3D	-3.03	122.59	129.46
82	ND	203	PEB	C2A-C1A-NA	3.03	110.89	108.27
82	XB	201	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	JD	201	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
87	52	611	CLA	C2A-C1A-CHA	3.03	129.16	123.86
82	TK	202	PEB	CAB-C3B-C4B	3.03	130.37	125.01
82	JF	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
82	HK	201	PEB	CHA-C1B-C2B	3.03	132.69	124.90
82	I5	202	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
85	IN	101	BCR	C38-C26-C27	3.03	119.44	113.62
95	C6	503	DGD	C2G-O2G-C1B	-3.03	110.33	117.79
82	NJ	201	PEB	CAB-C3B-C4B	3.03	130.37	125.01
82	R4	203	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	cE	201	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	aJ	203	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	AD	303	PEB	CHC-C4C-NC	3.03	125.25	121.15
82	YE	201	PEB	CHC-C4C-NC	3.03	125.25	121.15
82	tC	201	PEB	CHC-C4C-NC	3.03	125.25	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EF	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
87	DL	406	CLA	CHB-C4A-NA	3.03	128.70	124.51
87	B2	831	CLA	CHB-C4A-NA	3.03	128.70	124.51
82	WE	202	PEB	CMB-C2B-C1B	3.03	129.73	125.06
82	H1	1002	PEB	CMB-C2B-C1B	3.03	129.73	125.06
82	c4	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
82	GP	201	PEB	OD-C4D-C3D	-3.03	122.59	129.46
82	U4	202	PEB	C3B-C4B-NB	3.03	114.46	110.05
82	GQ	202	PEB	OD-C4D-ND	-3.03	121.44	125.93
87	C6	516	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
87	AN	852	CLA	CHB-C4A-NA	3.03	128.70	124.51
92	aL	611	LMG	C1-O6-C5	3.03	119.63	113.69
82	U4	201	PEB	C2B-C1B-NB	3.03	117.00	110.53
82	xF	302	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	bP	502	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	cO	201	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	PH	202	PEB	CAC-C2C-C1C	3.03	130.59	125.76
82	GQ	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
87	B2	815	CLA	O1D-CGD-CBD	3.03	130.68	124.48
87	A2	834	CLA	CHB-C4A-NA	3.03	128.70	124.51
82	jM	202	PEB	CHA-C1B-NB	-3.03	118.60	124.93
87	cL	512	CLA	CMC-C2C-C1C	-3.03	120.43	125.04
82	iK	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	UM	203	PEB	C3C-C4C-NC	3.03	111.06	108.33
82	RJ	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	S5	203	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	pK	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
87	72	606	CLA	C2A-C1A-CHA	3.03	129.15	123.86
82	a4	202	PEB	CAB-C3B-C4B	3.03	130.37	125.01
82	NA	203	PEB	C4C-C3C-C2C	-3.03	104.70	107.50
83	xK	306	PUB	CHB-C4B-NB	-3.03	118.38	125.32
82	sK	202	PEB	C1C-CHB-C4B	3.03	135.07	128.28
82	nF	202	PEB	C2A-C1A-NA	3.03	110.88	108.27
82	OQ	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	WM	202	PEB	OD-C4D-ND	-3.03	121.44	125.93
82	N9	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	K5	202	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	R5	202	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	sF	201	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
82	CD	201	PEB	OA-C1A-C2A	-3.03	123.77	126.17
82	SF	203	PEB	CHA-C4A-NA	3.03	128.80	125.20
82	JJ	201	PEB	CHA-C4A-NA	3.03	128.80	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aG	201	PEB	OD-C4D-ND	-3.03	121.45	125.93
82	YI	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	lF	201	PEB	C3B-C4B-NB	3.03	114.45	110.05
87	BN	821	CLA	C3B-C4B-NB	-3.03	107.71	110.52
82	CI	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	WQ	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
87	M2	101	CLA	CHB-C4A-NA	3.03	128.70	124.51
87	cL	509	CLA	CHB-C4A-NA	3.03	128.70	124.51
82	k1	201	PEB	OD-C4D-ND	-3.03	121.45	125.93
82	CA	201	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	G9	201	PEB	CMB-C2B-C1B	3.03	129.72	125.06
87	AN	811	CLA	C2A-C1A-CHA	3.03	129.15	123.86
82	cB	401	PEB	CHC-C4C-NC	3.03	125.24	121.15
82	YJ	202	PEB	CMA-C2A-C1A	-3.03	105.88	112.40
82	WH	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
82	NG	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
82	dO	201	PEB	CHB-C1C-C2C	-3.03	120.32	127.15
85	KN	101	BCR	C15-C14-C13	3.03	131.63	127.31
82	FA	201	PEB	OD-C4D-ND	-3.03	121.45	125.93
82	U9	204	PEB	OD-C4D-ND	-3.03	121.45	125.93
82	HD	201	PEB	C3B-C4B-NB	3.03	114.45	110.05
82	XM	202	PEB	CHB-C4B-NB	-3.03	118.28	124.58
82	pC	202	PEB	CMB-C2B-C1B	3.03	129.72	125.06
85	B2	802	BCR	C21-C20-C19	3.03	132.66	123.22
82	B7	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
82	uC	203	PEB	C2A-C1A-NA	3.03	110.88	108.27
82	uF	203	PEB	C2A-C1A-NA	3.03	110.88	108.27
82	CI	201	PEB	CHC-C1D-ND	-3.03	109.90	113.72
87	32	313	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
82	eE	202	PEB	OD-C4D-ND	-3.02	121.45	125.93
82	BD	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	KI	201	PEB	CMB-C2B-C1B	3.02	129.72	125.06
87	CL	509	CLA	C3B-C4B-NB	-3.02	107.71	110.52
82	T5	202	PEB	C1B-C2B-C3B	-3.02	103.03	106.51
82	jH	202	PEB	C1B-C2B-C3B	-3.02	103.03	106.51
82	aM	204	PEB	CHA-C1B-NB	-3.02	118.61	124.93
82	YG	201	PEB	CHC-C4C-NC	3.02	125.24	121.15
82	PJ	202	PEB	CHC-C4C-NC	3.02	125.24	121.15
87	A2	817	CLA	CHB-C4A-NA	3.02	128.69	124.51
87	2N	302	CLA	CHB-C4A-NA	3.02	128.69	124.51
82	jE	202	PEB	CHA-C1B-NB	-3.02	118.61	124.93
87	5N	611	CLA	C2A-C1A-CHA	3.02	129.15	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	c1	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
82	dH	203	PEB	C3B-C4B-NB	3.02	114.45	110.05
96	VL	201	HEM	C4B-C3B-C2B	-3.02	104.71	107.11
82	OK	203	PEB	C1D-CHC-C4C	-3.02	108.80	113.26
85	I2	101	BCR	C38-C26-C27	3.02	119.42	113.62
82	Q9	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
87	32	312	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
84	GO	1001	CYC	CHB-C4A-NA	-3.02	118.61	124.93
82	OJ	201	PEB	OA-C1A-C2A	-3.02	123.77	126.17
82	sK	203	PEB	CHB-C4B-NB	-3.02	118.28	124.58
82	m1	202	PEB	OD-C4D-ND	-3.02	121.45	125.93
82	P7	203	PEB	C3B-C4B-NB	3.02	114.45	110.05
82	jE	202	PEB	C3B-C4B-NB	3.02	114.45	110.05
82	Y1	201	PEB	C1D-CHC-C4C	3.02	117.71	113.26
82	DG	1002	PEB	C2A-C1A-NA	3.02	110.88	108.27
82	j1	203	PEB	C2A-C1A-NA	3.02	110.88	108.27
82	WF	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	YH	201	PEB	CAB-CBB-CGB	-3.02	107.10	113.60
82	AO	304	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	BP	201	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	L4	1002	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	KD	201	PEB	OD-C4D-ND	-3.02	121.45	125.93
82	vK	201	PEB	OD-C4D-ND	-3.02	121.45	125.93
82	tF	202	PEB	CHC-C4C-NC	3.02	125.24	121.15
82	aG	201	PEB	CHC-C4C-NC	3.02	125.24	121.15
82	lE	201	PEB	CHA-C1B-NB	-3.02	118.61	124.93
82	HB	203	PEB	CHC-C1D-ND	-3.02	109.90	113.72
87	A2	832	CLA	O2D-CGD-CBD	3.02	116.64	111.27
82	JD	203	PEB	OD-C4D-C3D	-3.02	122.61	129.46
82	tF	202	PEB	OD-C4D-C3D	-3.02	122.61	129.46
94	AL	413	PL9	C53-C6-C1	3.02	121.17	114.99
82	BQ	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	uC	203	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
92	J6	102	LMG	O8-C28-O10	-3.02	115.97	123.59
82	QP	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	lK	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	PG	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
87	7N	606	CLA	C2A-C1A-CHA	3.02	129.14	123.86
82	kK	201	PEB	CHB-C1C-C2C	-3.02	120.33	127.15
82	UQ	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
85	BN	803	BCR	C21-C20-C19	3.02	132.65	123.22
85	CL	516	BCR	C28-C27-C26	-3.02	108.68	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	817	CLA	CHB-C4A-NA	3.02	128.69	124.51
87	AN	836	CLA	CHB-C4A-NA	3.02	128.69	124.51
82	WH	203	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
82	QA	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	WK	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	T1	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	OK	201	PEB	C1C-CHB-C4B	3.02	135.06	128.28
82	QJ	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	TJ	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
82	cB	402	PEB	CHA-C1B-NB	-3.02	118.61	124.93
82	XK	203	PEB	CAB-C3B-C4B	3.02	130.35	125.01
85	AN	848	BCR	C23-C24-C25	3.02	135.69	127.20
92	a6	614	LMG	C8-O7-C10	-3.02	110.35	117.79
85	A2	845	BCR	C20-C21-C22	-3.02	123.00	127.31
82	XQ	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	W7	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	CK	201	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
82	MQ	202	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
87	AN	832	CLA	O2D-CGD-CBD	3.02	116.64	111.27
82	j1	202	PEB	CHA-C4A-NA	-3.02	121.61	125.20
82	gF	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	dM	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	UI	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	V1	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
95	C6	504	DGD	O1G-C1A-O1A	-3.02	115.97	123.59
82	lH	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
84	H4	1001	CYC	C2D-C1D-ND	3.02	111.64	107.40
82	tK	202	PEB	CHC-C4C-NC	3.02	125.24	121.15
82	eM	202	PEB	OA-C1A-C2A	-3.02	123.77	126.17
82	FJ	201	PEB	OD-C4D-C3D	-3.02	122.62	129.46
82	jH	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
82	YP	503	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	cG	201	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	FO	1002	PEB	CMD-C2D-C3D	3.02	134.32	130.06
82	WE	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	IJ	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
87	BL	603	CLA	CMD-C2D-C1D	-3.02	119.39	124.71
83	xK	301	PUB	CAC-CBC-CGC	-3.02	107.11	113.60
82	ZB	201	PEB	CHC-C4C-NC	3.02	125.23	121.15
82	g4	203	PEB	CBB-CAB-C3B	3.02	121.02	112.63
87	A2	819	CLA	CHB-C1B-NB	3.02	127.45	124.26
82	xF	304	PEB	CHA-C1B-NB	-3.02	118.62	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	M7	201	PEB	CMB-C2B-C1B	3.02	129.71	125.06
82	AM	302	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	HK	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	GJ	202	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
82	XD	201	PEB	CHA-C1B-NB	-3.02	118.62	124.93
82	fK	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	FA	202	PEB	OD-C4D-C3D	-3.02	122.62	129.46
82	HJ	202	PEB	CAA-C3A-C2A	-3.02	106.72	114.26
84	EE	1001	CYC	C1B-NB-C4B	-3.02	106.83	110.67
82	EI	201	PEB	CHC-C1D-ND	-3.02	109.91	113.72
82	GI	202	PEB	CHC-C1D-ND	-3.02	109.91	113.72
82	KI	202	PEB	CHC-C1D-ND	-3.02	109.91	113.72
82	PI	201	PEB	CHC-C1D-ND	-3.02	109.91	113.72
85	H6	101	BCR	C38-C26-C25	-3.02	121.14	124.53
82	HD	201	PEB	OD-C4D-C3D	-3.02	122.62	129.46
82	TF	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	OP	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	bP	502	PEB	C3B-C4B-NB	3.02	114.44	110.05
87	AN	852	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
82	FD	203	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
82	dB	202	PEB	OD-C4D-C3D	-3.02	122.62	129.46
82	fJ	202	PEB	C4C-C3C-C2C	-3.02	104.72	107.50
87	AN	833	CLA	C3B-C4B-NB	-3.02	107.72	110.52
82	EM	203	PEB	C3C-C4C-NC	3.02	111.05	108.33
87	R2	201	CLA	CHB-C4A-NA	3.02	128.68	124.51
82	KB	304	PEB	CMB-C2B-C1B	3.02	129.71	125.06
82	VG	202	PEB	CHB-C1C-NC	-3.02	118.41	125.32
82	DF	201	PEB	CHC-C4C-NC	3.02	125.23	121.15
85	B2	841	BCR	C34-C9-C10	-3.02	118.70	122.92
92	m6	101	LMG	O8-C28-C29	3.02	121.38	111.91
82	TO	203	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	YO	203	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	D5	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
82	cE	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	rC	201	PEB	CMC-C3C-C4C	-3.02	123.86	127.06
82	O4	202	PEB	C1D-CHC-C4C	3.02	117.70	113.26
82	WF	201	PEB	CHC-C1D-ND	-3.02	109.91	113.72
82	iK	201	PEB	C1C-CHB-C4B	3.02	135.05	128.28
82	rC	201	PEB	CHA-C1B-NB	-3.02	118.62	124.93
82	jG	202	PEB	CHA-C1B-NB	-3.02	118.62	124.93
82	c4	203	PEB	C2A-C1A-NA	3.02	110.87	108.27
82	u8	203	PEB	C2A-C1A-NA	3.02	110.87	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HP	201	PEB	CAC-CBC-CGC	-3.02	107.11	113.60
82	dJ	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
82	kJ	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
84	DG	1001	CYC	C2A-C1A-NA	3.02	114.44	110.05
83	Z5	302	PUB	CHB-C1C-NC	3.02	130.85	124.58
82	KM	202	PEB	OD-C4D-C3D	-3.02	122.63	129.46
82	QB	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	QJ	204	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
82	XP	202	PEB	CAC-CBC-CGC	-3.02	107.11	113.60
82	m1	202	PEB	CHC-C4C-NC	3.02	125.23	121.15
82	18	203	PEB	CHC-C4C-NC	3.02	125.23	121.15
82	sC	201	PEB	CHB-C4B-C3B	-3.02	118.34	125.32
82	WA	201	PEB	CHA-C4A-NA	3.02	128.79	125.20
92	JL	102	LMG	C8-O7-C10	-3.02	110.37	117.79
82	QO	201	PEB	C2B-C1B-NB	3.02	116.97	110.53
82	WJ	203	PEB	CMB-C2B-C1B	3.01	129.71	125.06
87	A2	803	CLA	C3B-C4B-NB	-3.01	107.72	110.52
96	VL	201	HEM	CAA-CBA-CGA	-3.01	107.11	113.60
85	c6	602	BCR	C10-C11-C12	-3.01	113.81	123.22
82	XP	202	PEB	OD-C4D-ND	-3.01	121.46	125.93
82	WF	203	PEB	CHC-C4C-NC	3.01	125.23	121.15
82	zC	201	PEB	C1D-CHC-C4C	-3.01	108.81	113.26
82	tC	201	PEB	CAC-C2C-C1C	3.01	130.56	125.76
87	D6	402	CLA	C1-C2-C3	-3.01	120.83	126.04
87	4N	604	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
82	JP	202	PEB	CHC-C1D-ND	-3.01	109.91	113.72
84	KH	1001	CYC	C1A-C2A-C3A	-3.01	103.45	106.78
82	JQ	203	PEB	CAC-C2C-C1C	3.01	130.56	125.76
82	yC	202	PEB	CMC-C3C-C4C	3.01	130.25	127.06
82	O4	202	PEB	CMB-C2B-C1B	3.01	129.71	125.06
82	p8	201	PEB	CMB-C2B-C1B	3.01	129.71	125.06
82	U1	201	PEB	C2A-C1A-NA	3.01	110.87	108.27
82	L5	203	PEB	CHA-C1B-NB	-3.01	118.63	124.93
82	xK	304	PEB	CHA-C1B-NB	-3.01	118.63	124.93
82	UO	201	PEB	C2B-C1B-NB	3.01	116.96	110.53
82	M7	201	PEB	CAB-C3B-C4B	3.01	130.34	125.01
82	O7	201	PEB	OA-C1A-C2A	-3.01	123.78	126.17
92	B6	618	LMG	C7-O1-C1	-3.01	107.85	113.74
87	AN	823	CLA	CHB-C4A-NA	3.01	128.68	124.51
87	6N	607	CLA	CHB-C4A-NA	3.01	128.68	124.51
82	DE	1002	PEB	CHB-C4B-NB	-3.01	118.31	124.58
84	GO	1001	CYC	C4A-C3A-C2A	-3.01	103.05	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XD	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	YM	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	J9	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	e7	301	PEB	CHC-C1D-ND	-3.01	109.91	113.72
82	WE	201	PEB	CHC-C4C-NC	3.01	125.23	121.15
82	PM	201	PEB	C3B-C4B-NB	3.01	114.43	110.05
82	NE	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
82	eJ	201	PEB	CMB-C2B-C1B	3.01	129.70	125.06
82	EP	203	PEB	C2C-C1C-NC	3.01	111.63	107.57
82	DM	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	MF	203	PEB	C1C-CHB-C4B	3.01	135.04	128.28
82	UJ	203	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
82	YJ	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
82	XQ	203	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
82	aM	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
84	LG	1001	CYC	C4A-C3A-C2A	-3.01	103.05	106.51
82	XD	202	PEB	CHC-C4C-NC	3.01	125.23	121.15
87	5N	607	CLA	CHC-C4B-NB	3.01	127.45	124.26
82	MP	201	PEB	CAA-C3A-C4A	-3.01	104.94	112.67
82	W1	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
82	aM	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
87	72	601	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
82	iJ	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
87	A2	837	CLA	CHB-C4A-NA	3.01	128.68	124.51
82	F9	201	PEB	CHB-C4B-C3B	-3.01	118.35	125.32
82	EQ	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
82	a4	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
82	hK	201	PEB	OA-C1A-NA	3.01	128.59	124.94
82	cO	203	PEB	C2A-C1A-NA	3.01	110.87	108.27
82	W1	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	pK	201	PEB	CHB-C1C-NC	-3.01	118.42	125.32
82	NO	1002	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
82	IJ	202	PEB	CHA-C1B-C2B	3.01	132.64	124.90
82	OB	201	PEB	OD-C4D-C3D	-3.01	122.64	129.46
82	W1	201	PEB	CAC-C2C-C3C	3.01	133.97	127.07
82	y8	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
82	18	203	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
87	AN	808	CLA	CHB-C4A-NA	3.01	128.68	124.51
85	F6	101	BCR	C36-C18-C17	-3.01	118.71	122.92
82	JJ	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
82	iK	202	PEB	CHA-C1B-NB	-3.01	118.64	124.93
82	mM	202	PEB	C1C-CHB-C4B	-3.01	121.53	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lG	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
82	TM	202	PEB	CAB-C3B-C4B	3.01	130.33	125.01
82	U9	201	PEB	CAA-C3A-C2A	-3.01	106.74	114.26
92	m6	103	LMG	O8-C28-C29	3.01	121.35	111.91
82	SP	202	PEB	CHB-C4B-C3B	-3.01	118.36	125.32
82	hF	202	PEB	OA-C1A-C2A	-3.01	123.78	126.17
95	a6	603	DGD	O1G-C1A-C2A	3.01	121.35	111.91
96	vL	201	HEM	C4C-NC-C1C	3.01	108.30	105.35
82	DF	201	PEB	CHA-C1B-NB	-3.01	118.64	124.93
82	F5	202	PEB	CHA-C4A-NA	-3.01	121.63	125.20
85	A2	848	BCR	C23-C24-C25	3.01	135.65	127.20
82	WI	201	PEB	CAA-C3A-C2A	-3.01	106.74	114.26
82	hF	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
82	XB	201	PEB	C3B-C4B-NB	3.01	114.43	110.05
82	OH	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
82	bB	201	PEB	CHA-C1B-NB	-3.01	118.64	124.93
84	DH	1003	CYC	C1D-C2D-C3D	-3.01	103.96	107.79
94	DL	401	PL9	C20-C19-C18	-3.01	115.96	123.68
82	ZF	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
84	CO	1001	CYC	C1A-C2A-C3A	-3.01	103.45	106.78
84	y3	1001	CYC	CHD-C4C-NC	3.01	128.78	125.20
87	BL	621	CLA	CHB-C4A-NA	3.01	128.67	124.51
82	RM	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	eO	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
82	HG	1002	PEB	OD-C4D-C3D	-3.01	122.64	129.46
82	B7	202	PEB	C1D-CHC-C4C	-3.01	108.82	113.26
82	WM	202	PEB	C3B-C4B-NB	3.01	114.42	110.05
85	BN	841	BCR	C34-C9-C10	-3.01	118.71	122.92
82	S7	201	PEB	CBB-CAB-C3B	-3.01	104.27	112.63
87	K6	101	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
87	A2	852	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
82	dF	201	PEB	OA-C1A-NA	3.01	128.58	124.94
82	DP	202	PEB	CHC-C4C-NC	3.01	125.22	121.15
82	P5	202	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
84	FE	1001	CYC	C1B-NB-C4B	-3.01	106.84	110.67
87	BN	816	CLA	O1D-CGD-CBD	3.01	130.64	124.48
82	MJ	202	PEB	CHA-C1B-C2B	3.01	132.63	124.90
82	JI	202	PEB	OA-C1A-C2A	-3.01	123.78	126.17
82	TA	203	PEB	CAC-CBC-CGC	-3.01	107.13	113.60
96	vL	201	HEM	CAA-CBA-CGA	-3.01	107.13	113.60
82	QE	201	PEB	CHA-C1B-NB	-3.01	118.64	124.93
82	DK	201	PEB	CHA-C1B-NB	-3.01	118.64	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OM	203	PEB	C3B-C4B-NB	3.01	114.42	110.05
87	AL	405	CLA	CHB-C4A-NA	3.01	128.67	124.51
87	A2	809	CLA	CHB-C4A-NA	3.01	128.67	124.51
82	JP	201	PEB	CAB-C3B-C4B	3.01	130.33	125.01
82	iJ	202	PEB	CHB-C4B-NB	-3.01	118.32	124.58
82	KK	203	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
82	L7	203	PEB	OD-C4D-ND	-3.01	121.48	125.93
82	mH	202	PEB	OD-C4D-ND	-3.01	121.48	125.93
82	cJ	202	PEB	OD-C4D-ND	-3.01	121.48	125.93
82	DI	202	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
82	FP	202	PEB	OD-C4D-ND	-3.01	121.48	125.93
82	k4	201	PEB	OD-C4D-ND	-3.01	121.48	125.93
85	FN	202	BCR	C24-C23-C22	-3.01	121.69	126.23
82	XJ	202	PEB	CAC-CBC-CGC	-3.01	107.14	113.60
82	iF	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
82	NQ	203	PEB	C2A-C1A-NA	3.01	110.86	108.27
82	gE	202	PEB	CHA-C1B-NB	-3.01	118.65	124.93
82	fJ	202	PEB	C3B-C4B-NB	3.01	114.42	110.05
82	YA	304	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
82	ZE	203	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
82	C5	202	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
82	1C	202	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
87	22	601	CLA	CHB-C4A-NA	3.01	128.67	124.51
87	c6	610	CLA	C3B-C4B-NB	-3.01	107.73	110.52
82	B7	203	PEB	CMB-C2B-C1B	3.01	129.69	125.06
82	T7	202	PEB	C2B-C1B-NB	3.01	116.94	110.53
82	L9	203	PEB	CHA-C1B-NB	-3.01	118.65	124.93
82	cO	201	PEB	CHA-C1B-NB	-3.01	118.65	124.93
82	GF	201	PEB	CAA-C3A-C2A	3.01	121.77	114.26
84	JH	1001	CYC	C4D-CHA-C1A	3.00	135.02	128.28
84	D1	1003	CYC	C1D-C2D-C3D	-3.00	103.96	107.79
82	MK	203	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
82	EP	203	PEB	OD-C4D-C3D	-3.00	122.65	129.46
82	X5	202	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
82	UB	303	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	EJ	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	IJ	203	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	JA	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	GP	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	D7	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
87	b6	614	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
82	iO	201	PEB	C3B-C4B-NB	3.00	114.42	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	S7	202	PEB	CMB-C2B-C1B	3.00	129.69	125.06
82	TQ	203	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
84	C1	1001	CYC	CHA-C4D-C3D	-3.00	120.37	127.15
82	HK	201	PEB	C1C-NC-C4C	-3.00	104.25	109.60
82	iJ	202	PEB	C3B-C4B-NB	3.00	114.42	110.05
84	EO	1001	CYC	C2A-C1A-NA	3.00	114.42	110.05
82	O1	201	PEB	CHB-C1C-C2C	-3.00	120.37	127.15
82	SM	201	PEB	CMB-C2B-C1B	3.00	129.69	125.06
82	YH	202	PEB	CHB-C4B-C3B	-3.00	118.37	125.32
82	YF	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	eB	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	KI	201	PEB	CAC-C2C-C1C	3.00	130.54	125.76
87	B6	606	CLA	C3B-C4B-NB	-3.00	107.73	110.52
82	JH	1002	PEB	CAB-CBB-CGB	-3.00	107.14	113.60
82	FM	202	PEB	CHC-C4C-NC	3.00	125.21	121.15
82	OO	201	PEB	CHC-C4C-NC	3.00	125.21	121.15
82	GF	203	PEB	CBB-CAB-C3B	3.00	120.97	112.63
82	gO	202	PEB	C3B-C4B-NB	3.00	114.42	110.05
82	LI	201	PEB	CMB-C2B-C1B	3.00	129.69	125.06
82	XP	201	PEB	CMB-C2B-C1B	3.00	129.69	125.06
82	UJ	201	PEB	C3C-C4C-NC	3.00	111.04	108.33
85	L2	201	BCR	C34-C9-C10	-3.00	118.72	122.92
82	aM	202	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	VI	201	PEB	CHC-C1D-ND	-3.00	109.93	113.72
82	XI	201	PEB	CHC-C1D-ND	-3.00	109.93	113.72
82	F9	202	PEB	CAB-C3B-C4B	3.00	130.32	125.01
82	CB	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
84	K4	1001	CYC	C1A-C2A-C3A	-3.00	103.46	106.78
84	HE	1001	CYC	C2A-C1A-NA	3.00	114.42	110.05
82	gJ	202	PEB	CHC-C4C-NC	3.00	125.21	121.15
87	A2	817	CLA	C3B-C4B-NB	-3.00	107.73	110.52
82	DB	202	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
82	BA	203	PEB	CMB-C2B-C1B	3.00	129.69	125.06
87	B2	822	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
82	D7	203	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	eM	202	PEB	CHB-C4B-NB	-3.00	118.33	124.58
82	L5	203	PEB	OD-C4D-C3D	-3.00	122.66	129.46
82	iG	201	PEB	OD-C4D-C3D	-3.00	122.66	129.46
82	Q4	201	PEB	C2B-C1B-NB	3.00	116.94	110.53
82	dG	204	PEB	C3B-C4B-NB	3.00	114.42	110.05
82	LQ	203	PEB	CMB-C2B-C1B	3.00	129.69	125.06
82	QJ	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HF	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	DG	1002	PEB	OD-C4D-C3D	-3.00	122.66	129.46
82	dG	203	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
82	gO	203	PEB	CBB-CAB-C3B	3.00	120.97	112.63
87	bL	608	CLA	C3B-C4B-NB	-3.00	107.73	110.52
82	AP	202	PEB	OD-C4D-ND	-3.00	121.48	125.93
82	IJ	201	PEB	C3C-C4C-NC	3.00	111.03	108.33
82	RA	203	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
82	PD	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
82	lG	203	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
96	vL	201	HEM	C4B-C3B-C2B	-3.00	104.73	107.11
84	W3	1001	CYC	CHD-C4C-NC	3.00	128.77	125.20
87	BN	823	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
87	22	604	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
82	H4	1002	PEB	OD-C4D-ND	-3.00	121.49	125.93
82	gE	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
82	JQ	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	eE	201	PEB	OA-C1A-C2A	-3.00	123.79	126.17
82	IA	202	PEB	C3B-C4B-NB	3.00	114.41	110.05
82	dE	204	PEB	C3B-C4B-NB	3.00	114.41	110.05
82	OM	202	PEB	C3C-C4C-NC	3.00	111.03	108.33
87	D6	403	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
85	BN	838	BCR	C1-C6-C5	-3.00	118.39	122.61
85	B2	838	BCR	C1-C6-C5	-3.00	118.39	122.61
82	DA	203	PEB	OD-C4D-ND	-3.00	121.49	125.93
83	AJ	304	PUB	OA-C1A-NA	-3.00	121.49	125.93
82	Y1	201	PEB	CAB-CBB-CGB	-3.00	107.15	113.60
94	AL	413	PL9	C35-C34-C36	3.00	120.32	115.27
82	jO	201	PEB	CHB-C1C-C2C	-3.00	120.38	127.15
82	WG	202	PEB	CMB-C2B-C1B	3.00	129.68	125.06
82	uC	201	PEB	C1C-CHB-C4B	3.00	135.01	128.28
82	KM	202	PEB	C3B-C4B-NB	3.00	114.41	110.05
82	pF	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	Q7	202	PEB	CHB-C1C-C2C	-3.00	120.39	127.15
82	EA	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
82	P5	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
95	BL	613	DGD	O1G-C1A-C2A	3.00	121.31	111.91
82	BI	201	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
82	DK	203	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
82	QG	203	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
82	fJ	203	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
82	Y5	201	PEB	CHB-C4B-C3B	-3.00	118.38	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jH	202	PEB	CHA-C4A-NA	-3.00	121.64	125.20
84	G4	1001	CYC	CMA-C3A-C4A	3.00	129.68	125.06
82	u8	201	PEB	C1C-CHB-C4B	3.00	135.00	128.28
82	SA	201	PEB	CMA-C2A-C1A	-3.00	105.94	112.40
82	NO	1002	PEB	C3B-C4B-NB	3.00	114.41	110.05
84	BE	1001	CYC	C2A-C1A-NA	3.00	114.41	110.05
82	H7	203	PEB	CAB-C3B-C2B	-3.00	122.30	127.88
84	BE	1002	CYC	CAB-C3B-C4B	3.00	126.11	121.38
84	M1	201	CYC	CMB-C2B-C1B	3.00	127.91	124.17
82	LK	201	PEB	CAB-C3B-C4B	3.00	130.31	125.01
82	D7	203	PEB	CMB-C2B-C1B	3.00	129.68	125.06
82	aJ	203	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
82	bK	201	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
82	W7	201	PEB	CHA-C4A-NA	3.00	128.77	125.20
82	kK	203	PEB	CHA-C4A-NA	-3.00	121.64	125.20
82	TD	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
82	p8	201	PEB	C3B-C4B-NB	3.00	114.41	110.05
82	jJ	203	PEB	CHA-C1B-NB	-3.00	118.67	124.93
82	YD	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	UH	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	e1	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	t8	201	PEB	CAC-C2C-C1C	3.00	130.53	125.76
87	K2	101	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
82	PA	202	PEB	C1C-NC-C4C	-3.00	104.27	109.60
84	n3	1001	CYC	C1B-CHB-C4A	3.00	135.40	128.08
96	VL	201	HEM	C4C-NC-C1C	3.00	108.28	105.35
82	O5	202	PEB	C1C-CHB-C4B	3.00	135.00	128.28
82	OD	201	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
82	yC	202	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
84	CG	1001	CYC	C2A-C1A-NA	3.00	114.41	110.05
82	EB	501	PEB	OD-C4D-C3D	-3.00	122.67	129.46
82	YJ	202	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
82	J7	203	PEB	CHB-C4B-NB	-3.00	118.34	124.58
87	A2	811	CLA	C2A-C1A-CHA	3.00	129.10	123.86
82	GB	201	PEB	CMA-C2A-C1A	-3.00	105.95	112.40
84	H1	1001	CYC	CMC-C2C-C1C	-3.00	105.95	112.40
82	L5	201	PEB	OD-C4D-C3D	-3.00	122.67	129.46
82	KP	201	PEB	CAC-CBC-CGC	-3.00	107.16	113.60
87	AN	809	CLA	CHB-C1B-NB	3.00	127.43	124.26
82	IJ	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
82	FQ	203	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
82	ZK	201	PEB	CAB-CBB-CGB	-2.99	107.16	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hO	202	PEB	CHC-C4C-NC	2.99	125.20	121.15
82	DG	1002	PEB	CHB-C4B-NB	-2.99	118.34	124.58
87	A2	810	CLA	CHB-C4A-NA	2.99	128.65	124.51
82	XQ	201	PEB	CHA-C1B-NB	-2.99	118.67	124.93
82	S9	203	PEB	C3B-C4B-NB	2.99	114.41	110.05
82	BQ	203	PEB	C1C-NC-C4C	-2.99	104.27	109.60
82	P7	202	PEB	C1C-NC-C4C	-2.99	104.27	109.60
82	XK	202	PEB	OD-C4D-C3D	-2.99	122.68	129.46
87	AN	850	CLA	CMB-C2B-C3B	2.99	133.84	126.59
82	PE	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	wK	303	PEB	CAB-C3B-C2B	2.99	133.45	127.88
92	m6	101	LMG	C8-O7-C10	-2.99	110.42	117.79
82	HP	201	PEB	C2A-C1A-NA	2.99	110.85	108.27
87	BN	832	CLA	CHB-C4A-NA	2.99	128.65	124.51
87	MN	101	CLA	CHB-C4A-NA	2.99	128.65	124.51
84	73	1002	CYC	C1B-NB-C4B	-2.99	106.86	110.67
82	fM	201	PEB	C3B-C4B-NB	2.99	114.40	110.05
82	VF	201	PEB	C1C-CHB-C4B	2.99	135.00	128.28
84	NO	1001	CYC	CHB-C1B-NB	-2.99	119.63	126.06
82	RH	201	PEB	CMB-C2B-C1B	2.99	129.67	125.06
82	O5	202	PEB	CBA-CAA-C3A	-2.99	106.80	113.47
82	RD	202	PEB	CHC-C1D-ND	-2.99	109.94	113.72
82	AG	301	PEB	C3B-C4B-NB	2.99	114.40	110.05
87	BL	606	CLA	CHB-C4A-NA	2.99	128.65	124.51
82	Q9	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	CP	201	PEB	C2A-C1A-NA	2.99	110.85	108.27
82	yC	203	PEB	OD-C4D-C3D	-2.99	122.68	129.46
82	J5	202	PEB	CHC-C1D-ND	-2.99	109.94	113.72
82	XQ	201	PEB	C3C-C4C-NC	2.99	111.03	108.33
82	fM	203	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	P1	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	a1	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	DP	201	PEB	CHA-C1B-NB	-2.99	118.67	124.93
87	C6	509	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
82	NK	202	PEB	OA-C1A-C2A	-2.99	123.79	126.17
85	c6	602	BCR	C15-C16-C17	-2.99	117.34	123.47
82	RI	201	PEB	CHC-C1D-ND	-2.99	109.94	113.72
82	D7	202	PEB	CHA-C4A-NA	2.99	128.76	125.20
82	QP	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
82	VK	201	PEB	C1C-CHB-C4B	2.99	134.99	128.28
82	MD	202	PEB	C1B-C2B-C3B	-2.99	103.07	106.51
82	ZE	201	PEB	C1B-C2B-C3B	-2.99	103.07	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	v8	202	PEB	C1B-C2B-C3B	-2.99	103.07	106.51
82	cO	202	PEB	C1B-C2B-C3B	-2.99	103.07	106.51
87	A2	809	CLA	CHB-C1B-NB	2.99	127.42	124.26
82	GQ	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	NQ	204	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
85	CL	501	BCR	C11-C10-C9	-2.99	123.04	127.31
88	i6	101	LHG	O7-C7-C8	2.99	117.95	111.50
82	R5	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	wK	301	PEB	CHC-C4C-NC	2.99	125.20	121.15
87	BN	831	CLA	CHB-C4A-NA	2.99	128.65	124.51
82	kE	202	PEB	CAC-CBC-CGC	-2.99	107.17	113.60
84	BG	1001	CYC	C4A-C3A-C2A	-2.99	103.07	106.51
82	TF	201	PEB	CHB-C1C-C2C	-2.99	120.40	127.15
82	F7	202	PEB	OD-C4D-C3D	-2.99	122.68	129.46
87	AL	403	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
87	3N	312	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
82	RE	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	VG	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	TP	201	PEB	C3B-C4B-NB	2.99	114.40	110.05
82	E7	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
82	sF	203	PEB	CHB-C4B-NB	-2.99	118.35	124.58
87	DL	403	CLA	CHB-C4A-NA	2.99	128.65	124.51
87	A2	823	CLA	CHB-C4A-NA	2.99	128.65	124.51
82	YK	201	PEB	C4C-C3C-C2C	-2.99	104.74	107.50
82	A5	202	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
82	yK	301	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
85	B6	601	BCR	C8-C7-C6	-2.99	118.81	127.20
91	d6	404	PHO	CGD-CBD-CAD	-2.99	101.05	110.73
82	m4	203	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	kH	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	SE	201	PEB	CMB-C2B-C1B	2.99	129.67	125.06
87	A2	836	CLA	CHB-C4A-NA	2.99	128.65	124.51
82	i4	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
82	BD	203	PEB	C1C-NC-C4C	-2.99	104.28	109.60
82	EQ	201	PEB	CHA-C1B-NB	-2.99	118.68	124.93
82	T1	202	PEB	OD-C4D-C3D	-2.99	122.69	129.46
82	y8	203	PEB	CHA-C4A-NA	-2.99	121.65	125.20
82	zK	501	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	WA	202	PEB	CMB-C2B-C1B	2.99	129.67	125.06
82	HQ	201	PEB	C3B-C4B-NB	2.99	114.40	110.05
82	O7	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
82	cJ	202	PEB	C3B-C4B-NB	2.99	114.40	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RI	203	PEB	C1C-NC-C4C	-2.99	104.28	109.60
82	QP	203	PEB	CHA-C1B-NB	-2.99	118.68	124.93
87	AN	822	CLA	CHB-C4A-NA	2.99	128.65	124.51
87	bL	608	CLA	CHB-C4A-NA	2.99	128.65	124.51
82	II	201	PEB	CHC-C1D-ND	-2.99	109.94	113.72
82	QQ	202	PEB	CHC-C1D-ND	-2.99	109.94	113.72
94	AL	413	PL9	C8-C7-C3	2.99	120.43	111.98
82	HJ	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	P1	202	PEB	OD-C4D-ND	-2.99	121.50	125.93
84	BG	1001	CYC	C2A-C1A-NA	2.99	114.40	110.05
82	AI	203	PEB	C1C-NC-C4C	-2.99	104.28	109.60
82	C7	201	PEB	CHA-C4A-NA	2.99	128.76	125.20
82	aB	202	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
82	XQ	202	PEB	CHC-C4C-NC	2.99	125.19	121.15
82	P1	202	PEB	CHC-C4C-NC	2.99	125.19	121.15
87	FN	203	CLA	C3B-C4B-NB	-2.99	107.74	110.52
87	A2	833	CLA	C3B-C4B-NB	-2.99	107.74	110.52
87	6N	608	CLA	CGD-CBD-CAD	-2.99	101.06	110.73
87	4N	605	CLA	O2A-CGA-O1A	-2.99	115.85	123.30
82	18	203	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
82	zC	202	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	YA	304	PEB	C3B-C4B-NB	2.99	114.39	110.05
82	SM	202	PEB	OD-C4D-C3D	-2.99	122.69	129.46
82	fM	202	PEB	OD-C4D-C3D	-2.99	122.69	129.46
84	EE	1001	CYC	CHA-C4D-C3D	-2.99	120.41	127.15
87	BN	836	CLA	C4D-C3D-CAD	-2.99	104.58	108.10
82	R1	202	PEB	CMC-C3C-C4C	2.99	130.23	127.06
82	pK	202	PEB	CMC-C3C-C4C	2.99	130.23	127.06
82	MB	202	PEB	CBA-CAA-C3A	-2.99	106.82	113.47
82	H4	1002	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
82	A1	302	PEB	OD-C4D-ND	-2.99	121.50	125.93
82	WH	203	PEB	OA-C1A-C2A	-2.99	123.80	126.17
82	JK	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
82	UQ	202	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
82	r8	201	PEB	CMC-C3C-C4C	-2.99	123.90	127.06
82	RQ	202	PEB	CHC-C1D-ND	-2.99	109.95	113.72
85	hL	102	BCR	C20-C21-C22	-2.99	123.05	127.31
82	DI	202	PEB	C3B-C4B-NB	2.99	114.39	110.05
82	pK	201	PEB	C3B-C4B-NB	2.99	114.39	110.05
82	AJ	302	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
82	AQ	303	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
87	B2	820	CLA	C3B-C4B-NB	-2.99	107.75	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iK	201	PEB	CHA-C1B-C2B	2.99	132.58	124.90
82	QQ	201	PEB	OD-C4D-ND	-2.99	121.51	125.93
82	b4	202	PEB	OD-C4D-ND	-2.99	121.51	125.93
92	d6	409	LMG	O1-C7-C8	-2.99	103.69	110.90
82	I7	202	PEB	C3B-C4B-NB	2.99	114.39	110.05
82	FD	203	PEB	CHB-C4B-C3B	2.99	132.22	125.32
82	dG	201	PEB	CHA-C1B-NB	-2.99	118.69	124.93
82	EA	201	PEB	CHA-C1B-C2B	2.99	132.58	124.90
82	iM	201	PEB	C1C-CHB-C4B	-2.99	121.59	128.28
82	H5	203	PEB	CMB-C2B-C1B	2.99	129.66	125.06
82	WH	201	PEB	CAC-C2C-C3C	2.99	133.91	127.07
82	A5	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
82	PG	202	PEB	C2A-C1A-NA	2.98	110.85	108.27
82	uK	202	PEB	C2A-C1A-NA	2.98	110.85	108.27
82	BI	203	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
82	hJ	201	PEB	C1C-CHB-C4B	2.98	134.97	128.28
85	c6	603	BCR	C4-C5-C6	-2.98	118.40	122.73
84	BE	1001	CYC	CMB-C2B-C1B	2.98	127.89	124.17
82	DO	1002	PEB	OD-C4D-ND	-2.98	121.51	125.93
82	N5	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
82	iG	202	PEB	OD-C4D-ND	-2.98	121.51	125.93
82	hO	202	PEB	OD-C4D-ND	-2.98	121.51	125.93
85	BN	841	BCR	C10-C11-C12	-2.98	113.90	123.22
82	MD	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
82	MQ	201	PEB	C3B-C4B-NB	2.98	114.39	110.05
82	HA	203	PEB	CAB-C3B-C2B	-2.98	122.32	127.88
87	A2	850	CLA	CMB-C2B-C3B	2.98	133.81	126.59
84	BE	1001	CYC	C4A-C3A-C2A	-2.98	103.08	106.51
82	h4	201	PEB	C2B-C1B-NB	2.98	116.90	110.53
84	LE	1001	CYC	C1B-NB-C4B	-2.98	106.87	110.67
84	BG	1001	CYC	CMB-C2B-C1B	2.98	127.89	124.17
85	AN	845	BCR	C20-C21-C22	-2.98	123.05	127.31
82	eM	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
82	PA	203	PEB	OD-C4D-C3D	-2.98	122.70	129.46
87	42	605	CLA	O2A-CGA-O1A	-2.98	115.86	123.30
85	F6	101	BCR	C19-C18-C17	2.98	123.52	118.94
82	gF	203	PEB	OA-C1A-C2A	-2.98	123.80	126.17
92	BL	611	LMG	C7-O1-C1	-2.98	107.91	113.74
82	OF	201	PEB	C1C-CHB-C4B	2.98	134.97	128.28
82	HF	201	PEB	CHA-C1B-C2B	2.98	132.57	124.90
82	IP	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
82	FQ	203	PEB	CHB-C4B-C3B	2.98	132.22	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	KN	103	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
84	JO	1001	CYC	C2A-C1A-NA	2.98	114.39	110.05
82	OK	201	PEB	CAC-CBC-CGC	-2.98	107.19	113.60
87	RN	201	CLA	CHB-C4A-NA	2.98	128.64	124.51
82	XQ	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
85	kL	100	BCR	C30-C25-C26	-2.98	118.41	122.61
82	NB	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
82	SM	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
82	MQ	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
85	hL	102	BCR	C15-C14-C13	-2.98	123.05	127.31
82	Y1	202	PEB	CHA-C1B-NB	-2.98	118.69	124.93
84	63	901	CYC	C4A-C3A-C2A	-2.98	103.08	106.51
82	ZF	201	PEB	CAB-CBB-CGB	-2.98	107.19	113.60
82	EM	203	PEB	OD-C4D-C3D	-2.98	122.70	129.46
82	JQ	202	PEB	OD-C4D-C3D	-2.98	122.70	129.46
82	JQ	203	PEB	OD-C4D-C3D	-2.98	122.70	129.46
82	I5	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
87	b6	615	CLA	C3B-C4B-NB	-2.98	107.75	110.52
82	lM	201	PEB	C3C-C4C-NC	2.98	111.02	108.33
82	a4	203	PEB	CAB-CBB-CGB	2.98	120.02	113.60
84	B3	1001	CYC	C1B-CHB-C4A	2.98	135.37	128.08
82	QO	201	PEB	CHC-C4C-NC	2.98	125.18	121.15
82	sF	202	PEB	C1C-CHB-C4B	2.98	134.97	128.28
82	gG	202	PEB	CHA-C1B-NB	-2.98	118.70	124.93
84	LE	1001	CYC	C4A-C3A-C2A	-2.98	103.08	106.51
82	T7	203	PEB	CAC-CBC-CGC	-2.98	107.19	113.60
82	OK	203	PEB	OD-C4D-ND	-2.98	121.51	125.93
87	AN	813	CLA	CHB-C4A-NA	2.98	128.63	124.51
87	A2	808	CLA	CHB-C4A-NA	2.98	128.63	124.51
84	EG	1001	CYC	CHA-C4D-C3D	-2.98	120.42	127.15
82	QD	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
82	YD	201	PEB	CHC-C4C-NC	2.98	125.18	121.15
84	U3	1001	CYC	C1B-CHB-C4A	2.98	135.36	128.08
82	RK	202	PEB	C1D-CHC-C4C	2.98	117.65	113.26
87	B2	836	CLA	C4D-C3D-CAD	-2.98	104.58	108.10
82	d4	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
92	a6	614	LMG	O8-C28-C29	2.98	121.26	111.91
82	W4	201	PEB	C1C-CHB-C4B	2.98	134.97	128.28
82	QA	202	PEB	CHB-C1C-C2C	-2.98	120.43	127.15
82	F4	1002	PEB	CMD-C2D-C3D	2.98	134.27	130.06
82	MB	201	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	WQ	202	PEB	C1B-C2B-C3B	-2.98	103.09	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B9	202	PEB	CHB-C4B-NB	-2.98	118.38	124.58
87	ON	203	CLA	C2A-C1A-CHA	2.98	129.07	123.86
82	GK	203	PEB	CBB-CAB-C3B	2.98	120.91	112.63
82	J9	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
85	H6	101	BCR	C7-C8-C9	-2.98	121.73	126.23
82	AI	201	PEB	CHC-C1D-ND	-2.98	109.95	113.72
84	CH	1001	CYC	CHA-C4D-C3D	-2.98	120.43	127.15
82	QF	201	PEB	CHC-C4C-NC	2.98	125.18	121.15
82	lF	202	PEB	CHC-C4C-NC	2.98	125.18	121.15
82	bK	202	PEB	C1D-CHC-C4C	2.98	117.65	113.26
85	d6	405	BCR	C38-C26-C27	2.98	119.34	113.62
82	CK	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
87	62	309	CLA	CGD-CBD-CAD	-2.98	101.08	110.73
82	b4	201	PEB	OD-C4D-C3D	-2.98	122.71	129.46
82	HH	1002	PEB	OA-C1A-C2A	-2.98	123.80	126.17
82	RO	201	PEB	CHB-C4B-C3B	-2.98	118.43	125.32
82	NQ	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	A4	304	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	BQ	203	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	BA	202	PEB	C3C-C4C-NC	2.98	111.02	108.33
82	dK	201	PEB	OA-C1A-NA	2.98	128.55	124.94
82	PG	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	mE	203	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	pF	201	PEB	CHB-C1C-NC	-2.98	118.50	125.32
82	MD	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	dB	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	W9	202	PEB	CAB-CBB-CGB	-2.98	107.19	113.60
82	iG	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	W7	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
82	YP	503	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	IF	202	PEB	CHC-C1D-ND	-2.98	109.96	113.72
82	XP	201	PEB	CHA-C1B-NB	-2.98	118.70	124.93
82	QF	203	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	OG	203	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	K5	201	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	LQ	201	PEB	OA-C1A-C2A	-2.98	123.81	126.17
84	F3	1001	CYC	C1B-CHB-C4A	2.98	135.36	128.08
82	JM	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	eO	203	PEB	CMB-C2B-C1B	2.98	129.65	125.06
82	JF	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	lE	203	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	lE	202	PEB	CHC-C1D-ND	-2.98	109.96	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QM	202	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	OQ	201	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	V4	202	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	g4	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	F7	203	PEB	CHA-C4A-NA	-2.98	121.67	125.20
82	dB	201	PEB	OD-C4D-C3D	-2.98	122.71	129.46
82	dE	201	PEB	CHA-C1B-NB	-2.98	118.70	124.93
84	f3	1001	CYC	C1B-CHB-C4A	2.98	135.35	128.08
83	xK	301	PUB	C2C-C1C-NC	2.98	114.38	110.05
82	jG	201	PEB	CAB-CBB-CGB	-2.98	107.20	113.60
87	AN	852	CLA	C1D-ND-C4D	2.98	108.45	106.33
87	CL	506	CLA	CHD-C1D-ND	-2.98	121.72	124.45
82	Z4	201	PEB	C1D-CHC-C4C	-2.98	108.87	113.26
87	2N	305	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
82	z8	201	PEB	CHC-C4C-NC	2.98	125.18	121.15
82	O1	202	PEB	CHC-C1D-ND	-2.98	109.96	113.72
82	WO	201	PEB	OD-C4D-C3D	-2.98	122.72	129.46
82	T4	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	I5	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	O5	201	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
87	3N	308	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
82	ND	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	wF	302	PEB	C3B-C4B-NB	2.98	114.38	110.05
85	B2	841	BCR	C10-C11-C12	-2.98	113.93	123.22
82	CP	203	PEB	C2A-C1A-NA	2.98	110.84	108.27
82	OO	202	PEB	C1D-CHC-C4C	2.98	117.64	113.26
84	I3	1001	CYC	C1B-CHB-C4A	2.98	135.35	128.08
87	BN	818	CLA	CMB-C2B-C1B	-2.98	120.84	125.37
82	JM	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	SB	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	C7	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	kG	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	XD	203	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	dE	203	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
82	P4	202	PEB	CAB-C3B-C4B	2.98	130.27	125.01
82	CB	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	iH	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
82	Q4	201	PEB	CHB-C4B-NB	2.98	130.77	124.58
82	PG	201	PEB	CHB-C1C-NC	-2.98	118.50	125.32
82	GQ	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
82	j4	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
87	AN	817	CLA	C3B-C4B-NB	-2.98	107.75	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	KL	100	BCR	C30-C25-C26	-2.98	118.42	122.61
82	gF	201	PEB	CMC-C3C-C4C	2.98	130.21	127.06
87	AN	837	CLA	CHB-C4A-NA	2.98	128.63	124.51
87	A2	822	CLA	CHB-C4A-NA	2.98	128.63	124.51
82	V5	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	jK	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
82	XD	203	PEB	C3B-C4B-NB	2.97	114.38	110.05
82	H5	203	PEB	C3B-C4B-NB	2.97	114.38	110.05
87	2N	309	CLA	CHB-C1B-NB	2.97	127.41	124.26
82	z8	201	PEB	C1D-CHC-C4C	-2.97	108.87	113.26
82	XF	202	PEB	C2A-C1A-NA	2.97	110.84	108.27
87	7N	601	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
82	PH	202	PEB	OD-C4D-ND	-2.97	121.52	125.93
82	fM	201	PEB	OD-C4D-ND	-2.97	121.52	125.93
82	A1	301	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
82	FI	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	BD	202	PEB	CHC-C4C-NC	2.97	125.17	121.15
82	WG	201	PEB	CHC-C4C-NC	2.97	125.17	121.15
82	D9	203	PEB	CHC-C1D-ND	-2.97	109.96	113.72
87	a6	608	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
82	UQ	201	PEB	CHA-C1B-NB	-2.97	118.71	124.93
82	FO	1002	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	NE	202	PEB	OD-C4D-C3D	-2.97	122.72	129.46
82	MA	201	PEB	CAB-C3B-C4B	2.97	130.27	125.01
82	18	202	PEB	C1B-C2B-C3B	-2.97	103.09	106.51
82	WD	201	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
84	k3	1001	CYC	C1B-CHB-C4A	2.97	135.34	128.08
83	xF	301	PUB	C2C-C1C-NC	2.97	114.37	110.05
82	QB	203	PEB	C2A-C1A-NA	2.97	110.84	108.27
82	WD	201	PEB	C2A-C1A-NA	2.97	110.84	108.27
82	Q1	201	PEB	C2A-C1A-NA	2.97	110.84	108.27
84	63	901	CYC	C2C-C1C-NC	2.97	110.84	108.27
82	hK	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	NM	201	PEB	CAB-C3B-C4B	2.97	130.27	125.01
82	jE	201	PEB	CAB-CBB-CGB	-2.97	107.21	113.60
82	SJ	203	PEB	CHA-C1B-NB	-2.97	118.72	124.93
82	ZJ	202	PEB	CHB-C4B-NB	-2.97	118.39	124.58
82	W4	201	PEB	CHC-C4C-NC	2.97	125.17	121.15
82	PJ	202	PEB	C1C-CHB-C4B	-2.97	121.62	128.28
82	UO	202	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
88	CL	521	LHG	O8-C23-C24	2.97	121.23	111.91
82	NK	202	PEB	OD-C4D-ND	-2.97	121.53	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TQ	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
82	TH	201	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	O7	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
84	DH	1003	CYC	CHB-C4A-NA	-2.97	118.72	124.93
82	j4	201	PEB	CHB-C1C-C2C	-2.97	120.44	127.15
82	YQ	201	PEB	C2A-C1A-NA	2.97	110.83	108.27
82	iJ	202	PEB	CAB-C3B-C4B	2.97	130.27	125.01
82	mF	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
82	m4	202	PEB	C3C-C4C-NC	2.97	111.01	108.33
82	lO	201	PEB	C1C-CHB-C4B	2.97	134.95	128.28
82	CA	201	PEB	CHA-C4A-NA	2.97	128.74	125.20
82	QF	202	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
82	IM	202	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
82	XP	202	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
82	vC	201	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
82	UP	203	PEB	CAC-CBC-CGC	-2.97	107.21	113.60
85	AN	847	BCR	C2-C1-C6	2.97	115.06	110.48
82	bO	201	PEB	OD-C4D-C3D	-2.97	122.73	129.46
82	BD	203	PEB	CAC-C2C-C1C	2.97	130.49	125.76
82	JM	202	PEB	CHB-C4B-NB	-2.97	118.39	124.58
83	Y7	302	PUB	CHA-C1B-NB	2.97	125.17	121.15
82	TB	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	MD	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	PE	201	PEB	C2A-C1A-NA	2.97	110.83	108.27
87	62	308	CLA	CHB-C4A-NA	2.97	128.62	124.51
82	MF	201	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	YE	201	PEB	CAC-C2C-C1C	2.97	130.49	125.76
82	R7	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
87	cL	509	CLA	CMB-C2B-C1B	-2.97	120.84	125.37
82	XA	203	PEB	C1D-CHC-C4C	-2.97	108.88	113.26
82	qK	201	PEB	C3C-C4C-NC	2.97	111.01	108.33
87	BN	815	CLA	O2D-CGD-CBD	2.97	116.55	111.27
82	a4	203	PEB	OD-C4D-ND	-2.97	121.53	125.93
84	j3	1001	CYC	C1B-CHB-C4A	2.97	135.34	128.08
82	dE	201	PEB	CAC-C2C-C1C	2.97	130.49	125.76
87	52	607	CLA	CHC-C4B-NB	2.97	127.40	124.26
82	Z1	203	PEB	CHA-C1B-C2B	2.97	132.54	124.90
82	bE	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
82	LI	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
82	aM	203	PEB	C3B-C4B-NB	2.97	114.37	110.05
82	AO	305	PEB	CHA-C1B-NB	-2.97	118.72	124.93
82	C5	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	d3	1001	CYC	C1B-CHB-C4A	2.97	135.34	128.08
82	p8	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
82	RJ	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
82	iE	201	PEB	OD-C4D-C3D	-2.97	122.73	129.46
82	WM	202	PEB	CMC-C3C-C2C	2.97	132.03	125.61
82	EJ	201	PEB	CHA-C1B-NB	-2.97	118.72	124.93
82	eG	203	PEB	CHB-C4B-NB	-2.97	118.40	124.58
82	WO	201	PEB	CHC-C4C-NC	2.97	125.17	121.15
82	MF	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
82	uC	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
83	AG	302	PUB	OA-C1A-NA	-2.97	121.53	125.93
84	O3	1001	CYC	C1B-CHB-C4A	2.97	135.33	128.08
87	F2	201	CLA	C3B-C4B-NB	-2.97	107.76	110.52
82	GK	201	PEB	CAA-C3A-C2A	2.97	121.68	114.26
82	VM	201	PEB	OD-C4D-C3D	-2.97	122.73	129.46
82	y8	203	PEB	OD-C4D-C3D	-2.97	122.73	129.46
82	KB	304	PEB	C3B-C4B-NB	2.97	114.37	110.05
82	QB	204	PEB	C1C-CHB-C4B	2.97	134.94	128.28
82	YH	202	PEB	CHA-C1B-NB	-2.97	118.72	124.93
82	LD	201	PEB	OA-C1A-C2A	-2.97	123.81	126.17
82	ZJ	202	PEB	OA-C1A-C2A	-2.97	123.81	126.17
82	c4	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
82	W5	203	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
84	KO	1001	CYC	C4A-C3A-C2A	-2.97	103.10	106.51
82	OF	201	PEB	CAC-CBC-CGC	-2.97	107.22	113.60
87	LN	206	CLA	CHB-C1B-NB	2.97	127.40	124.26
82	T5	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	ZK	202	PEB	CHB-C4B-C3B	-2.97	118.45	125.32
82	WI	203	PEB	C3B-C4B-NB	2.97	114.37	110.05
84	E4	1001	CYC	C2A-C1A-NA	2.97	114.37	110.05
95	AL	416	DGD	C6D-C5D-C4D	-2.97	105.90	112.09
87	FN	205	CLA	C2A-C1A-CHA	2.97	129.05	123.86
87	BN	835	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
84	u3	1001	CYC	C1B-CHB-C4A	2.97	135.33	128.08
95	AL	416	DGD	O1G-C1A-C2A	2.97	121.22	111.91
82	RQ	201	PEB	C2A-C1A-NA	2.97	110.83	108.27
82	TH	202	PEB	OD-C4D-C3D	-2.97	122.74	129.46
82	F5	201	PEB	CAC-C2C-C3C	2.97	133.87	127.07
84	D3	1001	CYC	C1B-CHB-C4A	2.97	135.33	128.08
82	E7	201	PEB	CHB-C1C-C2C	-2.97	120.46	127.15
87	B6	606	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
82	QQ	202	PEB	C3B-C4B-NB	2.97	114.36	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	FE	1001	CYC	C2A-C1A-NA	2.97	114.36	110.05
87	O2	203	CLA	C2A-C1A-CHA	2.97	129.05	123.86
92	j6	101	LMG	O8-C28-O10	-2.97	116.10	123.59
82	VA	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	MF	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	EJ	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	V1	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	E5	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
82	UG	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
83	AM	303	PUB	OD-C4D-ND	-2.97	121.53	125.93
84	L3	1001	CYC	C1B-CHB-C4A	2.97	135.33	128.08
82	wF	303	PEB	CAB-C3B-C2B	2.97	133.40	127.88
87	BL	602	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
87	J2	101	CLA	C3B-C4B-NB	-2.97	107.76	110.52
84	D1	1003	CYC	CHB-C4A-NA	-2.97	118.73	124.93
82	jG	202	PEB	C3B-C4B-NB	2.97	114.36	110.05
82	JB	202	PEB	CMB-C2B-C1B	2.97	129.63	125.06
85	F2	203	BCR	C24-C23-C22	-2.97	121.75	126.23
82	QP	202	PEB	OD-C4D-ND	-2.97	121.54	125.93
82	E5	201	PEB	OD-C4D-ND	-2.97	121.54	125.93
91	d6	404	PHO	CBC-CAC-C3C	-2.97	108.54	112.88
82	AH	301	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
84	M1	201	CYC	C1A-C2A-C3A	-2.97	103.50	106.78
82	TI	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
82	RM	202	PEB	CHB-C4B-NB	-2.97	118.41	124.58
82	e4	203	PEB	CMB-C2B-C1B	2.97	129.63	125.06
82	WJ	202	PEB	C3B-C4B-NB	2.97	114.36	110.05
82	V7	202	PEB	C3B-C4B-NB	2.97	114.36	110.05
82	yC	203	PEB	C3B-C4B-NB	2.97	114.36	110.05
85	AN	845	BCR	C11-C10-C9	-2.97	123.08	127.31
82	iE	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
84	q3	1001	CYC	C1B-CHB-C4A	2.97	135.32	128.08
87	K2	104	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
82	KK	201	PEB	CHA-C1B-NB	-2.96	118.73	124.93
84	LG	1001	CYC	C1B-NB-C4B	-2.96	106.89	110.67
82	e4	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
83	NQ	201	PUB	OD-C4D-ND	-2.96	121.54	125.93
82	bH	202	PEB	CMD-C2D-C3D	2.96	134.25	130.06
84	o3	1001	CYC	C1B-CHB-C4A	2.96	135.32	128.08
82	dG	201	PEB	C1B-C2B-C3B	-2.96	103.10	106.51
82	mK	202	PEB	C1B-C2B-C3B	-2.96	103.10	106.51
84	F1	1001	CYC	C4A-C3A-C2A	-2.96	103.10	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	832	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
84	K4	1001	CYC	C4D-CHA-C1A	2.96	134.93	128.28
82	WP	202	PEB	C1D-CHC-C4C	-2.96	108.89	113.26
82	O1	203	PEB	C3B-C4B-NB	2.96	114.36	110.05
82	hM	201	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
85	IN	101	BCR	C15-C14-C13	-2.96	123.08	127.31
103	82	310	ZEX	C31-C32-C33	-2.96	118.09	126.42
82	cE	202	PEB	OD-C4D-C3D	-2.96	122.75	129.46
82	HG	1002	PEB	CAA-C3A-C4A	-2.96	105.06	112.67
82	hO	201	PEB	C2B-C1B-NB	2.96	116.86	110.53
87	B2	813	CLA	CHB-C4A-NA	2.96	128.61	124.51
87	C6	518	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
87	3N	305	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
82	OF	203	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	X5	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	v8	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	Q9	202	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	gG	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
95	BL	613	DGD	C6D-C5D-C4D	-2.96	105.91	112.09
87	B6	603	CLA	C3B-C4B-NB	-2.96	107.77	110.52
82	Q5	202	PEB	OA-C1A-C2A	-2.96	123.82	126.17
82	TH	201	PEB	C4C-C3C-C2C	-2.96	104.77	107.50
82	QG	201	PEB	CHA-C1B-NB	-2.96	118.73	124.93
82	CD	201	PEB	CAC-C2C-C1C	2.96	130.48	125.76
82	iF	203	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
87	L2	203	CLA	CHB-C4A-NA	2.96	128.61	124.51
87	d6	401	CLA	C1-C2-C3	-2.96	120.92	126.04
82	AA	202	PEB	C2A-C1A-NA	2.96	110.83	108.27
82	WG	203	PEB	C2A-C1A-NA	2.96	110.83	108.27
91	D6	404	PHO	CMB-C2B-C3B	2.96	130.22	124.68
85	bL	602	BCR	C34-C9-C10	-2.96	118.77	122.92
82	FJ	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
82	lG	202	PEB	CHC-C4C-NC	2.96	125.16	121.15
84	w3	1001	CYC	C1B-CHB-C4A	2.96	135.32	128.08
82	XJ	202	PEB	CAB-C3B-C4B	2.96	130.25	125.01
82	YB	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	O5	202	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	mF	202	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	VK	202	PEB	CHB-C4B-NB	2.96	130.74	124.58
85	cL	518	BCR	C33-C5-C4	2.96	119.31	113.62
87	7N	604	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
82	mJ	202	PEB	OA-C1A-C2A	-2.96	123.82	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AB	501	PEB	CMB-C2B-C1B	2.96	129.62	125.06
82	hF	202	PEB	C1C-CHB-C4B	2.96	134.92	128.28
82	TO	202	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
82	Q7	202	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
82	T7	201	PEB	CAB-C3B-C4B	2.96	130.25	125.01
82	WJ	203	PEB	C2A-C1A-NA	2.96	110.83	108.27
82	YM	201	PEB	C2A-C1A-NA	2.96	110.83	108.27
82	uK	201	PEB	C2A-C1A-NA	2.96	110.83	108.27
84	73	1001	CYC	C1B-CHB-C4A	2.96	135.32	128.08
84	FG	1001	CYC	C4D-CHA-C1A	2.96	134.92	128.28
82	XP	202	PEB	CHC-C1D-ND	-2.96	109.98	113.72
82	DF	203	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
82	S9	202	PEB	C1D-CHC-C4C	2.96	117.62	113.26
87	32	307	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
82	GB	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
82	P5	202	PEB	C3B-C4B-NB	2.96	114.36	110.05
95	C6	503	DGD	O1G-C1A-C2A	2.96	121.20	111.91
82	A5	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	J5	202	PEB	OD-C4D-ND	-2.96	121.54	125.93
82	MB	202	PEB	C3D-C4D-ND	2.96	113.07	107.26
84	Q3	1001	CYC	C1B-CHB-C4A	2.96	135.31	128.08
82	E7	201	PEB	CHA-C1B-C2B	2.96	132.51	124.90
84	F4	1001	CYC	CAB-C3B-C4B	2.96	126.05	121.38
84	H3	1001	CYC	C1B-CHB-C4A	2.96	135.31	128.08
82	M9	302	PEB	OD-C4D-C3D	-2.96	122.75	129.46
87	F2	205	CLA	C2A-C1A-CHA	2.96	129.03	123.86
82	aJ	204	PEB	CAA-C3A-C4A	-2.96	105.07	112.67
84	IO	1001	CYC	C4D-C3D-C2D	-2.96	104.12	107.62
82	BJ	301	PEB	OD-C4D-ND	-2.96	121.55	125.93
87	72	609	CLA	CHB-C4A-NA	2.96	128.60	124.51
82	W5	201	PEB	C2B-C1B-NB	2.96	116.85	110.53
87	aL	606	CLA	C4-C3-C5	2.96	120.25	115.27
82	SI	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	fM	203	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	DP	202	PEB	CAC-CBC-CGC	-2.96	107.23	113.60
82	PJ	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	HP	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	BP	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	LQ	203	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	PD	201	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
82	T1	202	PEB	CAA-C3A-C4A	2.96	120.27	112.67
84	M3	1001	CYC	C1B-CHB-C4A	2.96	135.31	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	D5	203	PEB	C2A-C1A-NA	2.96	110.82	108.27
82	M9	304	PEB	C2A-C1A-NA	2.96	110.82	108.27
87	CL	513	CLA	CHB-C4A-NA	2.96	128.60	124.51
87	LN	203	CLA	CHB-C4A-NA	2.96	128.60	124.51
82	PG	202	PEB	CMC-C3C-C4C	-2.96	123.92	127.06
85	bL	603	BCR	C4-C5-C6	-2.96	118.44	122.73
87	IN	103	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
82	RQ	201	PEB	OD-C4D-C3D	-2.96	122.76	129.46
82	MA	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	KB	301	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	W9	203	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	kF	203	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	xK	303	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	T4	201	PEB	CHC-C1D-ND	-2.96	109.98	113.72
82	A4	305	PEB	CHA-C1B-NB	-2.96	118.74	124.93
82	ZH	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	aO	203	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	YI	201	PEB	C2C-C1C-NC	2.96	111.56	107.57
82	jE	202	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
82	UK	202	PEB	CHB-C1C-C2C	-2.96	120.48	127.15
85	F6	101	BCR	C24-C23-C22	2.96	130.71	126.23
82	CQ	201	PEB	OA-C1A-C2A	-2.96	123.82	126.17
82	VA	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	HF	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	UE	201	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	XA	203	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	DI	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	WQ	201	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	gK	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
87	c6	609	CLA	C3B-C4B-NB	-2.96	107.77	110.52
82	PA	201	PEB	CAB-CBB-CGB	-2.96	107.24	113.60
82	cE	201	PEB	CHA-C1B-NB	-2.96	118.75	124.93
82	IQ	202	PEB	C4C-C3C-C2C	-2.96	104.77	107.50
82	JA	203	PEB	CHB-C4B-NB	-2.96	118.42	124.58
82	QJ	204	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
82	dE	201	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
82	XF	203	PEB	CAB-C3B-C4B	2.96	130.24	125.01
82	PE	201	PEB	CHB-C1C-NC	-2.96	118.55	125.32
82	Y5	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
84	KO	1001	CYC	C2A-C1A-NA	2.96	114.35	110.05
82	EK	202	PEB	CHB-C1C-C2C	-2.96	120.48	127.15
82	vC	201	PEB	OD-C4D-ND	-2.96	121.55	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eF	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	CB	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
82	SA	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	h1	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	M7	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	kF	201	PEB	CHA-C1B-C2B	2.96	132.50	124.90
82	HI	203	PEB	C2A-C1A-NA	2.96	110.82	108.27
82	aK	203	PEB	C2A-C1A-NA	2.96	110.82	108.27
82	eG	201	PEB	OA-C1A-C2A	-2.96	123.82	126.17
82	hK	202	PEB	C1C-CHB-C4B	2.96	134.91	128.28
87	B2	814	CLA	O2D-CGD-CBD	2.96	116.52	111.27
82	CF	203	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	mK	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
82	LD	203	PEB	CMB-C2B-C1B	2.96	129.62	125.06
82	q8	203	PEB	CAB-C3B-C4B	2.96	130.24	125.01
82	eO	202	PEB	CHA-C1B-NB	-2.96	118.75	124.93
87	62	311	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
85	A2	845	BCR	C11-C10-C9	-2.96	123.09	127.31
82	X7	203	PEB	C1D-CHC-C4C	-2.96	108.90	113.26
82	XF	202	PEB	OD-C4D-C3D	-2.96	122.76	129.46
82	RB	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
82	BD	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	G7	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	dM	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
82	CJ	202	PEB	C3C-C4C-NC	2.96	110.99	108.33
84	J1	1001	CYC	C4D-CHA-C1A	2.96	134.91	128.28
82	LA	203	PEB	CMB-C2B-C1B	2.96	129.62	125.06
82	NG	201	PEB	CMB-C2B-C1B	2.96	129.62	125.06
82	MA	201	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
84	G4	1001	CYC	C4A-C3A-C2A	-2.96	103.11	106.51
82	nF	202	PEB	OD-C4D-C3D	-2.96	122.76	129.46
82	A7	202	PEB	OA-C1A-C2A	-2.96	123.82	126.17
82	VP	201	PEB	CHC-C4C-NC	2.96	125.15	121.15
82	ID	202	PEB	C4C-C3C-C2C	-2.96	104.77	107.50
82	lG	203	PEB	C1D-CHC-C4C	-2.96	108.90	113.26
87	AN	811	CLA	C2D-C1D-ND	-2.96	107.93	110.10
82	N5	202	PEB	CAA-C3A-C4A	-2.96	105.08	112.67
82	pF	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
83	AJ	304	PUB	OD-C4D-ND	-2.96	121.55	125.93
82	ZH	203	PEB	CHA-C1B-C2B	2.96	132.50	124.90
82	YM	203	PEB	C3C-C4C-NC	2.95	110.99	108.33
84	S3	1001	CYC	C1B-CHB-C4A	2.95	135.30	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YA	303	PEB	CHC-C4C-NC	2.95	125.15	121.15
82	PH	202	PEB	CHC-C4C-NC	2.95	125.15	121.15
82	F9	203	PEB	CHC-C1D-ND	-2.95	109.99	113.72
82	iF	202	PEB	CHC-C1D-ND	-2.95	109.99	113.72
87	6N	610	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
82	PG	201	PEB	CAB-C3B-C4B	2.95	130.24	125.01
82	R1	201	PEB	CMB-C2B-C1B	2.95	129.61	125.06
87	BN	808	CLA	C3B-C4B-NB	-2.95	107.77	110.52
82	QG	201	PEB	C1C-NC-C4C	-2.95	104.34	109.60
82	iK	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	D9	202	PEB	CBA-CAA-C3A	-2.95	106.89	113.47
92	CL	519	LMG	O8-C28-C29	2.95	121.18	111.91
82	OM	203	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
82	B9	201	PEB	CAB-C3B-C4B	2.95	130.24	125.01
82	S5	202	PEB	CHC-C1D-ND	-2.95	109.99	113.72
82	cK	203	PEB	C3B-C4B-NB	2.95	114.35	110.05
83	AE	302	PUB	OA-C1A-NA	-2.95	121.55	125.93
82	NJ	201	PEB	CHA-C1B-NB	-2.95	118.75	124.93
82	cG	201	PEB	CHA-C1B-NB	-2.95	118.75	124.93
82	GM	201	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
82	X5	202	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
82	G7	202	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
82	OE	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	XF	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	eK	202	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	FI	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	YI	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	JM	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
87	BN	817	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
83	BJ	302	PUB	CHA-C4A-NA	-2.95	109.99	113.72
85	A2	847	BCR	C2-C1-C6	2.95	115.03	110.48
82	EA	201	PEB	CHB-C1C-C2C	-2.95	120.49	127.15
82	bF	202	PEB	C1D-CHC-C4C	2.95	117.61	113.26
82	BQ	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	C9	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
84	h3	1001	CYC	C1B-CHB-C4A	2.95	135.29	128.08
82	GF	201	PEB	C1C-NC-C4C	-2.95	104.34	109.60
84	JH	1003	CYC	CHB-C1B-NB	-2.95	119.72	126.06
82	J7	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
87	A2	813	CLA	CHB-C4A-NA	2.95	128.59	124.51
82	kO	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	gO	202	PEB	OD-C4D-ND	-2.95	121.56	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CQ	202	PEB	OD-C4D-C3D	-2.95	122.77	129.46
82	kG	202	PEB	CAC-CBC-CGC	-2.95	107.25	113.60
85	bL	602	BCR	C8-C7-C6	2.95	135.49	127.20
84	LO	1001	CYC	CAB-C3B-C4B	2.95	126.04	121.38
82	hH	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
84	JH	1003	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
87	1N	609	CLA	C2A-C1A-CHA	2.95	129.02	123.86
82	iF	202	PEB	CHA-C1B-NB	-2.95	118.76	124.93
84	HG	1001	CYC	CHB-C1B-NB	-2.95	119.72	126.06
82	XB	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	FP	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
87	BL	603	CLA	CHB-C4A-NA	2.95	128.59	124.51
87	AN	823	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
87	B2	835	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
82	jH	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	eO	202	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	HO	1002	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	EA	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	mO	202	PEB	C3C-C4C-NC	2.95	110.99	108.33
82	HF	201	PEB	C1C-NC-C4C	-2.95	104.35	109.60
87	6N	608	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
83	AO	302	PUB	OA-C1A-NA	-2.95	121.56	125.93
82	NB	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
82	YM	203	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
82	R5	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
87	R2	204	CLA	CHB-C4A-NA	2.95	128.59	124.51
82	TH	201	PEB	CHC-C4C-NC	2.95	125.14	121.15
87	B2	816	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
82	WF	201	PEB	OD-C4D-C3D	-2.95	122.78	129.46
85	cL	503	BCR	C21-C20-C19	-2.95	114.01	123.22
82	QE	203	PEB	OA-C1A-C2A	-2.95	123.83	126.17
82	D4	1002	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	V5	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
83	YA	302	PUB	OA-C1A-NA	-2.95	121.56	125.93
103	8N	310	ZEX	C31-C32-C33	-2.95	118.13	126.42
87	82	301	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
87	7N	609	CLA	CHB-C4A-NA	2.95	128.59	124.51
82	fB	301	PEB	CAC-CBC-CGC	-2.95	107.26	113.60
82	IA	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
82	j1	203	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
82	U4	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
82	G5	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	JO	1001	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
82	RB	202	PEB	C1C-CHB-C4B	2.95	134.90	128.28
82	DB	203	PEB	C2A-C1A-NA	2.95	110.81	108.27
82	CD	202	PEB	OD-C4D-C3D	-2.95	122.78	129.46
82	VP	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	G5	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	T5	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	W1	203	PEB	CAC-C2C-C1C	2.95	130.46	125.76
82	UF	202	PEB	CHB-C1C-C2C	-2.95	120.50	127.15
82	E5	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	pF	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	XJ	201	PEB	C1C-CHB-C4B	-2.95	121.67	128.28
82	RD	203	PEB	C1C-CHB-C4B	2.95	134.89	128.28
82	P7	203	PEB	CHC-C4C-NC	2.95	125.14	121.15
91	DL	405	PHO	C4B-NB-C1B	-2.95	104.27	108.83
87	72	604	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
82	kK	201	PEB	CHA-C1B-C2B	2.95	132.48	124.90
82	UG	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
82	tC	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
82	eH	202	PEB	CHA-C4A-NA	2.95	128.71	125.20
82	PM	201	PEB	C1C-CHB-C4B	-2.95	121.67	128.28
82	SH	203	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	mO	203	PEB	OD-C4D-ND	-2.95	121.56	125.93
82	HM	202	PEB	CAB-C3B-C2B	2.95	133.37	127.88
82	DQ	201	PEB	OD-C4D-C3D	-2.95	122.78	129.46
82	TK	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	SF	203	PEB	CMC-C3C-C4C	2.95	130.19	127.06
82	TK	201	PEB	CHB-C1C-C2C	-2.95	120.50	127.15
82	BQ	202	PEB	CHC-C4C-NC	2.95	125.14	121.15
84	NH	1001	CYC	C4D-C3D-C2D	-2.95	104.14	107.62
82	I5	202	PEB	CAA-C3A-C4A	-2.95	105.11	112.67
82	WM	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
82	i4	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
82	RA	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
82	e1	202	PEB	CHA-C4A-NA	2.95	128.71	125.20
82	eH	203	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
82	lJ	203	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
82	cG	202	PEB	OD-C4D-C3D	-2.95	122.78	129.46
82	X5	202	PEB	CAA-C3A-C4A	-2.95	105.11	112.67
82	iK	202	PEB	CMB-C2B-C1B	2.95	129.60	125.06
84	FE	1002	CYC	CMA-C3A-C4A	2.95	129.60	125.06
82	cF	201	PEB	CAB-C3B-C4B	2.95	130.22	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	D6	407	LMG	O6-C1-O1	2.95	116.95	109.97
82	iE	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
82	aM	201	PEB	CMB-C2B-C1B	2.95	129.60	125.06
82	v8	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
95	b6	621	DGD	O1G-C1A-C2A	2.95	121.15	111.91
82	RM	202	PEB	OD-C4D-ND	-2.95	121.57	125.93
82	zF	501	PEB	OD-C4D-ND	-2.95	121.57	125.93
82	jM	201	PEB	OD-C4D-ND	-2.95	121.57	125.93
82	IB	202	PEB	CHA-C1B-NB	-2.95	118.77	124.93
82	l1	202	PEB	C3B-C4B-NB	2.95	114.33	110.05
82	MQ	202	PEB	CMB-C2B-C1B	2.95	129.60	125.06
82	sK	201	PEB	C1B-C2B-C3B	-2.95	103.13	106.51
82	WJ	203	PEB	CAA-C3A-C4A	-2.95	105.11	112.67
82	YB	202	PEB	CHC-C1D-ND	-2.95	110.00	113.72
82	yC	201	PEB	CHC-C1D-ND	-2.95	110.00	113.72
82	aH	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
82	v8	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
82	PP	202	PEB	CAC-CBC-CGC	-2.95	107.27	113.60
82	UJ	202	PEB	CHC-C4C-NC	2.95	125.14	121.15
82	VE	201	PEB	OD-C4D-ND	-2.95	121.57	125.93
82	FP	201	PEB	OD-C4D-ND	-2.95	121.57	125.93
82	IK	201	PEB	CAB-C3B-C4B	2.95	130.22	125.01
82	BB	202	PEB	C3B-C4B-NB	2.95	114.33	110.05
82	KG	201	PEB	C3B-C4B-NB	2.95	114.33	110.05
82	G5	202	PEB	C3B-C4B-NB	2.95	114.33	110.05
87	K2	104	CLA	CAA-C2A-C3A	-2.94	106.90	114.26
82	R5	202	PEB	CAA-C3A-C4A	-2.94	105.11	112.67
85	FL	101	BCR	C19-C18-C17	-2.94	114.42	118.94
82	zC	202	PEB	CAB-C3B-C4B	2.94	130.22	125.01
82	U5	203	PEB	OA-C1A-C2A	-2.94	123.83	126.17
82	GA	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	dE	203	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	IF	201	PEB	CAB-C3B-C4B	2.94	130.22	125.01
85	a6	605	BCR	C23-C24-C25	-2.94	118.93	127.20
82	NG	201	PEB	OD-C4D-C3D	-2.94	122.79	129.46
82	WK	201	PEB	CHC-C1D-ND	-2.94	110.00	113.72
82	QG	203	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
82	SB	203	PEB	CMB-C2B-C1B	2.94	129.60	125.06
82	R4	201	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
84	J4	1001	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
82	FJ	202	PEB	OD-C4D-C3D	-2.94	122.79	129.46
94	a6	601	PL9	C12-C13-C14	-2.94	120.57	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	62	309	CLA	O2A-CGA-O1A	-2.94	116.16	123.59
88	AN	843	LHG	O8-C23-C24	2.94	121.14	111.91
82	J4	1002	PEB	CMC-C3C-C4C	2.94	130.18	127.06
82	zC	201	PEB	CHC-C4C-NC	2.94	125.13	121.15
82	R7	203	PEB	OD-C4D-C3D	-2.94	122.79	129.46
82	D5	202	PEB	CHC-C1D-ND	-2.94	110.00	113.72
82	fF	201	PEB	CMB-C2B-C1B	2.94	129.60	125.06
82	KD	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
84	HE	1001	CYC	CHB-C1B-NB	-2.94	119.74	126.06
84	N4	1001	CYC	CHB-C1B-NB	-2.94	119.74	126.06
82	x8	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
92	DL	402	LMG	O6-C1-C2	2.94	116.58	110.35
82	P5	202	PEB	CAA-C3A-C4A	-2.94	105.12	112.67
94	a6	601	PL9	C25-C24-C26	2.94	120.22	115.27
82	Z4	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
84	FE	1002	CYC	C4D-CHA-C1A	2.94	134.88	128.28
82	hB	301	PEB	CAC-CBC-CGC	-2.94	107.27	113.60
82	TQ	203	PEB	C3B-C4B-NB	2.94	114.33	110.05
82	W4	201	PEB	OD-C4D-C3D	-2.94	122.79	129.46
82	hM	201	PEB	C1D-CHC-C4C	-2.94	108.92	113.26
82	bG	201	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
87	AN	819	CLA	CHB-C1B-NB	2.94	127.37	124.26
87	CL	508	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
85	c6	603	BCR	C35-C13-C14	-2.94	118.80	122.92
82	AH	302	PEB	OD-C4D-ND	-2.94	121.57	125.93
82	Z1	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
87	22	604	CLA	CHB-C4A-NA	2.94	128.58	124.51
87	B2	836	CLA	CHB-C4A-NA	2.94	128.58	124.51
82	t8	201	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
87	6N	603	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
82	T5	202	PEB	C3B-C4B-NB	2.94	114.33	110.05
82	UO	201	PEB	CMA-C2A-C1A	-2.94	106.06	112.40
87	12	609	CLA	C2A-C1A-CHA	2.94	129.00	123.86
82	J7	201	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	dG	203	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	OH	202	PEB	CHC-C1D-ND	-2.94	110.00	113.72
82	IK	202	PEB	CHC-C1D-ND	-2.94	110.00	113.72
82	iO	202	PEB	CHA-C1B-NB	-2.94	118.78	124.93
82	H5	202	PEB	OA-C1A-C2A	-2.94	123.83	126.17
87	AN	841	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
82	hE	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
82	V5	202	PEB	CAA-C3A-C4A	-2.94	105.12	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PF	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
82	EF	202	PEB	CHB-C1C-C2C	-2.94	120.52	127.15
82	hM	203	PEB	CHB-C1C-NC	-2.94	118.58	125.32
82	T7	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	z8	202	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	OA	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
82	EP	203	PEB	CMB-C2B-C1B	2.94	129.59	125.06
82	D7	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
82	XF	201	PEB	CHB-C1C-C2C	-2.94	120.52	127.15
82	R5	202	PEB	C3B-C4B-NB	2.94	114.33	110.05
87	a6	608	CLA	C3B-C4B-NB	-2.94	107.79	110.52
82	C5	202	PEB	CAA-C3A-C4A	-2.94	105.12	112.67
82	LG	1002	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
92	qL	301	LMG	C8-O7-C10	-2.94	110.56	117.79
82	NF	202	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	aG	202	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	lM	203	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	QD	202	PEB	CHC-C1D-ND	-2.94	110.01	113.72
87	8N	302	CLA	C2A-C1A-CHA	2.94	129.00	123.86
84	FG	1001	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
87	BN	836	CLA	CHB-C4A-NA	2.94	128.58	124.51
82	UP	201	PEB	C4B-NB-C1B	-2.94	100.97	106.51
82	BI	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
82	dJ	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
82	ZI	401	PEB	OD-C4D-C3D	-2.94	122.80	129.46
82	IQ	202	PEB	OD-C4D-C3D	-2.94	122.80	129.46
84	HH	1001	CYC	CMC-C2C-C1C	-2.94	106.07	112.40
82	S5	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	QA	202	PEB	CBA-CAA-C3A	-2.94	106.92	113.47
82	UB	303	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	DE	1002	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	vK	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	qK	202	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
82	A5	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
84	FG	1001	CYC	C4D-C3D-C2D	-2.94	104.15	107.62
82	VE	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	SJ	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	K5	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
85	BN	838	BCR	C33-C5-C4	2.94	119.26	113.62
85	d6	405	BCR	C11-C10-C9	-2.94	123.12	127.31
82	VQ	202	PEB	OA-C1A-C2A	-2.94	123.84	126.17
82	YG	201	PEB	CAC-C2C-C1C	2.94	130.44	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FA	203	PEB	CHA-C4A-NA	-2.94	121.71	125.20
82	b1	202	PEB	CMD-C2D-C3D	2.94	134.21	130.06
82	HQ	202	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	CB	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
82	O9	203	PEB	C3B-C4B-NB	2.94	114.32	110.05
87	22	609	CLA	CHB-C4A-NA	2.94	128.57	124.51
85	I2	101	BCR	C15-C14-C13	-2.94	123.12	127.31
82	SP	201	PEB	CHA-C1B-NB	-2.94	118.79	124.93
87	cL	508	CLA	C3C-C4C-NC	-2.94	107.28	110.57
82	WE	203	PEB	C2A-C1A-NA	2.94	110.81	108.27
82	VF	201	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	cB	403	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	hO	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
84	BE	1001	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
84	DG	1001	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
82	CD	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	fK	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	FM	201	PEB	CBC-CAC-C2C	-2.94	104.47	112.63
82	TP	202	PEB	CAC-CBC-CGC	-2.94	107.28	113.60
82	TA	201	PEB	CAB-C3B-C4B	2.94	130.20	125.01
83	BM	302	PUB	CHA-C4A-NA	-2.94	110.01	113.72
85	HL	103	BCR	C20-C21-C22	-2.94	123.12	127.31
82	QO	201	PEB	CHB-C4B-NB	2.94	130.69	124.58
82	TA	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	A5	202	PEB	CAA-C3A-C4A	-2.94	105.13	112.67
87	c6	614	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
82	XP	201	PEB	CHC-C4C-NC	2.94	125.12	121.15
82	GP	202	PEB	C1C-CHB-C4B	2.94	134.87	128.28
82	QM	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	N5	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	qF	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
82	aJ	204	PEB	C2A-C1A-NA	2.94	110.80	108.27
82	gM	202	PEB	C2A-C1A-NA	2.94	110.80	108.27
82	qF	201	PEB	C3C-C4C-NC	2.94	110.98	108.33
84	K1	1001	CYC	CHB-C1B-NB	-2.94	119.75	126.06
82	DF	203	PEB	CMB-C2B-C1B	2.94	129.59	125.06
82	MK	203	PEB	OD-C4D-ND	-2.94	121.58	125.93
83	YA	302	PUB	CHA-C1B-NB	2.94	125.12	121.15
82	AA	202	PEB	OA-C1A-C2A	-2.94	123.84	126.17
82	AK	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
82	CM	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
84	H1	1001	CYC	C2A-C1A-NA	2.94	114.32	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	814	CLA	CHB-C4A-NA	2.94	128.57	124.51
82	CI	201	PEB	CHA-C1B-NB	-2.94	118.79	124.93
87	AN	840	CLA	C3B-C4B-NB	-2.94	107.79	110.52
82	mH	202	PEB	CMB-C2B-C1B	2.94	129.58	125.06
82	PB	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	Q1	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	e1	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	P5	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
82	fK	202	PEB	CAC-CBC-CGC	-2.93	107.29	113.60
82	cO	201	PEB	CAB-CBB-CGB	-2.93	107.29	113.60
87	CL	506	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
82	UE	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	gK	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	QM	202	PEB	C3B-C4B-NB	2.93	114.32	110.05
82	Q1	203	PEB	C3B-C4B-NB	2.93	114.32	110.05
82	HF	202	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
82	QP	201	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
82	HQ	203	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
82	gG	201	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
82	mE	201	PEB	OD-C4D-ND	-2.93	121.58	125.93
82	BB	202	PEB	CHC-C1D-ND	-2.93	110.01	113.72
82	N7	203	PEB	OD-C4D-C3D	-2.93	122.81	129.46
82	G5	202	PEB	CAA-C3A-C4A	-2.93	105.14	112.67
85	B2	838	BCR	C33-C5-C4	2.93	119.25	113.62
82	B7	202	PEB	C3C-C4C-NC	2.93	110.97	108.33
87	AN	825	CLA	CMB-C2B-C1B	-2.93	120.90	125.37
82	ZO	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
82	b4	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
82	YI	201	PEB	CHC-C4C-NC	2.93	125.12	121.15
82	gM	202	PEB	C3B-C4B-NB	2.93	114.32	110.05
82	OD	201	PEB	OD-C4D-C3D	-2.93	122.81	129.46
82	aJ	201	PEB	OD-C4D-C3D	-2.93	122.81	129.46
82	MM	203	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
82	zF	501	PEB	CAC-CBC-CGC	2.93	119.92	113.60
84	r3	1001	CYC	CMB-C2B-C1B	2.93	127.83	124.17
87	72	602	CLA	CHB-C4A-NA	2.93	128.57	124.51
82	i4	202	PEB	CHA-C1B-NB	-2.93	118.80	124.93
82	IJ	201	PEB	OD-C4D-C3D	-2.93	122.81	129.46
82	JJ	202	PEB	CAB-C3B-C4B	2.93	130.20	125.01
82	z8	202	PEB	CAB-C3B-C4B	2.93	130.20	125.01
82	qC	203	PEB	CAB-C3B-C4B	2.93	130.20	125.01
82	d1	202	PEB	CAB-CBB-CGB	-2.93	107.29	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IB	202	PEB	C3B-C4B-NB	2.93	114.31	110.05
87	2N	305	CLA	CHB-C4A-NA	2.93	128.57	124.51
83	A4	302	PUB	OD-C4D-ND	-2.93	121.59	125.93
82	m4	202	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
87	bL	616	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
85	BL	617	BCR	C8-C7-C6	2.93	135.44	127.20
87	B6	609	CLA	C3B-C4B-NB	-2.93	107.80	110.52
87	7N	603	CLA	O2D-CGD-CBD	2.93	116.48	111.27
82	PA	203	PEB	CHC-C4C-NC	2.93	125.12	121.15
84	L1	1001	CYC	CHB-C1B-C2B	2.93	132.76	126.95
82	CK	202	PEB	CAC-CBC-CGC	2.93	119.91	113.60
82	aE	201	PEB	CAB-CBB-CGB	-2.93	107.29	113.60
82	HE	1002	PEB	CAA-C3A-C4A	-2.93	105.14	112.67
82	JD	203	PEB	OA-C1A-C2A	-2.93	123.84	126.17
82	Y9	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	O5	203	PEB	OD-C4D-C3D	-2.93	122.82	129.46
82	NI	201	PEB	CHA-C1B-NB	-2.93	118.80	124.93
82	S9	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
87	CL	513	CLA	CMD-C2D-C1D	2.93	129.88	124.71
82	UA	202	PEB	CMB-C2B-C1B	2.93	129.58	125.06
87	L2	206	CLA	CHB-C1B-NB	2.93	127.36	124.26
82	MM	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	CQ	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	NQ	204	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	18	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	UM	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
82	gE	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
82	YH	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
82	wC	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
82	WP	201	PEB	OD-C4D-C3D	-2.93	122.82	129.46
82	AG	304	PEB	OA-C1A-C2A	-2.93	123.84	126.17
82	H9	202	PEB	CAB-C3B-C4B	2.93	130.19	125.01
87	B2	817	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
82	LA	203	PEB	OD-C4D-ND	-2.93	121.59	125.93
87	I2	103	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
82	X5	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	i4	201	PEB	CMB-C2B-C1B	2.93	129.58	125.06
82	CK	203	PEB	C3B-C4B-NB	2.93	114.31	110.05
82	VH	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
82	bH	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
87	A2	821	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
87	b6	607	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dG	201	PEB	CAC-C2C-C1C	2.93	130.43	125.76
82	HI	202	PEB	C3C-C4C-NC	2.93	110.97	108.33
82	LG	1002	PEB	OD-C4D-C3D	-2.93	122.82	129.46
87	82	301	CLA	C2A-C1A-CHA	2.93	128.98	123.86
83	xK	301	PUB	CBA-CAA-C3A	-2.93	108.54	112.98
82	aK	203	PEB	OA-C1A-C2A	-2.93	123.84	126.17
82	CQ	201	PEB	CAC-C2C-C1C	2.93	130.43	125.76
82	FM	201	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	b1	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
82	V9	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
84	BG	1001	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
82	cO	203	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	O4	201	PEB	CHC-C4C-NC	2.93	125.11	121.15
82	u8	203	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
82	U9	204	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
82	uK	201	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
84	K4	1001	CYC	C4A-C3A-C2A	-2.93	103.14	106.51
87	dL	409	CLA	CHB-C4A-NA	2.93	128.56	124.51
82	TH	202	PEB	CAA-C3A-C4A	2.93	120.19	112.67
82	T5	202	PEB	CAA-C3A-C4A	-2.93	105.15	112.67
87	AN	821	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
82	1C	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
91	A6	407	PHO	C4-C3-C5	2.93	120.20	115.27
82	L5	201	PEB	CHC-C4C-NC	2.93	125.11	121.15
87	RN	204	CLA	CHB-C4A-NA	2.93	128.56	124.51
87	A2	841	CLA	CHB-C4A-NA	2.93	128.56	124.51
82	TH	201	PEB	CBB-CAB-C3B	2.93	120.76	112.63
82	PD	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	UG	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	DO	1002	PEB	C1D-CHC-C4C	2.93	117.57	113.26
82	PI	201	PEB	CHA-C1B-NB	-2.93	118.81	124.93
82	LD	203	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	kM	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
87	KN	103	CLA	CAA-C2A-C3A	-2.93	106.94	114.26
87	bL	620	CLA	CHB-C4A-NA	2.93	128.56	124.51
92	ML	101	LMG	O8-C28-C29	2.93	121.09	111.91
87	8N	302	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
84	L1	1001	CYC	C4A-C3A-C2A	-2.93	103.15	106.51
82	L9	202	PEB	C3C-C4C-NC	2.93	110.97	108.33
82	iE	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
88	A2	843	LHG	O8-C23-C24	2.93	121.09	111.91
82	hG	203	PEB	CHC-C4C-NC	2.93	125.11	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XI	201	PEB	CHA-C1B-NB	-2.93	118.81	124.93
87	AN	841	CLA	CHB-C4A-NA	2.93	128.56	124.51
87	bL	614	CLA	C3B-C4B-NB	-2.93	107.80	110.52
82	AF	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
82	CK	203	PEB	OD-C4D-ND	-2.93	121.59	125.93
82	jG	202	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
82	aG	201	PEB	CAB-CBB-CGB	-2.93	107.31	113.60
82	iM	202	PEB	CAB-C3B-C4B	2.93	130.19	125.01
82	lG	202	PEB	C3B-C4B-NB	2.93	114.31	110.05
87	B6	610	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
82	YI	202	PEB	OD-C4D-ND	-2.93	121.60	125.93
82	CK	203	PEB	C1C-CHB-C4B	2.93	134.84	128.28
82	WO	201	PEB	C1C-CHB-C4B	2.93	134.84	128.28
82	QQ	201	PEB	C2A-C1A-NA	2.93	110.80	108.27
82	vC	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
87	82	305	CLA	CED-O2D-CGD	2.93	122.55	115.94
84	LH	1001	CYC	CHD-C1D-C2D	2.93	134.67	127.49
82	cH	201	PEB	CHB-C4B-C3B	-2.93	118.55	125.32
82	DA	202	PEB	CMB-C2B-C1B	2.93	129.57	125.06
82	eK	201	PEB	CMB-C2B-C1B	2.93	129.57	125.06
82	cK	203	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
82	GD	202	PEB	C4B-C3B-C2B	-2.93	103.55	106.78
82	ND	204	PEB	C4B-C3B-C2B	-2.93	103.55	106.78
82	GK	201	PEB	C1C-NC-C4C	-2.93	104.39	109.60
82	nK	202	PEB	OD-C4D-C3D	-2.93	122.83	129.46
82	HP	201	PEB	CHC-C4C-NC	2.93	125.11	121.15
82	zK	501	PEB	CAC-CBC-CGC	2.93	119.90	113.60
87	32	304	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
82	pF	202	PEB	CMC-C3C-C4C	2.93	130.16	127.06
82	GI	202	PEB	CHA-C1B-NB	-2.92	118.81	124.93
82	RI	201	PEB	CHA-C1B-NB	-2.92	118.81	124.93
82	N4	1002	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
82	X7	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
82	A9	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
87	nL	101	CLA	CHB-C4A-NA	2.92	128.56	124.51
87	7N	602	CLA	CHB-C4A-NA	2.92	128.56	124.51
82	X5	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
82	QE	203	PEB	C2A-C1A-NA	2.92	110.79	108.27
82	FM	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
82	eG	201	PEB	OD-C4D-ND	-2.92	121.60	125.93
83	Z5	302	PUB	OD-C4D-ND	-2.92	121.60	125.93
82	L7	201	PEB	C4C-C3C-C2C	-2.92	104.80	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	E5	202	PEB	CAA-C3A-C4A	-2.92	105.17	112.67
82	EI	201	PEB	CHA-C1B-NB	-2.92	118.82	124.93
82	bG	201	PEB	CHC-C4C-NC	2.92	125.11	121.15
87	CL	507	CLA	CHB-C4A-NA	2.92	128.56	124.51
82	Y9	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
82	UP	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
82	aE	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
87	A2	841	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
87	B2	832	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
82	JB	202	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	Z9	301	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	kF	203	PEB	CHA-C4A-NA	-2.92	121.73	125.20
82	fF	202	PEB	CAC-CBC-CGC	-2.92	107.31	113.60
82	BQ	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
82	ZO	201	PEB	CHC-C1D-ND	-2.92	110.03	113.72
82	DD	201	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	g1	201	PEB	OD-C4D-C3D	-2.92	122.84	129.46
98	BN	837	PQN	C11-C3-C4	-2.92	115.37	118.50
87	b6	610	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
82	dH	202	PEB	CAB-CBB-CGB	-2.92	107.31	113.60
82	K7	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
82	QB	202	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	fJ	202	PEB	C3C-C4C-NC	2.92	110.96	108.33
82	VF	202	PEB	CHB-C4B-NB	2.92	130.66	124.58
82	QE	201	PEB	C1C-NC-C4C	-2.92	104.40	109.60
87	C6	517	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
85	B2	843	BCR	C7-C8-C9	-2.92	121.82	126.23
82	PM	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
82	j4	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
84	K4	1001	CYC	C2A-C1A-NA	2.92	114.30	110.05
82	hE	203	PEB	CHC-C4C-NC	2.92	125.10	121.15
82	fE	201	PEB	OD-C4D-ND	-2.92	121.60	125.93
82	pK	201	PEB	OD-C4D-ND	-2.92	121.60	125.93
83	BJ	302	PUB	OD-C4D-ND	-2.92	121.60	125.93
82	B7	202	PEB	OA-C1A-NA	2.92	128.48	124.94
82	U4	201	PEB	CMA-C2A-C1A	-2.92	106.10	112.40
82	T4	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
82	Q9	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
87	b6	605	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
82	K5	202	PEB	CAA-C3A-C4A	-2.92	105.17	112.67
85	HL	103	BCR	C15-C14-C13	-2.92	123.14	127.31
82	yC	203	PEB	CHA-C4A-NA	-2.92	121.73	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	T1	201	PEB	CBB-CAB-C3B	2.92	120.75	112.63
85	cL	518	BCR	C33-C5-C6	-2.92	121.25	124.53
96	fL	102	HEM	CHA-C4D-ND	2.92	127.98	124.37
82	bG	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
82	iO	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
82	YP	502	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	IB	201	PEB	CMB-C2B-C1B	2.92	129.56	125.06
87	AN	839	CLA	CMB-C2B-C3B	2.92	133.66	126.59
82	BA	202	PEB	OA-C1A-NA	2.92	128.48	124.94
82	OQ	201	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	D7	203	PEB	CHB-C1C-NC	-2.92	118.63	125.32
82	S5	201	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
82	OH	203	PEB	C3B-C4B-NB	2.92	114.30	110.05
82	lE	203	PEB	C1D-CHC-C4C	-2.92	108.95	113.26
82	GB	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
82	hM	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
82	RP	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
82	SH	203	PEB	CMB-C2B-C1B	2.92	129.56	125.06
82	Y7	303	PEB	CHC-C4C-NC	2.92	125.10	121.15
87	2N	308	CLA	C2B-C1B-NB	2.92	112.19	110.23
82	II	201	PEB	CHA-C1B-NB	-2.92	118.82	124.93
82	NM	202	PEB	CHA-C1B-NB	-2.92	118.82	124.93
82	KE	201	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	AJ	302	PEB	OD-C4D-C3D	-2.92	122.84	129.46
82	WF	203	PEB	OA-C1A-C2A	-2.92	123.85	126.17
82	UA	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
88	BL	615	LHG	O8-C23-C24	2.92	121.07	111.91
82	c4	203	PEB	OD-C4D-ND	-2.92	121.60	125.93
82	h4	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
82	eH	201	PEB	OD-C4D-ND	-2.92	121.60	125.93
87	JN	101	CLA	C3B-C4B-NB	-2.92	107.81	110.52
94	A6	410	PL9	C37-C38-C39	-2.92	120.63	127.66
82	ZJ	201	PEB	CHB-C1C-NC	-2.92	118.63	125.32
82	CK	203	PEB	C4C-C3C-C2C	-2.92	104.81	107.50
82	aM	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
82	VG	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	Q7	202	PEB	CBA-CAA-C3A	-2.92	106.97	113.47
87	B2	812	CLA	CHB-C4A-NA	2.92	128.55	124.51
87	cL	513	CLA	CHB-C4A-NA	2.92	128.55	124.51
82	KD	201	PEB	CHC-C4C-NC	2.92	125.10	121.15
82	LB	201	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
82	BP	201	PEB	C1B-C2B-C3B	-2.92	103.16	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	DL	404	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
82	wC	203	PEB	OD-C4D-C3D	-2.92	122.85	129.46
82	UG	203	PEB	OA-C1A-C2A	-2.92	123.85	126.17
82	VO	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
87	BL	605	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
82	QB	204	PEB	CHB-C4B-C3B	-2.92	118.57	125.32
82	V5	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
83	xK	305	PUB	C2C-C1C-NC	2.92	114.30	110.05
82	dM	203	PEB	C1D-CHC-C4C	2.92	117.56	113.26
83	AO	302	PUB	OD-C4D-ND	-2.92	121.61	125.93
82	NB	203	PEB	C4C-C3C-C2C	-2.92	104.81	107.50
82	w8	203	PEB	OD-C4D-C3D	-2.92	122.85	129.46
82	mO	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
82	DM	202	PEB	CAA-C3A-C2A	-2.92	106.97	114.26
82	f4	202	PEB	CHC-C1D-ND	-2.92	110.03	113.72
84	FH	1001	CYC	C4A-C3A-C2A	-2.92	103.16	106.51
82	AM	302	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	wK	302	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	HD	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	QH	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	HK	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	JM	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	VQ	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	aH	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
84	FO	1001	CYC	CAB-C3B-C4B	2.92	125.99	121.38
87	22	609	CLA	CHB-C1B-NB	2.92	127.35	124.26
82	fH	202	PEB	OA-C1A-C2A	-2.92	123.85	126.17
82	kG	201	PEB	CAC-CBC-CGC	-2.92	107.32	113.60
82	TI	202	PEB	CHA-C1B-NB	-2.92	118.83	124.93
82	q8	203	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	CP	203	PEB	OD-C4D-ND	-2.92	121.61	125.93
87	62	304	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
82	GK	202	PEB	OD-C4D-C3D	-2.92	122.85	129.46
82	qF	202	PEB	CAB-CBB-CGB	-2.92	107.33	113.60
87	IN	103	CLA	CHB-C4A-NA	2.92	128.55	124.51
82	RQ	203	PEB	C1C-CHB-C4B	2.92	134.82	128.28
82	WK	201	PEB	C3C-C4C-NC	2.92	110.96	108.33
84	DH	1001	CYC	C4D-C3D-C2D	-2.92	104.17	107.62
84	I1	1001	CYC	CHD-C1D-C2D	2.92	134.65	127.49
82	j1	202	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	LA	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
82	fK	202	PEB	OD-C4D-ND	-2.92	121.61	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BL	622	CLA	O2D-CGD-CBD	2.92	116.45	111.27
82	QK	202	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
87	B6	608	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
82	KQ	201	PEB	CHC-C4C-NC	2.92	125.10	121.15
82	A1	302	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
82	V1	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
82	I7	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
82	N9	201	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
82	vF	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
82	XD	201	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	GM	202	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	JP	202	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	SP	201	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	UK	202	PEB	CHC-C1D-ND	-2.92	110.03	113.72
82	kE	201	PEB	CAC-CBC-CGC	-2.92	107.33	113.60
87	A2	823	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
82	c1	201	PEB	CHB-C4B-C3B	-2.92	118.57	125.32
82	M7	201	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
82	cK	202	PEB	C3D-C4D-ND	2.92	112.98	107.26
82	UD	201	PEB	CHA-C1B-NB	-2.92	118.83	124.93
82	VI	201	PEB	CHA-C1B-NB	-2.92	118.83	124.93
82	AP	203	PEB	CMB-C2B-C1B	2.92	129.55	125.06
83	A4	302	PUB	OA-C1A-NA	-2.92	121.61	125.93
82	c4	201	PEB	CAB-CBB-CGB	-2.92	107.33	113.60
82	OA	202	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	NM	202	PEB	C3B-C4B-NB	2.92	114.29	110.05
82	WM	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
84	M1	201	CYC	CHB-C1B-NB	-2.92	119.80	126.06
82	PK	201	PEB	CHC-C1D-ND	-2.92	110.04	113.72
82	jE	201	PEB	CHA-C1B-NB	-2.92	118.83	124.93
82	jG	201	PEB	CHA-C1B-NB	-2.92	118.83	124.93
87	B2	819	CLA	CHB-C4A-NA	2.92	128.54	124.51
92	bL	624	LMG	O8-C28-C29	2.91	121.06	111.91
82	FB	201	PEB	C3B-C4B-NB	2.91	114.29	110.05
82	eH	202	PEB	OD-C4D-C3D	-2.91	122.86	129.46
82	SK	203	PEB	CMC-C3C-C4C	2.91	130.15	127.06
82	OP	202	PEB	CHB-C4B-C3B	-2.91	118.58	125.32
85	BN	843	BCR	C7-C8-C9	-2.91	121.83	126.23
82	LQ	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
87	bL	617	CLA	CHB-C4A-NA	2.91	128.54	124.51
82	gK	202	PEB	CHA-C1B-NB	-2.91	118.84	124.93
82	Z5	304	PEB	CHC-C4C-NC	2.91	125.09	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	M9	303	PUB	CMA-C2A-C1A	2.91	128.25	121.39
87	8N	306	CLA	CED-O2D-CGD	2.91	122.53	115.94
82	YF	203	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	TO	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	jK	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	eE	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
82	GJ	202	PEB	CHC-C1D-ND	-2.91	110.04	113.72
82	c4	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
82	I9	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
84	L4	1001	CYC	CAB-C3B-C4B	2.91	125.98	121.38
84	DG	1001	CYC	CHB-C1B-NB	-2.91	119.80	126.06
82	PO	202	PEB	CAB-C3B-C4B	2.91	130.16	125.01
82	VG	201	PEB	OD-C4D-ND	-2.91	121.61	125.93
82	bE	201	PEB	CHC-C4C-NC	2.91	125.09	121.15
82	DA	202	PEB	CHA-C4A-NA	2.91	128.67	125.20
82	PG	202	PEB	C3B-C4B-NB	2.91	114.29	110.05
82	C5	202	PEB	C3B-C4B-NB	2.91	114.29	110.05
84	BE	1002	CYC	C2A-C1A-NA	2.91	114.29	110.05
82	NA	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
82	EB	501	PEB	C1B-C2B-C3B	-2.91	103.16	106.51
82	AM	302	PEB	C1B-C2B-C3B	-2.91	103.16	106.51
82	L7	203	PEB	CMB-C2B-C1B	2.91	129.55	125.06
82	vF	201	PEB	CAA-C3A-C2A	-2.91	106.98	114.26
82	e1	202	PEB	OD-C4D-C3D	-2.91	122.86	129.46
82	gM	202	PEB	CAB-C3B-C4B	2.91	130.16	125.01
87	B2	814	CLA	CHB-C4A-NA	2.91	128.54	124.51
82	KF	201	PEB	CHA-C1B-NB	-2.91	118.84	124.93
82	TF	202	PEB	CHA-C1B-NB	-2.91	118.84	124.93
82	i1	202	PEB	OD-C4D-ND	-2.91	121.61	125.93
82	bH	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	K9	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
82	1C	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
82	MF	201	PEB	C3B-C4B-NB	2.91	114.29	110.05
82	a1	201	PEB	C3B-C4B-NB	2.91	114.29	110.05
82	ZI	401	PEB	CHC-C4C-NC	2.91	125.09	121.15
82	XK	201	PEB	CHB-C1C-C2C	-2.91	120.58	127.15
87	b6	610	CLA	C3B-C4B-NB	-2.91	107.81	110.52
82	HI	202	PEB	C1C-NC-C4C	-2.91	104.42	109.60
82	QE	203	PEB	C1B-C2B-C3B	-2.91	103.16	106.51
82	P7	201	PEB	CAB-CBB-CGB	-2.91	107.34	113.60
82	AA	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	L7	202	PEB	OD-C4D-ND	-2.91	121.62	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	N5	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	KI	202	PEB	CHA-C1B-NB	-2.91	118.84	124.93
82	E9	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
82	YP	501	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	QO	201	PEB	OA-C1A-C2A	-2.91	123.86	126.17
87	B2	807	CLA	C3B-C4B-NB	-2.91	107.81	110.52
82	QF	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	u8	203	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	AH	305	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	hK	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
87	62	307	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
82	LA	201	PEB	CHA-C1B-C2B	2.91	132.39	124.90
82	A7	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
85	KN	104	BCR	C11-C12-C13	-2.91	118.24	126.42
82	e4	203	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	K5	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	QI	201	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	YM	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	a4	203	PEB	CHC-C1D-ND	-2.91	110.04	113.72
82	UD	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	dE	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	gM	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	T5	202	PEB	OD-C4D-C3D	-2.91	122.87	129.46
82	W5	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	z8	201	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	cM	201	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	qC	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
83	Z9	302	PUB	CMA-C2A-C1A	2.91	128.24	121.39
84	NE	201	CYC	CHA-C4D-C3D	-2.91	120.58	127.15
82	RD	201	PEB	OD-C4D-C3D	-2.91	122.87	129.46
82	TK	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	bK	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	g4	202	PEB	CHA-C1B-NB	-2.91	118.85	124.93
82	OE	203	PEB	OD-C4D-ND	-2.91	121.62	125.93
87	A2	825	CLA	CMB-C2B-C1B	-2.91	120.94	125.37
87	b6	614	CLA	C3B-C4B-NB	-2.91	107.82	110.52
82	PG	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	QG	203	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	tC	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	X9	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
82	E5	202	PEB	OD-C4D-C3D	-2.91	122.87	129.46
82	kF	201	PEB	OD-C4D-C3D	-2.91	122.87	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cF	203	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	iJ	201	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	jM	201	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	MM	203	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	I5	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	dG	203	PEB	CHC-C4C-NC	2.91	125.08	121.15
87	A2	839	CLA	CMB-C2B-C3B	2.91	133.63	126.59
82	S7	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
82	LM	202	PEB	C1C-CHB-C4B	-2.91	121.76	128.28
82	U5	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	qK	203	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	ID	202	PEB	OD-C4D-C3D	-2.91	122.87	129.46
82	PE	202	PEB	CMC-C3C-C4C	-2.91	123.98	127.06
82	f4	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	ZO	201	PEB	C1D-CHC-C4C	-2.91	108.97	113.26
82	aK	203	PEB	CHA-C1B-C2B	2.91	132.38	124.90
84	NO	1001	CYC	C4A-C3A-C2A	-2.91	103.17	106.51
82	YF	201	PEB	C4C-C3C-C2C	-2.91	104.82	107.50
82	h4	202	PEB	CMB-C2B-C1B	2.91	129.54	125.06
87	b6	604	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
82	HP	201	PEB	CHA-C1B-NB	-2.91	118.85	124.93
84	CG	1001	CYC	C1B-NB-C4B	-2.91	106.97	110.67
82	jJ	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
84	CG	1001	CYC	C1A-C2A-C3A	-2.91	103.56	106.78
82	EA	201	PEB	CMD-C2D-C3D	2.91	134.16	130.06
82	cF	203	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	TB	202	PEB	OD-C4D-C3D	-2.91	122.87	129.46
82	OK	202	PEB	OD-C4D-C3D	-2.91	122.87	129.46
87	C6	514	CLA	C3B-C4B-NB	-2.91	107.82	110.52
82	BD	203	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	BA	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	fH	203	PEB	OD-C4D-C3D	-2.91	122.87	129.46
82	YH	201	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	LP	202	PEB	CAC-CBC-CGC	-2.91	107.35	113.60
83	AO	302	PUB	CHC-C1D-ND	-2.91	110.05	113.72
82	XQ	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	aB	202	PEB	OA-C1A-C2A	-2.91	123.86	126.17
83	Z5	302	PUB	CMB-C2B-C3B	2.91	131.89	125.61
84	KO	1001	CYC	C4D-CHA-C1A	2.91	134.80	128.28
103	8N	310	ZEX	C1-C2-C3	-2.91	107.08	113.64
82	y8	203	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	kE	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	LH	1002	CYC	C4A-C3A-C2A	-2.91	103.17	106.51
82	aO	203	PEB	CAB-CBB-CGB	2.91	119.86	113.60
87	d6	406	CLA	C3B-C4B-NB	-2.91	107.82	110.52
84	w3	1001	CYC	C2D-C1D-ND	2.91	111.48	107.40
82	AE	301	PEB	OD-C4D-ND	-2.91	121.62	125.93
82	LD	201	PEB	C3C-C4C-NC	2.91	110.95	108.33
92	b6	620	LMG	C4-C3-C2	2.91	115.90	110.82
84	x3	1001	CYC	CAD-C3D-C4D	2.91	130.39	125.76
82	I5	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
82	QK	201	PEB	C2A-C1A-NA	-2.91	105.77	108.27
82	iK	202	PEB	CHC-C1D-ND	-2.91	110.05	113.72
85	cL	503	BCR	C15-C14-C13	-2.91	123.16	127.31
87	AN	839	CLA	CHB-C4A-NA	2.91	128.53	124.51
84	LH	1002	CYC	CHB-C1B-C2B	2.91	132.71	126.95
82	CB	202	PEB	C3D-C4D-ND	2.91	112.96	107.26
82	tC	202	PEB	CHB-C4B-C3B	2.91	132.04	125.32
82	AA	202	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
82	WI	202	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
82	uF	203	PEB	OD-C4D-ND	-2.91	121.63	125.93
82	UE	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
82	XJ	201	PEB	CMC-C3C-C4C	2.91	130.14	127.06
84	V3	1001	CYC	CAD-C3D-C4D	2.91	130.39	125.76
82	OM	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
82	cK	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
84	FO	1001	CYC	CAB-C3B-C2B	2.91	132.50	127.53
84	D1	1001	CYC	C4D-C3D-C2D	-2.91	104.19	107.62
82	e4	201	PEB	CHB-C4B-C3B	-2.91	118.60	125.32
82	Z4	201	PEB	CHC-C1D-ND	-2.90	110.05	113.72
82	lJ	203	PEB	CHA-C1B-NB	-2.90	118.86	124.93
82	C5	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
82	DK	203	PEB	CMB-C2B-C1B	2.90	129.54	125.06
82	GA	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	KJ	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
85	A2	848	BCR	C12-C13-C14	-2.90	114.48	118.94
82	IQ	201	PEB	CAB-C3B-C2B	-2.90	122.47	127.88
95	a6	602	DGD	C2G-O2G-C1B	-2.90	110.64	117.79
82	aO	203	PEB	CHC-C1D-ND	-2.90	110.05	113.72
82	RA	203	PEB	OD-C4D-C3D	-2.90	122.88	129.46
85	CL	516	BCR	C33-C5-C6	-2.90	121.27	124.53
82	HP	201	PEB	CAB-C3B-C4B	2.90	130.15	125.01
82	AI	201	PEB	CHA-C1B-NB	-2.90	118.86	124.93
82	gF	202	PEB	CHA-C1B-NB	-2.90	118.86	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NB	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
87	6N	606	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
82	YE	201	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
82	IJ	203	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
82	S1	202	PEB	C2A-C1A-NA	2.90	110.78	108.27
82	b1	201	PEB	C2A-C1A-NA	2.90	110.78	108.27
82	uF	202	PEB	C2A-C1A-NA	2.90	110.78	108.27
84	V3	1001	CYC	CBA-CAA-C2A	-2.90	104.56	112.63
83	A4	302	PUB	CHC-C1D-ND	-2.90	110.05	113.72
82	HI	203	PEB	OD-C4D-ND	-2.90	121.63	125.93
82	AO	305	PEB	OD-C4D-ND	-2.90	121.63	125.93
82	S9	201	PEB	CAA-C3A-C4A	-2.90	105.22	112.67
82	A5	202	PEB	OD-C4D-C3D	-2.90	122.88	129.46
82	U5	201	PEB	OD-C4D-C3D	-2.90	122.88	129.46
82	fM	203	PEB	C3B-C4B-NB	2.90	114.27	110.05
87	BN	815	CLA	CHB-C4A-NA	2.90	128.53	124.51
82	mG	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
83	xF	306	PUB	OD-C4D-ND	-2.90	121.63	125.93
82	RF	202	PEB	C1D-CHC-C4C	2.90	117.54	113.26
87	42	607	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
82	SI	201	PEB	CHC-C4C-NC	2.90	125.08	121.15
82	lO	201	PEB	CHC-C4C-NC	2.90	125.08	121.15
82	wC	202	PEB	OD-C4D-C3D	-2.90	122.88	129.46
82	AB	501	PEB	C2A-C1A-NA	2.90	110.78	108.27
82	aF	203	PEB	C2A-C1A-NA	2.90	110.78	108.27
82	UJ	201	PEB	CHA-C1B-NB	-2.90	118.86	124.93
82	kG	201	PEB	CAB-C3B-C4B	2.90	130.14	125.01
87	A2	824	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
87	7N	610	CLA	CHB-C4A-NA	2.90	128.53	124.51
82	QE	203	PEB	CMB-C2B-C1B	2.90	129.53	125.06
82	e1	201	PEB	CBA-CAA-C3A	-2.90	107.01	113.47
82	xF	303	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	kH	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	bO	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	UE	201	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	hG	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	L7	201	PEB	CHA-C1B-C2B	2.90	132.36	124.90
85	AN	848	BCR	C35-C13-C12	2.90	122.65	118.08
82	GM	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
82	GM	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
82	AE	301	PEB	C1C-CHB-C4B	-2.90	121.78	128.28
82	cM	202	PEB	C3B-C4B-NB	2.90	114.27	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YB	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	OI	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	R5	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
87	2N	312	CLA	CHB-C4A-NA	2.90	128.52	124.51
82	PE	201	PEB	CAB-C3B-C4B	2.90	130.14	125.01
83	M5	302	PUB	CMB-C2B-C3B	2.90	131.88	125.61
84	u3	1001	CYC	C2D-C1D-ND	2.90	111.48	107.40
82	jJ	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
82	aK	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
92	j6	101	LMG	O1-C7-C8	-2.90	103.90	110.90
82	KQ	202	PEB	CHC-C1D-ND	-2.90	110.06	113.72
82	SE	202	PEB	OA-C1A-C2A	-2.90	123.87	126.17
82	D5	203	PEB	OA-C1A-C2A	-2.90	123.87	126.17
85	AN	847	BCR	C15-C16-C17	-2.90	117.53	123.47
82	J1	1002	PEB	CAB-CBB-CGB	-2.90	107.36	113.60
82	YP	502	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	xC	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	FA	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	R9	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	bF	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	eO	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	MP	202	PEB	CMB-C2B-C1B	2.90	129.53	125.06
82	JA	201	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	K5	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	V5	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	OM	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
82	eE	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
82	RA	201	PEB	CHA-C1B-NB	-2.90	118.87	124.93
85	k6	102	BCR	C15-C16-C17	-2.90	117.53	123.47
82	DI	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
82	H5	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
84	HH	1001	CYC	C2A-C1A-NA	2.90	114.27	110.05
87	bL	618	CLA	CMB-C2B-C3B	2.90	133.61	126.59
87	bL	613	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
82	MP	203	PEB	CMB-C2B-C1B	2.90	129.53	125.06
82	uK	201	PEB	CHC-C4C-NC	2.90	125.07	121.15
82	fH	203	PEB	CHB-C1C-C2C	-2.90	120.61	127.15
82	YK	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
82	kK	201	PEB	OD-C4D-C3D	-2.90	122.89	129.46
82	UM	203	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	xK	304	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	mO	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	FE	1002	CYC	C4D-C3D-C2D	-2.90	104.19	107.62
82	MF	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
82	eG	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
87	22	601	CLA	CHC-C4B-NB	2.90	127.33	124.26
82	U7	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
87	7N	602	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
82	T5	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	w8	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
82	LD	202	PEB	CHB-C1C-C2C	-2.90	120.61	127.15
82	WG	201	PEB	CBA-CAA-C3A	-2.90	107.01	113.47
84	L3	1001	CYC	C2D-C1D-ND	2.90	111.47	107.40
92	bL	623	LMG	C7-O1-C1	-2.90	108.08	113.74
82	M5	304	PEB	CHC-C4C-NC	2.90	125.07	121.15
82	gH	203	PEB	CAC-C2C-C1C	2.90	130.38	125.76
82	cH	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	TJ	202	PEB	CAB-C3B-C4B	2.90	130.13	125.01
82	ZM	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
82	BD	202	PEB	CHA-C1B-NB	-2.90	118.87	124.93
82	ZG	203	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	i4	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
82	N5	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
82	V1	202	PEB	CMB-C2B-C1B	2.90	129.53	125.06
82	SK	203	PEB	CHA-C4A-NA	2.90	128.65	125.20
95	DL	408	DGD	O2G-C1B-C2B	2.90	117.75	111.50
82	T1	201	PEB	CHC-C4C-NC	2.90	125.07	121.15
82	tK	202	PEB	CHB-C1C-C2C	-2.90	120.61	127.15
103	82	310	ZEX	C1-C2-C3	-2.90	107.10	113.64
96	E6	101	HEM	C1B-NB-C4B	2.90	108.06	105.07
82	zC	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
83	AJ	303	PUB	OD-C4D-ND	-2.90	121.64	125.93
82	eH	201	PEB	CBA-CAA-C3A	-2.90	107.02	113.47
82	j1	201	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	jF	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
87	4N	607	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
82	LD	203	PEB	CHC-C4C-NC	2.90	125.07	121.15
82	FJ	201	PEB	CHA-C1B-C2B	2.90	132.35	124.90
82	F7	202	PEB	CHC-C1D-ND	-2.90	110.06	113.72
82	SI	202	PEB	CHA-C1B-NB	-2.90	118.88	124.93
82	D4	1002	PEB	C1D-CHC-C4C	2.90	117.53	113.26
82	FI	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
82	iO	201	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
84	CO	1001	CYC	C4A-C3A-C2A	-2.90	103.18	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	P5	202	PEB	OD-C4D-C3D	-2.90	122.90	129.46
82	lK	203	PEB	C1C-CHB-C4B	2.90	134.78	128.28
82	aF	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
82	HB	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
82	JD	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
95	BL	614	DGD	O6D-C5D-C4D	-2.90	104.44	109.69
87	C6	510	CLA	C3B-C4B-NB	-2.90	107.83	110.52
82	KJ	201	PEB	CHB-C1C-C2C	-2.90	120.62	127.15
92	J6	102	LMG	O1-C7-C8	-2.90	103.91	110.90
82	PE	202	PEB	OD-C4D-ND	-2.90	121.64	125.93
82	mK	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
82	iM	202	PEB	CHA-C1B-NB	-2.90	118.88	124.93
82	UO	201	PEB	CHC-C4C-NC	2.89	125.07	121.15
82	WD	202	PEB	C1B-C2B-C3B	-2.89	103.18	106.51
82	kH	203	PEB	CMC-C3C-C4C	2.89	130.13	127.06
82	y8	203	PEB	C3B-C4B-NB	2.89	114.26	110.05
82	aH	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
85	A2	848	BCR	C35-C13-C12	2.89	122.64	118.08
82	QK	202	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
82	q8	202	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
82	CF	202	PEB	CAC-CBC-CGC	2.89	119.83	113.60
82	fF	202	PEB	OD-C4D-ND	-2.89	121.64	125.93
82	M9	305	PEB	C1D-CHC-C4C	-2.89	108.99	113.26
82	GB	203	PEB	OD-C4D-C3D	-2.89	122.90	129.46
84	KG	202	CYC	CHA-C4D-C3D	-2.89	120.62	127.15
82	MQ	202	PEB	CHC-C4C-NC	2.89	125.07	121.15
82	FA	202	PEB	CHC-C1D-ND	-2.89	110.06	113.72
82	RM	202	PEB	CHC-C1D-ND	-2.89	110.06	113.72
82	TO	201	PEB	CAC-C2C-C1C	2.89	130.37	125.76
82	vF	202	PEB	CAC-C2C-C1C	2.89	130.37	125.76
82	PE	202	PEB	C3B-C4B-NB	2.89	114.26	110.05
82	mF	201	PEB	OD-C4D-ND	-2.89	121.64	125.93
82	KA	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	KJ	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	H7	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	S5	201	PEB	OD-C4D-C3D	-2.89	122.91	129.46
82	ID	201	PEB	CAB-C3B-C2B	-2.89	122.49	127.88
82	PG	201	PEB	CMC-C3C-C4C	2.89	130.13	127.06
82	OI	202	PEB	CMC-C3C-C4C	2.89	130.13	127.06
85	H6	101	BCR	C10-C11-C12	-2.89	114.19	123.22
87	A2	818	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
82	bE	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	uF	202	PEB	CHC-C4C-NC	2.89	125.06	121.15
82	ZB	202	PEB	CHA-C1B-NB	-2.89	118.88	124.93
82	TQ	203	PEB	CHA-C1B-NB	-2.89	118.88	124.93
82	Z9	304	PEB	C1D-CHC-C4C	-2.89	108.99	113.26
82	HA	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	SJ	203	PEB	CMB-C2B-C1B	2.89	129.52	125.06
82	m1	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
82	Y5	203	PEB	CMB-C2B-C1B	2.89	129.52	125.06
82	U7	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
82	V4	202	PEB	C1C-CHB-C4B	2.89	134.77	128.28
82	BJ	301	PEB	C3B-C4B-NB	2.89	114.26	110.05
84	N1	1001	CYC	C1B-C2B-C3B	-2.89	104.85	107.87
82	WJ	202	PEB	CBA-CAA-C3A	-2.89	107.03	113.47
82	h1	201	PEB	CAC-C2C-C1C	2.89	130.37	125.76
82	LQ	203	PEB	CHC-C4C-NC	2.89	125.06	121.15
82	F7	202	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
82	T9	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
82	CB	201	PEB	C2A-C1A-NA	2.89	110.77	108.27
82	fO	202	PEB	OD-C4D-ND	-2.89	121.65	125.93
82	TE	201	PEB	CAC-CBC-CGC	-2.89	107.38	113.60
82	LE	1002	PEB	OD-C4D-C3D	-2.89	122.91	129.46
82	OF	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
82	YJ	202	PEB	C1D-CHC-C4C	-2.89	108.99	113.26
82	hF	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
82	iO	201	PEB	CMB-C2B-C1B	2.89	129.52	125.06
82	VO	202	PEB	C3C-C4C-NC	2.89	110.94	108.33
82	QB	203	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	A4	305	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	WJ	202	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
84	LE	1001	CYC	C1A-C2A-C3A	-2.89	103.58	106.78
82	f1	203	PEB	OD-C4D-C3D	-2.89	122.91	129.46
82	NJ	202	PEB	CHB-C4B-NB	-2.89	118.56	124.58
82	j1	201	PEB	CHB-C4B-C3B	-2.89	118.63	125.32
82	t8	202	PEB	CHB-C4B-C3B	2.89	132.00	125.32
82	FA	203	PEB	CAC-C2C-C1C	2.89	130.37	125.76
82	mO	201	PEB	CHC-C1D-ND	-2.89	110.07	113.72
82	nF	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
91	D6	404	PHO	CGD-CBD-CAD	-2.89	101.37	110.73
82	NO	1002	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	BP	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	EJ	202	PEB	OD-C4D-ND	-2.89	121.65	125.93
82	gB	203	PEB	OD-C4D-ND	-2.89	121.65	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	nK	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
87	72	604	CLA	CHB-C4A-NA	2.89	128.51	124.51
82	FJ	201	PEB	CAB-CBB-CGB	-2.89	107.38	113.60
82	hG	202	PEB	CMB-C2B-C1B	2.89	129.51	125.06
87	B2	819	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
82	LD	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
82	gK	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
82	U5	203	PEB	CAC-C2C-C1C	2.89	130.37	125.76
85	L2	201	BCR	C20-C19-C18	-2.89	118.30	126.42
82	KE	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
87	c6	606	CLA	C3B-C4B-NB	-2.89	107.83	110.52
82	OJ	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
82	A7	202	PEB	OD-C4D-ND	-2.89	121.65	125.93
83	xF	301	PUB	OA-C1A-NA	-2.89	121.65	125.93
82	kG	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	VD	201	PEB	C2A-C1A-NA	2.89	110.76	108.27
82	RB	201	PEB	OD-C4D-C3D	-2.89	122.91	129.46
82	V5	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
82	CF	203	PEB	C4C-C3C-C2C	-2.89	104.83	107.50
82	PM	201	PEB	C4C-C3C-C2C	-2.89	104.83	107.50
82	e4	202	PEB	CHA-C1B-NB	-2.89	118.89	124.93
82	QJ	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
82	x8	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
82	f1	203	PEB	CHB-C1C-C2C	-2.89	120.63	127.15
82	IM	203	PEB	CMB-C2B-C1B	2.89	129.51	125.06
82	vK	201	PEB	CAA-C3A-C2A	-2.89	107.04	114.26
82	WK	203	PEB	OA-C1A-C2A	-2.89	123.88	126.17
82	UI	202	PEB	CHA-C1B-NB	-2.89	118.89	124.93
82	NA	202	PEB	C1C-NC-C4C	-2.89	104.46	109.60
82	NE	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	K5	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
82	jH	201	PEB	CHB-C4B-C3B	-2.89	118.64	125.32
87	BL	621	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
94	A6	410	PL9	C42-C43-C44	-2.89	120.70	127.66
82	f4	201	PEB	C2A-C1A-NA	2.89	110.76	108.27
82	zC	201	PEB	C2A-C1A-NA	2.89	110.76	108.27
82	hG	203	PEB	C2A-C1A-NA	2.89	110.76	108.27
82	sK	201	PEB	C2A-C1A-NA	2.89	110.76	108.27
82	UE	203	PEB	CMB-C2B-C1B	2.89	129.51	125.06
87	72	602	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
84	x3	1001	CYC	CBA-CAA-C2A	-2.89	104.60	112.63
82	ZB	201	PEB	C4B-C3B-C2B	-2.89	103.59	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	A6	407	PHO	CMB-C2B-C3B	2.89	130.08	124.68
82	MD	202	PEB	CHC-C4C-NC	2.89	125.06	121.15
87	BN	813	CLA	CHB-C4A-NA	2.89	128.51	124.51
87	2N	309	CLA	CHB-C4A-NA	2.89	128.51	124.51
87	AN	824	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
82	YI	201	PEB	CAB-CBB-CGB	-2.89	107.39	113.60
82	pC	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
85	K2	105	BCR	C11-C12-C13	-2.89	118.30	126.42
84	I3	1001	CYC	C2D-C1D-ND	2.89	111.46	107.40
82	DK	201	PEB	CHC-C4C-NC	2.89	125.06	121.15
82	AM	302	PEB	CHC-C4C-NC	2.89	125.06	121.15
87	cL	517	CLA	CHB-C4A-NA	2.89	128.50	124.51
85	A2	847	BCR	C15-C16-C17	-2.89	117.56	123.47
82	gJ	201	PEB	CHA-C1B-NB	-2.89	118.89	124.93
82	kG	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
82	fK	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	aK	201	PEB	C1C-CHB-C4B	2.89	134.76	128.28
87	BN	801	CLA	CMB-C2B-C3B	2.89	133.58	126.59
82	B9	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
83	AM	304	PUB	OA-C1A-NA	-2.89	121.65	125.93
82	FB	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	yC	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
84	t3	1001	CYC	C1D-C2D-C3D	-2.89	104.11	107.79
82	EQ	202	PEB	CHA-C1B-NB	-2.89	118.89	124.93
82	YD	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
82	I5	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
82	JB	202	PEB	CHC-C4C-NC	-2.89	117.24	121.15
82	r8	202	PEB	CBA-CAA-C3A	-2.89	107.04	113.47
85	BL	618	BCR	C4-C5-C6	-2.89	118.54	122.73
82	CJ	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	kJ	201	PEB	CMB-C2B-C1B	2.89	129.51	125.06
87	22	608	CLA	C2B-C1B-NB	2.89	112.17	110.23
82	mJ	202	PEB	CAC-C2C-C1C	2.89	130.36	125.76
82	mF	201	PEB	C4C-C3C-C2C	-2.89	104.84	107.50
87	2N	311	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
87	5N	601	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
82	uK	201	PEB	CBA-CAA-C3A	2.89	119.89	113.47
84	B3	1001	CYC	C2D-C1D-ND	2.89	111.46	107.40
84	d3	1001	CYC	C2D-C1D-ND	2.89	111.46	107.40
87	B2	830	CLA	CHB-C4A-NA	2.89	128.50	124.51
82	SH	202	PEB	C2A-C1A-NA	2.89	110.76	108.27
82	lM	202	PEB	C2A-C1A-NA	2.89	110.76	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ED	202	PEB	CHA-C1B-NB	-2.89	118.90	124.93
82	HI	203	PEB	CHA-C1B-NB	-2.89	118.90	124.93
82	W9	203	PEB	CHA-C1B-NB	-2.89	118.90	124.93
82	EK	202	PEB	CHC-C1D-ND	-2.89	110.07	113.72
82	DA	203	PEB	CHB-C1C-NC	-2.89	118.71	125.32
82	UB	303	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	hO	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	XP	202	PEB	CHA-C1B-C2B	2.89	132.32	124.90
87	3N	303	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
82	WG	202	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
82	DK	203	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
82	fF	201	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
82	W9	201	PEB	OD-C4D-C3D	-2.89	122.92	129.46
82	gH	201	PEB	OD-C4D-C3D	-2.89	122.92	129.46
82	NG	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	H5	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
82	E7	201	PEB	CMD-C2D-C3D	2.89	134.13	130.06
82	EF	202	PEB	CHC-C1D-ND	-2.89	110.07	113.72
82	WA	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
82	YK	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
85	b6	601	BCR	C23-C24-C25	-2.89	119.10	127.20
82	F9	202	PEB	OD-C4D-ND	-2.89	121.66	125.93
82	fG	201	PEB	OD-C4D-ND	-2.89	121.66	125.93
82	bO	202	PEB	OD-C4D-ND	-2.89	121.66	125.93
87	B2	825	CLA	CMB-C2B-C3B	2.89	133.58	126.59
82	C5	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	G7	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	ZO	201	PEB	C3C-C4C-NC	2.88	110.93	108.33
82	dE	202	PEB	C3C-C4C-NC	2.88	110.93	108.33
82	WK	201	PEB	OD-C4D-C3D	-2.88	122.92	129.46
82	X7	203	PEB	OD-C4D-C3D	-2.88	122.92	129.46
87	82	305	CLA	C3B-C4B-NB	-2.88	107.84	110.52
87	BN	820	CLA	CHB-C4A-NA	2.88	128.50	124.51
87	3N	307	CLA	CHB-C4A-NA	2.88	128.50	124.51
82	PG	201	PEB	CHB-C4B-C3B	-2.88	118.65	125.32
82	A1	302	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	v8	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	f4	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
82	m4	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	G5	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	AG	301	PEB	OD-C4D-ND	-2.88	121.66	125.93
82	rK	202	PEB	OD-C4D-ND	-2.88	121.66	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aO	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
94	a6	601	PL9	C15-C14-C16	2.88	120.12	115.27
87	B2	814	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
85	K6	102	BCR	C15-C16-C17	-2.88	117.57	123.47
82	XD	202	PEB	OD-C4D-C3D	-2.88	122.93	129.46
82	mM	201	PEB	CHB-C1C-NC	-2.88	118.72	125.32
82	gO	202	PEB	CHA-C1B-NB	-2.88	118.90	124.93
82	PK	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	O9	203	PEB	CHC-C4C-NC	2.88	125.05	121.15
82	UB	302	PEB	C3D-C4D-ND	2.88	112.92	107.26
82	D5	201	PEB	OD-C4D-ND	-2.88	121.66	125.93
82	dO	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
82	BQ	202	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
98	B2	837	PQN	C11-C3-C4	-2.88	115.42	118.50
82	eF	202	PEB	CHC-C1D-ND	-2.88	110.08	113.72
82	IP	201	PEB	C1C-CHB-C4B	2.88	134.75	128.28
82	GP	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
84	F3	1001	CYC	C2D-C1D-ND	2.88	111.45	107.40
84	o3	1001	CYC	C2D-C1D-ND	2.88	111.45	107.40
82	EJ	201	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	KQ	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	GI	201	PEB	C3C-C4C-NC	2.88	110.93	108.33
82	F4	1002	PEB	CMB-C2B-C1B	2.88	129.50	125.06
82	iO	203	PEB	OD-C4D-C3D	-2.88	122.93	129.46
82	WM	202	PEB	CHB-C1C-NC	-2.88	118.72	125.32
82	l4	201	PEB	CHC-C4C-NC	2.88	125.05	121.15
82	VE	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
87	R2	204	CLA	C3B-C4B-NB	-2.88	107.84	110.52
84	KH	1001	CYC	CHB-C1B-NB	-2.88	119.87	126.06
84	N3	1001	CYC	C1D-C2D-C3D	-2.88	104.12	107.79
82	QM	204	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
82	cK	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
87	72	603	CLA	O2D-CGD-CBD	2.88	116.39	111.27
82	GF	203	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	lF	201	PEB	OA-C1A-NA	2.88	128.43	124.94
82	lH	201	PEB	CHA-C1B-NB	-2.88	118.91	124.93
82	HP	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
82	S1	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
82	kH	201	PEB	OD-C4D-C3D	-2.88	122.93	129.46
82	nF	201	PEB	CAB-CBB-CGB	-2.88	107.40	113.60
82	dG	202	PEB	C3C-C4C-NC	2.88	110.93	108.33
82	XK	203	PEB	C2A-C1A-NA	2.88	110.76	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	A4	301	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	F9	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	fO	201	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	QF	201	PEB	C2A-C1A-NA	-2.88	105.79	108.27
88	d6	402	LHG	O8-C23-C24	2.88	120.95	111.91
87	A2	832	CLA	C3B-C4B-NB	-2.88	107.84	110.52
82	PM	202	PEB	CHC-C1D-ND	-2.88	110.08	113.72
82	HJ	201	PEB	CHA-C1B-NB	-2.88	118.91	124.93
82	l1	202	PEB	CHA-C1B-NB	-2.88	118.91	124.93
82	iF	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
84	f3	1001	CYC	C2D-C1D-ND	2.88	111.45	107.40
82	UA	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
82	b1	202	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
82	fK	202	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
84	FE	1001	CYC	C1A-C2A-C3A	-2.88	103.59	106.78
82	CF	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	Y1	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	qC	203	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	lK	201	PEB	CAB-CBB-CGB	-2.88	107.40	113.60
82	CF	203	PEB	C1C-CHB-C4B	2.88	134.74	128.28
82	hO	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
87	CL	514	CLA	CHB-C4A-NA	2.88	128.50	124.51
82	vF	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
82	P9	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
94	A6	410	PL9	C27-C28-C29	-2.88	120.72	127.66
82	lF	203	PEB	C1C-CHB-C4B	2.88	134.74	128.28
82	S5	203	PEB	CAC-C2C-C1C	2.88	130.35	125.76
82	WF	202	PEB	CHC-C1D-ND	-2.88	110.08	113.72
82	m4	201	PEB	CHC-C1D-ND	-2.88	110.08	113.72
82	iE	201	PEB	CAB-CBB-CGB	-2.88	107.41	113.60
85	FN	204	BCR	C2-C1-C6	2.88	114.91	110.48
87	CL	504	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
82	C5	202	PEB	OD-C4D-C3D	-2.88	122.94	129.46
82	R7	201	PEB	CHA-C1B-NB	-2.88	118.91	124.93
82	SE	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
82	QG	203	PEB	CMB-C2B-C1B	2.88	129.50	125.06
82	nK	201	PEB	CAB-CBB-CGB	-2.88	107.41	113.60
84	N4	1001	CYC	C4A-C3A-C2A	-2.88	103.20	106.51
85	B6	601	BCR	C38-C26-C27	2.88	119.15	113.62
87	2N	302	CLA	CHC-C4B-NB	2.88	127.31	124.26
87	BN	820	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
87	12	605	CLA	O2D-CGD-O1D	-2.88	118.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	M3	1001	CYC	C2D-C1D-ND	2.88	111.45	107.40
82	O4	202	PEB	OD-C4D-ND	-2.88	121.67	125.93
82	cB	403	PEB	C3B-C4B-NB	2.88	114.24	110.05
82	AH	305	PEB	CHA-C1B-NB	-2.88	118.91	124.93
82	MD	201	PEB	CHB-C4B-C3B	-2.88	118.66	125.32
82	ZF	202	PEB	CHB-C4B-C3B	-2.88	118.66	125.32
82	LQ	202	PEB	CHB-C1C-C2C	-2.88	120.66	127.15
82	RG	202	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
82	fJ	202	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
82	I7	202	PEB	C1D-CHC-C4C	-2.88	109.01	113.26
82	SD	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
82	bO	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
82	TB	202	PEB	CHC-C4C-NC	-2.88	117.25	121.15
84	NH	1001	CYC	C1B-C2B-C3B	-2.88	104.87	107.87
82	XA	203	PEB	OD-C4D-C3D	-2.88	122.94	129.46
85	CL	501	BCR	C21-C20-C19	-2.88	114.24	123.22
87	BN	815	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
82	KE	201	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
82	KP	201	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
87	22	612	CLA	CHB-C4A-NA	2.88	128.49	124.51
82	AG	301	PEB	C1C-CHB-C4B	-2.88	121.83	128.28
87	BN	802	CLA	CHB-C1B-NB	2.88	127.30	124.26
85	BL	618	BCR	C20-C21-C22	-2.88	123.20	127.31
87	AN	818	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
82	fO	201	PEB	OD-C4D-ND	-2.88	121.67	125.93
84	U3	1001	CYC	C2D-C1D-ND	2.88	111.44	107.40
84	73	1001	CYC	C2D-C1D-ND	2.88	111.44	107.40
82	dQ	401	PEB	C2A-C1A-NA	2.88	110.75	108.27
82	CP	201	PEB	OD-C4D-C3D	-2.88	122.94	129.46
82	l1	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
82	r8	202	PEB	CHB-C4B-C3B	2.88	131.97	125.32
82	FI	201	PEB	CAC-CBC-CGC	-2.88	107.41	113.60
82	G5	202	PEB	OD-C4D-C3D	-2.88	122.94	129.46
82	1C	203	PEB	C3B-C4B-NB	2.88	114.23	110.05
84	n3	1001	CYC	C2D-C1D-ND	2.88	111.44	107.40
82	QQ	201	PEB	CHB-C4B-C3B	-2.88	118.67	125.32
82	WP	201	PEB	C3D-C4D-ND	2.88	112.90	107.26
82	VD	202	PEB	OD-C4D-ND	-2.88	121.67	125.93
82	m4	202	PEB	CAB-C3B-C4B	2.88	130.10	125.01
95	lL	101	DGD	C4D-C3D-C2D	2.88	115.84	110.82
82	DB	201	PEB	C4C-C3C-C2C	-2.88	104.85	107.50
82	sC	203	PEB	CMB-C2B-C1B	2.88	129.49	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	T1	201	PEB	CHC-C1D-ND	-2.87	110.09	113.72
82	WH	203	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
84	Q3	1001	CYC	C2D-C1D-ND	2.87	111.44	107.40
95	C6	523	DGD	O1G-C1A-C2A	2.87	120.93	111.91
84	y3	1001	CYC	CAD-CBD-CGD	-2.87	107.42	113.60
82	T4	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
82	fE	203	PEB	C1C-CHB-C4B	2.87	134.73	128.28
82	YM	203	PEB	C3B-C4B-NB	2.87	114.23	110.05
82	AO	301	PEB	C3B-C4B-NB	2.87	114.23	110.05
82	Y5	203	PEB	CMC-C3C-C4C	2.87	130.11	127.06
82	aJ	201	PEB	CMB-C2B-C1B	2.87	129.49	125.06
82	SD	202	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
82	iK	201	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
84	L4	1001	CYC	C4A-C3A-C2A	-2.87	103.21	106.51
87	52	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
87	1N	605	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
82	KK	203	PEB	OA-C1A-C2A	-2.87	123.89	126.17
84	R3	1001	CYC	OC-C1C-C2C	-2.87	123.89	126.17
87	C6	518	CLA	C3B-C4B-NB	-2.87	107.85	110.52
85	LN	201	BCR	C20-C19-C18	-2.87	118.34	126.42
82	aF	203	PEB	OD-C4D-C3D	-2.87	122.95	129.46
82	dO	202	PEB	OD-C4D-C3D	-2.87	122.95	129.46
82	RD	203	PEB	CHC-C1D-ND	-2.87	110.09	113.72
82	A5	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
82	ZB	203	PEB	C4C-C3C-C2C	-2.87	104.85	107.50
82	hJ	201	PEB	OD-C4D-C3D	-2.87	122.95	129.46
82	k4	201	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
84	LO	1001	CYC	C4A-C3A-C2A	-2.87	103.21	106.51
87	A2	839	CLA	CHB-C4A-NA	2.87	128.49	124.51
82	MB	202	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
82	dO	202	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
82	SD	202	PEB	C1C-CHB-C4B	2.87	134.72	128.28
83	M5	302	PUB	OD-C4D-ND	-2.87	121.67	125.93
87	C6	510	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
82	fK	202	PEB	CMB-C2B-C1B	2.87	129.49	125.06
82	rF	201	PEB	OA-C1A-NA	2.87	128.42	124.94
82	FA	201	PEB	CHA-C1B-NB	-2.87	118.92	124.93
82	FP	202	PEB	CHC-C1D-ND	-2.87	110.09	113.72
82	UF	202	PEB	OA-C1A-C2A	-2.87	123.89	126.17
82	aF	203	PEB	OA-C1A-C2A	-2.87	123.89	126.17
88	DL	407	LHG	O8-C23-C24	2.87	120.92	111.91
82	IJ	203	PEB	CMC-C3C-C4C	-2.87	124.02	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OG	203	PEB	CMC-C3C-C4C	2.87	130.10	127.06
82	aF	203	PEB	CHA-C1B-C2B	2.87	132.29	124.90
82	LP	201	PEB	CHA-C1B-NB	-2.87	118.92	124.93
82	kJ	202	PEB	C3B-C4B-NB	2.87	114.23	110.05
82	nK	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
82	GK	201	PEB	CMB-C2B-C1B	2.87	129.49	125.06
82	aM	202	PEB	CAA-C3A-C2A	-2.87	107.08	114.26
82	SP	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
85	F2	204	BCR	C2-C1-C6	2.87	114.90	110.48
87	B2	820	CLA	CHB-C4A-NA	2.87	128.48	124.51
82	F5	203	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	AD	303	PEB	CHB-C1C-NC	-2.87	118.74	125.32
87	42	610	CLA	C2A-C1A-CHA	2.87	128.88	123.86
82	AO	305	PEB	C3B-C4B-NB	2.87	114.23	110.05
82	18	203	PEB	C3B-C4B-NB	2.87	114.23	110.05
82	PE	201	PEB	CHB-C4B-C3B	-2.87	118.68	125.32
82	T1	201	PEB	OA-C1A-C2A	-2.87	123.89	126.17
82	HD	203	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	X5	202	PEB	OD-C4D-C3D	-2.87	122.95	129.46
82	z8	201	PEB	C2A-C1A-NA	2.87	110.75	108.27
87	72	610	CLA	CHB-C4A-NA	2.87	128.48	124.51
87	A2	820	CLA	CHB-C4A-NA	2.87	128.48	124.51
87	BL	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
82	EP	203	PEB	C1C-NC-C4C	2.87	114.70	109.60
82	YE	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	bO	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	JK	201	PEB	CAC-C2C-C1C	2.87	130.33	125.76
82	HJ	201	PEB	CHB-C1C-NC	-2.87	118.74	125.32
82	YQ	202	PEB	OD-C4D-C3D	-2.87	122.96	129.46
87	A2	825	CLA	C3B-C4B-NB	-2.87	107.85	110.52
84	N1	1001	CYC	C4D-C3D-C2D	-2.87	104.23	107.62
87	A2	836	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
82	WE	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	SH	203	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	T7	203	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	FP	201	PEB	CMB-C2B-C1B	2.87	129.48	125.06
94	A6	410	PL9	C53-C6-C1	2.87	120.86	114.99
82	IB	203	PEB	CAA-C3A-C4A	-2.87	105.30	112.67
82	JQ	203	PEB	OA-C1A-C2A	-2.87	123.89	126.17
85	AN	848	BCR	C12-C13-C14	-2.87	114.54	118.94
84	S3	1001	CYC	C2D-C1D-ND	2.87	111.43	107.40
84	T3	1001	CYC	C1D-C2D-C3D	-2.87	104.13	107.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KG	201	PEB	OD-C4D-C3D	-2.87	122.96	129.46
82	MP	203	PEB	OD-C4D-C3D	-2.87	122.96	129.46
82	HB	202	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
82	ND	204	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	O9	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	MK	201	PEB	CHB-C1C-C2C	-2.87	120.68	127.15
82	SG	201	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	MK	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
87	B6	607	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
82	N7	203	PEB	C3C-C4C-NC	2.87	110.92	108.33
82	SH	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	CJ	202	PEB	CMB-C2B-C1B	2.87	129.48	125.06
94	A6	410	PL9	C30-C29-C31	2.87	120.10	115.27
82	z8	201	PEB	CHB-C4B-NB	2.87	130.55	124.58
82	PQ	201	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
87	cL	512	CLA	CHB-C4A-NA	2.87	128.48	124.51
82	GF	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	SJ	203	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	GP	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	M5	305	PEB	C2A-C1A-NA	2.87	110.75	108.27
82	DF	203	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	gO	201	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	OP	201	PEB	OD-C4D-C3D	-2.87	122.96	129.46
82	qK	203	PEB	CAB-C3B-C4B	2.87	130.08	125.01
82	RG	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	WG	203	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	VM	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	iK	201	PEB	C3C-C4C-NC	2.87	110.92	108.33
82	GK	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	hB	301	PEB	C3B-C4B-NB	2.87	114.22	110.05
84	k3	1001	CYC	C2D-C1D-ND	2.87	111.43	107.40
84	q3	1001	CYC	C2D-C1D-ND	2.87	111.43	107.40
82	h1	201	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
87	32	306	CLA	CHB-C4A-NA	2.87	128.48	124.51
87	82	301	CLA	CHB-C4A-NA	2.87	128.48	124.51
82	bF	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
82	AP	203	PEB	CHA-C1B-NB	-2.87	118.94	124.93
82	WE	201	PEB	CBA-CAA-C3A	-2.87	107.08	113.47
82	CM	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
82	a1	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
82	G9	201	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
84	FE	1002	CYC	C1A-C2A-C3A	-2.87	103.61	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LM	201	PEB	C1D-CHC-C4C	2.87	117.48	113.26
82	DJ	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	QD	201	PEB	CHB-C4B-C3B	-2.87	118.69	125.32
82	TK	202	PEB	CHA-C1B-NB	-2.87	118.94	124.93
91	dL	403	PHO	O2A-CGA-CBA	2.87	120.90	111.91
82	mJ	201	PEB	CHB-C4B-NB	-2.87	118.61	124.58
82	R5	202	PEB	C2A-C1A-NA	2.87	110.74	108.27
82	fF	202	PEB	CMB-C2B-C1B	2.87	129.48	125.06
82	fO	202	PEB	CHC-C1D-ND	-2.87	110.10	113.72
82	TG	201	PEB	CAC-CBC-CGC	-2.87	107.44	113.60
82	f4	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
83	xK	301	PUB	OA-C1A-NA	-2.87	121.68	125.93
82	vF	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
87	32	306	CLA	CAA-C2A-C3A	-2.87	107.10	114.26
85	BN	839	BCR	C15-C16-C17	-2.87	117.60	123.47
82	eA	301	PEB	C1D-CHC-C4C	2.87	117.48	113.26
82	UM	203	PEB	CHA-C1B-NB	-2.87	118.94	124.93
82	S5	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	dM	203	PEB	C3B-C4B-NB	2.87	114.22	110.05
82	WH	201	PEB	OD-C4D-C3D	-2.87	122.97	129.46
82	fB	301	PEB	OD-C4D-C3D	-2.87	122.97	129.46
82	hB	301	PEB	OD-C4D-C3D	-2.87	122.97	129.46
82	cK	201	PEB	CAB-C3B-C4B	2.87	130.08	125.01
82	QB	201	PEB	CMC-C3C-C2C	-2.87	119.41	125.61
82	NQ	203	PEB	C1D-CHC-C4C	-2.87	109.03	113.26
82	V7	201	PEB	OD-C4D-C3D	-2.87	122.97	129.46
82	kO	201	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
82	QH	201	PEB	C2A-C1A-NA	2.87	110.74	108.27
82	wK	301	PEB	OA-C1A-C2A	-2.87	123.89	126.17
82	oF	201	PEB	CHB-C4B-NB	-2.86	118.61	124.58
82	iK	202	PEB	CHB-C4B-C3B	-2.86	118.69	125.32
82	BM	301	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
82	XM	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	hM	201	PEB	OD-C4D-C3D	-2.86	122.97	129.46
84	H3	1001	CYC	C2D-C1D-ND	2.86	111.43	107.40
85	C6	507	BCR	C3-C4-C5	-2.86	108.96	114.08
87	cL	516	CLA	CHB-C4A-NA	2.86	128.47	124.51
84	K3	1001	CYC	C1D-C2D-C3D	-2.86	104.14	107.79
87	AN	836	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
82	WA	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	PE	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	H9	203	PEB	OD-C4D-ND	-2.86	121.69	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	rF	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
84	O3	1001	CYC	C2D-C1D-ND	2.86	111.42	107.40
82	hJ	202	PEB	C2A-C1A-NA	2.86	110.74	108.27
85	hL	102	BCR	C29-C30-C25	2.86	114.89	110.48
87	AN	811	CLA	CHC-C4B-NB	2.86	127.29	124.26
82	U7	201	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
82	fO	201	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
82	JA	202	PEB	CAC-C2C-C1C	2.86	130.32	125.76
82	jO	201	PEB	OA-C1A-C2A	-2.86	123.90	126.17
87	BN	830	CLA	CHB-C4A-NA	2.86	128.47	124.51
82	HB	203	PEB	CHB-C4B-C3B	-2.86	118.69	125.32
82	BQ	202	PEB	CHA-C1B-NB	-2.86	118.94	124.93
82	QP	202	PEB	C4C-C3C-C2C	-2.86	104.86	107.50
82	Z5	304	PEB	OD-C4D-ND	-2.86	121.69	125.93
84	D3	1001	CYC	C2D-C1D-ND	2.86	111.42	107.40
82	QK	203	PEB	CAA-C3A-C2A	2.86	121.41	114.26
82	hF	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
82	CQ	201	PEB	CHA-C1B-NB	-2.86	118.94	124.93
82	B9	202	PEB	CHA-C4A-NA	-2.86	121.80	125.20
82	sC	202	PEB	C2A-C1A-NA	2.86	110.74	108.27
82	jH	201	PEB	C2A-C1A-NA	2.86	110.74	108.27
84	A3	1001	CYC	C1D-C2D-C3D	-2.86	104.14	107.79
84	C3	1001	CYC	C1D-C2D-C3D	-2.86	104.14	107.79
82	VA	201	PEB	OD-C4D-C3D	-2.86	122.97	129.46
82	w8	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
84	P3	1001	CYC	OC-C1C-C2C	-2.86	123.90	126.17
82	T1	201	PEB	C4C-C3C-C2C	-2.86	104.86	107.50
82	LQ	201	PEB	CMB-C2B-C1B	2.86	129.47	125.06
87	22	604	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
82	UJ	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	UH	202	PEB	CAB-CBB-CGB	-2.86	107.44	113.60
82	T4	201	PEB	CAC-C2C-C1C	2.86	130.32	125.76
82	J4	1002	PEB	OD-C4D-C3D	-2.86	122.98	129.46
82	kE	202	PEB	OD-C4D-C3D	-2.86	122.98	129.46
87	A2	817	CLA	CAA-C2A-C3A	-2.86	107.11	114.26
82	UH	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
82	MJ	201	PEB	C2A-C1A-NA	2.86	110.74	108.27
82	AQ	303	PEB	C2A-C1A-NA	2.86	110.74	108.27
82	P5	202	PEB	C2A-C1A-NA	2.86	110.74	108.27
95	c6	620	DGD	O1G-C1A-C2A	2.86	120.89	111.91
82	M9	301	PEB	CHC-C1D-ND	-2.86	110.10	113.72
82	TA	203	PEB	OD-C4D-ND	-2.86	121.69	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	D5	201	PEB	CHB-C4B-C3B	-2.86	118.70	125.32
82	gF	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
84	P3	1001	CYC	C1D-C2D-C3D	-2.86	104.14	107.79
84	p3	1001	CYC	C1D-C2D-C3D	-2.86	104.14	107.79
82	EJ	201	PEB	CMB-C2B-C1B	2.86	129.47	125.06
82	zC	201	PEB	CHB-C4B-NB	2.86	130.53	124.58
82	PO	203	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	TO	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
87	I2	103	CLA	CHB-C4A-NA	2.86	128.47	124.51
82	J7	202	PEB	CAC-C2C-C1C	2.86	130.32	125.76
82	eE	201	PEB	C2A-C1A-NA	2.86	110.74	108.27
82	hK	202	PEB	C2A-C1A-NA	2.86	110.74	108.27
91	d6	404	PHO	C4-C3-C5	2.86	120.08	115.27
82	YM	203	PEB	OD-C4D-C3D	-2.86	122.98	129.46
82	L7	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	VB	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
82	eB	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
82	F7	203	PEB	CAC-C2C-C1C	2.86	130.32	125.76
82	dG	202	PEB	C1D-CHC-C4C	-2.86	109.04	113.26
82	AH	302	PEB	C3B-C4B-NB	2.86	114.21	110.05
82	KI	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
87	3N	307	CLA	CAA-C2A-C3A	-2.86	107.11	114.26
82	VO	202	PEB	C1C-CHB-C4B	2.86	134.69	128.28
84	G3	1001	CYC	C1D-C2D-C3D	-2.86	104.15	107.79
84	l3	1001	CYC	C1D-C2D-C3D	-2.86	104.15	107.79
87	4N	605	CLA	C3A-C2A-C1A	2.86	105.62	101.34
82	Y9	201	PEB	O2B-CGB-CBB	2.86	123.22	114.03
82	Q7	202	PEB	C2A-C1A-NA	2.86	110.74	108.27
87	AN	820	CLA	CHB-C4A-NA	2.86	128.47	124.51
82	NJ	201	PEB	CAB-CBB-CGB	-2.86	107.45	113.60
82	mO	202	PEB	CAB-C3B-C4B	2.86	130.07	125.01
82	PA	202	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
82	LE	1002	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
82	gF	201	PEB	CMB-C2B-C3B	-2.86	118.36	126.12
87	BN	817	CLA	CMB-C2B-C1B	-2.86	121.02	125.37
82	WE	203	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	OO	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	O7	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
82	hO	201	PEB	C4B-NB-C1B	-2.86	101.12	106.51
87	22	610	CLA	C3B-C4B-NB	-2.86	107.86	110.52
82	OJ	203	PEB	CAA-C3A-C4A	-2.86	105.33	112.67
82	QJ	203	PEB	C3B-C4B-NB	2.86	114.21	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YJ	203	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
82	ZF	202	PEB	C1C-CHB-C4B	2.86	134.69	128.28
84	LG	1001	CYC	C4D-CHA-C1A	2.86	134.69	128.28
82	N1	1002	PEB	C2A-C1A-NA	2.86	110.74	108.27
82	OE	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
82	gH	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
87	B2	813	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
87	A2	840	CLA	C3B-C4B-NB	-2.86	107.86	110.52
82	RQ	203	PEB	CHC-C1D-ND	-2.86	110.11	113.72
82	B9	201	PEB	OD-C4D-ND	-2.86	121.70	125.93
82	uC	203	PEB	OD-C4D-ND	-2.86	121.70	125.93
82	HJ	201	PEB	OD-C4D-C3D	-2.86	122.99	129.46
82	jJ	203	PEB	OD-C4D-C3D	-2.86	122.99	129.46
82	vC	201	PEB	C3B-C4B-NB	2.86	114.20	110.05
82	SJ	202	PEB	C3C-C4C-NC	2.86	110.91	108.33
82	hJ	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
82	UG	201	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
82	HI	203	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
82	r8	201	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
82	GF	201	PEB	CMB-C2B-C1B	2.86	129.46	125.06
87	2N	310	CLA	C3B-C4B-NB	-2.86	107.86	110.52
82	iG	201	PEB	CAB-CBB-CGB	-2.86	107.46	113.60
84	i3	1001	CYC	C1D-C2D-C3D	-2.86	104.15	107.79
87	dL	402	CLA	CMB-C2B-C1B	-2.86	121.02	125.37
82	AE	304	PEB	OD-C4D-ND	-2.86	121.70	125.93
82	gO	203	PEB	OD-C4D-C3D	-2.86	122.99	129.46
85	LN	201	BCR	C11-C10-C9	-2.86	123.23	127.31
82	U1	202	PEB	CAB-CBB-CGB	-2.86	107.46	113.60
88	I6	101	LHG	O2-C2-C3	2.86	119.57	109.56
82	UQ	202	PEB	C2A-C1A-NA	2.86	110.73	108.27
82	FA	202	PEB	CMB-C2B-C1B	2.86	129.46	125.06
82	WQ	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
82	h4	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
84	DE	1001	CYC	CHB-C1B-NB	-2.86	119.93	126.06
85	bL	603	BCR	C16-C15-C14	-2.86	117.62	123.47
82	F9	203	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
82	GA	202	PEB	C3B-C4B-NB	2.86	114.20	110.05
82	MK	202	PEB	C3B-C4B-NB	2.86	114.20	110.05
84	W3	1001	CYC	CAD-CBD-CGD	-2.86	107.46	113.60
82	Y7	304	PEB	OD-C4D-C3D	-2.86	122.99	129.46
87	32	302	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
82	vK	202	PEB	CAC-C2C-C1C	2.85	130.31	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CD	201	PEB	CHA-C1B-NB	-2.85	118.96	124.93
82	MD	202	PEB	C4B-C3B-C2B	-2.85	103.62	106.78
84	R3	1001	CYC	C1D-C2D-C3D	-2.85	104.15	107.79
82	rC	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
82	hM	202	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
82	wC	204	PEB	OD-C4D-ND	-2.85	121.70	125.93
83	Y7	302	PUB	OA-C1A-NA	-2.85	121.70	125.93
87	22	611	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
87	32	309	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
82	OE	203	PEB	CHA-C1B-NB	-2.85	118.96	124.93
82	V1	203	PEB	CHA-C1B-NB	-2.85	118.96	124.93
82	z8	201	PEB	CHC-C1D-ND	-2.85	110.11	113.72
82	d4	202	PEB	OD-C4D-C3D	-2.85	122.99	129.46
82	MF	201	PEB	CHB-C1C-C2C	-2.85	120.71	127.15
82	M9	301	PEB	OD-C4D-ND	-2.85	121.70	125.93
82	R7	201	PEB	C4B-C3B-C2B	-2.85	103.62	106.78
82	bP	501	PEB	CHA-C1B-NB	-2.85	118.96	124.93
82	tK	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
82	GB	203	PEB	CMB-C2B-C1B	2.85	129.46	125.06
82	eH	201	PEB	CMB-C2B-C1B	2.85	129.46	125.06
82	jM	201	PEB	CHA-C1B-C2B	2.85	132.24	124.90
82	O1	203	PEB	CAC-C2C-C1C	2.85	130.31	125.76
82	QA	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
82	YG	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
84	h3	1001	CYC	C2D-C1D-ND	2.85	111.41	107.40
82	rC	202	PEB	CBA-CAA-C3A	-2.85	107.11	113.47
82	EF	202	PEB	CMB-C2B-C1B	2.85	129.46	125.06
87	A2	810	CLA	C3B-C4B-NB	-2.85	107.87	110.52
87	K6	101	CLA	C3B-C4B-NB	-2.85	107.87	110.52
84	63	901	CYC	C1A-C2A-C3A	-2.85	103.62	106.78
82	YG	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
82	VH	202	PEB	CHA-C1B-NB	-2.85	118.97	124.93
82	F7	202	PEB	CHA-C1B-NB	-2.85	118.97	124.93
95	hL	101	DGD	C2G-O2G-C1B	-2.85	110.77	117.79
82	CF	203	PEB	C3B-C4B-NB	2.85	114.20	110.05
82	UP	201	PEB	CAA-C3A-C4A	-2.85	105.35	112.67
82	V4	202	PEB	C3C-C4C-NC	2.85	110.90	108.33
82	SH	202	PEB	C3D-C4D-ND	2.85	112.86	107.26
87	BN	814	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
82	fG	203	PEB	C1C-CHB-C4B	2.85	134.68	128.28
82	ZG	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
82	hM	202	PEB	CHB-C4B-NB	-2.85	118.64	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dG	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
82	TK	202	PEB	CAA-C3A-C4A	-2.85	105.35	112.67
82	VG	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
82	lH	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	HQ	203	PEB	C3B-C4B-NB	2.85	114.20	110.05
95	J6	101	DGD	C2G-O2G-C1B	-2.85	110.77	117.79
82	H9	201	PEB	CHC-C4C-NC	2.85	125.01	121.15
82	DB	202	PEB	OD-C4D-ND	-2.85	121.70	125.93
82	lE	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
82	LK	202	PEB	CHB-C4B-NB	2.85	130.51	124.58
85	K6	102	BCR	C35-C13-C14	-2.85	118.93	122.92
82	MK	203	PEB	C1C-NC-C4C	-2.85	104.52	109.60
82	eG	203	PEB	OD-C4D-C3D	-2.85	123.00	129.46
87	4N	610	CLA	C2A-C1A-CHA	2.85	128.84	123.86
87	4N	601	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
82	Q5	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
82	mG	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
82	gH	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	VB	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
82	E5	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
82	W5	203	PEB	CAC-C2C-C1C	2.85	130.30	125.76
82	AP	201	PEB	OA-C1A-C2A	-2.85	123.91	126.17
82	lO	201	PEB	OD-C4D-C3D	-2.85	123.00	129.46
87	AN	832	CLA	C3B-C4B-NB	-2.85	107.87	110.52
83	AJ	304	PUB	CMD-C2D-C3D	2.85	132.05	127.77
82	EF	201	PEB	CHB-C4B-C3B	-2.85	118.72	125.32
82	W1	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
82	b4	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
82	W7	201	PEB	C3B-C4B-NB	2.85	114.20	110.05
82	NJ	202	PEB	O2B-CGB-CBB	2.85	123.19	114.03
82	UG	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06
82	QM	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
82	a4	202	PEB	OD-C4D-ND	-2.85	121.71	125.93
87	12	605	CLA	CHB-C4A-NA	2.85	128.45	124.51
82	EK	201	PEB	CHB-C4B-C3B	-2.85	118.72	125.32
82	GE	1002	PEB	CHC-C1D-ND	-2.85	110.12	113.72
82	U9	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	qK	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	hH	201	PEB	C1D-CHC-C4C	2.85	117.46	113.26
82	OJ	203	PEB	CMA-C2A-C1A	-2.85	106.26	112.40
82	dD	401	PEB	C2A-C1A-NA	2.85	110.73	108.27
82	WM	203	PEB	OD-C4D-ND	-2.85	121.71	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	B2	824	CLA	CHB-C4A-NA	2.85	128.45	124.51
85	k6	102	BCR	C35-C13-C14	-2.85	118.93	122.92
82	OG	203	PEB	CHA-C1B-NB	-2.85	118.97	124.93
82	dF	201	PEB	C1D-CHC-C4C	-2.85	109.05	113.26
82	KD	202	PEB	CHC-C1D-ND	-2.85	110.12	113.72
84	63	901	CYC	CHB-C1B-C2B	-2.85	121.30	126.95
82	QF	202	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	SH	201	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	CK	201	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	A4	301	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	rK	201	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	LA	201	PEB	C4C-C3C-C2C	-2.85	104.87	107.50
82	lJ	203	PEB	OD-C4D-ND	-2.85	121.71	125.93
82	lJ	203	PEB	CHB-C1C-NC	-2.85	118.79	125.32
82	SE	201	PEB	C1D-CHC-C4C	-2.85	109.06	113.26
82	lK	203	PEB	C1D-CHC-C4C	2.85	117.46	113.26
87	AN	841	CLA	C3B-C4B-NB	-2.85	107.87	110.52
87	A2	841	CLA	C3B-C4B-NB	-2.85	107.87	110.52
82	WI	202	PEB	C2B-C1B-NB	2.85	116.61	110.53
82	jH	202	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	fM	203	PEB	CHA-C1B-NB	-2.85	118.97	124.93
82	eF	201	PEB	CMB-C2B-C1B	2.85	129.45	125.06
82	mO	203	PEB	OA-C1A-C2A	-2.85	123.91	126.17
82	w8	204	PEB	OD-C4D-ND	-2.85	121.71	125.93
85	A2	848	BCR	C30-C25-C24	2.85	123.84	115.78
84	e3	1001	CYC	C1D-C2D-C3D	-2.85	104.16	107.79
84	v3	1001	CYC	C1D-C2D-C3D	-2.85	104.16	107.79
82	QF	203	PEB	CAA-C3A-C2A	2.85	121.38	114.26
82	aO	201	PEB	CHC-C4C-NC	2.85	125.00	121.15
87	B6	616	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
82	JA	203	PEB	CHC-C1D-ND	-2.85	110.12	113.72
82	yF	301	PEB	CAC-C2C-C1C	2.85	130.30	125.76
82	rC	202	PEB	CHB-C4B-C3B	2.85	131.91	125.32
82	FM	202	PEB	OD-C4D-ND	-2.85	121.71	125.93
87	BN	812	CLA	C3B-C4B-NB	-2.85	107.87	110.52
87	3N	309	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
82	Y9	202	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
82	UM	202	PEB	CHA-C1B-C2B	2.85	132.22	124.90
82	qF	201	PEB	CHA-C1B-C2B	2.85	132.22	124.90
82	H9	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
82	XF	202	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	bF	202	PEB	C3B-C4B-NB	2.85	114.19	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AH	301	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
87	dL	402	CLA	O2D-CGD-CBD	2.85	116.33	111.27
82	P1	201	PEB	CHC-C4C-NC	2.85	125.00	121.15
82	l1	201	PEB	CMC-C3C-C4C	2.85	130.08	127.06
82	S1	201	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	A1	305	PEB	C3B-C4B-NB	2.85	114.19	110.05
82	R7	201	PEB	CAC-CBC-CGC	-2.85	107.48	113.60
82	d4	202	PEB	OD-C4D-ND	-2.85	121.71	125.93
92	B6	622	LMG	C8-O7-C10	-2.85	110.78	117.79
87	7N	604	CLA	CHB-C4A-NA	2.85	128.45	124.51
87	42	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
84	LE	1001	CYC	C4D-CHA-C1A	2.85	134.66	128.28
82	KF	203	PEB	OA-C1A-C2A	-2.85	123.91	126.17
82	m4	203	PEB	OA-C1A-C2A	-2.85	123.91	126.17
85	AN	848	BCR	C30-C25-C24	2.85	123.83	115.78
87	AN	817	CLA	CAA-C2A-C3A	-2.85	107.15	114.26
82	QB	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	AH	302	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	aF	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	tF	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
82	KQ	202	PEB	OD-C4D-C3D	-2.85	123.01	129.46
82	t8	202	PEB	OD-C4D-C3D	-2.85	123.01	129.46
87	KN	102	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
87	A2	840	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
87	8N	306	CLA	C3B-C4B-NB	-2.85	107.88	110.52
82	b4	201	PEB	CMA-C2A-C1A	-2.85	106.27	112.40
82	XD	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
82	AP	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
82	NB	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
82	fE	203	PEB	OD-C4D-C3D	-2.85	123.01	129.46
82	PA	203	PEB	CHB-C4B-C3B	-2.85	118.74	125.32
82	FA	202	PEB	CHA-C1B-NB	-2.85	118.98	124.93
82	kK	203	PEB	C3B-C4B-NB	2.85	114.19	110.05
83	xF	305	PUB	C2C-C1C-NC	2.85	114.19	110.05
82	OA	202	PEB	OD-C4D-ND	-2.85	121.72	125.93
85	hL	102	BCR	C2-C1-C6	2.85	114.86	110.48
87	BL	606	CLA	C2A-C1A-CHA	2.85	128.83	123.86
82	EJ	203	PEB	OD-C4D-C3D	-2.84	123.01	129.46
82	YP	502	PEB	C4B-C3B-C2B	-2.84	103.63	106.78
84	DE	1001	CYC	C1A-C2A-C3A	-2.84	103.63	106.78
82	KJ	202	PEB	CAC-C2C-C1C	2.84	130.29	125.76
82	UK	202	PEB	OA-C1A-C2A	-2.84	123.91	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HD	203	PEB	C3B-C4B-NB	2.84	114.19	110.05
87	AL	405	CLA	C3B-C4B-NB	-2.84	107.88	110.52
82	Y5	202	PEB	CAA-C3A-C4A	-2.84	105.37	112.67
82	Z1	202	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
84	F4	1001	CYC	CHA-C4D-C3D	-2.84	120.73	127.15
82	DP	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
82	aH	201	PEB	C2A-C1A-NA	2.84	110.72	108.27
87	CL	511	CLA	CHB-C4A-NA	2.84	128.44	124.51
87	cL	511	CLA	CHB-C4A-NA	2.84	128.44	124.51
82	VJ	201	PEB	CHC-C1D-ND	2.84	117.32	113.72
82	WK	202	PEB	CHC-C1D-ND	-2.84	110.13	113.72
82	MB	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
82	J9	202	PEB	CAB-C3B-C4B	2.84	130.04	125.01
82	MF	202	PEB	C3B-C4B-NB	2.84	114.19	110.05
84	DO	1001	CYC	CAD-CBD-CGD	-2.84	107.48	113.60
82	iF	202	PEB	CHB-C4B-C3B	-2.84	118.74	125.32
82	LF	202	PEB	OD-C4D-C3D	-2.84	123.02	129.46
82	M5	304	PEB	OD-C4D-C3D	-2.84	123.02	129.46
82	Q5	201	PEB	OA-C1A-C2A	-2.84	123.91	126.17
84	K3	1001	CYC	OC-C1C-C2C	-2.84	123.91	126.17
84	v3	1001	CYC	OC-C1C-C2C	-2.84	123.91	126.17
82	WF	203	PEB	CMB-C2B-C1B	2.84	129.44	125.06
82	s8	203	PEB	CMB-C2B-C1B	2.84	129.44	125.06
82	GG	1002	PEB	CHC-C1D-ND	-2.84	110.13	113.72
84	C4	1001	CYC	C2A-C1A-NA	2.84	114.19	110.05
82	eO	201	PEB	CHB-C4B-C3B	-2.84	118.74	125.32
82	LI	202	PEB	OD-C4D-ND	-2.84	121.72	125.93
84	NH	1001	CYC	C2B-C1B-NB	2.84	111.15	106.99
82	O9	201	PEB	C2A-C1A-NA	2.84	110.72	108.27
82	J5	203	PEB	CAC-C2C-C1C	2.84	130.29	125.76
82	TD	203	PEB	CHA-C1B-NB	-2.84	118.99	124.93
82	YA	304	PEB	OD-C4D-C3D	-2.84	123.02	129.46
87	A2	811	CLA	CHB-C4A-NA	2.84	128.44	124.51
82	AH	305	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
82	UD	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
82	WE	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
82	HD	203	PEB	CHA-C1B-NB	-2.84	118.99	124.93
82	bO	201	PEB	CMA-C2A-C1A	-2.84	106.28	112.40
84	t3	1001	CYC	OC-C1C-C2C	-2.84	123.91	126.17
82	A9	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
82	fG	203	PEB	OD-C4D-C3D	-2.84	123.02	129.46
87	B2	801	CLA	CHB-C1B-NB	2.84	127.27	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WD	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
82	JM	202	PEB	CAB-C3B-C4B	2.84	130.04	125.01
82	M9	302	PEB	CMB-C2B-C1B	2.84	129.44	125.06
84	E3	1001	CYC	C1D-C2D-C3D	-2.84	104.17	107.79
84	L1	1001	CYC	OB-C4B-C3B	-2.84	124.96	128.04
95	cL	502	DGD	O1G-C1A-C2A	2.84	120.83	111.91
96	FL	102	HEM	CHD-C1D-C2D	-2.84	120.54	124.98
82	N5	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
82	V1	201	PEB	CHB-C4B-C3B	-2.84	118.74	125.32
82	VE	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	mE	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	NB	203	PEB	CBB-CAB-C3B	-2.84	104.73	112.63
94	A6	410	PL9	C15-C14-C16	2.84	120.05	115.27
82	aK	203	PEB	OD-C4D-C3D	-2.84	123.02	129.46
82	RA	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
82	VQ	201	PEB	C1C-CHB-C4B	-2.84	121.91	128.28
95	CL	523	DGD	O1G-C1A-C2A	2.84	120.82	111.91
84	g3	1001	CYC	OC-C1C-C2C	-2.84	123.91	126.17
87	42	608	CLA	CMA-C3A-C4A	-2.84	104.14	111.77
82	Q9	203	PEB	CHC-C4C-NC	2.84	124.99	121.15
82	UJ	203	PEB	OD-C4D-C3D	-2.84	123.02	129.46
82	GJ	203	PEB	CAA-C3A-C4A	-2.84	105.38	112.67
82	OG	201	PEB	CAA-C3A-C2A	-2.84	107.16	114.26
82	XP	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	r8	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	OH	203	PEB	C1D-CHC-C4C	2.84	117.44	113.26
84	j3	1001	CYC	C2D-C1D-ND	2.84	111.39	107.40
87	BN	821	CLA	CHB-C4A-NA	2.84	128.44	124.51
82	eO	203	PEB	C3B-C4B-NB	2.84	114.18	110.05
82	RO	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
82	cO	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
85	bL	601	BCR	C7-C8-C9	-2.84	121.94	126.23
82	d1	201	PEB	C3C-C4C-NC	2.84	110.89	108.33
87	7N	605	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
82	H7	203	PEB	CAC-CBC-CGC	-2.84	107.49	113.60
84	LO	1001	CYC	CHD-C1D-ND	-2.84	118.81	125.32
82	p8	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	YP	501	PEB	OD-C4D-ND	-2.84	121.72	125.93
82	UH	202	PEB	OA-C1A-C2A	-2.84	123.92	126.17
82	EI	201	PEB	OA-C1A-C2A	-2.84	123.92	126.17
82	h4	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
82	fB	301	PEB	C3B-C4B-NB	2.84	114.18	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	1N	605	CLA	CHB-C4A-NA	2.84	128.44	124.51
82	iF	203	PEB	C2A-C1A-NA	2.84	110.72	108.27
85	C6	507	BCR	C33-C5-C4	2.84	119.07	113.62
82	SO	201	PEB	CHC-C1D-ND	-2.84	110.13	113.72
82	mF	202	PEB	CHC-C1D-ND	-2.84	110.13	113.72
87	BN	831	CLA	C3B-C4B-NB	-2.84	107.88	110.52
82	jM	203	PEB	C3C-C4C-NC	2.84	110.89	108.33
82	uK	202	PEB	OD-C4D-ND	-2.84	121.72	125.93
82	H9	201	PEB	O2B-CGB-CBB	2.84	123.15	114.03
82	OB	201	PEB	CHA-C1B-NB	-2.84	118.99	124.93
84	g3	1001	CYC	C1D-C2D-C3D	-2.84	104.17	107.79
87	K2	101	CLA	CHB-C4A-NA	2.84	128.44	124.51
82	Y5	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	Y7	303	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	G9	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	SM	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
87	2N	305	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
82	zC	201	PEB	CHC-C1D-ND	-2.84	110.13	113.72
82	xC	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
82	ZB	203	PEB	C3B-C4B-NB	2.84	114.18	110.05
82	PM	201	PEB	CMB-C2B-C1B	2.84	129.44	125.06
82	b1	201	PEB	C3C-C4C-NC	2.84	110.89	108.33
82	lF	201	PEB	CAB-CBB-CGB	-2.84	107.50	113.60
82	O1	201	PEB	OD-C4D-ND	-2.84	121.73	125.93
82	nF	201	PEB	OD-C4D-ND	-2.84	121.73	125.93
82	hJ	201	PEB	CAA-C3A-C4A	-2.84	105.39	112.67
87	cL	508	CLA	CMB-C2B-C1B	-2.84	121.05	125.37
82	F7	201	PEB	CHA-C1B-NB	-2.84	119.00	124.93
82	A4	301	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
82	Q4	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	mO	202	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	AD	304	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	GJ	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	hE	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
82	pF	201	PEB	CAB-CBB-CGB	-2.84	107.50	113.60
84	e3	1001	CYC	OC-C1C-C2C	-2.84	123.92	126.17
82	OE	203	PEB	CMC-C3C-C4C	2.84	130.07	127.06
82	KK	202	PEB	OD-C4D-ND	-2.84	121.73	125.93
82	A4	305	PEB	OD-C4D-ND	-2.84	121.73	125.93
87	AN	810	CLA	C3B-C4B-NB	-2.84	107.88	110.52
82	JB	201	PEB	C3B-C4B-NB	2.84	114.18	110.05
82	WH	202	PEB	C3B-C4B-NB	2.84	114.18	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WB	402	PEB	CMB-C2B-C1B	2.84	129.43	125.06
83	xK	305	PUB	CHB-C1C-NC	-2.84	118.67	124.58
82	cK	203	PEB	CHC-C1D-ND	-2.84	110.14	113.72
87	4N	608	CLA	CMA-C3A-C4A	-2.84	104.15	111.77
82	JP	201	PEB	CHA-C1B-NB	-2.84	119.00	124.93
82	H5	201	PEB	CHA-C1B-NB	-2.84	119.00	124.93
82	QO	201	PEB	CHB-C1C-C2C	-2.84	120.75	127.15
82	S1	202	PEB	C3D-C4D-ND	2.84	112.83	107.26
82	AQ	303	PEB	CHB-C1C-NC	-2.84	118.82	125.32
82	AA	202	PEB	C3B-C4B-NB	2.84	114.17	110.05
84	D1	1001	CYC	CHB-C4A-NA	-2.84	119.00	124.93
82	QK	201	PEB	CHC-C1D-ND	-2.84	110.14	113.72
82	k1	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	WH	203	PEB	CAC-C2C-C1C	2.84	130.28	125.76
82	O5	201	PEB	CAC-C2C-C1C	2.84	130.28	125.76
82	lF	203	PEB	C1D-CHC-C4C	2.84	117.44	113.26
87	AN	840	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
82	i4	203	PEB	OA-C1A-C2A	-2.84	123.92	126.17
84	c3	1001	CYC	OC-C1C-C2C	-2.84	123.92	126.17
87	CL	518	CLA	C3B-C4B-NB	-2.84	107.88	110.52
82	Q7	201	PEB	C1C-NC-C4C	-2.84	104.55	109.60
83	yF	303	PUB	OD-C4D-ND	-2.84	121.73	125.93
82	W1	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
82	HQ	202	PEB	C3B-C4B-NB	2.84	114.17	110.05
87	c6	604	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
94	D6	408	PL9	C35-C34-C36	2.84	120.04	115.27
82	DM	202	PEB	CAB-C3B-C4B	2.84	130.03	125.01
82	tC	202	PEB	OD-C4D-C3D	-2.84	123.04	129.46
82	bP	502	PEB	OD-C4D-C3D	-2.84	123.04	129.46
84	m3	1001	CYC	C1D-C2D-C3D	-2.84	104.18	107.79
82	ZI	401	PEB	OD-C4D-ND	-2.84	121.73	125.93
82	H9	203	PEB	CMB-C2B-C1B	2.84	129.43	125.06
87	cL	506	CLA	C3B-C4B-NB	-2.83	107.89	110.52
82	SG	201	PEB	CHA-C1B-NB	-2.83	119.00	124.93
82	BB	201	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
82	CP	203	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
84	F4	1001	CYC	C4D-CHA-C1A	2.83	134.64	128.28
82	MQ	201	PEB	CHB-C4B-C3B	-2.83	118.76	125.32
87	AN	810	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
82	AB	501	PEB	OD-C4D-ND	-2.83	121.73	125.93
87	32	302	CLA	CHD-C1D-C2D	2.83	131.43	125.48
82	SB	202	PEB	CHA-C1B-NB	-2.83	119.00	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jO	201	PEB	OD-C4D-C3D	-2.83	123.04	129.46
82	MD	201	PEB	CHC-C4C-NC	2.83	124.98	121.15
82	U4	201	PEB	CHC-C4C-NC	2.83	124.98	121.15
82	eB	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	pK	201	PEB	CAB-CBB-CGB	-2.83	107.50	113.60
87	72	605	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
82	AQ	304	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
82	j1	202	PEB	C2A-C1A-NA	2.83	110.72	108.27
83	yF	302	PUB	CAD-C3D-C4D	2.83	125.85	121.38
82	Z9	301	PEB	CMB-C2B-C1B	2.83	129.43	125.06
82	PH	201	PEB	CHC-C4C-NC	2.83	124.98	121.15
84	J3	1001	CYC	C1D-C2D-C3D	-2.83	104.18	107.79
95	b6	621	DGD	O6E-C1E-C2E	2.83	116.35	110.35
82	VD	202	PEB	OA-C1A-C2A	-2.83	123.92	126.17
82	NB	203	PEB	CMC-C3C-C4C	2.83	130.06	127.06
82	U4	202	PEB	OD-C4D-C3D	-2.83	123.04	129.46
87	HL	102	CLA	CHB-C4A-NA	2.83	128.43	124.51
82	pF	201	PEB	OD-C4D-ND	-2.83	121.73	125.93
82	GK	203	PEB	CHC-C1D-ND	-2.83	110.14	113.72
82	OP	201	PEB	CHA-C1B-NB	-2.83	119.01	124.93
82	YE	202	PEB	CAC-C2C-C3C	2.83	133.56	127.07
82	hE	203	PEB	C2A-C1A-NA	2.83	110.72	108.27
82	D7	201	PEB	CHA-C4A-NA	2.83	128.57	125.20
82	RP	202	PEB	OD-C4D-C3D	-2.83	123.04	129.46
82	iF	201	PEB	OD-C4D-C3D	-2.83	123.04	129.46
87	BN	825	CLA	CHB-C4A-NA	2.83	128.43	124.51
85	JN	102	BCR	C37-C22-C23	2.83	122.54	118.08
82	NA	203	PEB	C3C-C4C-NC	2.83	110.88	108.33
82	fO	202	PEB	CHA-C1B-NB	-2.83	119.01	124.93
82	dH	201	PEB	OD-C4D-ND	-2.83	121.73	125.93
82	YF	203	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	TB	201	PEB	C3B-C4B-NB	2.83	114.17	110.05
82	YP	503	PEB	C3B-C4B-NB	2.83	114.17	110.05
83	yK	303	PUB	C2C-C1C-NC	2.83	114.17	110.05
82	DA	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	YQ	202	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	aF	203	PEB	C4C-C3C-C2C	-2.83	104.89	107.50
87	BN	830	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
87	B2	830	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
82	NH	1002	PEB	OD-C4D-ND	-2.83	121.73	125.93
82	QH	202	PEB	OD-C4D-ND	-2.83	121.73	125.93
82	HI	202	PEB	CHB-C4B-NB	-2.83	118.68	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LK	202	PEB	OD-C4D-C3D	-2.83	123.04	129.46
82	Z5	304	PEB	OD-C4D-C3D	-2.83	123.04	129.46
82	K9	201	PEB	OD-C4D-C3D	-2.83	123.04	129.46
82	mJ	202	PEB	CAA-C3A-C2A	-2.83	107.18	114.26
84	N1	1001	CYC	C2B-C1B-NB	2.83	111.13	106.99
82	RK	201	PEB	C3B-C4B-NB	2.83	114.17	110.05
82	A1	305	PEB	CHA-C1B-NB	-2.83	119.01	124.93
82	F5	203	PEB	CHA-C1B-NB	-2.83	119.01	124.93
82	qF	203	PEB	CAB-C3B-C4B	2.83	130.02	125.01
87	42	601	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
87	B6	612	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
82	eB	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	RB	202	PEB	CHC-C4C-NC	2.83	124.98	121.15
82	kF	201	PEB	CHC-C4C-NC	2.83	124.98	121.15
82	IA	202	PEB	C1D-CHC-C4C	-2.83	109.08	113.26
83	yK	302	PUB	CAD-C3D-C4D	2.83	125.85	121.38
82	UE	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
84	G3	1001	CYC	OC-C1C-C2C	-2.83	123.92	126.17
87	5N	606	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
82	mG	203	PEB	CAB-C3B-C4B	2.83	130.02	125.01
82	R9	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
96	GN	201	HEM	C4C-NC-C1C	2.83	108.12	105.35
84	HG	1001	CYC	C1A-C2A-C3A	-2.83	103.65	106.78
82	JF	201	PEB	CAC-C2C-C1C	2.83	130.27	125.76
82	KG	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	iF	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
83	xK	306	PUB	OD-C4D-ND	-2.83	121.74	125.93
82	O7	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
82	BM	301	PEB	C2A-C1A-NA	2.83	110.71	108.27
82	e4	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
82	Z5	305	PEB	C2A-C1A-NA	2.83	110.71	108.27
82	N7	202	PEB	C1C-NC-C4C	-2.83	104.56	109.60
82	gK	201	PEB	CMB-C2B-C3B	-2.83	118.43	126.12
82	SE	201	PEB	CHA-C1B-NB	-2.83	119.01	124.93
85	a6	605	BCR	C20-C21-C22	-2.83	123.27	127.31
82	OI	202	PEB	C1D-CHC-C4C	-2.83	109.08	113.26
82	HI	201	PEB	CHC-C4C-NC	2.83	124.98	121.15
82	IP	203	PEB	CMB-C2B-C1B	2.83	129.42	125.06
82	f1	202	PEB	OA-C1A-C2A	-2.83	123.92	126.17
82	z8	202	PEB	OA-C1A-C2A	-2.83	123.92	126.17
82	ZG	203	PEB	OD-C4D-ND	-2.83	121.74	125.93
84	FO	1001	CYC	C4D-CHA-C1A	2.83	134.63	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MJ	203	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	P7	202	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	bF	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	aG	202	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	KF	202	PEB	OD-C4D-C3D	-2.83	123.05	129.46
82	aE	201	PEB	CAB-C3B-C4B	2.83	130.01	125.01
82	GP	201	PEB	CHA-C1B-NB	-2.83	119.02	124.93
82	l4	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
82	hJ	203	PEB	OD-C4D-C3D	-2.83	123.05	129.46
82	EP	202	PEB	OD-C4D-ND	-2.83	121.74	125.93
82	M5	304	PEB	OD-C4D-ND	-2.83	121.74	125.93
87	AN	811	CLA	CHB-C4A-NA	2.83	128.42	124.51
87	B2	820	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
87	4N	611	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
84	BG	1002	CYC	C2A-C1A-NA	2.83	114.16	110.05
85	J2	102	BCR	C37-C22-C23	2.83	122.53	118.08
82	aG	201	PEB	CAB-C3B-C4B	2.83	130.01	125.01
82	eH	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	OB	201	PEB	CMB-C2B-C1B	2.83	129.42	125.06
82	a4	201	PEB	CHC-C4C-NC	2.83	124.98	121.15
82	DM	202	PEB	CHC-C1D-ND	-2.83	110.15	113.72
87	A2	840	CLA	CHB-C4A-NA	2.83	128.42	124.51
82	OA	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
82	kE	201	PEB	CAB-C3B-C4B	2.83	130.01	125.01
82	V1	203	PEB	C3B-C4B-NB	2.83	114.16	110.05
82	tF	202	PEB	CHB-C1C-C2C	-2.83	120.77	127.15
82	L9	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	KA	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	cK	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	U5	201	PEB	CHA-C1B-NB	-2.83	119.02	124.93
82	QJ	204	PEB	C3B-C4B-NB	2.83	114.16	110.05
82	SP	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
82	m4	202	PEB	OD-C4D-C3D	-2.83	123.05	129.46
84	m3	1001	CYC	OC-C1C-C2C	-2.83	123.92	126.17
84	IO	1001	CYC	C4D-CHA-C1A	2.83	134.62	128.28
87	62	309	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
82	bP	501	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
82	VQ	201	PEB	C2A-C1A-NA	2.83	110.71	108.27
82	fE	201	PEB	C2A-C1A-NA	2.83	110.71	108.27
87	AN	840	CLA	CHB-C4A-NA	2.83	128.42	124.51
95	cL	520	DGD	O1G-C1A-C2A	2.83	120.78	111.91
84	K4	1001	CYC	C4D-C3D-C2D	-2.83	104.28	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aM	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
87	AN	802	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
87	6N	608	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
82	VB	201	PEB	CHA-C1B-NB	-2.83	119.02	124.93
82	FP	201	PEB	CAC-C2C-C1C	2.83	130.26	125.76
82	A1	301	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
82	II	201	PEB	OA-C1A-C2A	-2.83	123.93	126.17
82	NI	201	PEB	OA-C1A-C2A	-2.83	123.93	126.17
82	U1	202	PEB	OA-C1A-C2A	-2.83	123.93	126.17
82	ZF	201	PEB	CHB-C4B-NB	-2.83	118.70	124.58
82	iM	201	PEB	CHA-C1B-C2B	2.83	132.17	124.90
82	YE	201	PEB	CAB-CBB-CGB	-2.83	107.52	113.60
82	M9	301	PEB	CAC-CBC-CGC	-2.83	107.52	113.60
82	a1	201	PEB	C2A-C1A-NA	2.83	110.71	108.27
82	YG	202	PEB	CAC-C2C-C3C	2.83	133.54	127.07
84	JO	1001	CYC	C1B-NB-C4B	-2.83	107.07	110.67
84	J4	1001	CYC	C1B-NB-C4B	-2.83	107.07	110.67
84	FO	1001	CYC	CHA-C4D-C3D	-2.83	120.78	127.15
82	ZO	201	PEB	CHC-C4C-NC	2.83	124.97	121.15
87	42	605	CLA	C3A-C2A-C1A	2.83	105.57	101.34
82	k1	201	PEB	CAB-C3B-C4B	2.83	130.01	125.01
82	L9	203	PEB	CAB-C3B-C4B	2.83	130.01	125.01
82	h4	201	PEB	C4B-NB-C1B	-2.83	101.19	106.51
82	S5	201	PEB	CAC-C2C-C3C	2.83	133.54	127.07
82	MJ	202	PEB	CHB-C1C-C2C	-2.83	120.78	127.15
82	BD	202	PEB	C4B-C3B-C2B	-2.83	103.66	106.78
82	kJ	201	PEB	CHB-C4B-NB	-2.83	118.70	124.58
82	Y1	201	PEB	OD-C4D-ND	-2.83	121.75	125.93
82	kF	201	PEB	CMC-C3C-C4C	2.83	130.06	127.06
82	GG	1002	PEB	CBB-CAB-C3B	2.82	120.48	112.63
82	HA	203	PEB	CAC-CBC-CGC	-2.82	107.52	113.60
87	A2	810	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
82	QB	201	PEB	CMB-C2B-C1B	2.82	129.41	125.06
82	Y5	203	PEB	C3B-C4B-NB	2.82	114.16	110.05
82	P9	201	PEB	OD-C4D-C3D	-2.82	123.06	129.46
82	VH	201	PEB	CHB-C4B-C3B	-2.82	118.78	125.32
82	oK	202	PEB	C2A-C1A-NA	2.82	110.71	108.27
84	L4	1001	CYC	CHD-C1D-ND	-2.82	118.85	125.32
82	SQ	202	PEB	C1C-CHB-C4B	2.82	134.62	128.28
82	UG	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
87	L2	206	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
82	T9	201	PEB	OD-C4D-C3D	-2.82	123.06	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W1	203	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
82	aK	203	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
87	AN	825	CLA	C3B-C4B-NB	-2.82	107.89	110.52
87	RN	204	CLA	C3B-C4B-NB	-2.82	107.89	110.52
87	K2	104	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
82	eK	202	PEB	C1D-CHC-C4C	-2.82	109.09	113.26
87	A2	852	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
83	AG	302	PUB	C2B-C1B-NB	2.82	110.88	108.33
82	J7	203	PEB	CHC-C1D-ND	-2.82	110.15	113.72
85	B2	839	BCR	C15-C16-C17	-2.82	117.69	123.47
82	Q4	201	PEB	OA-C1A-C2A	-2.82	123.93	126.17
82	TA	203	PEB	C4C-C3C-C2C	-2.82	104.89	107.50
83	K7	203	PUB	CAC-CBC-CGC	-2.82	107.53	113.60
82	OH	201	PEB	C2A-C1A-NA	2.82	110.71	108.27
82	OD	202	PEB	OD-C4D-C3D	-2.82	123.06	129.46
82	TQ	202	PEB	C3B-C4B-NB	2.82	114.16	110.05
82	A7	202	PEB	C3B-C4B-NB	2.82	114.16	110.05
87	a6	607	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
82	AO	301	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
82	dE	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
82	tK	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
82	dK	201	PEB	C1D-CHC-C4C	-2.82	109.09	113.26
82	GE	1002	PEB	CBB-CAB-C3B	2.82	120.47	112.63
82	gK	201	PEB	CMC-C3C-C4C	2.82	130.05	127.06
87	B2	811	CLA	C3B-C4B-NB	-2.82	107.90	110.52
83	xK	306	PUB	OA-C1A-NA	-2.82	121.75	125.93
82	sC	202	PEB	CMA-C2A-C1A	-2.82	106.32	112.40
82	RP	201	PEB	CHC-C1D-ND	-2.82	110.15	113.72
87	B2	824	CLA	CHA-C1A-NA	-2.82	119.93	126.40
95	AL	416	DGD	O5D-C6D-C5D	2.82	114.27	109.05
82	G7	201	PEB	C3C-C4C-NC	2.82	110.87	108.33
85	kL	100	BCR	C1-C6-C5	-2.82	118.64	122.61
82	MK	201	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
82	jO	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
82	Q5	202	PEB	C4C-C3C-C2C	-2.82	104.89	107.50
82	KB	304	PEB	C2A-C1A-NA	2.82	110.71	108.27
82	PQ	203	PEB	C2A-C1A-NA	2.82	110.71	108.27
82	s8	202	PEB	C2A-C1A-NA	2.82	110.71	108.27
82	EJ	202	PEB	CMA-C2A-C1A	-2.82	106.32	112.40
87	8N	302	CLA	CHB-C4A-NA	2.82	128.41	124.51
82	SF	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	g4	201	PEB	OD-C4D-ND	-2.82	121.75	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	CL	511	CLA	CMB-C2B-C3B	2.82	133.42	126.59
82	eE	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
87	AN	852	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
82	UQ	201	PEB	C4C-C3C-C2C	-2.82	104.90	107.50
82	Q4	201	PEB	C4C-C3C-C2C	-2.82	104.90	107.50
82	SH	202	PEB	CHB-C1C-NC	-2.82	118.86	125.32
82	LM	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
91	a6	613	PHO	CMA-C3A-C4A	-2.82	108.20	114.38
82	AQ	301	PEB	CAC-CBC-CGC	-2.82	107.53	113.60
84	D4	1001	CYC	CAD-CBD-CGD	-2.82	107.53	113.60
82	TP	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
84	c3	1001	CYC	C1D-C2D-C3D	-2.82	104.20	107.79
82	SQ	202	PEB	OA-C1A-C2A	-2.82	123.93	126.17
87	BL	601	CLA	C3B-C4B-NB	-2.82	107.90	110.52
87	D6	405	CLA	C3B-C4B-NB	-2.82	107.90	110.52
82	BD	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	I7	201	PEB	CHB-C1C-C2C	-2.82	120.79	127.15
94	DL	401	PL9	C53-C6-C1	2.82	120.76	114.99
87	b6	617	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
87	B2	816	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
82	kE	201	PEB	OD-C4D-C3D	-2.82	123.07	129.46
82	GK	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
87	72	602	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
87	6N	612	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
82	YG	202	PEB	CHC-C1D-ND	-2.82	110.16	113.72
82	s8	202	PEB	CHC-C1D-ND	-2.82	110.16	113.72
87	42	611	CLA	CHB-C4A-NA	2.82	128.41	124.51
82	cM	202	PEB	OD-C4D-C3D	-2.82	123.07	129.46
82	T1	202	PEB	CMB-C2B-C1B	2.82	129.41	125.06
82	SI	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	e1	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	lJ	203	PEB	CAC-C2C-C1C	2.82	130.25	125.76
92	D6	407	LMG	O6-C5-C6	2.82	113.45	106.44
85	b6	602	BCR	C35-C13-C14	-2.82	118.97	122.92
85	L2	205	BCR	C4-C5-C6	-2.82	118.64	122.73
82	D7	201	PEB	OD-C4D-C3D	-2.82	123.07	129.46
82	D9	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
84	FH	1001	CYC	C2A-C1A-NA	2.82	114.15	110.05
82	dM	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	VB	201	PEB	CHB-C4B-C3B	-2.82	118.80	125.32
82	F7	203	PEB	OD-C4D-C3D	-2.82	123.07	129.46
82	V9	201	PEB	OD-C4D-C3D	-2.82	123.07	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GB	201	PEB	CHC-C1D-ND	-2.82	110.16	113.72
94	dL	406	PL9	C53-C6-C1	2.82	120.75	114.99
82	RA	201	PEB	CAC-CBC-CGC	-2.82	107.54	113.60
83	KA	203	PUB	CAC-CBC-CGC	-2.82	107.54	113.60
82	f1	203	PEB	C2A-C1A-NA	2.82	110.70	108.27
82	jF	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
87	22	612	CLA	C3B-C4B-NB	-2.82	107.90	110.52
87	A2	811	CLA	CHC-C4B-NB	2.82	127.24	124.26
87	b6	609	CLA	CHB-C1B-NB	2.82	127.24	124.26
87	2N	303	CLA	CHB-C1B-NB	2.82	127.24	124.26
82	YI	202	PEB	CHA-C1B-NB	-2.82	119.04	124.93
82	z8	202	PEB	CHB-C4B-C3B	2.82	131.84	125.32
84	DO	1001	CYC	C4D-CHA-C1A	2.82	134.60	128.28
82	KD	202	PEB	OD-C4D-C3D	-2.82	123.07	129.46
82	AE	304	PEB	OA-C1A-C2A	-2.82	123.93	126.17
84	T3	1001	CYC	OC-C1C-C2C	-2.82	123.93	126.17
82	PO	203	PEB	CAC-CBC-CGC	-2.82	107.54	113.60
82	MM	203	PEB	OD-C4D-ND	-2.82	121.75	125.93
82	D1	1002	PEB	OD-C4D-ND	-2.82	121.75	125.93
82	YD	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	Q9	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
87	c6	616	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
82	H9	203	PEB	CHC-C4C-NC	2.82	124.96	121.15
82	hK	202	PEB	CHA-C1B-NB	-2.82	119.04	124.93
87	52	606	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
82	BI	203	PEB	OD-C4D-C3D	-2.82	123.08	129.46
82	E9	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
82	LP	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
82	eB	201	PEB	C2A-C1A-NA	2.82	110.70	108.27
95	DL	408	DGD	O1G-C1A-C2A	2.82	120.75	111.91
82	PG	201	PEB	OD-C4D-ND	-2.82	121.76	125.93
83	yK	303	PUB	OD-C4D-ND	-2.82	121.76	125.93
82	H9	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
82	OG	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
82	dE	202	PEB	C1D-CHC-C4C	-2.82	109.10	113.26
82	QG	203	PEB	C4C-C3C-C2C	-2.82	104.90	107.50
87	CL	504	CLA	CHB-C1B-NB	2.82	127.24	124.26
82	VA	202	PEB	CHA-C4A-NA	2.82	128.55	125.20
87	BN	821	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
87	BN	825	CLA	CHA-C1A-NA	-2.82	119.95	126.40
82	DD	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
82	AK	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	w8	203	PEB	C2A-C1A-NA	2.82	110.70	108.27
82	oF	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
82	SO	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
82	H9	203	PEB	CHB-C4B-NB	-2.82	118.72	124.58
87	2N	312	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
87	b6	609	CLA	CMB-C2B-C1B	-2.82	121.08	125.37
87	BN	819	CLA	CHB-C4A-NA	2.82	128.41	124.51
94	a6	601	PL9	C20-C19-C21	2.82	120.01	115.27
82	RJ	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
82	mE	203	PEB	CAB-C3B-C4B	2.82	129.99	125.01
87	cL	506	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
82	H5	202	PEB	C1B-C2B-C3B	-2.82	103.28	106.51
103	82	310	ZEX	C16-C1-C17	2.82	117.17	108.53
82	OE	201	PEB	CAA-C3A-C2A	-2.82	107.22	114.26
82	S7	201	PEB	C1C-NC-C4C	-2.82	104.59	109.60
87	FN	205	CLA	CAA-C2A-C3A	-2.82	105.07	112.78
87	K2	103	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
87	bL	617	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
82	UM	201	PEB	C3B-C4B-NB	2.82	114.14	110.05
82	NB	202	PEB	CMB-C2B-C1B	2.81	129.40	125.06
83	QM	201	PUB	OD-C4D-ND	-2.81	121.76	125.93
82	QF	201	PEB	CHC-C1D-ND	-2.81	110.16	113.72
82	xC	201	PEB	C4C-C3C-C2C	-2.81	104.90	107.50
82	PE	201	PEB	CMC-C3C-C4C	2.81	130.04	127.06
87	A2	812	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
82	GF	202	PEB	OD-C4D-C3D	-2.81	123.08	129.46
82	GD	202	PEB	CHC-C4C-NC	2.81	124.96	121.15
82	vC	201	PEB	CHC-C4C-NC	2.81	124.96	121.15
82	XM	201	PEB	C1D-CHC-C4C	2.81	117.41	113.26
82	L5	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
87	3N	303	CLA	CHD-C1D-C2D	2.81	131.38	125.48
87	DL	403	CLA	CMB-C2B-C1B	-2.81	121.08	125.37
82	KK	202	PEB	OD-C4D-C3D	-2.81	123.08	129.46
82	aF	201	PEB	C1C-CHB-C4B	2.81	134.59	128.28
84	MG	1001	CYC	CMB-C2B-C1B	2.81	127.68	124.17
87	B2	807	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
82	RE	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
82	W5	201	PEB	CHA-C1B-NB	-2.81	119.05	124.93
87	2N	312	CLA	C3B-C4B-NB	-2.81	107.91	110.52
87	4N	607	CLA	C3B-C4B-NB	-2.81	107.91	110.52
82	TH	201	PEB	CHC-C1D-ND	-2.81	110.17	113.72
82	g4	203	PEB	OD-C4D-C3D	-2.81	123.09	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gB	203	PEB	CBB-CAB-C3B	-2.81	104.81	112.63
87	8N	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
82	DQ	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
82	rC	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
82	dE	203	PEB	CHC-C4C-NC	2.81	124.96	121.15
82	UQ	201	PEB	OD-C4D-ND	-2.81	121.76	125.93
96	G2	201	HEM	CBB-CAB-C3B	-2.81	113.62	127.62
82	UO	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	eB	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
87	A2	801	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
87	6N	610	CLA	C2A-C1A-CHA	2.81	128.78	123.86
85	L2	201	BCR	C11-C10-C9	-2.81	123.30	127.31
88	l6	101	LHG	O8-C23-C24	2.81	120.73	111.91
82	qK	202	PEB	CAB-C3B-C2B	-2.81	122.64	127.88
82	UP	202	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
82	g4	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
82	iE	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
84	CO	1001	CYC	C2A-C1A-NA	2.81	114.14	110.05
82	ZK	202	PEB	C1C-CHB-C4B	2.81	134.59	128.28
82	YG	201	PEB	CAB-CBB-CGB	-2.81	107.55	113.60
82	W7	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
85	A2	847	BCR	C23-C22-C21	-2.81	114.63	118.94
82	t8	201	PEB	C2A-C1A-NA	2.81	110.70	108.27
82	eG	201	PEB	C2A-C1A-NA	2.81	110.70	108.27
82	eK	202	PEB	CHC-C1D-ND	-2.81	110.17	113.72
82	ND	203	PEB	C1D-CHC-C4C	-2.81	109.11	113.26
82	O4	201	PEB	C1D-CHC-C4C	-2.81	109.11	113.26
82	KK	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
85	c6	617	BCR	C36-C18-C19	2.81	122.51	118.08
87	AL	403	CLA	C2D-C1D-ND	-2.81	108.03	110.10
87	AN	831	CLA	C2D-C1D-ND	-2.81	108.03	110.10
82	C9	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	N9	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
84	J4	1001	CYC	C4D-CHA-C1A	2.81	134.59	128.28
82	TF	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
87	A2	849	CLA	CHB-C1B-NB	2.81	127.23	124.26
82	j4	203	PEB	CMB-C2B-C1B	2.81	129.39	125.06
82	SG	201	PEB	C1D-CHC-C4C	-2.81	109.11	113.26
82	I9	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
84	GO	1001	CYC	C2A-C1A-NA	2.81	114.14	110.05
84	G4	1001	CYC	C2A-C1A-NA	2.81	114.14	110.05
82	MP	202	PEB	CHC-C1D-ND	-2.81	110.17	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	j4	201	PEB	OA-C1A-C2A	-2.81	123.94	126.17
84	E3	1001	CYC	OC-C1C-C2C	-2.81	123.94	126.17
85	LN	205	BCR	C4-C5-C6	-2.81	118.65	122.73
82	uF	203	PEB	CHA-C4A-NA	2.81	128.55	125.20
82	iF	203	PEB	CHC-C4C-NC	2.81	124.95	121.15
82	OJ	202	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
82	D9	202	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
82	ZK	202	PEB	CAB-C3B-C4B	2.81	129.98	125.01
82	j4	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	xC	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	QJ	204	PEB	C4C-C3C-C2C	-2.81	104.91	107.50
82	QO	201	PEB	C4C-C3C-C2C	-2.81	104.91	107.50
82	AD	301	PEB	CAC-CBC-CGC	-2.81	107.56	113.60
82	F7	202	PEB	CMB-C2B-C1B	2.81	129.39	125.06
82	iG	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
82	P7	203	PEB	CHB-C4B-C3B	-2.81	118.82	125.32
82	PG	202	PEB	C1D-CHC-C4C	2.81	117.40	113.26
82	BB	203	PEB	OD-C4D-ND	-2.81	121.77	125.93
82	gB	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
82	DF	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	iO	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
95	BL	614	DGD	O6E-C1E-C2E	2.81	116.30	110.35
82	rK	201	PEB	OA-C1A-NA	2.81	128.34	124.94
82	AA	201	PEB	CMB-C2B-C1B	2.81	129.39	125.06
82	FF	201	PEB	CHA-C1B-NB	-2.81	119.06	124.93
82	FO	1002	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
82	SI	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
82	YK	203	PEB	C2A-C1A-NA	2.81	110.69	108.27
87	BN	835	CLA	CHB-C4A-NA	2.81	128.40	124.51
82	OK	203	PEB	C4C-C3C-C2C	-2.81	104.91	107.50
82	iG	202	PEB	CHC-C4C-NC	2.81	124.95	121.15
82	OQ	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	B9	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
82	SK	201	PEB	C3C-C4C-NC	2.81	110.86	108.33
82	M7	201	PEB	C3C-C4C-NC	2.81	110.86	108.33
84	I4	1001	CYC	C4D-CHA-C1A	2.81	134.58	128.28
82	UQ	201	PEB	CHA-C4A-NA	2.81	128.54	125.20
85	BL	616	BCR	C20-C21-C22	-2.81	123.30	127.31
84	LH	1002	CYC	OB-C4B-C3B	-2.81	124.99	128.04
82	SP	202	PEB	CMA-C2A-C1A	-2.81	106.35	112.40
82	A4	305	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
84	J1	1001	CYC	CHA-C4D-C3D	-2.81	120.81	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U4	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
82	ZH	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
82	cK	202	PEB	CHC-C1D-ND	-2.81	110.17	113.72
94	dL	406	PL9	C11-C12-C13	-2.81	102.65	111.88
82	QA	201	PEB	C1C-NC-C4C	-2.81	104.60	109.60
87	62	309	CLA	C2C-C1C-NC	2.81	112.60	109.97
84	J3	1001	CYC	OC-C1C-C2C	-2.81	123.94	126.17
84	d3	1001	CYC	CHA-C4D-C3D	-2.81	120.81	127.15
82	ZB	203	PEB	C2A-C1A-NA	2.81	110.69	108.27
82	CM	203	PEB	C2A-C1A-NA	2.81	110.69	108.27
82	qF	203	PEB	C2A-C1A-NA	2.81	110.69	108.27
82	cB	403	PEB	C4C-C3C-C2C	-2.81	104.91	107.50
87	8N	301	CLA	CMB-C2B-C3B	2.81	133.39	126.59
87	AN	849	CLA	CHB-C1B-NB	2.81	127.23	124.26
82	VH	202	PEB	C3B-C4B-NB	2.81	114.13	110.05
82	bP	501	PEB	C3B-C4B-NB	2.81	114.13	110.05
82	GF	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
103	8N	310	ZEX	C16-C1-C17	2.81	117.15	108.53
87	A2	851	CLA	C3B-C4B-NB	-2.81	107.91	110.52
82	MF	203	PEB	C1C-NC-C4C	-2.81	104.60	109.60
84	FG	1001	CYC	CMA-C3A-C4A	2.81	129.39	125.06
82	VM	201	PEB	CHC-C1D-ND	2.81	117.28	113.72
87	A2	831	CLA	C2D-C1D-ND	-2.81	108.03	110.10
82	IA	201	PEB	CHB-C1C-C2C	-2.81	120.82	127.15
82	S1	202	PEB	CHB-C1C-NC	-2.81	118.89	125.32
85	c6	603	BCR	C20-C19-C18	-2.81	118.53	126.42
84	C3	1001	CYC	OC-C1C-C2C	-2.81	123.94	126.17
82	ID	202	PEB	CMC-C3C-C4C	2.81	130.04	127.06
82	QI	201	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
82	ZK	202	PEB	CHC-C1D-ND	2.81	117.28	113.72
82	Y1	202	PEB	C3B-C4B-NB	2.81	114.13	110.05
82	bH	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
83	xF	301	PUB	CBA-CAA-C3A	-2.81	108.72	112.98
82	bK	201	PEB	CHC-C4C-NC	2.81	124.95	121.15
87	6N	608	CLA	C2C-C1C-NC	2.81	112.60	109.97
84	o3	1001	CYC	CHA-C4D-C3D	-2.81	120.82	127.15
82	DA	201	PEB	OD-C4D-C3D	-2.81	123.10	129.46
82	ZE	203	PEB	C3B-C4B-NB	2.81	114.13	110.05
82	eG	202	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
84	LG	1001	CYC	C1A-C2A-C3A	-2.81	103.68	106.78
82	BD	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
82	qK	201	PEB	CHA-C1B-C2B	2.81	132.12	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VD	201	PEB	C1C-CHB-C4B	-2.81	121.99	128.28
82	XA	203	PEB	C1B-C2B-C3B	-2.81	103.29	106.51
82	qF	202	PEB	CAB-C3B-C2B	-2.81	122.65	127.88
82	RD	202	PEB	OA-C1A-C2A	-2.81	123.94	126.17
82	GA	201	PEB	C3C-C4C-NC	2.81	110.86	108.33
87	4N	611	CLA	CHB-C4A-NA	2.81	128.39	124.51
82	i4	201	PEB	OD-C4D-C3D	-2.81	123.10	129.46
82	gB	202	PEB	OD-C4D-C3D	-2.81	123.10	129.46
82	N9	201	PEB	CHC-C4C-NC	2.81	124.95	121.15
82	lG	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
84	L3	1001	CYC	CHA-C4D-C3D	-2.81	120.82	127.15
82	MJ	203	PEB	OD-C4D-C3D	-2.81	123.10	129.46
82	O4	202	PEB	OD-C4D-C3D	-2.81	123.10	129.46
82	eK	201	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
85	k6	102	BCR	C38-C26-C25	-2.81	121.38	124.53
82	TF	202	PEB	CAA-C3A-C4A	-2.81	105.47	112.67
82	DA	201	PEB	CHA-C4A-NA	2.80	128.54	125.20
82	OO	202	PEB	OD-C4D-C3D	-2.80	123.11	129.46
82	QK	202	PEB	C3B-C4B-NB	2.80	114.13	110.05
82	KA	202	PEB	CMB-C2B-C1B	2.80	129.38	125.06
82	vC	202	PEB	CMB-C2B-C1B	2.80	129.38	125.06
82	YO	202	PEB	CAB-C3B-C4B	2.80	129.97	125.01
82	kK	203	PEB	OD-C4D-C3D	-2.80	123.11	129.46
87	AN	807	CLA	CHB-C4A-NA	2.80	128.39	124.51
82	QK	203	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
82	fF	202	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
88	L6	101	LHG	O8-C23-C24	2.80	120.71	111.91
82	Z4	201	PEB	CHC-C4C-NC	2.80	124.94	121.15
87	c6	613	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
82	IB	202	PEB	CAB-C3B-C4B	2.80	129.97	125.01
84	L1	1001	CYC	C1B-CHB-C4A	-2.80	121.23	128.08
82	ZB	201	PEB	C2A-C1A-NA	2.80	110.69	108.27
82	wC	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
87	b6	617	CLA	C3B-C4B-NB	-2.80	107.91	110.52
84	q3	1001	CYC	CHA-C4D-C3D	-2.80	120.83	127.15
82	SI	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
82	XQ	202	PEB	OD-C4D-C3D	-2.80	123.11	129.46
82	i1	201	PEB	CHB-C4B-C3B	-2.80	118.83	125.32
82	ZF	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
82	aJ	204	PEB	C3B-C4B-NB	2.80	114.13	110.05
84	73	1002	CYC	C1B-CHB-C4A	2.80	134.93	128.08
85	B6	602	BCR	C33-C5-C6	-2.80	121.38	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GM	203	PEB	CHA-C1B-NB	-2.80	119.07	124.93
87	A2	825	CLA	CHB-C4A-NA	2.80	128.39	124.51
82	LJ	201	PEB	C4C-C3C-C2C	-2.80	104.91	107.50
82	x8	201	PEB	C4C-C3C-C2C	-2.80	104.91	107.50
87	BN	810	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
82	ND	202	PEB	C1D-CHC-C4C	2.80	117.39	113.26
82	KA	202	PEB	C3B-C4B-NB	2.80	114.13	110.05
82	W5	203	PEB	CMB-C2B-C1B	2.80	129.38	125.06
82	QG	203	PEB	CHC-C4C-NC	2.80	124.94	121.15
82	ZB	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
82	hF	202	PEB	C2A-C1A-NA	2.80	110.69	108.27
82	Q1	201	PEB	CAC-CBC-CGC	-2.80	107.57	113.60
82	Q9	201	PEB	CHA-C1B-C2B	-2.80	117.69	124.90
82	GI	202	PEB	OA-C1A-C2A	-2.80	123.94	126.17
84	p3	1001	CYC	OC-C1C-C2C	-2.80	123.94	126.17
82	WO	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
82	bF	201	PEB	CHC-C4C-NC	2.80	124.94	121.15
82	D9	201	PEB	CBA-CAA-C3A	-2.80	107.23	113.47
82	OG	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
82	aJ	204	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
82	L1	1002	PEB	CHA-C4A-NA	2.80	128.54	125.20
87	B2	821	CLA	C3B-C4B-NB	-2.80	107.92	110.52
82	HD	203	PEB	CMC-C3C-C4C	2.80	130.03	127.06
82	PB	201	PEB	C3C-C4C-NC	2.80	110.86	108.33
82	UO	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
82	GK	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
82	MK	201	PEB	C3B-C4B-NB	2.80	114.12	110.05
87	AN	812	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
87	A2	817	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
87	8N	308	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
84	u3	1001	CYC	CHA-C4D-C3D	-2.80	120.83	127.15
82	D9	202	PEB	OD-C4D-C3D	-2.80	123.11	129.46
87	F2	205	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
82	eH	203	PEB	CAA-C3A-C4A	-2.80	105.48	112.67
82	YB	202	PEB	CAB-CBB-CGB	-2.80	107.58	113.60
82	X9	201	PEB	CHC-C4C-NC	2.80	124.94	121.15
82	s8	202	PEB	CMA-C2A-C1A	-2.80	106.36	112.40
82	OK	202	PEB	CHA-C1B-C2B	2.80	132.10	124.90
82	cF	201	PEB	C1D-CHC-C4C	2.80	117.39	113.26
82	SG	203	PEB	OA-C1A-C2A	-2.80	123.95	126.17
82	AF	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
87	B2	828	CLA	CHB-C4A-NA	2.80	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bF	201	PEB	C4C-C3C-C2C	-2.80	104.92	107.50
82	AA	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
83	xF	306	PUB	OA-C1A-NA	-2.80	121.78	125.93
87	1N	602	CLA	CMC-C2C-C3C	2.80	133.72	126.12
82	D1	1002	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
84	JH	1003	CYC	C4D-CHA-C1A	2.80	134.56	128.28
87	32	309	CLA	CAA-C2A-C1A	2.80	121.15	111.97
82	kF	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
87	BL	601	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
82	SI	201	PEB	CHA-C1B-NB	-2.80	119.08	124.93
82	MA	201	PEB	C3C-C4C-NC	2.80	110.85	108.33
87	BL	621	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
87	B2	818	CLA	CHB-C4A-NA	2.80	128.38	124.51
85	Z6	101	BCR	C33-C5-C4	2.80	119.00	113.62
96	G2	201	HEM	C4C-NC-C1C	2.80	108.09	105.35
87	KN	103	CLA	CMB-C2B-C1B	-2.80	121.11	125.37
82	aO	203	PEB	OA-C1A-C2A	-2.80	123.95	126.17
82	FA	203	PEB	OD-C4D-C3D	-2.80	123.12	129.46
82	hM	201	PEB	CHA-C1B-NB	-2.80	119.08	124.93
82	TH	202	PEB	CMB-C2B-C1B	2.80	129.38	125.06
82	jE	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
87	AN	851	CLA	C3B-C4B-NB	-2.80	107.92	110.52
82	J9	201	PEB	O2B-CGB-CBB	2.80	123.02	114.03
87	B2	835	CLA	CHB-C4A-NA	2.80	128.38	124.51
87	82	308	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
82	O4	201	PEB	C2B-C1B-NB	2.80	116.50	110.53
82	bH	201	PEB	C3C-C4C-NC	2.80	110.85	108.33
82	ZO	201	PEB	OA-C1A-NA	2.80	128.33	124.94
82	PG	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
82	GD	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
82	JQ	203	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
82	KI	201	PEB	C1D-CHC-C4C	-2.80	109.13	113.26
82	EK	202	PEB	CMB-C2B-C1B	2.80	129.37	125.06
82	e4	203	PEB	OD-C4D-ND	-2.80	121.78	125.93
82	dM	203	PEB	OD-C4D-ND	-2.80	121.78	125.93
82	g1	201	PEB	C3B-C4B-NB	2.80	114.12	110.05
84	LE	1001	CYC	C2A-C1A-NA	2.80	114.12	110.05
82	OK	202	PEB	CMB-C2B-C3B	-2.80	118.52	126.12
87	A2	830	CLA	C3B-C4B-NB	-2.80	107.92	110.52
87	b6	618	CLA	C3B-C4B-NB	-2.80	107.92	110.52
82	V7	202	PEB	CHA-C4A-NA	2.80	128.53	125.20
82	SP	203	PEB	CHC-C4C-NC	2.80	124.94	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MQ	201	PEB	CHC-C4C-NC	2.80	124.94	121.15
82	gO	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
82	e1	202	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
82	M5	301	PEB	C2A-C1A-NA	2.80	110.69	108.27
82	F9	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
82	X9	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
84	K4	1001	CYC	CHA-C4D-C3D	-2.80	120.84	127.15
82	MM	202	PEB	CHA-C1B-C2B	2.80	132.09	124.90
82	AO	301	PEB	CAC-CBC-CGC	-2.80	107.58	113.60
82	A1	305	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
82	fF	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
87	52	607	CLA	CHB-C4A-NA	2.80	128.38	124.51
87	5N	607	CLA	CHB-C4A-NA	2.80	128.38	124.51
82	QA	202	PEB	CHA-C1B-NB	-2.80	119.08	124.93
82	x8	201	PEB	OA-C1A-C2A	-2.80	123.95	126.17
84	KH	1001	CYC	CHA-C1A-C2A	-2.80	118.85	125.32
82	YA	303	PEB	OD-C4D-C3D	-2.80	123.12	129.46
82	VJ	201	PEB	C1D-CHC-C4C	2.80	117.38	113.26
82	A7	201	PEB	OD-C4D-ND	-2.80	121.79	125.93
95	C6	502	DGD	O5E-C6E-C5E	-2.80	101.70	111.29
82	hH	201	PEB	C3B-C4B-NB	2.80	114.12	110.05
82	KP	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
84	B3	1001	CYC	CHA-C4D-C3D	-2.80	120.84	127.15
84	f3	1001	CYC	CHA-C4D-C3D	-2.80	120.84	127.15
87	LN	206	CLA	CHB-C4A-NA	2.80	128.38	124.51
82	uF	202	PEB	CBA-CAA-C3A	2.80	119.69	113.47
85	K6	102	BCR	C38-C26-C25	-2.80	121.39	124.53
82	TB	201	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
87	B6	603	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
82	NP	201	PEB	CHA-C1B-NB	-2.80	119.08	124.93
87	C6	509	CLA	C3B-C4B-NB	-2.80	107.92	110.52
87	a6	607	CLA	C3B-C4B-NB	-2.80	107.92	110.52
82	D5	203	PEB	CAC-CBC-CGC	-2.80	107.59	113.60
83	QJ	201	PUB	OA-C1A-NA	-2.80	121.79	125.93
82	QD	201	PEB	CHC-C1D-ND	-2.80	110.19	113.72
82	iF	201	PEB	C3C-C4C-NC	2.80	110.85	108.33
82	bK	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
82	zC	202	PEB	OA-C1A-C2A	-2.80	123.95	126.17
82	W5	201	PEB	CHB-C4B-C3B	-2.80	118.85	125.32
82	X7	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
82	kO	202	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
96	GN	201	HEM	CBB-CAB-C3B	-2.80	113.71	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W1	202	PEB	C2A-C1A-NA	2.80	110.68	108.27
82	d4	201	PEB	CAB-CBB-CGB	-2.80	107.59	113.60
82	IP	202	PEB	CMB-C2B-C1B	2.80	129.37	125.06
82	O1	203	PEB	C1D-CHC-C4C	2.80	117.38	113.26
88	AL	406	LHG	C5-O7-C7	-2.80	110.91	117.79
82	PB	201	PEB	OD-C4D-C3D	-2.80	123.13	129.46
84	U3	1001	CYC	CHA-C4D-C3D	-2.80	120.84	127.15
84	73	1001	CYC	CHA-C4D-C3D	-2.80	120.84	127.15
87	82	306	CLA	CMB-C2B-C3B	2.80	133.36	126.59
87	AN	807	CLA	C3B-C4B-NB	-2.80	107.92	110.52
87	B6	614	CLA	C3B-C4B-NB	-2.80	107.92	110.52
96	f6	101	HEM	C1B-NB-C4B	2.80	107.96	105.07
82	OO	201	PEB	C2B-C1B-NB	2.80	116.50	110.53
82	CF	201	PEB	CMB-C2B-C1B	2.79	129.37	125.06
82	kO	202	PEB	CMB-C2B-C1B	2.79	129.37	125.06
84	K1	1001	CYC	CHA-C1A-C2A	-2.79	118.85	125.32
82	OP	202	PEB	CHA-C1B-NB	-2.79	119.09	124.93
82	KB	304	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	YD	201	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	O5	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	PD	202	PEB	OD-C4D-C3D	-2.79	123.13	129.46
82	DK	202	PEB	OD-C4D-C3D	-2.79	123.13	129.46
87	AN	817	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
84	S3	1001	CYC	CHA-C4D-C3D	-2.79	120.84	127.15
84	l3	1001	CYC	OC-C1C-C2C	-2.79	123.95	126.17
82	v8	201	PEB	CHC-C4C-NC	2.79	124.93	121.15
82	q8	201	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	UM	202	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
82	bK	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
87	3N	309	CLA	CAA-C2A-C1A	2.79	121.13	111.97
82	QF	201	PEB	C4C-C3C-C2C	-2.79	104.92	107.50
84	D3	1001	CYC	CHA-C4D-C3D	-2.79	120.85	127.15
82	QB	203	PEB	CMB-C2B-C1B	2.79	129.37	125.06
82	IM	201	PEB	CMB-C2B-C1B	2.79	129.37	125.06
87	82	307	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
82	NQ	202	PEB	C1D-CHC-C4C	2.79	117.38	113.26
82	h1	202	PEB	C1D-CHC-C4C	2.79	117.38	113.26
82	BQ	202	PEB	OD-C4D-ND	-2.79	121.79	125.93
84	LH	1002	CYC	C1B-CHB-C4A	-2.79	121.25	128.08
85	AN	846	BCR	C29-C30-C25	2.79	114.78	110.48
82	ZE	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
84	I3	1001	CYC	CHA-C4D-C3D	-2.79	120.85	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TD	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	MJ	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	VM	202	PEB	CHC-C4C-NC	2.79	124.93	121.15
82	J1	1002	PEB	C3C-C4C-NC	2.79	110.85	108.33
82	JH	1002	PEB	CMB-C2B-C1B	2.79	129.37	125.06
82	c1	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
82	LJ	202	PEB	O2B-CGB-CBB	2.79	123.00	114.03
87	B2	809	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
87	7N	602	CLA	C3D-C2D-C1D	-2.79	102.02	105.83
82	QH	201	PEB	CAC-CBC-CGC	-2.79	107.59	113.60
84	CH	1001	CYC	C4D-CHA-C1A	2.79	134.55	128.28
82	kH	201	PEB	CAB-C3B-C4B	2.79	129.95	125.01
82	j4	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	vK	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
87	AN	830	CLA	C3B-C4B-NB	-2.79	107.92	110.52
82	Q4	201	PEB	CHB-C1C-C2C	-2.79	120.85	127.15
84	j3	1001	CYC	CHA-C4D-C3D	-2.79	120.85	127.15
82	sC	201	PEB	CHA-C1B-C2B	2.79	132.08	124.90
82	IP	203	PEB	CHA-C1B-NB	-2.79	119.09	124.93
87	L2	206	CLA	CHB-C4A-NA	2.79	128.37	124.51
83	AM	303	PUB	OA-C1A-NA	-2.79	121.79	125.93
87	8N	307	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
82	l1	203	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
87	32	302	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
82	RF	201	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	OH	203	PEB	CAC-C2C-C1C	2.79	130.21	125.76
82	DD	203	PEB	C2B-C1B-NB	2.79	116.49	110.53
82	eK	202	PEB	CAC-C2C-C3C	2.79	133.46	127.07
82	dH	202	PEB	CHB-C1C-C2C	-2.79	120.85	127.15
82	S5	203	PEB	OD-C4D-ND	-2.79	121.79	125.93
82	YH	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	UH	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
82	WK	203	PEB	CMB-C2B-C1B	2.79	129.36	125.06
84	H3	1001	CYC	CHA-C4D-C3D	-2.79	120.85	127.15
82	PP	201	PEB	CHC-C4C-NC	2.79	124.93	121.15
82	iE	202	PEB	CHC-C4C-NC	2.79	124.93	121.15
82	D5	201	PEB	CAB-CBB-CGB	-2.79	107.60	113.60
82	PE	201	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	SQ	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	wC	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	xF	304	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	u8	203	PEB	CHC-C1D-ND	-2.79	110.19	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DM	201	PEB	CHB-C1C-NC	-2.79	118.93	125.32
87	cL	511	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
82	MM	203	PEB	C4C-C3C-C2C	-2.79	104.92	107.50
82	HD	202	PEB	C1C-CHB-C4B	2.79	134.54	128.28
82	U5	202	PEB	OA-C1A-C2A	-2.79	123.95	126.17
82	wF	302	PEB	CHC-C4C-NC	2.79	124.93	121.15
82	BB	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
87	AN	825	CLA	CHB-C4A-NA	2.79	128.37	124.51
82	AG	304	PEB	OD-C4D-ND	-2.79	121.80	125.93
84	F4	1001	CYC	CAB-C3B-C2B	2.79	132.30	127.53
82	WP	202	PEB	CHB-C4B-C3B	-2.79	118.86	125.32
82	OE	202	PEB	CHC-C1D-ND	-2.79	110.19	113.72
82	U5	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
82	M9	301	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	SM	202	PEB	CAC-C2C-C1C	2.79	130.21	125.76
82	CK	201	PEB	CMB-C2B-C1B	2.79	129.36	125.06
82	RE	202	PEB	OD-C4D-C3D	-2.79	123.14	129.46
87	5N	609	CLA	C2A-C1A-CHA	2.79	128.74	123.86
84	Q3	1001	CYC	CHA-C4D-C3D	-2.79	120.86	127.15
85	A2	848	BCR	C4-C5-C6	-2.79	118.68	122.73
84	FE	1001	CYC	CHB-C1B-NB	-2.79	120.07	126.06
82	Q5	203	PEB	OD-C4D-ND	-2.79	121.80	125.93
82	UD	201	PEB	C4C-C3C-C2C	-2.79	104.92	107.50
82	SG	203	PEB	C1C-NC-C4C	-2.79	104.63	109.60
82	HA	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
82	UE	202	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
82	JQ	203	PEB	C2A-C1A-NA	2.79	110.68	108.27
82	wF	302	PEB	C2A-C1A-NA	2.79	110.68	108.27
82	gO	203	PEB	C2A-C1A-NA	2.79	110.68	108.27
82	O4	201	PEB	CHA-C4A-NA	2.79	128.52	125.20
82	gM	202	PEB	CHA-C4A-NA	-2.79	121.89	125.20
82	YM	202	PEB	CHA-C1B-C2B	2.79	132.07	124.90
82	SP	202	PEB	CBB-CAB-C3B	-2.79	104.88	112.63
87	BN	822	CLA	C3B-C4B-NB	-2.79	107.93	110.52
82	uC	203	PEB	CMB-C2B-C1B	2.79	129.36	125.06
82	sC	202	PEB	CHC-C1D-ND	-2.79	110.19	113.72
82	PM	202	PEB	C1C-CHB-C4B	-2.79	122.03	128.28
87	BN	808	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
82	cG	201	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
84	C4	1001	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
82	FI	202	PEB	CHA-C1B-NB	-2.79	119.10	124.93
87	B2	824	CLA	C2B-C1B-NB	2.79	112.10	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CP	201	PEB	C1C-NC-C4C	2.79	114.56	109.60
82	R7	201	PEB	CHC-C4C-NC	2.79	124.92	121.15
87	62	313	CLA	CHD-C1D-C2D	2.79	131.33	125.48
87	B2	804	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
82	iM	201	PEB	C3B-C4B-NB	2.79	114.11	110.05
82	OF	202	PEB	CMB-C2B-C3B	-2.79	118.55	126.12
84	M3	1001	CYC	CHA-C4D-C3D	-2.79	120.86	127.15
87	AN	826	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
82	uC	203	PEB	CHC-C1D-ND	-2.79	110.20	113.72
82	ZK	202	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
82	BP	202	PEB	C2A-C1A-NA	2.79	110.68	108.27
82	sF	201	PEB	C2A-C1A-NA	2.79	110.68	108.27
82	hG	202	PEB	OD-C4D-ND	-2.79	121.80	125.93
82	KB	304	PEB	OD-C4D-C3D	-2.79	123.14	129.46
82	TM	201	PEB	CMB-C2B-C1B	2.79	129.36	125.06
82	cB	402	PEB	CMB-C2B-C1B	2.79	129.36	125.06
82	KI	202	PEB	OA-C1A-C2A	-2.79	123.96	126.17
87	3N	303	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
83	AE	302	PUB	C2B-C1B-NB	2.79	110.84	108.33
82	MM	202	PEB	OD-C4D-C3D	-2.79	123.14	129.46
82	MK	202	PEB	CHB-C1C-C2C	-2.79	120.86	127.15
82	AO	301	PEB	C1D-CHC-C4C	-2.79	109.14	113.26
82	zC	202	PEB	CHB-C4B-C3B	2.79	131.77	125.32
82	d1	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
85	AN	847	BCR	C23-C22-C21	-2.79	114.66	118.94
82	RI	203	PEB	C1C-CHB-C4B	2.79	134.53	128.28
82	YH	201	PEB	C4C-C3C-C2C	-2.79	104.93	107.50
82	XK	202	PEB	C3B-C4B-NB	2.79	114.10	110.05
84	KO	1001	CYC	C4D-C3D-C2D	-2.79	104.33	107.62
87	cL	510	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
82	Y5	203	PEB	C2A-C1A-NA	2.79	110.68	108.27
92	j6	102	LMG	O8-C28-C29	2.79	120.66	111.91
82	kF	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
82	RD	203	PEB	OD-C4D-C3D	-2.79	123.14	129.46
82	p8	202	PEB	CAC-C2C-C1C	2.79	130.20	125.76
82	DH	1002	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
82	TG	201	PEB	CHC-C4C-NC	2.79	124.92	121.15
87	HL	101	CLA	CHB-C4A-NA	2.79	128.37	124.51
82	TI	202	PEB	OA-C1A-C2A	-2.79	123.96	126.17
84	A3	1001	CYC	OC-C1C-C2C	-2.79	123.96	126.17
87	22	612	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
82	SQ	202	PEB	CAA-C3A-C4A	2.79	119.83	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	f1	201	PEB	OD-C4D-C3D	-2.79	123.15	129.46
82	O5	201	PEB	OD-C4D-C3D	-2.79	123.15	129.46
85	A2	846	BCR	C29-C30-C25	2.79	114.77	110.48
82	D5	203	PEB	CHA-C1B-NB	-2.79	119.10	124.93
87	HL	102	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
87	82	306	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
87	cL	513	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
82	i4	201	PEB	CHC-C1D-ND	-2.79	110.20	113.72
82	eG	202	PEB	CMC-C3C-C4C	2.79	130.01	127.06
82	T4	203	PEB	CAB-CBB-CGB	2.79	119.60	113.60
82	vC	202	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
94	D6	408	PL9	C45-C44-C46	2.79	119.96	115.27
95	c6	601	DGD	O5E-C6E-C5E	-2.79	101.73	111.29
84	JH	1003	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
84	M1	201	CYC	C4D-CHA-C1A	2.79	134.53	128.28
82	PE	202	PEB	C1D-CHC-C4C	2.79	117.36	113.26
82	YM	203	PEB	CAC-C2C-C1C	2.79	130.20	125.76
92	dL	407	LMG	O6-C1-C2	2.79	116.25	110.35
82	WE	203	PEB	C3C-C4C-NC	2.79	110.84	108.33
84	k3	1001	CYC	CHA-C4D-C3D	-2.79	120.86	127.15
82	XB	202	PEB	C1C-CHB-C4B	2.79	134.53	128.28
82	rF	201	PEB	C3B-C4B-NB	2.79	114.10	110.05
88	AL	407	LHG	O8-C23-C24	2.79	120.65	111.91
84	w3	1001	CYC	CHA-C4D-C3D	-2.79	120.87	127.15
82	BI	202	PEB	C1D-CHC-C4C	-2.79	109.15	113.26
82	Y7	303	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
82	aE	202	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
82	KM	201	PEB	C2A-C1A-NA	2.79	110.67	108.27
87	62	311	CLA	C2A-C1A-CHA	2.79	128.73	123.86
82	x8	202	PEB	OD-C4D-C3D	-2.78	123.15	129.46
84	JH	1001	CYC	CHA-C4D-C3D	-2.78	120.87	127.15
82	GQ	202	PEB	CHC-C4C-NC	2.78	124.92	121.15
83	K7	203	PUB	CHA-C1B-NB	2.78	124.92	121.15
87	BN	828	CLA	CHB-C4A-NA	2.78	128.36	124.51
87	82	302	CLA	CAA-C2A-C3A	-2.78	105.15	112.78
82	YB	202	PEB	C3B-C4B-NB	2.78	114.10	110.05
82	IM	202	PEB	C3B-C4B-NB	2.78	114.10	110.05
82	EM	201	PEB	C3C-C4C-NC	2.78	110.84	108.33
82	yK	301	PEB	CAC-C2C-C1C	2.78	130.20	125.76
83	xF	306	PUB	CAB-C3B-C4B	2.78	130.20	125.76
82	U4	201	PEB	C1C-CHB-C4B	2.78	134.53	128.28
82	eF	202	PEB	CAB-C3B-C4B	2.78	129.94	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jO	202	PEB	C1D-CHC-C4C	2.78	117.36	113.26
84	n3	1001	CYC	CHA-C4D-C3D	-2.78	120.87	127.15
82	EP	202	PEB	CMB-C2B-C1B	2.78	129.35	125.06
87	8N	301	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
87	42	607	CLA	C3B-C4B-NB	-2.78	107.93	110.52
82	HQ	203	PEB	CHA-C1B-NB	-2.78	119.11	124.93
82	iK	201	PEB	OD-C4D-C3D	-2.78	123.15	129.46
82	eK	202	PEB	CAB-C3B-C4B	2.78	129.93	125.01
82	K7	202	PEB	CMB-C2B-C1B	2.78	129.35	125.06
82	KF	202	PEB	C3B-C4B-NB	2.78	114.10	110.05
84	NH	1001	CYC	C2A-C1A-NA	2.78	114.10	110.05
82	K9	201	PEB	CHC-C4C-NC	2.78	124.92	121.15
87	52	606	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
82	NM	202	PEB	CHB-C4B-NB	-2.78	118.78	124.58
82	jK	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
82	A7	201	PEB	CMB-C2B-C1B	2.78	129.35	125.06
95	C6	523	DGD	C2G-O2G-C1B	-2.78	110.94	117.79
82	iF	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	eJ	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
87	52	609	CLA	C2A-C1A-CHA	2.78	128.72	123.86
82	dB	201	PEB	CHA-C1B-NB	-2.78	119.11	124.93
82	JO	1002	PEB	OD-C4D-C3D	-2.78	123.16	129.46
82	PP	202	PEB	C3B-C4B-NB	2.78	114.10	110.05
82	QF	203	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
82	dO	201	PEB	CAB-CBB-CGB	-2.78	107.61	113.60
82	WF	201	PEB	C3C-C4C-NC	2.78	110.84	108.33
82	JM	201	PEB	C1C-CHB-C4B	-2.78	122.04	128.28
82	SJ	203	PEB	OD-C4D-C3D	-2.78	123.16	129.46
82	B7	201	PEB	OD-C4D-C3D	-2.78	123.16	129.46
84	DO	1001	CYC	CHB-C1B-NB	-2.78	120.08	126.06
82	UI	201	PEB	CAC-C2C-C1C	2.78	130.19	125.76
82	SD	202	PEB	CAA-C3A-C4A	2.78	119.82	112.67
87	A2	807	CLA	C3B-C4B-NB	-2.78	107.93	110.52
82	xC	201	PEB	OA-C1A-C2A	-2.78	123.96	126.17
87	BL	608	CLA	CHB-C4A-NA	2.78	128.36	124.51
82	aJ	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
82	sK	203	PEB	OD-C4D-ND	-2.78	121.81	125.93
84	DH	1001	CYC	CHB-C4A-NA	-2.78	119.11	124.93
82	AO	305	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
82	MQ	202	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
82	tF	201	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
82	j4	203	PEB	C2A-C1A-NA	2.78	110.67	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	v8	201	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
82	hF	201	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
82	wF	301	PEB	C1C-CHB-C4B	-2.78	122.04	128.28
82	ZB	201	PEB	OD-C4D-C3D	-2.78	123.16	129.46
82	iJ	201	PEB	CBC-CAC-C2C	-2.78	104.90	112.63
82	PF	202	PEB	CAB-C3B-C4B	2.78	129.93	125.01
87	5N	605	CLA	CHB-C4A-NA	2.78	128.36	124.51
82	FI	201	PEB	CAB-CBB-CGB	2.78	119.59	113.60
82	TO	203	PEB	CAB-CBB-CGB	2.78	119.59	113.60
82	d1	203	PEB	OD-C4D-ND	-2.78	121.81	125.93
83	M5	303	PUB	C1C-C2C-C3C	-2.78	103.70	106.78
82	VO	201	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
82	AI	201	PEB	OA-C1A-C2A	-2.78	123.96	126.17
82	O5	203	PEB	CAC-CBC-CGC	-2.78	107.62	113.60
82	PK	202	PEB	CAB-C3B-C4B	2.78	129.93	125.01
82	kK	201	PEB	CMC-C3C-C4C	2.78	130.01	127.06
82	T7	202	PEB	CHA-C4A-NA	2.78	128.51	125.20
87	12	602	CLA	CMC-C2C-C3C	2.78	133.66	126.12
87	5N	606	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
87	LN	206	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
82	WO	201	PEB	C3C-C4C-NC	2.78	110.84	108.33
82	dH	201	PEB	C3C-C4C-NC	2.78	110.84	108.33
82	BJ	301	PEB	OD-C4D-C3D	-2.78	123.16	129.46
82	lM	202	PEB	OD-C4D-C3D	-2.78	123.16	129.46
87	62	313	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
84	F3	1001	CYC	CHA-C4D-C3D	-2.78	120.88	127.15
87	H6	102	CLA	C3B-C4B-NB	-2.78	107.94	110.52
82	K7	202	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
82	TA	203	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
82	CP	203	PEB	CMB-C2B-C1B	2.78	129.34	125.06
85	B2	843	BCR	C39-C30-C25	-2.78	105.79	110.30
82	Z1	201	PEB	C1D-CHC-C4C	2.78	117.36	113.26
83	Z5	302	PUB	OA-C1A-NA	-2.78	121.81	125.93
82	A9	201	PEB	CHC-C4C-NC	2.78	124.91	121.15
82	JQ	201	PEB	OD-C4D-C3D	-2.78	123.16	129.46
82	WI	201	PEB	CAB-C3B-C4B	2.78	129.93	125.01
82	JM	202	PEB	CHC-C1D-ND	-2.78	110.21	113.72
82	QH	202	PEB	CAB-CBB-CGB	-2.78	107.62	113.60
82	HP	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
82	U1	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
84	M1	201	CYC	C4A-C3A-C2A	-2.78	103.32	106.51
87	A2	826	CLA	C2D-C1D-ND	-2.78	108.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	B2	822	CLA	CHB-C1B-NB	2.78	127.20	124.26
82	G9	201	PEB	CHC-C4C-NC	2.78	124.91	121.15
82	QJ	202	PEB	CHA-C1B-NB	-2.78	119.12	124.93
82	xK	304	PEB	CHA-C4A-NA	2.78	128.51	125.20
87	22	609	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
82	M7	202	PEB	C3B-C4B-NB	2.78	114.09	110.05
87	32	304	CLA	CMA-C3A-C4A	2.78	119.24	111.77
82	PQ	202	PEB	OD-C4D-C3D	-2.78	123.17	129.46
84	KO	1001	CYC	CHA-C4D-C3D	-2.78	120.88	127.15
82	Y5	201	PEB	CHC-C4C-NC	2.78	124.91	121.15
82	iK	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	XQ	201	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
82	SF	201	PEB	C3C-C4C-NC	2.78	110.83	108.33
82	bF	201	PEB	C3B-C4B-NB	2.78	114.09	110.05
83	AM	303	PUB	CHB-C1C-NC	-2.78	118.80	124.58
82	BB	202	PEB	C1D-CHC-C4C	-2.78	109.16	113.26
82	eO	203	PEB	OD-C4D-ND	-2.78	121.81	125.93
82	VF	201	PEB	CAA-C3A-C2A	-2.78	107.32	114.26
82	iH	201	PEB	CHB-C4B-C3B	-2.78	118.89	125.32
82	SK	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
82	VO	202	PEB	CAB-C3B-C4B	2.78	129.92	125.01
82	hJ	201	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
84	h3	1001	CYC	C1B-C2B-C3B	-2.78	104.97	107.87
82	CJ	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	f1	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	fG	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	LF	202	PEB	CHB-C4B-NB	2.78	130.36	124.58
82	RI	201	PEB	OA-C1A-C2A	-2.78	123.97	126.17
82	R9	201	PEB	CHC-C4C-NC	2.78	124.91	121.15
82	QO	201	PEB	OD-C4D-C3D	-2.78	123.17	129.46
82	BM	301	PEB	C3B-C4B-NB	2.78	114.09	110.05
82	kM	201	PEB	CHB-C4B-NB	-2.78	118.80	124.58
82	aG	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
82	sF	203	PEB	OD-C4D-ND	-2.78	121.82	125.93
82	dG	202	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
83	Z5	303	PUB	C1C-C2C-C3C	-2.78	103.71	106.78
85	KL	100	BCR	C1-C6-C5	-2.78	118.70	122.61
87	bL	615	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
95	c6	620	DGD	C2G-O2G-C1B	-2.78	110.96	117.79
82	HM	201	PEB	CHA-C1B-NB	-2.78	119.13	124.93
87	8N	303	CLA	CAA-C2A-C3A	-2.78	105.18	112.78
82	VK	201	PEB	CAA-C3A-C2A	-2.78	107.32	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	J4	1001	CYC	CAD-CBD-CGD	-2.78	107.63	113.60
82	T9	201	PEB	CHC-C4C-NC	2.78	124.91	121.15
82	WH	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	WJ	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	SK	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
82	GA	202	PEB	C4C-C3C-C2C	-2.78	104.94	107.50
82	eF	203	PEB	C4C-C3C-C2C	-2.78	104.94	107.50
82	dH	203	PEB	OD-C4D-ND	-2.78	121.82	125.93
82	kK	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
85	AN	848	BCR	C4-C5-C6	-2.78	118.70	122.73
82	QE	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
82	QD	202	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
82	cH	201	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
82	1C	203	PEB	OD-C4D-C3D	-2.78	123.17	129.46
87	BL	608	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
82	Z1	202	PEB	CHA-C1B-NB	-2.78	119.13	124.93
82	XF	203	PEB	CMC-C3C-C4C	2.78	130.00	127.06
82	BA	201	PEB	OD-C4D-C3D	-2.77	123.17	129.46
82	QQ	202	PEB	OD-C4D-C3D	-2.77	123.17	129.46
82	CM	202	PEB	C4C-C3C-C2C	-2.77	104.94	107.50
87	82	304	CLA	CHB-C4A-NA	2.77	128.35	124.51
82	U1	203	PEB	C2A-C1A-NA	2.77	110.67	108.27
82	mM	201	PEB	C2A-C1A-NA	2.77	110.67	108.27
82	kO	202	PEB	C2A-C1A-NA	2.77	110.67	108.27
82	PG	201	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
82	BQ	201	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
82	l1	202	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
82	tF	201	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
82	QQ	201	PEB	CHC-C1D-ND	-2.77	110.21	113.72
82	HQ	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
91	aL	610	PHO	C1A-C2A-C3A	-2.77	100.20	102.84
87	82	302	CLA	O2D-CGD-CBD	2.77	116.20	111.27
98	B2	837	PQN	C14-C13-C15	2.77	119.94	115.27
87	A2	814	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
82	fO	201	PEB	CMB-C2B-C1B	2.77	129.34	125.06
82	uF	202	PEB	OD-C4D-C3D	-2.77	123.17	129.46
82	eB	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	b4	201	PEB	C4B-NB-C1B	-2.77	101.28	106.51
82	WI	201	PEB	CHC-C4C-NC	2.77	124.90	121.15
82	Y1	202	PEB	OD-C4D-ND	-2.77	121.82	125.93
82	XA	201	PEB	CMA-C2A-C1A	-2.77	106.42	112.40
82	JH	1002	PEB	C3C-C4C-NC	2.77	110.83	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gK	203	PEB	OA-C1A-C2A	-2.77	123.97	126.17
82	AF	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	YO	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	DM	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46
82	UD	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
82	kM	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
82	SJ	202	PEB	CHC-C1D-ND	-2.77	110.22	113.72
82	GK	203	PEB	CMA-C2A-C1A	-2.77	106.43	112.40
82	JK	202	PEB	CAB-C3B-C4B	2.77	129.91	125.01
82	aJ	202	PEB	CAB-C3B-C4B	2.77	129.91	125.01
82	HA	201	PEB	CMB-C2B-C1B	2.77	129.33	125.06
82	TQ	202	PEB	OD-C4D-C3D	-2.77	123.18	129.46
88	BL	615	LHG	O7-C7-C8	2.77	117.48	111.50
82	WJ	202	PEB	C3C-C4C-NC	2.77	110.83	108.33
84	h3	1001	CYC	CHA-C4D-C3D	-2.77	120.89	127.15
82	J9	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	DM	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
82	hO	201	PEB	CHA-C1B-NB	-2.77	119.13	124.93
85	B6	601	BCR	C27-C26-C25	-2.77	118.71	122.73
82	ZF	202	PEB	CHC-C1D-ND	2.77	117.23	113.72
82	Y4	202	PEB	CAB-C3B-C4B	2.77	129.91	125.01
82	fH	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46
87	CL	511	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
82	NQ	203	PEB	CHA-C1B-NB	-2.77	119.14	124.93
85	F2	203	BCR	C2-C1-C6	2.77	114.75	110.48
82	WQ	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
94	aL	601	PL9	C3-C4-C5	-2.77	115.00	118.60
82	JP	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
82	kK	201	PEB	CHC-C4C-NC	2.77	124.90	121.15
87	A2	826	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
82	DD	203	PEB	CHA-C1B-NB	-2.77	119.14	124.93
82	YP	501	PEB	CHA-C1B-NB	-2.77	119.14	124.93
82	TA	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46
82	DI	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46
82	DJ	201	PEB	CHB-C4B-NB	-2.77	118.81	124.58
82	DP	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
84	LG	1001	CYC	C2A-C1A-NA	2.77	114.08	110.05
85	c6	617	BCR	C3-C4-C5	-2.77	109.13	114.08
82	AM	301	PEB	OD-C4D-ND	-2.77	121.83	125.93
82	QQ	201	PEB	C1D-CHC-C4C	-2.77	109.17	113.26
82	c4	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
82	O7	202	PEB	C4B-C3B-C2B	-2.77	103.72	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QD	202	PEB	OD-C4D-C3D	-2.77	123.18	129.46
95	J6	101	DGD	O1G-C1A-C2A	2.77	120.60	111.91
98	BN	837	PQN	C14-C13-C15	2.77	119.93	115.27
87	AN	806	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
85	F2	203	BCR	C28-C27-C26	-2.77	109.13	114.08
82	QE	203	PEB	C4C-C3C-C2C	-2.77	104.94	107.50
87	72	603	CLA	CHB-C4A-NA	2.77	128.34	124.51
82	OO	201	PEB	C1D-CHC-C4C	-2.77	109.17	113.26
87	B2	831	CLA	C3B-C4B-NB	-2.77	107.94	110.52
87	72	605	CLA	CBA-CAA-C2A	-2.77	105.69	113.86
82	GJ	202	PEB	OD-C4D-C3D	-2.77	123.18	129.46
82	GF	203	PEB	CHC-C1D-ND	-2.77	110.22	113.72
82	XA	203	PEB	CHB-C4B-C3B	-2.77	118.91	125.32
82	HH	1002	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	iF	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	GF	203	PEB	CMA-C2A-C1A	-2.77	106.43	112.40
82	f4	201	PEB	CMB-C2B-C1B	2.77	129.33	125.06
82	OF	202	PEB	C4C-C3C-C2C	-2.77	104.94	107.50
82	TI	201	PEB	CHB-C4B-NB	-2.77	118.81	124.58
82	zC	201	PEB	CAA-C3A-C2A	-2.77	107.34	114.26
87	c6	608	CLA	C3B-C4B-NB	-2.77	107.95	110.52
82	l1	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
82	lH	201	PEB	OD-C4D-C3D	-2.77	123.19	129.46
87	BN	805	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
82	NM	202	PEB	CAC-CBC-CGC	-2.77	107.64	113.60
82	jJ	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
82	BM	301	PEB	OD-C4D-ND	-2.77	121.83	125.93
82	b4	202	PEB	CMB-C2B-C1B	2.77	129.33	125.06
82	1C	201	PEB	CAB-C3B-C4B	2.77	129.91	125.01
82	TM	202	PEB	CHA-C4A-NA	-2.77	121.91	125.20
82	JD	201	PEB	OD-C4D-C3D	-2.77	123.19	129.46
82	Q1	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
82	b1	203	PEB	OD-C4D-C3D	-2.77	123.19	129.46
87	22	602	CLA	CHB-C1B-NB	2.77	127.19	124.26
82	B5	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
82	lE	203	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
82	JB	201	PEB	C4C-C3C-C2C	-2.77	104.94	107.50
95	cL	519	DGD	O1G-C1A-C2A	2.77	120.59	111.91
87	A2	816	CLA	CHB-C4A-NA	2.77	128.34	124.51
85	BN	843	BCR	C39-C30-C25	-2.77	105.81	110.30
84	i3	1001	CYC	OC-C1C-C2C	-2.77	123.97	126.17
82	EQ	201	PEB	CAB-CBB-CGB	-2.77	107.65	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	A2	824	CLA	C3B-C4B-NB	-2.77	107.95	110.52
82	SA	201	PEB	C1C-NC-C4C	-2.77	104.67	109.60
82	OF	202	PEB	CHA-C1B-C2B	2.77	132.02	124.90
82	ED	201	PEB	C2A-C1A-NA	2.77	110.66	108.27
82	RP	202	PEB	C2A-C1A-NA	2.77	110.66	108.27
82	IB	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
82	A4	301	PEB	CAC-CBC-CGC	-2.77	107.65	113.60
87	6N	612	CLA	CHD-C1D-C2D	2.77	131.28	125.48
82	NG	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
84	O3	1001	CYC	CHA-C4D-C3D	-2.77	120.91	127.15
82	e1	201	PEB	CMB-C2B-C1B	2.77	129.33	125.06
87	1N	603	CLA	CHB-C4A-NA	2.77	128.34	124.51
82	Q7	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
82	KJ	203	PEB	CAA-C3A-C4A	-2.77	105.57	112.67
82	v8	202	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
82	R1	201	PEB	CBA-CAA-C3A	-2.77	107.31	113.47
82	A1	305	PEB	CHC-C4C-NC	2.77	124.89	121.15
82	R7	203	PEB	CHC-C4C-NC	2.77	124.89	121.15
87	L2	206	CLA	C3B-C4B-NB	-2.77	107.95	110.52
87	b6	613	CLA	C3B-C4B-NB	-2.77	107.95	110.52
82	J5	203	PEB	CHA-C1B-NB	-2.77	119.14	124.93
82	mG	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
82	UA	201	PEB	C3B-C4B-NB	2.77	114.07	110.05
82	HD	202	PEB	C3B-C4B-NB	2.77	114.07	110.05
82	KJ	202	PEB	CMB-C2B-C1B	2.77	129.32	125.06
82	BI	201	PEB	C2B-C1B-NB	2.77	116.44	110.53
82	IM	202	PEB	OA-C1A-C2A	-2.77	123.97	126.17
82	WQ	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
82	AO	301	PEB	C2A-C1A-NA	2.77	110.66	108.27
82	BP	202	PEB	CAA-C3A-C4A	-2.77	105.57	112.67
82	WE	203	PEB	CHA-C1B-NB	-2.77	119.15	124.93
82	DQ	203	PEB	C2B-C1B-NB	2.77	116.43	110.53
83	yF	303	PUB	C2C-C1C-NC	2.77	114.07	110.05
84	FG	1001	CYC	C2A-C1A-NA	2.77	114.07	110.05
82	TA	202	PEB	CHA-C4A-NA	2.77	128.49	125.20
82	F1	1002	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
82	U7	201	PEB	CBB-CAB-C3B	-2.77	104.94	112.63
82	L9	202	PEB	C1D-CHC-C4C	-2.77	109.18	113.26
82	LP	202	PEB	C3B-C4B-NB	2.77	114.07	110.05
87	A2	806	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
87	B2	826	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
82	U1	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FJ	202	PEB	CAA-C3A-C2A	-2.77	107.35	114.26
87	6N	605	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
82	hE	202	PEB	OD-C4D-ND	-2.76	121.83	125.93
83	QJ	201	PUB	OD-C4D-ND	-2.76	121.83	125.93
82	DM	201	PEB	C1D-CHC-C4C	2.76	117.33	113.26
82	SI	202	PEB	OD-C4D-C3D	-2.76	123.20	129.46
84	D4	1001	CYC	C4D-CHA-C1A	2.76	134.48	128.28
82	ZK	201	PEB	CHB-C4B-NB	-2.76	118.82	124.58
87	2N	302	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
82	lF	202	PEB	CAC-CBC-CGC	-2.76	107.65	113.60
82	Z5	301	PEB	C2A-C1A-NA	2.76	110.66	108.27
82	BB	203	PEB	OD-C4D-C3D	-2.76	123.20	129.46
82	F7	203	PEB	CHC-C4C-NC	2.76	124.89	121.15
84	JO	1001	CYC	C4D-CHA-C1A	2.76	134.48	128.28
85	C6	507	BCR	C15-C16-C17	-2.76	117.81	123.47
82	KM	202	PEB	CAC-C2C-C1C	2.76	130.16	125.76
82	O5	203	PEB	CAC-C2C-C1C	2.76	130.16	125.76
87	bL	608	CLA	CHD-C1D-ND	-2.76	121.91	124.45
83	M5	302	PUB	C1D-CHC-C4C	-2.76	107.35	113.37
87	b6	604	CLA	C3B-C4B-NB	-2.76	107.95	110.52
82	LA	203	PEB	C4B-C3B-C2B	-2.76	103.72	106.78
82	CP	203	PEB	C3B-C4B-NB	2.76	114.07	110.05
82	S4	202	PEB	C3B-C4B-NB	2.76	114.07	110.05
82	JA	202	PEB	CHC-C1D-ND	-2.76	110.23	113.72
82	QE	203	PEB	CHC-C4C-NC	2.76	124.89	121.15
82	I9	201	PEB	CHC-C4C-NC	2.76	124.89	121.15
88	d6	407	LHG	O8-C23-C24	2.76	120.58	111.91
95	JL	101	DGD	O1G-C1A-C2A	2.76	120.58	111.91
82	WI	203	PEB	CAA-C3A-C4A	2.76	119.77	112.67
82	fM	201	PEB	C1B-C2B-C3B	-2.76	103.33	106.51
82	V4	201	PEB	CHB-C4B-C3B	-2.76	118.93	125.32
82	CI	201	PEB	OA-C1A-C2A	-2.76	123.98	126.17
82	Q1	202	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
82	SQ	202	PEB	CMB-C2B-C1B	2.76	129.32	125.06
87	CL	511	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
82	G7	202	PEB	C4C-C3C-C2C	-2.76	104.95	107.50
82	VP	202	PEB	C3B-C4B-NB	2.76	114.07	110.05
82	K7	202	PEB	C3B-C4B-NB	2.76	114.07	110.05
85	H6	101	BCR	C15-C14-C13	-2.76	123.37	127.31
82	TD	202	PEB	C4B-C3B-C2B	-2.76	103.72	106.78
82	ED	201	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
87	8N	303	CLA	O2D-CGD-CBD	2.76	116.18	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YQ	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
82	D7	203	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
84	LH	1001	CYC	C4A-C3A-C2A	-2.76	103.34	106.51
83	Z5	302	PUB	C1D-CHC-C4C	-2.76	107.36	113.37
82	W5	203	PEB	OD-C4D-ND	-2.76	121.84	125.93
82	ZH	202	PEB	CHA-C1B-NB	-2.76	119.16	124.93
85	AN	848	BCR	C10-C11-C12	-2.76	114.60	123.22
82	hJ	202	PEB	C3B-C4B-NB	2.76	114.07	110.05
82	U1	203	PEB	CHC-C4C-NC	2.76	124.89	121.15
85	c6	603	BCR	C36-C18-C17	-2.76	119.05	122.92
82	RD	202	PEB	C2A-C1A-NA	2.76	110.65	108.27
84	FH	1001	CYC	C2C-C1C-NC	2.76	110.65	108.27
87	62	302	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
82	XI	201	PEB	OA-C1A-C2A	-2.76	123.98	126.17
84	N3	1001	CYC	OC-C1C-C2C	-2.76	123.98	126.17
82	D7	203	PEB	C4C-C3C-C2C	-2.76	104.95	107.50
82	cH	201	PEB	C4C-C3C-C2C	-2.76	104.95	107.50
82	M9	302	PEB	C4C-C3C-C2C	-2.76	104.95	107.50
87	12	603	CLA	CHB-C4A-NA	2.76	128.33	124.51
84	JO	1001	CYC	CAD-CBD-CGD	-2.76	107.66	113.60
87	DL	406	CLA	C3B-C4B-NB	-2.76	107.95	110.52
87	I2	102	CLA	C3B-C4B-NB	-2.76	107.95	110.52
82	RO	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
82	wC	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
82	WO	201	PEB	CHB-C4B-NB	2.76	130.33	124.58
82	kG	201	PEB	OD-C4D-C3D	-2.76	123.20	129.46
82	sC	203	PEB	C1C-CHB-C4B	2.76	134.47	128.28
82	kJ	201	PEB	CAB-C3B-C4B	2.76	129.89	125.01
82	d1	202	PEB	CHB-C1C-C2C	-2.76	120.92	127.15
82	LQ	201	PEB	C3C-C4C-NC	2.76	110.82	108.33
82	fJ	201	PEB	CHA-C1B-NB	-2.76	119.16	124.93
82	oK	201	PEB	CHB-C4B-NB	-2.76	118.83	124.58
82	S4	201	PEB	CHB-C4B-NB	2.76	130.32	124.58
87	AN	801	CLA	CHB-C4A-NA	2.76	128.33	124.51
87	AN	816	CLA	CHB-C4A-NA	2.76	128.33	124.51
82	QQ	202	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
82	VF	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
82	OH	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
82	F7	203	PEB	OD-C4D-ND	-2.76	121.84	125.93
82	jG	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
87	FN	201	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
82	O1	201	PEB	C2A-C1A-NA	2.76	110.65	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UQ	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	X7	201	PEB	CMA-C2A-C1A	-2.76	106.45	112.40
82	CJ	203	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
87	AN	834	CLA	C3B-C4B-NB	-2.76	107.95	110.52
82	bO	201	PEB	C4B-NB-C1B	-2.76	101.31	106.51
87	CL	510	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
82	qC	202	PEB	CMB-C2B-C1B	2.76	129.31	125.06
82	lK	201	PEB	OA-C1A-NA	2.76	128.28	124.94
82	HD	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
82	mE	202	PEB	OD-C4D-ND	-2.76	121.84	125.93
83	wK	304	PUB	OA-C1A-NA	-2.76	121.84	125.93
82	MA	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	yC	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
84	D1	1003	CYC	C4A-C3A-C2A	-2.76	103.34	106.51
82	h4	202	PEB	CHA-C1B-NB	-2.76	119.16	124.93
82	1C	202	PEB	OD-C4D-C3D	-2.76	123.21	129.46
84	u3	1001	CYC	C1B-C2B-C3B	-2.76	104.99	107.87
82	O4	202	PEB	CHC-C4C-NC	2.76	124.88	121.15
85	A2	848	BCR	C10-C11-C12	-2.76	114.61	123.22
82	QB	202	PEB	CHC-C1D-ND	-2.76	110.23	113.72
82	iK	203	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	ZH	203	PEB	OA-C1A-C2A	-2.76	123.98	126.17
83	xF	305	PUB	CHB-C1C-NC	-2.76	118.83	124.58
82	iO	203	PEB	CBB-CAB-C3B	2.76	120.29	112.63
95	D6	410	DGD	O1G-C1A-C2A	2.76	120.57	111.91
82	hF	202	PEB	CHA-C1B-NB	-2.76	119.16	124.93
82	s8	203	PEB	C1C-CHB-C4B	2.76	134.47	128.28
82	PE	201	PEB	OD-C4D-C3D	-2.76	123.21	129.46
82	LJ	201	PEB	CHB-C1C-NC	-2.76	119.00	125.32
87	C6	519	CLA	C3B-C4B-NB	-2.76	107.96	110.52
87	CL	514	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
87	dL	401	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
87	A2	820	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
82	wK	302	PEB	CHC-C4C-NC	2.76	124.88	121.15
87	bL	614	CLA	CHB-C1B-NB	2.76	127.18	124.26
82	UP	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
82	cE	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
82	UA	201	PEB	CBB-CAB-C3B	-2.76	104.96	112.63
82	wF	301	PEB	CHB-C1C-NC	-2.76	119.00	125.32
82	dM	203	PEB	CHB-C1C-NC	-2.76	119.00	125.32
82	iO	201	PEB	CHC-C1D-ND	-2.76	110.23	113.72
82	JO	1002	PEB	CHA-C1B-NB	-2.76	119.16	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ZJ	201	PEB	C1C-CHB-C4B	-2.76	122.10	128.28
87	BN	817	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
87	cL	512	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
87	2N	309	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
82	Q5	202	PEB	OD-C4D-C3D	-2.76	123.21	129.46
87	7N	605	CLA	CBA-CAA-C2A	-2.76	105.72	113.86
82	J7	201	PEB	CHB-C1C-NC	-2.76	119.00	125.32
82	R5	202	PEB	C4C-C3C-C2C	-2.76	104.95	107.50
82	eF	202	PEB	C1D-CHC-C4C	-2.76	109.19	113.26
87	cL	508	CLA	CHD-C1D-ND	-2.76	121.92	124.45
87	7N	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
82	XD	201	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
82	VQ	202	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
82	b1	203	PEB	CAA-C3A-C4A	-2.76	105.59	112.67
82	v8	202	PEB	CMB-C2B-C1B	2.76	129.31	125.06
82	fM	203	PEB	CMB-C2B-C1B	2.76	129.31	125.06
82	WG	203	PEB	C3C-C4C-NC	2.76	110.81	108.33
82	PI	201	PEB	OA-C1A-C2A	-2.76	123.98	126.17
82	a4	203	PEB	OA-C1A-C2A	-2.76	123.98	126.17
82	18	202	PEB	OD-C4D-C3D	-2.76	123.21	129.46
82	kF	203	PEB	OD-C4D-C3D	-2.76	123.21	129.46
82	SE	202	PEB	C1C-NC-C4C	-2.76	104.69	109.60
87	A2	807	CLA	CHB-C4A-NA	2.76	128.32	124.51
82	GB	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	AD	303	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	BP	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
84	BG	1001	CYC	C1D-C2D-C3D	-2.76	104.28	107.79
82	Z9	301	PEB	C4C-C3C-C2C	-2.76	104.96	107.50
87	3N	305	CLA	CMA-C3A-C4A	2.76	119.18	111.77
82	gB	203	PEB	C2A-C1A-NA	2.76	110.65	108.27
82	Q1	202	PEB	CHA-C4A-NA	2.76	128.48	125.20
82	PB	201	PEB	CAC-CBC-CGC	-2.76	107.67	113.60
82	ND	203	PEB	CHA-C1B-NB	-2.76	119.17	124.93
82	mJ	201	PEB	CHA-C1B-C2B	2.76	131.99	124.90
82	CM	202	PEB	OD-C4D-C3D	-2.76	123.22	129.46
83	AJ	304	PUB	CHB-C4B-NB	-2.76	119.01	125.32
85	CL	516	BCR	C1-C6-C5	-2.76	118.73	122.61
82	SB	201	PEB	CAB-CBB-CGB	-2.76	107.67	113.60
82	H9	201	PEB	OA-C1A-C2A	-2.76	123.98	126.17
82	SH	203	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
82	b1	202	PEB	OD-C4D-ND	-2.76	121.85	125.93
83	M5	302	PUB	OA-C1A-NA	-2.76	121.85	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RA	203	PEB	CHC-C4C-NC	2.76	124.88	121.15
87	BN	826	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
82	iJ	201	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	gM	201	PEB	C3B-C4B-NB	2.76	114.06	110.05
82	z8	202	PEB	CAA-C3A-C2A	-2.76	107.38	114.26
82	DM	201	PEB	CAB-CBB-CGB	-2.76	107.67	113.60
82	h4	201	PEB	CHA-C1B-NB	-2.76	119.17	124.93
82	LA	201	PEB	OD-C4D-ND	-2.75	121.85	125.93
82	Q1	202	PEB	OD-C4D-ND	-2.75	121.85	125.93
84	IE	1001	CYC	CHA-C4D-C3D	-2.75	120.94	127.15
87	B2	816	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
82	JF	202	PEB	CAB-C3B-C4B	2.75	129.88	125.01
82	FF	202	PEB	C1B-C2B-C3B	-2.75	103.34	106.51
82	NP	202	PEB	C1B-C2B-C3B	-2.75	103.34	106.51
82	GQ	202	PEB	C1B-C2B-C3B	-2.75	103.34	106.51
82	ZG	201	PEB	CMB-C2B-C1B	2.75	129.31	125.06
82	OG	202	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	GP	203	PEB	CMB-C2B-C1B	2.75	129.31	125.06
87	32	309	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
82	XA	203	PEB	C3B-C4B-NB	2.75	114.06	110.05
82	PO	203	PEB	C3B-C4B-NB	2.75	114.06	110.05
82	SG	203	PEB	C2A-C1A-NA	2.75	110.65	108.27
82	AH	302	PEB	C2A-C1A-NA	2.75	110.65	108.27
84	E1	1001	CYC	CMB-C2B-C1B	2.75	127.61	124.17
82	RG	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	U5	203	PEB	C4B-C3B-C2B	-2.75	103.73	106.78
82	eF	202	PEB	CAC-C2C-C3C	2.75	133.38	127.07
82	DA	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
87	82	306	CLA	C2A-C1A-CHA	2.75	128.67	123.86
82	wK	301	PEB	CHB-C1C-NC	-2.75	119.01	125.32
82	ZG	201	PEB	CHA-C1B-NB	-2.75	119.17	124.93
87	O2	202	CLA	C2B-C1B-NB	2.75	112.08	110.23
82	QH	202	PEB	CHA-C4A-NA	2.75	128.48	125.20
82	18	201	PEB	CAB-C3B-C4B	2.75	129.88	125.01
82	ZE	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
82	tK	202	PEB	OD-C4D-ND	-2.75	121.85	125.93
82	NJ	201	PEB	CMB-C2B-C1B	2.75	129.30	125.06
82	J1	1002	PEB	CMB-C2B-C1B	2.75	129.30	125.06
82	PO	202	PEB	CAC-CBC-CGC	-2.75	107.68	113.60
82	R4	203	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	RH	201	PEB	CBA-CAA-C3A	-2.75	107.34	113.47
82	MK	203	PEB	OD-C4D-C3D	-2.75	123.22	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bK	201	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	T7	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
87	aL	605	CLA	C4-C3-C5	2.75	119.90	115.27
82	Q5	201	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
82	DH	1002	PEB	OD-C4D-ND	-2.75	121.85	125.93
82	D7	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
82	18	203	PEB	OD-C4D-C3D	-2.75	123.22	129.46
87	62	306	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
82	HI	201	PEB	C1D-CHC-C4C	-2.75	109.20	113.26
82	aJ	203	PEB	CAC-C2C-C1C	2.75	130.15	125.76
82	tC	202	PEB	CMB-C2B-C1B	2.75	129.30	125.06
84	F1	1001	CYC	C2A-C1A-NA	2.75	114.05	110.05
82	BD	202	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	VO	202	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	S4	201	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	IK	201	PEB	OD-C4D-C3D	-2.75	123.22	129.46
82	O9	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
87	32	305	CLA	CHB-C4A-NA	2.75	128.32	124.51
87	ON	202	CLA	C2B-C1B-NB	2.75	112.08	110.23
82	W5	202	PEB	CMA-C2A-C1A	-2.75	106.47	112.40
84	JH	1001	CYC	CHB-C1B-NB	-2.75	120.15	126.06
82	FK	201	PEB	CHA-C1B-NB	-2.75	119.18	124.93
85	c6	603	BCR	C33-C5-C6	-2.75	121.44	124.53
82	yC	202	PEB	C1C-CHB-C4B	2.75	134.45	128.28
82	PO	203	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	AH	305	PEB	CHC-C4C-NC	2.75	124.87	121.15
87	bL	617	CLA	CHB-C1B-NB	2.75	127.17	124.26
82	Z1	203	PEB	CHB-C4B-NB	-2.75	118.85	124.58
82	BI	203	PEB	C3C-C4C-NC	2.75	110.81	108.33
82	OM	203	PEB	C3C-C4C-NC	2.75	110.81	108.33
103	8N	310	ZEX	C32-C33-C34	2.75	123.16	118.94
84	F3	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
84	o3	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
87	d6	401	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
82	Q9	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	e4	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	RJ	202	PEB	CHB-C4B-NB	-2.75	118.85	124.58
82	RA	201	PEB	CHC-C4C-NC	2.75	124.87	121.15
82	gG	202	PEB	CHC-C1D-ND	-2.75	110.24	113.72
82	MF	202	PEB	CHB-C1C-C2C	-2.75	120.94	127.15
82	HQ	202	PEB	C1C-CHB-C4B	2.75	134.45	128.28
87	bL	607	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eE	202	PEB	CMC-C3C-C4C	2.75	129.98	127.06
82	H9	203	PEB	C3B-C4B-NB	2.75	114.05	110.05
85	FN	202	BCR	C2-C1-C6	2.75	114.72	110.48
82	OG	203	PEB	C1C-CHB-C4B	2.75	134.45	128.28
82	kF	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	P7	203	PEB	C3C-C4C-NC	2.75	110.81	108.33
87	CL	510	CLA	CHB-C4A-NA	2.75	128.31	124.51
82	B5	203	PEB	OD-C4D-C3D	-2.75	123.23	129.46
82	KB	304	PEB	OD-C4D-ND	-2.75	121.86	125.93
82	cK	203	PEB	CAC-CBC-CGC	-2.75	107.69	113.60
82	FM	202	PEB	C1D-CHC-C4C	-2.75	109.20	113.26
82	X7	202	PEB	C1C-NC-C4C	-2.75	104.70	109.60
87	a6	608	CLA	CAC-C3C-C4C	2.75	128.38	124.81
85	c6	603	BCR	C3-C4-C5	-2.75	109.17	114.08
87	LN	206	CLA	C3B-C4B-NB	-2.75	107.96	110.52
87	dL	401	CLA	C3B-C4B-NB	-2.75	107.96	110.52
82	SM	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	h1	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	WD	202	PEB	OD-C4D-C3D	-2.75	123.23	129.46
82	SJ	201	PEB	OD-C4D-C3D	-2.75	123.23	129.46
82	E7	202	PEB	OD-C4D-C3D	-2.75	123.23	129.46
82	IJ	202	PEB	CAB-C3B-C4B	2.75	129.87	125.01
82	FD	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	F4	1002	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	C9	201	PEB	CHC-C4C-NC	2.75	124.87	121.15
82	VF	202	PEB	C4B-NB-C1B	-2.75	101.33	106.51
87	22	601	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
82	XF	201	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	TJ	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	iG	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	FI	201	PEB	CHA-C1B-NB	-2.75	119.18	124.93
82	N1	1002	PEB	OD-C4D-C3D	-2.75	123.23	129.46
82	A5	202	PEB	C4C-C3C-C2C	-2.75	104.96	107.50
82	LD	201	PEB	CMB-C2B-C1B	2.75	129.30	125.06
82	uK	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
84	I1	1001	CYC	C4A-C3A-C2A	-2.75	103.35	106.51
82	lJ	202	PEB	CHA-C4A-NA	2.75	128.47	125.20
82	J7	203	PEB	CHA-C4A-NA	-2.75	121.94	125.20
84	IG	1001	CYC	CHA-C4D-C3D	-2.75	120.95	127.15
82	VE	202	PEB	CHC-C1D-ND	-2.75	110.25	113.72
82	YK	203	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
82	TQ	202	PEB	C4B-C3B-C2B	-2.75	103.74	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	L7	201	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
82	TI	201	PEB	CAC-C2C-C1C	2.75	130.14	125.76
82	VH	202	PEB	OD-C4D-ND	-2.75	121.86	125.93
87	A2	802	CLA	CHB-C4A-NA	2.75	128.31	124.51
87	4N	604	CLA	C3D-C4D-CHA	2.75	119.01	112.72
87	AN	828	CLA	C2A-C1A-CHA	2.75	128.66	123.86
87	AN	820	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
87	LN	203	CLA	CHC-C4B-NB	2.75	127.17	124.26
82	UE	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
82	NF	201	PEB	C3B-C4B-NB	2.75	114.05	110.05
83	AJ	303	PUB	C2C-C1C-NC	2.75	114.05	110.05
82	ND	204	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	w8	201	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	W9	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	RJ	202	PEB	O2B-CGB-CBB	2.75	122.86	114.03
87	B6	607	CLA	C3B-C4B-NB	-2.75	107.97	110.52
82	Q1	203	PEB	OD-C4D-ND	-2.75	121.86	125.93
82	f4	202	PEB	CHA-C1B-NB	-2.75	119.19	124.93
84	f3	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
82	O5	201	PEB	CAB-C3B-C4B	2.75	129.87	125.01
87	52	605	CLA	CHB-C4A-NA	2.75	128.31	124.51
82	wK	301	PEB	C1C-CHB-C4B	-2.75	122.12	128.28
82	jE	202	PEB	OD-C4D-C3D	-2.75	123.24	129.46
82	DQ	203	PEB	CHA-C1B-NB	-2.75	119.19	124.93
83	xF	305	PUB	CHA-C4A-NA	-2.75	110.25	113.72
87	A2	841	CLA	CHB-C1B-NB	2.75	127.17	124.26
82	V1	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	gE	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
82	l4	202	PEB	CMB-C2B-C1B	2.75	129.29	125.06
82	hJ	201	PEB	CMB-C2B-C1B	2.75	129.29	125.06
82	TB	201	PEB	C4C-C3C-C2C	-2.75	104.97	107.50
88	D6	406	LHG	C5-O7-C7	-2.75	111.03	117.79
87	32	303	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
87	b6	612	CLA	C3B-C4B-NB	-2.75	107.97	110.52
98	BN	837	PQN	C9-C10-C5	-2.75	116.21	119.26
82	b1	201	PEB	C3B-C4B-NB	2.75	114.04	110.05
82	X7	203	PEB	C3B-C4B-NB	2.75	114.04	110.05
82	XK	203	PEB	CAA-C3A-C4A	-2.75	105.62	112.67
82	JA	201	PEB	CHB-C1C-NC	-2.75	119.03	125.32
82	NQ	202	PEB	OD-C4D-C3D	-2.75	123.24	129.46
82	T4	202	PEB	OD-C4D-C3D	-2.75	123.24	129.46
82	aH	202	PEB	OD-C4D-C3D	-2.75	123.24	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cM	201	PEB	OD-C4D-C3D	-2.75	123.24	129.46
82	VQ	202	PEB	CMB-C2B-C1B	2.75	129.29	125.06
82	VG	202	PEB	CHC-C1D-ND	-2.75	110.25	113.72
82	uK	201	PEB	OD-C4D-ND	-2.75	121.86	125.93
87	BN	823	CLA	CHB-C1B-NB	2.75	127.16	124.26
82	f4	201	PEB	C2B-C1B-NB	2.75	116.39	110.53
82	GI	203	PEB	C3C-C4C-NC	2.75	110.81	108.33
82	JI	202	PEB	CHC-C4C-NC	2.75	124.86	121.15
82	hE	202	PEB	OD-C4D-C3D	-2.75	123.24	129.46
82	Z9	304	PEB	OD-C4D-C3D	-2.75	123.24	129.46
87	dL	409	CLA	O2D-CGD-CBD	2.75	116.15	111.27
82	DO	1002	PEB	C3B-C4B-NB	2.75	114.04	110.05
82	zC	201	PEB	C4C-C3C-C2C	-2.75	104.97	107.50
91	AL	410	PHO	C4D-CHA-CBD	-2.75	107.28	108.52
82	iF	202	PEB	OA-C1A-C2A	-2.75	123.99	126.17
85	c6	602	BCR	C28-C27-C26	-2.75	109.17	114.08
82	gB	201	PEB	OD-C4D-C3D	-2.74	123.24	129.46
82	KF	202	PEB	OD-C4D-ND	-2.74	121.86	125.93
92	C6	501	LMG	O8-C28-C29	2.74	120.52	111.91
82	L5	202	PEB	C2A-C1A-NA	2.74	110.64	108.27
82	y8	202	PEB	C1C-CHB-C4B	2.74	134.44	128.28
87	8N	301	CLA	C2A-C1A-CHA	2.74	128.66	123.86
82	LH	1003	PEB	CHA-C4A-NA	2.74	128.47	125.20
82	dE	202	PEB	C3B-C4B-NB	2.74	114.04	110.05
82	jJ	202	PEB	C3B-C4B-NB	2.74	114.04	110.05
82	OO	201	PEB	OA-C1A-C2A	-2.74	123.99	126.17
82	E9	201	PEB	CHC-C4C-NC	2.74	124.86	121.15
82	S9	203	PEB	CHC-C4C-NC	2.74	124.86	121.15
82	VD	202	PEB	CMB-C2B-C1B	2.74	129.29	125.06
82	FJ	202	PEB	C1C-CHB-C4B	-2.74	122.13	128.28
82	UO	201	PEB	C1C-CHB-C4B	2.74	134.44	128.28
87	cL	509	CLA	CBC-CAC-C3C	2.74	120.00	112.43
87	L2	203	CLA	CHC-C4B-NB	2.74	127.16	124.26
87	c6	607	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
82	YG	202	PEB	OD-C4D-C3D	-2.74	123.24	129.46
82	cO	201	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
85	FN	202	BCR	C28-C27-C26	-2.74	109.18	114.08
82	TA	201	PEB	CMA-C2A-C1A	-2.74	106.49	112.40
82	jJ	202	PEB	CMB-C2B-C1B	2.74	129.29	125.06
84	w3	1001	CYC	C1B-C2B-C3B	-2.74	105.01	107.87
82	V9	201	PEB	CHC-C4C-NC	2.74	124.86	121.15
82	aJ	202	PEB	OD-C4D-C3D	-2.74	123.24	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	M9	305	PEB	OD-C4D-C3D	-2.74	123.24	129.46
94	A6	410	PL9	C35-C34-C36	2.74	119.89	115.27
82	PM	202	PEB	CAB-C3B-C4B	2.74	129.86	125.01
82	xK	304	PEB	CAB-C3B-C4B	2.74	129.86	125.01
82	RA	203	PEB	C2A-C1A-NA	2.74	110.64	108.27
82	B9	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
82	OE	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
82	uF	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
82	L5	201	PEB	CAB-CBB-CGB	-2.74	107.70	113.60
82	UE	203	PEB	OA-C1A-C2A	-2.74	123.99	126.17
82	VI	201	PEB	OA-C1A-C2A	-2.74	123.99	126.17
87	4N	603	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
82	BQ	202	PEB	CHC-C1D-ND	-2.74	110.25	113.72
82	iJ	201	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
82	H1	1002	PEB	CHC-C4C-NC	2.74	124.86	121.15
82	JI	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
85	h6	102	BCR	C38-C26-C27	2.74	118.88	113.62
82	H7	201	PEB	CMB-C2B-C1B	2.74	129.29	125.06
82	SE	202	PEB	C2A-C1A-NA	2.74	110.64	108.27
82	QM	204	PEB	C3B-C4B-NB	2.74	114.04	110.05
87	42	602	CLA	CHB-C4A-NA	2.74	128.30	124.51
82	JB	201	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
82	JA	203	PEB	CHA-C4A-NA	-2.74	121.94	125.20
82	YE	202	PEB	OD-C4D-C3D	-2.74	123.25	129.46
82	LP	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
82	J5	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
87	3N	309	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
87	AN	849	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
82	SM	203	PEB	C3C-C4C-NC	2.74	110.80	108.33
82	TF	201	PEB	CHA-C1B-NB	-2.74	119.20	124.93
87	AN	826	CLA	C2D-C1D-ND	-2.74	108.08	110.10
82	XF	203	PEB	CAA-C3A-C4A	-2.74	105.64	112.67
82	QD	201	PEB	C1D-CHC-C4C	-2.74	109.22	113.26
87	CL	503	CLA	C2A-C1A-CHA	2.74	128.65	123.86
84	73	1002	CYC	OC-C1C-C2C	-2.74	123.99	126.17
82	HA	203	PEB	OD-C4D-C3D	-2.74	123.25	129.46
82	GJ	201	PEB	CMA-C2A-C1A	-2.74	106.50	112.40
82	HJ	202	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	H1	1002	PEB	C3B-C4B-NB	2.74	114.03	110.05
83	xK	306	PUB	CAB-C3B-C4B	2.74	130.13	125.76
87	AN	824	CLA	C3B-C4B-NB	-2.74	107.97	110.52
87	A2	835	CLA	C3B-C4B-NB	-2.74	107.97	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	a6	605	BCR	C21-C20-C19	-2.74	114.67	123.22
87	C6	520	CLA	CHB-C4A-NA	2.74	128.30	124.51
82	a4	202	PEB	OD-C4D-C3D	-2.74	123.25	129.46
82	18	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
82	qC	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
82	oF	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
82	j4	202	PEB	C1D-CHC-C4C	2.74	117.30	113.26
82	MP	201	PEB	CHA-C1B-NB	-2.74	119.20	124.93
87	42	604	CLA	C3D-C4D-CHA	2.74	118.99	112.72
82	q8	202	PEB	CMB-C2B-C1B	2.74	129.28	125.06
85	BL	617	BCR	C11-C12-C13	-2.74	118.72	126.42
87	3N	304	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
87	AN	819	CLA	CMB-C2B-C3B	2.74	133.22	126.59
84	CG	1001	CYC	CHB-C1B-NB	-2.74	120.18	126.06
82	SJ	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
82	jF	201	PEB	OD-C4D-ND	-2.74	121.87	125.93
82	S5	203	PEB	CHA-C1B-NB	-2.74	119.20	124.93
82	iO	203	PEB	OA-C1A-C2A	-2.74	124.00	126.17
82	T7	203	PEB	C4C-C3C-C2C	-2.74	104.97	107.50
82	VK	201	PEB	CAB-CBB-CGB	-2.74	107.71	113.60
82	YF	201	PEB	CAC-C2C-C3C	2.74	133.34	127.07
82	TK	201	PEB	CHA-C1B-NB	-2.74	119.20	124.93
82	QI	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	y8	202	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	fH	202	PEB	C2A-C1A-NA	2.74	110.63	108.27
85	B6	621	BCR	C33-C5-C4	2.74	118.88	113.62
84	HE	1001	CYC	C1A-C2A-C3A	-2.74	103.75	106.78
82	V4	202	PEB	CAB-C3B-C4B	2.74	129.85	125.01
82	j4	203	PEB	C1C-CHB-C4B	2.74	134.42	128.28
82	YE	202	PEB	CHC-C1D-ND	-2.74	110.26	113.72
82	NI	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
82	CB	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
82	BI	202	PEB	CHB-C4B-NB	-2.74	118.88	124.58
96	E6	101	HEM	CHD-C1D-ND	2.74	127.39	124.42
82	PA	203	PEB	C3C-C4C-NC	2.74	110.80	108.33
82	A1	301	PEB	C4C-C3C-C2C	-2.74	104.97	107.50
83	yF	302	PUB	OA-C1A-NA	-2.74	121.87	125.93
82	BJ	301	PEB	CAC-CBC-CGC	-2.74	107.71	113.60
82	D5	201	PEB	CHB-C1C-NC	-2.74	119.05	125.32
82	QH	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
82	F7	203	PEB	CAA-C3A-C4A	-2.74	105.64	112.67
92	JL	102	LMG	O1-C1-C2	2.74	112.58	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lK	202	PEB	CAC-CBC-CGC	-2.74	107.71	113.60
82	CD	202	PEB	CHC-C1D-ND	-2.74	110.26	113.72
82	F5	201	PEB	CHC-C1D-ND	-2.74	110.26	113.72
82	D4	1002	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	U7	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
87	A2	849	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
82	uK	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
82	RK	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
87	A2	815	CLA	CHB-C4A-NA	2.74	128.30	124.51
84	D4	1001	CYC	CHB-C1B-NB	-2.74	120.18	126.06
82	L7	201	PEB	C3C-C4C-NC	2.74	110.80	108.33
82	T5	202	PEB	C4C-C3C-C2C	-2.74	104.97	107.50
87	F2	202	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
87	52	602	CLA	C3B-C4B-NB	-2.74	107.98	110.52
82	XA	203	PEB	OA-C1A-C2A	-2.74	124.00	126.17
82	TH	201	PEB	OA-C1A-C2A	-2.74	124.00	126.17
82	J9	201	PEB	OA-C1A-C2A	-2.74	124.00	126.17
82	1C	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	mK	202	PEB	CHC-C1D-ND	-2.74	110.26	113.72
94	aL	601	PL9	C2-C3-C4	2.74	122.57	118.80
82	VF	201	PEB	CAB-CBB-CGB	-2.74	107.71	113.60
82	P4	202	PEB	CAC-CBC-CGC	-2.74	107.71	113.60
82	XQ	202	PEB	CMB-C2B-C1B	2.74	129.28	125.06
82	b1	201	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
82	HQ	203	PEB	CMC-C3C-C4C	2.74	129.96	127.06
85	b6	601	BCR	C15-C16-C17	-2.74	117.87	123.47
82	lG	202	PEB	CAB-CBB-CGB	-2.74	107.72	113.60
82	Y4	203	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	18	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	N1	1002	PEB	OD-C4D-ND	-2.74	121.88	125.93
82	BQ	203	PEB	CMB-C2B-C1B	2.74	129.28	125.06
98	AN	842	PQN	C14-C13-C15	2.74	119.87	115.27
82	XI	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
82	BQ	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
82	YA	303	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
82	PB	201	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
82	A4	301	PEB	CHA-C1B-NB	-2.74	119.21	124.93
82	OO	202	PEB	CHC-C4C-NC	2.74	124.85	121.15
82	DD	201	PEB	C1C-NC-C4C	-2.74	104.73	109.60
87	5N	606	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
82	QH	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
82	xF	303	PEB	C3B-C4B-NB	2.74	114.03	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SO	201	PEB	CHB-C4B-NB	2.74	130.27	124.58
94	DL	401	PL9	C37-C38-C39	-2.74	121.07	127.66
82	gH	201	PEB	CMB-C2B-C1B	2.74	129.28	125.06
82	YP	501	PEB	CHA-C4A-NA	2.74	128.46	125.20
84	LH	1002	CYC	CAD-C3D-C4D	2.74	130.12	125.76
82	OI	203	PEB	CHC-C1D-ND	-2.74	110.26	113.72
95	AL	414	DGD	O3G-C1D-C2D	2.73	112.57	108.30
87	bL	618	CLA	CMD-C2D-C1D	-2.73	119.89	124.71
82	vC	202	PEB	CAA-C3A-C2A	-2.73	107.43	114.26
87	62	306	CLA	C3B-C4B-NB	-2.73	107.98	110.52
82	kK	203	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
84	DH	1003	CYC	C4A-C3A-C2A	-2.73	103.37	106.51
82	Y5	201	PEB	OD-C4D-ND	-2.73	121.88	125.93
87	42	603	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
82	XJ	202	PEB	C1C-CHB-C4B	-2.73	122.15	128.28
82	rF	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	Z5	304	PEB	CAA-C3A-C4A	-2.73	105.65	112.67
82	hJ	203	PEB	CHA-C1B-NB	-2.73	119.21	124.93
82	BK	201	PEB	C3B-C4B-NB	2.73	114.03	110.05
85	F6	101	BCR	C38-C26-C27	2.73	118.87	113.62
82	VD	202	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
82	eF	203	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
85	b6	602	BCR	C38-C26-C25	-2.73	121.46	124.53
82	cJ	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
84	BE	1001	CYC	C1D-C2D-C3D	-2.73	104.31	107.79
82	V4	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
82	cK	201	PEB	C1D-CHC-C4C	2.73	117.29	113.26
82	z8	201	PEB	CAA-C3A-C2A	-2.73	107.43	114.26
82	JI	202	PEB	CHC-C1D-ND	-2.73	110.27	113.72
85	cL	504	BCR	C38-C26-C27	2.73	118.87	113.62
82	RQ	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	Q9	203	PEB	C3B-C4B-NB	2.73	114.03	110.05
82	V1	203	PEB	OD-C4D-ND	-2.73	121.88	125.93
82	aF	203	PEB	CHC-C4C-NC	2.73	124.85	121.15
82	SF	202	PEB	CHB-C1C-C2C	-2.73	120.98	127.15
82	LF	202	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
82	DH	1002	PEB	C2A-C1A-NA	2.73	110.63	108.27
82	OI	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	H7	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	KM	201	PEB	CAA-C3A-C2A	-2.73	107.43	114.26
87	3N	306	CLA	CHB-C4A-NA	2.73	128.29	124.51
87	4N	609	CLA	O2D-CGD-CBD	2.73	116.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XK	203	PEB	CMC-C3C-C4C	2.73	129.96	127.06
87	5N	602	CLA	C3B-C4B-NB	-2.73	107.98	110.52
82	RG	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	TI	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	eO	202	PEB	C1D-CHC-C4C	-2.73	109.23	113.26
82	kG	201	PEB	CHB-C1C-NC	-2.73	119.06	125.32
82	XB	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	YD	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	GI	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	XQ	201	PEB	CAC-C2C-C1C	2.73	130.11	125.76
82	ZB	201	PEB	OD-C4D-ND	-2.73	121.88	125.93
82	YE	202	PEB	OD-C4D-ND	-2.73	121.88	125.93
87	bL	607	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
85	c6	617	BCR	C38-C26-C27	2.73	118.86	113.62
82	1C	201	PEB	C2A-C1A-NA	2.73	110.63	108.27
87	BN	828	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
82	P9	201	PEB	CHC-C4C-NC	2.73	124.85	121.15
92	b6	619	LMG	O8-C28-C29	2.73	120.48	111.91
87	AN	835	CLA	C3B-C4B-NB	-2.73	107.98	110.52
87	B6	604	CLA	C3B-C4B-NB	-2.73	107.98	110.52
85	d6	405	BCR	C35-C13-C14	-2.73	119.10	122.92
82	BB	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	QQ	201	PEB	CHA-C1B-NB	-2.73	119.22	124.93
82	fG	203	PEB	CHA-C1B-NB	-2.73	119.22	124.93
82	KD	202	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
82	tK	203	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
82	bO	202	PEB	CHC-C1D-ND	-2.73	110.27	113.72
82	XJ	201	PEB	CAB-CBB-CGB	-2.73	107.73	113.60
82	VO	201	PEB	CHB-C4B-C3B	-2.73	119.00	125.32
82	X7	203	PEB	CHB-C4B-C3B	-2.73	119.00	125.32
82	T7	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	hG	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
82	Z4	201	PEB	OA-C1A-NA	2.73	128.25	124.94
87	c6	614	CLA	CHB-C4A-NA	2.73	128.29	124.51
82	lO	202	PEB	CMB-C2B-C1B	2.73	129.27	125.06
82	S9	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	lM	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
87	A2	834	CLA	C3B-C4B-NB	-2.73	107.98	110.52
82	aE	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
82	DQ	202	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
82	WH	202	PEB	CHC-C4C-NC	2.73	124.84	121.15
82	T7	201	PEB	CMA-C2A-C1A	-2.73	106.52	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	N7	201	PEB	CHA-C4A-NA	2.73	128.45	125.20
82	t8	201	PEB	CAC-CBC-CGC	-2.73	107.73	113.60
82	VD	201	PEB	CHB-C4B-NB	-2.73	118.90	124.58
82	xF	304	PEB	CAB-C3B-C4B	2.73	129.84	125.01
82	VM	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
87	a6	607	CLA	C1-C2-C3	-2.73	121.32	126.04
82	EB	501	PEB	CHC-C1D-ND	-2.73	110.27	113.72
85	cL	503	BCR	C10-C11-C12	-2.73	114.70	123.22
82	LP	201	PEB	CHC-C4C-NC	2.73	124.84	121.15
82	B9	202	PEB	C2A-C1A-NA	2.73	110.63	108.27
82	iE	201	PEB	C2A-C1A-NA	2.73	110.63	108.27
82	jE	202	PEB	C2A-C1A-NA	2.73	110.63	108.27
82	PO	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
82	zC	202	PEB	CAA-C3A-C2A	-2.73	107.44	114.26
87	A2	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
82	VI	202	PEB	OD-C4D-C3D	-2.73	123.28	129.46
87	B2	810	CLA	CHC-C4B-NB	2.73	127.15	124.26
82	i4	203	PEB	CBB-CAB-C3B	2.73	120.21	112.63
82	b1	201	PEB	CHA-C1B-NB	-2.73	119.22	124.93
82	NI	203	PEB	CHA-C1B-C2B	2.73	131.92	124.90
82	IP	203	PEB	C1C-NC-C4C	2.73	114.45	109.60
82	DJ	201	PEB	CMB-C2B-C1B	2.73	129.27	125.06
82	FK	202	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
82	cM	201	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
82	WG	201	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	QH	203	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	eO	203	PEB	OD-C4D-C3D	-2.73	123.28	129.46
82	OA	202	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
82	H5	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
87	B2	808	CLA	CHB-C4A-NA	2.73	128.28	124.51
87	B2	828	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
82	dJ	202	PEB	CBC-CAC-C2C	2.73	120.21	112.63
82	UF	201	PEB	C3C-C4C-NC	2.73	110.79	108.33
87	A2	801	CLA	C3C-C4C-NC	-2.73	107.51	110.57
82	gJ	202	PEB	CHA-C1B-NB	-2.73	119.23	124.93
84	JO	1001	CYC	CHB-C1B-NB	-2.73	120.20	126.06
82	JO	1002	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	JQ	201	PEB	C2A-C1A-NA	2.73	110.62	108.27
82	VK	202	PEB	C4B-NB-C1B	-2.73	101.37	106.51
82	xK	303	PEB	C3B-C4B-NB	2.73	114.02	110.05
82	kM	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
87	2N	310	CLA	CHB-C4A-NA	2.73	128.28	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	h6	102	BCR	C33-C5-C6	-2.73	121.47	124.53
82	sC	202	PEB	C4B-C3B-C2B	-2.73	103.77	106.78
87	BL	619	CLA	O2D-CGD-CBD	2.73	116.11	111.27
82	TI	201	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	FA	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
82	mM	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
82	sF	203	PEB	CHC-C1D-ND	-2.73	110.28	113.72
82	gB	203	PEB	OD-C4D-C3D	-2.73	123.28	129.46
84	J4	1001	CYC	CHB-C1B-NB	-2.73	120.20	126.06
82	pC	202	PEB	CAC-C2C-C1C	2.73	130.10	125.76
82	P7	203	PEB	C4C-C3C-C2C	-2.73	104.98	107.50
82	M5	304	PEB	CAA-C3A-C4A	-2.73	105.67	112.67
82	nK	202	PEB	CMB-C2B-C1B	2.73	129.26	125.06
82	SK	203	PEB	CHA-C1B-NB	-2.73	119.23	124.93
82	J4	1002	PEB	CHA-C1B-NB	-2.73	119.23	124.93
87	c6	614	CLA	CHD-C1D-ND	-2.73	121.95	124.45
82	YH	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	kO	202	PEB	C1C-CHB-C4B	2.73	134.40	128.28
82	CQ	202	PEB	C3B-C4B-NB	2.73	114.01	110.05
82	lE	203	PEB	C3B-C4B-NB	2.73	114.01	110.05
83	xF	306	PUB	CHB-C1C-C2C	-2.73	119.01	125.32
85	bL	603	BCR	C29-C30-C25	2.73	114.68	110.48
87	A2	828	CLA	C2A-C1A-CHA	2.73	128.62	123.86
87	6N	601	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
82	A4	305	PEB	OD-C4D-C3D	-2.73	123.28	129.46
82	kG	202	PEB	CHA-C1B-NB	-2.73	119.23	124.93
82	OI	202	PEB	C2B-C1B-NB	2.73	116.35	110.53
82	DJ	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
82	NB	202	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
82	OF	203	PEB	C4C-C3C-C2C	-2.73	104.98	107.50
82	E5	202	PEB	C4C-C3C-C2C	-2.73	104.98	107.50
82	K5	202	PEB	C4C-C3C-C2C	-2.73	104.98	107.50
82	CI	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
82	YM	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
82	gB	201	PEB	CHA-C1B-NB	-2.72	119.23	124.93
85	c6	603	BCR	C38-C26-C27	2.72	118.85	113.62
82	RH	201	PEB	OD-C4D-C3D	-2.72	123.29	129.46
82	hO	202	PEB	CHA-C1B-NB	-2.72	119.23	124.93
82	qC	201	PEB	C3B-C4B-NB	2.72	114.01	110.05
82	Z4	201	PEB	CHB-C1C-C2C	-2.72	121.00	127.15
82	v8	202	PEB	CAA-C3A-C2A	-2.72	107.45	114.26
103	82	310	ZEX	C32-C33-C34	2.72	123.12	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jJ	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
87	BN	821	CLA	C1D-ND-C4D	-2.72	104.40	106.33
82	QG	203	PEB	CHB-C1C-C2C	-2.72	121.00	127.15
82	OJ	202	PEB	C1D-CHC-C4C	2.72	117.27	113.26
82	FA	203	PEB	CHA-C1B-NB	-2.72	119.24	124.93
82	cB	401	PEB	CMB-C2B-C1B	2.72	129.26	125.06
84	M3	1001	CYC	C1B-C2B-C3B	-2.72	105.03	107.87
82	FA	203	PEB	OD-C4D-ND	-2.72	121.90	125.93
82	tF	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
82	IP	202	PEB	CHB-C4B-C3B	-2.72	119.02	125.32
82	AO	301	PEB	CHA-C1B-NB	-2.72	119.24	124.93
82	EP	203	PEB	CHA-C1B-NB	-2.72	119.24	124.93
82	BF	201	PEB	C3B-C4B-NB	2.72	114.01	110.05
82	AQ	303	PEB	C3B-C4B-NB	2.72	114.01	110.05
82	X7	203	PEB	OA-C1A-C2A	-2.72	124.01	126.17
85	FL	101	BCR	C15-C14-C13	-2.72	123.42	127.31
82	Y1	201	PEB	C4C-C3C-C2C	-2.72	104.99	107.50
82	EI	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
87	AN	826	CLA	CHB-C4A-NA	2.72	128.28	124.51
82	dG	203	PEB	CAB-CBB-CGB	-2.72	107.74	113.60
84	EH	1001	CYC	CMB-C2B-C1B	2.72	127.57	124.17
84	L1	1001	CYC	CAD-C3D-C4D	2.72	130.10	125.76
82	JD	201	PEB	C2A-C1A-NA	2.72	110.62	108.27
82	PD	201	PEB	C3C-C4C-NC	2.72	110.78	108.33
82	s8	201	PEB	CHA-C1B-C2B	2.72	131.90	124.90
82	WB	401	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
82	vC	201	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
84	C1	1001	CYC	C4D-CHA-C1A	2.72	134.39	128.28
82	MQ	201	PEB	CHB-C1C-NC	-2.72	119.08	125.32
87	CL	509	CLA	C2A-C1A-CHA	2.72	128.62	123.86
82	D9	203	PEB	CHC-C4C-NC	2.72	124.83	121.15
87	AN	815	CLA	CHB-C4A-NA	2.72	128.28	124.51
82	XF	201	PEB	CAB-C3B-C4B	2.72	129.82	125.01
82	hJ	202	PEB	CAB-C3B-C4B	2.72	129.82	125.01
94	d6	408	PL9	C27-C28-C29	-2.72	121.11	127.66
82	lH	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
82	YP	501	PEB	CAB-CBB-CGB	-2.72	107.75	113.60
82	CM	202	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
82	bH	201	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
84	n3	1001	CYC	C1B-C2B-C3B	-2.72	105.03	107.87
82	ZE	201	PEB	CMB-C2B-C1B	2.72	129.25	125.06
82	F9	202	PEB	CMB-C2B-C1B	2.72	129.25	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gK	202	PEB	CMB-C2B-C1B	2.72	129.25	125.06
82	RI	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
82	J5	203	PEB	OD-C4D-C3D	-2.72	123.29	129.46
82	SP	201	PEB	C1C-NC-C4C	2.72	114.44	109.60
82	Y5	201	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
87	A2	819	CLA	CMB-C2B-C3B	2.72	133.18	126.59
85	BN	843	BCR	C29-C30-C25	2.72	114.67	110.48
84	ME	1001	CYC	CMB-C2B-C1B	2.72	127.56	124.17
87	52	606	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
94	A6	410	PL9	C40-C39-C41	2.72	119.85	115.27
87	c6	614	CLA	C3B-C4B-NB	-2.72	107.99	110.52
87	aL	606	CLA	C3B-C4B-NB	-2.72	107.99	110.52
82	XM	202	PEB	CHA-C1B-NB	-2.72	119.24	124.93
82	SK	202	PEB	CHB-C1C-C2C	-2.72	121.01	127.15
87	A6	404	CLA	C1-C2-C3	-2.72	122.35	126.75
87	DL	403	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
82	VM	202	PEB	C1C-CHB-C4B	-2.72	122.18	128.28
83	QJ	201	PUB	CHB-C1C-NC	-2.72	118.92	124.58
82	NE	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
82	V1	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
87	32	310	CLA	CHB-C4A-NA	2.72	128.27	124.51
82	DB	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	AI	202	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	XA	202	PEB	C1C-NC-C4C	-2.72	104.76	109.60
82	KI	201	PEB	C1C-NC-C4C	-2.72	104.76	109.60
94	aL	601	PL9	C10-C9-C11	2.72	119.85	115.27
83	xK	306	PUB	CHB-C1C-C2C	-2.72	119.03	125.32
87	bL	622	CLA	C3B-C4B-NB	-2.72	107.99	110.52
84	S3	1001	CYC	C1B-C2B-C3B	-2.72	105.03	107.87
82	lM	203	PEB	C3B-C4B-NB	2.72	114.00	110.05
82	SO	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
87	82	302	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
82	AI	202	PEB	C3C-C4C-NC	2.72	110.78	108.33
82	cF	201	PEB	OA-C1A-C2A	-2.72	124.01	126.17
82	F5	202	PEB	CAB-C3B-C4B	2.72	129.82	125.01
82	wK	302	PEB	C2A-C1A-NA	2.72	110.62	108.27
82	JD	203	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
82	UI	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
82	NP	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
85	C6	508	BCR	C37-C22-C23	2.72	122.36	118.08
82	tC	201	PEB	CAC-CBC-CGC	-2.72	107.75	113.60
85	cL	504	BCR	C39-C30-C25	-2.72	105.89	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OJ	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	A4	301	PEB	C1D-CHC-C4C	-2.72	109.25	113.26
82	wF	303	PEB	C1D-CHC-C4C	2.72	117.27	113.26
82	II	203	PEB	C2B-C1B-NB	2.72	116.33	110.53
88	L6	101	LHG	C5-O7-C7	-2.72	111.10	117.79
82	BF	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
82	gH	201	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
82	QP	203	PEB	C1C-NC-C4C	2.72	114.43	109.60
82	OK	202	PEB	C4C-C3C-C2C	-2.72	104.99	107.50
87	F2	205	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
82	VK	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	OO	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	fG	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
87	22	610	CLA	CHB-C4A-NA	2.72	128.27	124.51
87	3N	310	CLA	CHB-C4A-NA	2.72	128.27	124.51
82	UD	201	PEB	CHA-C4A-NA	2.72	128.44	125.20
82	OP	201	PEB	CMB-C2B-C1B	2.72	129.25	125.06
82	u8	203	PEB	CMB-C2B-C1B	2.72	129.25	125.06
87	b6	605	CLA	C1D-ND-C4D	-2.72	104.40	106.33
82	SK	202	PEB	C3B-C4B-NB	2.72	114.00	110.05
82	PA	202	PEB	C1D-CHC-C4C	-2.72	109.25	113.26
82	q8	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
87	AN	814	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
82	OP	202	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	eH	203	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	r8	201	PEB	OD-C4D-ND	-2.72	121.90	125.93
84	D3	1001	CYC	C1B-C2B-C3B	-2.72	105.03	107.87
84	FH	1001	CYC	C1A-C2A-C3A	-2.72	103.78	106.78
87	AN	803	CLA	CHB-C4A-NA	2.72	128.27	124.51
82	aJ	204	PEB	OD-C4D-C3D	-2.72	123.30	129.46
84	FE	1002	CYC	C2A-C1A-NA	2.72	114.00	110.05
87	BL	603	CLA	C3B-C4B-NB	-2.72	107.99	110.52
82	BD	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
82	RB	201	PEB	OD-C4D-ND	-2.72	121.91	125.93
82	H5	203	PEB	OD-C4D-ND	-2.72	121.91	125.93
82	lM	201	PEB	CMB-C2B-C1B	2.72	129.25	125.06
87	AN	807	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
82	HO	1002	PEB	CAC-C2C-C1C	2.72	130.09	125.76
82	E7	202	PEB	CHA-C1B-NB	-2.72	119.25	124.93
82	YA	303	PEB	C3B-C4B-NB	2.72	114.00	110.05
82	ZH	201	PEB	C1D-CHC-C4C	2.72	117.26	113.26
82	IP	202	PEB	C4B-C3B-C2B	-2.72	103.78	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	g1	201	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
82	p8	201	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
82	dO	201	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
85	fL	101	BCR	C29-C30-C25	2.72	114.66	110.48
82	OI	202	PEB	CHB-C4B-NB	-2.72	118.92	124.58
82	sK	203	PEB	C1C-CHB-C4B	2.72	134.37	128.28
82	BB	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
82	EA	202	PEB	CHA-C1B-NB	-2.72	119.25	124.93
82	FK	202	PEB	CHA-C1B-NB	-2.72	119.25	124.93
82	PO	202	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
82	gG	202	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
82	V5	202	PEB	C4C-C3C-C2C	-2.72	104.99	107.50
82	H4	1002	PEB	CAC-C2C-C1C	2.72	130.09	125.76
82	dK	202	PEB	OD-C4D-C3D	-2.72	123.31	129.46
87	AN	830	CLA	CHB-C4A-NA	2.72	128.27	124.51
87	BN	818	CLA	CHB-C4A-NA	2.72	128.27	124.51
88	l6	101	LHG	C5-O7-C7	-2.72	111.10	117.79
82	RB	202	PEB	CAC-CBC-CGC	-2.72	107.76	113.60
82	S9	202	PEB	C3B-C4B-NB	2.72	114.00	110.05
82	j4	202	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
82	qF	201	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
82	sK	202	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
84	M4	1001	CYC	CHA-C4D-C3D	-2.72	121.02	127.15
84	H3	1001	CYC	C1B-C2B-C3B	-2.72	105.04	107.87
84	q3	1001	CYC	C1B-C2B-C3B	-2.72	105.04	107.87
82	hH	201	PEB	OD-C4D-ND	-2.72	121.91	125.93
82	gH	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
94	a6	601	PL9	C45-C44-C46	2.72	119.84	115.27
87	4N	602	CLA	CHB-C4A-NA	2.72	128.27	124.51
87	42	609	CLA	O2D-CGD-CBD	2.72	116.09	111.27
82	C5	202	PEB	C4C-C3C-C2C	-2.72	104.99	107.50
82	iM	201	PEB	CHB-C1C-NC	-2.72	119.10	125.32
82	XQ	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
87	FN	203	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
87	bL	621	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
85	K6	102	BCR	C34-C9-C10	-2.71	119.12	122.92
84	l3	1001	CYC	CBC-CAC-C3C	2.71	119.51	113.47
82	R4	201	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
82	eE	203	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
82	W4	201	PEB	CHB-C4B-NB	2.71	130.23	124.58
82	b4	202	PEB	CHC-C1D-ND	-2.71	110.29	113.72
82	TD	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	HL	101	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
82	eM	202	PEB	CAC-CBC-CGC	-2.71	107.76	113.60
82	DI	202	PEB	C4C-C3C-C2C	-2.71	105.00	107.50
82	VK	201	PEB	C4C-C3C-C2C	-2.71	105.00	107.50
82	aO	203	PEB	CBB-CAB-C3B	2.71	120.17	112.63
82	ZH	203	PEB	CHB-C4B-NB	-2.71	118.93	124.58
82	AK	202	PEB	C3B-C4B-NB	2.71	114.00	110.05
82	eE	203	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
95	C6	504	DGD	C4D-C3D-C2D	-2.71	106.08	110.82
82	TO	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
82	OH	203	PEB	CHA-C1B-NB	-2.71	119.26	124.93
94	aL	601	PL9	O1-C4-C3	2.71	123.71	120.72
82	cF	203	PEB	CAC-CBC-CGC	-2.71	107.76	113.60
82	t8	202	PEB	CMB-C2B-C1B	2.71	129.24	125.06
82	YG	202	PEB	OD-C4D-ND	-2.71	121.91	125.93
82	YQ	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
87	cL	505	CLA	C1-C2-C3	-2.71	121.35	126.04
85	k6	102	BCR	C34-C9-C10	-2.71	119.12	122.92
87	AN	852	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
87	A2	852	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
82	GF	203	PEB	C2A-C1A-NA	2.71	110.61	108.27
82	LI	201	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
82	HD	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
82	II	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
82	aO	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
87	BN	805	CLA	CHB-C1B-NB	2.71	127.13	124.26
82	kF	202	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
87	FN	205	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
82	iH	201	PEB	OA-C1A-C2A	-2.71	124.02	126.17
82	JD	203	PEB	C3B-C4B-NB	2.71	114.00	110.05
82	ZG	203	PEB	C3B-C4B-NB	2.71	114.00	110.05
82	EA	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
82	PI	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
82	ZE	201	PEB	CHA-C1B-NB	-2.71	119.26	124.93
82	L5	202	PEB	C1C-CHB-C4B	2.71	134.37	128.28
82	rC	201	PEB	OD-C4D-ND	-2.71	121.91	125.93
82	g1	201	PEB	CHB-C4B-C3B	-2.71	119.04	125.32
82	LM	202	PEB	O2B-CGB-CBB	2.71	122.74	114.03
82	BJ	301	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
82	eF	201	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
82	AO	305	PEB	OD-C4D-C3D	-2.71	123.31	129.46
82	a1	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	d6	401	CLA	C3B-C4B-NB	-2.71	108.00	110.52
82	fE	203	PEB	CHA-C1B-NB	-2.71	119.26	124.93
82	oK	202	PEB	C4C-C3C-C2C	-2.71	105.00	107.50
82	OE	203	PEB	C1C-CHB-C4B	2.71	134.36	128.28
82	MB	201	PEB	C3B-C4B-NB	2.71	113.99	110.05
82	WD	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
85	J2	102	BCR	C33-C5-C6	-2.71	121.48	124.53
84	T3	1001	CYC	CBC-CAC-C3C	2.71	119.50	113.47
82	V7	203	PEB	CHC-C1D-ND	-2.71	110.29	113.72
82	pF	201	PEB	CHC-C1D-ND	-2.71	110.29	113.72
82	MJ	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
82	pC	201	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
87	AN	828	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
87	A2	833	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
87	C6	511	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
82	SF	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
84	N1	1001	CYC	C2A-C1A-NA	2.71	113.99	110.05
82	yC	203	PEB	CAB-C3B-C4B	2.71	129.81	125.01
82	dE	203	PEB	CAB-C3B-C4B	2.71	129.81	125.01
87	B2	820	CLA	C1D-ND-C4D	-2.71	104.41	106.33
82	UH	201	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
87	3N	313	CLA	CHB-C4A-NA	2.71	128.26	124.51
82	e4	202	PEB	CAC-CBC-CGC	-2.71	107.77	113.60
87	B6	612	CLA	C3B-C4B-NB	-2.71	108.00	110.52
84	Q3	1001	CYC	C1B-C2B-C3B	-2.71	105.04	107.87
82	RQ	202	PEB	C2A-C1A-NA	2.71	110.61	108.27
82	A1	302	PEB	C2A-C1A-NA	2.71	110.61	108.27
82	fH	201	PEB	CHA-C1B-NB	-2.71	119.26	124.93
87	CL	506	CLA	CAC-C3C-C2C	-2.71	122.89	127.53
82	MF	203	PEB	OD-C4D-C3D	-2.71	123.32	129.46
87	AN	826	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
82	W4	201	PEB	OD-C4D-ND	-2.71	121.92	125.93
82	HH	1002	PEB	CHC-C4C-NC	2.71	124.82	121.15
85	BL	616	BCR	C21-C20-C19	-2.71	114.76	123.22
82	aM	204	PEB	C3C-C4C-NC	2.71	110.77	108.33
82	QG	201	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	IP	201	PEB	OD-C4D-C3D	-2.71	123.32	129.46
82	R1	201	PEB	OD-C4D-C3D	-2.71	123.32	129.46
82	rK	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
82	xF	304	PEB	C3B-C4B-NB	2.71	113.99	110.05
87	B6	610	CLA	C3B-C4B-NB	-2.71	108.00	110.52
82	AH	301	PEB	C4C-C3C-C2C	-2.71	105.00	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	ME	1001	CYC	CBC-CAC-C3C	-2.71	107.43	113.47
83	QM	201	PUB	OA-C1A-NA	-2.71	121.92	125.93
82	j1	201	PEB	CAB-CBB-CGB	-2.71	107.77	113.60
82	UH	203	PEB	CHC-C4C-NC	2.71	124.82	121.15
82	cB	403	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	WG	203	PEB	CHA-C1B-NB	-2.71	119.27	124.93
82	EJ	203	PEB	C3C-C4C-NC	2.71	110.77	108.33
82	W1	202	PEB	C3C-C4C-NC	2.71	110.77	108.33
84	HO	1001	CYC	CAD-CBD-CGD	-2.71	107.77	113.60
82	kF	203	PEB	OA-C1A-C2A	-2.71	124.02	126.17
87	A2	826	CLA	CHB-C4A-NA	2.71	128.26	124.51
82	R7	202	PEB	C2B-C1B-NB	2.71	116.31	110.53
82	SD	202	PEB	CHC-C4C-NC	2.71	124.81	121.15
82	jH	201	PEB	CAB-CBB-CGB	-2.71	107.77	113.60
82	VH	201	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	hK	201	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	OA	201	PEB	CMA-C2A-C1A	-2.71	106.56	112.40
82	b1	202	PEB	CHA-C4A-NA	-2.71	121.98	125.20
85	BN	838	BCR	C23-C24-C25	2.71	134.81	127.20
82	P7	202	PEB	C1D-CHC-C4C	-2.71	109.26	113.26
82	Q5	202	PEB	CBA-CAA-C3A	-2.71	107.44	113.47
84	MG	1001	CYC	CBC-CAC-C3C	-2.71	107.44	113.47
82	F7	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
87	52	604	CLA	C3B-C4B-NB	-2.71	108.00	110.52
94	A6	410	PL9	C20-C19-C21	2.71	119.83	115.27
82	VK	202	PEB	C4B-C3B-C2B	-2.71	103.79	106.78
82	FQ	202	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	J5	202	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
94	aL	601	PL9	C31-C32-C33	-2.71	102.98	111.88
82	jG	202	PEB	C2A-C1A-NA	2.71	110.61	108.27
82	mE	201	PEB	CHA-C1B-NB	-2.71	119.27	124.93
87	3N	303	CLA	C3D-C2D-C1D	-2.71	102.14	105.83
82	XD	201	PEB	CAC-C2C-C1C	2.71	130.07	125.76
82	UO	201	PEB	C4B-C3B-C2B	-2.71	103.79	106.78
82	U4	201	PEB	C4B-C3B-C2B	-2.71	103.79	106.78
82	lG	202	PEB	C4B-C3B-C2B	-2.71	103.79	106.78
82	GB	202	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
87	BN	807	CLA	C3B-C4B-NB	-2.71	108.00	110.52
87	B2	806	CLA	C3B-C4B-NB	-2.71	108.00	110.52
87	b6	616	CLA	C3B-C4B-NB	-2.71	108.00	110.52
82	I5	202	PEB	C4C-C3C-C2C	-2.71	105.00	107.50
82	H9	201	PEB	C4C-C3C-C2C	-2.71	105.00	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	Z5	302	PUB	C1B-C2B-C3B	-2.71	105.00	107.50
82	T4	203	PEB	C3B-C4B-NB	2.71	113.99	110.05
82	PQ	203	PEB	CHA-C1B-NB	-2.71	119.27	124.93
82	D7	202	PEB	OD-C4D-ND	-2.71	121.92	125.93
82	x8	202	PEB	OD-C4D-ND	-2.71	121.92	125.93
82	C9	202	PEB	C1C-CHB-C4B	2.71	134.35	128.28
84	O3	1001	CYC	C1B-C2B-C3B	-2.71	105.05	107.87
82	SA	201	PEB	CAB-C3B-C4B	2.71	129.80	125.01
82	fO	201	PEB	C2B-C1B-NB	2.71	116.31	110.53
87	A2	803	CLA	CHB-C4A-NA	2.71	128.25	124.51
82	U1	202	PEB	CHB-C1C-C2C	-2.71	121.05	127.15
82	lO	201	PEB	CMA-C2A-C1A	-2.71	106.57	112.40
82	BK	202	PEB	C4B-C3B-C2B	-2.71	103.79	106.78
82	F9	203	PEB	CHC-C4C-NC	2.71	124.81	121.15
83	KA	203	PUB	CHA-C1B-NB	2.71	124.81	121.15
82	O9	201	PEB	CHC-C1D-ND	-2.71	110.30	113.72
82	OH	201	PEB	C3B-C4B-NB	2.71	113.98	110.05
94	d6	408	PL9	C12-C13-C14	-2.71	121.14	127.66
87	72	606	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
82	aH	201	PEB	C4C-C3C-C2C	-2.71	105.00	107.50
87	AN	802	CLA	C3C-C4C-NC	-2.71	107.54	110.57
87	8N	301	CLA	CAC-C3C-C4C	-2.71	121.30	124.81
87	A2	838	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
82	c4	201	PEB	OD-C4D-C3D	-2.71	123.33	129.46
82	bB	201	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	oK	202	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
82	s8	202	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
82	hJ	203	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
82	AH	301	PEB	CHA-C4A-NA	2.70	128.42	125.20
84	J3	1001	CYC	CBC-CAC-C3C	2.70	119.49	113.47
82	nF	202	PEB	CMB-C2B-C1B	2.70	129.23	125.06
82	PA	203	PEB	C4C-C3C-C2C	-2.70	105.00	107.50
82	a1	201	PEB	C4C-C3C-C2C	-2.70	105.00	107.50
98	B2	837	PQN	C9-C10-C5	-2.70	116.25	119.26
85	B2	838	BCR	C23-C24-C25	2.70	134.80	127.20
82	TQ	202	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
82	eG	203	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
84	DH	1003	CYC	C2C-C1C-NC	2.70	110.60	108.27
82	M7	202	PEB	CMB-C2B-C1B	2.70	129.23	125.06
82	YM	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
82	OM	202	PEB	CHB-C1C-NC	-2.70	119.13	125.32
84	x3	1001	CYC	CBC-CAC-C3C	2.70	119.49	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NK	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
82	VG	201	PEB	CHC-C4C-NC	2.70	124.81	121.15
82	T4	201	PEB	CAC-CBC-CGC	-2.70	107.78	113.60
82	X9	202	PEB	C1C-CHB-C4B	2.70	134.34	128.28
87	52	605	CLA	C3B-C4B-NB	-2.70	108.01	110.52
87	D6	402	CLA	C3B-C4B-NB	-2.70	108.01	110.52
82	U9	204	PEB	CHA-C1B-C2B	2.70	131.85	124.90
82	CK	203	PEB	CMB-C2B-C1B	2.70	129.23	125.06
82	g1	202	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
82	DH	1002	PEB	C3B-C4B-NB	2.70	113.98	110.05
82	VQ	201	PEB	CHB-C4B-NB	-2.70	118.95	124.58
82	aM	203	PEB	CHA-C1B-NB	-2.70	119.28	124.93
82	l1	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
82	kK	203	PEB	CHB-C4B-C3B	-2.70	119.07	125.32
87	AN	838	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
87	cL	507	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
82	H9	203	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	LA	201	PEB	C3C-C4C-NC	2.70	110.77	108.33
87	A2	830	CLA	CHB-C4A-NA	2.70	128.25	124.51
82	jG	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
84	d3	1001	CYC	C1B-C2B-C3B	-2.70	105.05	107.87
82	eH	202	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
82	HO	1002	PEB	CMB-C2B-C1B	2.70	129.22	125.06
82	sK	203	PEB	CHC-C1D-ND	-2.70	110.31	113.72
82	DK	203	PEB	C2A-C1A-NA	2.70	110.60	108.27
84	F1	1001	CYC	C2C-C1C-NC	2.70	110.60	108.27
84	y3	1001	CYC	C2C-C1C-NC	-2.70	105.94	108.27
82	e4	203	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	U7	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	cO	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	NM	201	PEB	CHB-C4B-NB	-2.70	118.95	124.58
82	aM	202	PEB	CHA-C1B-NB	-2.70	119.28	124.93
82	fJ	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
82	GB	202	PEB	CAC-CBC-CGC	-2.70	107.79	113.60
82	z8	201	PEB	C4C-C3C-C2C	-2.70	105.01	107.50
82	KI	203	PEB	C1D-CHC-C4C	-2.70	109.27	113.26
82	J7	202	PEB	CHC-C1D-ND	-2.70	110.31	113.72
87	a6	609	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
82	bH	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
82	SB	202	PEB	CAB-C3B-C4B	2.70	129.79	125.01
85	B2	843	BCR	C29-C30-C25	2.70	114.64	110.48
82	LQ	202	PEB	C3B-C4B-NB	2.70	113.98	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iG	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
82	X5	202	PEB	OD-C4D-ND	-2.70	121.93	125.93
82	W9	201	PEB	OD-C4D-ND	-2.70	121.93	125.93
84	HE	1001	CYC	CAD-CBD-CGD	-2.70	107.79	113.60
82	YJ	202	PEB	CHB-C1C-C2C	-2.70	121.06	127.15
82	SK	203	PEB	CHB-C1C-C2C	-2.70	121.06	127.15
82	J7	202	PEB	CMB-C2B-C1B	2.70	129.22	125.06
82	UG	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
82	kE	202	PEB	CHA-C1B-NB	-2.70	119.28	124.93
82	IQ	202	PEB	CMC-C3C-C4C	2.70	129.92	127.06
84	I3	1001	CYC	C1B-C2B-C3B	-2.70	105.05	107.87
84	k3	1001	CYC	C1B-C2B-C3B	-2.70	105.05	107.87
92	bL	611	LMG	O1-C1-C2	2.70	112.52	108.30
82	FA	203	PEB	CAA-C3A-C4A	-2.70	105.74	112.67
85	LN	205	BCR	C2-C1-C6	2.70	114.64	110.48
82	KI	203	PEB	OD-C4D-C3D	-2.70	123.34	129.46
84	c3	1001	CYC	CBC-CAC-C3C	2.70	119.48	113.47
82	U9	204	PEB	C4C-C3C-C2C	-2.70	105.01	107.50
82	QF	202	PEB	CMB-C2B-C1B	2.70	129.22	125.06
82	HM	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	HQ	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	kK	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
82	gE	202	PEB	C1D-CHC-C4C	2.70	117.24	113.26
82	VF	202	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	QI	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
82	eJ	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
82	SB	202	PEB	C3B-C4B-NB	2.70	113.98	110.05
94	A6	410	PL9	C17-C18-C19	-2.70	121.16	127.66
84	H4	1001	CYC	CAD-CBD-CGD	-2.70	107.79	113.60
87	CL	505	CLA	C3B-C4B-NB	-2.70	108.01	110.52
87	5N	604	CLA	C3B-C4B-NB	-2.70	108.01	110.52
87	6N	605	CLA	C3B-C4B-NB	-2.70	108.01	110.52
82	SI	201	PEB	C4C-C3C-C2C	-2.70	105.01	107.50
82	G5	202	PEB	C4C-C3C-C2C	-2.70	105.01	107.50
82	RM	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	DP	202	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	hM	203	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	FA	202	PEB	C3B-C4B-NB	2.70	113.97	110.05
82	QM	203	PEB	C3B-C4B-NB	2.70	113.97	110.05
84	g3	1001	CYC	CBC-CAC-C3C	2.70	119.48	113.47
82	LH	1003	PEB	CMB-C2B-C1B	2.70	129.22	125.06
87	AN	841	CLA	CHB-C1B-NB	2.70	127.11	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cK	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
82	MD	201	PEB	CHB-C1C-NC	-2.70	119.14	125.32
82	QB	202	PEB	OD-C4D-ND	-2.70	121.93	125.93
82	YD	202	PEB	OD-C4D-ND	-2.70	121.93	125.93
85	CL	501	BCR	C15-C16-C17	-2.70	117.95	123.47
82	oK	201	PEB	CMB-C2B-C1B	2.70	129.22	125.06
87	42	607	CLA	CHB-C4A-NA	2.70	128.24	124.51
87	4N	607	CLA	CHB-C4A-NA	2.70	128.24	124.51
82	L4	1002	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	fE	202	PEB	C4C-C3C-C2C	-2.70	105.01	107.50
82	QG	202	PEB	C1D-CHC-C4C	-2.70	109.28	113.26
82	WM	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
84	B3	1001	CYC	C1B-C2B-C3B	-2.70	105.06	107.87
82	lM	201	PEB	C3B-C4B-NB	2.70	113.97	110.05
82	V5	202	PEB	OD-C4D-ND	-2.70	121.93	125.93
85	K2	102	BCR	C24-C23-C22	-2.70	122.16	126.23
83	AE	302	PUB	CMD-C2D-C3D	2.70	131.82	127.77
82	x8	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
82	fE	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
82	lH	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	hB	301	PEB	CAB-C3B-C4B	2.70	129.78	125.01
87	b6	608	CLA	C3B-C4B-NB	-2.70	108.01	110.52
82	lK	203	PEB	C3C-C4C-NC	2.70	110.76	108.33
82	sF	202	PEB	C4B-C3B-C2B	-2.70	103.80	106.78
84	FO	1001	CYC	C1A-C2A-C3A	-2.70	103.80	106.78
82	EB	501	PEB	OD-C4D-ND	-2.70	121.94	125.93
82	Y9	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
82	dO	202	PEB	CHA-C1B-NB	-2.70	119.29	124.93
82	M9	305	PEB	CAB-C3B-C4B	2.70	129.78	125.01
82	i1	201	PEB	OA-C1A-C2A	-2.70	124.03	126.17
82	JD	201	PEB	C1D-CHC-C4C	2.70	117.23	113.26
82	ZG	202	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
87	A2	849	CLA	CMD-C2D-C1D	-2.70	119.96	124.71
82	GI	201	PEB	CHB-C4B-NB	-2.70	118.97	124.58
82	OG	203	PEB	CMB-C2B-C1B	2.70	129.22	125.06
82	H7	201	PEB	C4B-C3B-C2B	-2.70	103.80	106.78
87	BN	811	CLA	CHC-C4B-NB	2.70	127.11	124.26
82	W4	201	PEB	C3C-C4C-NC	2.70	110.76	108.33
82	W5	201	PEB	C4B-NB-C1B	-2.70	101.43	106.51
82	CB	201	PEB	C4C-C3C-C2C	-2.70	105.01	107.50
84	N3	1001	CYC	CBC-CAC-C3C	2.70	119.47	113.47
87	CL	507	CLA	CMB-C2B-C3B	2.70	133.12	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	KN	101	BCR	C24-C23-C22	-2.70	122.16	126.23
82	Q1	201	PEB	C3B-C4B-NB	2.70	113.97	110.05
82	dG	202	PEB	C3B-C4B-NB	2.70	113.97	110.05
82	O9	202	PEB	OD-C4D-ND	-2.70	121.94	125.93
82	TQ	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
82	OF	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
82	UG	202	PEB	C4B-C3B-C2B	-2.70	103.80	106.78
82	TH	201	PEB	C1C-CHB-C4B	2.70	134.33	128.28
82	B9	202	PEB	CMA-C2A-C1A	-2.69	106.59	112.40
85	B2	802	BCR	C11-C10-C9	-2.69	123.46	127.31
82	VK	202	PEB	C1B-C2B-C3B	-2.69	103.41	106.51
82	KQ	202	PEB	C1B-C2B-C3B	-2.69	103.41	106.51
82	OK	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	FP	202	PEB	CAA-C3A-C4A	-2.69	105.75	112.67
87	32	313	CLA	CHB-C4A-NA	2.69	128.24	124.51
82	l4	201	PEB	CMA-C2A-C1A	-2.69	106.59	112.40
82	gG	202	PEB	C1D-CHC-C4C	2.69	117.23	113.26
82	NI	203	PEB	C1C-NC-C4C	-2.69	104.80	109.60
82	kJ	202	PEB	CAB-C3B-C4B	2.69	129.78	125.01
82	L1	1002	PEB	CMB-C2B-C1B	2.69	129.21	125.06
82	L7	203	PEB	C4B-C3B-C2B	-2.69	103.80	106.78
82	TA	203	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	jG	202	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	dH	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	SA	201	PEB	C3B-C4B-NB	2.69	113.97	110.05
82	lG	203	PEB	C3B-C4B-NB	2.69	113.97	110.05
96	fL	102	HEM	C4C-NC-C1C	2.69	107.99	105.35
87	BN	809	CLA	CHB-C4A-NA	2.69	128.24	124.51
87	LN	204	CLA	CHB-C4A-NA	2.69	128.24	124.51
82	P4	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	w8	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	kJ	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	mH	201	PEB	CHB-C4B-C3B	-2.69	119.09	125.32
82	DA	203	PEB	C4C-C3C-C2C	-2.69	105.01	107.50
82	UI	201	PEB	C4C-C3C-C2C	-2.69	105.01	107.50
82	T4	202	PEB	C3C-C4C-NC	2.69	110.76	108.33
87	B2	823	CLA	C2D-C1D-ND	-2.69	108.12	110.10
82	AD	303	PEB	C2A-C1A-NA	2.69	110.59	108.27
87	BN	813	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
82	dE	203	PEB	CAB-CBB-CGB	-2.69	107.81	113.60
82	a4	203	PEB	CBB-CAB-C3B	2.69	120.11	112.63
82	U9	202	PEB	C1C-CHB-C4B	2.69	134.32	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OM	201	PEB	C4B-C3B-C2B	-2.69	103.80	106.78
82	YK	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
84	J1	1001	CYC	CHB-C1B-NB	-2.69	120.28	126.06
82	QE	202	PEB	OA-C1A-C2A	-2.69	124.03	126.17
87	B2	835	CLA	C3B-C4B-NB	-2.69	108.02	110.52
84	m3	1001	CYC	CBC-CAC-C3C	2.69	119.46	113.47
82	CI	202	PEB	C3C-C4C-NC	2.69	110.76	108.33
87	A2	828	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
82	y8	202	PEB	C2A-C1A-NA	2.69	110.59	108.27
82	fO	202	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	ZG	202	PEB	C4B-C3B-C2B	-2.69	103.80	106.78
87	5N	611	CLA	CHB-C4A-NA	2.69	128.24	124.51
82	VG	201	PEB	CAB-C3B-C4B	2.69	129.77	125.01
82	SF	203	PEB	CHA-C1B-NB	-2.69	119.30	124.93
84	73	1001	CYC	C1B-C2B-C3B	-2.69	105.06	107.87
82	N5	202	PEB	C4C-C3C-C2C	-2.69	105.02	107.50
82	jH	201	PEB	OA-C1A-C2A	-2.69	124.03	126.17
82	NI	202	PEB	C3C-C4C-NC	2.69	110.76	108.33
82	FF	202	PEB	C2A-C1A-NA	2.69	110.59	108.27
82	I7	201	PEB	C2A-C1A-NA	2.69	110.59	108.27
82	YH	202	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	T7	203	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	DQ	201	PEB	C1C-NC-C4C	-2.69	104.81	109.60
87	42	603	CLA	CHB-C4A-NA	2.69	128.23	124.51
87	BN	824	CLA	C2D-C1D-ND	-2.69	108.12	110.10
87	F2	201	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
82	kM	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
82	F7	203	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
82	eK	203	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
82	A1	301	PEB	CHA-C4A-NA	2.69	128.40	125.20
82	NQ	204	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	O1	203	PEB	CHA-C1B-NB	-2.69	119.31	124.93
82	mG	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
82	J9	201	PEB	OD-C4D-ND	-2.69	121.94	125.93
82	dF	202	PEB	OD-C4D-ND	-2.69	121.94	125.93
82	NM	202	PEB	CHC-C1D-ND	-2.69	110.32	113.72
84	JH	1003	CYC	C2C-C1C-NC	2.69	110.59	108.27
83	AJ	303	PUB	CHB-C4B-NB	-2.69	119.16	125.32
84	L3	1001	CYC	C1B-C2B-C3B	-2.69	105.06	107.87
82	fF	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
82	fK	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
82	rK	201	PEB	CAB-CBB-CGB	-2.69	107.81	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QD	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
82	CJ	202	PEB	OD-C4D-ND	-2.69	121.95	125.93
82	P4	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	LJ	202	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	LM	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	iE	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	xC	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
84	C3	1001	CYC	CBC-CAC-C3C	2.69	119.45	113.47
83	Z9	305	PUB	CBC-CAC-C2C	2.69	120.10	112.63
82	bH	202	PEB	CHA-C4A-NA	-2.69	122.01	125.20
82	HQ	202	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
82	xC	202	PEB	OD-C4D-ND	-2.69	121.95	125.93
84	A3	1001	CYC	CBC-CAC-C3C	2.69	119.45	113.47
84	R3	1001	CYC	CBC-CAC-C3C	2.69	119.45	113.47
82	SP	203	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	Z1	203	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	Y4	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	UM	202	PEB	CHC-C1D-ND	-2.69	110.32	113.72
82	QJ	203	PEB	CMB-C2B-C1B	2.69	129.20	125.06
87	62	301	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
87	1N	608	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
82	SE	201	PEB	CAC-CBC-CGC	-2.69	107.82	113.60
84	K3	1001	CYC	CBC-CAC-C3C	2.69	119.45	113.47
82	oK	202	PEB	C3C-C4C-NC	2.69	110.75	108.33
87	B2	817	CLA	CHB-C4A-NA	2.69	128.23	124.51
87	1N	607	CLA	CHB-C4A-NA	2.69	128.23	124.51
82	VJ	202	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	TM	202	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	c1	202	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
82	ND	203	PEB	CMB-C2B-C1B	2.69	129.20	125.06
82	f1	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
82	YM	201	PEB	C1C-NC-C4C	-2.69	104.81	109.60
88	C6	522	LHG	O7-C7-O9	-2.69	117.21	123.70
82	NH	1002	PEB	OD-C4D-C3D	-2.69	123.37	129.46
82	BM	301	PEB	OD-C4D-C3D	-2.69	123.37	129.46
84	MO	1001	CYC	CHA-C4D-C3D	-2.69	121.09	127.15
82	TE	201	PEB	CHC-C4C-NC	2.69	124.79	121.15
87	12	607	CLA	CHB-C4A-NA	2.69	128.23	124.51
82	gH	201	PEB	CHB-C4B-C3B	-2.69	119.10	125.32
82	VF	201	PEB	OD-C4D-C3D	-2.69	123.37	129.46
84	j3	1001	CYC	C1B-C2B-C3B	-2.69	105.07	107.87
82	QE	203	PEB	CHB-C1C-C2C	-2.69	121.09	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OE	202	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
82	PQ	202	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
84	W3	1001	CYC	C1A-C2A-C3A	-2.69	103.81	106.78
82	PI	202	PEB	C3C-C4C-NC	2.69	110.75	108.33
87	7N	606	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
82	jJ	203	PEB	OD-C4D-ND	-2.69	121.95	125.93
82	D1	1002	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	q8	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
87	AN	833	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
87	bL	620	CLA	C3B-C4B-NB	-2.69	108.02	110.52
82	FP	201	PEB	OD-C4D-C3D	-2.69	123.37	129.46
82	bK	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
82	sF	203	PEB	C1C-CHB-C4B	2.69	134.31	128.28
83	M5	302	PUB	C1B-C2B-C3B	-2.69	105.02	107.50
82	cF	201	PEB	OD-C4D-ND	-2.69	121.95	125.93
83	AG	302	PUB	CMD-C2D-C3D	2.69	131.80	127.77
82	q8	201	PEB	CAB-CBB-CGB	-2.69	107.82	113.60
84	e3	1001	CYC	CBC-CAC-C3C	2.69	119.45	113.47
82	UD	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
82	eF	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
82	JA	202	PEB	CMB-C2B-C1B	2.69	129.20	125.06
82	DK	202	PEB	CMB-C2B-C1B	2.69	129.20	125.06
98	A2	842	PQN	C14-C13-C15	2.69	119.79	115.27
82	GA	202	PEB	OD-C4D-C3D	-2.69	123.38	129.46
82	UH	202	PEB	CHB-C1C-C2C	-2.69	121.09	127.15
82	eO	202	PEB	CAC-CBC-CGC	-2.69	107.82	113.60
82	UP	202	PEB	OD-C4D-C3D	-2.69	123.38	129.46
82	LA	201	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
87	c6	605	CLA	C3B-C4B-NB	-2.69	108.02	110.52
82	vF	201	PEB	CAB-CBB-CGB	-2.68	107.83	113.60
84	E3	1001	CYC	CBC-CAC-C3C	2.68	119.44	113.47
82	pF	201	PEB	OD-C4D-C3D	-2.68	123.38	129.46
82	EI	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	O7	201	PEB	CMA-C2A-C1A	-2.68	106.62	112.40
82	MA	202	PEB	OD-C4D-ND	-2.68	121.95	125.93
82	C5	202	PEB	OD-C4D-ND	-2.68	121.95	125.93
84	G3	1001	CYC	CBC-CAC-C3C	2.68	119.44	113.47
82	TF	202	PEB	CHC-C4C-NC	-2.68	117.51	121.15
82	G7	202	PEB	OD-C4D-C3D	-2.68	123.38	129.46
84	GO	1001	CYC	C4D-C3D-C2D	-2.68	104.45	107.62
87	KN	102	CLA	CHB-C4A-NA	2.68	128.22	124.51
82	RI	203	PEB	CAC-C2C-C1C	2.68	130.04	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	U3	1001	CYC	C1B-C2B-C3B	-2.68	105.07	107.87
87	BL	621	CLA	C2D-C1D-ND	-2.68	108.13	110.10
82	vK	201	PEB	CAB-CBB-CGB	-2.68	107.83	113.60
82	dJ	202	PEB	OA-C1A-C2A	-2.68	124.04	126.17
82	X5	202	PEB	C4C-C3C-C2C	-2.68	105.02	107.50
82	PD	203	PEB	CHA-C1B-NB	-2.68	119.32	124.93
82	Z9	304	PEB	CAB-C3B-C4B	2.68	129.76	125.01
82	YA	304	PEB	OD-C4D-ND	-2.68	121.95	125.93
82	VG	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
82	SI	201	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
82	IM	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
84	GE	1001	CYC	C4A-C3A-C2A	-2.68	103.43	106.51
82	GK	202	PEB	CMB-C2B-C3B	-2.68	118.83	126.12
84	p3	1001	CYC	CBC-CAC-C3C	2.68	119.44	113.47
82	YK	202	PEB	OD-C4D-C3D	-2.68	123.38	129.46
87	BN	832	CLA	C3B-C4B-NB	-2.68	108.03	110.52
87	82	306	CLA	CMC-C2C-C3C	2.68	133.40	126.12
82	FI	201	PEB	C4C-C3C-C2C	-2.68	105.02	107.50
82	SG	201	PEB	CAC-CBC-CGC	-2.68	107.83	113.60
82	r8	201	PEB	OD-C4D-C3D	-2.68	123.38	129.46
82	WJ	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
82	CB	201	PEB	CMC-C3C-C4C	2.68	129.90	127.06
84	HH	1001	CYC	CHD-C1D-ND	-2.68	119.17	125.32
82	WH	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	II	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	RI	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	FF	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
82	LD	202	PEB	C3B-C4B-NB	2.68	113.95	110.05
82	V1	203	PEB	OD-C4D-C3D	-2.68	123.38	129.46
82	CQ	202	PEB	CHC-C1D-ND	-2.68	110.33	113.72
87	82	306	CLA	CAC-C3C-C4C	-2.68	121.33	124.81
82	Y9	202	PEB	C2A-C1A-NA	2.68	110.58	108.27
82	DF	202	PEB	CMB-C2B-C1B	2.68	129.19	125.06
82	WJ	201	PEB	OD-C4D-C3D	-2.68	123.38	129.46
82	Q1	202	PEB	C3B-C4B-NB	2.68	113.95	110.05
87	BL	609	CLA	CHB-C1B-NB	2.68	127.10	124.26
82	vK	202	PEB	CHB-C1C-NC	-2.68	119.18	125.32
82	S4	202	PEB	C4B-C3B-C2B	-2.68	103.81	106.78
84	t3	1001	CYC	CBC-CAC-C3C	2.68	119.44	113.47
82	sF	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	OJ	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
87	6N	613	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	L9	203	PEB	C3B-C4B-NB	2.68	113.95	110.05
92	bL	624	LMG	C6-C5-C4	-2.68	106.72	113.00
82	ZK	201	PEB	C2A-C1A-NA	2.68	110.58	108.27
82	YK	201	PEB	CHC-C4C-NC	2.68	124.78	121.15
82	RE	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
82	bK	201	PEB	C4C-C3C-C2C	-2.68	105.03	107.50
88	D6	401	LHG	O8-C23-C24	2.68	120.32	111.91
82	bP	501	PEB	OD-C4D-ND	-2.68	121.96	125.93
83	AH	304	PUB	OD-C4D-ND	-2.68	121.96	125.93
82	BB	203	PEB	CMB-C2B-C1B	2.68	129.19	125.06
82	VI	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	S5	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
82	iK	202	PEB	OA-C1A-C2A	-2.68	124.04	126.17
82	lM	202	PEB	CHA-C1B-C2B	2.68	131.79	124.90
84	v3	1001	CYC	CBC-CAC-C3C	2.68	119.43	113.47
82	AG	304	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	NK	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	mM	201	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	TO	201	PEB	CAC-CBC-CGC	-2.68	107.84	113.60
82	h4	201	PEB	CHB-C1C-C2C	-2.68	121.10	127.15
82	SD	202	PEB	CMC-C3C-C4C	2.68	129.90	127.06
87	5N	605	CLA	C3B-C4B-NB	-2.68	108.03	110.52
82	OM	201	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	jM	203	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	H4	1002	PEB	CMB-C2B-C1B	2.68	129.19	125.06
82	KA	201	PEB	OD-C4D-ND	-2.68	121.96	125.93
82	QI	201	PEB	CHC-C4C-NC	2.68	124.78	121.15
82	D5	203	PEB	CAC-C2C-C1C	2.68	130.03	125.76
82	XI	202	PEB	C3C-C4C-NC	2.68	110.75	108.33
87	R2	203	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
82	ZF	202	PEB	CAB-C3B-C4B	2.68	129.75	125.01
82	BA	203	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
84	y3	1001	CYC	C1A-C2A-C3A	-2.68	103.82	106.78
87	A2	808	CLA	C3B-C4B-NB	-2.68	108.03	110.52
82	uF	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
82	fG	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
87	B2	821	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
87	c6	612	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
87	B2	805	CLA	CHB-C4A-NA	2.68	128.22	124.51
82	J5	201	PEB	CHB-C4B-C3B	-2.68	119.12	125.32
82	SP	203	PEB	C2A-C1A-NA	2.68	110.58	108.27
82	CD	202	PEB	C3B-C4B-NB	2.68	113.94	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NF	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
95	C6	521	DGD	O6D-C5D-C6D	2.68	112.07	106.67
82	SF	203	PEB	CHB-C1C-C2C	-2.68	121.11	127.15
82	UG	202	PEB	C3B-C4B-NB	2.68	113.94	110.05
82	O1	201	PEB	C3B-C4B-NB	2.68	113.94	110.05
87	7N	610	CLA	C3B-C4B-NB	-2.68	108.03	110.52
92	AL	411	LMG	C8-O7-C10	-2.68	111.20	117.79
87	12	608	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
82	Y1	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	cB	401	PEB	OD-C4D-C3D	-2.68	123.39	129.46
82	W1	203	PEB	C2A-C1A-NA	2.68	110.58	108.27
82	m1	201	PEB	CHB-C4B-C3B	-2.68	119.12	125.32
82	lM	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
82	TD	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
84	ME	1001	CYC	C4A-C3A-C2A	-2.68	103.43	106.51
88	m6	102	LHG	O8-C23-C24	2.68	120.31	111.91
92	jL	101	LMG	C7-O1-C1	-2.68	108.51	113.74
87	cL	506	CLA	CHB-C1B-NB	2.68	127.09	124.26
84	V3	1001	CYC	CHB-C1B-NB	2.68	131.81	126.06
94	d6	408	PL9	C35-C34-C36	2.68	119.77	115.27
82	I9	202	PEB	C1C-CHB-C4B	2.68	134.28	128.28
82	JQ	201	PEB	C1D-CHC-C4C	2.68	117.20	113.26
82	dG	203	PEB	CAB-C3B-C4B	2.68	129.74	125.01
82	UE	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
82	V4	202	PEB	CHC-C1D-ND	-2.68	110.34	113.72
84	P3	1001	CYC	CBC-CAC-C3C	2.68	119.43	113.47
82	FA	203	PEB	CHC-C4C-NC	2.68	124.77	121.15
94	dL	406	PL9	C37-C38-C39	-2.68	121.22	127.66
82	c1	201	PEB	C2A-C1A-NA	2.68	110.58	108.27
82	SH	202	PEB	CHB-C4B-NB	-2.68	119.01	124.58
82	a4	202	PEB	CAC-C2C-C1C	2.68	130.02	125.76
82	gB	201	PEB	OD-C4D-ND	-2.68	121.97	125.93
82	XF	202	PEB	CHA-C1B-C2B	2.68	131.78	124.90
82	AB	501	PEB	OD-C4D-C3D	-2.68	123.40	129.46
82	lG	203	PEB	C4C-C3C-C2C	-2.68	105.03	107.50
82	K7	201	PEB	OD-C4D-ND	-2.68	121.97	125.93
85	BL	616	BCR	C15-C16-C17	-2.68	117.99	123.47
87	52	609	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
82	SI	202	PEB	C2A-C1A-NA	2.67	110.58	108.27
91	D6	404	PHO	O2A-CGA-CBA	2.67	120.30	111.91
82	F7	203	PEB	CHA-C1B-NB	-2.67	119.34	124.93
87	AN	849	CLA	CMD-C2D-C1D	-2.67	120.00	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	C6	503	DGD	O5D-C1E-C2E	2.67	112.48	108.30
82	e4	202	PEB	C1D-CHC-C4C	-2.67	109.31	113.26
82	MA	202	PEB	CMB-C2B-C1B	2.67	129.18	125.06
82	XQ	203	PEB	OD-C4D-C3D	-2.67	123.40	129.46
84	V3	1001	CYC	CBC-CAC-C3C	2.67	119.42	113.47
87	aL	605	CLA	CMB-C2B-C3B	2.67	133.07	126.59
82	A7	201	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
82	ZO	201	PEB	CHB-C1C-C2C	-2.67	121.12	127.15
82	VK	201	PEB	OD-C4D-ND	-2.67	121.97	125.93
82	wF	302	PEB	OD-C4D-ND	-2.67	121.97	125.93
82	V9	202	PEB	C1C-CHB-C4B	2.67	134.28	128.28
87	1N	602	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
85	L2	205	BCR	C2-C1-C6	2.67	114.60	110.48
87	B2	830	CLA	C3B-C4B-NB	-2.67	108.03	110.52
82	KB	304	PEB	CHA-C1B-NB	-2.67	119.34	124.93
82	LK	202	PEB	C4B-C3B-C2B	-2.67	103.82	106.78
82	f4	202	PEB	OD-C4D-C3D	-2.67	123.40	129.46
82	lJ	203	PEB	OD-C4D-C3D	-2.67	123.40	129.46
82	cF	203	PEB	CHC-C1D-ND	-2.67	110.34	113.72
82	ZB	201	PEB	C3B-C4B-NB	2.67	113.94	110.05
82	SI	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
82	eO	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
82	P7	202	PEB	C4C-C3C-C2C	-2.67	105.03	107.50
82	PO	201	PEB	CHC-C4C-NC	2.67	124.77	121.15
82	mM	201	PEB	CMC-C3C-C4C	2.67	129.90	127.06
87	7N	602	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
82	DA	202	PEB	OD-C4D-ND	-2.67	121.97	125.93
82	K5	202	PEB	OD-C4D-ND	-2.67	121.97	125.93
82	FA	203	PEB	OA-C1A-C2A	-2.67	124.05	126.17
82	rC	201	PEB	OD-C4D-C3D	-2.67	123.40	129.46
82	FK	202	PEB	C2A-C1A-NA	2.67	110.58	108.27
82	dB	202	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
85	FN	202	BCR	C8-C7-C6	2.67	134.71	127.20
87	22	602	CLA	C2A-C1A-CHA	2.67	128.53	123.86
82	k1	202	PEB	C4B-C3B-C2B	-2.67	103.82	106.78
82	NB	203	PEB	CHB-C4B-C3B	-2.67	119.13	125.32
82	hG	201	PEB	CHB-C1C-NC	2.67	131.44	125.32
82	YK	203	PEB	CBA-CAA-C3A	-2.67	107.52	113.47
87	AN	818	CLA	C3B-C4B-NB	-2.67	108.03	110.52
87	BN	830	CLA	C3B-C4B-NB	-2.67	108.03	110.52
87	IN	102	CLA	C3B-C4B-NB	-2.67	108.03	110.52
82	r8	202	PEB	CHB-C1C-C2C	2.67	133.18	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	P9	202	PEB	C1C-CHB-C4B	2.67	134.28	128.28
82	VJ	202	PEB	CAC-C2C-C1C	2.67	130.02	125.76
82	BB	202	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
82	J9	202	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
84	W3	1001	CYC	CAA-C2A-C1A	2.67	129.74	125.01
87	4N	606	CLA	CHB-C4A-NA	2.67	128.21	124.51
82	g4	203	PEB	C2A-C1A-NA	2.67	110.58	108.27
82	GB	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	O4	201	PEB	OD-C4D-C3D	-2.67	123.41	129.46
87	2N	303	CLA	C2A-C1A-CHA	2.67	128.53	123.86
82	dB	201	PEB	CAC-CBC-CGC	-2.67	107.85	113.60
87	I2	102	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
87	A2	818	CLA	C3B-C4B-NB	-2.67	108.04	110.52
95	L6	102	DGD	C1D-O6D-C5D	-2.67	108.44	113.69
91	dL	403	PHO	C4-C3-C5	2.67	119.77	115.27
94	a6	601	PL9	C40-C39-C41	2.67	119.77	115.27
85	b6	602	BCR	C36-C18-C17	-2.67	119.18	122.92
82	VO	202	PEB	C1C-NC-C4C	-2.67	104.84	109.60
82	AF	202	PEB	CHC-C4C-NC	2.67	124.77	121.15
82	gK	202	PEB	OD-C4D-ND	-2.67	121.97	125.93
82	SJ	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	BD	203	PEB	CMB-C2B-C1B	2.67	129.18	125.06
82	TH	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
82	a4	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
82	S7	201	PEB	C3B-C4B-NB	2.67	113.94	110.05
82	b4	201	PEB	C2B-C1B-NB	2.67	116.23	110.53
82	O4	201	PEB	OA-C1A-C2A	-2.67	124.05	126.17
82	RO	203	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	18	201	PEB	O2B-CGB-CBB	2.67	122.61	114.03
87	HL	101	CLA	C3B-C4B-NB	-2.67	108.04	110.52
87	8N	301	CLA	CMC-C2C-C3C	2.67	133.37	126.12
82	I9	202	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
82	1C	201	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
84	i3	1001	CYC	CBC-CAC-C3C	2.67	119.41	113.47
84	HO	1001	CYC	C1D-C2D-C3D	-2.67	104.39	107.79
84	G4	1001	CYC	C4D-C3D-C2D	-2.67	104.46	107.62
82	WF	203	PEB	CHB-C4B-NB	-2.67	119.02	124.58
82	Y7	303	PEB	C3B-C4B-NB	2.67	113.93	110.05
87	A2	808	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
82	S7	201	PEB	CAB-C3B-C4B	2.67	129.73	125.01
82	1C	201	PEB	O2B-CGB-CBB	2.67	122.61	114.03
82	M7	202	PEB	OD-C4D-ND	-2.67	121.97	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y9	203	PEB	CHC-C4C-NC	2.67	124.76	121.15
82	OO	201	PEB	CHA-C4A-NA	2.67	128.38	125.20
85	BN	803	BCR	C11-C10-C9	-2.67	123.50	127.31
82	iM	202	PEB	C2A-C1A-NA	2.67	110.58	108.27
82	NB	201	PEB	CMA-C2A-C1A	-2.67	106.65	112.40
82	mK	201	PEB	CMC-C3C-C4C	2.67	129.89	127.06
82	VA	203	PEB	CHC-C1D-ND	-2.67	110.35	113.72
85	A6	401	BCR	C28-C27-C26	-2.67	109.31	114.08
82	uF	203	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
84	MG	1001	CYC	C4A-C3A-C2A	-2.67	103.44	106.51
87	BN	825	CLA	C2B-C1B-NB	2.67	112.02	110.23
82	Z5	305	PEB	C2A-C3A-C4A	-2.67	97.34	101.34
82	wC	201	PEB	CAA-C3A-C2A	-2.67	107.59	114.26
82	RI	202	PEB	C1D-CHC-C4C	-2.67	109.32	113.26
82	wK	303	PEB	C1D-CHC-C4C	2.67	117.19	113.26
85	d6	405	BCR	C36-C18-C17	-2.67	119.18	122.92
87	A2	833	CLA	CHB-C4A-NA	2.67	128.20	124.51
84	H1	1001	CYC	CHD-C1D-ND	-2.67	119.20	125.32
82	YH	202	PEB	C4C-C3C-C2C	-2.67	105.04	107.50
85	HL	103	BCR	C2-C1-C6	2.67	114.59	110.48
91	d6	404	PHO	CMB-C2B-C3B	2.67	129.67	124.68
85	F2	203	BCR	C8-C7-C6	2.67	134.70	127.20
82	J7	203	PEB	CHC-C4C-NC	2.67	124.76	121.15
82	aK	203	PEB	CHC-C4C-NC	2.67	124.76	121.15
82	NB	202	PEB	CHA-C1B-NB	-2.67	119.35	124.93
82	IJ	203	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	ZO	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	bO	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	eJ	201	PEB	CHB-C1C-NC	-2.67	119.20	125.32
82	DM	201	PEB	C3B-C4B-NB	2.67	113.93	110.05
82	D7	201	PEB	C3B-C4B-NB	2.67	113.93	110.05
82	F7	201	PEB	C3B-C4B-NB	2.67	113.93	110.05
82	bH	201	PEB	C3B-C4B-NB	2.67	113.93	110.05
85	hL	102	BCR	C16-C15-C14	-2.67	118.01	123.47
82	E9	202	PEB	C1C-CHB-C4B	2.67	134.27	128.28
82	qC	201	PEB	CAB-CBB-CGB	-2.67	107.86	113.60
82	OG	203	PEB	CAC-C2C-C1C	2.67	130.01	125.76
84	W3	1001	CYC	C2C-C1C-NC	-2.67	105.97	108.27
82	aF	201	PEB	C3C-C4C-NC	2.67	110.74	108.33
87	AN	837	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
82	bO	202	PEB	CHA-C1B-NB	-2.67	119.35	124.93
95	lL	101	DGD	C2G-O2G-C1B	-2.67	111.22	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ND	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	GM	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	S1	202	PEB	CHB-C4B-NB	-2.67	119.02	124.58
82	B7	201	PEB	CMB-C2B-C1B	2.67	129.17	125.06
82	d4	201	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
82	GF	202	PEB	CMB-C2B-C3B	-2.67	118.87	126.12
87	BN	822	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
82	Y9	202	PEB	CAB-C3B-C4B	2.67	129.73	125.01
82	T9	202	PEB	C1C-CHB-C4B	2.67	134.27	128.28
82	JH	1002	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	bP	501	PEB	OD-C4D-C3D	-2.67	123.41	129.46
82	UP	203	PEB	C1C-NC-C4C	2.67	114.34	109.60
87	A2	832	CLA	CHC-C4B-NB	2.67	127.08	124.26
83	AH	303	PUB	OD-C4D-ND	-2.67	121.98	125.93
82	WK	203	PEB	CHB-C4B-NB	-2.67	119.02	124.58
94	A6	410	PL9	C12-C13-C14	-2.67	121.23	127.66
82	kE	201	PEB	CHB-C1C-NC	-2.67	119.21	125.32
91	A6	407	PHO	CGD-CBD-CAD	-2.67	102.09	110.73
82	MJ	201	PEB	CAA-C3A-C4A	-2.67	105.82	112.67
87	AN	808	CLA	C3B-C4B-NB	-2.67	108.04	110.52
82	R5	202	PEB	OD-C4D-ND	-2.67	121.98	125.93
82	AP	202	PEB	CHA-C1B-NB	-2.67	119.35	124.93
82	S9	203	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
82	J5	203	PEB	CHC-C4C-NC	2.67	124.76	121.15
87	8N	303	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
82	CM	203	PEB	C1C-NC-C4C	-2.67	104.85	109.60
82	aM	204	PEB	C3B-C4B-NB	2.67	113.93	110.05
82	WF	201	PEB	C1D-CHC-C4C	-2.67	109.32	113.26
82	z8	201	PEB	CHA-C1B-C2B	-2.67	118.04	124.90
82	XM	201	PEB	OD-C4D-C3D	-2.67	123.42	129.46
83	xK	305	PUB	CHA-C4A-NA	-2.67	110.35	113.72
87	B2	832	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
87	5N	603	CLA	CHB-C4A-NA	2.67	128.20	124.51
92	BL	612	LMG	O8-C28-C29	2.67	120.28	111.91
82	OG	203	PEB	C3C-C4C-NC	2.67	110.73	108.33
82	rF	201	PEB	CAB-CBB-CGB	-2.67	107.86	113.60
82	LA	203	PEB	C2A-C1A-NA	2.67	110.57	108.27
87	RN	203	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
87	cL	517	CLA	C3B-C4B-NB	-2.67	108.04	110.52
84	J1	1001	CYC	C4D-ND-C1D	-2.67	105.03	109.79
82	18	201	PEB	C1B-C2B-C3B	-2.67	103.45	106.51
82	UD	202	PEB	CHC-C4C-NC	2.67	124.76	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	832	CLA	CHC-C4B-NB	2.67	127.08	124.26
82	D9	201	PEB	OD-C4D-ND	-2.67	121.98	125.93
82	ND	204	PEB	CHC-C1D-ND	-2.67	110.35	113.72
82	HK	201	PEB	OD-C4D-C3D	-2.67	123.42	129.46
82	AM	301	PEB	OD-C4D-C3D	-2.67	123.42	129.46
82	FA	203	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
82	KP	202	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
84	F4	1001	CYC	C1A-C2A-C3A	-2.67	103.83	106.78
82	VE	201	PEB	CAB-C3B-C4B	2.67	129.72	125.01
82	CI	202	PEB	C1D-CHC-C4C	-2.67	109.33	113.26
82	EI	202	PEB	C1D-CHC-C4C	-2.67	109.33	113.26
82	aM	203	PEB	OD-C4D-C3D	-2.67	123.42	129.46
82	SO	201	PEB	C2B-C1B-NB	2.67	116.22	110.53
87	AN	808	CLA	CAA-C2A-C3A	-2.67	105.48	112.78
84	x3	1001	CYC	CHB-C1B-NB	2.67	131.78	126.06
87	BN	820	CLA	C3B-C4B-NB	-2.67	108.04	110.52
82	zC	201	PEB	CHA-C1B-C2B	-2.67	118.05	124.90
82	d4	202	PEB	CHA-C1B-NB	-2.67	119.36	124.93
84	V3	1001	CYC	CMA-C3A-C4A	2.67	129.17	125.06
87	B2	823	CLA	CAA-CBA-CGA	-2.67	105.46	113.25
84	NO	1001	CYC	CAA-C2A-C3A	2.67	132.84	127.88
83	AJ	303	PUB	CMD-C2D-C3D	2.67	131.77	127.77
82	qF	203	PEB	CHA-C4A-NA	2.67	128.37	125.20
87	AN	837	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
82	gH	202	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
82	VI	202	PEB	C1D-CHC-C4C	-2.67	109.33	113.26
82	vF	202	PEB	CHB-C1C-NC	-2.67	119.22	125.32
82	A9	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
85	b6	602	BCR	C37-C22-C21	-2.66	119.19	122.92
82	kM	201	PEB	C1C-CHB-C4B	-2.66	122.31	128.28
82	DJ	202	PEB	OD-C4D-C3D	-2.66	123.42	129.46
82	NB	201	PEB	CAB-CBB-CGB	-2.66	107.87	113.60
82	VE	201	PEB	CHC-C4C-NC	2.66	124.75	121.15
82	kF	203	PEB	OD-C4D-ND	-2.66	121.98	125.93
82	BQ	202	PEB	C4C-C3C-C2C	-2.66	105.04	107.50
87	B2	812	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
87	nL	101	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
82	YK	201	PEB	CAC-C2C-C3C	2.66	133.17	127.07
82	FK	202	PEB	CHB-C1C-NC	-2.66	119.22	125.32
87	BN	806	CLA	C2B-C1B-NB	2.66	112.02	110.23
87	42	604	CLA	C2B-C1B-NB	2.66	112.02	110.23
82	sC	202	PEB	OD-C4D-C3D	-2.66	123.42	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	4N	603	CLA	CHB-C4A-NA	2.66	128.20	124.51
82	lG	203	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
82	eO	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
82	RP	202	PEB	CAC-CBC-CGC	-2.66	107.87	113.60
87	bL	607	CLA	CAA-CBA-CGA	-2.66	105.47	113.25
85	B6	601	BCR	C20-C21-C22	-2.66	123.51	127.31
82	NB	202	PEB	CHC-C1D-ND	-2.66	110.35	113.72
82	f1	203	PEB	CHC-C1D-ND	-2.66	110.35	113.72
87	HL	101	CLA	CMB-C2B-C3B	2.66	133.04	126.59
82	WG	201	PEB	CMA-C2A-C1A	-2.66	106.66	112.40
82	IP	201	PEB	OA-C1A-C2A	-2.66	124.06	126.17
82	qC	201	PEB	CHA-C1B-NB	-2.66	119.36	124.93
82	RH	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
87	12	602	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
82	hH	201	PEB	CMB-C2B-C1B	2.66	129.17	125.06
82	R7	201	PEB	CAC-C2C-C1C	2.66	130.00	125.76
82	IA	201	PEB	C2A-C1A-NA	2.66	110.57	108.27
82	V7	201	PEB	C4C-C3C-C2C	-2.66	105.04	107.50
87	72	602	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
87	bL	618	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
82	WQ	202	PEB	OD-C4D-ND	-2.66	121.98	125.93
82	I5	202	PEB	OD-C4D-ND	-2.66	121.98	125.93
82	aK	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
84	L1	1001	CYC	O2D-CGD-CBD	2.66	122.59	114.03
87	BN	824	CLA	CAA-CBA-CGA	-2.66	105.47	113.25
82	c1	202	PEB	CHC-C4C-NC	2.66	124.75	121.15
87	BL	603	CLA	CMB-C2B-C3B	2.66	133.04	126.59
82	R9	202	PEB	C1C-CHB-C4B	2.66	134.25	128.28
82	SQ	202	PEB	CMC-C3C-C4C	2.66	129.88	127.06
87	IN	102	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
87	3N	309	CLA	C2B-C1B-NB	2.66	112.02	110.23
82	YB	202	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
87	cL	507	CLA	C3B-C4B-NB	-2.66	108.05	110.52
82	R7	203	PEB	C3C-C4C-NC	2.66	110.73	108.33
82	BA	201	PEB	OD-C4D-ND	-2.66	121.99	125.93
82	wK	302	PEB	OD-C4D-ND	-2.66	121.99	125.93
82	B7	203	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
82	lF	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
82	DJ	202	PEB	CHA-C1B-NB	-2.66	119.36	124.93
82	P4	201	PEB	CHC-C4C-NC	2.66	124.75	121.15
82	Z4	202	PEB	OD-C4D-C3D	-2.66	123.43	129.46
82	lG	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PI	202	PEB	C1D-CHC-C4C	-2.66	109.33	113.26
82	VD	203	PEB	C3B-C4B-NB	2.66	113.92	110.05
82	mG	203	PEB	C3B-C4B-NB	2.66	113.92	110.05
82	aO	202	PEB	C3B-C4B-NB	2.66	113.92	110.05
82	CB	201	PEB	CAB-CBB-CGB	-2.66	107.88	113.60
82	sK	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
82	rC	202	PEB	CHB-C1C-C2C	2.66	133.16	127.15
87	B2	806	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
82	T1	201	PEB	C1C-CHB-C4B	2.66	134.25	128.28
82	BJ	301	PEB	CHC-C4C-NC	2.66	124.75	121.15
82	uF	203	PEB	CHC-C4C-NC	2.66	124.75	121.15
82	pK	202	PEB	CHC-C4C-NC	2.66	124.75	121.15
82	XK	203	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
84	GG	1001	CYC	C4A-C3A-C2A	-2.66	103.45	106.51
87	A6	402	CLA	C3B-C4B-NB	-2.66	108.05	110.52
82	Z1	201	PEB	OA-C1A-NA	2.66	128.16	124.94
87	52	611	CLA	CHB-C4A-NA	2.66	128.19	124.51
87	B2	810	CLA	CHB-C4A-NA	2.66	128.19	124.51
87	BL	602	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
82	GI	203	PEB	C1D-CHC-C4C	-2.66	109.33	113.26
85	bL	602	BCR	C33-C5-C4	2.66	118.73	113.62
82	GK	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
82	OP	203	PEB	C2A-C1A-NA	2.66	110.57	108.27
82	JA	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
82	IF	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
82	bG	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
85	JN	102	BCR	C33-C5-C6	-2.66	121.54	124.53
82	PK	202	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
82	WI	202	PEB	CHB-C4B-NB	-2.66	119.04	124.58
82	A9	202	PEB	C1C-CHB-C4B	2.66	134.25	128.28
84	J1	1001	CYC	CHD-C1D-ND	-2.66	119.22	125.32
82	d1	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
82	R4	203	PEB	OD-C4D-C3D	-2.66	123.43	129.46
82	mM	202	PEB	O2B-CGB-CBB	2.66	122.58	114.03
87	A2	826	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
82	YE	202	PEB	CMB-C2B-C1B	2.66	129.16	125.06
82	QK	201	PEB	C4C-C3C-C2C	-2.66	105.05	107.50
82	dF	202	PEB	C4C-C3C-C2C	-2.66	105.05	107.50
83	M9	303	PUB	CMD-C2D-C3D	2.66	131.76	127.77
83	AH	303	PUB	CHC-C1D-ND	-2.66	110.36	113.72
87	32	302	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
82	DF	201	PEB	CMC-C3C-C4C	2.66	129.88	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	b6	603	BCR	C34-C9-C10	-2.66	119.20	122.92
84	HG	1001	CYC	CAD-CBD-CGD	-2.66	107.88	113.60
87	BN	807	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
82	UJ	202	PEB	CHB-C1C-C2C	-2.66	121.15	127.15
83	BM	302	PUB	CBA-CAA-C3A	-2.66	108.94	112.98
82	SF	202	PEB	CBB-CAB-C3B	-2.66	105.24	112.63
87	R2	203	CLA	C3B-C4B-NB	-2.66	108.05	110.52
87	A6	403	CLA	C3B-C4B-NB	-2.66	108.05	110.52
82	UK	201	PEB	C3C-C4C-NC	2.66	110.73	108.33
82	hJ	201	PEB	OD-C4D-ND	-2.66	121.99	125.93
82	b4	202	PEB	CHA-C1B-NB	-2.66	119.37	124.93
82	GI	202	PEB	CHB-C1C-NC	-2.66	119.23	125.32
82	TD	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
82	MM	203	PEB	OD-C4D-C3D	-2.66	123.44	129.46
95	C6	504	DGD	O3G-C3G-C2G	-2.66	104.48	110.90
82	WB	401	PEB	C1C-CHB-C4B	-2.66	122.32	128.28
82	p8	201	PEB	OD-C4D-C3D	-2.66	123.44	129.46
82	N5	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
87	BN	806	CLA	CHB-C4A-NA	2.66	128.19	124.51
87	2N	312	CLA	C2A-C1A-CHA	2.66	128.51	123.86
87	K6	101	CLA	CHB-C1B-NB	2.66	127.07	124.26
82	Y9	203	PEB	CAB-C3B-C4B	2.66	129.71	125.01
82	yC	202	PEB	CAB-C3B-C4B	2.66	129.71	125.01
82	wF	302	PEB	CHB-C1C-NC	-2.66	119.23	125.32
82	ZG	203	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
82	E9	202	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
82	gB	202	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
82	P5	202	PEB	C4C-C3C-C2C	-2.66	105.05	107.50
87	A2	837	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
82	TH	202	PEB	CAC-C2C-C1C	2.66	130.00	125.76
82	DP	201	PEB	CHC-C4C-NC	2.66	124.75	121.15
87	2N	301	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
82	WB	402	PEB	CAB-CBB-CGB	-2.66	107.88	113.60
82	y8	203	PEB	CAB-C3B-C4B	2.66	129.71	125.01
82	s8	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
82	LI	202	PEB	OA-C1A-C2A	-2.66	124.06	126.17
82	mM	202	PEB	CHB-C4B-NB	-2.66	119.05	124.58
84	JH	1001	CYC	C4D-ND-C1D	-2.66	105.05	109.79
82	SD	201	PEB	CMB-C2B-C1B	2.66	129.16	125.06
82	lJ	201	PEB	CMB-C2B-C1B	2.66	129.16	125.06
82	iK	203	PEB	CMB-C2B-C1B	2.66	129.16	125.06
84	JH	1001	CYC	C1A-C2A-C3A	-2.66	103.84	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dO	202	PEB	CHC-C4C-NC	2.66	124.75	121.15
82	lJ	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
82	E5	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
82	W7	202	PEB	C3C-C4C-NC	2.66	110.72	108.33
87	A2	838	CLA	CHB-C4A-NA	2.66	128.19	124.51
87	B2	833	CLA	CHB-C4A-NA	2.66	128.19	124.51
82	c1	201	PEB	C4C-C3C-C2C	-2.66	105.05	107.50
82	YK	203	PEB	C1C-CHB-C4B	2.66	134.24	128.28
82	RA	201	PEB	CAC-C2C-C1C	2.66	129.99	125.76
82	DO	1002	PEB	CAB-C3B-C4B	2.66	129.71	125.01
82	yC	202	PEB	C2A-C1A-NA	2.66	110.56	108.27
82	NA	203	PEB	CHB-C1C-NC	-2.66	119.23	125.32
82	XK	201	PEB	C3B-C4B-NB	2.66	113.91	110.05
87	82	303	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
82	X9	202	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
82	DD	202	PEB	OA-C1A-C2A	-2.66	124.06	126.17
82	Q1	202	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
87	32	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
87	5N	609	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
82	W5	202	PEB	CHC-C1D-ND	-2.66	110.36	113.72
82	lE	203	PEB	CHC-C1D-ND	-2.66	110.36	113.72
87	B6	608	CLA	C3B-C4B-NB	-2.66	108.05	110.52
84	EO	1001	CYC	CHB-C1B-NB	-2.66	120.36	126.06
82	RA	202	PEB	C2B-C1B-NB	2.66	116.20	110.53
82	AM	302	PEB	CMB-C2B-C1B	2.66	129.15	125.06
82	G9	202	PEB	C1C-CHB-C4B	2.66	134.24	128.28
82	II	202	PEB	C1D-CHC-C4C	-2.66	109.34	113.26
82	pC	201	PEB	OD-C4D-C3D	-2.66	123.44	129.46
82	fE	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
82	T7	203	PEB	CHC-C4C-NC	2.66	124.74	121.15
82	fO	202	PEB	C3B-C4B-NB	2.66	113.91	110.05
84	E4	1001	CYC	CHB-C1B-NB	-2.66	120.36	126.06
82	LA	202	PEB	OA-C1A-NA	2.66	128.16	124.94
87	AN	833	CLA	CHB-C4A-NA	2.66	128.18	124.51
82	AA	201	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
82	K9	202	PEB	C1C-CHB-C4B	2.66	134.24	128.28
82	ZE	203	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
82	Y5	203	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
82	qK	201	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
82	fB	301	PEB	CAB-C3B-C4B	2.66	129.71	125.01
82	DA	203	PEB	CAC-CBC-CGC	-2.66	107.89	113.60
84	D1	1003	CYC	C2C-C1C-NC	2.66	110.56	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FJ	202	PEB	C3B-C4B-NB	2.65	113.91	110.05
82	R1	201	PEB	CHC-C4C-NC	2.65	124.74	121.15
82	HF	202	PEB	OD-C4D-C3D	-2.65	123.44	129.46
82	FK	202	PEB	CAA-C3A-C4A	-2.65	105.86	112.67
82	H1	1002	PEB	CAC-CBC-CGC	-2.65	107.89	113.60
82	T7	202	PEB	CAB-C3B-C4B	2.65	129.71	125.01
87	CL	510	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
82	DP	201	PEB	C1B-C2B-C3B	-2.65	103.46	106.51
82	ZO	201	PEB	OD-C4D-C3D	-2.65	123.45	129.46
82	w8	201	PEB	CAA-C3A-C2A	-2.65	107.63	114.26
82	JQ	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
83	yK	302	PUB	OA-C1A-NA	-2.65	122.00	125.93
82	OI	201	PEB	CAB-C3B-C4B	2.65	129.70	125.01
82	HK	202	PEB	CAB-C3B-C4B	2.65	129.70	125.01
82	VJ	201	PEB	CHB-C1C-NC	-2.65	119.24	125.32
87	8N	304	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
82	R7	203	PEB	C2A-C1A-NA	2.65	110.56	108.27
82	OP	202	PEB	C1C-CHB-C4B	2.65	134.23	128.28
87	1N	610	CLA	CHB-C4A-NA	2.65	128.18	124.51
82	XI	202	PEB	CMB-C2B-C1B	2.65	129.15	125.06
82	T1	201	PEB	CHA-C1B-NB	-2.65	119.38	124.93
82	L5	202	PEB	OA-C1A-C2A	-2.65	124.06	126.17
83	A4	302	PUB	CHA-C4A-NA	-2.65	110.37	113.72
82	wK	302	PEB	CHB-C1C-NC	-2.65	119.24	125.32
82	TO	201	PEB	C1B-C2B-C3B	-2.65	103.46	106.51
82	kK	202	PEB	C1B-C2B-C3B	-2.65	103.46	106.51
82	GJ	202	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	BQ	203	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	T5	202	PEB	OD-C4D-ND	-2.65	122.00	125.93
92	b6	619	LMG	C8-O7-C10	-2.65	111.26	117.79
82	cJ	201	PEB	C1C-CHB-C4B	-2.65	122.33	128.28
82	XF	201	PEB	C4C-C3C-C2C	-2.65	105.05	107.50
84	CH	1001	CYC	C2A-C1A-NA	2.65	113.91	110.05
82	J1	1002	PEB	OD-C4D-C3D	-2.65	123.45	129.46
82	cH	202	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
87	3N	311	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
82	V4	202	PEB	C1C-NC-C4C	-2.65	104.88	109.60
87	AN	838	CLA	CHB-C4A-NA	2.65	128.18	124.51
84	FE	1002	CYC	CHB-C1B-NB	-2.65	120.36	126.06
82	YF	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
82	AI	202	PEB	C1D-CHC-C4C	-2.65	109.34	113.26
87	7N	610	CLA	O2D-CGD-O1D	-2.65	118.65	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gF	202	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	RE	202	PEB	C3B-C4B-NB	2.65	113.91	110.05
87	12	605	CLA	C3B-C4B-NB	-2.65	108.05	110.52
87	c6	615	CLA	C3B-C4B-NB	-2.65	108.05	110.52
82	J9	202	PEB	CHA-C4A-NA	-2.65	122.05	125.20
82	BA	201	PEB	CMB-C2B-C1B	2.65	129.15	125.06
82	G7	202	PEB	CMB-C2B-C1B	2.65	129.15	125.06
82	aK	203	PEB	C4C-C3C-C2C	-2.65	105.05	107.50
82	D7	203	PEB	CAC-CBC-CGC	-2.65	107.89	113.60
87	BL	602	CLA	CHB-C1B-NB	2.65	127.06	124.26
82	cH	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	pK	201	PEB	OD-C4D-C3D	-2.65	123.45	129.46
82	oF	201	PEB	CMB-C2B-C1B	2.65	129.15	125.06
82	M5	305	PEB	C2A-C3A-C4A	-2.65	97.37	101.34
82	NI	201	PEB	CHB-C1C-NC	-2.65	119.25	125.32
82	TP	201	PEB	CHC-C4C-NC	2.65	124.74	121.15
82	NA	201	PEB	CHA-C4A-NA	2.65	128.36	125.20
87	cL	509	CLA	O2D-CGD-CBD	2.65	115.98	111.27
82	qF	201	PEB	CAC-C2C-C1C	2.65	129.99	125.76
82	xK	304	PEB	C3B-C4B-NB	2.65	113.91	110.05
82	pK	201	PEB	CHC-C1D-ND	-2.65	110.37	113.72
82	X7	203	PEB	CBA-CAA-C3A	2.65	119.37	113.47
82	TA	203	PEB	CHC-C4C-NC	2.65	124.74	121.15
85	K2	105	BCR	C38-C26-C27	2.65	118.71	113.62
82	g1	201	PEB	C1B-C2B-C3B	-2.65	103.46	106.51
82	eK	201	PEB	C3B-C4B-NB	2.65	113.91	110.05
83	AM	304	PUB	C2C-C1C-NC	2.65	113.91	110.05
82	PQ	202	PEB	CAA-C3A-C2A	-2.65	107.64	114.26
87	82	306	CLA	C2B-C1B-NB	2.65	112.01	110.23
84	JH	1001	CYC	CHD-C1D-ND	-2.65	119.25	125.32
83	A1	303	PUB	CHC-C1D-ND	-2.65	110.37	113.72
85	a6	605	BCR	C7-C8-C9	-2.65	122.23	126.23
82	MJ	203	PEB	CMC-C3C-C4C	-2.65	124.25	127.06
82	N9	202	PEB	C1C-CHB-C4B	2.65	134.23	128.28
82	gO	201	PEB	OD-C4D-C3D	-2.65	123.45	129.46
91	d6	404	PHO	C1A-C2A-C3A	-2.65	100.32	102.84
87	BN	811	CLA	CHB-C4A-NA	2.65	128.18	124.51
87	4N	609	CLA	CHB-C4A-NA	2.65	128.18	124.51
82	iJ	202	PEB	CAC-C2C-C1C	2.65	129.98	125.76
82	VA	202	PEB	C4C-C3C-C2C	-2.65	105.05	107.50
82	TM	201	PEB	C4C-C3C-C2C	-2.65	105.05	107.50
82	fG	202	PEB	C4C-C3C-C2C	-2.65	105.05	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	BL	618	BCR	C29-C30-C25	2.65	114.56	110.48
85	cL	503	BCR	C16-C15-C14	-2.65	118.05	123.47
82	B7	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	kK	203	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	KI	203	PEB	C3C-C4C-NC	2.65	110.72	108.33
82	JQ	203	PEB	C3C-C4C-NC	2.65	110.72	108.33
82	VE	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	kK	203	PEB	OA-C1A-C2A	-2.65	124.07	126.17
82	S4	201	PEB	C2B-C1B-NB	2.65	116.19	110.53
84	NE	201	CYC	CMB-C2B-C1B	2.65	127.47	124.17
82	LH	1003	PEB	CAB-CBB-CGB	-2.65	107.90	113.60
87	BN	833	CLA	CHB-C4A-NA	2.65	128.18	124.51
87	42	606	CLA	CHB-C4A-NA	2.65	128.18	124.51
87	K2	103	CLA	CHB-C4A-NA	2.65	128.18	124.51
87	L2	204	CLA	CHB-C4A-NA	2.65	128.18	124.51
82	JB	202	PEB	OD-C4D-ND	-2.65	122.00	125.93
82	b4	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
82	UD	202	PEB	CMC-C3C-C4C	2.65	129.87	127.06
82	WB	402	PEB	CHA-C1B-NB	-2.65	119.39	124.93
87	22	605	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
82	PP	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	N9	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	P9	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	RA	203	PEB	C3C-C4C-NC	2.65	110.72	108.33
82	qK	201	PEB	CAC-C2C-C1C	2.65	129.98	125.76
87	A2	810	CLA	CMD-C2D-C3D	2.65	133.71	127.61
87	32	304	CLA	C2A-C1A-CHA	2.65	128.49	123.86
82	UP	203	PEB	CHC-C1D-ND	-2.65	110.37	113.72
82	Z1	201	PEB	OD-C4D-ND	-2.65	122.01	125.93
82	eK	201	PEB	OD-C4D-ND	-2.65	122.01	125.93
82	TI	202	PEB	CHB-C1C-NC	-2.65	119.25	125.32
82	g1	201	PEB	CMB-C2B-C1B	2.65	129.14	125.06
82	SD	202	PEB	OA-C1A-C2A	-2.65	124.07	126.17
82	sF	203	PEB	OA-C1A-C2A	-2.65	124.07	126.17
82	aM	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
94	d6	408	PL9	C53-C6-C1	2.65	120.41	114.99
82	QO	201	PEB	CMD-C2D-C3D	2.65	133.80	130.06
92	JL	102	LMG	C7-O1-C1	-2.65	108.56	113.74
82	HB	202	PEB	CAC-CBC-CGC	-2.65	107.90	113.60
82	kF	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
82	jM	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
82	GB	203	PEB	OD-C4D-ND	-2.65	122.01	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PJ	201	PEB	C4C-C3C-C2C	-2.65	105.06	107.50
82	gM	201	PEB	CHC-C1D-ND	2.65	117.08	113.72
82	PD	202	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
82	V1	201	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
82	P1	202	PEB	C3B-C4B-NB	2.65	113.90	110.05
82	tK	201	PEB	CHA-C1B-NB	-2.65	119.39	124.93
87	3N	305	CLA	C2A-C1A-CHA	2.65	128.49	123.86
82	NF	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
82	XI	202	PEB	C1D-CHC-C4C	-2.65	109.35	113.26
83	A1	304	PUB	OD-C4D-ND	-2.65	122.01	125.93
87	L2	203	CLA	CHD-C1D-ND	-2.65	122.02	124.45
82	aM	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
84	F1	1001	CYC	C1A-C2A-C3A	-2.65	103.85	106.78
82	hE	201	PEB	CHB-C1C-NC	2.65	131.38	125.32
82	ZE	201	PEB	C4C-C3C-C2C	-2.65	105.06	107.50
82	hO	201	PEB	CHB-C1C-C2C	-2.65	121.18	127.15
82	RD	201	PEB	CHA-C1B-NB	-2.65	119.40	124.93
82	wF	303	PEB	OD-C4D-C3D	-2.65	123.46	129.46
82	DD	202	PEB	C3C-C4C-NC	2.65	110.72	108.33
82	oF	202	PEB	C3C-C4C-NC	2.65	110.72	108.33
82	YE	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	VH	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
82	EJ	202	PEB	OD-C4D-C3D	-2.65	123.46	129.46
87	42	607	CLA	C4D-C3D-CAD	-2.65	104.98	108.10
82	NI	202	PEB	C1D-CHC-C4C	-2.65	109.35	113.26
84	LH	1002	CYC	O2D-CGD-CBD	2.65	122.53	114.03
82	bF	202	PEB	OD-C4D-C3D	-2.65	123.47	129.46
82	MJ	201	PEB	CAA-C3A-C2A	-2.65	107.65	114.26
82	MB	202	PEB	C3B-C4B-NB	2.65	113.90	110.05
82	RG	202	PEB	C3B-C4B-NB	2.65	113.90	110.05
85	B6	601	BCR	C33-C5-C4	2.65	118.70	113.62
82	OJ	203	PEB	C2A-C1A-NA	2.65	110.55	108.27
84	L4	1001	CYC	CAD-CBD-CGD	-2.65	107.91	113.60
82	LO	1002	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	C9	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
82	IJ	202	PEB	OD-C4D-C3D	-2.65	123.47	129.46
82	JM	201	PEB	OD-C4D-C3D	-2.65	123.47	129.46
87	A2	806	CLA	CMB-C2B-C3B	2.65	133.00	126.59
82	VG	201	PEB	CHA-C1B-NB	-2.65	119.40	124.93
82	YJ	201	PEB	CAC-CBC-CGC	-2.65	107.91	113.60
82	F4	1002	PEB	CAB-CBB-CGB	-2.65	107.91	113.60
82	bP	502	PEB	CMB-C2B-C1B	2.64	129.14	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LG	1002	PEB	OD-C4D-ND	-2.64	122.01	125.93
82	G5	202	PEB	OD-C4D-ND	-2.64	122.01	125.93
82	T7	203	PEB	CMC-C3C-C4C	2.64	129.86	127.06
87	12	606	CLA	C2D-C1D-ND	-2.64	108.16	110.10
82	D5	203	PEB	OD-C4D-C3D	-2.64	123.47	129.46
82	BK	202	PEB	CAA-C3A-C4A	-2.64	105.88	112.67
82	NB	201	PEB	C3B-C4B-NB	2.64	113.90	110.05
82	QH	202	PEB	C3B-C4B-NB	2.64	113.90	110.05
82	hM	201	PEB	C3B-C4B-NB	2.64	113.90	110.05
82	VK	202	PEB	CAB-C3B-C4B	2.64	129.69	125.01
84	EO	1001	CYC	C1A-C2A-C3A	-2.64	103.86	106.78
82	CF	202	PEB	CBB-CAB-C3B	-2.64	105.28	112.63
82	SM	203	PEB	CAA-C3A-C4A	-2.64	105.88	112.67
82	gK	203	PEB	OD-C4D-C3D	-2.64	123.47	129.46
82	Y5	202	PEB	CHC-C1D-ND	-2.64	110.38	113.72
87	BL	622	CLA	C3B-C4B-NB	-2.64	108.06	110.52
82	MM	201	PEB	C1B-C2B-C3B	-2.64	103.47	106.51
82	l1	203	PEB	CAC-C2C-C1C	2.64	129.97	125.76
87	CL	509	CLA	CHB-C4A-NA	2.64	128.17	124.51
82	AH	301	PEB	OD-C4D-C3D	-2.64	123.47	129.46
82	UJ	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
85	FN	204	BCR	C29-C30-C25	2.64	114.55	110.48
82	iK	203	PEB	CHC-C4C-NC	2.64	124.73	121.15
82	RQ	202	PEB	OA-C1A-C2A	-2.64	124.07	126.17
82	NH	1002	PEB	C2A-C1A-NA	2.64	110.55	108.27
87	AN	806	CLA	CMB-C2B-C3B	2.64	132.99	126.59
82	P5	202	PEB	OD-C4D-ND	-2.64	122.01	125.93
82	eE	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
82	SD	202	PEB	CMA-C2A-C1A	-2.64	106.70	112.40
87	B2	801	CLA	C2D-C1D-ND	-2.64	108.16	110.10
82	GQ	202	PEB	C3B-C4B-NB	2.64	113.89	110.05
87	RN	203	CLA	C3B-C4B-NB	-2.64	108.06	110.52
87	c6	604	CLA	C3B-C4B-NB	-2.64	108.06	110.52
82	TK	202	PEB	CHC-C4C-NC	-2.64	117.57	121.15
82	D9	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
87	4N	607	CLA	C4D-C3D-CAD	-2.64	104.98	108.10
82	dK	202	PEB	OD-C4D-ND	-2.64	122.02	125.93
87	22	604	CLA	CMB-C2B-C3B	2.64	132.99	126.59
82	RI	201	PEB	CHB-C1C-NC	-2.64	119.27	125.32
82	xF	304	PEB	CHA-C4A-NA	2.64	128.35	125.20
82	UM	202	PEB	CMA-C2A-C1A	-2.64	106.71	112.40
82	AP	201	PEB	CMA-C2A-C1A	-2.64	106.71	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	62	312	CLA	CHB-C4A-NA	2.64	128.17	124.51
82	k1	201	PEB	CAA-C3A-C4A	2.64	119.46	112.67
82	KB	301	PEB	CHC-C4C-NC	2.64	124.72	121.15
82	UB	303	PEB	CAC-C2C-C1C	2.64	129.97	125.76
82	cK	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
82	UA	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
82	bO	201	PEB	C2B-C1B-NB	2.64	116.17	110.53
82	JQ	203	PEB	C3B-C4B-NB	2.64	113.89	110.05
82	dB	202	PEB	CHC-C1D-ND	-2.64	110.38	113.72
82	VF	202	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
87	32	309	CLA	C2B-C1B-NB	2.64	112.00	110.23
87	12	610	CLA	CHB-C4A-NA	2.64	128.16	124.51
82	DF	202	PEB	C1C-NC-C4C	-2.64	104.90	109.60
82	JD	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
82	p8	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
82	VI	201	PEB	CHB-C1C-NC	-2.64	119.27	125.32
82	JF	202	PEB	C1B-C2B-C3B	-2.64	103.47	106.51
82	TI	203	PEB	C3C-C4C-NC	2.64	110.71	108.33
82	HH	1002	PEB	CAC-CBC-CGC	-2.64	107.92	113.60
85	A2	848	BCR	C38-C26-C25	-2.64	121.56	124.53
82	F7	203	PEB	OA-C1A-C2A	-2.64	124.07	126.17
82	AI	201	PEB	CHB-C1C-NC	-2.64	119.27	125.32
82	CF	203	PEB	CMB-C2B-C1B	2.64	129.13	125.06
82	RP	202	PEB	OD-C4D-ND	-2.64	122.02	125.93
82	wK	303	PEB	OD-C4D-C3D	-2.64	123.48	129.46
87	1N	606	CLA	C2D-C1D-ND	-2.64	108.16	110.10
82	OO	201	PEB	CHB-C4B-NB	2.64	130.07	124.58
82	FF	202	PEB	CAA-C3A-C4A	-2.64	105.89	112.67
82	QP	203	PEB	CMB-C2B-C1B	2.64	129.13	125.06
82	WE	203	PEB	OD-C4D-C3D	-2.64	123.48	129.46
82	SQ	202	PEB	CMA-C2A-C1A	-2.64	106.71	112.40
82	AP	201	PEB	CHB-C4B-C3B	-2.64	119.21	125.32
82	JJ	201	PEB	CHA-C1B-C2B	2.64	131.69	124.90
84	GO	1001	CYC	CHA-C4D-C3D	-2.64	121.19	127.15
87	62	303	CLA	C3B-C4B-NB	-2.64	108.07	110.52
87	3N	307	CLA	C3B-C4B-NB	-2.64	108.07	110.52
82	DA	202	PEB	C3B-C4B-NB	2.64	113.89	110.05
84	73	1002	CYC	C4A-C3A-C2A	-2.64	103.48	106.51
84	C4	1001	CYC	CBC-CAC-C3C	-2.64	107.59	113.47
82	LH	1003	PEB	C1D-CHC-C4C	2.64	117.15	113.26
83	AH	304	PUB	CHC-C1D-ND	-2.64	110.39	113.72
82	XD	202	PEB	OD-C4D-ND	-2.64	122.02	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EJ	203	PEB	OD-C4D-ND	-2.64	122.02	125.93
82	UO	202	PEB	OD-C4D-ND	-2.64	122.02	125.93
87	bL	607	CLA	C2A-C1A-CHA	2.64	128.47	123.86
85	b6	602	BCR	C11-C12-C13	-2.64	119.00	126.42
82	s8	201	PEB	C3B-C4B-NB	2.64	113.89	110.05
82	XD	202	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
82	EI	202	PEB	CMB-C2B-C1B	2.64	129.13	125.06
82	iF	203	PEB	CMB-C2B-C1B	2.64	129.13	125.06
82	lJ	203	PEB	CMB-C2B-C1B	2.64	129.13	125.06
82	SF	201	PEB	C2A-C1A-NA	2.64	110.55	108.27
82	rF	201	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
82	TI	203	PEB	C1D-CHC-C4C	-2.64	109.36	113.26
87	4N	604	CLA	CHD-C1D-ND	-2.64	122.03	124.45
82	NG	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
85	H6	101	BCR	C33-C5-C4	2.64	118.69	113.62
82	L5	201	PEB	OA-C1A-C2A	-2.64	124.08	126.17
82	lJ	201	PEB	CHA-C1B-NB	-2.64	119.41	124.93
87	B2	812	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
82	OM	202	PEB	CMB-C2B-C1B	2.64	129.13	125.06
87	82	305	CLA	CHA-C1A-NA	-2.64	120.36	126.40
82	IJ	202	PEB	CHB-C1C-C2C	-2.64	121.20	127.15
82	ZE	202	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
82	aM	203	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
82	pC	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
83	wF	304	PUB	OA-C1A-NA	-2.64	122.02	125.93
82	Y9	202	PEB	C3C-C4C-NC	2.64	110.71	108.33
82	WK	201	PEB	C1C-CHB-C4B	2.64	134.20	128.28
82	XJ	201	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
82	AO	304	PEB	CHC-C1D-ND	-2.64	110.39	113.72
82	DF	203	PEB	C2A-C1A-NA	2.64	110.55	108.27
84	M1	201	CYC	C2C-C1C-NC	2.64	110.55	108.27
82	DA	201	PEB	C3B-C4B-NB	2.64	113.89	110.05
82	dM	202	PEB	C3B-C4B-NB	2.64	113.89	110.05
82	VI	202	PEB	CMB-C2B-C1B	2.64	129.13	125.06
82	EI	201	PEB	CHB-C1C-NC	-2.64	119.28	125.32
87	BL	602	CLA	CHB-C4A-NA	2.64	128.16	124.51
84	G4	1001	CYC	CHA-C4D-C3D	-2.64	121.20	127.15
82	NQ	204	PEB	CMC-C3C-C4C	2.64	129.86	127.06
82	SM	201	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
87	AN	829	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
87	BN	809	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
82	FJ	201	PEB	C1B-C2B-C3B	-2.64	103.48	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RO	203	PEB	CHC-C1D-ND	-2.64	110.39	113.72
82	UE	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
82	U9	204	PEB	OD-C4D-C3D	-2.64	123.49	129.46
82	fH	203	PEB	C2A-C1A-NA	2.64	110.55	108.27
82	cH	201	PEB	C2A-C1A-NA	2.64	110.55	108.27
87	AN	849	CLA	C3B-C4B-NB	-2.64	108.07	110.52
87	MN	101	CLA	C3B-C4B-NB	-2.64	108.07	110.52
87	72	610	CLA	C3B-C4B-NB	-2.64	108.07	110.52
87	B6	607	CLA	C1-C2-C3	-2.64	121.48	126.04
84	FG	1001	CYC	CHB-C1B-NB	-2.64	120.40	126.06
82	cB	401	PEB	C3B-C4B-NB	2.64	113.88	110.05
82	lK	203	PEB	OD-C4D-C3D	-2.64	123.49	129.46
82	M9	305	PEB	C4C-C3C-C2C	-2.64	105.07	107.50
82	L5	203	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
82	G9	202	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
82	B5	201	PEB	OA-C1A-C2A	-2.64	124.08	126.17
91	D6	404	PHO	C4B-NB-C1B	-2.64	104.75	108.83
82	F7	202	PEB	C1C-NC-C4C	-2.64	104.91	109.60
82	NA	202	PEB	CAC-C2C-C1C	2.64	129.96	125.76
82	cJ	202	PEB	OD-C4D-C3D	-2.64	123.49	129.46
82	mO	203	PEB	OD-C4D-C3D	-2.64	123.49	129.46
87	A2	851	CLA	CAC-C3C-C4C	2.64	128.23	124.81
91	a6	613	PHO	C4-C3-C5	2.64	119.70	115.27
82	QQ	202	PEB	CMB-C2B-C1B	2.64	129.12	125.06
82	VA	201	PEB	CAB-CBB-CGB	-2.64	107.93	113.60
82	PH	202	PEB	C3B-C4B-NB	2.64	113.88	110.05
87	KN	102	CLA	C3B-C4B-NB	-2.64	108.07	110.52
83	AO	302	PUB	CHA-C4A-NA	-2.64	110.39	113.72
82	i1	202	PEB	OD-C4D-C3D	-2.64	123.49	129.46
87	B2	804	CLA	CHB-C1B-NB	2.64	127.05	124.26
82	NK	202	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
82	m4	201	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
84	LO	1001	CYC	CAD-CBD-CGD	-2.64	107.93	113.60
82	M5	301	PEB	C4C-C3C-C2C	-2.64	105.07	107.50
82	XA	203	PEB	CBA-CAA-C3A	2.64	119.33	113.47
82	GI	203	PEB	CMB-C2B-C1B	2.64	129.12	125.06
82	IB	201	PEB	C3B-C4B-NB	2.63	113.88	110.05
82	uK	202	PEB	CHC-C4C-NC	2.63	124.72	121.15
82	BP	202	PEB	CHC-C1D-ND	-2.63	110.39	113.72
82	YJ	201	PEB	C3C-C4C-NC	2.63	110.70	108.33
87	cL	505	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
82	PO	203	PEB	OD-C4D-C3D	-2.63	123.49	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	j4	201	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
82	jG	201	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
82	FF	202	PEB	CHB-C1C-NC	-2.63	119.28	125.32
82	Z1	201	PEB	CHB-C1C-NC	2.63	131.35	125.32
82	D9	201	PEB	CHB-C4B-C3B	-2.63	119.22	125.32
87	DL	403	CLA	C3B-C4B-NB	-2.63	108.07	110.52
95	C6	504	DGD	O5D-C1E-C2E	2.63	112.42	108.30
87	bL	616	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
85	c6	603	BCR	C37-C22-C21	-2.63	119.23	122.92
82	kH	201	PEB	CAA-C3A-C4A	2.63	119.44	112.67
82	A1	301	PEB	OD-C4D-C3D	-2.63	123.49	129.46
82	cG	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
82	GF	202	PEB	C4C-C3C-C2C	-2.63	105.07	107.50
82	PI	201	PEB	CHB-C1C-NC	-2.63	119.29	125.32
82	mE	202	PEB	CHB-C4B-C3B	-2.63	119.22	125.32
82	kF	203	PEB	CHB-C4B-C3B	-2.63	119.22	125.32
82	YF	203	PEB	C1C-CHB-C4B	2.63	134.19	128.28
82	H5	203	PEB	CAC-CBC-CGC	-2.63	107.94	113.60
82	pF	202	PEB	CHA-C1B-NB	-2.63	119.42	124.93
82	PF	202	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
82	mE	203	PEB	C3B-C4B-NB	2.63	113.88	110.05
87	BN	832	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
82	ZH	201	PEB	C3C-C4C-NC	2.63	110.70	108.33
82	VO	201	PEB	CAB-CBB-CGB	-2.63	107.94	113.60
82	a1	202	PEB	OD-C4D-ND	-2.63	122.03	125.93
87	B6	605	CLA	C3B-C4B-NB	-2.63	108.07	110.52
82	YJ	202	PEB	OD-C4D-C3D	-2.63	123.49	129.46
82	dF	202	PEB	OD-C4D-C3D	-2.63	123.49	129.46
82	lM	203	PEB	OD-C4D-C3D	-2.63	123.49	129.46
82	JD	203	PEB	C2A-C1A-NA	2.63	110.54	108.27
82	iG	201	PEB	C2A-C1A-NA	2.63	110.54	108.27
84	N4	1001	CYC	CAA-C2A-C3A	2.63	132.78	127.88
82	GD	202	PEB	CHC-C1D-ND	-2.63	110.39	113.72
87	22	612	CLA	C2A-C1A-CHA	2.63	128.46	123.86
82	iF	201	PEB	C3B-C4B-NB	2.63	113.88	110.05
82	aE	202	PEB	OD-C4D-C3D	-2.63	123.50	129.46
82	ZH	201	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
82	R4	202	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
82	KI	202	PEB	CHB-C1C-NC	-2.63	119.29	125.32
85	BN	803	BCR	C35-C13-C12	2.63	122.22	118.08
82	QK	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
82	RI	203	PEB	CHB-C4B-NB	-2.63	119.10	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WG	203	PEB	OD-C4D-C3D	-2.63	123.50	129.46
82	NQ	204	PEB	CHC-C1D-ND	-2.63	110.39	113.72
87	BN	835	CLA	C3B-C4B-NB	-2.63	108.07	110.52
87	b6	607	CLA	C3B-C4B-NB	-2.63	108.07	110.52
87	A2	818	CLA	CHB-C4A-NA	2.63	128.15	124.51
82	ID	202	PEB	C3B-C4B-NB	2.63	113.88	110.05
82	TO	203	PEB	C3B-C4B-NB	2.63	113.88	110.05
82	aO	202	PEB	CAC-C2C-C1C	2.63	129.95	125.76
82	L7	203	PEB	C2A-C1A-NA	2.63	110.54	108.27
82	cH	202	PEB	CHC-C4C-NC	2.63	124.71	121.15
82	HI	201	PEB	C4C-C3C-C2C	-2.63	105.07	107.50
82	ZH	203	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
82	XK	202	PEB	CHA-C1B-C2B	2.63	131.67	124.90
82	hM	201	PEB	CMB-C2B-C1B	2.63	129.12	125.06
82	OG	202	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
87	8N	306	CLA	CHA-C1A-NA	-2.63	120.37	126.40
82	lG	203	PEB	CHC-C1D-ND	-2.63	110.39	113.72
83	A1	303	PUB	CHA-C4A-NA	-2.63	110.39	113.72
82	YF	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
82	lF	203	PEB	C3C-C4C-NC	2.63	110.70	108.33
85	a6	605	BCR	C8-C7-C6	-2.63	119.81	127.20
82	X7	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
82	F7	201	PEB	CHB-C1C-C2C	-2.63	121.21	127.15
82	O9	202	PEB	OA-C1A-C2A	-2.63	124.08	126.17
82	EK	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
82	YI	202	PEB	CAB-C3B-C4B	2.63	129.66	125.01
82	PF	202	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
82	DF	201	PEB	C4C-C3C-C2C	-2.63	105.07	107.50
87	3N	303	CLA	CHB-C4A-NA	2.63	128.15	124.51
82	J4	1002	PEB	OD-C4D-ND	-2.63	122.03	125.93
82	Y7	304	PEB	OD-C4D-ND	-2.63	122.03	125.93
82	XA	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
82	ZG	202	PEB	CHC-C4C-NC	2.63	124.71	121.15
82	XK	201	PEB	CAB-C3B-C4B	2.63	129.66	125.01
87	AN	810	CLA	CMD-C2D-C3D	2.63	133.66	127.61
85	KN	104	BCR	C38-C26-C27	2.63	118.67	113.62
82	VE	201	PEB	CHA-C1B-NB	-2.63	119.43	124.93
82	TO	202	PEB	C3C-C4C-NC	2.63	110.70	108.33
82	cH	202	PEB	C3B-C4B-NB	2.63	113.88	110.05
82	C5	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
87	B2	832	CLA	C3B-C4B-NB	-2.63	108.08	110.52
82	lK	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B9	202	PEB	CHB-C1C-NC	2.63	131.34	125.32
82	UM	201	PEB	CHA-C1B-NB	-2.63	119.43	124.93
82	xC	201	PEB	CHC-C4C-NC	2.63	124.71	121.15
82	OE	203	PEB	CAC-C2C-C1C	2.63	129.95	125.76
82	CK	202	PEB	CBB-CAB-C3B	-2.63	105.32	112.63
82	SG	203	PEB	CMB-C2B-C1B	2.63	129.11	125.06
82	NQ	203	PEB	CMB-C2B-C1B	2.63	129.11	125.06
82	RO	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
82	R9	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
82	M7	201	PEB	CAB-CBB-CGB	-2.63	107.94	113.60
85	A6	401	BCR	C20-C19-C18	-2.63	119.03	126.42
87	2N	305	CLA	CMB-C2B-C3B	2.63	132.96	126.59
82	hE	201	PEB	C3C-C4C-NC	2.63	110.70	108.33
82	sK	202	PEB	C3C-C4C-NC	2.63	110.70	108.33
82	RJ	201	PEB	C1C-CHB-C4B	-2.63	122.39	128.28
82	W1	202	PEB	CHC-C4C-NC	2.63	124.71	121.15
87	A2	837	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
82	dK	201	PEB	C3B-C4B-NB	2.63	113.87	110.05
85	AN	804	BCR	C8-C7-C6	-2.63	119.82	127.20
82	sC	203	PEB	C4C-C3C-C2C	-2.63	105.07	107.50
94	AL	413	PL9	C15-C14-C16	2.63	119.69	115.27
85	A2	846	BCR	C1-C6-C5	-2.63	118.91	122.61
82	QD	202	PEB	CMB-C2B-C1B	2.63	129.11	125.06
82	QG	202	PEB	OA-C1A-C2A	-2.63	124.08	126.17
82	Z1	203	PEB	OA-C1A-C2A	-2.63	124.08	126.17
82	EQ	201	PEB	C2A-C1A-NA	2.63	110.54	108.27
82	FH	1002	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
82	U5	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
82	CM	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
87	BL	623	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
82	J5	201	PEB	CHC-C4C-NC	2.63	124.71	121.15
94	DL	401	PL9	C32-C33-C34	-2.63	121.33	127.66
87	CL	515	CLA	C3B-C4B-NB	-2.63	108.08	110.52
87	B2	819	CLA	C3B-C4B-NB	-2.63	108.08	110.52
82	BQ	203	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	QE	202	PEB	C1D-CHC-C4C	-2.63	109.38	113.26
85	A2	804	BCR	C8-C7-C6	-2.63	119.82	127.20
82	IF	203	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	cE	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	N7	203	PEB	CHB-C1C-NC	-2.63	119.30	125.32
82	tK	201	PEB	C4B-C3B-C2B	-2.63	103.88	106.78
82	W1	202	PEB	CHB-C4B-NB	-2.63	119.11	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lF	203	PEB	OD-C4D-C3D	-2.63	123.51	129.46
87	A2	809	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
91	aL	610	PHO	C4B-NB-C1B	-2.63	104.76	108.83
82	WF	201	PEB	C1C-CHB-C4B	2.63	134.17	128.28
82	UQ	202	PEB	CHC-C4C-NC	2.63	124.70	121.15
83	Z9	302	PUB	CMD-C2D-C3D	2.63	131.71	127.77
82	nK	202	PEB	OD-C4D-ND	-2.63	122.04	125.93
82	GQ	202	PEB	C4C-C3C-C2C	-2.63	105.08	107.50
82	eK	203	PEB	C4C-C3C-C2C	-2.63	105.08	107.50
87	52	602	CLA	CHB-C4A-NA	2.63	128.14	124.51
87	62	301	CLA	CHB-C4A-NA	2.63	128.14	124.51
82	QJ	204	PEB	CAC-C2C-C1C	2.63	129.94	125.76
82	nK	202	PEB	C4B-C3B-C2B	-2.63	103.88	106.78
84	CG	1001	CYC	C4D-CHA-C1A	2.63	134.17	128.28
87	BN	813	CLA	CAA-C2A-C3A	-2.63	105.59	112.78
82	SK	202	PEB	CBB-CAB-C3B	-2.63	105.33	112.63
82	Z4	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	L7	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	II	201	PEB	CHB-C1C-NC	-2.63	119.30	125.32
82	hJ	203	PEB	CHB-C1C-NC	-2.63	119.30	125.32
85	B2	842	BCR	C33-C5-C6	-2.63	121.58	124.53
82	FI	201	PEB	CHC-C4C-NC	2.63	124.70	121.15
82	OQ	202	PEB	CHC-C4C-NC	2.63	124.70	121.15
82	GA	202	PEB	CMB-C2B-C1B	2.63	129.11	125.06
82	DQ	201	PEB	CHA-C1B-NB	-2.63	119.44	124.93
82	ZH	201	PEB	OD-C4D-ND	-2.63	122.04	125.93
82	J9	203	PEB	CMC-C3C-C4C	2.63	129.84	127.06
84	y3	1001	CYC	CAA-C2A-C1A	2.63	129.65	125.01
87	C6	520	CLA	C3B-C4B-NB	-2.63	108.08	110.52
87	bL	605	CLA	O2D-CGD-CBD	2.63	115.93	111.27
82	RF	201	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
82	LA	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	iH	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	gK	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
87	8N	303	CLA	CHD-C1D-ND	-2.63	122.04	124.45
82	PA	202	PEB	C4C-C3C-C2C	-2.63	105.08	107.50
87	H6	103	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
82	DJ	202	PEB	C3B-C4B-NB	2.63	113.87	110.05
82	JA	203	PEB	CHC-C4C-NC	2.63	124.70	121.15
82	eG	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
82	NF	201	PEB	CHC-C1D-ND	-2.63	110.40	113.72
82	AH	305	PEB	CHB-C4B-NB	-2.63	119.11	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	B2	825	CLA	CHB-C4A-NA	2.63	128.14	124.51
87	6N	611	CLA	CHB-C4A-NA	2.63	128.14	124.51
85	AN	847	BCR	C8-C9-C10	2.62	122.97	118.94
87	72	610	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
82	XD	203	PEB	OD-C4D-C3D	-2.62	123.51	129.46
82	AE	304	PEB	OD-C4D-C3D	-2.62	123.51	129.46
82	DO	1002	PEB	OD-C4D-C3D	-2.62	123.51	129.46
82	OJ	202	PEB	C3B-C4B-NB	2.62	113.87	110.05
82	UP	201	PEB	C2B-C1B-NB	2.62	116.13	110.53
82	JI	201	PEB	CAC-CBC-CGC	-2.62	107.95	113.60
82	eF	201	PEB	CAC-CBC-CGC	-2.62	107.95	113.60
87	c6	606	CLA	O2D-CGD-CBD	2.62	115.93	111.27
82	V7	201	PEB	CAB-CBB-CGB	-2.62	107.96	113.60
82	GB	203	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
82	iK	201	PEB	C3B-C4B-NB	2.62	113.87	110.05
82	RM	202	PEB	CAA-C3A-C2A	-2.62	107.70	114.26
82	Z9	301	PEB	C2A-C1A-NA	2.62	110.53	108.27
87	FN	203	CLA	O2A-CGA-O1A	-2.62	116.76	123.30
82	QH	202	PEB	C4B-C3B-C2B	-2.62	103.88	106.78
82	KM	201	PEB	C4B-C3B-C2B	-2.62	103.88	106.78
82	y8	202	PEB	CAB-C3B-C4B	2.62	129.65	125.01
92	JL	103	LMG	O8-C28-C29	2.62	120.14	111.91
82	OJ	202	PEB	C3C-C4C-NC	2.62	110.69	108.33
82	UG	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
82	QH	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
82	PJ	201	PEB	C3B-C4B-NB	2.62	113.86	110.05
82	uC	202	PEB	C3B-C4B-NB	2.62	113.86	110.05
82	A5	202	PEB	OD-C4D-ND	-2.62	122.04	125.93
82	K9	202	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
82	R1	201	PEB	CHA-C1B-NB	-2.62	119.45	124.93
84	LH	1002	CYC	CHA-C4D-C3D	-2.62	121.23	127.15
82	g4	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
82	fG	202	PEB	CAB-C3B-C4B	2.62	129.65	125.01
82	QA	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
82	YG	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
82	II	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
82	iH	202	PEB	CAC-CBC-CGC	-2.62	107.96	113.60
82	AA	201	PEB	CHB-C1C-C2C	-2.62	121.23	127.15
82	ND	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
84	CO	1001	CYC	CBC-CAC-C3C	-2.62	107.63	113.47
82	cO	202	PEB	C3C-C4C-NC	2.62	110.69	108.33
82	CI	201	PEB	CHB-C1C-NC	-2.62	119.31	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QF	202	PEB	CHB-C1C-C2C	-2.62	121.23	127.15
82	IA	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
82	GM	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	iJ	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	TA	203	PEB	CMC-C3C-C4C	2.62	129.84	127.06
82	H9	203	PEB	CMC-C3C-C4C	2.62	129.84	127.06
87	52	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
87	7N	605	CLA	CHB-C4A-NA	2.62	128.14	124.51
82	T4	201	PEB	CHB-C4B-C3B	-2.62	119.25	125.32
91	dL	403	PHO	O2A-CGA-O1A	-2.62	116.97	123.59
82	zF	501	PEB	CBB-CAB-C3B	-2.62	105.34	112.63
84	DG	1001	CYC	CAB-C3B-C2B	2.62	132.01	127.53
87	6N	608	CLA	C3B-C4B-NB	-2.62	108.08	110.52
82	fJ	201	PEB	CMB-C2B-C1B	2.62	129.10	125.06
84	H4	1001	CYC	C1D-C2D-C3D	-2.62	104.45	107.79
82	HF	202	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
82	UQ	201	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
84	HO	1001	CYC	C4A-C3A-C2A	-2.62	103.50	106.51
82	RB	201	PEB	C3C-C4C-NC	2.62	110.69	108.33
82	DB	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
82	aG	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
87	A2	829	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
82	NE	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
82	AM	302	PEB	C4C-C3C-C2C	-2.62	105.08	107.50
82	jO	201	PEB	C4B-C3B-C2B	-2.62	103.88	106.78
82	TA	203	PEB	CHB-C1C-C2C	-2.62	121.24	127.15
82	SQ	202	PEB	CHC-C4C-NC	2.62	124.70	121.15
82	cF	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
82	EM	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
87	cL	517	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
82	OJ	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	T9	202	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
82	fJ	203	PEB	OD-C4D-C3D	-2.62	123.52	129.46
87	M2	101	CLA	C3B-C4B-NB	-2.62	108.08	110.52
82	ID	201	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	WA	201	PEB	C4B-C3B-C2B	-2.62	103.88	106.78
82	FA	201	PEB	CHB-C1C-C2C	-2.62	121.24	127.15
82	dE	202	PEB	C4C-C3C-C2C	-2.62	105.08	107.50
82	PQ	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
82	fB	301	PEB	OD-C4D-ND	-2.62	122.05	125.93
84	C1	1001	CYC	C2A-C1A-NA	2.62	113.86	110.05
82	TO	201	PEB	CHB-C4B-C3B	-2.62	119.26	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	CL	503	CLA	CMB-C2B-C3B	2.62	132.93	126.59
82	T1	202	PEB	CAC-C2C-C1C	2.62	129.93	125.76
82	WF	201	PEB	C2A-C3A-C4A	-2.62	97.42	101.34
87	BN	801	CLA	CHB-C4A-NA	2.62	128.13	124.51
87	BN	822	CLA	CHB-C4A-NA	2.62	128.13	124.51
82	r8	201	PEB	CAC-C2C-C3C	2.62	133.07	127.07
82	YQ	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
82	PQ	201	PEB	C3B-C4B-NB	2.62	113.86	110.05
82	jE	201	PEB	C3B-C4B-NB	2.62	113.86	110.05
103	82	309	ZEX	C8-C7-C6	-2.62	119.85	127.20
82	DH	1002	PEB	OD-C4D-C3D	-2.62	123.53	129.46
82	TP	201	PEB	CAB-C3B-C4B	2.62	129.64	125.01
82	X7	202	PEB	CHA-C4A-NA	2.62	128.32	125.20
83	BM	302	PUB	CAB-C3B-C4B	2.62	129.93	125.76
82	O5	202	PEB	C4C-C3C-C2C	-2.62	105.08	107.50
82	v8	202	PEB	C4C-C3C-C2C	-2.62	105.08	107.50
84	x3	1001	CYC	CMA-C3A-C4A	2.62	129.10	125.06
82	BK	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	BM	301	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	RQ	201	PEB	CHA-C1B-NB	-2.62	119.45	124.93
82	jF	202	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
82	D5	203	PEB	CHC-C4C-NC	2.62	124.69	121.15
87	AN	818	CLA	CHB-C4A-NA	2.62	128.13	124.51
82	MA	201	PEB	CAB-CBB-CGB	-2.62	107.97	113.60
82	WI	203	PEB	CHB-C4B-C3B	-2.62	119.26	125.32
82	WK	201	PEB	C1D-CHC-C4C	-2.62	109.39	113.26
82	F9	202	PEB	CHA-C1B-NB	-2.62	119.46	124.93
87	5N	604	CLA	CAA-C2A-C3A	-2.62	107.72	114.26
82	aM	204	PEB	C4B-C3B-C2B	-2.62	103.89	106.78
82	Z1	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
82	A4	304	PEB	CHC-C1D-ND	-2.62	110.41	113.72
82	AB	501	PEB	C3C-C4C-NC	2.62	110.69	108.33
85	K6	102	BCR	C4-C5-C6	-2.62	118.93	122.73
82	gE	202	PEB	CHB-C4B-NB	-2.62	119.13	124.58
82	fH	203	PEB	CHA-C1B-NB	-2.62	119.46	124.93
83	AO	303	PUB	OA-C1A-NA	-2.62	122.05	125.93
87	AN	835	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
82	i1	202	PEB	OA-C1A-NA	2.62	128.11	124.94
82	uK	201	PEB	C4B-C3B-C2B	-2.62	103.89	106.78
87	LN	204	CLA	C3B-C4B-NB	-2.62	108.09	110.52
87	K2	103	CLA	C3B-C4B-NB	-2.62	108.09	110.52
87	6N	611	CLA	O2D-CGD-O1D	-2.62	118.72	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	D5	203	PEB	OD-C4D-ND	-2.62	122.05	125.93
82	sF	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
87	5N	602	CLA	CHB-C4A-NA	2.62	128.13	124.51
82	XI	201	PEB	CHB-C1C-NC	-2.62	119.33	125.32
82	VQ	203	PEB	C2A-C1A-NA	2.62	110.53	108.27
82	OE	203	PEB	CMB-C2B-C1B	2.62	129.09	125.06
82	Z9	304	PEB	C4C-C3C-C2C	-2.62	105.08	107.50
82	O9	203	PEB	CHA-C4A-NA	-2.62	122.09	125.20
82	DI	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
83	A1	303	PUB	OD-C4D-ND	-2.62	122.05	125.93
82	HD	202	PEB	C4B-C3B-C2B	-2.62	103.89	106.78
82	UQ	201	PEB	CHC-C4C-NC	2.62	124.69	121.15
82	RP	202	PEB	C3B-C4B-NB	2.62	113.86	110.05
82	L1	1002	PEB	C1D-CHC-C4C	2.62	117.11	113.26
103	8N	309	ZEX	C8-C7-C6	-2.62	119.85	127.20
82	KI	203	PEB	CMB-C2B-C1B	2.62	129.09	125.06
82	AM	301	PEB	CMB-C2B-C1B	2.62	129.09	125.06
82	mF	201	PEB	CBC-CAC-C2C	-2.62	105.36	112.63
82	cE	202	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
87	BL	606	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
85	B2	802	BCR	C35-C13-C12	2.62	122.20	118.08
87	C6	516	CLA	C3B-C4B-NB	-2.62	108.09	110.52
82	J7	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
82	PD	202	PEB	CAA-C3A-C2A	-2.62	107.72	114.26
87	bL	607	CLA	CAC-C3C-C4C	2.62	128.20	124.81
82	gE	202	PEB	CHC-C1D-ND	-2.62	110.42	113.72
82	x8	201	PEB	CHC-C4C-NC	2.62	124.69	121.15
82	VQ	203	PEB	C3B-C4B-NB	2.62	113.85	110.05
82	NI	202	PEB	CMB-C2B-C1B	2.62	129.09	125.06
95	c6	618	DGD	O1G-C1A-C2A	2.62	120.12	111.91
87	cL	508	CLA	CHB-C1B-NB	2.62	127.03	124.26
82	pK	202	PEB	CHA-C1B-NB	-2.62	119.46	124.93
96	VL	201	HEM	CMB-C2B-C1B	-2.62	121.06	125.04
84	IE	1001	CYC	CBC-CAC-C3C	-2.62	107.64	113.47
82	H7	202	PEB	CAC-C2C-C1C	2.62	129.93	125.76
82	T7	203	PEB	CHB-C1C-C2C	-2.62	121.25	127.15
82	D1	1002	PEB	OD-C4D-C3D	-2.62	123.53	129.46
82	D4	1002	PEB	OD-C4D-C3D	-2.62	123.53	129.46
82	fG	202	PEB	OD-C4D-C3D	-2.62	123.53	129.46
82	kO	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
82	c4	201	PEB	OD-C4D-ND	-2.62	122.06	125.93
83	M5	303	PUB	OA-C1A-NA	-2.62	122.06	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	F2	201	CLA	O2A-CGA-O1A	-2.62	116.78	123.30
82	SF	201	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	wC	203	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	Z5	305	PEB	C2B-C1B-NB	2.61	116.11	110.53
82	j1	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
82	CK	203	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
82	dH	202	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
87	RN	204	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
82	mJ	201	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
83	AE	302	PUB	CAC-C2C-C1C	2.61	129.63	125.01
83	Z9	302	PUB	OD-C4D-ND	-2.61	122.06	125.93
82	YI	201	PEB	CHB-C1C-NC	-2.61	119.33	125.32
82	D7	202	PEB	C3B-C4B-NB	2.61	113.85	110.05
82	XB	202	PEB	CAB-CBB-CGB	-2.61	107.98	113.60
82	lK	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
82	e1	202	PEB	CHC-C4C-NC	2.61	124.69	121.15
82	e1	201	PEB	CHC-C1D-ND	-2.61	110.42	113.72
82	FM	201	PEB	CHB-C4B-NB	-2.61	119.14	124.58
82	zK	501	PEB	CBB-CAB-C3B	-2.61	105.36	112.63
82	D4	1002	PEB	CAB-C3B-C4B	2.61	129.63	125.01
82	WJ	201	PEB	CHA-C4A-NA	2.61	128.31	125.20
87	A6	404	CLA	C3B-C4B-NB	-2.61	108.09	110.52
87	22	602	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
82	CJ	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
82	F5	202	PEB	CMA-C2A-C1A	-2.61	106.77	112.40
82	CI	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	Q7	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	DK	201	PEB	CMC-C3C-C4C	2.61	129.83	127.06
85	AN	848	BCR	C38-C26-C25	-2.61	121.59	124.53
82	WA	202	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
87	BN	802	CLA	C2D-C1D-ND	-2.61	108.18	110.10
83	wK	304	PUB	CMD-C2D-C3D	2.61	131.69	127.77
82	BK	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
82	sK	203	PEB	OD-C4D-C3D	-2.61	123.54	129.46
82	U5	203	PEB	CHC-C1D-ND	-2.61	110.42	113.72
85	FL	101	BCR	C2-C1-C6	2.61	114.50	110.48
82	TB	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
103	8N	310	ZEX	O3-C3-C2	-2.61	104.61	109.80
82	lE	201	PEB	OD-C4D-C3D	-2.61	123.54	129.46
87	1N	605	CLA	C3B-C4B-NB	-2.61	108.09	110.52
82	jE	201	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
82	MP	203	PEB	C1C-NC-C4C	2.61	114.25	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AK	202	PEB	CHC-C4C-NC	2.61	124.69	121.15
87	AN	809	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
85	A2	847	BCR	C8-C9-C10	2.61	122.95	118.94
82	aB	202	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
82	RI	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
82	M9	301	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	PJ	202	PEB	CAA-C3A-C2A	-2.61	107.73	114.26
82	HF	202	PEB	CAB-C3B-C4B	2.61	129.63	125.01
82	lG	202	PEB	C2A-C1A-NA	2.61	110.53	108.27
82	Q4	201	PEB	CMD-C2D-C3D	2.61	133.75	130.06
84	IO	1001	CYC	CBC-CAC-C3C	-2.61	107.65	113.47
82	ZE	202	PEB	OA-C1A-C2A	-2.61	124.10	126.17
82	LI	201	PEB	CHB-C1C-NC	-2.61	119.34	125.32
82	SM	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
82	m4	203	PEB	OD-C4D-C3D	-2.61	123.54	129.46
82	d4	202	PEB	CHC-C4C-NC	2.61	124.68	121.15
82	MJ	201	PEB	CAC-CBC-CGC	-2.61	107.98	113.60
87	B2	805	CLA	C2B-C1B-NB	2.61	111.98	110.23
84	H4	1001	CYC	C4A-C3A-C2A	-2.61	103.51	106.51
82	WD	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
82	SJ	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	SQ	201	PEB	CMB-C2B-C1B	2.61	129.09	125.06
82	OM	201	PEB	C3B-C4B-NB	2.61	113.85	110.05
87	42	604	CLA	CHD-C1D-ND	-2.61	122.05	124.45
82	DD	203	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
82	H9	202	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
87	B2	821	CLA	CHB-C4A-NA	2.61	128.12	124.51
83	K7	203	PUB	CHB-C1C-NC	-2.61	119.14	124.58
82	TA	202	PEB	CAB-C3B-C4B	2.61	129.63	125.01
87	CL	506	CLA	CAC-C3C-C4C	2.61	128.20	124.81
87	AN	851	CLA	CAC-C3C-C4C	2.61	128.20	124.81
82	iO	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
87	CL	503	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
82	UJ	203	PEB	CHB-C1C-NC	-2.61	119.34	125.32
84	I4	1001	CYC	CBC-CAC-C3C	-2.61	107.65	113.47
94	A6	410	PL9	C25-C24-C26	2.61	119.66	115.27
82	TM	202	PEB	CAA-C3A-C4A	2.61	119.38	112.67
82	T5	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	M7	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
84	x3	1001	CYC	CAA-CBA-CGA	2.61	119.22	113.60
87	BL	601	CLA	CHB-C4A-NA	2.61	128.12	124.51
82	EJ	203	PEB	CMB-C2B-C1B	2.61	129.08	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eF	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
82	P5	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
83	A1	304	PUB	CHC-C1D-ND	-2.61	110.42	113.72
82	WA	202	PEB	C3C-C4C-NC	2.61	110.68	108.33
82	c1	202	PEB	CAC-C2C-C1C	2.61	129.92	125.76
85	F2	204	BCR	C29-C30-C25	2.61	114.50	110.48
87	b6	614	CLA	CHB-C4A-NA	2.61	128.12	124.51
82	CJ	202	PEB	CHA-C1B-NB	-2.61	119.47	124.93
83	Z5	303	PUB	OA-C1A-NA	-2.61	122.06	125.93
82	cK	201	PEB	OA-C1A-C2A	-2.61	124.10	126.17
82	ZH	201	PEB	CHB-C1C-NC	2.61	131.30	125.32
87	32	309	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
82	I7	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
95	b6	622	DGD	O1G-C1A-C2A	2.61	120.10	111.91
82	KQ	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
82	Y1	202	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
87	3N	309	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
82	SE	202	PEB	CMB-C2B-C1B	2.61	129.08	125.06
82	JH	1002	PEB	OD-C4D-ND	-2.61	122.06	125.93
87	ON	202	CLA	CHB-C1B-NB	2.61	127.02	124.26
82	ZJ	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	gG	202	PEB	CHB-C4B-NB	-2.61	119.15	124.58
87	52	604	CLA	CAA-C2A-C3A	-2.61	107.74	114.26
82	GP	202	PEB	CHB-C1C-C2C	-2.61	121.27	127.15
82	AI	202	PEB	CMB-C2B-C1B	2.61	129.08	125.06
82	RI	202	PEB	CMB-C2B-C1B	2.61	129.08	125.06
87	42	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
87	72	605	CLA	CHB-C4A-NA	2.61	128.12	124.51
87	B2	816	CLA	CHB-C4A-NA	2.61	128.12	124.51
83	Z9	305	PUB	OA-C1A-NA	-2.61	122.07	125.93
84	W3	1001	CYC	CMD-C2D-C3D	-2.61	119.96	125.61
82	S5	203	PEB	CAC-CBC-CGC	-2.61	107.99	113.60
82	XJ	202	PEB	C1D-CHC-C4C	-2.61	109.41	113.26
82	WE	201	PEB	CMA-C2A-C1A	-2.61	106.78	112.40
82	O5	202	PEB	CMA-C2A-C1A	-2.61	106.78	112.40
82	SJ	202	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
82	LD	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	jH	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	hM	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	BF	202	PEB	CAA-C3A-C4A	-2.61	105.98	112.67
82	DJ	201	PEB	CMC-C3C-C4C	2.61	129.82	127.06
87	B2	808	CLA	O2D-CGD-O1D	-2.61	118.74	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BD	203	PEB	OD-C4D-ND	-2.61	122.07	125.93
82	R1	201	PEB	OD-C4D-ND	-2.61	122.07	125.93
82	eB	202	PEB	OD-C4D-ND	-2.61	122.07	125.93
82	M9	302	PEB	C2A-C1A-NA	2.61	110.52	108.27
82	NE	202	PEB	CAC-C2C-C1C	2.61	129.91	125.76
82	FJ	202	PEB	O2B-CGB-CBB	2.61	122.41	114.03
82	V5	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	x8	202	PEB	CAA-C3A-C2A	-2.61	107.74	114.26
87	dL	404	CLA	C3B-C4B-NB	-2.61	108.10	110.52
84	V3	1001	CYC	CAA-CBA-CGA	2.61	119.21	113.60
82	ZM	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	N5	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	DA	201	PEB	OD-C4D-ND	-2.61	122.07	125.93
82	H5	201	PEB	CAC-C2C-C1C	2.61	129.91	125.76
87	B6	616	CLA	CHB-C4A-NA	2.61	128.12	124.51
82	Y7	301	PEB	CHB-C1C-NC	-2.61	119.35	125.32
82	DQ	202	PEB	C3C-C4C-NC	2.61	110.68	108.33
82	GD	202	PEB	C3B-C4B-NB	2.61	113.84	110.05
82	HO	1002	PEB	OD-C4D-C3D	-2.61	123.55	129.46
82	VH	202	PEB	C1B-C2B-C3B	-2.61	103.52	106.51
82	BM	301	PEB	C1B-C2B-C3B	-2.61	103.52	106.51
82	w8	203	PEB	CMB-C2B-C1B	2.61	129.08	125.06
82	CD	202	PEB	OD-C4D-ND	-2.61	122.07	125.93
82	LE	1002	PEB	OD-C4D-ND	-2.61	122.07	125.93
82	C9	201	PEB	OD-C4D-ND	-2.61	122.07	125.93
83	M9	303	PUB	OD-C4D-ND	-2.61	122.07	125.93
85	C6	507	BCR	C8-C7-C6	-2.61	119.88	127.20
82	GQ	202	PEB	CBC-CAC-C2C	2.61	119.87	112.63
82	aO	202	PEB	C1C-NC-C4C	-2.61	104.96	109.60
82	FF	202	PEB	C4B-NB-C1B	-2.61	101.60	106.51
82	W9	201	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
82	vC	202	PEB	C4C-C3C-C2C	-2.61	105.09	107.50
82	pK	201	PEB	OA-C1A-NA	2.61	128.10	124.94
82	DA	203	PEB	CHA-C1B-NB	-2.61	119.48	124.93
82	BF	202	PEB	CHA-C1B-NB	-2.61	119.48	124.93
95	DL	408	DGD	C1E-O6E-C5E	2.61	118.80	113.69
82	JB	201	PEB	CMA-C2A-C1A	-2.61	106.79	112.40
82	TD	202	PEB	CHA-C4A-NA	2.61	128.30	125.20
94	A6	410	PL9	C45-C44-C46	2.61	119.65	115.27
82	lJ	203	PEB	CHB-C4B-NB	-2.61	119.16	124.58
82	eG	203	PEB	CHC-C4C-NC	2.61	124.67	121.15
87	42	606	CLA	C2D-C1D-ND	-2.61	108.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	l1	201	PEB	CMB-C2B-C1B	2.61	129.08	125.06
82	GI	203	PEB	OD-C4D-ND	-2.61	122.07	125.93
87	32	311	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
82	HM	202	PEB	CAA-C3A-C2A	-2.60	107.75	114.26
82	AQ	304	PEB	C3B-C4B-NB	2.60	113.84	110.05
82	O4	202	PEB	C3B-C4B-NB	2.60	113.84	110.05
82	u8	202	PEB	C3B-C4B-NB	2.60	113.84	110.05
82	SB	202	PEB	CAC-CBC-CGC	-2.60	108.00	113.60
82	MA	202	PEB	OD-C4D-C3D	-2.60	123.56	129.46
87	LN	203	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
82	RG	201	PEB	C2A-C1A-NA	2.60	110.52	108.27
82	WB	402	PEB	CAC-CBC-CGC	-2.60	108.00	113.60
82	k4	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	G5	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	eB	202	PEB	CHA-C1B-NB	-2.60	119.49	124.93
82	cG	202	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	SK	201	PEB	CMB-C2B-C1B	2.60	129.07	125.06
82	YF	201	PEB	CHC-C4C-NC	2.60	124.67	121.15
82	NG	201	PEB	CAC-C2C-C1C	2.60	129.91	125.76
82	fE	202	PEB	CAB-C3B-C4B	2.60	129.62	125.01
82	lF	202	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	l1	201	PEB	C3B-C4B-NB	2.60	113.84	110.05
82	X5	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
87	bL	616	CLA	C3B-C4B-NB	-2.60	108.10	110.52
82	fJ	201	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	rC	201	PEB	CAC-C2C-C3C	2.60	133.03	127.07
82	N9	201	PEB	OD-C4D-ND	-2.60	122.07	125.93
83	xK	305	PUB	OD-C4D-ND	-2.60	122.07	125.93
82	DD	202	PEB	C4B-C3B-C2B	-2.60	103.90	106.78
95	c6	601	DGD	O1G-C1A-O1A	-2.60	117.02	123.59
82	PE	202	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	K5	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	Z5	301	PEB	C4C-C3C-C2C	-2.60	105.10	107.50
82	RD	203	PEB	C3B-C4B-NB	2.60	113.83	110.05
84	M1	201	CYC	CAD-C3D-C4D	2.60	129.91	125.76
82	BD	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
87	CL	508	CLA	CMC-C2C-C1C	-2.60	121.08	125.04
82	V9	202	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	H7	202	PEB	CBB-CAB-C3B	-2.60	105.40	112.63
85	BN	842	BCR	C33-C5-C6	-2.60	121.61	124.53
87	A2	837	CLA	CHA-C1A-NA	-2.60	120.44	126.40
87	M2	101	CLA	CMB-C2B-C1B	-2.60	121.41	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RJ	202	PEB	CAC-C2C-C1C	2.60	129.91	125.76
82	PI	202	PEB	CMB-C2B-C1B	2.60	129.07	125.06
82	A5	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	kM	202	PEB	OD-C4D-C3D	-2.60	123.56	129.46
82	YF	203	PEB	CBA-CAA-C3A	-2.60	107.67	113.47
84	y3	1001	CYC	CMD-C2D-C3D	-2.60	119.98	125.61
82	JP	201	PEB	CHC-C1D-ND	-2.60	110.43	113.72
82	M9	301	PEB	OD-C4D-C3D	-2.60	123.57	129.46
82	Z1	201	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	RK	201	PEB	CAB-CBB-CGB	-2.60	108.00	113.60
82	eK	201	PEB	CAC-CBC-CGC	-2.60	108.00	113.60
82	jJ	203	PEB	C3C-C4C-NC	2.60	110.67	108.33
82	wC	203	PEB	C3B-C4B-NB	2.60	113.83	110.05
82	tF	202	PEB	C3B-C4B-NB	2.60	113.83	110.05
82	R9	202	PEB	CAB-C3B-C4B	2.60	129.61	125.01
82	HK	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
82	LQ	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
82	E5	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
82	pF	201	PEB	OA-C1A-NA	2.60	128.09	124.94
87	cL	510	CLA	CMC-C2C-C1C	-2.60	121.08	125.04
85	BN	842	BCR	C1-C6-C5	-2.60	118.95	122.61
85	kL	100	BCR	C23-C22-C21	2.60	122.93	118.94
87	BN	834	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
82	YI	202	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	D4	1002	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	GP	201	PEB	C1C-NC-C4C	2.60	114.22	109.60
82	NQ	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	XQ	203	PEB	CHC-C4C-NC	2.60	124.67	121.15
82	UB	302	PEB	OD-C4D-C3D	-2.60	123.57	129.46
84	FE	1001	CYC	C4D-CHA-C1A	2.60	134.11	128.28
85	bL	602	BCR	C11-C12-C13	-2.60	119.11	126.42
82	AK	201	PEB	CHC-C1D-ND	-2.60	110.44	113.72
82	eH	201	PEB	CHC-C1D-ND	-2.60	110.44	113.72
82	i1	202	PEB	CAC-CBC-CGC	-2.60	108.01	113.60
82	tK	201	PEB	CAB-CBB-CGB	-2.60	108.01	113.60
82	w8	203	PEB	C3B-C4B-NB	2.60	113.83	110.05
87	AN	837	CLA	CHA-C1A-NA	-2.60	120.44	126.40
82	WH	202	PEB	CHB-C4B-NB	-2.60	119.17	124.58
82	OQ	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	T4	202	PEB	CMC-C3C-C4C	2.60	129.82	127.06
82	g1	201	PEB	CHC-C4C-NC	2.60	124.67	121.15
82	BA	203	PEB	CAB-CBB-CGB	-2.60	108.01	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AF	201	PEB	C4C-C3C-C2C	-2.60	105.10	107.50
82	DK	202	PEB	C1C-NC-C4C	-2.60	104.97	109.60
82	OI	203	PEB	C3B-C4B-NB	2.60	113.83	110.05
82	D9	202	PEB	C3C-C4C-NC	2.60	110.67	108.33
82	lM	203	PEB	C3C-C4C-NC	2.60	110.67	108.33
82	KI	203	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	WI	202	PEB	CAC-C2C-C1C	2.60	129.90	125.76
82	YP	501	PEB	CMA-C2A-C1A	-2.60	106.80	112.40
85	AN	846	BCR	C1-C6-C5	-2.60	118.95	122.61
87	MN	101	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
87	A2	835	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
82	UB	303	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	wC	203	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
82	P9	202	PEB	CAB-C3B-C4B	2.60	129.61	125.01
82	SP	203	PEB	CMB-C2B-C1B	2.60	129.07	125.06
82	eE	203	PEB	CHC-C4C-NC	2.60	124.67	121.15
87	AN	851	CLA	C2D-C1D-ND	-2.60	108.19	110.10
82	N7	202	PEB	CHB-C4B-C3B	-2.60	119.31	125.32
82	YP	501	PEB	C3B-C4B-NB	2.60	113.83	110.05
82	jF	201	PEB	CHA-C1B-C2B	2.60	131.58	124.90
82	bO	201	PEB	C4B-C3B-C2B	-2.60	103.91	106.78
82	JI	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
82	GQ	201	PEB	C4C-C3C-C2C	-2.60	105.10	107.50
82	AF	201	PEB	CHC-C1D-ND	-2.60	110.44	113.72
82	NK	201	PEB	CHC-C1D-ND	-2.60	110.44	113.72
87	12	604	CLA	CAA-C2A-C3A	-2.60	107.77	114.26
87	BN	817	CLA	CHB-C4A-NA	2.60	128.10	124.51
82	mE	202	PEB	CMB-C2B-C1B	2.60	129.06	125.06
82	gF	202	PEB	CMB-C2B-C1B	2.60	129.06	125.06
82	hG	201	PEB	C3C-C4C-NC	2.60	110.67	108.33
82	SO	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
82	f4	202	PEB	C3B-C4B-NB	2.60	113.83	110.05
87	62	312	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
95	CL	520	DGD	C1E-O6E-C5E	2.60	118.79	113.69
82	YA	303	PEB	CAB-C3B-C4B	2.60	129.60	125.01
82	lH	202	PEB	CAC-C2C-C1C	2.60	129.90	125.76
82	h1	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	i4	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	X9	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	VH	201	PEB	CHC-C1D-ND	-2.60	110.44	113.72
85	F6	101	BCR	C20-C21-C22	-2.60	123.60	127.31
82	GB	202	PEB	CHA-C1B-NB	-2.60	119.50	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	nF	201	PEB	C4C-C3C-C2C	-2.60	105.10	107.50
82	PH	201	PEB	CAB-CBB-CGB	-2.60	108.01	113.60
82	EF	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
82	HA	202	PEB	CAC-C2C-C1C	2.60	129.90	125.76
85	BN	841	BCR	C24-C23-C22	-2.60	122.31	126.23
87	b6	613	CLA	CHB-C4A-NA	2.60	128.10	124.51
83	KA	203	PUB	CHB-C1C-NC	-2.60	119.17	124.58
83	K7	203	PUB	CHB-C4B-NB	-2.60	119.37	125.32
82	aJ	202	PEB	CHA-C1B-NB	-2.60	119.50	124.93
82	xC	202	PEB	CAA-C3A-C2A	-2.60	107.77	114.26
82	OD	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	dK	202	PEB	C4C-C3C-C2C	-2.60	105.10	107.50
87	R2	204	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
82	jK	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
82	NM	202	PEB	O2B-CGB-CBB	2.60	122.37	114.03
82	FK	202	PEB	C4B-NB-C1B	-2.60	101.62	106.51
82	RJ	202	PEB	CHC-C1D-ND	-2.60	110.44	113.72
82	Z5	304	PEB	CHC-C1D-ND	-2.60	110.44	113.72
87	AL	405	CLA	O2D-CGD-CBD	2.60	115.88	111.27
82	LQ	201	PEB	CAB-C3B-C4B	2.60	129.60	125.01
82	WM	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
87	bL	621	CLA	C2A-C1A-CHA	2.60	128.40	123.86
87	c6	607	CLA	C3B-C4B-NB	-2.60	108.11	110.52
82	IP	201	PEB	CMA-C2A-C1A	-2.60	106.81	112.40
82	GE	1002	PEB	OD-C4D-ND	-2.60	122.08	125.93
82	XI	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
87	D6	405	CLA	C1-C2-C3	-2.60	121.55	126.04
82	f1	202	PEB	CHA-C4A-NA	-2.60	122.12	125.20
82	OJ	203	PEB	C1C-NC-C4C	-2.60	104.98	109.60
83	wF	304	PUB	CMD-C2D-C3D	2.60	131.66	127.77
82	C9	202	PEB	CAB-C3B-C4B	2.60	129.60	125.01
82	W5	202	PEB	OD-C4D-C3D	-2.60	123.58	129.46
95	C6	502	DGD	O1G-C1A-O1A	-2.60	117.04	123.59
87	A2	820	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
82	V7	202	PEB	C4C-C3C-C2C	-2.60	105.11	107.50
82	PI	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	GP	202	PEB	OD-C4D-C3D	-2.59	123.58	129.46
82	XQ	202	PEB	C4B-C3B-C2B	-2.59	103.91	106.78
83	yF	302	PUB	CHB-C4B-C3B	-2.59	121.30	127.15
82	VD	201	PEB	C3C-C4C-NC	2.59	110.67	108.33
82	mK	201	PEB	CBC-CAC-C2C	-2.59	105.42	112.63
82	QB	203	PEB	CHA-C1B-NB	-2.59	119.51	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	a6	604	DGD	C2G-O2G-C1B	-2.59	111.40	117.79
82	PD	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	RK	201	PEB	CMB-C2B-C1B	2.59	129.06	125.06
82	SJ	203	PEB	CAA-C3A-C4A	-2.59	106.01	112.67
82	IQ	201	PEB	CHA-C1B-NB	-2.59	119.51	124.93
82	R5	201	PEB	OD-C4D-C3D	-2.59	123.58	129.46
85	LN	205	BCR	C33-C5-C4	2.59	118.60	113.62
82	oK	202	PEB	C4B-C3B-C2B	-2.59	103.91	106.78
82	OO	202	PEB	C3B-C4B-NB	2.59	113.82	110.05
82	sC	201	PEB	C3B-C4B-NB	2.59	113.82	110.05
87	4N	605	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
82	WK	201	PEB	C2A-C3A-C4A	-2.59	97.45	101.34
82	HB	203	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
82	ZH	202	PEB	CMB-C2B-C1B	2.59	129.06	125.06
82	g4	203	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	cE	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	QF	201	PEB	C3C-C4C-NC	2.59	110.67	108.33
82	D7	203	PEB	CHA-C1B-NB	-2.59	119.51	124.93
87	bL	618	CLA	C3B-C4B-NB	-2.59	108.11	110.52
82	QK	202	PEB	CHB-C1C-C2C	-2.59	121.30	127.15
82	sK	203	PEB	OA-C1A-C2A	-2.59	124.11	126.17
87	52	606	CLA	CHB-C4A-NA	2.59	128.10	124.51
87	bL	616	CLA	CHB-C4A-NA	2.59	128.10	124.51
84	M1	201	CYC	CHB-C4A-NA	-2.59	119.51	124.93
82	VJ	202	PEB	CHB-C1C-NC	-2.59	119.38	125.32
82	Y9	202	PEB	CHA-C4A-NA	-2.59	122.12	125.20
82	VF	201	PEB	C4C-C3C-C2C	-2.59	105.11	107.50
82	QI	201	PEB	C4C-C3C-C2C	-2.59	105.11	107.50
82	s8	203	PEB	C4C-C3C-C2C	-2.59	105.11	107.50
82	BJ	301	PEB	CAB-CBB-CGB	-2.59	108.02	113.60
82	NI	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	I9	201	PEB	OD-C4D-ND	-2.59	122.09	125.93
83	A4	303	PUB	OA-C1A-NA	-2.59	122.09	125.93
82	DG	1002	PEB	CAA-C3A-C4A	-2.59	106.02	112.67
82	OK	202	PEB	CHC-C1D-ND	-2.59	110.44	113.72
82	S4	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
82	H5	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
82	ZF	201	PEB	C2A-C1A-NA	2.59	110.51	108.27
87	6N	612	CLA	CHB-C4A-NA	2.59	128.10	124.51
87	6N	613	CLA	CHB-C4A-NA	2.59	128.10	124.51
82	Z1	201	PEB	C3C-C4C-NC	2.59	110.67	108.33
87	A2	849	CLA	C3B-C4B-NB	-2.59	108.11	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	2N	302	CLA	C2A-C1A-CHA	2.59	128.39	123.86
82	II	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	BD	202	PEB	C4C-C3C-C2C	-2.59	105.11	107.50
82	PK	202	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
82	UB	303	PEB	OD-C4D-C3D	-2.59	123.59	129.46
82	lJ	203	PEB	C3B-C4B-NB	2.59	113.82	110.05
83	wK	304	PUB	C2C-C1C-NC	2.59	113.82	110.05
82	E9	202	PEB	CAB-C3B-C4B	2.59	129.59	125.01
85	LN	201	BCR	C10-C11-C12	-2.59	115.13	123.22
83	QM	201	PUB	CAB-C3B-C4B	2.59	129.89	125.76
87	32	306	CLA	C3B-C4B-NB	-2.59	108.11	110.52
82	H4	1002	PEB	OD-C4D-C3D	-2.59	123.59	129.46
82	Q5	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
82	IF	201	PEB	C3C-C4C-NC	2.59	110.67	108.33
82	hJ	203	PEB	C3C-C4C-NC	2.59	110.67	108.33
82	VH	201	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
87	B2	831	CLA	CAC-C3C-C4C	2.59	128.17	124.81
82	RG	202	PEB	CHA-C1B-NB	-2.59	119.51	124.93
82	ZB	201	PEB	CAB-CBB-CGB	-2.59	108.03	113.60
87	AN	831	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
85	K2	102	BCR	C20-C21-C22	-2.59	123.61	127.31
82	OI	201	PEB	CAA-C3A-C2A	-2.59	107.79	114.26
83	A4	303	PUB	C2C-C1C-NC	2.59	113.82	110.05
82	Y1	201	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
82	UH	203	PEB	C1C-CHB-C4B	-2.59	122.47	128.28
82	UG	203	PEB	CBA-CAA-C3A	-2.59	107.70	113.47
82	DB	201	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	D5	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
84	L1	1001	CYC	CHA-C4D-C3D	-2.59	121.31	127.15
84	EE	1001	CYC	CMB-C2B-C1B	2.59	127.40	124.17
87	BN	831	CLA	CAC-C3C-C4C	2.59	128.17	124.81
87	42	605	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
82	WP	202	PEB	CMA-C2A-C1A	-2.59	106.82	112.40
84	HO	1001	CYC	CHD-C1D-ND	-2.59	119.39	125.32
84	H4	1001	CYC	CHD-C1D-ND	-2.59	119.39	125.32
82	f1	203	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
84	IG	1001	CYC	CBC-CAC-C3C	-2.59	107.70	113.47
82	V4	202	PEB	CAC-CBC-CGC	-2.59	108.03	113.60
84	LH	1002	CYC	CHB-C4A-NA	-2.59	119.52	124.93
84	DE	1001	CYC	C2C-C1C-NC	2.59	110.50	108.27
82	L5	202	PEB	C3C-C4C-NC	2.59	110.66	108.33
87	LN	204	CLA	C2D-C1D-ND	-2.59	108.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	bL	605	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
82	cM	202	PEB	C1C-CHB-C4B	-2.59	122.48	128.28
85	B2	842	BCR	C36-C18-C19	2.59	122.16	118.08
82	B9	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
82	N7	202	PEB	CAC-C2C-C1C	2.59	129.88	125.76
87	22	607	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
85	a6	605	BCR	C28-C27-C26	-2.59	109.45	114.08
82	CA	201	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
82	TI	203	PEB	CMB-C2B-C1B	2.59	129.05	125.06
82	eB	202	PEB	C1B-C2B-C3B	-2.59	103.54	106.51
82	YO	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
82	LF	201	PEB	C3B-C4B-NB	2.59	113.81	110.05
82	IQ	202	PEB	C3B-C4B-NB	2.59	113.81	110.05
82	J1	1002	PEB	OD-C4D-ND	-2.59	122.10	125.93
82	A7	201	PEB	CHB-C1C-C2C	-2.59	121.31	127.15
87	A2	830	CLA	O2D-CGD-CBD	2.59	115.87	111.27
82	dJ	201	PEB	CHC-C1D-ND	-2.59	110.45	113.72
87	cL	507	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
82	18	202	PEB	C3C-C4C-NC	2.59	110.66	108.33
88	D6	406	LHG	O8-C23-C24	2.59	120.03	111.91
85	KL	100	BCR	C23-C22-C21	2.59	122.91	118.94
82	TP	201	PEB	CHA-C1B-NB	-2.59	119.52	124.93
82	iJ	202	PEB	CHB-C1C-NC	-2.59	119.39	125.32
82	KK	203	PEB	CHC-C4C-NC	2.59	124.65	121.15
85	L2	205	BCR	C33-C5-C4	2.59	118.59	113.62
85	KN	101	BCR	C20-C21-C22	-2.59	123.62	127.31
83	wF	304	PUB	C2C-C1C-NC	2.59	113.81	110.05
82	aF	201	PEB	OD-C4D-ND	-2.59	122.10	125.93
82	v8	202	PEB	CHB-C4B-C3B	2.59	131.30	125.32
82	GQ	202	PEB	CHC-C1D-ND	-2.59	110.45	113.72
82	WB	401	PEB	CHA-C1B-NB	-2.59	119.52	124.93
82	KB	301	PEB	CMC-C3C-C4C	-2.59	124.32	127.06
87	22	601	CLA	C2A-C1A-CHA	2.59	128.38	123.86
82	gF	203	PEB	C1C-CHB-C4B	2.59	134.08	128.28
82	kH	203	PEB	CMB-C2B-C1B	2.59	129.05	125.06
87	1N	609	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
91	dL	403	PHO	C4B-NB-C1B	-2.59	104.82	108.83
85	BN	842	BCR	C36-C18-C19	2.59	122.15	118.08
82	D9	201	PEB	CAC-C2C-C1C	2.59	129.88	125.76
82	A9	202	PEB	CAB-C3B-C4B	2.59	129.59	125.01
82	OB	201	PEB	C3B-C4B-NB	2.59	113.81	110.05
82	QM	203	PEB	C2A-C1A-NA	2.59	110.50	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	b6	606	CLA	CHB-C4A-NA	2.59	128.09	124.51
87	bL	619	CLA	CHB-C4A-NA	2.59	128.09	124.51
82	W7	201	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
84	EE	1001	CYC	C4A-C3A-C2A	-2.59	103.54	106.51
82	I5	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
82	m4	201	PEB	CAB-CBB-CGB	-2.59	108.04	113.60
82	F5	201	PEB	CMB-C2B-C1B	2.59	129.05	125.06
82	x8	201	PEB	C3B-C4B-NB	2.59	113.81	110.05
82	WM	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
82	jF	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
82	HD	201	PEB	C1C-NC-C4C	-2.59	105.00	109.60
82	T4	201	PEB	C1B-C2B-C3B	-2.59	103.54	106.51
82	RM	202	PEB	C3B-C4B-NB	2.59	113.81	110.05
83	AG	303	PUB	OD-C4D-ND	-2.59	122.10	125.93
82	ZE	202	PEB	CHC-C4C-NC	2.59	124.65	121.15
82	ZG	201	PEB	C4C-C3C-C2C	-2.59	105.11	107.50
82	AJ	302	PEB	CMC-C3C-C4C	2.59	129.80	127.06
82	CB	201	PEB	C1D-CHC-C4C	-2.59	109.44	113.26
82	HA	202	PEB	CBB-CAB-C3B	-2.58	105.44	112.63
82	RM	202	PEB	CHA-C1B-NB	-2.58	119.53	124.93
87	a6	609	CLA	C3B-C4B-NB	-2.58	108.12	110.52
82	XM	201	PEB	C1B-C2B-C3B	-2.58	103.54	106.51
82	uF	203	PEB	C3B-C4B-NB	2.58	113.81	110.05
82	gJ	202	PEB	C3B-C4B-NB	2.58	113.81	110.05
82	FA	202	PEB	C1C-NC-C4C	-2.58	105.00	109.60
82	HF	201	PEB	OD-C4D-C3D	-2.58	123.60	129.46
82	c4	202	PEB	C3C-C4C-NC	2.58	110.66	108.33
82	D1	1002	PEB	C2A-C1A-NA	2.58	110.50	108.27
82	LQ	203	PEB	C1C-CHB-C4B	2.58	134.08	128.28
87	AN	820	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
91	d6	404	PHO	O2D-CGD-O1D	-2.58	118.78	123.84
85	FL	101	BCR	C37-C22-C23	2.58	122.15	118.08
87	cL	510	CLA	CMB-C2B-C1B	-2.58	121.43	125.37
82	OM	202	PEB	CHB-C4B-NB	-2.58	119.20	124.58
82	dD	401	PEB	CAC-C2C-C3C	2.58	132.99	127.07
82	oF	202	PEB	C4C-C3C-C2C	-2.58	105.11	107.50
82	sF	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
82	hK	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
84	DE	1001	CYC	CAB-C3B-C2B	2.58	131.95	127.53
82	PD	201	PEB	C3B-C4B-NB	2.58	113.81	110.05
82	R9	201	PEB	OD-C4D-ND	-2.58	122.10	125.93
82	jO	201	PEB	OD-C4D-ND	-2.58	122.10	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jK	201	PEB	CHA-C1B-C2B	2.58	131.54	124.90
82	AD	301	PEB	CHB-C1C-NC	-2.58	119.40	125.32
83	yK	303	PUB	CHB-C4B-C3B	-2.58	121.32	127.15
82	R4	203	PEB	C3B-C4B-NB	2.58	113.81	110.05
82	LA	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
82	B7	203	PEB	C2A-C1A-NA	2.58	110.50	108.27
82	WF	202	PEB	OA-C1A-C2A	-2.58	124.12	126.17
82	gF	201	PEB	C4C-C3C-C2C	-2.58	105.12	107.50
82	KF	203	PEB	CHC-C4C-NC	2.58	124.64	121.15
82	PA	202	PEB	CAC-CBC-CGC	-2.58	108.04	113.60
82	mG	202	PEB	CMB-C2B-C1B	2.58	129.04	125.06
82	YO	201	PEB	C1B-C2B-C3B	-2.58	103.54	106.51
82	SA	201	PEB	C4B-C3B-C2B	-2.58	103.92	106.78
82	RD	201	PEB	CAB-C3B-C4B	2.58	129.58	125.01
82	I9	202	PEB	CAB-C3B-C4B	2.58	129.58	125.01
82	J9	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
87	3N	306	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
96	G2	201	HEM	C3C-C2C-C1C	2.58	109.54	107.08
92	b6	624	LMG	C9-C8-C7	-2.58	105.68	111.79
92	jL	101	LMG	O8-C28-C29	2.58	120.01	111.91
82	SI	202	PEB	OD-C4D-ND	-2.58	122.10	125.93
82	U4	202	PEB	OD-C4D-ND	-2.58	122.10	125.93
82	RH	202	PEB	CAC-CBC-CGC	-2.58	108.05	113.60
82	lM	203	PEB	C1C-CHB-C4B	-2.58	122.49	128.28
82	OI	202	PEB	CHC-C1D-ND	2.58	116.99	113.72
82	AQ	301	PEB	CHB-C1C-NC	-2.58	119.40	125.32
82	lH	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
82	UD	201	PEB	CHC-C4C-NC	2.58	124.64	121.15
82	bP	502	PEB	C3C-C4C-NC	2.58	110.66	108.33
87	AN	832	CLA	CHB-C4A-NA	2.58	128.08	124.51
87	A2	828	CLA	CHB-C4A-NA	2.58	128.08	124.51
103	82	310	ZEX	O3-C3-C2	-2.58	104.67	109.80
82	C7	201	PEB	C4B-C3B-C2B	-2.58	103.92	106.78
82	RE	201	PEB	C2A-C1A-NA	2.58	110.50	108.27
82	TB	201	PEB	CMA-C2A-C1A	-2.58	106.84	112.40
82	mO	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	e1	202	PEB	OA-C1A-C2A	-2.58	124.12	126.17
82	M5	305	PEB	C2B-C1B-NB	2.58	116.04	110.53
85	CL	516	BCR	C33-C5-C4	2.58	118.58	113.62
82	SM	203	PEB	CMB-C2B-C1B	2.58	129.04	125.06
82	PJ	201	PEB	CAB-CBB-CGB	-2.58	108.05	113.60
84	73	1002	CYC	C2D-C1D-ND	2.58	111.03	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OD	202	PEB	CHC-C4C-NC	2.58	124.64	121.15
82	IP	201	PEB	CHB-C4B-C3B	-2.58	119.35	125.32
82	FJ	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	K9	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
87	AN	815	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
82	U1	203	PEB	C1C-CHB-C4B	-2.58	122.49	128.28
82	h1	202	PEB	CMB-C2B-C1B	2.58	129.04	125.06
85	AL	401	BCR	C20-C19-C18	-2.58	119.17	126.42
85	B2	842	BCR	C1-C6-C5	-2.58	118.98	122.61
87	2N	303	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
82	JH	1002	PEB	C4C-C3C-C2C	-2.58	105.12	107.50
83	KA	203	PUB	CHB-C4B-NB	-2.58	119.41	125.32
82	YG	201	PEB	CMA-C2A-C1A	-2.58	106.84	112.40
82	X9	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
82	cE	202	PEB	C3B-C4B-NB	2.58	113.80	110.05
82	lG	201	PEB	C3B-C4B-NB	2.58	113.80	110.05
85	cL	504	BCR	C36-C18-C19	-2.58	114.01	118.08
82	OD	202	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
82	JK	202	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
82	QM	204	PEB	C1D-CHC-C4C	-2.58	109.45	113.26
82	aE	202	PEB	CAC-CBC-CGC	-2.58	108.05	113.60
82	BF	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
87	aL	605	CLA	CHB-C4A-NA	2.58	128.08	124.51
87	6N	603	CLA	CHB-C4A-NA	2.58	128.08	124.51
82	OG	203	PEB	CAB-C3B-C4B	2.58	129.57	125.01
82	V9	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
82	TI	203	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	E9	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	QQ	202	PEB	CAC-C2C-C1C	2.58	129.87	125.76
82	UB	302	PEB	C4C-C3C-C2C	-2.58	105.12	107.50
82	IF	201	PEB	C4C-C3C-C2C	-2.58	105.12	107.50
85	L2	201	BCR	C10-C11-C12	-2.58	115.17	123.22
82	ZG	202	PEB	CHA-C1B-C2B	2.58	131.53	124.90
87	A2	838	CLA	O2D-CGD-CBD	2.58	115.85	111.27
82	DO	1002	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
82	gH	201	PEB	CHC-C4C-NC	2.58	124.64	121.15
87	62	309	CLA	C3B-C4B-NB	-2.58	108.12	110.52
82	u8	203	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
85	JN	102	BCR	C23-C22-C21	-2.58	114.98	118.94
82	AH	301	PEB	C3B-C4B-NB	2.58	113.80	110.05
82	fJ	203	PEB	C3B-C4B-NB	2.58	113.80	110.05
82	YP	503	PEB	CMB-C2B-C1B	2.58	129.04	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lM	202	PEB	CAA-C3A-C2A	-2.58	107.81	114.26
82	cB	403	PEB	CAC-CBC-CGC	-2.58	108.05	113.60
82	VM	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
87	A2	831	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
87	L2	203	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
87	BL	620	CLA	CHB-C4A-NA	2.58	128.08	124.51
82	YG	202	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
87	C6	511	CLA	C1-C2-C3	-2.58	121.58	126.04
82	B9	201	PEB	O2B-CGB-CBB	2.58	122.31	114.03
82	AI	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	D7	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
83	wF	304	PUB	CHB-C1C-C2C	-2.58	119.35	125.32
82	VG	202	PEB	C3B-C4B-NB	2.58	113.80	110.05
82	xC	201	PEB	C3B-C4B-NB	2.58	113.80	110.05
82	aO	203	PEB	OD-C4D-C3D	-2.58	123.62	129.46
94	DL	401	PL9	C11-C12-C13	-2.58	103.41	111.88
82	RM	201	PEB	CHB-C1C-C2C	-2.58	121.33	127.15
82	NA	202	PEB	CHB-C4B-C3B	-2.58	119.35	125.32
83	YA	302	PUB	CAC-CBC-CGC	-2.58	108.06	113.60
82	S1	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	DE	1002	PEB	CAA-C3A-C4A	-2.58	106.05	112.67
82	D7	203	PEB	C3C-C4C-NC	2.58	110.65	108.33
82	CB	201	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
82	dQ	401	PEB	CAC-C2C-C3C	2.58	132.97	127.07
82	CF	203	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
82	O4	201	PEB	CHB-C4B-NB	2.58	129.94	124.58
87	1N	604	CLA	CAA-C2A-C3A	-2.58	107.82	114.26
82	YE	201	PEB	CMA-C2A-C1A	-2.58	106.85	112.40
91	D6	404	PHO	CMA-C3A-C4A	-2.58	108.73	114.38
82	hB	301	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	fE	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	cO	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
87	22	603	CLA	CHB-C4A-NA	2.58	128.08	124.51
87	A2	832	CLA	CHB-C4A-NA	2.58	128.08	124.51
82	TA	202	PEB	CMB-C2B-C1B	2.58	129.03	125.06
82	NQ	204	PEB	CMB-C2B-C1B	2.58	129.03	125.06
82	OE	203	PEB	CAB-C3B-C4B	2.58	129.57	125.01
87	AN	823	CLA	CMB-C2B-C3B	2.58	132.83	126.59
82	EP	201	PEB	CHC-C1D-ND	-2.58	110.46	113.72
82	RH	201	PEB	CHB-C4B-C3B	-2.58	119.36	125.32
82	mM	202	PEB	CAC-C2C-C1C	2.58	129.87	125.76
83	AM	304	PUB	CAB-C3B-C4B	2.58	129.87	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	c6	611	CLA	CHB-C1B-NB	2.58	126.98	124.26
82	c4	203	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	mG	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	kM	201	PEB	CAB-C3B-C4B	2.58	129.57	125.01
82	WP	202	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
82	oF	202	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
87	62	305	CLA	C4D-C3D-CAD	-2.58	105.06	108.10
87	42	604	CLA	C1D-CHD-C4C	2.58	131.62	126.06
95	CL	520	DGD	O5D-C6D-C5D	2.58	113.81	109.05
82	CI	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	EI	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	ND	204	PEB	CMB-C2B-C1B	2.58	129.03	125.06
85	BL	617	BCR	C34-C9-C10	-2.58	119.31	122.92
87	AN	820	CLA	C2A-C1A-CHA	2.58	128.36	123.86
82	F5	201	PEB	CHA-C1B-NB	-2.58	119.54	124.93
87	AN	801	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
82	WE	203	PEB	CAC-C2C-C1C	2.58	129.87	125.76
82	TA	201	PEB	CHA-C1B-C2B	2.58	131.53	124.90
82	L1	1002	PEB	CAB-CBB-CGB	-2.58	108.06	113.60
83	AJ	303	PUB	CAC-CBC-CGC	-2.58	108.06	113.60
82	UB	302	PEB	CHB-C1C-C2C	-2.58	121.34	127.15
88	ML	102	LHG	O8-C23-C24	2.58	119.99	111.91
82	Q1	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	bE	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
87	CL	518	CLA	CHB-C4A-NA	2.58	128.07	124.51
87	62	304	CLA	CHB-C4A-NA	2.58	128.07	124.51
87	6N	604	CLA	C4D-C3D-CAD	-2.58	105.06	108.10
82	E7	201	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
82	V4	201	PEB	CAB-CBB-CGB	-2.58	108.06	113.60
82	j1	201	PEB	OA-C1A-C2A	-2.58	124.12	126.17
87	A2	820	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
82	FH	1002	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	TK	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	O9	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
82	ZH	201	PEB	OA-C1A-NA	2.58	128.06	124.94
82	GA	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	lO	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
82	aG	202	PEB	CAC-CBC-CGC	-2.58	108.06	113.60
82	QH	202	PEB	C2A-C1A-NA	2.58	110.49	108.27
82	AJ	302	PEB	C2A-C1A-NA	2.58	110.49	108.27
82	SF	203	PEB	CHC-C4C-NC	2.58	124.63	121.15
82	R1	201	PEB	CHB-C4B-C3B	-2.57	119.36	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	hL	101	DGD	C3G-O3G-C1D	-2.57	108.71	113.74
83	AH	303	PUB	CHA-C4A-NA	-2.57	110.47	113.72
82	dG	202	PEB	C4C-C3C-C2C	-2.57	105.12	107.50
82	BK	201	PEB	CAB-C3B-C4B	2.57	129.56	125.01
84	EG	1001	CYC	CMB-C2B-C1B	2.57	127.38	124.17
82	fJ	201	PEB	CHB-C1C-C2C	-2.57	121.34	127.15
87	B2	834	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
87	bL	614	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
82	RJ	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
82	qF	201	PEB	OD-C4D-C3D	-2.57	123.63	129.46
82	OO	201	PEB	C4B-C3B-C2B	-2.57	103.93	106.78
82	QD	202	PEB	OD-C4D-ND	-2.57	122.12	125.93
82	V9	201	PEB	OD-C4D-ND	-2.57	122.12	125.93
87	cL	515	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
83	AJ	304	PUB	C2C-C1C-NC	2.57	113.79	110.05
87	5N	607	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
87	62	303	CLA	CHB-C4A-NA	2.57	128.07	124.51
82	gF	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
82	qF	201	PEB	CBA-CAA-C3A	2.57	119.20	113.47
82	ID	202	PEB	C3C-C4C-NC	2.57	110.65	108.33
83	YA	302	PUB	C1B-C2B-C3B	-2.57	105.12	107.50
82	VF	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
82	TA	203	PEB	CMA-C2A-C1A	-2.57	106.86	112.40
82	QJ	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
82	fM	201	PEB	OD-C4D-C3D	-2.57	123.63	129.46
87	A2	823	CLA	CMB-C2B-C3B	2.57	132.82	126.59
87	HL	102	CLA	C3B-C4B-NB	-2.57	108.13	110.52
82	K9	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
82	sC	201	PEB	CHA-C4A-NA	2.57	128.26	125.20
82	m4	202	PEB	OD-C4D-ND	-2.57	122.12	125.93
82	TI	201	PEB	C2B-C1B-NB	2.57	116.02	110.53
82	cB	403	PEB	CAB-CBB-CGB	-2.57	108.07	113.60
82	tF	201	PEB	CHA-C1B-NB	-2.57	119.55	124.93
82	cM	201	PEB	CHA-C1B-NB	-2.57	119.55	124.93
82	GK	202	PEB	C4C-C3C-C2C	-2.57	105.13	107.50
82	l1	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
82	RQ	201	PEB	CAB-C3B-C4B	2.57	129.56	125.01
82	eF	203	PEB	CHB-C1C-C2C	-2.57	121.35	127.15
84	DE	1001	CYC	C4D-CHA-C1A	2.57	134.05	128.28
95	C6	503	DGD	O1G-C1A-O1A	-2.57	117.10	123.59
82	KE	201	PEB	CAC-C2C-C1C	2.57	129.86	125.76
82	P7	202	PEB	CAC-C2C-C1C	2.57	129.86	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	A1	301	PEB	C3B-C4B-NB	2.57	113.79	110.05
82	B7	203	PEB	CAB-CBB-CGB	-2.57	108.07	113.60
87	c6	607	CLA	CHB-C4A-NA	2.57	128.07	124.51
82	DD	201	PEB	CHA-C1B-NB	-2.57	119.55	124.93
82	RH	201	PEB	CHA-C1B-NB	-2.57	119.55	124.93
82	XK	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
84	H1	1001	CYC	OB-C4B-C3B	-2.57	125.25	128.04
82	S7	201	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
82	DA	203	PEB	C3C-C4C-NC	2.57	110.65	108.33
82	G9	201	PEB	OD-C4D-ND	-2.57	122.12	125.93
83	xF	305	PUB	OD-C4D-ND	-2.57	122.12	125.93
87	A2	820	CLA	C2A-C1A-CHA	2.57	128.35	123.86
82	NA	201	PEB	CHA-C1B-C2B	2.57	131.51	124.90
82	QP	203	PEB	CAC-CBC-CGC	-2.57	108.07	113.60
82	XA	202	PEB	CHA-C4A-NA	2.57	128.26	125.20
83	AO	303	PUB	C2C-C1C-NC	2.57	113.79	110.05
82	B7	201	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
87	cL	505	CLA	C3B-C4B-NB	-2.57	108.13	110.52
87	2N	307	CLA	CHB-C4A-NA	2.57	128.07	124.51
82	M5	301	PEB	CHC-C1D-ND	-2.57	110.47	113.72
92	bL	611	LMG	O8-C9-C8	2.57	115.92	108.43
82	b1	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
82	RE	202	PEB	CHA-C1B-NB	-2.57	119.56	124.93
82	YE	202	PEB	CHA-C1B-NB	-2.57	119.56	124.93
82	WH	203	PEB	C2A-C1A-NA	2.57	110.49	108.27
84	73	1002	CYC	CAA-C2A-C1A	2.57	129.56	125.01
82	jJ	202	PEB	C1D-CHC-C4C	2.57	117.05	113.26
82	gM	202	PEB	CMB-C2B-C1B	2.57	129.02	125.06
82	C7	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
87	A2	851	CLA	C2D-C1D-ND	-2.57	108.21	110.10
87	4N	606	CLA	C2D-C1D-ND	-2.57	108.21	110.10
82	lO	201	PEB	CHB-C1C-C2C	-2.57	121.35	127.15
84	E4	1001	CYC	CHA-C4D-C3D	-2.57	121.35	127.15
82	VI	202	PEB	OD-C4D-ND	-2.57	122.12	125.93
82	P9	201	PEB	OD-C4D-ND	-2.57	122.12	125.93
87	K2	106	CLA	CHA-C1A-NA	-2.57	120.51	126.40
88	aL	607	LHG	O8-C23-C24	2.57	119.97	111.91
84	GG	1001	CYC	CMB-C2B-C1B	2.57	127.38	124.17
82	E7	202	PEB	C1D-CHC-C4C	-2.57	109.47	113.26
82	XQ	201	PEB	CMB-C2B-C1B	2.57	129.02	125.06
82	jO	201	PEB	C2A-C1A-NA	2.57	110.49	108.27
82	MB	202	PEB	C2A-C1A-NA	-2.57	106.06	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gK	203	PEB	C1C-CHB-C4B	2.57	134.04	128.28
82	R1	202	PEB	CAC-CBC-CGC	-2.57	108.07	113.60
82	W5	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
82	mE	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
85	c6	602	BCR	C36-C18-C19	2.57	122.12	118.08
87	4N	608	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
95	L6	102	DGD	O1G-C1A-C2A	2.57	119.97	111.91
82	TM	201	PEB	CHB-C4B-NB	-2.57	119.23	124.58
82	RF	201	PEB	CAB-CBB-CGB	-2.57	108.08	113.60
82	mO	201	PEB	CAB-CBB-CGB	-2.57	108.08	113.60
84	JH	1003	CYC	CAD-C3D-C4D	2.57	129.85	125.76
82	OJ	201	PEB	CHB-C1C-C2C	-2.57	121.36	127.15
84	HH	1001	CYC	OB-C4B-C3B	-2.57	125.25	128.04
82	B5	203	PEB	OD-C4D-ND	-2.57	122.12	125.93
91	a6	613	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
82	dQ	401	PEB	OD-C4D-C3D	-2.57	123.64	129.46
82	XF	203	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
82	FI	201	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
82	dF	202	PEB	C3B-C4B-NB	2.57	113.78	110.05
82	xF	303	PEB	C2A-C1A-NA	2.57	110.49	108.27
96	vL	201	HEM	CMB-C2B-C1B	-2.57	121.13	125.04
82	B5	201	PEB	O2B-CGB-CBB	2.57	122.28	114.03
82	cH	202	PEB	CAC-C2C-C1C	2.57	129.85	125.76
82	T7	201	PEB	CHA-C1B-C2B	2.57	131.50	124.90
82	qK	203	PEB	C4C-C3C-C2C	-2.57	105.13	107.50
87	KN	105	CLA	CHA-C1A-NA	-2.57	120.52	126.40
87	BL	620	CLA	O2D-CGD-CBD	2.57	115.83	111.27
82	GJ	202	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
82	l1	202	PEB	C1D-CHC-C4C	2.57	117.04	113.26
82	ZJ	202	PEB	CAC-C2C-C1C	2.57	129.85	125.76
87	HL	101	CLA	CHB-C1B-NB	2.57	126.97	124.26
82	ZH	202	PEB	CHB-C1C-C2C	-2.57	121.36	127.15
84	KG	202	CYC	CMB-C2B-C1B	2.57	127.37	124.17
82	uC	201	PEB	CHB-C1C-NC	-2.57	119.44	125.32
82	iH	202	PEB	OA-C1A-NA	2.57	128.05	124.94
84	IE	1001	CYC	C4D-CHA-C1A	2.57	134.04	128.28
82	Y5	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
82	eO	201	PEB	CHC-C4C-NC	2.57	124.62	121.15
82	lE	201	PEB	C3B-C4B-NB	2.57	113.78	110.05
82	qK	203	PEB	CHA-C4A-NA	2.57	128.26	125.20
82	aK	201	PEB	C3C-C4C-NC	2.57	110.64	108.33
82	B5	201	PEB	CMA-C2A-C1A	-2.57	106.87	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KJ	203	PEB	C1C-NC-C4C	-2.57	105.03	109.60
82	EJ	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
82	d4	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
82	UB	301	PEB	OD-C4D-ND	-2.57	122.13	125.93
82	LQ	202	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
82	YO	201	PEB	CHA-C1B-NB	-2.57	119.56	124.93
82	RQ	203	PEB	C1D-CHC-C4C	2.57	117.04	113.26
87	AN	820	CLA	O2A-CGA-O1A	-2.57	117.12	123.59
82	V1	201	PEB	CHC-C1D-ND	-2.57	110.48	113.72
82	J5	203	PEB	C4C-C3C-C2C	-2.57	105.13	107.50
87	A6	404	CLA	CHB-C4A-NA	2.57	128.06	124.51
82	F5	203	PEB	OD-C4D-C3D	-2.57	123.65	129.46
82	S9	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
82	eO	201	PEB	OD-C4D-C3D	-2.57	123.65	129.46
82	OB	201	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
87	4N	604	CLA	C2B-C1B-NB	2.57	111.95	110.23
91	d6	404	PHO	O2A-CGA-CBA	2.57	119.96	111.91
87	12	609	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
82	u8	201	PEB	CHB-C1C-NC	-2.57	119.44	125.32
84	L1	1001	CYC	CHB-C4A-NA	-2.57	119.57	124.93
82	dM	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
87	12	608	CLA	CMD-C2D-C1D	2.57	129.23	124.71
82	AO	301	PEB	CHC-C1D-ND	-2.57	110.48	113.72
82	QD	201	PEB	CBA-CAA-C3A	-2.57	107.76	113.47
87	AN	816	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
82	kH	202	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
84	DG	1001	CYC	CAA-C2A-C1A	2.56	129.55	125.01
82	UA	202	PEB	C4C-C3C-C2C	-2.56	105.13	107.50
82	OQ	202	PEB	C1B-C2B-C3B	-2.56	103.56	106.51
82	JJ	202	PEB	CHC-C4C-NC	2.56	124.62	121.15
82	B5	203	PEB	C3C-C4C-NC	2.56	110.64	108.33
82	WJ	202	PEB	CMC-C3C-C4C	-2.56	124.34	127.06
82	kE	202	PEB	OD-C4D-ND	-2.56	122.13	125.93
82	T7	203	PEB	CMA-C2A-C1A	-2.56	106.88	112.40
82	c1	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
82	MP	201	PEB	CHC-C1D-ND	-2.56	110.48	113.72
87	B2	836	CLA	C2A-C1A-CHA	2.56	128.34	123.86
82	DI	201	PEB	CHB-C1C-C2C	2.56	132.94	127.15
87	8N	301	CLA	C2B-C1B-NB	2.56	111.95	110.23
82	NA	201	PEB	C3B-C4B-NB	2.56	113.78	110.05
96	GN	201	HEM	C3C-C2C-C1C	2.56	109.52	107.08
82	j4	202	PEB	CHC-C4C-NC	2.56	124.62	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ZH	203	PEB	C1C-CHB-C4B	-2.56	122.53	128.28
82	c1	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
82	dB	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
87	62	309	CLA	C3D-C4D-ND	2.56	114.39	110.24
82	T9	202	PEB	CAB-C3B-C4B	2.56	129.54	125.01
82	L5	203	PEB	CMC-C3C-C4C	2.56	129.78	127.06
87	12	602	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
82	WB	401	PEB	OD-C4D-C3D	-2.56	123.65	129.46
82	PG	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
82	J9	202	PEB	C3C-C4C-NC	2.56	110.64	108.33
82	eG	202	PEB	C3C-C4C-NC	2.56	110.64	108.33
82	N7	201	PEB	CHA-C1B-C2B	2.56	131.49	124.90
82	FO	1002	PEB	CAB-CBB-CGB	-2.56	108.09	113.60
82	D9	203	PEB	CAB-C3B-C4B	2.56	129.54	125.01
91	A6	407	PHO	O1D-CGD-CBD	-2.56	120.47	124.74
82	WM	203	PEB	CHB-C4B-C3B	-2.56	119.39	125.32
82	mG	202	PEB	CHB-C4B-C3B	-2.56	119.39	125.32
82	xC	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
82	Y9	201	PEB	CAA-C3A-C4A	-2.56	106.09	112.67
87	AN	830	CLA	O2D-CGD-CBD	2.56	115.82	111.27
83	Y7	302	PUB	CAC-CBC-CGC	-2.56	108.09	113.60
82	OP	203	PEB	OD-C4D-C3D	-2.56	123.65	129.46
82	VM	202	PEB	CAB-C3B-C4B	2.56	129.54	125.01
87	c6	615	CLA	C1-C2-C3	-2.56	121.61	126.04
82	JI	201	PEB	CHC-C4C-NC	2.56	124.62	121.15
82	eH	202	PEB	CHC-C4C-NC	2.56	124.62	121.15
82	j4	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
82	A9	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
82	T9	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
82	kK	202	PEB	OD-C4D-ND	-2.56	122.13	125.93
82	uC	203	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
82	mO	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
84	IG	1001	CYC	C4D-CHA-C1A	2.56	134.03	128.28
82	CQ	202	PEB	OD-C4D-ND	-2.56	122.14	125.93
82	pF	202	PEB	CHC-C4C-NC	2.56	124.62	121.15
82	IK	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
82	RM	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
84	73	1002	CYC	CHD-C1D-C2D	-2.56	121.20	127.49
82	N1	1002	PEB	CHB-C1C-C2C	-2.56	121.37	127.15
82	eE	202	PEB	C3B-C4B-NB	2.56	113.78	110.05
87	B6	611	CLA	CHB-C4A-NA	2.56	128.05	124.51
87	cL	506	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	J1	1001	CYC	C1A-C2A-C3A	-2.56	103.95	106.78
82	FP	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
82	LP	202	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
82	gG	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
82	hF	201	PEB	C3C-C4C-NC	2.56	110.64	108.33
87	AN	838	CLA	O2D-CGD-CBD	2.56	115.82	111.27
82	ID	201	PEB	CHB-C1C-C2C	2.56	132.93	127.15
82	GD	202	PEB	CBC-CAC-C2C	2.56	119.74	112.63
82	uK	202	PEB	C3B-C4B-NB	2.56	113.77	110.05
82	U4	201	PEB	C1C-NC-C4C	-2.56	105.04	109.60
82	lM	201	PEB	CHA-C1B-NB	-2.56	119.58	124.93
82	PH	201	PEB	CHB-C4B-C3B	-2.56	119.39	125.32
82	gK	202	PEB	C4C-C3C-C2C	-2.56	105.14	107.50
82	V7	201	PEB	OD-C4D-ND	-2.56	122.14	125.93
85	K2	105	BCR	C33-C5-C6	-2.56	121.65	124.53
82	kH	203	PEB	C3B-C4B-NB	2.56	113.77	110.05
87	BN	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
87	B6	612	CLA	CHB-C4A-NA	2.56	128.05	124.51
82	WG	203	PEB	CAC-C2C-C1C	2.56	129.84	125.76
87	A2	815	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
85	BN	841	BCR	C36-C18-C19	2.56	122.11	118.08
82	m4	203	PEB	CAB-C3B-C2B	2.56	132.65	127.88
82	EP	203	PEB	CAC-CBC-CGC	-2.56	108.09	113.60
82	e4	202	PEB	C4C-C3C-C2C	-2.56	105.14	107.50
82	cK	202	PEB	C4C-C3C-C2C	-2.56	105.14	107.50
87	BL	619	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
82	EP	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
82	L9	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
82	PQ	201	PEB	C3C-C4C-NC	2.56	110.64	108.33
82	NP	202	PEB	C2A-C1A-NA	2.56	110.48	108.27
82	iH	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
82	mF	201	PEB	CMC-C3C-C4C	2.56	129.77	127.06
87	42	606	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
82	UA	202	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
82	U7	202	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
82	IJ	203	PEB	C3B-C4B-NB	2.56	113.77	110.05
87	cL	507	CLA	C2A-C1A-CHA	2.56	128.33	123.86
87	4N	603	CLA	CMB-C2B-C3B	2.56	132.78	126.59
82	jM	202	PEB	CMB-C2B-C1B	2.56	129.00	125.06
82	aH	202	PEB	OD-C4D-ND	-2.56	122.14	125.93
85	BN	839	BCR	C1-C6-C5	-2.56	119.01	122.61
87	LN	203	CLA	CHD-C1D-ND	-2.56	122.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CA	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
82	JA	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
82	OE	201	PEB	CHC-C4C-NC	2.56	124.61	121.15
83	xF	301	PUB	CHA-C4A-NA	-2.56	110.49	113.72
82	N7	201	PEB	C3B-C4B-NB	2.56	113.77	110.05
92	AL	411	LMG	O8-C28-C29	2.56	119.94	111.91
87	BL	621	CLA	C4-C3-C5	2.56	119.57	115.27
87	6N	602	CLA	C3B-C4B-NB	-2.56	108.14	110.52
82	jK	202	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
82	dO	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
87	AN	831	CLA	CHB-C4A-NA	2.56	128.05	124.51
82	WI	202	PEB	C1C-NC-C4C	-2.56	105.05	109.60
82	b4	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
82	ZE	201	PEB	CAC-CBC-CGC	-2.56	108.10	113.60
82	uK	202	PEB	CHA-C4A-NA	2.56	128.25	125.20
83	AM	303	PUB	CHB-C4B-NB	-2.56	119.46	125.32
82	ZE	202	PEB	CHA-C1B-C2B	2.56	131.48	124.90
82	vC	202	PEB	CHB-C4B-C3B	2.56	131.23	125.32
82	SH	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
95	C6	521	DGD	O1G-C1A-C2A	2.56	119.93	111.91
82	BI	203	PEB	OD-C4D-ND	-2.56	122.14	125.93
82	i1	202	PEB	CMC-C3C-C4C	2.56	129.77	127.06
82	B5	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
82	mG	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
87	A2	839	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
82	AG	301	PEB	CHA-C1B-NB	-2.56	119.58	124.93
82	OP	201	PEB	C1C-NC-C4C	2.56	114.15	109.60
83	QJ	201	PUB	C1D-CHC-C4C	-2.56	107.81	113.37
82	M5	304	PEB	CHC-C1D-ND	-2.56	110.49	113.72
82	g1	201	PEB	C1C-CHB-C4B	2.56	134.01	128.28
82	H9	202	PEB	C1C-CHB-C4B	2.56	134.01	128.28
82	R7	202	PEB	CHB-C1C-NC	2.56	131.18	125.32
87	BN	825	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
87	J2	101	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
82	Y4	201	PEB	CHA-C1B-NB	-2.56	119.59	124.93
82	UQ	202	PEB	CMC-C3C-C4C	2.56	129.77	127.06
82	YG	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
82	JK	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
82	Q5	203	PEB	OD-C4D-C3D	-2.56	123.67	129.46
82	PQ	202	PEB	C1C-CHB-C4B	2.56	134.01	128.28
82	PO	203	PEB	CMB-C2B-C1B	2.56	129.00	125.06
87	2N	307	CLA	O2D-CGD-O1D	-2.56	118.84	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BQ	201	PEB	OD-C4D-ND	-2.56	122.14	125.93
82	w8	203	PEB	OD-C4D-ND	-2.56	122.14	125.93
82	A7	202	PEB	C3C-C4C-NC	2.56	110.63	108.33
82	d1	202	PEB	CMA-C2A-C1A	-2.56	106.89	112.40
82	H1	1002	PEB	CHA-C1B-C2B	2.56	131.47	124.90
87	2N	304	CLA	CHB-C4A-NA	2.56	128.05	124.51
82	DF	202	PEB	CBD-CAD-C3D	-2.56	114.91	127.62
82	KD	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
82	fM	203	PEB	OD-C4D-C3D	-2.56	123.67	129.46
82	WI	203	PEB	CAC-C2C-C1C	2.56	129.83	125.76
82	Y7	301	PEB	CHB-C4B-NB	-2.56	119.26	124.58
82	P7	203	PEB	C1C-CHB-C4B	2.56	134.01	128.28
82	cM	202	PEB	C2A-C1A-NA	2.56	110.48	108.27
82	IJ	201	PEB	C1D-CHC-C4C	-2.56	109.49	113.26
82	H4	1002	PEB	CAC-CBC-CGC	-2.56	108.10	113.60
82	HI	202	PEB	C2B-C1B-NB	2.56	115.98	110.53
87	12	606	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
84	E4	1001	CYC	CMB-C2B-C1B	2.56	127.36	124.17
84	EG	1001	CYC	C4A-C3A-C2A	-2.56	103.57	106.51
82	M7	201	PEB	C3B-C4B-NB	2.56	113.77	110.05
82	L7	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
82	KA	202	PEB	C4C-C3C-C2C	-2.56	105.14	107.50
82	P4	202	PEB	C4C-C3C-C2C	-2.56	105.14	107.50
82	K7	202	PEB	C4C-C3C-C2C	-2.56	105.14	107.50
82	jM	202	PEB	OD-C4D-ND	-2.56	122.14	125.93
82	DJ	202	PEB	CAC-C2C-C1C	2.55	129.83	125.76
87	O2	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
82	P1	201	PEB	CAB-CBB-CGB	-2.55	108.11	113.60
82	P7	202	PEB	CAC-CBC-CGC	-2.55	108.11	113.60
82	f1	203	PEB	CHA-C1B-NB	-2.55	119.59	124.93
82	a4	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
82	hF	201	PEB	OD-C4D-C3D	-2.55	123.67	129.46
82	bH	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
87	L2	204	CLA	C3B-C4B-NB	-2.55	108.14	110.52
82	cB	403	PEB	CHC-C4C-NC	2.55	124.61	121.15
82	BD	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
82	KD	202	PEB	OD-C4D-ND	-2.55	122.15	125.93
82	bP	502	PEB	OD-C4D-ND	-2.55	122.15	125.93
82	RM	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
87	A2	815	CLA	CHB-C1B-NB	2.55	126.96	124.26
82	AI	203	PEB	CHC-C1D-ND	2.55	116.96	113.72
82	rK	202	PEB	C1D-CHC-C4C	2.55	117.02	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HQ	201	PEB	C4C-C3C-C2C	-2.55	105.14	107.50
82	ZI	401	PEB	OA-C1A-NA	2.55	128.03	124.94
91	a6	613	PHO	CGD-CBD-CAD	-2.55	102.46	110.73
87	4N	608	CLA	C2D-C1D-ND	-2.55	108.22	110.10
82	l4	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
82	Y5	203	PEB	CHB-C1C-NC	-2.55	119.47	125.32
82	DK	202	PEB	CBD-CAD-C3D	-2.55	114.92	127.62
87	4N	604	CLA	C1D-CHD-C4C	2.55	131.56	126.06
87	42	607	CLA	C2A-C1A-CHA	2.55	128.32	123.86
87	B2	822	CLA	CHB-C4A-NA	2.55	128.04	124.51
82	eK	201	PEB	OD-C4D-C3D	-2.55	123.67	129.46
82	FK	201	PEB	CMA-C2A-C1A	-2.55	106.90	112.40
82	IJ	201	PEB	CHA-C1B-NB	-2.55	119.59	124.93
82	fH	203	PEB	CHC-C1D-ND	-2.55	110.49	113.72
87	O2	202	CLA	CHB-C1B-NB	2.55	126.96	124.26
82	AG	304	PEB	C2A-C1A-NA	2.55	110.47	108.27
82	bO	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
87	82	302	CLA	CHD-C1D-ND	-2.55	122.11	124.45
82	RM	201	PEB	CAA-C3A-C4A	2.55	119.23	112.67
87	1N	606	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
87	12	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
87	62	302	CLA	CHB-C4A-NA	2.55	128.04	124.51
87	D6	403	CLA	C3B-C4B-NB	-2.55	108.15	110.52
87	8N	302	CLA	C3B-C4B-NB	-2.55	108.15	110.52
92	bL	611	LMG	C9-C8-C7	-2.55	105.75	111.79
84	JH	1003	CYC	CHB-C4A-NA	-2.55	119.59	124.93
85	cL	503	BCR	C29-C28-C27	2.55	117.08	111.38
82	YE	201	PEB	OD-C4D-C3D	-2.55	123.68	129.46
87	5N	606	CLA	CHB-C4A-NA	2.55	128.04	124.51
82	qF	203	PEB	C4C-C3C-C2C	-2.55	105.14	107.50
82	MD	201	PEB	OA-C1A-C2A	-2.55	124.14	126.17
84	F4	1001	CYC	C2A-C1A-NA	2.55	113.76	110.05
84	EO	1001	CYC	CHA-C4D-C3D	-2.55	121.39	127.15
87	JN	101	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
82	ID	202	PEB	OD-C4D-ND	-2.55	122.15	125.93
82	DJ	201	PEB	CMA-C2A-C1A	-2.55	106.90	112.40
82	dH	202	PEB	CMA-C2A-C1A	-2.55	106.90	112.40
96	v6	201	HEM	CHD-C4C-NC	2.55	127.20	124.44
82	YH	201	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
82	iH	202	PEB	CMC-C3C-C4C	2.55	129.76	127.06
82	N7	203	PEB	CMB-C2B-C1B	2.55	128.99	125.06
82	SM	202	PEB	C3C-C4C-NC	2.55	110.63	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	6N	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
82	VQ	203	PEB	CHB-C4B-NB	-2.55	119.27	124.58
82	AH	302	PEB	OD-C4D-C3D	-2.55	123.68	129.46
84	E1	1001	CYC	CHB-C1B-NB	-2.55	120.58	126.06
82	VO	202	PEB	CAC-CBC-CGC	-2.55	108.11	113.60
82	qK	201	PEB	CBA-CAA-C3A	2.55	119.15	113.47
87	L2	204	CLA	C2D-C1D-ND	-2.55	108.22	110.10
82	GK	203	PEB	CAB-C3B-C2B	-2.55	123.13	127.88
87	A6	403	CLA	C1-C2-C3	-2.55	121.63	126.04
82	O9	203	PEB	CHC-C1D-ND	-2.55	110.50	113.72
82	s8	201	PEB	CHA-C4A-NA	2.55	128.24	125.20
82	LI	202	PEB	CHB-C1C-C2C	-2.55	121.39	127.15
82	JP	202	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
82	Q1	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
82	G9	202	PEB	CAB-C3B-C4B	2.55	129.52	125.01
82	TO	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
82	mG	202	PEB	CAC-C2C-C1C	2.55	129.82	125.76
82	a4	202	PEB	C1C-NC-C4C	-2.55	105.06	109.60
84	C4	1001	CYC	CMB-C2B-C1B	2.55	127.35	124.17
87	BL	621	CLA	CAA-CBA-CGA	-2.55	105.80	113.25
87	62	309	CLA	CAA-C2A-C3A	2.55	119.76	112.78
82	DI	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
82	XB	202	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
83	yK	303	PUB	CAB-C3B-C4B	2.55	129.82	125.76
82	hF	201	PEB	C4C-C3C-C2C	-2.55	105.15	107.50
82	uF	202	PEB	C4C-C3C-C2C	-2.55	105.15	107.50
82	eO	202	PEB	C4C-C3C-C2C	-2.55	105.15	107.50
82	mE	201	PEB	C2A-C1A-NA	2.55	110.47	108.27
82	OK	203	PEB	CHB-C1C-C2C	-2.55	121.40	127.15
88	B6	617	LHG	O8-C23-C24	2.55	119.91	111.91
95	a6	604	DGD	O1G-C1A-C2A	2.55	119.91	111.91
82	DI	202	PEB	CHC-C4C-NC	2.55	124.60	121.15
85	cL	518	BCR	C20-C19-C18	-2.55	119.25	126.42
82	VQ	201	PEB	C3C-C4C-NC	2.55	110.63	108.33
82	LK	201	PEB	C3B-C4B-NB	2.55	113.76	110.05
82	EP	201	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
87	A2	821	CLA	O2D-CGD-CBD	2.55	115.80	111.27
96	VL	201	HEM	CHD-C4C-NC	2.55	127.20	124.44
82	Z9	303	PEB	CHA-C1B-C2B	2.55	131.45	124.90
82	HP	202	PEB	CHC-C1D-ND	-2.55	110.50	113.72
87	b6	612	CLA	CHB-C1B-NB	2.55	126.95	124.26
82	jO	202	PEB	CHC-C4C-NC	2.55	124.60	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	6N	601	CLA	CHB-C4A-NA	2.55	128.04	124.51
82	VQ	202	PEB	C3B-C4B-NB	2.55	113.76	110.05
82	hJ	201	PEB	C3B-C4B-NB	2.55	113.76	110.05
82	L9	203	PEB	CHB-C4B-NB	-2.55	119.27	124.58
87	42	603	CLA	CMB-C2B-C3B	2.55	132.76	126.59
87	AN	813	CLA	C3B-C4B-NB	-2.55	108.15	110.52
87	62	308	CLA	C3B-C4B-NB	-2.55	108.15	110.52
82	QK	202	PEB	OD-C4D-C3D	-2.55	123.69	129.46
85	J2	102	BCR	C23-C22-C21	-2.55	115.03	118.94
82	RA	202	PEB	CHB-C1C-NC	2.55	131.16	125.32
82	YA	301	PEB	CHB-C1C-NC	-2.55	119.48	125.32
82	K5	202	PEB	C3C-C4C-NC	2.55	110.63	108.33
82	N5	202	PEB	C3C-C4C-NC	2.55	110.63	108.33
82	OK	202	PEB	C1C-CHB-C4B	2.55	134.00	128.28
82	EJ	201	PEB	C1C-NC-C4C	-2.55	105.06	109.60
87	62	313	CLA	CHB-C4A-NA	2.55	128.03	124.51
87	A2	831	CLA	CHB-C4A-NA	2.55	128.03	124.51
87	B2	823	CLA	CHB-C4A-NA	2.55	128.03	124.51
87	B6	603	CLA	CHB-C4A-NA	2.55	128.03	124.51
82	VP	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
82	DF	203	PEB	CHB-C1C-NC	-2.55	119.48	125.32
82	J1	1002	PEB	C4C-C3C-C2C	-2.55	105.15	107.50
82	N9	202	PEB	CAB-C3B-C4B	2.55	129.51	125.01
87	42	608	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
91	DL	405	PHO	C4-C3-C5	2.55	119.56	115.27
82	rF	202	PEB	C1D-CHC-C4C	2.55	117.01	113.26
87	A2	802	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
82	VI	201	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
82	z8	201	PEB	OA-C1A-C2A	-2.55	124.15	126.17
82	MF	202	PEB	CMB-C2B-C1B	2.55	128.99	125.06
82	CK	201	PEB	CAC-C2C-C1C	2.55	129.82	125.76
82	PQ	203	PEB	CHB-C1C-NC	-2.55	119.49	125.32
87	42	610	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
87	cL	509	CLA	CMB-C2B-C3B	2.55	132.76	126.59
82	OG	201	PEB	CAC-CBC-CGC	-2.55	108.12	113.60
82	IK	203	PEB	CAC-CBC-CGC	-2.55	108.12	113.60
83	yK	302	PUB	CHB-C4B-C3B	-2.55	121.41	127.15
82	gK	201	PEB	C4C-C3C-C2C	-2.55	105.15	107.50
82	QQ	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
87	42	603	CLA	C3B-C4B-NB	-2.55	108.15	110.52
82	M9	304	PEB	CHA-C1B-C2B	2.55	131.45	124.90
82	Y1	201	PEB	CHA-C4A-NA	2.55	128.23	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	cL	518	BCR	C8-C7-C6	-2.55	120.05	127.20
82	JD	203	PEB	C3C-C4C-NC	2.55	110.62	108.33
82	J5	202	PEB	C3C-C4C-NC	2.55	110.62	108.33
82	QO	201	PEB	OA-C1A-NA	2.55	128.03	124.94
82	dK	202	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
84	IE	1001	CYC	C4A-C3A-C2A	-2.55	103.58	106.51
82	kF	202	PEB	OD-C4D-ND	-2.55	122.16	125.93
82	qC	202	PEB	C3B-C4B-NB	2.55	113.75	110.05
82	tK	202	PEB	C3B-C4B-NB	2.55	113.75	110.05
87	4N	610	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
82	mF	202	PEB	C4C-C3C-C2C	-2.55	105.15	107.50
85	B2	841	BCR	C24-C23-C22	-2.55	122.39	126.23
82	PJ	201	PEB	C1C-CHB-C4B	-2.55	122.57	128.28
82	ZO	201	PEB	C4B-C3B-C2B	-2.55	103.97	106.78
82	S5	201	PEB	CAB-CBB-CGB	-2.55	108.13	113.60
87	5N	603	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
82	LQ	201	PEB	C2A-C1A-NA	2.55	110.47	108.27
82	kG	202	PEB	OD-C4D-ND	-2.54	122.16	125.93
82	UE	201	PEB	CMB-C2B-C1B	2.54	128.98	125.06
87	1N	608	CLA	CMD-C2D-C1D	2.54	129.20	124.71
82	LD	203	PEB	C1C-CHB-C4B	2.54	133.99	128.28
82	DM	202	PEB	OD-C4D-C3D	-2.54	123.69	129.46
82	mH	202	PEB	OD-C4D-C3D	-2.54	123.69	129.46
82	vK	202	PEB	CHB-C4B-C3B	-2.54	119.43	125.32
84	BE	1001	CYC	C1B-NB-C4B	-2.54	107.43	110.67
82	j1	202	PEB	OD-C4D-ND	-2.54	122.16	125.93
85	k6	102	BCR	C4-C5-C6	-2.54	119.04	122.73
82	cJ	201	PEB	CHA-C1B-NB	-2.54	119.61	124.93
82	jK	202	PEB	C4C-C3C-C2C	-2.54	105.15	107.50
82	Z1	202	PEB	CHB-C1C-C2C	-2.54	121.41	127.15
82	kH	201	PEB	CAB-CBB-CGB	-2.54	108.13	113.60
87	1N	602	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
82	WK	202	PEB	CAC-C2C-C3C	2.54	132.90	127.07
82	ZG	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
92	JL	102	LMG	O8-C28-C29	2.54	119.89	111.91
87	8N	303	CLA	C3B-C4B-NB	-2.54	108.16	110.52
82	aK	202	PEB	C1C-CHB-C4B	2.54	133.99	128.28
84	DG	1001	CYC	C4D-CHA-C1A	2.54	133.99	128.28
87	3N	305	CLA	CHB-C1B-C2B	-2.54	120.05	127.24
82	lH	201	PEB	C1D-CHC-C4C	2.54	117.01	113.26
82	F1	1002	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	eB	201	PEB	C3B-C4B-NB	2.54	113.75	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	R5	202	PEB	C3C-C4C-NC	2.54	110.62	108.33
85	B2	839	BCR	C1-C6-C5	-2.54	119.03	122.61
82	u8	201	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
87	AN	837	CLA	CAA-CBA-CGA	-2.54	105.82	113.25
82	U5	203	PEB	C3B-C4B-NB	2.54	113.75	110.05
87	8N	306	CLA	O2A-CGA-O1A	-2.54	116.96	123.30
82	U9	202	PEB	CAB-CBB-CGB	-2.54	108.13	113.60
84	C1	1001	CYC	C2C-C1C-NC	2.54	110.47	108.27
87	32	304	CLA	CHB-C1B-C2B	-2.54	120.06	127.24
82	z8	202	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	w8	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
87	BL	603	CLA	CMD-C2D-C3D	2.54	133.46	127.61
85	b6	602	BCR	C28-C27-C26	-2.54	109.54	114.08
87	AN	815	CLA	CHB-C1B-NB	2.54	126.95	124.26
82	e4	201	PEB	CHC-C4C-NC	2.54	124.59	121.15
85	C6	508	BCR	C2-C1-C6	2.54	114.39	110.48
87	6N	608	CLA	C2B-C1B-NB	2.54	111.94	110.23
82	mJ	201	PEB	CBB-CAB-C3B	2.54	119.69	112.63
82	RF	201	PEB	CMB-C2B-C1B	2.54	128.98	125.06
82	BA	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
83	wK	304	PUB	CHB-C1C-C2C	-2.54	119.44	125.32
87	B2	824	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
87	BN	836	CLA	C2A-C1A-CHA	2.54	128.30	123.86
82	AE	301	PEB	CHA-C1B-NB	-2.54	119.62	124.93
82	BA	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
87	cL	509	CLA	CMC-C2C-C1C	-2.54	121.17	125.04
82	W9	201	PEB	CHB-C1C-NC	-2.54	119.50	125.32
82	ZE	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	cH	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	VA	201	PEB	C4C-C3C-C2C	-2.54	105.16	107.50
82	tF	201	PEB	CAB-CBB-CGB	-2.54	108.14	113.60
87	A2	837	CLA	CAA-CBA-CGA	-2.54	105.83	113.25
82	VD	202	PEB	C3B-C4B-NB	2.54	113.75	110.05
87	6N	610	CLA	C3B-C4B-NB	-2.54	108.16	110.52
82	TF	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	hF	202	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	aK	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
82	lM	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
87	32	305	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
82	TG	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
82	V1	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
82	j4	201	PEB	C2A-C1A-NA	2.54	110.46	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HQ	203	PEB	CBA-CAA-C3A	-2.54	107.81	113.47
82	EK	202	PEB	CAA-C3A-C4A	-2.54	106.15	112.67
82	D5	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
87	MN	101	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
82	HA	203	PEB	C3B-C4B-NB	2.54	113.74	110.05
82	QQ	201	PEB	CBA-CAA-C3A	-2.54	107.81	113.47
82	B9	203	PEB	CHC-C1D-ND	-2.54	110.51	113.72
82	LO	1002	PEB	C1C-CHB-C4B	2.54	133.98	128.28
82	J5	201	PEB	CAC-C2C-C1C	2.54	129.81	125.76
82	gF	203	PEB	OD-C4D-C3D	-2.54	123.71	129.46
82	RH	201	PEB	CHC-C4C-NC	2.54	124.59	121.15
82	fH	201	PEB	OD-C4D-ND	-2.54	122.17	125.93
82	RA	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
82	AD	304	PEB	C3B-C4B-NB	2.54	113.74	110.05
82	zC	201	PEB	OA-C1A-C2A	-2.54	124.15	126.17
82	QD	202	PEB	CAC-C2C-C1C	2.54	129.81	125.76
82	aE	202	PEB	CHB-C4B-NB	-2.54	119.29	124.58
82	B7	201	PEB	CAB-CBB-CGB	-2.54	108.14	113.60
82	GD	202	PEB	CMB-C2B-C1B	2.54	128.97	125.06
87	72	607	CLA	CHB-C4A-NA	2.54	128.02	124.51
94	d6	408	PL9	C45-C44-C46	2.54	119.54	115.27
82	Y7	303	PEB	CAB-C3B-C4B	2.54	129.50	125.01
82	GD	202	PEB	C4C-C3C-C2C	-2.54	105.16	107.50
82	fG	201	PEB	C4C-C3C-C2C	-2.54	105.16	107.50
82	PI	201	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
82	aH	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
82	rK	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
82	UJ	203	PEB	CHA-C1B-NB	-2.54	119.62	124.93
82	B9	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
82	NA	203	PEB	CMB-C2B-C1B	2.54	128.97	125.06
82	DD	201	PEB	CMB-C2B-C1B	2.54	128.97	125.06
87	M2	101	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
82	TB	202	PEB	CHB-C4B-NB	-2.54	119.30	124.58
82	VD	203	PEB	CHB-C4B-NB	-2.54	119.30	124.58
87	AN	820	CLA	CHB-C1B-NB	2.54	126.94	124.26
82	xF	303	PEB	OA-C1A-C2A	-2.54	124.16	126.17
82	EP	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
87	c6	609	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
82	XI	201	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
82	O4	201	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
82	MK	202	PEB	C4C-C3C-C2C	-2.54	105.16	107.50
82	dB	202	PEB	C4C-C3C-C2C	-2.54	105.16	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eK	203	PEB	CHB-C1C-C2C	-2.54	121.42	127.15
82	VA	202	PEB	CHC-C1D-ND	-2.54	110.51	113.72
82	FF	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
82	T4	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
82	A1	305	PEB	CHB-C4B-NB	-2.54	119.30	124.58
82	BI	201	PEB	CMB-C2B-C1B	2.54	128.97	125.06
82	bH	202	PEB	CMB-C2B-C1B	2.54	128.97	125.06
82	eJ	202	PEB	CMB-C2B-C1B	2.54	128.97	125.06
82	R7	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
82	FJ	202	PEB	C2A-C1A-NA	2.54	110.46	108.27
82	nF	202	PEB	OD-C4D-ND	-2.54	122.17	125.93
87	6N	608	CLA	CAA-C2A-C3A	2.54	119.72	112.78
87	22	607	CLA	CHB-C4A-NA	2.54	128.02	124.51
82	EQ	202	PEB	C4C-C3C-C2C	-2.54	105.16	107.50
82	fE	201	PEB	C4C-C3C-C2C	-2.54	105.16	107.50
82	XD	203	PEB	CHC-C4C-NC	2.54	124.58	121.15
82	f1	201	PEB	C3B-C4B-NB	2.54	113.74	110.05
87	A6	404	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
87	4N	601	CLA	C1D-ND-C4D	-2.54	104.53	106.33
82	iM	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
82	NO	1002	PEB	CMD-C2D-C3D	2.54	133.64	130.06
83	NQ	201	PUB	C4A-CHA-C1B	2.54	117.00	113.26
87	22	610	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
87	CL	504	CLA	C3B-C4B-NB	-2.54	108.16	110.52
82	NH	1002	PEB	CHB-C1C-C2C	-2.54	121.43	127.15
82	JF	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
82	cO	203	PEB	OD-C4D-C3D	-2.54	123.71	129.46
95	C6	503	DGD	C3E-C4E-C5E	2.54	114.76	110.24
82	e4	201	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
87	82	305	CLA	O2A-CGA-O1A	-2.54	116.98	123.30
82	q8	202	PEB	C3B-C4B-NB	2.54	113.74	110.05
82	TK	201	PEB	C1C-CHB-C4B	2.54	133.97	128.28
82	gH	201	PEB	C1C-CHB-C4B	2.54	133.97	128.28
82	WG	201	PEB	CHA-C1B-C2B	2.54	131.42	124.90
82	YA	301	PEB	CHB-C4B-NB	-2.54	119.30	124.58
82	TO	201	PEB	CAB-CBB-CGB	-2.54	108.15	113.60
82	OE	203	PEB	C3C-C4C-NC	2.54	110.62	108.33
87	b6	608	CLA	CBA-CAA-C2A	2.54	121.35	113.86
83	AG	302	PUB	CAC-C2C-C1C	2.54	129.49	125.01
85	H6	101	BCR	C27-C26-C25	-2.54	119.05	122.73
82	HQ	201	PEB	C1C-NC-C4C	-2.54	105.09	109.60
82	c1	202	PEB	C3B-C4B-NB	2.54	113.74	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y4	202	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
82	fG	202	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
82	h4	201	PEB	C4B-C3B-C2B	-2.54	103.98	106.78
82	LD	201	PEB	CAB-C3B-C4B	2.53	129.49	125.01
82	mO	203	PEB	CAB-C3B-C2B	2.53	132.60	127.88
87	82	303	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
82	YG	202	PEB	CHA-C1B-NB	-2.53	119.63	124.93
87	7N	607	CLA	CHB-C4A-NA	2.53	128.02	124.51
82	O9	202	PEB	C3C-C4C-NC	2.53	110.61	108.33
82	OK	201	PEB	C3B-C4B-NB	2.53	113.74	110.05
82	FD	202	PEB	C4C-C3C-C2C	-2.53	105.16	107.50
82	B5	203	PEB	C4C-C3C-C2C	-2.53	105.16	107.50
82	MP	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
87	4N	603	CLA	CHB-C1B-NB	2.53	126.94	124.26
82	MJ	201	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
82	PJ	201	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
87	22	605	CLA	CHD-C1D-ND	-2.53	122.12	124.45
84	E4	1001	CYC	C1A-C2A-C3A	-2.53	103.98	106.78
87	A2	829	CLA	C3B-C4B-NB	-2.53	108.16	110.52
82	L7	202	PEB	OA-C1A-NA	2.53	128.01	124.94
82	Y4	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
82	KD	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	dF	201	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	cG	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	HH	1002	PEB	CHA-C1B-C2B	2.53	131.42	124.90
82	k1	201	PEB	CMB-C2B-C1B	2.53	128.97	125.06
82	CF	201	PEB	CAC-C2C-C1C	2.53	129.80	125.76
82	WM	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
82	IA	201	PEB	CAB-CBB-CGB	-2.53	108.15	113.60
82	cG	202	PEB	OD-C4D-ND	-2.53	122.18	125.93
82	KD	201	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
82	AE	304	PEB	C2A-C1A-NA	2.53	110.46	108.27
82	d1	202	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
82	fO	202	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
96	f6	101	HEM	CHA-C4D-ND	2.53	127.50	124.37
82	YH	201	PEB	CHA-C4A-NA	2.53	128.22	125.20
82	AQ	304	PEB	CHA-C4A-NA	-2.53	122.19	125.20
87	KN	105	CLA	CHB-C4A-NA	2.53	128.01	124.51
87	LN	202	CLA	CHB-C4A-NA	2.53	128.01	124.51
82	IQ	201	PEB	CHB-C1C-C2C	2.53	132.87	127.15
87	32	312	CLA	C3B-C4B-NB	-2.53	108.17	110.52
87	B2	809	CLA	C3B-C4B-NB	-2.53	108.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	H6	103	CLA	C3B-C4B-NB	-2.53	108.17	110.52
92	B6	619	LMG	O8-C28-C29	2.53	119.86	111.91
82	eM	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
82	T1	202	PEB	OA-C1A-C2A	-2.53	124.16	126.17
82	RD	201	PEB	OD-C4D-ND	-2.53	122.18	125.93
87	52	610	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
82	zC	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
82	iJ	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
82	fO	201	PEB	CAB-CBB-CGB	-2.53	108.15	113.60
82	jK	202	PEB	CMC-C3C-C4C	2.53	129.75	127.06
87	AL	403	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
87	42	601	CLA	C1D-ND-C4D	-2.53	104.54	106.33
82	YB	201	PEB	CAC-C2C-C1C	2.53	129.79	125.76
82	H9	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
82	P1	201	PEB	CHB-C4B-C3B	-2.53	119.46	125.32
82	T4	203	PEB	CHC-C1D-ND	-2.53	110.52	113.72
82	OP	203	PEB	CAC-C2C-C3C	2.53	132.87	127.07
82	JD	201	PEB	CHA-C1B-C2B	2.53	131.41	124.90
82	TD	202	PEB	CHA-C1B-NB	-2.53	119.64	124.93
82	aF	202	PEB	C1C-CHB-C4B	2.53	133.96	128.28
96	FL	102	HEM	C4A-CHB-C1B	-2.53	120.33	126.34
82	BP	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
87	1N	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
87	6N	606	CLA	CHB-C4A-NA	2.53	128.01	124.51
87	cL	513	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
82	L9	202	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
82	NF	202	PEB	CMC-C3C-C2C	-2.53	120.13	125.61
82	mE	202	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
82	Y1	201	PEB	CHB-C4B-C3B	-2.53	119.46	125.32
82	NQ	202	PEB	CAB-C3B-C4B	2.53	129.49	125.01
82	t8	202	PEB	CHA-C1B-C2B	2.53	131.41	124.90
87	KN	105	CLA	CHC-C4B-NB	2.53	126.94	124.26
82	HA	201	PEB	C1C-CHB-C4B	2.53	133.96	128.28
87	CL	514	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
82	E5	202	PEB	C3C-C4C-NC	2.53	110.61	108.33
87	A2	816	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
82	JQ	201	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	jM	203	PEB	C3B-C4B-NB	2.53	113.73	110.05
87	AN	840	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
84	V3	1001	CYC	O2A-CGA-CBA	2.53	122.16	114.03
82	k1	201	PEB	CAC-C2C-C1C	2.53	129.79	125.76
87	AN	828	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	82	302	CLA	C3B-C4B-NB	-2.53	108.17	110.52
82	dD	401	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	HK	202	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
82	iO	203	PEB	OD-C4D-ND	-2.53	122.18	125.93
87	4N	606	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
87	8N	304	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
85	B6	602	BCR	C34-C9-C10	-2.53	119.38	122.92
87	J2	101	CLA	CHB-C1B-NB	2.53	126.94	124.26
87	b6	611	CLA	CHB-C1B-NB	2.53	126.94	124.26
82	H7	201	PEB	C1C-CHB-C4B	2.53	133.96	128.28
82	sC	201	PEB	CHB-C1C-C2C	-2.53	121.44	127.15
83	Z5	302	PUB	CAB-C3B-C4B	2.53	129.79	125.76
87	A2	833	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
82	C5	202	PEB	C3C-C4C-NC	2.53	110.61	108.33
82	M5	301	PEB	C3C-C4C-NC	2.53	110.61	108.33
82	WB	402	PEB	CHC-C4C-NC	2.53	124.57	121.15
82	QF	202	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	B9	203	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	eJ	201	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	PD	202	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
82	RP	202	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
84	IO	1001	CYC	C4A-C3A-C2A	-2.53	103.60	106.51
87	A2	840	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
82	TQ	202	PEB	CHA-C4A-NA	2.53	128.21	125.20
87	3N	312	CLA	C3B-C4B-NB	-2.53	108.17	110.52
82	RI	201	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
82	Z9	301	PEB	CAC-CBC-CGC	-2.53	108.16	113.60
82	gG	202	PEB	CHB-C1C-NC	-2.53	119.53	125.32
82	B9	201	PEB	CHA-C1B-C2B	-2.53	118.40	124.90
82	T4	203	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	UE	203	PEB	CBA-CAA-C3A	-2.53	107.84	113.47
82	EK	201	PEB	C4C-C3C-C2C	-2.53	105.17	107.50
82	TH	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	mE	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	fE	202	PEB	C3C-C4C-NC	2.53	110.61	108.33
82	BA	201	PEB	CAB-CBB-CGB	-2.53	108.16	113.60
87	1N	611	CLA	C3B-C4B-NB	-2.53	108.17	110.52
96	v6	201	HEM	C4D-ND-C1D	2.53	107.69	105.07
82	xK	303	PEB	C2A-C1A-NA	2.53	110.45	108.27
82	TA	202	PEB	CMC-C3C-C4C	2.53	129.74	127.06
82	SG	203	PEB	CAC-C2C-C1C	2.53	129.79	125.76
82	a1	201	PEB	CHB-C4B-C3B	-2.53	119.47	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	b6	602	BCR	C23-C22-C21	2.53	122.82	118.94
82	RO	203	PEB	CAC-CBC-CGC	-2.53	108.16	113.60
82	R4	203	PEB	CAC-CBC-CGC	-2.53	108.16	113.60
84	x3	1001	CYC	O2A-CGA-CBA	2.53	122.15	114.03
84	I4	1001	CYC	C4A-C3A-C2A	-2.53	103.61	106.51
87	BN	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
82	XK	201	PEB	C4C-C3C-C2C	-2.53	105.17	107.50
82	Z5	301	PEB	CHC-C1D-ND	-2.53	110.53	113.72
82	AP	201	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
82	fH	203	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
85	B2	841	BCR	C36-C18-C19	2.53	122.06	118.08
82	k1	201	PEB	CAB-CBB-CGB	-2.53	108.16	113.60
82	DM	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
82	RO	203	PEB	C3B-C4B-NB	2.53	113.73	110.05
87	B2	822	CLA	C3B-C4B-NB	-2.53	108.17	110.52
96	V6	201	HEM	CHD-C4C-NC	2.53	127.17	124.44
82	KQ	201	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	j4	203	PEB	OD-C4D-C3D	-2.53	123.73	129.46
85	L2	205	BCR	C38-C26-C27	2.53	118.47	113.62
84	KO	1001	CYC	CMB-C2B-C1B	2.53	127.32	124.17
87	cL	516	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
95	hL	101	DGD	O1G-C1A-O1A	-2.53	117.21	123.59
82	WI	203	PEB	CHC-C4C-NC	2.53	124.57	121.15
82	YJ	201	PEB	CHA-C1B-NB	-2.53	119.65	124.93
88	AN	844	LHG	O8-C23-C24	2.53	119.84	111.91
82	i4	203	PEB	CAC-CBC-CGC	-2.53	108.17	113.60
82	nK	201	PEB	C4C-C3C-C2C	-2.53	105.17	107.50
82	uK	201	PEB	C4C-C3C-C2C	-2.53	105.17	107.50
82	PA	203	PEB	C1C-CHB-C4B	2.53	133.95	128.28
82	DI	202	PEB	OD-C4D-C3D	-2.53	123.73	129.46
82	fE	202	PEB	CAA-C3A-C2A	-2.53	107.95	114.26
82	B5	202	PEB	CHB-C1C-NC	2.53	131.11	125.32
82	GQ	201	PEB	C1B-C2B-C3B	-2.53	103.61	106.51
82	hM	203	PEB	CMD-C2D-C3D	-2.53	126.50	130.06
82	AJ	301	PEB	OD-C4D-C3D	-2.53	123.74	129.46
82	MM	202	PEB	CMA-C2A-C1A	-2.53	106.96	112.40
82	WD	201	PEB	CHC-C4C-NC	2.53	124.57	121.15
82	VJ	202	PEB	CHC-C4C-NC	2.53	124.57	121.15
87	62	307	CLA	CHB-C4A-NA	2.53	128.00	124.51
82	QE	202	PEB	CBB-CAB-C3B	-2.53	105.61	112.63
87	AN	839	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
82	kG	201	PEB	C1C-CHB-C4B	2.53	133.95	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	aL	604	BCR	C20-C19-C18	-2.53	119.32	126.42
82	e4	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
82	kO	202	PEB	OD-C4D-C3D	-2.53	123.74	129.46
82	dG	202	PEB	CAC-CBC-CGC	-2.53	108.17	113.60
87	4N	603	CLA	C3B-C4B-NB	-2.53	108.17	110.52
82	RD	203	PEB	C1D-CHC-C4C	2.53	116.98	113.26
92	b6	620	LMG	O8-C28-C29	2.53	119.83	111.91
82	YF	202	PEB	OD-C4D-ND	-2.53	122.19	125.93
82	II	201	PEB	C4B-C3B-C2B	-2.53	103.99	106.78
82	KI	202	PEB	C4B-C3B-C2B	-2.53	103.99	106.78
83	AJ	303	PUB	CHB-C1C-NC	-2.53	119.32	124.58
82	s8	201	PEB	CHB-C1C-C2C	-2.53	121.45	127.15
82	XF	203	PEB	OD-C4D-C3D	-2.53	123.74	129.46
82	x8	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
82	mE	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
88	A2	844	LHG	O8-C23-C24	2.53	119.83	111.91
87	B2	801	CLA	CHA-C4D-ND	2.52	137.78	132.50
87	4N	607	CLA	C2A-C1A-CHA	2.52	128.27	123.86
82	hE	202	PEB	C4C-C3C-C2C	-2.52	105.17	107.50
82	OJ	201	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
82	PQ	202	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
82	J5	203	PEB	OD-C4D-ND	-2.52	122.19	125.93
82	G7	201	PEB	OD-C4D-ND	-2.52	122.19	125.93
82	JK	202	PEB	OD-C4D-C3D	-2.52	123.74	129.46
82	dM	203	PEB	OD-C4D-C3D	-2.52	123.74	129.46
82	IF	203	PEB	CAC-CBC-CGC	-2.52	108.17	113.60
84	EH	1001	CYC	CHB-C1B-NB	-2.52	120.64	126.06
87	CL	509	CLA	CHC-C4B-NB	2.52	126.93	124.26
82	MJ	202	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
92	BL	611	LMG	O8-C28-C29	2.52	119.83	111.91
82	TO	201	PEB	OD-C4D-C3D	-2.52	123.74	129.46
82	MP	202	PEB	CHA-C1B-NB	-2.52	119.65	124.93
84	DE	1001	CYC	CAA-C2A-C1A	2.52	129.47	125.01
87	52	603	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
87	52	607	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
82	hO	201	PEB	C4B-C3B-C2B	-2.52	103.99	106.78
85	BL	616	BCR	C7-C8-C9	-2.52	122.42	126.23
82	JQ	202	PEB	CMB-C2B-C1B	2.52	128.95	125.06
82	i1	201	PEB	CHB-C1C-C2C	-2.52	121.46	127.15
82	F9	203	PEB	CHA-C1B-C2B	2.52	131.39	124.90
82	f1	201	PEB	OD-C4D-ND	-2.52	122.19	125.93
82	YI	202	PEB	OD-C4D-C3D	-2.52	123.74	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	A1	302	PEB	OD-C4D-C3D	-2.52	123.74	129.46
82	EA	202	PEB	C1D-CHC-C4C	-2.52	109.54	113.26
82	f1	201	PEB	C1D-CHC-C4C	2.52	116.98	113.26
87	42	608	CLA	O2D-CGD-CBD	2.52	115.75	111.27
82	HO	1002	PEB	CAC-CBC-CGC	-2.52	108.17	113.60
92	aL	611	LMG	C8-O7-C10	-2.52	111.58	117.79
82	GG	1002	PEB	CHA-C1B-NB	-2.52	119.66	124.93
82	OF	202	PEB	C1C-CHB-C4B	2.52	133.94	128.28
87	6N	608	CLA	C3D-C4D-ND	2.52	114.32	110.24
87	b6	615	CLA	CHB-C4A-NA	2.52	128.00	124.51
87	L2	204	CLA	CHD-C1D-ND	-2.52	122.14	124.45
82	ZG	201	PEB	CAC-CBC-CGC	-2.52	108.17	113.60
82	CJ	201	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
82	fE	202	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
82	kH	201	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
82	O1	202	PEB	C1D-CHC-C4C	-2.52	109.54	113.26
82	PD	202	PEB	CHB-C1C-C2C	-2.52	121.46	127.15
87	2N	310	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
82	QQ	202	PEB	OD-C4D-ND	-2.52	122.19	125.93
85	KN	104	BCR	C33-C5-C6	-2.52	121.70	124.53
94	a6	601	PL9	C53-C6-C1	2.52	120.15	114.99
82	OG	201	PEB	CHC-C4C-NC	2.52	124.56	121.15
82	WF	202	PEB	CAC-C2C-C3C	2.52	132.84	127.07
82	M9	302	PEB	CAC-CBC-CGC	-2.52	108.18	113.60
87	AN	827	CLA	CHB-C4A-NA	2.52	128.00	124.51
82	jH	202	PEB	CHB-C1C-C2C	-2.52	121.46	127.15
82	IM	202	PEB	OD-C4D-C3D	-2.52	123.75	129.46
82	d1	203	PEB	OD-C4D-C3D	-2.52	123.75	129.46
82	aJ	201	PEB	CAA-C3A-C4A	-2.52	106.20	112.67
87	5N	610	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
87	7N	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
82	D5	203	PEB	CHA-C4A-NA	-2.52	122.21	125.20
82	OE	201	PEB	CAC-CBC-CGC	-2.52	108.18	113.60
82	I7	201	PEB	CAB-CBB-CGB	-2.52	108.18	113.60
82	AA	202	PEB	C3C-C4C-NC	2.52	110.60	108.33
85	KN	104	BCR	C16-C17-C18	-2.52	123.71	127.31
85	cL	504	BCR	C15-C16-C17	2.52	128.64	123.47
82	KM	202	PEB	CHA-C1B-NB	-2.52	119.66	124.93
87	AN	833	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
82	SK	203	PEB	CHC-C4C-NC	2.52	124.56	121.15
82	fG	202	PEB	OA-C1A-C2A	-2.52	124.17	126.17
82	OF	202	PEB	CAB-C3B-C4B	2.52	129.47	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UE	202	PEB	CHC-C1D-ND	-2.52	110.54	113.72
82	w8	204	PEB	C1D-CHC-C4C	2.52	116.97	113.26
87	72	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
82	gE	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
82	l1	202	PEB	CBB-CAB-C3B	-2.52	105.63	112.63
82	UO	201	PEB	C1C-NC-C4C	-2.52	105.11	109.60
82	LD	202	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
82	P7	203	PEB	CMB-C2B-C1B	2.52	128.94	125.06
82	KQ	202	PEB	C3B-C4B-NB	2.52	113.71	110.05
84	C4	1001	CYC	C4D-C3D-C2D	-2.52	104.64	107.62
82	pK	202	PEB	CBB-CAB-C3B	2.52	119.63	112.63
82	VH	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
87	42	603	CLA	CHB-C1B-NB	2.52	126.92	124.26
82	MQ	201	PEB	OA-C1A-C2A	-2.52	124.17	126.17
82	ND	202	PEB	CAB-C3B-C4B	2.52	129.47	125.01
82	P1	202	PEB	CAB-C3B-C4B	2.52	129.47	125.01
87	8N	307	CLA	CAA-C2A-C3A	-2.52	107.97	114.26
82	VJ	201	PEB	CHA-C1B-C2B	2.52	131.38	124.90
82	JM	202	PEB	OD-C4D-C3D	-2.52	123.75	129.46
82	eF	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
82	qK	203	PEB	OD-C4D-C3D	-2.52	123.75	129.46
82	N7	203	PEB	OD-C4D-ND	-2.52	122.20	125.93
82	jG	202	PEB	OD-C4D-ND	-2.52	122.20	125.93
82	dM	203	PEB	CAC-C2C-C1C	2.52	129.77	125.76
82	QP	202	PEB	C1C-CHB-C4B	2.52	133.93	128.28
82	AK	201	PEB	C4C-C3C-C2C	-2.52	105.18	107.50
82	W7	202	PEB	C4C-C3C-C2C	-2.52	105.18	107.50
82	cG	202	PEB	CAC-CBC-CGC	-2.52	108.18	113.60
82	NB	203	PEB	C1D-CHC-C4C	2.52	116.97	113.26
82	KI	201	PEB	CHB-C4B-NB	-2.52	119.34	124.58
82	CI	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
82	ZG	201	PEB	CAB-C3B-C4B	2.52	129.46	125.01
82	G5	202	PEB	C3C-C4C-NC	2.52	110.60	108.33
83	M5	302	PUB	CAB-C3B-C4B	2.52	129.77	125.76
82	DQ	202	PEB	OA-C1A-C2A	-2.52	124.17	126.17
82	VP	202	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
82	N4	1002	PEB	CHC-C1D-ND	-2.52	110.54	113.72
82	HM	201	PEB	CHB-C1C-NC	-2.52	119.55	125.32
85	c6	617	BCR	C8-C9-C10	-2.52	115.08	118.94
87	42	601	CLA	CHC-C4B-NB	2.52	126.92	124.26
82	WM	203	PEB	C1C-NC-C4C	-2.52	105.12	109.60
87	ON	203	CLA	CHB-C4A-NA	2.52	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dB	202	PEB	OD-C4D-ND	-2.52	122.20	125.93
83	AE	303	PUB	OD-C4D-ND	-2.52	122.20	125.93
82	NK	202	PEB	CMC-C3C-C2C	-2.52	120.16	125.61
82	HD	201	PEB	C4C-C3C-C2C	-2.52	105.18	107.50
82	DK	201	PEB	C4C-C3C-C2C	-2.52	105.18	107.50
82	JF	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	O7	202	PEB	CHB-C1C-C2C	-2.52	121.47	127.15
82	HK	201	PEB	CHB-C4B-NB	-2.52	119.34	124.58
82	JI	201	PEB	CHB-C1C-NC	-2.52	119.55	125.32
84	KH	1001	CYC	CMB-C2B-C1B	2.52	127.31	124.17
82	AM	302	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	WE	201	PEB	CHA-C1B-C2B	2.52	131.37	124.90
83	K7	203	PUB	C2C-C1C-NC	2.52	113.71	110.05
82	OH	202	PEB	C1D-CHC-C4C	-2.52	109.55	113.26
82	YK	203	PEB	CAC-C2C-C1C	2.52	129.77	125.76
82	AJ	302	PEB	OD-C4D-ND	-2.52	122.20	125.93
82	rF	202	PEB	CHB-C1C-NC	-2.52	119.56	125.32
82	MK	202	PEB	CMC-C3C-C4C	2.52	129.73	127.06
82	uC	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
82	lE	203	PEB	C4C-C3C-C2C	-2.52	105.18	107.50
82	cM	201	PEB	CHB-C4B-NB	-2.52	119.34	124.58
82	VE	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
87	BN	813	CLA	C3B-C4B-NB	-2.52	108.18	110.52
82	kE	201	PEB	C1C-CHB-C4B	2.52	133.92	128.28
85	cL	518	BCR	C1-C6-C5	-2.52	119.07	122.61
82	mJ	202	PEB	CHB-C1C-NC	-2.52	119.56	125.32
82	L7	202	PEB	CMB-C2B-C1B	2.52	128.94	125.06
82	AI	203	PEB	C2B-C1B-NB	2.52	115.90	110.53
82	AB	501	PEB	CBC-CAC-C2C	-2.52	105.64	112.63
82	S9	203	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	qK	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	A4	301	PEB	CHC-C1D-ND	-2.52	110.54	113.72
83	AO	302	PUB	CAB-C3B-C4B	2.52	129.77	125.76
82	wC	204	PEB	C1D-CHC-C4C	2.52	116.97	113.26
82	yK	301	PEB	CHC-C4C-NC	2.52	124.55	121.15
82	yC	203	PEB	OD-C4D-ND	-2.52	122.20	125.93
82	k1	201	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
87	82	307	CLA	CAA-C2A-C3A	-2.52	107.97	114.26
82	V1	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	X9	202	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	aF	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
82	jE	201	PEB	CAC-CBC-CGC	-2.51	108.19	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	LN	204	CLA	C2C-C1C-NC	-2.51	107.62	109.97
87	BN	826	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
82	fH	201	PEB	C1D-CHC-C4C	2.51	116.96	113.26
82	wC	202	PEB	C3C-C4C-NC	2.51	110.60	108.33
82	FK	202	PEB	OD-C4D-C3D	-2.51	123.76	129.46
82	iH	201	PEB	CHB-C1C-C2C	-2.51	121.48	127.15
82	WH	203	PEB	CAB-CBB-CGB	-2.51	108.19	113.60
82	HB	201	PEB	CMA-C2A-C1A	-2.51	106.98	112.40
82	SB	202	PEB	C1B-C2B-C3B	-2.51	103.62	106.51
82	CD	202	PEB	CAC-C2C-C1C	2.51	129.77	125.76
83	AH	304	PUB	CAB-C3B-C4B	2.51	129.77	125.76
85	K2	105	BCR	C16-C17-C18	-2.51	123.72	127.31
82	PH	202	PEB	CAB-C3B-C4B	2.51	129.46	125.01
82	PD	202	PEB	C1C-CHB-C4B	2.51	133.92	128.28
82	PD	203	PEB	CHB-C1C-NC	-2.51	119.56	125.32
92	bL	623	LMG	O8-C28-C29	2.51	119.80	111.91
82	GD	201	PEB	C4C-C3C-C2C	-2.51	105.18	107.50
82	FI	201	PEB	OD-C4D-ND	-2.51	122.21	125.93
87	12	604	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
82	lG	202	PEB	CHA-C1B-NB	-2.51	119.67	124.93
82	oK	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	e4	202	PEB	CMB-C2B-C1B	2.51	128.94	125.06
82	RF	201	PEB	CHB-C1C-C2C	-2.51	121.48	127.15
82	QA	201	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
84	H1	1001	CYC	C1A-C2A-C3A	-2.51	104.00	106.78
87	O2	202	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
87	B2	826	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
82	JB	202	PEB	CHB-C4B-NB	-2.51	119.35	124.58
87	CL	513	CLA	C2D-C1D-ND	-2.51	108.25	110.10
92	b6	624	LMG	O8-C28-O10	-2.51	117.25	123.59
87	A2	851	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
82	VE	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	S5	203	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	mF	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
84	DH	1003	CYC	C4D-ND-C1D	-2.51	105.31	109.79
82	OF	203	PEB	CHB-C1C-C2C	-2.51	121.48	127.15
82	ZB	203	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
82	W1	203	PEB	CAB-CBB-CGB	-2.51	108.20	113.60
82	aJ	202	PEB	CMA-C2A-C1A	-2.51	106.99	112.40
82	KJ	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
82	OP	203	PEB	CHB-C4B-C3B	-2.51	119.51	125.32
82	T7	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	sF	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
87	2N	309	CLA	CMB-C2B-C3B	2.51	132.67	126.59
82	OF	201	PEB	CHA-C4A-NA	2.51	128.19	125.20
82	NO	1002	PEB	CHC-C1D-ND	-2.51	110.55	113.72
95	CL	520	DGD	C1D-O6D-C5D	2.51	118.62	113.69
82	EF	202	PEB	CAA-C3A-C4A	-2.51	106.22	112.67
82	Q1	203	PEB	C4C-C3C-C2C	-2.51	105.18	107.50
82	wF	302	PEB	C1C-CHB-C4B	-2.51	122.65	128.28
87	RN	201	CLA	C2A-C1A-CHA	2.51	128.25	123.86
87	R2	201	CLA	C2A-C1A-CHA	2.51	128.25	123.86
82	UH	203	PEB	CMB-C2B-C1B	2.51	128.93	125.06
82	Z4	201	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
82	JQ	201	PEB	CHA-C1B-C2B	2.51	131.36	124.90
85	B6	602	BCR	C38-C26-C27	2.51	118.44	113.62
87	CL	504	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
82	T4	201	PEB	CAB-CBB-CGB	-2.51	108.20	113.60
82	TH	202	PEB	OA-C1A-C2A	-2.51	124.18	126.17
82	KP	202	PEB	OA-C1A-C2A	-2.51	124.18	126.17
82	N4	1002	PEB	CMD-C2D-C3D	2.51	133.61	130.06
87	AN	801	CLA	C3B-C4B-NB	-2.51	108.19	110.52
87	CL	505	CLA	O2D-CGD-CBD	2.51	115.73	111.27
82	V9	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	RK	201	PEB	CHB-C1C-C2C	-2.51	121.48	127.15
87	B6	606	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
82	WO	201	PEB	C1D-CHC-C4C	-2.51	109.55	113.26
82	hM	203	PEB	C1D-CHC-C4C	2.51	116.96	113.26
82	CP	202	PEB	CHB-C4B-C3B	-2.51	119.51	125.32
84	EO	1001	CYC	CMB-C2B-C1B	2.51	127.30	124.17
82	T1	202	PEB	C3B-C4B-NB	2.51	113.70	110.05
83	KA	203	PUB	C2C-C1C-NC	2.51	113.70	110.05
82	F7	202	PEB	OD-C4D-ND	-2.51	122.21	125.93
82	OK	202	PEB	CAB-C3B-C4B	2.51	129.45	125.01
82	NK	202	PEB	CAC-C2C-C1C	2.51	129.76	125.76
82	U1	203	PEB	CHB-C4B-NB	-2.51	119.35	124.58
82	OI	203	PEB	CHA-C1B-NB	-2.51	119.68	124.93
82	OI	203	PEB	C1B-C2B-C3B	-2.51	103.62	106.51
82	U9	201	PEB	C4C-C3C-C2C	-2.51	105.18	107.50
82	JK	201	PEB	CAB-C3B-C4B	2.51	129.45	125.01
82	OE	203	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	C9	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	WE	201	PEB	CHA-C4A-NA	2.51	128.19	125.20
82	W5	202	PEB	C3B-C4B-NB	2.51	113.70	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O4	201	PEB	CHB-C1C-C2C	-2.51	121.49	127.15
82	GG	1002	PEB	OD-C4D-ND	-2.51	122.21	125.93
82	FJ	202	PEB	CHB-C1C-NC	-2.51	119.57	125.32
87	B2	836	CLA	C3B-C4B-NB	-2.51	108.19	110.52
91	a6	613	PHO	CMB-C2B-C3B	2.51	129.38	124.68
82	P5	201	PEB	CHB-C4B-C3B	-2.51	119.51	125.32
82	V5	202	PEB	C3C-C4C-NC	2.51	110.59	108.33
82	lH	201	PEB	CBB-CAB-C3B	-2.51	105.65	112.63
82	rK	202	PEB	CHB-C1C-NC	-2.51	119.57	125.32
82	J5	203	PEB	CHC-C1D-ND	-2.51	110.55	113.72
87	22	607	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
87	4N	601	CLA	CHC-C4B-NB	2.51	126.91	124.26
82	m1	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
82	jM	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
85	LN	205	BCR	C38-C26-C27	2.51	118.44	113.62
82	A5	201	PEB	CHB-C4B-C3B	-2.51	119.51	125.32
87	BL	602	CLA	C3B-C4B-NB	-2.51	108.19	110.52
87	BN	810	CLA	C3B-C4B-NB	-2.51	108.19	110.52
87	12	611	CLA	C3B-C4B-NB	-2.51	108.19	110.52
82	tC	202	PEB	CHA-C1B-C2B	2.51	131.35	124.90
87	A6	403	CLA	CHB-C4A-NA	2.51	127.98	124.51
92	aL	611	LMG	C1-C2-C3	-2.51	104.77	110.00
87	LN	204	CLA	CHD-C1D-ND	-2.51	122.15	124.45
82	VA	201	PEB	OD-C4D-ND	-2.51	122.21	125.93
82	U1	203	PEB	CMB-C2B-C1B	2.51	128.93	125.06
82	vC	201	PEB	CAC-C2C-C1C	2.51	129.76	125.76
82	eF	201	PEB	C2A-C1A-NA	2.51	110.44	108.27
82	UI	202	PEB	C3C-C4C-NC	2.51	110.59	108.33
82	S4	201	PEB	C3C-C4C-NC	2.51	110.59	108.33
82	GI	202	PEB	C4B-C3B-C2B	-2.51	104.01	106.78
92	j6	102	LMG	C8-O7-C10	-2.51	111.61	117.79
82	TQ	201	PEB	CAB-C3B-C4B	2.51	129.45	125.01
82	RI	203	PEB	C2B-C1B-NB	2.51	115.88	110.53
82	iK	201	PEB	CAC-CBC-CGC	-2.51	108.20	113.60
103	82	310	ZEX	C38-C24-C23	-2.51	108.33	112.20
87	b6	610	CLA	CHB-C1B-NB	2.51	126.91	124.26
82	TM	202	PEB	CMA-C2A-C1A	-2.51	107.00	112.40
82	TJ	202	PEB	C1C-CHB-C4B	-2.51	122.66	128.28
82	OF	201	PEB	C3B-C4B-NB	2.51	113.70	110.05
82	PA	202	PEB	CAC-C2C-C1C	2.51	129.76	125.76
82	fO	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	Q9	201	PEB	CAA-C3A-C4A	-2.51	106.23	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UG	202	PEB	CHC-C1D-ND	-2.51	110.55	113.72
87	22	609	CLA	CMB-C2B-C3B	2.51	132.66	126.59
95	b6	622	DGD	C2G-O2G-C1B	-2.51	111.62	117.79
82	fH	202	PEB	CHA-C4A-NA	-2.51	122.22	125.20
82	O5	203	PEB	CHA-C1B-NB	-2.51	119.69	124.93
82	P9	202	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	QJ	202	PEB	CAC-CBC-CGC	-2.51	108.21	113.60
82	M9	304	PEB	CMA-C2A-C1A	-2.51	107.00	112.40
82	G5	201	PEB	CHB-C4B-C3B	-2.51	119.52	125.32
82	GF	203	PEB	CAB-C3B-C2B	-2.51	123.21	127.88
82	LP	202	PEB	CHC-C1D-ND	-2.51	110.55	113.72
82	jO	201	PEB	CMA-C2A-C1A	-2.51	107.00	112.40
82	f4	201	PEB	C4B-NB-C1B	-2.51	101.79	106.51
87	bL	613	CLA	C3B-C4B-NB	-2.51	108.19	110.52
83	A1	304	PUB	CAB-C3B-C4B	2.51	129.75	125.76
82	LA	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
82	QA	201	PEB	C3B-C4B-NB	2.51	113.70	110.05
82	vK	201	PEB	C3B-C4B-NB	2.51	113.70	110.05
82	XQ	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	I9	202	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	DB	203	PEB	CHB-C4B-C3B	-2.51	119.52	125.32
82	E5	201	PEB	CHB-C4B-C3B	-2.51	119.52	125.32
95	AL	414	DGD	C1E-C2E-C3E	2.51	115.22	110.00
82	dO	201	PEB	C3C-C4C-NC	2.51	110.59	108.33
87	ON	202	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
82	OF	202	PEB	CHC-C1D-ND	-2.51	110.55	113.72
82	PF	202	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	PM	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	N9	202	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	DK	203	PEB	CHB-C1C-NC	-2.51	119.58	125.32
82	eO	202	PEB	CMB-C2B-C1B	2.51	128.92	125.06
82	Z1	203	PEB	C1C-CHB-C4B	-2.51	122.66	128.28
82	hG	202	PEB	C4C-C3C-C2C	-2.51	105.19	107.50
82	gG	202	PEB	OD-C4D-C3D	-2.51	123.78	129.46
87	AN	829	CLA	C3B-C4B-NB	-2.51	108.19	110.52
82	l1	202	PEB	CHB-C1C-C2C	-2.51	121.50	127.15
82	BQ	202	PEB	CMC-C3C-C4C	2.51	129.72	127.06
83	AG	303	PUB	CHA-C4A-NA	-2.51	110.55	113.72
82	ZB	203	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	aE	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	hK	202	PEB	OD-C4D-C3D	-2.51	123.78	129.46
82	V1	202	PEB	C3B-C4B-NB	2.51	113.69	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	1N	604	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
96	FL	102	HEM	C1A-CHA-C4D	-2.51	120.39	126.34
82	L4	1002	PEB	C1C-CHB-C4B	2.51	133.90	128.28
82	TI	202	PEB	C4B-C3B-C2B	-2.51	104.01	106.78
82	c4	203	PEB	C4C-C3C-C2C	-2.51	105.19	107.50
82	eB	202	PEB	C4C-C3C-C2C	-2.51	105.19	107.50
82	KQ	202	PEB	OD-C4D-ND	-2.51	122.22	125.93
82	DH	1002	PEB	CHC-C1D-ND	-2.51	110.56	113.72
82	RQ	203	PEB	C3B-C4B-NB	2.51	113.69	110.05
82	eG	202	PEB	C3B-C4B-NB	2.51	113.69	110.05
87	6N	604	CLA	CHD-C1D-ND	-2.50	122.15	124.45
85	FL	101	BCR	C24-C23-C22	2.50	130.02	126.23
82	VG	201	PEB	OD-C4D-C3D	-2.50	123.78	129.46
82	VG	202	PEB	OD-C4D-C3D	-2.50	123.78	129.46
82	jG	201	PEB	OD-C4D-C3D	-2.50	123.78	129.46
82	lH	201	PEB	CHB-C1C-C2C	-2.50	121.50	127.15
87	2N	307	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
82	f4	201	PEB	CAB-CBB-CGB	-2.50	108.21	113.60
82	DD	202	PEB	CBB-CAB-C3B	-2.50	105.67	112.63
82	T5	202	PEB	C3C-C4C-NC	2.50	110.59	108.33
84	HH	1001	CYC	C1A-C2A-C3A	-2.50	104.01	106.78
82	MQ	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	jE	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	MA	201	PEB	C3B-C4B-NB	2.50	113.69	110.05
82	DM	201	PEB	CMC-C3C-C4C	2.50	129.72	127.06
82	yF	301	PEB	CHC-C4C-NC	2.50	124.54	121.15
87	1N	602	CLA	CHB-C1B-NB	-2.50	121.61	124.26
82	SG	203	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	J7	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	CM	201	PEB	C1B-C2B-C3B	-2.50	103.63	106.51
87	4N	608	CLA	O2D-CGD-CBD	2.50	115.72	111.27
82	YF	203	PEB	C3B-C4B-NB	2.50	113.69	110.05
87	4N	605	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
82	E7	202	PEB	C3C-C4C-NC	2.50	110.59	108.33
82	L5	201	PEB	CAC-C2C-C1C	2.50	129.75	125.76
82	ZJ	202	PEB	O2B-CGB-CBB	2.50	122.07	114.03
82	b1	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
82	dE	202	PEB	CAC-CBC-CGC	-2.50	108.22	113.60
82	aK	201	PEB	C2A-C1A-NA	2.50	110.43	108.27
95	c6	601	DGD	C4D-C3D-C2D	-2.50	106.45	110.82
82	VI	202	PEB	C4C-C3C-C2C	-2.50	105.19	107.50
87	AN	821	CLA	O2D-CGD-CBD	2.50	115.72	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	I5	201	PEB	CHB-C4B-C3B	-2.50	119.53	125.32
84	NH	1001	CYC	C1A-C2A-C3A	-2.50	104.01	106.78
82	XJ	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	VP	201	PEB	CMB-C2B-C1B	2.50	128.92	125.06
82	GQ	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
87	22	608	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
82	K5	201	PEB	CHB-C4B-C3B	-2.50	119.53	125.32
82	WJ	203	PEB	CMA-C2A-C1A	-2.50	107.01	112.40
82	SH	203	PEB	C3B-C4B-NB	2.50	113.69	110.05
82	Q9	202	PEB	C3B-C4B-NB	2.50	113.69	110.05
82	PJ	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	Q9	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	KG	201	PEB	CAC-C2C-C1C	2.50	129.75	125.76
87	nL	101	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
82	dJ	201	PEB	CAA-C3A-C4A	-2.50	106.25	112.67
82	i1	201	PEB	C2A-C1A-NA	2.50	110.43	108.27
82	qK	202	PEB	C2A-C1A-NA	2.50	110.43	108.27
91	A6	407	PHO	O2D-CGD-O1D	-2.50	118.95	123.84
87	L2	204	CLA	C2C-C1C-NC	-2.50	107.63	109.97
87	B2	814	CLA	C2A-C1A-CHA	2.50	128.23	123.86
87	K2	104	CLA	C2A-C1A-CHA	2.50	128.23	123.86
82	DK	201	PEB	CAB-CBB-CGB	-2.50	108.22	113.60
82	AI	201	PEB	C4B-C3B-C2B	-2.50	104.01	106.78
82	A9	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	PD	201	PEB	OD-C4D-ND	-2.50	122.22	125.93
82	T5	201	PEB	CHB-C4B-C3B	-2.50	119.53	125.32
82	iE	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	lG	203	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	SH	203	PEB	C3C-C4C-NC	2.50	110.58	108.33
82	R1	202	PEB	CHC-C4C-NC	2.50	124.53	121.15
82	DQ	202	PEB	CAA-C3A-C4A	-2.50	106.25	112.67
82	GP	202	PEB	CMA-C2A-C1A	-2.50	107.01	112.40
83	A4	302	PUB	CAB-C3B-C4B	2.50	129.75	125.76
83	QJ	201	PUB	C2C-C1C-NC	2.50	113.69	110.05
82	PH	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	iJ	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
82	X5	201	PEB	CHB-C4B-C3B	-2.50	119.53	125.32
96	E6	101	HEM	C4C-NC-C1C	2.50	107.80	105.35
82	jO	202	PEB	CHA-C1B-NB	-2.50	119.70	124.93
82	gK	201	PEB	CAC-C2C-C3C	2.50	132.80	127.07
95	C6	504	DGD	O2G-C1B-O1B	-2.50	117.66	123.70
82	R5	201	PEB	CHB-C4B-C3B	-2.50	119.53	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SJ	201	PEB	OD-C4D-ND	-2.50	122.23	125.93
82	wF	302	PEB	CBA-CAA-C3A	-2.50	107.90	113.47
82	eM	201	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
87	KN	103	CLA	C2A-C1A-CHA	2.50	128.23	123.86
82	ZE	202	PEB	CAC-C2C-C1C	2.50	129.74	125.76
82	FA	203	PEB	C3B-C4B-NB	2.50	113.69	110.05
84	FO	1001	CYC	C2A-C1A-NA	2.50	113.69	110.05
82	lJ	201	PEB	CAA-C3A-C4A	-2.50	106.25	112.67
87	AN	851	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
85	c6	602	BCR	C16-C17-C18	-2.50	123.74	127.31
87	B2	828	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
87	aL	606	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
82	UJ	202	PEB	CAB-C3B-C4B	2.50	129.43	125.01
82	CM	202	PEB	CAB-C3B-C4B	2.50	129.43	125.01
82	fK	202	PEB	CAB-C3B-C4B	2.50	129.43	125.01
82	cK	202	PEB	CHC-C4C-NC	2.50	124.53	121.15
82	I7	202	PEB	OD-C4D-ND	-2.50	122.23	125.93
82	TF	201	PEB	C1C-CHB-C4B	2.50	133.89	128.28
87	cL	505	CLA	C2A-C1A-CHA	2.50	128.23	123.86
85	b6	603	BCR	C33-C5-C6	-2.50	121.72	124.53
87	c6	611	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
82	AE	301	PEB	OD-C4D-C3D	-2.50	123.80	129.46
82	dE	203	PEB	C3B-C4B-NB	2.50	113.69	110.05
87	A2	820	CLA	CHB-C1B-NB	2.50	126.90	124.26
95	AL	414	DGD	O1G-C1A-C2A	2.50	119.75	111.91
82	gB	203	PEB	CHB-C1C-NC	-2.50	119.59	125.32
82	R9	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
82	GJ	203	PEB	CHA-C1B-NB	-2.50	119.71	124.93
82	oK	201	PEB	O1C-CGC-CBC	-2.50	115.05	123.08
82	CB	202	PEB	CAA-C3A-C2A	-2.50	108.02	114.26
82	GD	201	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
87	C6	512	CLA	CHB-C4A-NA	2.50	127.97	124.51
82	eH	203	PEB	OD-C4D-ND	-2.50	122.23	125.93
87	AN	837	CLA	O2A-CGA-CBA	2.50	119.75	111.91
87	nL	101	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
87	A2	837	CLA	O2A-CGA-CBA	2.50	119.75	111.91
87	5N	604	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
82	pK	201	PEB	CHB-C4B-NB	-2.50	119.38	124.58
82	gJ	201	PEB	OD-C4D-C3D	-2.50	123.80	129.46
87	L2	202	CLA	CHB-C4A-NA	2.50	127.97	124.51
82	nK	201	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
82	YJ	203	PEB	C4C-C3C-C2C	-2.50	105.19	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BL	620	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
82	hF	202	PEB	CMC-C3C-C4C	2.50	129.71	127.06
87	52	611	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
84	M1	201	CYC	CHA-C1A-C2A	-2.50	119.54	125.32
82	NK	201	PEB	OD-C4D-C3D	-2.50	123.80	129.46
82	K9	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
82	QH	203	PEB	C4B-C3B-C2B	-2.50	104.02	106.78
82	EI	201	PEB	C4B-C3B-C2B	-2.50	104.02	106.78
82	CB	201	PEB	CHB-C1C-C2C	-2.50	121.52	127.15
82	PA	203	PEB	CAC-CBC-CGC	-2.50	108.23	113.60
82	YP	502	PEB	CHC-C1D-ND	-2.50	110.56	113.72
82	WE	202	PEB	CHB-C4B-C3B	-2.50	119.54	125.32
82	WE	202	PEB	C3C-C4C-NC	2.50	110.58	108.33
82	Z5	301	PEB	C3C-C4C-NC	2.50	110.58	108.33
82	F7	203	PEB	C3B-C4B-NB	2.50	113.68	110.05
82	TO	202	PEB	CMC-C3C-C4C	2.50	129.71	127.06
82	LB	201	PEB	C4C-C3C-C2C	-2.50	105.20	107.50
82	NB	201	PEB	CAB-C3B-C4B	2.50	129.43	125.01
82	ZE	201	PEB	CAB-C3B-C4B	2.50	129.43	125.01
82	e4	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
87	AN	830	CLA	CMB-C2B-C1B	-2.50	121.57	125.37
82	gB	203	PEB	CAC-CBC-CGC	-2.50	108.23	113.60
87	2N	301	CLA	CHD-C1D-ND	-2.50	122.16	124.45
82	wK	302	PEB	C1C-CHB-C4B	-2.50	122.68	128.28
82	Q4	201	PEB	OA-C1A-NA	2.50	127.97	124.94
94	AL	413	PL9	C20-C19-C21	2.50	119.47	115.27
94	D6	408	PL9	C30-C29-C31	2.50	119.47	115.27
82	eH	201	PEB	CHC-C4C-NC	2.50	124.53	121.15
82	KM	203	PEB	OD-C4D-C3D	-2.50	123.81	129.46
84	K4	1001	CYC	CMB-C2B-C1B	2.50	127.28	124.17
82	U9	202	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
85	c6	602	BCR	C21-C20-C19	-2.50	115.43	123.22
82	KM	203	PEB	CAA-C3A-C4A	-2.50	106.26	112.67
82	jO	201	PEB	CAB-CBB-CGB	-2.50	108.23	113.60
82	YH	201	PEB	CHB-C4B-C3B	-2.50	119.55	125.32
87	AN	838	CLA	CHB-C1B-NB	2.50	126.90	124.26
82	MD	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
82	NJ	202	PEB	OD-C4D-C3D	-2.50	123.81	129.46
82	FM	202	PEB	OD-C4D-C3D	-2.50	123.81	129.46
82	E9	202	PEB	OD-C4D-C3D	-2.50	123.81	129.46
82	NI	201	PEB	C4B-C3B-C2B	-2.50	104.02	106.78
82	Q7	201	PEB	C4B-C3B-C2B	-2.50	104.02	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dK	202	PEB	C3B-C4B-NB	2.50	113.68	110.05
82	IQ	201	PEB	CHA-C4A-NA	2.50	128.17	125.20
87	A2	813	CLA	C3B-C4B-NB	-2.50	108.20	110.52
82	X7	203	PEB	CHC-C4C-NC	2.50	124.53	121.15
82	O7	202	PEB	CAC-C2C-C1C	2.50	129.74	125.76
82	kH	201	PEB	CAC-C2C-C1C	2.50	129.74	125.76
82	C5	201	PEB	CHB-C4B-C3B	-2.50	119.55	125.32
82	aH	201	PEB	CHB-C4B-C3B	-2.50	119.55	125.32
83	Y7	302	PUB	CHB-C1C-C2C	-2.50	119.55	125.32
82	WB	402	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
82	YJ	201	PEB	CAA-C3A-C4A	-2.50	106.27	112.67
96	vL	201	HEM	CHD-C4C-NC	2.50	127.14	124.44
82	NB	201	PEB	OD-C4D-ND	-2.50	122.23	125.93
82	S7	201	PEB	OD-C4D-ND	-2.50	122.23	125.93
82	D9	202	PEB	OD-C4D-ND	-2.50	122.23	125.93
87	A2	838	CLA	CHB-C1B-NB	2.49	126.90	124.26
87	62	310	CLA	O2D-CGD-CBD	2.49	115.70	111.27
82	LA	202	PEB	CAC-C2C-C1C	2.49	129.74	125.76
95	B6	620	DGD	O1G-C1A-C2A	2.49	119.74	111.91
82	HA	201	PEB	CAC-CBC-CGC	-2.49	108.23	113.60
82	iF	201	PEB	CAC-CBC-CGC	-2.49	108.23	113.60
82	jG	201	PEB	CAC-CBC-CGC	-2.49	108.23	113.60
87	B2	812	CLA	C3B-C4B-NB	-2.49	108.20	110.52
82	fJ	202	PEB	CMB-C2B-C1B	2.49	128.91	125.06
87	D6	402	CLA	CHB-C4A-NA	2.49	127.96	124.51
87	8N	307	CLA	CHB-C4A-NA	2.49	127.96	124.51
82	aG	202	PEB	CHB-C4B-NB	-2.49	119.39	124.58
82	AA	201	PEB	OA-C1A-C2A	-2.49	124.19	126.17
82	HK	201	PEB	C1C-CHB-C4B	2.49	133.88	128.28
87	LN	202	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
82	QD	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
84	BE	1001	CYC	CHB-C4A-C3A	2.49	131.31	124.90
82	Q1	201	PEB	C1C-NC-C4C	-2.49	105.16	109.60
83	yF	303	PUB	CHB-C4B-C3B	-2.49	121.52	127.15
82	jH	202	PEB	OD-C4D-ND	-2.49	122.24	125.93
82	D9	203	PEB	CMB-C2B-C1B	2.49	128.90	125.06
82	A5	202	PEB	C3C-C4C-NC	2.49	110.58	108.33
87	K2	106	CLA	CHB-C4A-NA	2.49	127.96	124.51
82	B5	202	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	a1	201	PEB	C1B-C2B-C3B	-2.49	103.64	106.51
82	f4	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
87	52	610	CLA	C3B-C4B-NB	-2.49	108.20	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	82	301	CLA	C3B-C4B-NB	-2.49	108.20	110.52
87	c6	611	CLA	C3B-C4B-NB	-2.49	108.20	110.52
84	HH	1001	CYC	C4D-ND-C1D	-2.49	105.34	109.79
85	HL	103	BCR	C29-C30-C25	2.49	114.32	110.48
82	PF	201	PEB	CAB-CBB-CGB	-2.49	108.24	113.60
82	Q9	203	PEB	C1C-CHB-C4B	-2.49	122.69	128.28
82	OI	203	PEB	OD-C4D-ND	-2.49	122.24	125.93
82	MJ	203	PEB	OD-C4D-ND	-2.49	122.24	125.93
82	mG	201	PEB	C2A-C1A-NA	2.49	110.42	108.27
82	aO	203	PEB	C2A-C1A-NA	2.49	110.42	108.27
82	HD	203	PEB	CBA-CAA-C3A	-2.49	107.92	113.47
82	WK	202	PEB	OA-C1A-C2A	-2.49	124.19	126.17
82	MM	202	PEB	OA-C1A-C2A	-2.49	124.19	126.17
87	a6	609	CLA	CHB-C4A-NA	2.49	127.96	124.51
82	fE	203	PEB	C3B-C4B-NB	2.49	113.67	110.05
82	qK	203	PEB	CHA-C1B-NB	-2.49	119.72	124.93
82	ZB	201	PEB	C1B-C2B-C3B	-2.49	103.65	106.51
82	v8	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
85	fL	101	BCR	C11-C12-C13	-2.49	119.41	126.42
82	TO	203	PEB	CHC-C1D-ND	-2.49	110.57	113.72
82	GP	203	PEB	CHC-C1D-ND	-2.49	110.57	113.72
82	pF	202	PEB	CBB-CAB-C3B	2.49	119.55	112.63
82	wC	203	PEB	OD-C4D-ND	-2.49	122.24	125.93
82	WB	401	PEB	C1D-CHC-C4C	2.49	116.93	113.26
82	WQ	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
82	JK	201	PEB	CAC-CBC-CGC	-2.49	108.24	113.60
82	P7	203	PEB	CAC-CBC-CGC	-2.49	108.24	113.60
82	WG	201	PEB	CHA-C4A-NA	2.49	128.17	125.20
82	AD	304	PEB	CHA-C4A-NA	-2.49	122.24	125.20
82	R4	202	PEB	C1C-NC-C4C	-2.49	105.16	109.60
82	F5	202	PEB	C1C-NC-C4C	-2.49	105.16	109.60
96	FL	102	HEM	C4D-ND-C1D	2.49	107.65	105.07
82	VE	202	PEB	C3B-C4B-NB	2.49	113.67	110.05
87	42	605	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
87	6N	609	CLA	O2D-CGD-CBD	2.49	115.70	111.27
87	12	602	CLA	CHB-C1B-NB	-2.49	121.62	124.26
82	gF	201	PEB	CAC-C2C-C3C	2.49	132.78	127.07
82	AD	301	PEB	CHA-C1B-NB	-2.49	119.72	124.93
85	Z6	101	BCR	C30-C25-C26	-2.49	119.10	122.61
82	S7	201	PEB	CHB-C4B-NB	-2.49	119.39	124.58
82	ZI	401	PEB	CHB-C1C-C2C	2.49	132.77	127.15
82	fE	202	PEB	OA-C1A-C2A	-2.49	124.19	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aO	201	PEB	CHB-C4B-C3B	-2.49	119.56	125.32
92	x6	601	LMG	O8-C28-C29	2.49	119.73	111.91
85	c6	617	BCR	C4-C5-C6	-2.49	119.11	122.73
82	LD	203	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	mE	203	PEB	CAB-CBB-CGB	-2.49	108.24	113.60
82	dM	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
87	d6	403	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
83	YA	302	PUB	CHA-C4A-NA	-2.49	110.57	113.72
82	g1	201	PEB	CAB-CBB-CGB	-2.49	108.24	113.60
87	cL	515	CLA	C2A-C1A-CHA	2.49	128.21	123.86
87	c6	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
82	Z1	203	PEB	CAA-C3A-C4A	2.49	119.07	112.67
95	BL	614	DGD	O1G-C1A-C2A	2.49	119.72	111.91
87	8N	305	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
82	fH	203	PEB	CMB-C2B-C1B	2.49	128.90	125.06
82	bB	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	sK	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	jF	202	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	fG	201	PEB	C4B-C3B-C2B	-2.49	104.03	106.78
87	42	608	CLA	C2D-C1D-ND	-2.49	108.27	110.10
87	BL	609	CLA	C3B-C4B-NB	-2.49	108.20	110.52
82	CK	201	PEB	CHB-C1C-NC	-2.49	119.62	125.32
82	GI	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	mF	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
87	BN	828	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
82	YJ	203	PEB	CAB-C3B-C4B	2.49	129.41	125.01
82	WE	202	PEB	C1D-CHC-C4C	-2.49	109.58	113.26
82	L7	203	PEB	C1D-CHC-C4C	-2.49	109.58	113.26
82	mH	202	PEB	CHA-C4A-NA	2.49	128.16	125.20
95	AL	416	DGD	C2G-O2G-C1B	-2.49	111.66	117.79
82	SI	201	PEB	CAB-CBB-CGB	2.49	118.96	113.60
82	oF	201	PEB	O1C-CGC-CBC	-2.49	115.08	123.08
82	CM	202	PEB	CMC-C3C-C4C	-2.49	124.42	127.06
82	hJ	203	PEB	CAC-C2C-C1C	2.49	129.73	125.76
82	gE	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	iJ	201	PEB	CAB-CBB-CGB	-2.49	108.25	113.60
87	B2	831	CLA	C2A-C1A-CHA	2.49	128.21	123.86
87	L2	204	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
82	V5	201	PEB	CHB-C4B-C3B	-2.49	119.56	125.32
82	RH	202	PEB	CHC-C4C-NC	2.49	124.52	121.15
82	UD	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
87	BL	604	CLA	CMB-C2B-C1B	-2.49	121.58	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RM	202	PEB	O2B-CGB-CBB	2.49	122.03	114.03
87	c6	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
82	PA	203	PEB	CMB-C2B-C1B	2.49	128.90	125.06
82	XD	201	PEB	CMB-C2B-C1B	2.49	128.90	125.06
83	YA	302	PUB	CHB-C1C-C2C	-2.49	119.56	125.32
87	BN	825	CLA	CHB-C1B-C2B	-2.49	120.21	127.24
82	UJ	203	PEB	C4B-C3B-C2B	-2.49	104.03	106.78
87	BN	802	CLA	CHA-C4D-ND	2.49	137.70	132.50
82	OH	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	WB	401	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	WQ	202	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
88	I6	101	LHG	O2-C2-C1	2.49	120.08	109.12
82	jJ	202	PEB	CHA-C1B-NB	-2.49	119.73	124.93
82	DQ	202	PEB	CBB-CAB-C3B	-2.49	105.72	112.63
82	vC	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	aG	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
82	c4	203	PEB	CAC-CBC-CGC	-2.49	108.25	113.60
82	WD	202	PEB	CHA-C1B-NB	-2.49	119.73	124.93
84	CO	1001	CYC	C4D-C3D-C2D	-2.49	104.68	107.62
87	52	605	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
82	ND	204	PEB	CMC-C3C-C4C	2.49	129.70	127.06
82	mK	201	PEB	OD-C4D-C3D	-2.49	123.83	129.46
82	LA	203	PEB	C3B-C4B-NB	2.49	113.67	110.05
82	FD	203	PEB	CAC-C2C-C1C	2.49	129.72	125.76
84	DG	1001	CYC	C2C-C1C-NC	2.49	110.42	108.27
83	AE	303	PUB	CHA-C4A-NA	-2.49	110.58	113.72
83	xK	301	PUB	CHA-C4A-NA	-2.49	110.58	113.72
82	QH	203	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	GI	203	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	NI	202	PEB	C4C-C3C-C2C	-2.49	105.20	107.50
82	UI	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
87	cL	513	CLA	C3B-C4B-NB	-2.49	108.21	110.52
82	dF	202	PEB	CHB-C4B-C3B	-2.49	119.57	125.32
87	CL	513	CLA	C2A-C1A-CHA	2.49	128.21	123.86
87	BN	815	CLA	C2A-C1A-CHA	2.49	128.21	123.86
92	B6	618	LMG	O8-C28-C29	2.49	119.71	111.91
82	HH	1002	PEB	CAC-C2C-C1C	2.49	129.72	125.76
82	fH	201	PEB	C3B-C4B-NB	2.49	113.67	110.05
82	WQ	201	PEB	CHC-C4C-NC	2.49	124.51	121.15
85	CL	502	BCR	C37-C22-C21	-2.49	119.44	122.92
82	TO	203	PEB	C1B-C2B-C3B	-2.49	103.65	106.51
82	JI	201	PEB	CAB-C3B-C4B	2.49	129.41	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EM	201	PEB	OD-C4D-C3D	-2.49	123.83	129.46
82	iG	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
82	mJ	201	PEB	OD-C4D-C3D	-2.49	123.83	129.46
82	LM	201	PEB	CMC-C3C-C4C	2.49	129.70	127.06
82	cE	202	PEB	CAC-CBC-CGC	-2.49	108.25	113.60
84	BG	1001	CYC	CHB-C4A-C3A	2.49	131.29	124.90
85	a6	605	BCR	C10-C11-C12	-2.49	115.46	123.22
82	sC	201	PEB	C4C-C3C-C2C	-2.49	105.21	107.50
82	GJ	202	PEB	C3B-C4B-NB	2.49	113.67	110.05
87	A2	802	CLA	C3B-C4B-NB	-2.49	108.21	110.52
82	P5	201	PEB	C4B-C3B-C2B	-2.49	104.03	106.78
82	NI	201	PEB	OD-C4D-C3D	-2.49	123.83	129.46
85	BL	616	BCR	C29-C28-C27	-2.49	105.82	111.38
82	pF	201	PEB	CHB-C4B-NB	-2.49	119.41	124.58
82	dG	203	PEB	CHC-C1D-ND	-2.49	110.58	113.72
84	FE	1001	CYC	CHA-C1A-C2A	-2.49	119.57	125.32
85	LN	205	BCR	C1-C6-C5	-2.49	119.11	122.61
87	5N	611	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
96	f6	101	HEM	C4C-C3C-C2C	-2.49	104.71	106.75
82	G9	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
82	W4	201	PEB	C1D-CHC-C4C	-2.48	109.59	113.26
82	PQ	202	PEB	CHB-C1C-C2C	-2.48	121.54	127.15
87	c6	609	CLA	CHB-C4A-NA	2.48	127.95	124.51
82	PK	201	PEB	CAB-CBB-CGB	-2.48	108.26	113.60
82	gB	201	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
82	l4	201	PEB	C4B-C3B-C2B	-2.48	104.03	106.78
82	nF	202	PEB	C4B-C3B-C2B	-2.48	104.03	106.78
82	EA	202	PEB	C3C-C4C-NC	2.48	110.57	108.33
82	w8	202	PEB	C3C-C4C-NC	2.48	110.57	108.33
82	hK	201	PEB	C3C-C4C-NC	2.48	110.57	108.33
94	dL	406	PL9	C32-C33-C34	-2.48	121.68	127.66
85	LN	201	BCR	C16-C15-C14	-2.48	118.39	123.47
82	Z9	303	PEB	CMA-C2A-C1A	-2.48	107.05	112.40
87	b6	605	CLA	C4B-CHC-C1C	-2.48	120.45	126.34
82	J5	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
82	z8	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
82	JF	201	PEB	CAB-C3B-C4B	2.48	129.40	125.01
82	DO	1002	PEB	CHA-C1B-NB	-2.48	119.74	124.93
82	JD	202	PEB	CMB-C2B-C1B	2.48	128.89	125.06
82	DF	201	PEB	CAB-CBB-CGB	-2.48	108.26	113.60
82	UB	302	PEB	C3B-C4B-NB	2.48	113.66	110.05
82	EA	201	PEB	C4B-C3B-C2B	-2.48	104.03	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	7N	602	CLA	CAD-C3D-C2D	2.48	152.78	140.80
87	62	309	CLA	C2B-C1B-NB	2.48	111.90	110.23
82	eK	201	PEB	C2A-C1A-NA	2.48	110.41	108.27
82	kG	201	PEB	OD-C4D-ND	-2.48	122.25	125.93
87	6N	607	CLA	C3B-C4B-NB	-2.48	108.21	110.52
82	cO	202	PEB	CAB-C3B-C4B	2.48	129.40	125.01
82	bB	201	PEB	C1D-CHC-C4C	2.48	116.92	113.26
82	I5	202	PEB	C3C-C4C-NC	2.48	110.57	108.33
82	X5	202	PEB	C3C-C4C-NC	2.48	110.57	108.33
82	1C	202	PEB	C3C-C4C-NC	2.48	110.57	108.33
82	cF	201	PEB	CHB-C4B-NB	-2.48	119.41	124.58
82	eE	202	PEB	OD-C4D-C3D	-2.48	123.83	129.46
87	d6	403	CLA	CHD-C1D-ND	-2.48	122.17	124.45
82	N5	201	PEB	CHB-C4B-C3B	-2.48	119.57	125.32
82	KB	301	PEB	CBC-CAC-C2C	2.48	119.53	112.63
82	cG	201	PEB	CAB-C3B-C4B	2.48	129.40	125.01
82	aF	202	PEB	C1D-CHC-C4C	-2.48	109.59	113.26
82	dG	202	PEB	OD-C4D-C3D	-2.48	123.83	129.46
84	JH	1003	CYC	CHA-C1A-C2A	-2.48	119.58	125.32
82	LJ	202	PEB	CAA-C3A-C2A	-2.48	108.06	114.26
82	JM	201	PEB	CHA-C1B-C2B	2.48	131.28	124.90
82	S9	202	PEB	CMB-C2B-C1B	2.48	128.89	125.06
87	52	601	CLA	C3B-C4B-NB	-2.48	108.21	110.52
87	72	607	CLA	CHB-C1B-NB	2.48	126.89	124.26
87	K2	106	CLA	CHC-C4B-NB	2.48	126.89	124.26
82	eA	301	PEB	C3B-C4B-NB	2.48	113.66	110.05
82	T9	202	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	fK	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	cK	202	PEB	OD-C4D-ND	-2.48	122.25	125.93
84	FH	1001	CYC	CHB-C1B-C2B	2.48	131.87	126.95
82	UJ	202	PEB	C1D-CHC-C4C	-2.48	109.60	113.26
85	CL	502	BCR	C39-C30-C25	-2.48	106.27	110.30
82	aO	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	KM	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06
82	OO	201	PEB	CHB-C1C-C2C	-2.48	121.55	127.15
82	IK	203	PEB	CHB-C1C-NC	2.48	131.00	125.32
83	A4	302	PUB	C2C-C1C-NC	2.48	113.66	110.05
84	CO	1001	CYC	CMB-C2B-C1B	2.48	127.27	124.17
82	dE	202	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	UI	202	PEB	CMA-C2A-C1A	-2.48	107.05	112.40
82	MP	201	PEB	CAC-CBC-CGC	-2.48	108.26	113.60
87	BN	834	CLA	CMB-C2B-C3B	2.48	132.60	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	12	603	CLA	CMB-C2B-C3B	2.48	132.60	126.59
88	d6	402	LHG	C5-O7-C7	-2.48	111.68	117.79
87	3N	301	CLA	CMD-C2D-C3D	2.48	133.32	127.61
82	RP	201	PEB	CMB-C2B-C1B	2.48	128.88	125.06
87	5N	605	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
82	mG	203	PEB	CAB-CBB-CGB	-2.48	108.26	113.60
82	OM	203	PEB	CAC-C2C-C1C	2.48	129.71	125.76
82	HA	203	PEB	OD-C4D-ND	-2.48	122.25	125.93
82	l1	202	PEB	OD-C4D-ND	-2.48	122.25	125.93
82	ZO	202	PEB	CHA-C1B-NB	-2.48	119.74	124.93
82	R4	202	PEB	CMC-C3C-C4C	2.48	129.69	127.06
87	5N	602	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
82	Q9	203	PEB	CMB-C2B-C1B	2.48	128.88	125.06
87	B2	824	CLA	CHB-C1B-C2B	-2.48	120.23	127.24
82	RK	202	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
82	fG	203	PEB	C3B-C4B-NB	2.48	113.66	110.05
87	BL	608	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
87	8N	305	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
85	L2	205	BCR	C27-C26-C25	-2.48	119.13	122.73
82	IA	202	PEB	OD-C4D-ND	-2.48	122.26	125.93
82	qK	203	PEB	OD-C4D-ND	-2.48	122.26	125.93
82	HP	202	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	eE	202	PEB	C3C-C4C-NC	2.48	110.57	108.33
82	UH	203	PEB	CHB-C4B-NB	-2.48	119.42	124.58
82	fE	201	PEB	CHB-C1C-C2C	-2.48	121.56	127.15
82	TP	201	PEB	CHB-C1C-NC	-2.48	119.64	125.32
82	VI	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	XI	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
87	bL	615	CLA	CHB-C4A-NA	2.48	127.94	124.51
82	j4	201	PEB	CMA-C2A-C1A	-2.48	107.06	112.40
87	52	604	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
82	gO	203	PEB	OD-C4D-ND	-2.48	122.26	125.93
83	ND	201	PUB	C4A-CHA-C1B	2.48	116.91	113.26
87	d6	403	CLA	C3B-C4B-NB	-2.48	108.22	110.52
82	SB	202	PEB	CHB-C1C-C2C	-2.48	121.56	127.15
82	IQ	202	PEB	C3C-C4C-NC	2.48	110.56	108.33
82	qC	203	PEB	CHC-C1D-ND	-2.48	110.59	113.72
82	mE	202	PEB	CAC-C2C-C1C	2.48	129.71	125.76
85	L2	201	BCR	C16-C15-C14	-2.48	118.40	123.47
82	WG	202	PEB	CHB-C4B-C3B	-2.48	119.58	125.32
82	KA	201	PEB	CHA-C1B-NB	-2.48	119.75	124.93
87	72	602	CLA	CAD-C3D-C2D	2.48	152.76	140.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	jJ	201	PEB	CHB-C1C-C2C	-2.48	121.56	127.15
82	CQ	202	PEB	CMB-C2B-C1B	2.48	128.88	125.06
82	mK	202	PEB	OD-C4D-C3D	-2.48	123.84	129.46
82	bF	202	PEB	C4B-C3B-C2B	-2.48	104.04	106.78
82	WD	202	PEB	C4C-C3C-C2C	-2.48	105.21	107.50
82	PI	202	PEB	C4C-C3C-C2C	-2.48	105.21	107.50
87	A2	827	CLA	CHB-C4A-NA	2.48	127.94	124.51
82	l4	201	PEB	CHB-C1C-C2C	-2.48	121.56	127.15
87	A2	830	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
82	UG	201	PEB	CMB-C2B-C1B	2.48	128.88	125.06
82	vF	202	PEB	CHB-C4B-C3B	-2.48	119.59	125.32
82	lE	203	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	hM	203	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	eO	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	cB	401	PEB	CHA-C1B-NB	-2.48	119.75	124.93
85	B2	841	BCR	C31-C1-C6	-2.48	106.28	110.30
82	SB	201	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
82	rF	202	PEB	CAC-C2C-C1C	2.48	129.71	125.76
94	d6	408	PL9	C25-C24-C26	2.48	119.44	115.27
87	JN	101	CLA	CHB-C1B-NB	2.48	126.88	124.26
84	F1	1001	CYC	CHB-C1B-C2B	2.48	131.86	126.95
87	BL	609	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
82	H7	203	PEB	C3B-C4B-NB	2.48	113.65	110.05
82	fJ	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	QF	202	PEB	OD-C4D-ND	-2.48	122.26	125.93
82	gK	201	PEB	C1C-CHB-C4B	2.48	133.84	128.28
82	IJ	203	PEB	C1D-CHC-C4C	-2.48	109.60	113.26
82	PH	201	PEB	C4C-C3C-C2C	-2.48	105.21	107.50
82	jE	201	PEB	CAC-C2C-C1C	2.48	129.71	125.76
82	eG	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	dH	203	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	j4	202	PEB	CHA-C1B-NB	-2.48	119.75	124.93
82	L5	203	PEB	CHC-C4C-NC	2.48	124.50	121.15
82	ZH	203	PEB	CAA-C3A-C4A	2.48	119.03	112.67
82	V1	202	PEB	C3C-C4C-NC	2.48	110.56	108.33
82	gH	201	PEB	CAB-CBB-CGB	-2.48	108.27	113.60
82	KF	203	PEB	CAB-C3B-C4B	2.48	129.39	125.01
82	dB	201	PEB	CHC-C1D-ND	-2.48	110.59	113.72
82	a4	201	PEB	CHB-C4B-C3B	-2.48	119.59	125.32
82	eF	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	FP	202	PEB	CAB-C3B-C4B	2.48	129.39	125.01
82	NP	202	PEB	C3B-C4B-NB	2.48	113.65	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NI	203	PEB	C4C-C3C-C2C	-2.48	105.22	107.50
87	LN	204	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
85	L2	205	BCR	C1-C6-C5	-2.48	119.13	122.61
82	HP	201	PEB	C1B-C2B-C3B	-2.48	103.67	106.51
94	D6	408	PL9	C53-C6-C1	2.48	120.05	114.99
82	UD	201	PEB	CBC-CAC-C2C	-2.48	105.75	112.63
83	ND	201	PUB	CHB-C1C-C2C	-2.48	119.59	125.32
82	fF	201	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	O5	203	PEB	CHB-C1C-NC	-2.48	119.65	125.32
82	M7	202	PEB	CHA-C1B-NB	-2.48	119.75	124.93
82	PI	201	PEB	OD-C4D-C3D	-2.48	123.85	129.46
82	YM	201	PEB	OD-C4D-C3D	-2.48	123.85	129.46
87	32	308	CLA	CMD-C2D-C3D	2.48	133.31	127.61
82	eH	202	PEB	OA-C1A-C2A	-2.48	124.20	126.17
82	TP	201	PEB	C1B-C2B-C3B	-2.48	103.67	106.51
82	IA	202	PEB	C4C-C3C-C2C	-2.48	105.22	107.50
82	RO	202	PEB	CMA-C2A-C1A	-2.47	107.07	112.40
82	CP	203	PEB	OD-C4D-C3D	-2.47	123.85	129.46
82	s8	202	PEB	C3B-C4B-NB	2.47	113.65	110.05
82	hM	202	PEB	C3B-C4B-NB	2.47	113.65	110.05
82	eH	202	PEB	OD-C4D-ND	-2.47	122.26	125.93
87	1N	603	CLA	CMB-C2B-C3B	2.47	132.58	126.59
82	f1	203	PEB	CMB-C2B-C1B	2.47	128.88	125.06
87	CL	513	CLA	CMB-C2B-C1B	-2.47	121.60	125.37
82	j1	202	PEB	CHB-C1C-C2C	-2.47	121.57	127.15
87	4N	601	CLA	CHB-C4A-NA	2.47	127.93	124.51
82	CA	201	PEB	CMA-C2A-C1A	-2.47	107.07	112.40
82	HF	201	PEB	CAB-C3B-C4B	2.47	129.39	125.01
82	GJ	201	PEB	CAB-C3B-C4B	2.47	129.39	125.01
87	82	304	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
82	QG	202	PEB	CBB-CAB-C3B	-2.47	105.75	112.63
82	qF	203	PEB	OD-C4D-C3D	-2.47	123.85	129.46
82	CB	202	PEB	CHB-C4B-NB	-2.47	119.43	124.58
82	gF	203	PEB	C3B-C4B-NB	2.47	113.65	110.05
82	NA	203	PEB	OD-C4D-ND	-2.47	122.27	125.93
98	BN	837	PQN	C10-C5-C4	-2.47	118.00	120.68
82	LA	203	PEB	C1D-CHC-C4C	-2.47	109.61	113.26
82	JJ	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
87	cL	514	CLA	CHB-C4A-NA	2.47	127.93	124.51
85	AN	804	BCR	C30-C25-C26	-2.47	119.13	122.61
82	JA	201	PEB	CHB-C4B-NB	-2.47	119.43	124.58
87	dL	409	CLA	C3B-C4B-NB	-2.47	108.22	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mM	202	PEB	CHB-C1C-NC	-2.47	119.65	125.32
82	SF	202	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
88	a6	610	LHG	C5-O7-C7	-2.47	111.70	117.79
84	K1	1001	CYC	CMB-C2B-C1B	2.47	127.25	124.17
82	OP	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
82	pC	201	PEB	CHA-C1B-NB	-2.47	119.76	124.93
82	OG	203	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	II	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	XJ	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	a4	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	J5	203	PEB	C3C-C4C-NC	2.47	110.56	108.33
82	kH	201	PEB	CMB-C2B-C1B	2.47	128.87	125.06
82	UE	203	PEB	CHB-C1C-NC	-2.47	119.65	125.32
87	A2	835	CLA	CHD-C1D-ND	-2.47	122.18	124.45
82	VQ	201	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
82	P7	201	PEB	CAB-C3B-C4B	2.47	129.38	125.01
82	rK	202	PEB	CAC-C2C-C1C	2.47	129.70	125.76
82	J9	201	PEB	CHC-C4C-NC	2.47	124.50	121.15
82	ZE	203	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	YP	501	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	TQ	202	PEB	CHA-C1B-NB	-2.47	119.76	124.93
87	RN	201	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
82	YM	202	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
82	B7	202	PEB	C4C-C3C-C2C	-2.47	105.22	107.50
82	D7	202	PEB	C4C-C3C-C2C	-2.47	105.22	107.50
83	Y7	302	PUB	C1B-C2B-C3B	-2.47	105.22	107.50
82	Z9	304	PEB	OD-C4D-ND	-2.47	122.27	125.93
82	H1	1002	PEB	CAC-C2C-C1C	2.47	129.70	125.76
82	eK	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	W9	201	PEB	OA-C1A-C2A	-2.47	124.21	126.17
87	2N	308	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
87	5N	606	CLA	CMB-C2B-C3B	2.47	132.58	126.59
82	FM	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	VA	202	PEB	CMC-C3C-C4C	2.47	129.68	127.06
82	VQ	203	PEB	CAC-C2C-C1C	2.47	129.70	125.76
103	8N	310	ZEX	C38-C24-C23	-2.47	108.38	112.20
82	gF	202	PEB	CHB-C1C-C2C	-2.47	121.57	127.15
84	EG	1001	CYC	CHB-C1B-NB	-2.47	120.75	126.06
87	ON	203	CLA	CHA-C1A-NA	-2.47	120.74	126.40
82	D1	1002	PEB	CHC-C1D-ND	-2.47	110.60	113.72
82	OK	201	PEB	CHA-C4A-NA	2.47	128.14	125.20
82	zC	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	c4	202	PEB	CAB-C3B-C4B	2.47	129.38	125.01
82	RM	201	PEB	CHA-C1B-C2B	2.47	131.26	124.90
82	VB	202	PEB	CMB-C2B-C1B	2.47	128.87	125.06
82	MP	202	PEB	CAC-C2C-C1C	2.47	129.70	125.76
87	CL	504	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
87	bL	619	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
82	T4	202	PEB	C3B-C4B-NB	2.47	113.64	110.05
82	NM	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	J9	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	fO	201	PEB	C4B-NB-C1B	-2.47	101.85	106.51
82	lJ	201	PEB	C1D-CHC-C4C	-2.47	109.61	113.26
82	XB	201	PEB	C3C-C4C-NC	2.47	110.56	108.33
82	WG	202	PEB	C3C-C4C-NC	2.47	110.56	108.33
82	j4	201	PEB	CAB-CBB-CGB	-2.47	108.28	113.60
82	J5	201	PEB	CAB-CBB-CGB	-2.47	108.28	113.60
82	AM	301	PEB	CHB-C1C-NC	-2.47	119.66	125.32
87	BN	833	CLA	CHB-C1B-NB	2.47	126.87	124.26
85	A2	804	BCR	C30-C25-C26	-2.47	119.13	122.61
82	aK	201	PEB	CHB-C4B-NB	-2.47	119.44	124.58
87	52	602	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
82	JI	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
84	H1	1001	CYC	C4D-ND-C1D	-2.47	105.38	109.79
82	RE	202	PEB	C4C-C3C-C2C	-2.47	105.22	107.50
82	JD	203	PEB	CHA-C1B-NB	-2.47	119.77	124.93
87	AL	403	CLA	C3B-C4B-NB	-2.47	108.22	110.52
87	IN	103	CLA	C3B-C4B-NB	-2.47	108.22	110.52
82	ZF	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	LP	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
87	82	304	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
96	f6	101	HEM	CMB-C2B-C1B	2.47	128.80	125.04
84	DO	1001	CYC	CBB-CAB-C3B	-2.47	105.62	112.43
82	L7	202	PEB	CAC-C2C-C1C	2.47	129.70	125.76
82	PQ	201	PEB	OD-C4D-ND	-2.47	122.27	125.93
82	aM	203	PEB	OD-C4D-ND	-2.47	122.27	125.93
87	BN	820	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
82	PQ	202	PEB	C3B-C4B-NB	2.47	113.64	110.05
82	YO	202	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
82	L7	203	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
82	pK	201	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
82	iO	203	PEB	CAC-CBC-CGC	-2.47	108.29	113.60
82	PH	201	PEB	C2A-C1A-NA	2.47	110.40	108.27
82	BA	202	PEB	C4C-C3C-C2C	-2.47	105.22	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EI	202	PEB	C4C-C3C-C2C	-2.47	105.22	107.50
82	YP	503	PEB	OD-C4D-C3D	-2.47	123.86	129.46
82	c4	202	PEB	CHC-C1D-ND	-2.47	110.60	113.72
82	QB	202	PEB	CAC-C2C-C1C	2.47	129.69	125.76
87	5N	603	CLA	C3B-C4B-NB	-2.47	108.22	110.52
87	5N	610	CLA	C3B-C4B-NB	-2.47	108.22	110.52
87	A2	808	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
82	BD	202	PEB	CMC-C3C-C4C	2.47	129.68	127.06
82	E5	201	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
82	cH	201	PEB	C1D-CHC-C4C	2.47	116.90	113.26
82	P5	202	PEB	C3C-C4C-NC	2.47	110.56	108.33
82	QH	201	PEB	C1C-NC-C4C	-2.47	105.20	109.60
85	BL	617	BCR	C33-C5-C4	2.47	118.36	113.62
82	SE	201	PEB	CAB-CBB-CGB	-2.47	108.29	113.60
95	CL	523	DGD	C4E-C3E-C2E	2.47	115.13	110.82
87	C6	509	CLA	CHB-C4A-NA	2.47	127.93	124.51
82	FA	202	PEB	OD-C4D-ND	-2.47	122.27	125.93
87	32	303	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
85	A2	846	BCR	C31-C1-C6	-2.47	106.30	110.30
82	cK	201	PEB	CHB-C4B-NB	-2.47	119.44	124.58
82	p8	202	PEB	CHA-C1B-C2B	2.47	131.25	124.90
87	cL	512	CLA	CHC-C1C-NC	2.47	127.95	124.20
82	wF	301	PEB	CAC-CBC-CGC	-2.47	108.29	113.60
82	FD	201	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
82	M9	302	PEB	CAC-C2C-C3C	2.47	132.72	127.07
82	gE	202	PEB	CHB-C1C-NC	-2.47	119.67	125.32
82	JQ	201	PEB	CHB-C4B-NB	-2.47	119.44	124.58
85	B2	840	BCR	C20-C21-C22	-2.47	123.79	127.31
82	CI	201	PEB	OD-C4D-C3D	-2.47	123.87	129.46
84	63	901	CYC	CBB-CAB-C3B	-2.47	105.63	112.43
82	SE	202	PEB	CAC-C2C-C1C	2.47	129.69	125.76
82	aB	201	PEB	CHA-C4A-NA	2.47	128.14	125.20
85	F6	101	BCR	C28-C27-C26	-2.47	109.67	114.08
84	D1	1003	CYC	C4D-ND-C1D	-2.47	105.39	109.79
87	ON	202	CLA	CHB-C4A-NA	2.47	127.92	124.51
82	PK	202	PEB	OD-C4D-C3D	-2.47	123.87	129.46
82	TM	202	PEB	OD-C4D-C3D	-2.47	123.87	129.46
87	bL	614	CLA	CMB-C2B-C3B	2.47	132.56	126.59
82	LD	201	PEB	C2A-C1A-NA	2.47	110.40	108.27
82	RF	202	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
85	H6	101	BCR	C23-C24-C25	-2.47	120.27	127.20
82	fG	202	PEB	CAA-C3A-C2A	-2.47	108.09	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JF	201	PEB	CAC-CBC-CGC	-2.47	108.29	113.60
82	vC	202	PEB	CAB-CBB-CGB	-2.47	108.29	113.60
82	Z9	301	PEB	CAC-C2C-C3C	2.47	132.72	127.07
84	BE	1001	CYC	CHB-C1B-NB	-2.47	120.76	126.06
82	uF	203	PEB	CHA-C1B-NB	-2.47	119.77	124.93
82	IF	203	PEB	CHB-C1C-NC	2.47	130.97	125.32
82	y8	202	PEB	CHB-C1C-NC	2.47	130.97	125.32
82	OG	201	PEB	CMA-C2A-C1A	-2.47	107.09	112.40
82	R4	202	PEB	CMA-C2A-C1A	-2.47	107.09	112.40
82	pC	202	PEB	CHA-C1B-C2B	2.47	131.24	124.90
82	KK	203	PEB	CAB-C3B-C4B	2.47	129.37	125.01
82	sC	202	PEB	C3B-C4B-NB	2.47	113.64	110.05
82	oF	202	PEB	C3B-C4B-NB	2.47	113.64	110.05
82	e1	201	PEB	CHC-C4C-NC	2.47	124.49	121.15
82	W5	203	PEB	CHC-C4C-NC	2.47	124.49	121.15
82	TI	202	PEB	OD-C4D-C3D	-2.47	123.87	129.46
82	LA	201	PEB	C1B-C2B-C3B	-2.47	103.68	106.51
82	Z4	202	PEB	CHA-C1B-NB	-2.47	119.77	124.93
82	DK	203	PEB	C2B-C1B-NB	2.47	115.79	110.53
87	1N	603	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
82	YA	301	PEB	CMB-C2B-C1B	2.47	128.86	125.06
82	wK	302	PEB	CBA-CAA-C3A	-2.47	107.98	113.47
84	FO	1001	CYC	CBD-CAD-C3D	-2.47	105.78	112.63
91	A6	407	PHO	C4B-NB-C1B	-2.47	105.01	108.83
85	BN	841	BCR	C31-C1-C6	-2.47	106.30	110.30
87	CL	511	CLA	C11-C12-C13	-2.47	107.95	115.92
82	IQ	202	PEB	OD-C4D-ND	-2.47	122.28	125.93
82	S5	201	PEB	CMC-C3C-C2C	2.47	130.94	125.61
82	vF	201	PEB	C3B-C4B-NB	2.47	113.64	110.05
83	BJ	302	PUB	C2C-C1C-NC	2.47	113.64	110.05
82	DJ	201	PEB	C1D-CHC-C4C	2.47	116.89	113.26
82	v8	201	PEB	CAC-C2C-C1C	2.47	129.69	125.76
87	3N	304	CLA	CAA-C2A-C3A	-2.47	106.03	112.78
82	Q1	203	PEB	OD-C4D-C3D	-2.47	123.87	129.46
82	nK	201	PEB	OD-C4D-C3D	-2.47	123.87	129.46
82	JQ	201	PEB	CAB-C3B-C4B	2.47	129.37	125.01
83	xK	305	PUB	CAC-C2C-C1C	2.47	129.37	125.01
82	kJ	201	PEB	C1D-CHC-C4C	2.47	116.89	113.26
84	73	1002	CYC	CAD-C3D-C4D	2.47	129.69	125.76
82	AP	201	PEB	OD-C4D-C3D	-2.47	123.88	129.46
82	TJ	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	DB	203	PEB	C1B-C2B-C3B	-2.46	103.68	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	IG	1001	CYC	C4A-C3A-C2A	-2.46	103.68	106.51
82	GM	202	PEB	C3C-C4C-NC	2.46	110.55	108.33
84	BG	1001	CYC	C1B-NB-C4B	-2.46	107.53	110.67
82	AE	301	PEB	CMB-C2B-C1B	2.46	128.86	125.06
82	JP	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
83	BM	302	PUB	CAB-CBB-CGB	-2.46	108.30	113.60
82	UJ	202	PEB	CHC-C1D-ND	-2.46	110.61	113.72
82	MJ	201	PEB	CHA-C1B-NB	-2.46	119.78	124.93
82	p8	201	PEB	CAA-C3A-C2A	-2.46	108.10	114.26
98	B2	837	PQN	C10-C5-C4	-2.46	118.01	120.68
82	NF	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	HI	203	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	LM	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	wK	302	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	aF	201	PEB	C2A-C1A-NA	2.46	110.40	108.27
82	wF	303	PEB	OA-C1A-C2A	-2.46	124.21	126.17
82	WB	401	PEB	CHB-C4B-NB	-2.46	119.45	124.58
87	A2	813	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
82	VJ	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
95	B2	844	DGD	O1G-C1A-C2A	2.46	119.64	111.91
82	b4	201	PEB	OD-C4D-ND	-2.46	122.28	125.93
82	UQ	201	PEB	CBC-CAC-C2C	-2.46	105.78	112.63
87	12	603	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
85	kL	100	BCR	C7-C8-C9	-2.46	122.51	126.23
82	RG	202	PEB	CAB-C3B-C4B	2.46	129.37	125.01
82	HI	201	PEB	CAB-C3B-C4B	2.46	129.37	125.01
82	lH	201	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
87	4N	606	CLA	C3B-C4B-NB	-2.46	108.23	110.52
82	YQ	201	PEB	CMB-C2B-C1B	2.46	128.86	125.06
82	GP	202	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
82	uF	202	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
82	YM	201	PEB	CMA-C2A-C1A	-2.46	107.09	112.40
82	VB	202	PEB	CAB-CBB-CGB	-2.46	108.30	113.60
82	SA	201	PEB	CHB-C4B-NB	-2.46	119.45	124.58
87	bL	619	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
82	UF	201	PEB	CHA-C1B-C2B	2.46	131.23	124.90
82	HQ	202	PEB	CHB-C1C-C2C	-2.46	121.59	127.15
82	KE	201	PEB	OD-C4D-ND	-2.46	122.28	125.93
87	BN	831	CLA	C2A-C1A-CHA	2.46	128.16	123.86
82	V7	202	PEB	CHC-C1D-ND	-2.46	110.61	113.72
82	FD	202	PEB	CMB-C2B-C1B	2.46	128.86	125.06
82	AM	302	PEB	C3C-C4C-NC	2.46	110.55	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	sK	203	PEB	C3C-C4C-NC	2.46	110.55	108.33
87	A2	828	CLA	CHA-C4D-ND	2.46	137.65	132.50
82	EI	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	RE	202	PEB	CAB-C3B-C4B	2.46	129.36	125.01
82	VJ	202	PEB	O2B-CGB-CBB	2.46	121.94	114.03
82	KG	201	PEB	OD-C4D-ND	-2.46	122.28	125.93
82	RD	203	PEB	CHA-C1B-C2B	2.46	131.23	124.90
84	V3	1001	CYC	CHD-C1D-C2D	2.46	133.53	127.49
83	AG	303	PUB	C2C-C1C-NC	2.46	113.63	110.05
82	RH	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
82	mG	203	PEB	CMB-C2B-C1B	2.46	128.85	125.06
85	Z6	101	BCR	C38-C26-C27	2.46	118.34	113.62
82	KI	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	xF	304	PEB	OD-C4D-C3D	-2.46	123.88	129.46
87	B2	819	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
87	cL	516	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
82	XJ	202	PEB	CHA-C1B-NB	-2.46	119.78	124.93
85	BN	841	BCR	C20-C21-C22	-2.46	123.80	127.31
82	fF	202	PEB	CAB-C3B-C4B	2.46	129.36	125.01
85	b6	601	BCR	C3-C4-C5	-2.46	109.68	114.08
82	fG	201	PEB	CHB-C1C-C2C	-2.46	121.60	127.15
82	PQ	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	mE	203	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	nF	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
82	iE	201	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
82	CI	202	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
82	cO	203	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
87	62	311	CLA	C3B-C4B-NB	-2.46	108.23	110.52
87	AL	403	CLA	CHB-C4A-NA	2.46	127.92	124.51
82	xF	304	PEB	CHB-C4B-NB	-2.46	119.46	124.58
82	D1	1002	PEB	CHA-C1B-C2B	2.46	131.23	124.90
82	JJ	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
87	L2	202	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
82	W1	201	PEB	OD-C4D-ND	-2.46	122.28	125.93
82	SG	201	PEB	CAB-CBB-CGB	-2.46	108.31	113.60
82	JD	201	PEB	CAB-C3B-C4B	2.46	129.36	125.01
82	TE	201	PEB	C1B-C2B-C3B	-2.46	103.68	106.51
82	O9	202	PEB	C1B-C2B-C3B	-2.46	103.68	106.51
82	kJ	202	PEB	C1B-C2B-C3B	-2.46	103.68	106.51
82	mM	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	GE	1002	PEB	CHA-C1B-NB	-2.46	119.79	124.93
82	AQ	303	PEB	C1C-CHB-C4B	-2.46	122.77	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UJ	203	PEB	CMC-C3C-C4C	-2.46	124.45	127.06
82	RI	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	Y1	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	MF	202	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
82	OI	203	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
87	62	313	CLA	C3B-C4B-NB	-2.46	108.23	110.52
82	mG	202	PEB	C3B-C4B-NB	2.46	113.63	110.05
82	oK	202	PEB	C3B-C4B-NB	2.46	113.63	110.05
82	tK	202	PEB	CHA-C1B-C2B	-2.46	118.58	124.90
85	bL	601	BCR	C21-C20-C19	-2.46	115.54	123.22
82	B7	201	PEB	CHC-C1D-ND	-2.46	110.61	113.72
87	A2	815	CLA	C2A-C1A-CHA	2.46	128.16	123.86
82	UI	201	PEB	CHC-C4C-NC	2.46	124.48	121.15
82	xK	304	PEB	CHB-C4B-NB	-2.46	119.46	124.58
82	DB	203	PEB	CMC-C3C-C4C	2.46	129.67	127.06
82	HJ	202	PEB	O2B-CGB-CBB	2.46	121.93	114.03
82	DJ	201	PEB	CAC-C2C-C1C	2.46	129.68	125.76
82	RI	202	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
82	AQ	301	PEB	CHA-C1B-NB	-2.46	119.79	124.93
82	v8	202	PEB	CAB-CBB-CGB	-2.46	108.31	113.60
82	cO	203	PEB	CAC-CBC-CGC	-2.46	108.31	113.60
82	W9	202	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
82	qF	202	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
85	bL	603	BCR	C33-C5-C4	2.46	118.34	113.62
82	GK	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	AP	203	PEB	C1C-NC-C4C	2.46	113.97	109.60
82	T4	203	PEB	CAC-CBC-CGC	-2.46	108.31	113.60
87	AN	808	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
82	ZG	203	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	J5	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	YG	202	PEB	CMC-C3C-C2C	2.46	130.92	125.61
87	82	307	CLA	CHB-C4A-NA	2.46	127.91	124.51
82	QG	201	PEB	CMC-C3C-C4C	2.46	129.67	127.06
82	XM	201	PEB	CMC-C3C-C4C	2.46	129.67	127.06
82	IK	201	PEB	C3C-C4C-NC	2.46	110.55	108.33
82	CD	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
82	YD	201	PEB	CMB-C2B-C1B	2.46	128.85	125.06
82	fM	201	PEB	CMB-C2B-C1B	2.46	128.85	125.06
82	z8	202	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
82	kG	201	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
87	B2	815	CLA	C3B-C4B-NB	-2.46	108.23	110.52
87	C6	511	CLA	C3B-C4B-NB	-2.46	108.23	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WG	201	PEB	CHB-C4B-C3B	-2.46	119.63	125.32
87	AN	828	CLA	CHA-C4D-ND	2.46	137.64	132.50
94	dL	406	PL9	C22-C23-C24	-2.46	121.74	127.66
82	B9	202	PEB	CHA-C1B-C2B	2.46	131.22	124.90
82	lJ	203	PEB	C1D-CHC-C4C	-2.46	109.63	113.26
82	PA	201	PEB	CAB-C3B-C4B	2.46	129.35	125.01
82	L7	203	PEB	C3B-C4B-NB	2.46	113.62	110.05
83	AE	303	PUB	C2C-C1C-NC	2.46	113.62	110.05
82	EP	202	PEB	CHC-C1D-ND	-2.46	110.62	113.72
82	FF	201	PEB	CMA-C2A-C1A	-2.46	107.11	112.40
82	yC	202	PEB	CHB-C1C-NC	2.46	130.95	125.32
82	fM	202	PEB	CHB-C1C-NC	-2.46	119.69	125.32
82	lM	203	PEB	CHB-C1C-NC	-2.46	119.69	125.32
85	C6	508	BCR	C23-C24-C25	2.46	134.10	127.20
96	fL	102	HEM	C4A-CHB-C1B	-2.46	120.51	126.34
82	f4	202	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
82	AI	202	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
87	B2	817	CLA	CMB-C2B-C3B	2.46	132.54	126.59
87	1N	609	CLA	C3B-C4B-NB	-2.46	108.24	110.52
87	B6	605	CLA	CHB-C4A-NA	2.46	127.91	124.51
82	O1	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
84	x3	1001	CYC	CHD-C1D-C2D	2.46	133.52	127.49
87	c6	610	CLA	O2D-CGD-CBD	2.46	115.63	111.27
82	ND	204	PEB	OD-C4D-C3D	-2.46	123.89	129.46
82	A7	201	PEB	OA-C1A-C2A	-2.46	124.22	126.17
82	YE	202	PEB	CMC-C3C-C2C	2.46	130.92	125.61
84	N4	1001	CYC	CHB-C4A-C3A	2.46	131.22	124.90
82	qK	202	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
82	iM	201	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
84	FE	1001	CYC	C4A-C3A-C2A	-2.46	103.69	106.51
82	O1	201	PEB	OD-C4D-C3D	-2.46	123.90	129.46
82	UP	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
82	Y7	301	PEB	CMB-C2B-C1B	2.46	128.85	125.06
82	DF	202	PEB	CAC-CBC-CGC	-2.46	108.32	113.60
87	bL	606	CLA	CHB-C4A-NA	2.46	127.91	124.51
82	FM	202	PEB	O2B-CGB-CBB	2.46	121.92	114.03
82	OA	202	PEB	CAC-C2C-C1C	2.46	129.67	125.76
82	OA	202	PEB	CHB-C1C-C2C	-2.46	121.61	127.15
82	HD	202	PEB	CHB-C1C-C2C	-2.46	121.61	127.15
82	cM	201	PEB	C4C-C3C-C2C	-2.46	105.23	107.50
82	MB	201	PEB	CMA-C2A-C1A	-2.46	107.11	112.40
82	AI	201	PEB	OD-C4D-C3D	-2.46	123.90	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	l1	201	PEB	OD-C4D-C3D	-2.46	123.90	129.46
82	YE	202	PEB	CAC-CBC-CGC	-2.46	108.32	113.60
82	XK	203	PEB	CAC-CBC-CGC	-2.46	108.32	113.60
82	DD	202	PEB	CAA-C3A-C4A	-2.46	106.37	112.67
82	KB	301	PEB	CHA-C1B-C2B	2.46	131.21	124.90
82	VD	201	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
84	CG	1001	CYC	CHA-C1A-C2A	-2.46	119.64	125.32
82	F7	201	PEB	OD-C4D-C3D	-2.46	123.90	129.46
82	D5	202	PEB	CAB-C3B-C4B	2.45	129.35	125.01
82	LJ	202	PEB	OD-C4D-C3D	-2.45	123.90	129.46
82	CK	203	PEB	OD-C4D-C3D	-2.45	123.90	129.46
82	UQ	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46
87	BL	621	CLA	C2A-C1A-CHA	2.45	128.15	123.86
82	eG	203	PEB	OD-C4D-ND	-2.45	122.29	125.93
82	BB	203	PEB	CAB-CBB-CGB	-2.45	108.32	113.60
82	TO	203	PEB	CAC-CBC-CGC	-2.45	108.32	113.60
82	B5	201	PEB	CAC-C2C-C1C	2.45	129.67	125.76
82	H5	203	PEB	CAC-C2C-C1C	2.45	129.67	125.76
87	12	609	CLA	C3B-C4B-NB	-2.45	108.24	110.52
87	52	603	CLA	C3B-C4B-NB	-2.45	108.24	110.52
95	DL	408	DGD	O3G-C1D-C2D	2.45	112.14	108.30
87	B6	607	CLA	CHB-C4A-NA	2.45	127.91	124.51
82	HE	1002	PEB	C1D-CHC-C4C	2.45	116.88	113.26
84	NO	1001	CYC	CHA-C4D-C3D	-2.45	121.61	127.15
82	J5	201	PEB	CHB-C1C-NC	-2.45	119.70	125.32
82	TP	202	PEB	C3B-C4B-NB	2.45	113.62	110.05
82	VJ	202	PEB	CHB-C4B-NB	-2.45	119.47	124.58
82	PD	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46
82	hO	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46
87	7N	607	CLA	CHB-C1B-NB	2.45	126.86	124.26
85	J2	102	BCR	C15-C16-C17	-2.45	118.45	123.47
82	BI	203	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
82	CJ	203	PEB	C1C-NC-C4C	-2.45	105.23	109.60
82	A4	304	PEB	OD-C4D-C3D	-2.45	123.90	129.46
83	NQ	201	PUB	CMD-C2D-C3D	2.45	131.45	127.77
82	fE	201	PEB	C3C-C4C-NC	2.45	110.54	108.33
82	CM	202	PEB	CHA-C1B-NB	-2.45	119.80	124.93
82	JQ	203	PEB	CHA-C1B-NB	-2.45	119.80	124.93
82	W9	201	PEB	O1B-CGB-CBB	-2.45	115.20	123.08
82	U5	203	PEB	C2A-C1A-NA	2.45	110.39	108.27
87	BN	823	CLA	C3B-C4B-NB	-2.45	108.24	110.52
87	BN	836	CLA	C3B-C4B-NB	-2.45	108.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	CL	510	CLA	CHC-C1C-NC	2.45	127.92	124.20
82	ZG	202	PEB	CAC-C2C-C1C	2.45	129.67	125.76
82	XA	203	PEB	CHC-C4C-NC	2.45	124.47	121.15
87	42	604	CLA	CHC-C4B-NB	2.45	126.85	124.26
82	a4	201	PEB	CAB-C3B-C4B	2.45	129.35	125.01
87	R2	201	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
82	oF	201	PEB	O2C-CGC-CBC	2.45	121.91	114.03
82	CF	201	PEB	CHB-C1C-NC	-2.45	119.70	125.32
82	FQ	203	PEB	CAC-C2C-C1C	2.45	129.67	125.76
82	HB	201	PEB	OD-C4D-ND	-2.45	122.30	125.93
82	dF	202	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
82	wF	302	PEB	OD-C4D-C3D	-2.45	123.90	129.46
82	GF	202	PEB	C3C-C4C-NC	2.45	110.54	108.33
82	hK	202	PEB	CMC-C3C-C4C	2.45	129.66	127.06
82	AD	304	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	dG	203	PEB	C3B-C4B-NB	2.45	113.62	110.05
82	T5	201	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
87	BN	818	CLA	CMB-C2B-C3B	2.45	132.53	126.59
82	SJ	203	PEB	OD-C4D-ND	-2.45	122.30	125.93
82	FP	201	PEB	CAC-CBC-CGC	-2.45	108.33	113.60
82	ID	201	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
82	pF	201	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
82	gK	202	PEB	CHB-C1C-C2C	-2.45	121.62	127.15
82	LM	202	PEB	CHA-C1B-NB	-2.45	119.81	124.93
82	dG	202	PEB	CAA-C3A-C4A	-2.45	106.38	112.67
82	V4	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	DF	203	PEB	C2B-C1B-NB	2.45	115.76	110.53
82	AG	301	PEB	CMB-C2B-C1B	2.45	128.84	125.06
82	jH	203	PEB	CMB-C2B-C1B	2.45	128.84	125.06
82	jJ	203	PEB	CMB-C2B-C1B	2.45	128.84	125.06
83	xF	305	PUB	CAC-C2C-C1C	2.45	129.34	125.01
82	GK	202	PEB	C3C-C4C-NC	2.45	110.54	108.33
82	WM	202	PEB	C3C-C4C-NC	2.45	110.54	108.33
82	SK	202	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
82	cJ	201	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	X7	203	PEB	OD-C4D-ND	-2.45	122.30	125.93
82	dE	202	PEB	CAA-C3A-C4A	-2.45	106.38	112.67
82	XD	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	UG	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	RP	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	F9	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
84	NO	1001	CYC	C1B-NB-C4B	-2.45	107.55	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	819	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
82	CB	201	PEB	CMA-C2A-C1A	-2.45	107.12	112.40
84	BE	1002	CYC	CMC-C2C-C1C	-2.45	107.12	112.40
82	HK	201	PEB	CAB-C3B-C4B	2.45	129.34	125.01
82	IM	202	PEB	CAB-C3B-C4B	2.45	129.34	125.01
82	B9	203	PEB	CAB-C3B-C4B	2.45	129.34	125.01
82	Q7	201	PEB	C3B-C4B-NB	2.45	113.61	110.05
82	GE	1002	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
82	BA	201	PEB	CAB-C3B-C2B	2.45	132.44	127.88
82	qF	203	PEB	CHA-C1B-NB	-2.45	119.81	124.93
82	HQ	202	PEB	CHC-C1D-ND	-2.45	110.62	113.72
82	y8	203	PEB	OD-C4D-ND	-2.45	122.30	125.93
103	8N	310	ZEX	C30-C31-C32	2.45	130.86	123.22
82	UG	203	PEB	CHB-C1C-NC	-2.45	119.71	125.32
82	PQ	202	PEB	CAB-C3B-C4B	2.45	129.34	125.01
82	UE	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	AG	301	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	IJ	203	PEB	CHA-C1B-NB	-2.45	119.81	124.93
87	B2	834	CLA	CMB-C2B-C3B	2.45	132.52	126.59
82	Q7	201	PEB	C2A-C1A-NA	2.45	110.39	108.27
84	N4	1001	CYC	CHA-C4D-C3D	-2.45	121.62	127.15
82	B7	201	PEB	CHB-C1C-NC	-2.45	119.71	125.32
87	CL	515	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
82	A1	305	PEB	CMB-C2B-C1B	2.45	128.84	125.06
82	CF	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	SK	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	NP	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	NQ	204	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	M5	305	PEB	OD-C4D-C3D	-2.45	123.91	129.46
94	aL	601	PL9	C35-C34-C33	-2.45	117.39	123.68
82	p8	201	PEB	CHA-C1B-NB	-2.45	119.81	124.93
82	ZF	202	PEB	C2B-C1B-NB	2.45	115.76	110.53
82	aJ	203	PEB	C3C-C4C-NC	2.45	110.54	108.33
82	cO	202	PEB	CHC-C1D-ND	-2.45	110.63	113.72
82	L7	201	PEB	C1B-C2B-C3B	-2.45	103.70	106.51
82	CB	202	PEB	CHB-C1C-NC	-2.45	119.71	125.32
82	SJ	201	PEB	CAB-CBB-CGB	-2.45	108.33	113.60
82	H7	201	PEB	CAC-CBC-CGC	-2.45	108.33	113.60
85	BN	840	BCR	C20-C21-C22	-2.45	123.81	127.31
82	VD	203	PEB	CAC-C2C-C1C	2.45	129.66	125.76
82	RB	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
82	XP	202	PEB	CAA-C3A-C4A	-2.45	106.39	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	rK	201	PEB	C2A-C1A-NA	2.45	110.38	108.27
82	jE	202	PEB	OD-C4D-ND	-2.45	122.30	125.93
82	M9	305	PEB	OD-C4D-ND	-2.45	122.30	125.93
87	O2	203	CLA	CHA-C1A-NA	-2.45	120.79	126.40
82	ID	201	PEB	CHA-C4A-NA	2.45	128.12	125.20
84	GE	1001	CYC	CMB-C2B-C1B	2.45	127.22	124.17
82	DB	203	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	ED	202	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	DQ	203	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	wC	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
85	K2	105	BCR	C3-C4-C5	-2.45	109.71	114.08
87	BL	603	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
84	73	1002	CYC	CBD-CAD-C3D	-2.45	105.83	112.63
82	DE	1002	PEB	O2B-CGB-CBB	2.45	121.89	114.03
82	kG	202	PEB	CAC-C2C-C3C	2.45	132.68	127.07
82	OG	201	PEB	CAC-C2C-C1C	2.45	129.66	125.76
82	UM	203	PEB	CAC-C2C-C1C	2.45	129.66	125.76
82	cG	202	PEB	CMB-C2B-C1B	2.45	128.83	125.06
82	ZJ	201	PEB	CBC-CAC-C2C	-2.45	105.83	112.63
82	uK	201	PEB	C3B-C4B-NB	2.45	113.61	110.05
84	BE	1001	CYC	CHA-C1A-C2A	-2.45	119.66	125.32
87	b6	618	CLA	CHB-C4A-NA	2.45	127.90	124.51
82	SA	201	PEB	OD-C4D-ND	-2.45	122.31	125.93
82	QH	203	PEB	OD-C4D-C3D	-2.45	123.92	129.46
82	gO	202	PEB	OD-C4D-C3D	-2.45	123.92	129.46
82	LA	202	PEB	C1C-NC-C4C	-2.45	105.24	109.60
82	WB	402	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	NK	202	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	k4	201	PEB	C4C-C3C-C2C	-2.45	105.24	107.50
82	HG	1002	PEB	C1D-CHC-C4C	2.45	116.86	113.26
82	KA	201	PEB	CAA-C3A-C4A	-2.45	106.39	112.67
84	EE	1001	CYC	CHB-C1B-NB	-2.45	120.81	126.06
82	S9	201	PEB	CAB-C3B-C4B	2.45	129.34	125.01
87	52	606	CLA	CMB-C2B-C3B	2.45	132.51	126.59
82	LB	201	PEB	C1C-CHB-C4B	2.45	133.77	128.28
82	B7	202	PEB	C3B-C4B-NB	2.45	113.61	110.05
87	F2	202	CLA	C2D-C1D-ND	-2.45	108.30	110.10
87	3N	312	CLA	C2A-C1A-CHA	2.45	128.14	123.86
82	uC	203	PEB	CAA-C3A-C4A	-2.45	106.39	112.67
82	hO	201	PEB	C2A-C1A-NA	2.45	110.38	108.27
82	SE	202	PEB	OD-C4D-C3D	-2.45	123.92	129.46
87	cL	508	CLA	CAC-C3C-C2C	-2.45	123.34	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YB	201	PEB	CAB-CBB-CGB	-2.45	108.34	113.60
82	WE	201	PEB	CHB-C4B-C3B	-2.45	119.66	125.32
82	UA	201	PEB	C1C-NC-C4C	-2.45	105.25	109.60
95	C6	502	DGD	C4D-C3D-C2D	-2.45	106.55	110.82
82	AD	303	PEB	C1C-CHB-C4B	-2.45	122.80	128.28
82	XM	202	PEB	OD-C4D-C3D	-2.45	123.92	129.46
87	BN	822	CLA	CBA-CAA-C2A	2.45	121.08	113.86
82	m1	202	PEB	C2A-C1A-NA	2.45	110.38	108.27
85	KN	104	BCR	C3-C4-C5	-2.45	109.71	114.08
82	DK	202	PEB	OD-C4D-ND	-2.45	122.31	125.93
87	42	601	CLA	CHB-C4A-NA	2.44	127.89	124.51
82	BD	202	PEB	OD-C4D-C3D	-2.44	123.92	129.46
82	xK	304	PEB	OD-C4D-C3D	-2.44	123.92	129.46
87	AN	815	CLA	C2A-C1A-CHA	2.44	128.13	123.86
82	jK	201	PEB	CMC-C3C-C4C	2.44	129.65	127.06
82	UI	202	PEB	C4C-C3C-C2C	-2.44	105.24	107.50
84	FH	1001	CYC	CHA-C1A-C2A	-2.44	119.66	125.32
87	B2	833	CLA	CHB-C1B-NB	2.44	126.84	124.26
87	C6	517	CLA	CHB-C1B-NB	2.44	126.84	124.26
84	T3	1001	CYC	C1B-C2B-C3B	-2.44	105.32	107.87
82	YK	203	PEB	C3B-C4B-NB	2.44	113.61	110.05
82	gK	203	PEB	C3B-C4B-NB	2.44	113.61	110.05
95	BN	844	DGD	O1G-C1A-C2A	2.44	119.58	111.91
83	yF	303	PUB	CAB-C3B-C4B	2.44	129.66	125.76
85	HL	103	BCR	C16-C15-C14	-2.44	118.47	123.47
82	R5	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
82	Q1	203	PEB	CMC-C3C-C4C	2.44	129.65	127.06
82	LA	203	PEB	C1B-C2B-C3B	-2.44	103.70	106.51
82	lK	203	PEB	OD-C4D-ND	-2.44	122.31	125.93
82	L7	202	PEB	C1C-NC-C4C	-2.44	105.25	109.60
87	BL	605	CLA	CAA-CBA-CGA	2.44	120.39	113.25
82	DA	202	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	VQ	202	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	iF	202	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
87	72	607	CLA	CHA-C1A-NA	-2.44	120.80	126.40
82	LI	202	PEB	OD-C4D-C3D	-2.44	123.92	129.46
82	ZK	202	PEB	OD-C4D-C3D	-2.44	123.92	129.46
87	cL	506	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
82	dK	202	PEB	CHB-C4B-C3B	-2.44	119.67	125.32
87	62	305	CLA	CHD-C1D-ND	-2.44	122.21	124.45
82	nF	201	PEB	CMC-C3C-C4C	2.44	129.65	127.06
82	IP	202	PEB	CAB-CBB-CGB	-2.44	108.35	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	JN	102	BCR	C15-C16-C17	-2.44	118.47	123.47
82	DA	201	PEB	C1D-CHC-C4C	2.44	116.86	113.26
85	A2	847	BCR	C30-C25-C26	-2.44	119.17	122.61
87	2N	303	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
82	VM	202	PEB	CAC-C2C-C1C	2.44	129.65	125.76
83	NQ	201	PUB	CAB-C3B-C4B	2.44	129.65	125.76
82	iK	202	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	BD	201	PEB	CMA-C2A-C1A	-2.44	107.14	112.40
82	K7	201	PEB	CHA-C1B-NB	-2.44	119.82	124.93
82	xK	303	PEB	OA-C1A-C2A	-2.44	124.23	126.17
82	TJ	202	PEB	CAA-C3A-C2A	-2.44	108.16	114.26
82	mE	203	PEB	CMB-C2B-C1B	2.44	128.82	125.06
82	H5	202	PEB	OD-C4D-C3D	-2.44	123.93	129.46
82	eB	202	PEB	C1D-CHC-C4C	-2.44	109.66	113.26
87	O2	202	CLA	CHB-C4A-NA	2.44	127.89	124.51
82	D4	1002	PEB	CHA-C1B-NB	-2.44	119.83	124.93
83	A4	303	PUB	CHC-C1D-ND	-2.44	110.64	113.72
82	tF	202	PEB	CHA-C1B-C2B	-2.44	118.62	124.90
82	aJ	201	PEB	OD-C4D-ND	-2.44	122.31	125.93
82	fG	202	PEB	C2A-C3A-C4A	-2.44	97.68	101.34
84	F1	1001	CYC	CHA-C1A-C2A	-2.44	119.67	125.32
82	TP	201	PEB	CMB-C2B-C1B	2.44	128.82	125.06
82	f1	201	PEB	CMB-C2B-C1B	2.44	128.82	125.06
82	BA	201	PEB	CHB-C1C-NC	-2.44	119.73	125.32
82	XD	203	PEB	CHA-C1B-NB	-2.44	119.83	124.93
84	V3	1001	CYC	CAB-C3B-C2B	2.44	131.71	127.53
82	HB	203	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
87	R2	203	CLA	CHB-C4A-NA	2.44	127.89	124.51
95	cL	520	DGD	C4E-C3E-C2E	2.44	115.08	110.82
82	h4	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46
82	UK	201	PEB	CHA-C1B-C2B	2.44	131.18	124.90
82	GG	1002	PEB	C1B-C2B-C3B	-2.44	103.70	106.51
82	KM	201	PEB	C3B-C4B-NB	2.44	113.60	110.05
103	82	310	ZEX	C30-C31-C32	2.44	130.84	123.22
82	SP	203	PEB	CBA-CAA-C3A	-2.44	108.03	113.47
85	LN	205	BCR	C27-C26-C25	-2.44	119.19	122.73
82	OM	201	PEB	CHB-C1C-C2C	-2.44	121.64	127.15
82	aB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
83	NQ	201	PUB	CHB-C1C-C2C	-2.44	119.67	125.32
82	ZF	201	PEB	CHA-C4A-NA	2.44	128.11	125.20
87	aL	606	CLA	C6-C7-C8	-2.44	108.03	115.92
82	BB	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HJ	202	PEB	OD-C4D-C3D	-2.44	123.93	129.46
82	CK	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46
87	C6	513	CLA	C3B-C4B-NB	-2.44	108.25	110.52
82	RG	202	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	DQ	201	PEB	CMB-C2B-C1B	2.44	128.82	125.06
87	BN	833	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
85	a6	605	BCR	C16-C15-C14	-2.44	118.48	123.47
85	a6	605	BCR	C11-C10-C9	-2.44	123.83	127.31
82	RO	202	PEB	C1C-NC-C4C	-2.44	105.26	109.60
82	SB	201	PEB	CMA-C2A-C1A	-2.44	107.14	112.40
82	UJ	203	PEB	OD-C4D-ND	-2.44	122.32	125.93
82	YJ	203	PEB	OD-C4D-ND	-2.44	122.32	125.93
82	j1	203	PEB	CMB-C2B-C1B	2.44	128.82	125.06
82	WB	402	PEB	CHB-C1C-C2C	-2.44	121.65	127.15
82	ZH	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46
82	Z1	202	PEB	OD-C4D-C3D	-2.44	123.93	129.46
82	II	202	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	EM	202	PEB	OD-C4D-C3D	-2.44	123.93	129.46
85	AN	847	BCR	C30-C25-C26	-2.44	119.18	122.61
82	FP	201	PEB	CHA-C4A-NA	2.44	128.10	125.20
82	KA	202	PEB	C3C-C4C-NC	2.44	110.53	108.33
82	b1	203	PEB	OD-C4D-ND	-2.44	122.32	125.93
82	w8	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
82	DH	1002	PEB	CHA-C1B-C2B	2.44	131.17	124.90
82	fJ	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	uK	202	PEB	CHA-C1B-NB	-2.44	119.83	124.93
82	G5	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
82	RP	201	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
96	E6	101	HEM	CHA-C4D-ND	2.44	127.38	124.37
82	BF	201	PEB	CAB-C3B-C4B	2.44	129.32	125.01
87	5N	601	CLA	C3B-C4B-NB	-2.44	108.25	110.52
82	pC	201	PEB	CAA-C3A-C2A	-2.44	108.17	114.26
82	PK	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	lJ	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	KI	203	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	ZE	201	PEB	CMC-C3C-C4C	2.44	129.65	127.06
82	QK	201	PEB	C3C-C4C-NC	2.44	110.53	108.33
82	w8	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	gF	201	PEB	C1C-CHB-C4B	2.44	133.75	128.28
85	FL	101	BCR	C32-C1-C6	-2.44	106.34	110.30
82	SB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
82	D9	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JD	201	PEB	C3B-C4B-NB	2.44	113.59	110.05
87	AN	813	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
82	X5	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
82	SO	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
82	NF	202	PEB	CAC-C2C-C1C	2.44	129.64	125.76
82	h1	202	PEB	OA-C1A-C2A	-2.44	124.23	126.17
82	wK	301	PEB	CAC-CBC-CGC	-2.44	108.36	113.60
82	MF	202	PEB	CMC-C3C-C4C	2.44	129.64	127.06
82	AM	302	PEB	CHB-C1C-NC	-2.44	119.74	125.32
87	B2	821	CLA	CBA-CAA-C2A	2.44	121.06	113.86
82	IK	201	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	LO	1002	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
92	m6	103	LMG	C8-O7-C10	-2.44	111.79	117.79
87	K6	101	CLA	CHB-C4A-NA	2.44	127.88	124.51
83	Z5	302	PUB	CMD-C2D-C3D	2.44	131.43	127.77
82	lE	201	PEB	C3C-C4C-NC	2.44	110.53	108.33
82	z8	202	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
82	QD	202	PEB	CHA-C4A-NA	-2.44	122.31	125.20
82	GF	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	wC	204	PEB	OD-C4D-C3D	-2.44	123.94	129.46
85	B6	601	BCR	C21-C20-C19	-2.44	115.61	123.22
82	aB	202	PEB	CMC-C3C-C4C	2.44	129.64	127.06
82	RQ	203	PEB	CHA-C1B-C2B	2.44	131.16	124.90
87	CL	504	CLA	C2A-C1A-CHA	2.44	128.12	123.86
85	A6	401	BCR	C33-C5-C4	2.44	118.30	113.62
87	BL	623	CLA	C3B-C4B-NB	-2.44	108.25	110.52
87	A2	801	CLA	C3B-C4B-NB	-2.44	108.25	110.52
87	I2	103	CLA	C3B-C4B-NB	-2.44	108.25	110.52
87	3N	304	CLA	C3B-C4B-NB	2.44	112.78	110.52
94	aL	601	PL9	C20-C19-C21	2.44	119.37	115.27
82	LQ	203	PEB	C4C-C3C-C2C	-2.44	105.25	107.50
82	TM	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	CB	201	PEB	CHB-C4B-C3B	-2.44	119.68	125.32
82	JJ	202	PEB	C1C-CHB-C4B	-2.44	122.82	128.28
82	eJ	202	PEB	CAA-C3A-C4A	2.44	118.93	112.67
82	gH	201	PEB	CAA-C3A-C2A	-2.44	108.17	114.26
82	BB	203	PEB	CHA-C1B-NB	-2.44	119.84	124.93
82	MK	202	PEB	CMB-C2B-C1B	2.44	128.81	125.06
87	dL	409	CLA	C2D-C1D-ND	-2.44	108.31	110.10
82	UB	301	PEB	CHA-C4A-NA	2.44	128.10	125.20
82	CF	203	PEB	C3C-C4C-NC	2.44	110.53	108.33
82	RQ	201	PEB	OD-C4D-ND	-2.44	122.32	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AO	304	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	aJ	202	PEB	CHC-C1D-ND	-2.44	110.64	113.72
82	eJ	202	PEB	CHC-C1D-ND	-2.44	110.64	113.72
87	8N	304	CLA	C3A-C2A-C1A	2.44	104.99	101.34
82	RK	201	PEB	CAB-C3B-C4B	2.44	129.32	125.01
85	B6	601	BCR	C15-C16-C17	-2.44	118.48	123.47
82	L5	201	PEB	C2B-C1B-NB	2.44	115.73	110.53
82	UI	201	PEB	CAC-CBC-CGC	-2.44	108.36	113.60
91	DL	405	PHO	O2A-CGA-O1A	-2.44	117.45	123.59
82	DA	203	PEB	OD-C4D-C3D	-2.44	123.94	129.46
82	PM	202	PEB	OD-C4D-C3D	-2.44	123.94	129.46
87	B2	831	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
82	SP	202	PEB	C4C-C3C-C2C	-2.43	105.25	107.50
83	AE	302	PUB	C2C-C1C-NC	2.43	113.59	110.05
82	Q9	203	PEB	CHC-C1D-ND	-2.43	110.64	113.72
82	oK	202	PEB	CHC-C1D-ND	-2.43	110.64	113.72
82	K7	202	PEB	C3C-C4C-NC	2.43	110.53	108.33
87	32	312	CLA	C2A-C1A-CHA	2.43	128.12	123.86
82	L7	202	PEB	CHB-C4B-C3B	-2.43	119.69	125.32
82	YP	502	PEB	OD-C4D-ND	-2.43	122.32	125.93
82	lH	201	PEB	OD-C4D-ND	-2.43	122.32	125.93
82	GP	203	PEB	OD-C4D-C3D	-2.43	123.94	129.46
82	lM	202	PEB	C1B-C2B-C3B	-2.43	103.71	106.51
82	C7	201	PEB	CMA-C2A-C1A	-2.43	107.16	112.40
84	L1	1001	CYC	O2A-CGA-O1A	-2.43	117.23	123.30
87	AN	822	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
82	RK	202	PEB	CAC-CBC-CGC	-2.43	108.36	113.60
82	fE	202	PEB	C2A-C3A-C4A	-2.43	97.69	101.34
82	CM	201	PEB	CHC-C1D-ND	-2.43	110.64	113.72
82	TG	201	PEB	CAB-C3B-C4B	2.43	129.31	125.01
82	W5	203	PEB	OA-C1A-C2A	-2.43	124.24	126.17
82	YK	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
87	82	303	CLA	C3A-C2A-C1A	2.43	104.98	101.34
87	A2	837	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
82	GM	203	PEB	C1D-CHC-C4C	-2.43	109.67	113.26
82	J5	202	PEB	CAB-C3B-C4B	2.43	129.31	125.01
83	Y7	302	PUB	CHC-C1D-ND	-2.43	110.65	113.72
82	cE	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
82	HF	202	PEB	CAC-CBC-CGC	-2.43	108.37	113.60
82	KA	201	PEB	OD-C4D-C3D	-2.43	123.95	129.46
82	18	201	PEB	OD-C4D-C3D	-2.43	123.95	129.46
82	O5	201	PEB	OD-C4D-ND	-2.43	122.33	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	313	CLA	C3B-C4B-NB	-2.43	108.26	110.52
82	TO	202	PEB	C3B-C4B-NB	2.43	113.59	110.05
82	U9	204	PEB	C3B-C4B-NB	2.43	113.59	110.05
82	mK	202	PEB	C4C-C3C-C2C	-2.43	105.25	107.50
82	IM	203	PEB	C1D-CHC-C4C	-2.43	109.67	113.26
82	P4	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
82	kH	203	PEB	OD-C4D-C3D	-2.43	123.95	129.46
87	C6	517	CLA	C1-C2-C3	-2.43	121.84	126.04
82	HI	202	PEB	C1C-CHB-C4B	2.43	133.74	128.28
82	QK	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
82	FQ	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
87	3N	304	CLA	CHA-C1A-NA	-2.43	120.83	126.40
82	tF	201	PEB	C3B-C4B-NB	2.43	113.59	110.05
82	QE	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
87	AN	835	CLA	CHD-C1D-ND	-2.43	122.22	124.45
82	PP	202	PEB	CAA-C3A-C4A	-2.43	106.43	112.67
87	b6	617	CLA	CHB-C4A-NA	2.43	127.88	124.51
82	EK	202	PEB	CHB-C4B-C3B	-2.43	119.69	125.32
82	vC	201	PEB	CHB-C4B-C3B	-2.43	119.69	125.32
82	lF	203	PEB	OD-C4D-ND	-2.43	122.33	125.93
82	VM	201	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
82	jM	203	PEB	CHA-C1B-NB	-2.43	119.85	124.93
82	RJ	202	PEB	CAA-C3A-C2A	-2.43	108.18	114.26
87	AN	837	CLA	O2A-C1-C2	-2.43	102.25	108.64
82	P1	201	PEB	C2A-C1A-NA	2.43	110.37	108.27
82	K7	201	PEB	CAA-C3A-C4A	-2.43	106.43	112.67
87	C6	514	CLA	CHB-C4A-NA	2.43	127.87	124.51
82	YE	202	PEB	C3C-C4C-NC	2.43	110.52	108.33
82	SO	201	PEB	C3C-C4C-NC	2.43	110.52	108.33
82	X9	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
82	CJ	201	PEB	OD-C4D-C3D	-2.43	123.95	129.46
82	wK	303	PEB	OA-C1A-C2A	-2.43	124.24	126.17
87	cL	514	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
82	wC	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
82	LK	201	PEB	CBA-CAA-C3A	2.43	118.88	113.47
82	ZM	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
82	QI	201	PEB	CMC-C3C-C4C	2.43	129.64	127.06
87	52	611	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
87	12	610	CLA	O1D-CGD-CBD	2.43	129.46	124.48
82	RM	201	PEB	CAC-CBC-CGC	-2.43	108.37	113.60
82	qF	203	PEB	OD-C4D-ND	-2.43	122.33	125.93
84	N3	1001	CYC	C1B-C2B-C3B	-2.43	105.33	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eE	202	PEB	CHA-C1B-NB	-2.43	119.85	124.93
82	bP	502	PEB	CHB-C1C-C2C	-2.43	121.67	127.15
82	VJ	201	PEB	OD-C4D-C3D	-2.43	123.95	129.46
82	MF	201	PEB	CAB-C3B-C4B	2.43	129.31	125.01
82	RA	203	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
82	DD	202	PEB	C1C-NC-C4C	-2.43	105.27	109.60
87	6N	612	CLA	C3B-C4B-NB	-2.43	108.26	110.52
82	oK	201	PEB	O2C-CGC-CBC	2.43	121.84	114.03
82	PD	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
82	XI	202	PEB	C4C-C3C-C2C	-2.43	105.26	107.50
82	WM	203	PEB	C4C-C3C-C2C	-2.43	105.26	107.50
85	H6	101	BCR	C35-C13-C12	2.43	121.91	118.08
82	BA	202	PEB	C4B-C3B-C2B	-2.43	104.09	106.78
87	B2	823	CLA	CHB-C1B-NB	2.43	126.83	124.26
87	A2	803	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
82	IM	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
82	oF	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
82	NA	202	PEB	C2B-C1B-NB	2.43	115.71	110.53
95	AL	415	DGD	C3G-O3G-C1D	-2.43	108.99	113.74
82	F9	201	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
82	RF	201	PEB	CAB-C3B-C4B	2.43	129.31	125.01
84	t3	1001	CYC	C1B-C2B-C3B	-2.43	105.34	107.87
87	32	303	CLA	CHA-C1A-NA	-2.43	120.83	126.40
87	2N	303	CLA	CHB-C1B-C2B	-2.43	120.38	127.24
82	w8	204	PEB	OD-C4D-C3D	-2.43	123.96	129.46
82	bF	201	PEB	CBA-CAA-C3A	-2.43	108.06	113.47
82	UE	202	PEB	CAB-CBB-CGB	-2.43	108.38	113.60
82	B7	203	PEB	CHB-C1C-NC	-2.43	119.76	125.32
82	vF	202	PEB	C1C-CHB-C4B	2.43	133.73	128.28
87	A2	826	CLA	C2A-C1A-CHA	2.43	128.11	123.86
87	7N	607	CLA	CHA-C1A-NA	-2.43	120.84	126.40
87	A2	837	CLA	O2A-C1-C2	-2.43	102.25	108.64
87	8N	305	CLA	C3B-C4B-NB	-2.43	108.26	110.52
82	uC	203	PEB	OD-C4D-C3D	-2.43	123.96	129.46
87	BN	827	CLA	CMB-C2B-C3B	2.43	132.47	126.59
82	YD	202	PEB	C4C-C3C-C2C	-2.43	105.26	107.50
87	BN	831	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
84	I4	1001	CYC	CHA-C4D-C3D	-2.43	121.67	127.15
87	AN	803	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
82	WB	402	PEB	CBC-CAC-C2C	2.43	119.37	112.63
82	FF	202	PEB	C2B-C1B-NB	2.43	115.71	110.53
82	K5	201	PEB	C4B-C3B-C2B	-2.43	104.10	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	bL	601	BCR	C16-C15-C14	-2.43	118.50	123.47
84	F4	1001	CYC	CBD-CAD-C3D	-2.43	105.88	112.63
87	BL	619	CLA	CHB-C4A-NA	2.43	127.87	124.51
82	DQ	203	PEB	CBA-CAA-C3A	-2.43	108.06	113.47
82	F7	202	PEB	CAB-C3B-C4B	2.43	129.30	125.01
82	kE	201	PEB	OD-C4D-ND	-2.43	122.33	125.93
87	c6	612	CLA	C3B-C4B-NB	-2.43	108.26	110.52
82	TI	203	PEB	C4C-C3C-C2C	-2.43	105.26	107.50
82	u8	203	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
82	dM	201	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
87	7N	602	CLA	CMB-C2B-C3B	2.43	132.47	126.59
87	5N	611	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
82	HI	202	PEB	CHB-C1C-NC	2.43	130.88	125.32
82	YG	202	PEB	CAC-CBC-CGC	-2.43	108.38	113.60
87	LN	204	CLA	CBC-CAC-C3C	2.43	119.12	112.43
96	V6	201	HEM	C4B-C3B-C2B	-2.43	105.19	107.11
82	fF	201	PEB	CHA-C1B-C2B	2.43	131.14	124.90
91	dL	403	PHO	CGD-CBD-CAD	-2.43	102.87	110.73
87	72	602	CLA	CMB-C2B-C3B	2.43	132.47	126.59
82	oF	202	PEB	CHC-C1D-ND	-2.43	110.65	113.72
82	WB	402	PEB	CMC-C3C-C4C	-2.43	124.49	127.06
82	QE	201	PEB	CMC-C3C-C4C	2.43	129.63	127.06
82	A5	201	PEB	C4B-C3B-C2B	-2.43	104.10	106.78
82	DF	203	PEB	OD-C4D-C3D	-2.43	123.96	129.46
82	X7	202	PEB	OA-C1A-NA	2.43	127.88	124.94
82	DA	201	PEB	CHB-C4B-NB	-2.43	119.53	124.58
83	AJ	304	PUB	CHB-C1C-NC	-2.43	119.53	124.58
91	d6	404	PHO	C4B-NB-C1B	-2.43	105.07	108.83
98	BN	837	PQN	C21-C22-C23	-2.43	108.08	115.92
84	d3	1001	CYC	C2A-C1A-NA	2.43	113.58	110.05
85	AN	846	BCR	C31-C1-C6	-2.43	106.36	110.30
82	VJ	201	PEB	C1C-CHB-C4B	-2.43	122.84	128.28
82	lK	202	PEB	C1D-CHC-C4C	2.43	116.83	113.26
82	I7	202	PEB	C4C-C3C-C2C	-2.43	105.26	107.50
84	N1	1001	CYC	CHD-C1D-ND	-2.43	119.76	125.32
87	AN	837	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
98	B2	837	PQN	C21-C22-C23	-2.43	108.08	115.92
84	LH	1002	CYC	C2B-C1B-NB	2.43	110.54	106.99
87	BL	604	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
82	OI	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
82	K7	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
82	1C	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	bL	616	CLA	CHB-C1B-NB	2.43	126.83	124.26
82	Q9	202	PEB	CAB-CBB-CGB	-2.43	108.38	113.60
83	ND	201	PUB	CAB-C3B-C4B	2.43	129.62	125.76
82	H7	203	PEB	OD-C4D-ND	-2.43	122.34	125.93
87	FN	203	CLA	CHB-C4A-NA	2.43	127.87	124.51
82	GE	1002	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
87	A2	819	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
82	A9	202	PEB	CMB-C2B-C1B	2.43	128.80	125.06
82	TD	201	PEB	CAB-C3B-C4B	2.43	129.30	125.01
87	1N	604	CLA	C3B-C4B-NB	-2.43	108.27	110.52
82	D7	201	PEB	CHB-C4B-NB	-2.43	119.53	124.58
82	DG	1002	PEB	O2B-CGB-CBB	2.43	121.82	114.03
82	vK	202	PEB	C1C-CHB-C4B	2.43	133.72	128.28
82	dF	202	PEB	C4B-C3B-C2B	-2.43	104.10	106.78
82	nK	201	PEB	CMC-C3C-C4C	2.42	129.63	127.06
82	J7	201	PEB	CHB-C4B-NB	-2.42	119.53	124.58
87	32	311	CLA	C2A-C1A-CHA	2.42	128.10	123.86
87	82	308	CLA	CHB-C1B-NB	2.42	126.82	124.26
82	V7	202	PEB	C2B-C1B-NB	2.42	115.70	110.53
82	DJ	202	PEB	CAA-C3A-C2A	-2.42	108.20	114.26
82	L9	202	PEB	C3B-C4B-NB	2.42	113.58	110.05
82	EQ	201	PEB	C1B-C2B-C3B	-2.42	103.72	106.51
82	R7	203	PEB	C1B-C2B-C3B	-2.42	103.72	106.51
82	U7	201	PEB	C1C-NC-C4C	-2.42	105.28	109.60
82	KE	201	PEB	CHC-C1D-ND	-2.42	110.66	113.72
84	g3	1001	CYC	C1B-C2B-C3B	-2.42	105.34	107.87
82	fH	202	PEB	CHC-C4C-NC	2.42	124.43	121.15
87	12	605	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
87	bL	622	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
82	XF	203	PEB	CAC-CBC-CGC	-2.42	108.39	113.60
82	Z5	305	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	YI	201	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
82	mG	202	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
82	LF	202	PEB	C4B-NB-C1B	-2.42	101.94	106.51
82	U5	201	PEB	CMC-C3C-C4C	-2.42	124.49	127.06
95	C6	502	DGD	O6E-C5E-C4E	2.42	114.10	109.69
82	N7	201	PEB	CMA-C2A-C1A	-2.42	107.18	112.40
82	cE	202	PEB	CHA-C4A-NA	-2.42	122.32	125.20
82	AA	201	PEB	CHB-C4B-NB	-2.42	119.53	124.58
87	A2	839	CLA	O2D-CGD-CBD	2.42	115.58	111.27
82	RH	201	PEB	C2B-C1B-NB	2.42	115.70	110.53
82	HI	201	PEB	CAC-C2C-C1C	2.42	129.62	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OJ	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	aO	201	PEB	CAB-C3B-C4B	2.42	129.30	125.01
82	HQ	202	PEB	OA-C1A-C2A	-2.42	124.25	126.17
82	DF	202	PEB	C1C-CHB-C4B	2.42	133.72	128.28
82	XA	203	PEB	OD-C4D-ND	-2.42	122.34	125.93
82	j4	202	PEB	OD-C4D-ND	-2.42	122.34	125.93
82	QJ	202	PEB	C3C-C4C-NC	2.42	110.52	108.33
82	d4	201	PEB	C3C-C4C-NC	2.42	110.52	108.33
87	B2	812	CLA	CBC-CAC-C3C	2.42	119.11	112.43
82	xK	303	PEB	CHA-C1B-NB	-2.42	119.86	124.93
82	QG	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	W9	203	PEB	C3B-C4B-NB	2.42	113.57	110.05
82	lO	201	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
87	12	604	CLA	C3B-C4B-NB	-2.42	108.27	110.52
82	FJ	202	PEB	CAC-C2C-C1C	2.42	129.62	125.76
82	r8	202	PEB	CAB-C3B-C4B	2.42	129.29	125.01
82	ZB	201	PEB	C4C-C3C-C2C	-2.42	105.26	107.50
85	k6	102	BCR	C1-C6-C7	2.42	122.63	115.78
82	BA	201	PEB	CHC-C1D-ND	-2.42	110.66	113.72
82	k1	201	PEB	CHC-C1D-ND	-2.42	110.66	113.72
82	O7	201	PEB	CHC-C1D-ND	-2.42	110.66	113.72
87	82	303	CLA	O2A-CGA-O1A	-2.42	117.26	123.30
87	a6	608	CLA	CHB-C1B-NB	2.42	126.82	124.26
82	X7	202	PEB	C2B-C1B-NB	2.42	115.70	110.53
82	BQ	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	R9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	UE	201	PEB	CHB-C1C-NC	2.42	130.87	125.32
82	v8	201	PEB	CHB-C4B-C3B	-2.42	119.71	125.32
84	BG	1002	CYC	C4D-ND-C1D	-2.42	105.47	109.79
84	M3	1001	CYC	C2A-C1A-NA	2.42	113.57	110.05
82	TJ	202	PEB	O2B-CGB-CBB	2.42	121.81	114.03
82	jG	201	PEB	CAC-C2C-C1C	2.42	129.62	125.76
82	QM	203	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	Q9	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	zF	501	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	S5	201	PEB	CHB-C1C-NC	-2.42	119.77	125.32
82	C5	201	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
82	I7	202	PEB	CHA-C4A-NA	-2.42	122.33	125.20
82	LA	202	PEB	CHB-C4B-C3B	-2.42	119.72	125.32
82	U7	202	PEB	C4C-C3C-C2C	-2.42	105.27	107.50
95	L6	102	DGD	O3G-C3G-C2G	-2.42	105.06	110.90
82	XM	201	PEB	CBC-CAC-C2C	-2.42	105.90	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QP	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
83	BM	302	PUB	C2C-C1C-NC	2.42	113.57	110.05
82	KB	302	PEB	CAC-C2C-C1C	2.42	129.62	125.76
82	RP	201	PEB	CAC-C2C-C1C	2.42	129.62	125.76
87	22	602	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
84	ME	1001	CYC	CHB-C1B-NB	-2.42	120.86	126.06
84	A3	1001	CYC	C1B-C2B-C3B	-2.42	105.34	107.87
82	fK	201	PEB	CAB-CBB-CGB	-2.42	108.39	113.60
82	U9	203	PEB	OD-C4D-C3D	-2.42	123.97	129.46
82	XQ	203	PEB	CHA-C1B-NB	-2.42	119.87	124.93
82	WB	401	PEB	CHC-C1D-ND	-2.42	110.66	113.72
82	QE	202	PEB	C3B-C4B-NB	2.42	113.57	110.05
83	AM	303	PUB	C2C-C1C-NC	2.42	113.57	110.05
82	Q5	202	PEB	CMA-C2A-C1A	-2.42	107.18	112.40
82	FO	1002	PEB	CAA-C3A-C2A	-2.42	108.21	114.26
82	GM	203	PEB	OD-C4D-C3D	-2.42	123.97	129.46
87	42	606	CLA	C3B-C4B-NB	-2.42	108.27	110.52
87	1N	601	CLA	C3B-C4B-NB	-2.42	108.27	110.52
82	UG	201	PEB	CHB-C1C-NC	2.42	130.87	125.32
87	4N	604	CLA	CHC-C4B-NB	2.42	126.82	124.26
82	HF	201	PEB	CHB-C4B-NB	-2.42	119.54	124.58
82	FI	202	PEB	C4C-C3C-C2C	-2.42	105.27	107.50
82	eO	201	PEB	C4C-C3C-C2C	-2.42	105.27	107.50
82	MP	202	PEB	CBA-CAA-C3A	-2.42	108.08	113.47
82	C9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
85	d6	405	BCR	C37-C22-C21	-2.42	119.53	122.92
82	PO	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	g4	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	mG	203	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	OE	201	PEB	CAC-C2C-C1C	2.42	129.62	125.76
82	RI	202	PEB	CHB-C1C-NC	-2.42	119.78	125.32
82	HD	202	PEB	CHC-C1D-ND	-2.42	110.66	113.72
83	Y7	302	PUB	CHA-C4A-NA	-2.42	110.66	113.72
85	CL	516	BCR	C29-C30-C25	2.42	114.21	110.48
87	A2	822	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
82	OF	201	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	I9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	K9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	YB	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	ZB	203	PEB	CHB-C1C-NC	-2.42	119.78	125.32
82	SQ	202	PEB	CHB-C4B-C3B	-2.42	119.72	125.32
82	gM	202	PEB	CHB-C4B-NB	-2.42	119.54	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	BN	843	BCR	C20-C19-C18	-2.42	119.62	126.42
82	kO	201	PEB	C4C-C3C-C2C	-2.42	105.27	107.50
82	OO	202	PEB	C4B-C3B-C2B	-2.42	104.11	106.78
82	XJ	202	PEB	CHB-C4B-NB	-2.42	119.54	124.58
82	A7	201	PEB	CHB-C4B-NB	-2.42	119.54	124.58
82	P9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
87	42	609	CLA	C2D-C1D-ND	-2.42	108.32	110.10
82	S4	202	PEB	OD-C4D-ND	-2.42	122.35	125.93
84	D4	1001	CYC	CBB-CAB-C3B	-2.42	105.76	112.43
82	PK	201	PEB	CMA-C2A-C1A	-2.42	107.19	112.40
82	FA	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	NI	202	PEB	CHB-C1C-NC	-2.42	119.78	125.32
82	HA	201	PEB	CHB-C1C-C2C	-2.42	121.69	127.15
82	ZF	201	PEB	CMB-C2B-C1B	2.42	128.79	125.06
87	FN	201	CLA	C3B-C4B-NB	-2.42	108.27	110.52
82	QB	204	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	CI	202	PEB	CHB-C1C-NC	-2.42	119.78	125.32
82	l4	202	PEB	OD-C4D-ND	-2.42	122.35	125.93
87	AN	811	CLA	CHA-C1A-NA	-2.42	120.86	126.40
82	Q5	202	PEB	C2A-C1A-NA	2.42	110.36	108.27
82	V7	203	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
82	AP	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	yK	301	PEB	CMC-C3C-C4C	2.42	129.62	127.06
82	Y7	301	PEB	CMC-C3C-C2C	-2.42	120.37	125.61
82	OK	201	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	YM	203	PEB	CMB-C2B-C1B	2.42	128.79	125.06
87	AN	850	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
87	B6	613	CLA	CHB-C1B-NB	2.42	126.82	124.26
82	IK	203	PEB	C1C-CHB-C4B	2.42	133.71	128.28
87	CL	511	CLA	C2D-C1D-ND	-2.42	108.32	110.10
83	Z9	305	PUB	CAB-C3B-C4B	2.42	129.61	125.76
82	rC	202	PEB	CAB-C3B-C4B	2.42	129.29	125.01
87	AN	826	CLA	C2A-C1A-CHA	2.42	128.09	123.86
82	FO	1002	PEB	C3C-C4C-NC	2.42	110.51	108.33
87	CL	514	CLA	C3B-C4B-NB	-2.42	108.27	110.52
87	AN	802	CLA	C3B-C4B-NB	-2.42	108.27	110.52
87	A2	814	CLA	C3B-C4B-NB	-2.42	108.27	110.52
84	l3	1001	CYC	C1B-C2B-C3B	-2.42	105.35	107.87
82	kF	201	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
82	fK	201	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
82	E9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	aB	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	RN	203	CLA	CHB-C4A-NA	2.42	127.86	124.51
82	OI	201	PEB	CAC-C2C-C1C	2.42	129.61	125.76
82	L9	203	PEB	CHC-C1D-ND	-2.42	110.67	113.72
82	KB	301	PEB	CAC-CBC-CGC	-2.42	108.40	113.60
82	N4	1002	PEB	CAB-CBB-CGB	-2.42	108.40	113.60
91	D6	404	PHO	CBA-CAA-C2A	-2.42	106.75	113.81
82	B7	201	PEB	CAB-C3B-C2B	2.42	132.38	127.88
82	DD	203	PEB	CBA-CAA-C3A	-2.42	108.08	113.47
82	GG	1002	PEB	CAA-C3A-C4A	-2.42	106.47	112.67
82	Y9	201	PEB	CHB-C1C-NC	-2.42	119.78	125.32
82	VF	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
84	L3	1001	CYC	C2A-C1A-NA	2.42	113.56	110.05
82	WG	202	PEB	C1D-CHC-C4C	-2.42	109.69	113.26
82	R1	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
82	DK	202	PEB	C1C-CHB-C4B	2.42	133.70	128.28
87	F2	201	CLA	CHB-C4A-NA	2.42	127.85	124.51
87	8N	304	CLA	CHB-C4A-NA	2.42	127.85	124.51
82	IQ	201	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
82	kK	201	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
82	i4	203	PEB	OD-C4D-ND	-2.42	122.35	125.93
82	eE	203	PEB	OD-C4D-ND	-2.42	122.35	125.93
87	BN	816	CLA	C3B-C4B-NB	-2.42	108.27	110.52
84	NH	1001	CYC	CHD-C1D-ND	-2.42	119.78	125.32
82	SG	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
82	gF	202	PEB	C4C-C3C-C2C	-2.42	105.27	107.50
85	BL	618	BCR	C33-C5-C4	2.42	118.26	113.62
82	FA	202	PEB	CAB-C3B-C4B	2.42	129.28	125.01
87	AL	405	CLA	CHB-C1B-NB	2.42	126.81	124.26
82	u8	203	PEB	OD-C4D-C3D	-2.42	123.99	129.46
82	SQ	202	PEB	CHB-C1C-C2C	-2.42	121.70	127.15
84	BG	1001	CYC	CHB-C1B-NB	-2.42	120.87	126.06
82	PF	201	PEB	CMA-C2A-C1A	-2.42	107.19	112.40
82	JQ	201	PEB	CMA-C2A-C1A	-2.42	107.19	112.40
82	HG	1002	PEB	OD-C4D-ND	-2.42	122.35	125.93
85	B2	843	BCR	C20-C19-C18	-2.42	119.63	126.42
84	G3	1001	CYC	C1B-C2B-C3B	-2.42	105.35	107.87
82	ZH	202	PEB	OD-C4D-C3D	-2.42	123.99	129.46
87	DL	404	CLA	CHD-C1D-ND	-2.42	122.23	124.45
87	B6	612	CLA	C1-C2-C3	-2.42	121.86	126.04
83	ND	201	PUB	CMD-C2D-C3D	2.42	131.39	127.77
85	hL	102	BCR	C31-C1-C6	-2.42	106.38	110.30
82	A4	301	PEB	C4C-C3C-C2C	-2.42	105.27	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	824	CLA	CHB-C1B-NB	2.42	126.81	124.26
87	B2	827	CLA	CMB-C2B-C3B	2.42	132.44	126.59
82	I5	201	PEB	C4B-C3B-C2B	-2.42	104.11	106.78
88	BL	615	LHG	C9-C8-C7	-2.41	104.84	113.62
82	q8	203	PEB	CHA-C1B-NB	-2.41	119.88	124.93
82	QQ	202	PEB	CHA-C4A-NA	-2.41	122.33	125.20
82	OB	201	PEB	CMA-C2A-C1A	-2.41	107.20	112.40
87	cL	508	CLA	CAC-C3C-C4C	2.41	127.94	124.81
82	y8	202	PEB	CAA-C3A-C2A	-2.41	108.23	114.26
87	B2	833	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
92	mL	101	LMG	O8-C28-O10	-2.41	117.50	123.59
82	xF	304	PEB	CAB-CBB-CGB	-2.41	108.41	113.60
85	CL	516	BCR	C10-C11-C12	-2.41	115.68	123.22
82	XI	202	PEB	CHB-C1C-NC	-2.41	119.79	125.32
82	VK	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
82	UM	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
82	L4	1002	PEB	C4C-C3C-C2C	-2.41	105.27	107.50
82	U9	203	PEB	C3B-C4B-NB	2.41	113.56	110.05
82	HF	201	PEB	C1C-CHB-C4B	2.41	133.70	128.28
87	AN	820	CLA	CMB-C2B-C3B	2.41	132.44	126.59
82	RF	202	PEB	CAC-CBC-CGC	-2.41	108.41	113.60
82	H9	201	PEB	OD-C4D-ND	-2.41	122.35	125.93
82	EI	202	PEB	CHB-C1C-NC	-2.41	119.79	125.32
82	CP	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
82	mK	202	PEB	C2A-C1A-NA	2.41	110.35	108.27
82	Q5	203	PEB	CHB-C1C-C2C	-2.41	121.70	127.15
84	J3	1001	CYC	C1B-C2B-C3B	-2.41	105.35	107.87
87	c6	616	CLA	CHB-C4A-NA	2.41	127.85	124.51
82	j4	201	PEB	CHA-C1B-NB	-2.41	119.88	124.93
91	AL	410	PHO	C16-C15-C13	-2.41	108.12	115.92
87	62	313	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
84	h3	1001	CYC	C2A-C1A-NA	2.41	113.56	110.05
82	HK	202	PEB	CAC-CBC-CGC	-2.41	108.41	113.60
87	A2	820	CLA	C7-C6-C5	-2.41	106.80	113.36
82	RE	201	PEB	OD-C4D-C3D	-2.41	123.99	129.46
87	82	304	CLA	C3B-C4B-NB	-2.41	108.28	110.52
87	b6	606	CLA	C3B-C4B-NB	-2.41	108.28	110.52
87	F2	201	CLA	CHB-C1B-NB	2.41	126.81	124.26
82	yC	202	PEB	CAA-C3A-C2A	-2.41	108.23	114.26
82	IJ	201	PEB	CAA-C3A-C4A	-2.41	106.48	112.67
84	NO	1001	CYC	CHB-C4A-C3A	2.41	131.11	124.90
84	N1	1001	CYC	C1A-C2A-C3A	-2.41	104.11	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
96	G2	201	HEM	CMD-C2D-C1D	2.41	128.71	125.04
82	VI	202	PEB	CHB-C1C-NC	-2.41	119.79	125.32
84	73	1002	CYC	CHA-C4D-C3D	-2.41	121.71	127.15
82	Y4	201	PEB	CHA-C4A-NA	2.41	128.07	125.20
87	K2	104	CLA	CMB-C2B-C3B	2.41	132.43	126.59
83	M5	303	PUB	CHB-C4B-NB	-2.41	119.79	125.32
82	T7	202	PEB	CMC-C3C-C4C	2.41	129.62	127.06
82	IJ	201	PEB	OD-C4D-ND	-2.41	122.36	125.93
82	P4	201	PEB	OD-C4D-C3D	-2.41	123.99	129.46
82	VA	202	PEB	C2B-C1B-NB	2.41	115.68	110.53
87	3N	305	CLA	CHC-C4B-NB	2.41	126.81	124.26
82	PP	201	PEB	CAC-C2C-C1C	2.41	129.60	125.76
82	EQ	202	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
82	fM	201	PEB	CHA-C1B-NB	-2.41	119.89	124.93
82	c1	201	PEB	C1D-CHC-C4C	2.41	116.81	113.26
82	XB	202	PEB	CHB-C4B-C3B	-2.41	119.74	125.32
84	EH	1001	CYC	CHA-C1A-C2A	-2.41	119.74	125.32
82	U4	201	PEB	CBA-CAA-C3A	-2.41	108.10	113.47
82	KM	202	PEB	CHC-C1D-ND	-2.41	110.67	113.72
96	GN	201	HEM	CMD-C2D-C1D	2.41	128.71	125.04
84	C4	1001	CYC	CBD-CAD-C3D	-2.41	105.93	112.63
82	PD	202	PEB	CAB-C3B-C4B	2.41	129.28	125.01
82	XF	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
87	B2	804	CLA	CHB-C4A-NA	2.41	127.85	124.51
82	QA	201	PEB	C2A-C1A-NA	2.41	110.35	108.27
82	nF	202	PEB	C1D-CHC-C4C	2.41	116.81	113.26
87	cL	508	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
82	L5	202	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
82	fE	201	PEB	C4B-C3B-C2B	-2.41	104.11	106.78
87	BN	813	CLA	CBC-CAC-C3C	2.41	119.08	112.43
82	XB	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	OJ	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	CK	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	Z1	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	e1	202	PEB	OD-C4D-ND	-2.41	122.36	125.93
82	D9	203	PEB	CHA-C4A-NA	-2.41	122.34	125.20
82	fG	202	PEB	C3C-C4C-NC	2.41	110.50	108.33
82	ZK	202	PEB	C2B-C1B-NB	2.41	115.67	110.53
82	YK	202	PEB	CMB-C2B-C1B	2.41	128.78	125.06
82	LF	201	PEB	CBA-CAA-C3A	2.41	118.83	113.47
82	W5	201	PEB	CAB-CBB-CGB	-2.41	108.42	113.60
95	c6	601	DGD	O6E-C5E-C4E	2.41	114.07	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	B2	843	BCR	C36-C18-C17	-2.41	119.55	122.92
82	a4	201	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
82	N7	202	PEB	C2B-C1B-NB	2.41	115.67	110.53
85	A6	401	BCR	C33-C5-C6	-2.41	121.82	124.53
82	BA	203	PEB	CHB-C1C-NC	-2.41	119.80	125.32
91	dL	403	PHO	O2D-CGD-O1D	-2.41	119.13	123.84
82	PO	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	DA	202	PEB	CAC-C2C-C1C	2.41	129.60	125.76
85	cL	504	BCR	C23-C22-C21	-2.41	115.24	118.94
84	NE	201	CYC	C4A-C3A-C2A	-2.41	103.74	106.51
82	G9	202	PEB	CMB-C2B-C1B	2.41	128.78	125.06
87	8N	308	CLA	CHB-C1B-NB	2.41	126.81	124.26
82	sC	203	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
82	QI	201	PEB	CBC-CAC-C2C	-2.41	105.93	112.63
82	YH	201	PEB	CHC-C4C-NC	2.41	124.41	121.15
82	T9	201	PEB	C1D-CHC-C4C	-2.41	109.70	113.26
87	c6	606	CLA	CHB-C4A-NA	2.41	127.84	124.51
82	a4	203	PEB	C2A-C1A-NA	2.41	110.35	108.27
82	DP	201	PEB	CAC-C2C-C1C	2.41	129.60	125.76
82	kK	203	PEB	CAC-C2C-C1C	2.41	129.60	125.76
85	K6	102	BCR	C1-C6-C7	2.41	122.59	115.78
82	FK	202	PEB	C2B-C1B-NB	2.41	115.67	110.53
84	BG	1001	CYC	CHA-C1A-C2A	-2.41	119.75	125.32
87	32	313	CLA	C3B-C4B-NB	-2.41	108.28	110.52
84	e3	1001	CYC	C1B-C2B-C3B	-2.41	105.36	107.87
82	e4	201	PEB	C4C-C3C-C2C	-2.41	105.28	107.50
82	lM	203	PEB	CHB-C4B-NB	-2.41	119.56	124.58
82	m4	203	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
87	d6	406	CLA	CHB-C4A-NA	2.41	127.84	124.51
87	3N	311	CLA	C2A-C1A-CHA	2.41	128.07	123.86
82	GB	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	OE	201	PEB	CMA-C2A-C1A	-2.41	107.21	112.40
84	63	901	CYC	C1D-C2D-C3D	-2.41	104.72	107.79
82	T9	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
83	M5	302	PUB	CMD-C2D-C3D	2.41	131.38	127.77
85	KL	100	BCR	C7-C8-C9	-2.41	122.60	126.23
85	F2	203	BCR	C20-C21-C22	-2.41	123.87	127.31
82	D7	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	YA	301	PEB	CMC-C3C-C2C	-2.41	120.40	125.61
82	m1	201	PEB	CHC-C4C-NC	2.41	124.41	121.15
84	K3	1001	CYC	C1B-C2B-C3B	-2.41	105.36	107.87
82	LK	202	PEB	C4B-NB-C1B	-2.41	101.97	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XP	202	PEB	C3B-C4B-NB	2.41	113.55	110.05
82	GJ	201	PEB	C4C-C3C-C2C	-2.41	105.28	107.50
82	dE	203	PEB	CHC-C1D-ND	-2.41	110.68	113.72
82	AH	305	PEB	CMB-C2B-C1B	2.41	128.77	125.06
82	PF	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	B7	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
82	RK	202	PEB	CHB-C1C-C2C	-2.41	121.72	127.15
82	KI	203	PEB	CHB-C1C-NC	-2.41	119.81	125.32
87	82	306	CLA	CHB-C1B-C2B	-2.41	120.44	127.24
82	T4	203	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
82	JF	202	PEB	CHA-C4A-NA	2.41	128.07	125.20
82	FM	201	PEB	CHA-C4A-NA	2.41	128.07	125.20
82	jO	201	PEB	CHA-C1B-NB	-2.41	119.90	124.93
82	SO	202	PEB	CBA-CAA-C3A	-2.41	108.11	113.47
82	B7	202	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
82	bK	202	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
82	BA	202	PEB	OD-C4D-C3D	-2.41	124.01	129.46
82	XP	202	PEB	OD-C4D-C3D	-2.41	124.01	129.46
82	WI	201	PEB	C4C-C3C-C2C	-2.41	105.28	107.50
82	dH	201	PEB	C4C-C3C-C2C	-2.41	105.28	107.50
82	II	202	PEB	CHB-C1C-NC	-2.41	119.81	125.32
82	SE	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
87	82	305	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
87	32	305	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
84	DE	1001	CYC	CBD-CAD-C3D	-2.41	105.94	112.63
84	JH	1001	CYC	CAC-C3C-C4C	-2.41	106.49	112.67
82	nK	202	PEB	C1D-CHC-C4C	2.41	116.80	113.26
82	D9	202	PEB	CAB-CBB-CGB	-2.41	108.42	113.60
82	fF	201	PEB	CAB-CBB-CGB	-2.41	108.42	113.60
82	PI	202	PEB	CHB-C1C-NC	-2.41	119.81	125.32
82	F9	202	PEB	OD-C4D-C3D	-2.41	124.01	129.46
82	TK	202	PEB	C2B-C1B-NB	2.41	115.66	110.53
82	WB	401	PEB	CMB-C2B-C1B	2.41	128.77	125.06
82	BQ	201	PEB	CMA-C2A-C1A	-2.41	107.22	112.40
84	BE	1002	CYC	C4D-ND-C1D	-2.41	105.50	109.79
82	XB	202	PEB	C4C-C3C-C2C	-2.41	105.28	107.50
82	xK	304	PEB	CAB-CBB-CGB	-2.41	108.43	113.60
82	aE	201	PEB	CHA-C1B-NB	-2.41	119.90	124.93
82	IF	203	PEB	C1C-CHB-C4B	2.41	133.68	128.28
91	AL	410	PHO	C1A-C2A-C3A	-2.41	100.55	102.84
84	M1	201	CYC	C1B-CHB-C4A	-2.41	122.20	128.08
82	K9	201	PEB	C1D-CHC-C4C	-2.41	109.71	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VA	203	PEB	C1B-C2B-C3B	-2.41	103.75	106.51
82	sF	202	PEB	C1B-C2B-C3B	-2.41	103.75	106.51
84	KG	202	CYC	C4A-C3A-C2A	-2.41	103.75	106.51
82	JD	201	PEB	CMA-C2A-C1A	-2.41	107.22	112.40
82	FD	201	PEB	C3B-C4B-NB	2.41	113.55	110.05
84	p3	1001	CYC	C1B-C2B-C3B	-2.41	105.36	107.87
85	JN	102	BCR	C10-C11-C12	-2.41	115.71	123.22
87	82	303	CLA	CHB-C4A-NA	2.41	127.84	124.51
87	c6	608	CLA	CHB-C4A-NA	2.41	127.84	124.51
87	CL	509	CLA	O2D-CGD-CBD	2.41	115.54	111.27
82	SK	202	PEB	OD-C4D-C3D	-2.41	124.01	129.46
85	BN	840	BCR	C33-C5-C4	2.40	118.24	113.62
82	IF	203	PEB	CAC-C2C-C1C	2.40	129.59	125.76
84	HO	1001	CYC	CHB-C4A-C3A	2.40	131.08	124.90
82	YI	201	PEB	CHA-C1B-NB	-2.40	119.90	124.93
84	73	1001	CYC	C2A-C1A-NA	2.40	113.55	110.05
82	XB	201	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
82	PO	202	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
82	MB	201	PEB	CHB-C1C-C2C	-2.40	121.72	127.15
87	3N	309	CLA	CMB-C2B-C3B	2.40	132.41	126.59
82	XP	202	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
82	F5	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
87	6N	606	CLA	C2D-C1D-ND	-2.40	108.33	110.10
82	RO	202	PEB	CAC-C2C-C1C	2.40	129.59	125.76
82	F4	1002	PEB	CAA-C3A-C2A	-2.40	108.25	114.26
82	N5	201	PEB	C4B-C3B-C2B	-2.40	104.12	106.78
87	3N	307	CLA	CHB-C1B-NB	2.40	126.80	124.26
82	NA	201	PEB	CMA-C2A-C1A	-2.40	107.22	112.40
82	lF	201	PEB	CBB-CAB-C3B	2.40	119.31	112.63
82	J9	203	PEB	CAB-C3B-C4B	2.40	129.26	125.01
87	B2	833	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
82	sK	202	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
82	P1	201	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
82	c1	202	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
87	1N	605	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
82	gM	201	PEB	CHB-C1C-NC	-2.40	119.81	125.32
82	m4	203	PEB	C1D-CHC-C4C	-2.40	109.71	113.26
82	CJ	203	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	YO	202	PEB	OD-C4D-C3D	-2.40	124.02	129.46
87	8N	306	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
82	VK	201	PEB	C3B-C4B-NB	2.40	113.55	110.05
87	B2	828	CLA	CHB-C1B-NB	2.40	126.80	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IK	203	PEB	CAC-C2C-C1C	2.40	129.59	125.76
82	eK	203	PEB	C1C-CHB-C4B	2.40	133.67	128.28
82	RA	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	hJ	202	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	zK	501	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	S9	201	PEB	O2B-CGB-CBB	2.40	121.75	114.03
82	SF	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
82	RJ	201	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
85	FN	202	BCR	C20-C21-C22	-2.40	123.88	127.31
82	N9	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
82	BA	202	PEB	C3B-C4B-NB	2.40	113.54	110.05
84	S3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05
84	k3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05
82	AQ	304	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
82	YB	201	PEB	C4B-C3B-C2B	-2.40	104.12	106.78
88	CL	522	LHG	O7-C7-O9	-2.40	117.90	123.70
84	v3	1001	CYC	C1B-C2B-C3B	-2.40	105.36	107.87
82	VD	203	PEB	C2A-C1A-NA	2.40	110.34	108.27
84	CH	1001	CYC	C2C-C1C-NC	2.40	110.34	108.27
82	ED	201	PEB	CMC-C3C-C4C	2.40	129.61	127.06
82	EM	202	PEB	O2C-CGC-CBC	2.40	121.75	114.03
82	jO	202	PEB	CHB-C1C-NC	-2.40	119.82	125.32
82	aK	202	PEB	C1D-CHC-C4C	-2.40	109.71	113.26
82	H9	203	PEB	C1C-CHB-C4B	-2.40	122.89	128.28
82	FQ	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
87	AL	404	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
82	eB	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
94	d6	408	PL9	C30-C29-C31	2.40	119.31	115.27
87	BN	805	CLA	CHB-C4A-NA	2.40	127.83	124.51
95	a6	602	DGD	O1G-C1A-O1A	-2.40	117.53	123.59
82	V5	201	PEB	C4B-C3B-C2B	-2.40	104.12	106.78
82	H7	202	PEB	C4B-C3B-C2B	-2.40	104.12	106.78
84	C3	1001	CYC	C1B-C2B-C3B	-2.40	105.36	107.87
82	d1	201	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
82	GI	203	PEB	CHB-C1C-NC	-2.40	119.82	125.32
82	TI	203	PEB	CHB-C1C-NC	-2.40	119.82	125.32
82	mJ	202	PEB	O2B-CGB-CBB	2.40	121.75	114.03
84	F3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05
82	GJ	202	PEB	C3C-C4C-NC	2.40	110.50	108.33
82	ZB	202	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	XK	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	aJ	203	PEB	OD-C4D-C3D	-2.40	124.02	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	32	304	CLA	CHC-C4B-NB	2.40	126.80	124.26
82	CQ	202	PEB	CAC-C2C-C1C	2.40	129.59	125.76
87	1N	610	CLA	O1D-CGD-CBD	2.40	129.40	124.48
87	8N	301	CLA	CHB-C1B-C2B	-2.40	120.46	127.24
82	S9	202	PEB	C1C-CHB-C4B	2.40	133.67	128.28
82	mK	201	PEB	CHB-C1C-C2C	-2.40	121.73	127.15
87	cL	515	CLA	CHD-C1D-C2D	2.40	130.51	125.48
82	cM	202	PEB	OD-C4D-ND	-2.40	122.37	125.93
82	XA	202	PEB	OA-C1A-NA	2.40	127.85	124.94
82	cH	202	PEB	C4C-C3C-C2C	-2.40	105.28	107.50
82	aF	201	PEB	CHB-C4B-NB	-2.40	119.58	124.58
94	D6	408	PL9	C42-C43-C44	-2.40	121.88	127.66
82	eM	202	PEB	OD-C4D-C3D	-2.40	124.02	129.46
82	XD	203	PEB	OD-C4D-ND	-2.40	122.38	125.93
82	GF	202	PEB	C1C-NC-C4C	-2.40	105.33	109.60
82	MJ	201	PEB	C1C-NC-C4C	-2.40	105.33	109.60
94	d6	408	PL9	C22-C21-C19	-2.40	105.08	112.98
82	UG	202	PEB	CAB-CBB-CGB	-2.40	108.44	113.60
82	OA	201	PEB	CMD-C2D-C3D	2.40	133.45	130.06
82	cG	202	PEB	CHA-C4A-NA	-2.40	122.35	125.20
82	CF	203	PEB	OD-C4D-C3D	-2.40	124.02	129.46
85	bL	603	BCR	C1-C6-C5	-2.40	119.23	122.61
82	M9	305	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
82	eJ	201	PEB	CHC-C1D-ND	2.40	116.76	113.72
85	d6	405	BCR	C3-C4-C5	-2.40	109.79	114.08
82	eO	203	PEB	CAB-CBB-CGB	2.40	118.77	113.60
84	U3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05
87	LN	204	CLA	CHD-C4C-NC	-2.40	120.43	124.20
96	V6	201	HEM	C4D-ND-C1D	2.40	107.55	105.07
83	AO	303	PUB	CMD-C2D-C3D	2.40	131.37	127.77
82	YK	203	PEB	C3C-C4C-NC	2.40	110.49	108.33
82	P1	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
82	MA	202	PEB	CHA-C1B-NB	-2.40	119.92	124.93
82	rF	201	PEB	C2A-C1A-NA	2.40	110.34	108.27
82	F7	201	PEB	CAC-CBC-CGC	-2.40	108.44	113.60
82	D7	201	PEB	C1D-CHC-C4C	2.40	116.79	113.26
82	R9	201	PEB	C1D-CHC-C4C	-2.40	109.72	113.26
82	GJ	201	PEB	CHA-C4A-NA	2.40	128.06	125.20
85	BN	843	BCR	C36-C18-C17	-2.40	119.56	122.92
82	mJ	202	PEB	CHC-C4C-NC	2.40	124.39	121.15
85	J2	102	BCR	C20-C19-C18	-2.40	119.68	126.42
84	D3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	dL	403	PHO	C4D-CHA-CBD	-2.40	107.43	108.52
82	1C	201	PEB	OA-C1A-C2A	-2.40	124.27	126.17
85	Z6	101	BCR	C16-C15-C14	-2.40	118.56	123.47
87	A2	849	CLA	CMD-C2D-C3D	2.40	133.13	127.61
82	gM	201	PEB	C4C-C3C-C2C	-2.40	105.29	107.50
85	A6	401	BCR	C11-C12-C13	-2.40	119.68	126.42
82	DP	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
82	bK	201	PEB	CBA-CAA-C3A	-2.40	108.13	113.47
82	aF	202	PEB	C4B-C3B-C2B	-2.40	104.13	106.78
87	AN	829	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
83	Z5	303	PUB	CHB-C4B-NB	-2.40	119.83	125.32
87	bL	618	CLA	CAA-CBA-CGA	-2.40	106.25	113.25
84	u3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05
82	F7	203	PEB	C2A-C1A-NA	2.40	110.34	108.27
87	L2	204	CLA	CBC-CAC-C3C	2.40	119.04	112.43
82	gM	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
82	YH	202	PEB	C1C-CHB-C4B	2.40	133.66	128.28
84	R3	1001	CYC	C1B-C2B-C3B	-2.40	105.37	107.87
95	C6	504	DGD	O4D-C4D-C3D	-2.40	104.81	110.35
87	A2	820	CLA	CMB-C2B-C3B	2.40	132.40	126.59
84	H4	1001	CYC	CHB-C4A-C3A	2.40	131.06	124.90
84	x3	1001	CYC	CAD-CBD-CGD	-2.40	108.44	113.60
87	12	601	CLA	C3B-C4B-NB	-2.40	108.29	110.52
87	3N	305	CLA	C1D-ND-C4D	-2.40	104.63	106.33
82	Y4	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
82	PD	202	PEB	C3B-C4B-NB	2.40	113.54	110.05
84	w3	1001	CYC	C2A-C1A-NA	2.40	113.54	110.05
82	b4	201	PEB	C4C-C3C-C2C	-2.40	105.29	107.50
82	L9	201	PEB	C4C-C3C-C2C	-2.40	105.29	107.50
82	GP	202	PEB	C2B-C1B-NB	2.40	115.64	110.53
82	UK	201	PEB	C1C-NC-C4C	-2.40	105.33	109.60
82	X7	201	PEB	CHA-C4A-NA	2.40	128.06	125.20
82	NJ	201	PEB	CHB-C4B-NB	-2.40	119.59	124.58
87	22	602	CLA	CHB-C1B-C2B	-2.40	120.47	127.24
87	A2	811	CLA	CHA-C1A-NA	-2.40	120.91	126.40
82	CF	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
82	aO	201	PEB	C1B-C2B-C3B	-2.40	103.76	106.51
82	C9	201	PEB	C1D-CHC-C4C	-2.40	109.72	113.26
82	jF	201	PEB	CMC-C3C-C4C	2.40	129.60	127.06
84	E3	1001	CYC	C1B-C2B-C3B	-2.40	105.37	107.87
84	c3	1001	CYC	C1B-C2B-C3B	-2.40	105.37	107.87
82	D9	202	PEB	CHA-C1B-NB	-2.40	119.92	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
96	f6	101	HEM	CHD-C1D-C2D	-2.40	121.23	124.98
82	L9	201	PEB	CHB-C1C-NC	-2.40	119.83	125.32
82	Z1	202	PEB	CAB-C3B-C4B	2.40	129.25	125.01
83	QM	201	PUB	C2C-C1C-NC	2.40	113.53	110.05
83	A4	303	PUB	CMD-C2D-C3D	2.40	131.36	127.77
82	KF	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
87	12	601	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
95	D6	410	DGD	C6D-C5D-C4D	-2.40	107.09	112.09
82	lG	201	PEB	CMB-C2B-C1B	2.40	128.75	125.06
82	p8	201	PEB	CHB-C1C-NC	-2.40	119.83	125.32
82	YQ	202	PEB	C4C-C3C-C2C	-2.40	105.29	107.50
82	G9	201	PEB	C1D-CHC-C4C	-2.40	109.72	113.26
82	VO	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
82	nF	201	PEB	C1B-C2B-C3B	-2.40	103.76	106.51
87	A2	850	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
87	6N	612	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
87	72	601	CLA	C2A-C1A-CHA	2.40	128.05	123.86
82	J7	202	PEB	C2B-C1B-NB	2.40	115.64	110.53
82	FJ	201	PEB	CMA-C2A-C1A	-2.40	107.24	112.40
85	d6	405	BCR	C20-C21-C22	-2.40	123.89	127.31
82	TP	202	PEB	CHA-C1B-C2B	2.40	131.06	124.90
82	mF	202	PEB	C2A-C1A-NA	2.40	110.34	108.27
82	m1	202	PEB	CHA-C4A-NA	2.40	128.05	125.20
82	H9	202	PEB	CHA-C4A-NA	-2.40	122.36	125.20
82	eO	201	PEB	CHA-C4A-NA	2.40	128.05	125.20
85	c6	603	BCR	C28-C27-C26	-2.40	109.80	114.08
82	cM	202	PEB	CHC-C1D-ND	-2.40	110.69	113.72
87	AN	814	CLA	C3B-C4B-NB	-2.40	108.29	110.52
85	K2	105	BCR	C1-C6-C5	-2.40	119.24	122.61
82	e1	201	PEB	C4C-C3C-C2C	-2.39	105.29	107.50
82	O4	201	PEB	C4C-C3C-C2C	-2.39	105.29	107.50
82	RO	202	PEB	CMC-C3C-C4C	2.39	129.60	127.06
84	m3	1001	CYC	C1B-C2B-C3B	-2.39	105.37	107.87
82	SD	202	PEB	CHB-C4B-C3B	-2.39	119.78	125.32
94	D6	408	PL9	C51-C49-C50	2.39	119.89	114.60
91	D6	404	PHO	CBC-CAC-C3C	-2.39	109.37	112.88
82	QG	202	PEB	C3B-C4B-NB	2.39	113.53	110.05
82	KM	203	PEB	C1C-NC-C4C	-2.39	105.34	109.60
82	lH	202	PEB	C2A-C1A-NA	2.39	110.34	108.27
82	LB	201	PEB	CHA-C1B-NB	-2.39	119.92	124.93
84	R3	1001	CYC	CAB-C3B-C2B	2.39	131.62	127.53
82	eH	201	PEB	OD-C4D-C3D	-2.39	124.04	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	fF	201	PEB	C1B-C2B-C3B	-2.39	103.76	106.51
87	12	601	CLA	O2A-CGA-O1A	-2.39	117.33	123.30
85	J2	102	BCR	C10-C11-C12	-2.39	115.75	123.22
82	j4	202	PEB	CHB-C1C-NC	-2.39	119.84	125.32
85	JN	102	BCR	C20-C19-C18	-2.39	119.69	126.42
82	YA	303	PEB	CMC-C3C-C4C	-2.39	124.52	127.06
87	AN	803	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
87	ON	201	CLA	CHB-C4A-NA	2.39	127.82	124.51
82	SM	201	PEB	CAB-CBB-CGB	-2.39	108.45	113.60
82	FM	202	PEB	CAC-C2C-C1C	2.39	129.57	125.76
87	32	309	CLA	CMB-C2B-C3B	2.39	132.38	126.59
82	QG	203	PEB	C3C-C4C-NC	2.39	110.49	108.33
82	aF	202	PEB	OA-C1A-C2A	-2.39	124.27	126.17
87	AN	831	CLA	CHC-C1C-NC	2.39	127.83	124.20
82	WH	201	PEB	OD-C4D-ND	-2.39	122.39	125.93
82	YM	203	PEB	OD-C4D-ND	-2.39	122.39	125.93
84	n3	1001	CYC	C2A-C1A-NA	2.39	113.53	110.05
84	N3	1001	CYC	CAD-C3D-C4D	2.39	129.57	125.76
87	AN	820	CLA	C7-C6-C5	-2.39	106.86	113.36
82	cF	203	PEB	CMC-C3C-C4C	2.39	129.60	127.06
82	ZF	202	PEB	C4C-C3C-C2C	-2.39	105.29	107.50
82	BB	202	PEB	CAC-CBC-CGC	-2.39	108.45	113.60
82	eB	202	PEB	CAB-CBB-CGB	-2.39	108.45	113.60
87	AN	826	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
87	A2	826	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
82	H7	201	PEB	CHB-C1C-C2C	-2.39	121.75	127.15
82	AI	202	PEB	CHB-C1C-NC	-2.39	119.84	125.32
87	bL	613	CLA	CMB-C2B-C3B	2.39	132.38	126.59
87	D6	403	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
84	H3	1001	CYC	C2A-C1A-NA	2.39	113.53	110.05
84	O3	1001	CYC	C2A-C1A-NA	2.39	113.53	110.05
82	F5	201	PEB	C1C-CHB-C4B	2.39	133.65	128.28
87	dL	402	CLA	CMB-C2B-C3B	2.39	132.38	126.59
84	CO	1001	CYC	CBD-CAD-C3D	-2.39	105.98	112.63
85	B2	840	BCR	C33-C5-C4	2.39	118.21	113.62
82	X9	201	PEB	C1D-CHC-C4C	-2.39	109.73	113.26
82	mO	203	PEB	C1D-CHC-C4C	-2.39	109.73	113.26
82	DK	203	PEB	OD-C4D-C3D	-2.39	124.04	129.46
82	FQ	202	PEB	C4C-C3C-C2C	-2.39	105.29	107.50
82	s8	201	PEB	C4C-C3C-C2C	-2.39	105.29	107.50
82	uF	203	PEB	C4C-C3C-C2C	-2.39	105.29	107.50
82	hK	201	PEB	C4C-C3C-C2C	-2.39	105.29	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	xF	305	PUB	C1B-C2B-C3B	-2.39	105.29	107.50
82	JD	201	PEB	CHB-C4B-NB	-2.39	119.60	124.58
82	XA	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
82	D5	201	PEB	C2B-C1B-NB	2.39	115.63	110.53
82	UF	201	PEB	C1C-NC-C4C	-2.39	105.34	109.60
87	KN	103	CLA	CMB-C2B-C3B	2.39	132.38	126.59
87	3N	306	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
82	e4	203	PEB	CAB-CBB-CGB	2.39	118.75	113.60
88	dL	408	LHG	O8-C23-O10	-2.39	117.56	123.59
82	XA	201	PEB	CHA-C4A-NA	2.39	128.05	125.20
84	DG	1001	CYC	CBD-CAD-C3D	-2.39	105.98	112.63
82	RF	202	PEB	CHB-C1C-C2C	-2.39	121.76	127.15
87	cL	514	CLA	C3B-C4B-NB	-2.39	108.30	110.52
84	J4	1001	CYC	C4D-ND-C1D	-2.39	105.52	109.79
82	SF	202	PEB	OD-C4D-C3D	-2.39	124.04	129.46
82	E9	201	PEB	C1D-CHC-C4C	-2.39	109.73	113.26
82	lF	202	PEB	C1D-CHC-C4C	2.39	116.78	113.26
82	DF	202	PEB	OD-C4D-ND	-2.39	122.39	125.93
83	AE	303	PUB	CMD-C2D-C3D	2.39	131.35	127.77
82	D9	202	PEB	C3B-C4B-NB	2.39	113.53	110.05
82	eF	202	PEB	C3C-C4C-NC	2.39	110.48	108.33
87	c6	615	CLA	CHB-C4A-NA	2.39	127.82	124.51
82	UJ	201	PEB	CAB-CBB-CGB	-2.39	108.46	113.60
82	R4	202	PEB	CAC-C2C-C1C	2.39	129.57	125.76
87	b6	605	CLA	C3B-C4B-NB	2.39	112.73	110.52
82	RG	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
82	aB	201	PEB	CHA-C1B-C2B	2.39	131.04	124.90
87	BN	833	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
82	SD	202	PEB	CHB-C1C-C2C	-2.39	121.76	127.15
82	lM	203	PEB	C4C-C3C-C2C	-2.39	105.30	107.50
87	AN	839	CLA	O2D-CGD-CBD	2.39	115.51	111.27
82	KB	301	PEB	CHA-C4A-NA	2.39	128.05	125.20
82	KM	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
82	SQ	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
82	F9	203	PEB	OD-C4D-C3D	-2.39	124.05	129.46
82	S4	202	PEB	CBA-CAA-C3A	-2.39	108.15	113.47
87	42	604	CLA	CGD-CBD-CAD	2.39	118.47	110.73
87	2N	307	CLA	C2A-C1A-CHA	2.39	128.04	123.86
85	B2	841	BCR	C20-C21-C22	-2.39	123.90	127.31
85	fL	101	BCR	C37-C22-C21	-2.39	119.58	122.92
82	BQ	201	PEB	CAB-C3B-C4B	2.39	129.23	125.01
85	FN	204	BCR	C16-C15-C14	-2.39	118.58	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	b6	616	CLA	CHB-C4A-NA	2.39	127.81	124.51
82	EF	202	PEB	CHB-C4B-C3B	-2.39	119.79	125.32
82	xF	303	PEB	CHA-C1B-NB	-2.39	119.94	124.93
82	aG	201	PEB	CHA-C1B-NB	-2.39	119.94	124.93
82	NQ	203	PEB	C4C-C3C-C2C	-2.39	105.30	107.50
82	DJ	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
84	x3	1001	CYC	CAB-C3B-C2B	2.39	131.61	127.53
82	eF	203	PEB	C1C-CHB-C4B	2.39	133.64	128.28
82	mH	201	PEB	CHC-C4C-NC	2.39	124.38	121.15
82	VI	203	PEB	C2B-C1B-NB	2.39	115.63	110.53
96	V6	201	HEM	CAA-CBA-CGA	-2.39	108.46	113.60
82	TG	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
84	e3	1001	CYC	CAD-C3D-C4D	2.39	129.56	125.76
87	BN	828	CLA	CHB-C1B-NB	2.39	126.78	124.26
82	JM	201	PEB	C1D-CHC-C4C	2.39	116.78	113.26
82	pC	201	PEB	CHB-C1C-NC	-2.39	119.85	125.32
82	KI	201	PEB	C2B-C1B-NB	2.39	115.62	110.53
87	2N	310	CLA	CMD-C2D-C1D	-2.39	120.50	124.71
87	BN	802	CLA	C2A-C1A-CHA	2.39	128.03	123.86
82	DA	203	PEB	CHB-C4B-C3B	-2.39	119.80	125.32
82	YH	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
82	MK	201	PEB	CAB-C3B-C4B	2.39	129.23	125.01
88	mL	102	LHG	O8-C23-C24	2.39	119.40	111.91
82	EF	201	PEB	C4C-C3C-C2C	-2.39	105.30	107.50
82	eH	201	PEB	C4C-C3C-C2C	-2.39	105.30	107.50
82	GB	201	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
82	V9	202	PEB	CMB-C2B-C1B	2.39	128.74	125.06
82	eA	301	PEB	OD-C4D-ND	-2.39	122.39	125.93
82	EF	201	PEB	CAC-C2C-C3C	2.39	132.54	127.07
82	IK	201	PEB	C1C-NC-C4C	-2.39	105.35	109.60
84	LH	1002	CYC	O2A-CGA-O1A	-2.39	117.35	123.30
94	d6	408	PL9	C42-C43-C44	-2.39	121.91	127.66
87	dL	409	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
82	YB	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
82	j1	203	PEB	CHC-C1D-ND	-2.39	110.70	113.72
85	B2	840	BCR	C39-C30-C25	-2.39	106.43	110.30
87	B6	604	CLA	CHB-C4A-NA	2.39	127.81	124.51
82	IK	203	PEB	CMB-C2B-C1B	2.39	128.74	125.06
87	62	303	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
84	BG	1002	CYC	CMC-C2C-C1C	-2.39	107.26	112.40
82	eA	301	PEB	CBA-CAA-C3A	-2.39	108.15	113.47
82	VB	201	PEB	C4C-C3C-C2C	-2.39	105.30	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lK	201	PEB	CBB-CAB-C3B	2.39	119.26	112.63
82	s8	203	PEB	C4B-C3B-C2B	-2.39	104.14	106.78
84	j3	1001	CYC	C2A-C1A-NA	2.39	113.52	110.05
84	q3	1001	CYC	C2A-C1A-NA	2.39	113.52	110.05
82	PQ	201	PEB	CHA-C1B-NB	-2.39	119.94	124.93
84	E3	1001	CYC	CAD-C3D-C4D	2.39	129.56	125.76
87	A2	825	CLA	CHB-C1B-NB	2.39	126.78	124.26
87	DL	404	CLA	CMB-C2B-C3B	2.39	132.37	126.59
82	D9	201	PEB	OA-C1A-C2A	-2.39	124.28	126.17
82	IF	201	PEB	C1C-NC-C4C	-2.39	105.35	109.60
82	CP	203	PEB	CHC-C1D-ND	-2.39	110.71	113.72
82	jH	203	PEB	CHC-C1D-ND	-2.39	110.71	113.72
84	V3	1001	CYC	CAD-CBD-CGD	-2.39	108.47	113.60
87	4N	609	CLA	C2D-C1D-ND	-2.39	108.35	110.10
87	bL	606	CLA	O2D-CGD-CBD	2.39	115.51	111.27
83	AO	302	PUB	C2C-C1C-NC	2.39	113.52	110.05
84	DH	1001	CYC	C2A-C1A-NA	2.39	113.52	110.05
84	P3	1001	CYC	CAB-C3B-C2B	2.39	131.61	127.53
84	i3	1001	CYC	CAB-C3B-C2B	2.39	131.61	127.53
85	F6	101	BCR	C20-C19-C18	-2.39	119.72	126.42
82	H5	202	PEB	CAB-C3B-C4B	2.39	129.23	125.01
92	qL	301	LMG	C4-C3-C2	2.39	114.99	110.82
82	RE	201	PEB	C4C-C3C-C2C	-2.39	105.30	107.50
96	G2	201	HEM	CBD-CAD-C3D	-2.39	106.00	112.63
82	N9	201	PEB	C1D-CHC-C4C	-2.39	109.74	113.26
82	D9	201	PEB	O1B-CGB-CBB	-2.38	115.42	123.08
87	7N	601	CLA	C2A-C1A-CHA	2.38	128.03	123.86
82	TK	202	PEB	C4B-NB-C1B	-2.38	102.02	106.51
82	TE	201	PEB	CAB-C3B-C4B	2.38	129.23	125.01
83	A1	304	PUB	CBB-CAB-C3B	-2.38	106.00	112.63
82	CP	202	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
82	FQ	201	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
82	iH	202	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
83	AG	303	PUB	CMD-C2D-C3D	2.38	131.35	127.77
85	FN	202	BCR	C29-C28-C27	-2.38	106.05	111.38
87	B2	801	CLA	C2A-C1A-CHA	2.38	128.03	123.86
84	L1	1001	CYC	CMA-C3A-C2A	-2.38	119.64	126.12
82	R7	201	PEB	OD-C4D-C3D	-2.38	124.06	129.46
82	XA	201	PEB	CAA-C3A-C2A	-2.38	108.30	114.26
82	UI	202	PEB	C1B-C2B-C3B	-2.38	103.77	106.51
82	t8	202	PEB	OD-C4D-ND	-2.38	122.40	125.93
82	JO	1002	PEB	CBA-CAA-C3A	-2.38	108.16	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IA	202	PEB	CHA-C4A-NA	-2.38	122.37	125.20
82	GE	1002	PEB	CAC-C2C-C1C	2.38	129.56	125.76
82	MF	201	PEB	OD-C4D-C3D	-2.38	124.06	129.46
82	UM	203	PEB	OD-C4D-C3D	-2.38	124.06	129.46
82	kE	202	PEB	CAC-C2C-C3C	2.38	132.53	127.07
82	KK	202	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
84	C1	1001	CYC	CHB-C4A-C3A	2.38	131.03	124.90
84	f3	1001	CYC	C2A-C1A-NA	2.38	113.52	110.05
82	B7	203	PEB	OA-C1A-C2A	-2.38	124.28	126.17
87	32	303	CLA	C3B-C4B-NB	2.38	112.73	110.52
87	BN	831	CLA	CHC-C4B-NB	2.38	126.78	124.26
82	YK	202	PEB	CHA-C1B-NB	-2.38	119.95	124.93
82	kK	203	PEB	C4C-C3C-C2C	-2.38	105.30	107.50
82	jJ	201	PEB	CAB-CBB-CGB	-2.38	108.47	113.60
82	CQ	202	PEB	C1B-C2B-C3B	-2.38	103.77	106.51
82	zC	202	PEB	C1B-C2B-C3B	-2.38	103.77	106.51
87	6N	602	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
82	h4	202	PEB	OD-C4D-C3D	-2.38	124.06	129.46
82	Z1	203	PEB	C2A-C1A-NA	2.38	110.33	108.27
82	RH	202	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
82	iG	201	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
85	b6	601	BCR	C33-C5-C4	2.38	118.19	113.62
82	zC	201	PEB	C2B-C1B-NB	2.38	115.61	110.53
83	yF	303	PUB	CMD-C2D-C3D	2.38	131.34	127.77
82	uC	202	PEB	C3C-C4C-NC	2.38	110.48	108.33
87	BL	621	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
82	R1	201	PEB	C2B-C1B-NB	2.38	115.61	110.53
82	sK	202	PEB	C3B-C4B-NB	2.38	113.51	110.05
87	L2	204	CLA	CHD-C4C-NC	-2.38	120.45	124.20
82	HD	203	PEB	C4C-C3C-C2C	-2.38	105.30	107.50
82	ZH	201	PEB	C4C-C3C-C2C	-2.38	105.30	107.50
82	OO	201	PEB	C4C-C3C-C2C	-2.38	105.30	107.50
82	mH	202	PEB	C4C-C3C-C2C	-2.38	105.30	107.50
87	BN	802	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
82	FQ	201	PEB	CHA-C4A-NA	2.38	128.04	125.20
82	N1	1002	PEB	CMB-C2B-C1B	2.38	128.73	125.06
82	F9	201	PEB	CAC-C2C-C3C	2.38	132.52	127.07
85	bL	601	BCR	C20-C21-C22	-2.38	123.91	127.31
82	VI	203	PEB	CHB-C4B-NB	-2.38	119.62	124.58
82	IJ	202	PEB	CAB-CBB-CGB	-2.38	108.48	113.60
82	NJ	202	PEB	CAC-CBC-CGC	-2.38	108.48	113.60
87	CL	505	CLA	C2A-C1A-CHA	2.38	128.02	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	22	607	CLA	C2A-C1A-CHA	2.38	128.02	123.86
85	BN	838	BCR	C37-C22-C23	2.38	121.83	118.08
82	hJ	203	PEB	C3B-C4B-NB	2.38	113.51	110.05
83	yF	302	PUB	C2C-C1C-NC	2.38	113.51	110.05
83	xK	306	PUB	C2C-C1C-NC	2.38	113.51	110.05
82	AA	201	PEB	CBB-CAB-C3B	2.38	119.24	112.63
82	NH	1002	PEB	CMB-C2B-C1B	2.38	128.73	125.06
84	MG	1001	CYC	CHB-C1B-NB	-2.38	120.95	126.06
83	AJ	304	PUB	CAC-CBC-CGC	-2.38	108.48	113.60
84	CG	1001	CYC	C4A-C3A-C2A	-2.38	103.77	106.51
87	C6	514	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
82	MP	202	PEB	OD-C4D-C3D	-2.38	124.07	129.46
82	dG	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
82	BA	203	PEB	OA-C1A-C2A	-2.38	124.28	126.17
82	lH	202	PEB	CHB-C4B-C3B	2.38	130.82	125.32
84	IO	1001	CYC	CHA-C4D-C3D	-2.38	121.78	127.15
82	U5	201	PEB	C2B-C1B-NB	2.38	115.61	110.53
82	UO	201	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
82	SF	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
82	fJ	202	PEB	CMD-C2D-C3D	2.38	133.42	130.06
82	P9	201	PEB	C1D-CHC-C4C	-2.38	109.75	113.26
87	ON	202	CLA	CHC-C4B-NB	2.38	126.78	124.26
84	P3	1001	CYC	C1B-C2B-C3B	-2.38	105.39	107.87
82	J9	202	PEB	C2A-C1A-NA	2.38	110.33	108.27
82	OB	201	PEB	OD-C4D-ND	-2.38	122.40	125.93
82	VP	201	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
82	F7	201	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
82	RH	202	PEB	CAB-C3B-C4B	2.38	129.22	125.01
82	DI	201	PEB	CAB-C3B-C4B	2.38	129.22	125.01
82	VQ	203	PEB	C3C-C4C-NC	2.38	110.48	108.33
87	AN	816	CLA	C3B-C4B-NB	-2.38	108.31	110.52
82	A4	301	PEB	OD-C4D-C3D	-2.38	124.07	129.46
96	FL	102	HEM	CBB-CAB-C3B	-2.38	115.78	127.62
82	FM	202	PEB	CMA-C2A-C1A	-2.38	107.27	112.40
84	J1	1001	CYC	CAC-C3C-C4C	-2.38	106.56	112.67
87	5N	608	CLA	CHD-C1D-ND	-2.38	122.27	124.45
82	I9	201	PEB	C1D-CHC-C4C	-2.38	109.75	113.26
87	4N	604	CLA	CGD-CBD-CAD	2.38	118.44	110.73
82	F9	201	PEB	CMC-C3C-C4C	2.38	129.58	127.06
82	yF	301	PEB	CMC-C3C-C4C	2.38	129.58	127.06
82	QP	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
82	CJ	201	PEB	CHA-C1B-C2B	2.38	131.02	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NO	1002	PEB	CAB-CBB-CGB	-2.38	108.48	113.60
82	DD	201	PEB	CAC-C2C-C1C	2.38	129.55	125.76
82	mH	202	PEB	C2A-C1A-NA	2.38	110.32	108.27
82	NB	203	PEB	CAB-C3B-C4B	2.38	129.22	125.01
82	BD	201	PEB	CAB-C3B-C4B	2.38	129.22	125.01
82	lO	202	PEB	OD-C4D-ND	-2.38	122.41	125.93
85	B2	838	BCR	C37-C22-C23	2.38	121.83	118.08
82	SB	203	PEB	CHB-C4B-NB	-2.38	119.63	124.58
85	d6	405	BCR	C28-C27-C26	-2.38	109.83	114.08
82	TF	202	PEB	C4B-NB-C1B	-2.38	102.03	106.51
82	U4	201	PEB	OA-C1A-C2A	-2.38	124.28	126.17
82	B5	203	PEB	OA-C1A-C2A	-2.38	124.28	126.17
87	RN	203	CLA	CMA-C3A-C2A	-2.38	104.23	113.83
82	i1	202	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
82	IF	203	PEB	CMB-C2B-C1B	2.38	128.73	125.06
82	fG	201	PEB	C3C-C4C-NC	2.38	110.47	108.33
85	CL	516	BCR	C20-C19-C18	-2.38	119.74	126.42
82	RK	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
87	B6	614	CLA	CHB-C4A-NA	2.38	127.80	124.51
82	V9	201	PEB	C1D-CHC-C4C	-2.38	109.75	113.26
82	VD	201	PEB	OD-C4D-ND	-2.38	122.41	125.93
82	WF	202	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
85	cL	503	BCR	C15-C16-C17	-2.38	118.60	123.47
82	KK	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
82	XB	202	PEB	CAB-C3B-C4B	2.38	129.21	125.01
82	O7	202	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
87	BN	836	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
82	SI	201	PEB	CBC-CAC-C2C	-2.38	106.02	112.63
96	GN	201	HEM	CBD-CAD-C3D	-2.38	106.02	112.63
82	uF	203	PEB	CHC-C1D-ND	-2.38	110.72	113.72
82	qC	203	PEB	CHA-C1B-NB	-2.38	119.96	124.93
82	NJ	201	PEB	OD-C4D-C3D	-2.38	124.08	129.46
82	MJ	203	PEB	CHB-C1C-NC	-2.38	119.88	125.32
87	1N	601	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
87	8N	304	CLA	O2A-CGA-O1A	-2.38	117.38	123.30
82	cE	201	PEB	CAB-C3B-C4B	2.38	129.21	125.01
82	Z9	304	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
82	YF	202	PEB	CMB-C2B-C1B	2.38	128.72	125.06
84	C3	1001	CYC	CAD-C3D-C4D	2.38	129.55	125.76
92	aL	611	LMG	O8-C28-O10	-2.38	117.59	123.59
84	B3	1001	CYC	C2A-C1A-NA	2.38	113.51	110.05
87	1N	601	CLA	O2A-CGA-O1A	-2.38	117.38	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	R2	203	CLA	CMA-C3A-C2A	-2.38	104.24	113.83
82	J5	203	PEB	C1D-CHC-C4C	-2.38	109.75	113.26
82	HA	202	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
85	BN	840	BCR	C39-C30-C25	-2.38	106.44	110.30
87	FN	201	CLA	C2D-C1D-ND	-2.38	108.35	110.10
87	62	307	CLA	C2D-C1D-ND	-2.38	108.35	110.10
82	eG	202	PEB	CHA-C1B-NB	-2.38	119.96	124.93
84	i3	1001	CYC	CAD-C3D-C4D	2.38	129.55	125.76
82	D7	203	PEB	CHB-C4B-C3B	-2.38	119.82	125.32
82	mO	203	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
84	o3	1001	CYC	C2A-C1A-NA	2.38	113.50	110.05
82	LD	202	PEB	OA-C1A-C2A	-2.38	124.28	126.17
82	TQ	201	PEB	C3C-C4C-NC	2.38	110.47	108.33
82	NF	201	PEB	CAB-C3B-C4B	2.38	129.21	125.01
82	WP	202	PEB	OD-C4D-C3D	-2.38	124.08	129.46
87	6N	609	CLA	CHB-C4A-NA	2.38	127.80	124.51
85	A2	804	BCR	C39-C30-C25	-2.38	106.45	110.30
82	ND	202	PEB	C4C-C3C-C2C	-2.38	105.31	107.50
82	JI	201	PEB	C4C-C3C-C2C	-2.38	105.31	107.50
87	L2	206	CLA	C4-C3-C5	2.38	119.27	115.27
84	E3	1001	CYC	CAB-C3B-C2B	2.38	131.59	127.53
84	v3	1001	CYC	CAB-C3B-C2B	2.38	131.59	127.53
82	NK	201	PEB	CMB-C2B-C1B	2.38	128.72	125.06
82	MM	202	PEB	CHB-C1C-C2C	-2.38	121.79	127.15
82	O9	202	PEB	CHB-C4B-NB	-2.38	119.63	124.58
82	DQ	202	PEB	C1C-NC-C4C	-2.38	105.37	109.60
82	qC	203	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
88	d6	407	LHG	C5-O7-C7	-2.37	111.94	117.79
84	T3	1001	CYC	CAD-C3D-C4D	2.37	129.54	125.76
87	B2	836	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
87	CL	504	CLA	CHA-C1A-NA	-2.37	120.96	126.40
83	xK	301	PUB	CAC-C2C-C1C	2.37	129.21	125.01
82	gB	203	PEB	C1C-CHB-C4B	-2.37	122.96	128.28
82	RG	201	PEB	CBB-CAB-C3B	2.37	119.22	112.63
82	UK	201	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	b1	201	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	iF	203	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	jF	201	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	jK	201	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	ZJ	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
87	A2	829	CLA	CMB-C2B-C1B	-2.37	121.75	125.37
87	cL	514	CLA	CMB-C2B-C1B	-2.37	121.75	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	NO	1002	PEB	CAC-C2C-C1C	2.37	129.54	125.76
82	JH	1002	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
82	kE	201	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
82	RO	203	PEB	CMB-C2B-C1B	2.37	128.72	125.06
82	lE	201	PEB	CMB-C2B-C1B	2.37	128.72	125.06
82	O7	201	PEB	CMD-C2D-C3D	2.37	133.41	130.06
82	CJ	201	PEB	CHB-C1C-C2C	-2.37	121.79	127.15
87	AN	852	CLA	CHA-C4D-ND	2.37	137.47	132.50
87	A2	851	CLA	CHB-C1B-NB	2.37	126.77	124.26
87	C6	510	CLA	CHB-C1B-NB	2.37	126.77	124.26
95	BL	607	DGD	C4D-C3D-C2D	2.37	114.97	110.82
87	72	608	CLA	C2A-C1A-CHA	2.37	128.00	123.85
84	H4	1001	CYC	O1A-CGA-CBA	-2.37	115.45	123.08
85	CL	501	BCR	C36-C18-C19	2.37	121.82	118.08
87	A6	403	CLA	O2D-CGD-CBD	2.37	115.49	111.27
82	fK	201	PEB	CHA-C1B-C2B	2.37	131.00	124.90
87	B2	808	CLA	C3B-C4B-NB	-2.37	108.31	110.52
82	cB	402	PEB	C1C-CHB-C4B	-2.37	122.96	128.28
84	G3	1001	CYC	CAD-C3D-C4D	2.37	129.54	125.76
84	63	901	CYC	CAD-C3D-C4D	2.37	129.54	125.76
82	UE	202	PEB	CAA-C3A-C2A	-2.37	108.33	114.26
87	O2	201	CLA	CHB-C4A-NA	2.37	127.79	124.51
82	AA	201	PEB	C2A-C1A-NA	2.37	110.32	108.27
87	32	304	CLA	C1D-ND-C4D	-2.37	104.65	106.33
82	zC	202	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
87	A2	827	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
82	iJ	202	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
82	q8	203	PEB	CHC-C1D-ND	-2.37	110.72	113.72
82	RD	202	PEB	CMC-C3C-C4C	2.37	129.58	127.06
82	DB	201	PEB	C3B-C4B-NB	2.37	113.50	110.05
87	AN	811	CLA	C1-O2A-CGA	2.37	122.67	116.44
82	SM	203	PEB	OD-C4D-C3D	-2.37	124.08	129.46
82	AP	202	PEB	C1D-CHC-C4C	-2.37	109.76	113.26
82	XF	202	PEB	C1C-NC-C4C	-2.37	105.38	109.60
87	FN	203	CLA	CHB-C1B-NB	2.37	126.77	124.26
82	M9	302	PEB	C2B-C1B-NB	2.37	115.59	110.53
84	x3	1001	CYC	C4D-CHA-C1A	2.37	133.60	128.28
82	Y7	301	PEB	CHA-C4A-NA	2.37	128.03	125.20
82	UM	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
82	dE	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
83	AH	304	PUB	CHB-C1C-C2C	2.37	130.81	125.32
82	UB	301	PEB	C3B-C4B-NB	2.37	113.50	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	308	CLA	O2A-CGA-O1A	-2.37	117.39	123.30
82	YM	202	PEB	C1D-CHC-C4C	-2.37	109.76	113.26
82	YF	202	PEB	CAC-C2C-C1C	2.37	129.54	125.76
84	y3	1001	CYC	CHB-C1B-C2B	-2.37	122.25	126.95
82	QH	201	PEB	CMB-C2B-C1B	2.37	128.72	125.06
82	TE	201	PEB	OD-C4D-C3D	-2.37	124.09	129.46
87	BN	812	CLA	O2D-CGD-CBD	2.37	115.48	111.27
82	VD	201	PEB	OA-C1A-C2A	-2.37	124.29	126.17
87	RN	202	CLA	C2D-C1D-ND	-2.37	108.36	110.10
82	LA	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
84	i3	1001	CYC	C1B-C2B-C3B	-2.37	105.40	107.87
82	DM	202	PEB	CHA-C1B-NB	-2.37	119.97	124.93
82	e1	202	PEB	C3B-C4B-NB	2.37	113.50	110.05
82	DQ	201	PEB	CAC-C2C-C1C	2.37	129.54	125.76
87	42	605	CLA	O1A-CGA-CBA	2.37	130.70	123.08
82	HM	201	PEB	CHB-C4B-NB	-2.37	119.64	124.58
87	7N	608	CLA	C3B-C4B-NB	-2.37	108.31	110.52
84	c3	1001	CYC	CAB-C3B-C2B	2.37	131.59	127.53
84	m3	1001	CYC	CAB-C3B-C2B	2.37	131.59	127.53
82	X7	201	PEB	CHA-C1B-C2B	2.37	131.00	124.90
82	GI	201	PEB	C2B-C1B-NB	2.37	115.59	110.53
94	AL	413	PL9	C45-C44-C46	2.37	119.26	115.27
82	YP	503	PEB	CHA-C1B-NB	-2.37	119.97	124.93
82	MK	201	PEB	OD-C4D-C3D	-2.37	124.09	129.46
82	YO	201	PEB	OD-C4D-C3D	-2.37	124.09	129.46
82	jK	202	PEB	OD-C4D-C3D	-2.37	124.09	129.46
82	TG	201	PEB	CHB-C4B-C3B	-2.37	119.83	125.32
82	P1	202	PEB	CMC-C3C-C4C	2.37	129.57	127.06
87	B2	801	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
91	AL	410	PHO	C4B-NB-C1B	-2.37	105.16	108.83
82	H5	202	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	jG	202	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	NG	201	PEB	CAB-C3B-C4B	2.37	129.20	125.01
82	ZH	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
82	eM	201	PEB	CHA-C4A-NA	2.37	128.02	125.20
82	PK	202	PEB	C1C-CHB-C4B	2.37	133.60	128.28
82	TF	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
82	iG	202	PEB	CMB-C2B-C1B	2.37	128.72	125.06
82	gM	202	PEB	OD-C4D-C3D	-2.37	124.09	129.46
87	B2	834	CLA	C2D-C1D-ND	-2.37	108.36	110.10
85	F6	101	BCR	C33-C5-C4	2.37	118.17	113.62
82	IB	203	PEB	CAC-CBC-CGC	-2.37	108.50	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JA	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
87	A2	811	CLA	C1-O2A-CGA	2.37	122.66	116.44
82	aF	202	PEB	OD-C4D-C3D	-2.37	124.09	129.46
96	V6	201	HEM	C1A-CHA-C4D	-2.37	120.72	126.34
82	kM	202	PEB	CHA-C1B-NB	-2.37	119.97	124.93
82	aJ	203	PEB	CMC-C3C-C4C	-2.37	124.55	127.06
84	y3	1001	CYC	CAB-C3B-C2B	2.37	131.58	127.53
82	LB	201	PEB	CMA-C2A-C1A	-2.37	107.29	112.40
82	YF	202	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	dB	201	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
87	52	608	CLA	CHD-C1D-ND	-2.37	122.28	124.45
82	W4	201	PEB	C4B-C3B-C2B	-2.37	104.16	106.78
82	L7	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
87	C6	517	CLA	CHB-C4A-NA	2.37	127.79	124.51
82	SK	203	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
82	WJ	201	PEB	CBB-CAB-C3B	-2.37	106.04	112.63
82	Y9	203	PEB	CBC-CAC-C2C	-2.37	106.04	112.63
84	HO	1001	CYC	O1A-CGA-CBA	-2.37	115.47	123.08
84	t3	1001	CYC	CAB-C3B-C2B	2.37	131.58	127.53
82	gH	203	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	XK	202	PEB	C1C-NC-C4C	-2.37	105.38	109.60
82	CB	201	PEB	CAC-CBC-CGC	-2.37	108.50	113.60
82	W1	202	PEB	CMC-C3C-C4C	-2.37	124.55	127.06
87	bL	604	CLA	C3B-C4B-NB	-2.37	108.32	110.52
87	R2	202	CLA	C2D-C1D-ND	-2.37	108.36	110.10
82	KG	201	PEB	CHC-C1D-ND	-2.37	110.73	113.72
83	BJ	302	PUB	CAB-C3B-C4B	2.37	129.53	125.76
87	A2	825	CLA	CMB-C2B-C3B	2.37	132.33	126.59
87	4N	607	CLA	CHB-C1B-NB	2.37	126.77	124.26
82	RG	201	PEB	C4C-C3C-C2C	-2.37	105.31	107.50
82	cF	203	PEB	C1C-NC-C4C	-2.37	105.38	109.60
82	Q9	202	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	ED	201	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
82	iF	203	PEB	CAB-C3B-C4B	2.37	129.20	125.01
87	62	313	CLA	C2A-C1A-CHA	2.37	128.00	123.86
84	V3	1001	CYC	C4D-CHA-C1A	2.37	133.59	128.28
87	AN	827	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
82	GJ	203	PEB	OD-C4D-C3D	-2.37	124.09	129.46
82	LA	203	PEB	CAB-CBB-CGB	-2.37	108.51	113.60
82	DK	202	PEB	CAC-CBC-CGC	-2.37	108.51	113.60
84	G3	1001	CYC	CAB-C3B-C2B	2.37	131.58	127.53
82	SJ	202	PEB	CHA-C1B-NB	-2.37	119.98	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YB	201	PEB	CMA-C2A-C1A	-2.37	107.30	112.40
82	KJ	201	PEB	CMA-C2A-C1A	-2.37	107.30	112.40
82	PQ	202	PEB	CMA-C2A-C1A	-2.37	107.30	112.40
82	G7	202	PEB	CHB-C1C-C2C	-2.37	121.81	127.15
82	sF	202	PEB	C3B-C4B-NB	2.37	113.49	110.05
82	CM	202	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	dJ	201	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	DM	201	PEB	CHA-C1B-C2B	2.37	130.99	124.90
82	O5	203	PEB	C1D-CHC-C4C	-2.37	109.76	113.26
84	E1	1001	CYC	CHA-C1A-C2A	-2.37	119.84	125.32
82	Q9	203	PEB	CHB-C4B-NB	-2.37	119.65	124.58
87	AN	836	CLA	CHB-C1B-NB	2.37	126.76	124.26
87	42	607	CLA	CHB-C1B-NB	2.37	126.76	124.26
87	B2	831	CLA	CHC-C4B-NB	2.37	126.76	124.26
82	QB	202	PEB	CAB-CBB-CGB	-2.37	108.51	113.60
87	62	303	CLA	C2D-C1D-ND	-2.37	108.36	110.10
82	mG	201	PEB	CAC-C2C-C1C	2.37	129.53	125.76
84	CG	1001	CYC	CHA-C4D-C3D	-2.37	121.81	127.15
82	g1	201	PEB	CAA-C3A-C2A	-2.37	108.34	114.26
82	QK	203	PEB	CHB-C4B-C3B	2.37	130.79	125.32
82	EJ	201	PEB	CAB-C3B-C4B	2.37	129.20	125.01
82	LK	201	PEB	O2B-CGB-CBB	2.37	121.64	114.03
82	m4	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	gH	201	PEB	CHC-C1D-ND	-2.37	110.73	113.72
82	f1	202	PEB	CHC-C4C-NC	2.37	124.35	121.15
82	WH	202	PEB	CMC-C3C-C4C	-2.37	124.55	127.06
82	DI	201	PEB	CMC-C3C-C4C	-2.37	124.55	127.06
87	AN	827	CLA	CAA-C2A-C1A	-2.37	104.22	111.97
84	g3	1001	CYC	CAD-C3D-C4D	2.37	129.53	125.76
82	OM	202	PEB	CBC-CAC-C2C	-2.37	106.05	112.63
87	6N	603	CLA	C3B-C4B-NB	-2.37	108.32	110.52
82	DK	201	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
87	52	607	CLA	C2A-C1A-CHA	2.37	128.00	123.86
82	YO	203	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	FM	201	PEB	CMA-C2A-C1A	-2.37	107.30	112.40
87	B6	613	CLA	CHB-C4A-NA	2.37	127.78	124.51
84	I3	1001	CYC	C2A-C1A-NA	2.37	113.49	110.05
88	ML	102	LHG	C5-O7-C7	-2.37	111.96	117.79
82	XQ	203	PEB	OD-C4D-ND	-2.37	122.42	125.93
82	cM	202	PEB	CHC-C4C-NC	2.37	124.35	121.15
82	kM	201	PEB	C4C-C3C-C2C	-2.37	105.32	107.50
82	SD	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	A2	827	CLA	CAA-C2A-C1A	-2.37	104.22	111.97
82	QE	203	PEB	C3C-C4C-NC	2.37	110.46	108.33
82	cB	402	PEB	CHB-C4B-NB	-2.37	119.65	124.58
84	W3	1001	CYC	CAB-C3B-C2B	2.37	131.58	127.53
85	A2	847	BCR	C27-C26-C25	-2.37	119.30	122.73
87	b6	608	CLA	C2D-C1D-ND	-2.37	108.36	110.10
85	F6	101	BCR	C37-C22-C21	-2.37	119.61	122.92
82	NQ	202	PEB	CHB-C1C-C2C	-2.37	121.81	127.15
82	LI	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	h1	202	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	cK	203	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	Y4	203	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	HM	202	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
82	TP	202	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
87	C6	516	CLA	CHC-C4B-NB	2.37	126.76	124.26
103	8N	310	ZEX	C10-C11-C12	2.37	130.60	123.22
87	F2	202	CLA	C3B-C4B-NB	-2.37	108.32	110.52
82	KB	304	PEB	CAB-C3B-C4B	2.37	129.19	125.01
82	i1	202	PEB	CAB-C3B-C4B	2.37	129.19	125.01
87	3N	313	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
82	SB	202	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	SP	202	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	e4	201	PEB	CHA-C4A-NA	2.37	128.02	125.20
82	XA	201	PEB	CHA-C1B-C2B	2.37	130.98	124.90
87	A2	852	CLA	CHA-C4D-ND	2.37	137.45	132.50
87	AN	825	CLA	CMB-C2B-C3B	2.37	132.32	126.59
82	UJ	202	PEB	C3C-C4C-NC	2.37	110.46	108.33
82	OD	202	PEB	CMB-C2B-C1B	2.37	128.71	125.06
82	SF	201	PEB	C1C-NC-C4C	-2.37	105.39	109.60
84	W3	1001	CYC	CHB-C1B-C2B	-2.37	122.26	126.95
94	a6	601	PL9	C51-C49-C50	2.37	119.83	114.60
82	Y4	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
82	U5	201	PEB	OD-C4D-ND	-2.37	122.43	125.93
87	B6	608	CLA	CHB-C4A-NA	2.37	127.78	124.51
82	pK	201	PEB	CAA-C3A-C2A	-2.37	108.35	114.26
82	KF	202	PEB	C4B-C3B-C2B	-2.37	104.17	106.78
87	22	611	CLA	C2A-C1A-CHA	2.37	128.00	123.86
82	U9	201	PEB	O1B-CGB-CBB	-2.37	115.48	123.08
87	AN	828	CLA	CHC-C4B-NB	2.37	126.76	124.26
87	AN	851	CLA	CHB-C1B-NB	2.37	126.76	124.26
96	v6	201	HEM	CAA-CBA-CGA	-2.37	108.51	113.60
82	UI	202	PEB	CHC-C1D-ND	-2.37	110.73	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	O9	202	PEB	C2A-C1A-NA	2.37	110.31	108.27
82	WK	201	PEB	CBA-CAA-C3A	2.37	118.73	113.47
91	A6	407	PHO	O2A-CGA-CBA	2.37	119.33	111.91
85	B2	843	BCR	C1-C6-C7	2.37	122.47	115.78
87	O2	202	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
87	b6	606	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
87	B6	604	CLA	O2D-CGD-CBD	2.36	115.47	111.27
82	gO	201	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
85	KN	104	BCR	C1-C6-C5	-2.36	119.28	122.61
87	7N	608	CLA	C2A-C1A-CHA	2.36	127.98	123.85
87	52	602	CLA	CAA-C2A-C3A	-2.36	106.30	112.78
82	zF	501	PEB	CHC-C1D-ND	-2.36	110.73	113.72
82	ZK	201	PEB	CMB-C2B-C1B	2.36	128.71	125.06
82	OA	202	PEB	CBA-CAA-C3A	-2.36	108.20	113.47
82	W4	201	PEB	CHB-C1C-C2C	-2.36	121.82	127.15
94	dL	406	PL9	C16-C17-C18	-2.36	104.11	111.88
82	VF	201	PEB	C3B-C4B-NB	2.36	113.49	110.05
82	YF	203	PEB	CAC-C2C-C1C	2.36	129.53	125.76
82	aK	201	PEB	C2B-C1B-NB	2.36	115.57	110.53
82	IF	201	PEB	CHB-C4B-NB	2.36	129.50	124.58
82	hO	202	PEB	OD-C4D-C3D	-2.36	124.11	129.46
85	BN	843	BCR	C1-C6-C7	2.36	122.47	115.78
82	QB	201	PEB	C1B-C2B-C3B	-2.36	103.79	106.51
87	C6	515	CLA	O2D-CGD-CBD	2.36	115.47	111.27
82	BB	203	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
84	FE	1001	CYC	CHA-C4D-C3D	-2.36	121.82	127.15
85	A2	848	BCR	C34-C9-C10	-2.36	119.61	122.92
82	U5	201	PEB	C1C-CHB-C4B	2.36	133.58	128.28
85	F2	203	BCR	C29-C28-C27	-2.36	106.10	111.38
84	Q3	1001	CYC	C2A-C1A-NA	2.36	113.49	110.05
82	jJ	203	PEB	CAA-C3A-C4A	-2.36	106.61	112.67
82	WG	201	PEB	C4B-C3B-C2B	-2.36	104.17	106.78
87	22	610	CLA	CMD-C2D-C1D	-2.36	120.55	124.71
87	A2	839	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
84	l3	1001	CYC	CAB-C3B-C2B	2.36	131.57	127.53
82	CQ	201	PEB	C4B-NB-C1B	-2.36	102.06	106.51
82	TK	202	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	OI	202	PEB	CHB-C1C-NC	2.36	130.73	125.32
82	XK	202	PEB	OD-C4D-ND	-2.36	122.43	125.93
82	r8	202	PEB	C3B-C4B-NB	2.36	113.48	110.05
82	sC	203	PEB	C3B-C4B-NB	2.36	113.48	110.05
82	WO	201	PEB	CHB-C1C-C2C	-2.36	121.82	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aK	202	PEB	OD-C4D-C3D	-2.36	124.11	129.46
87	3N	303	CLA	C2A-C1A-CHA	2.36	127.99	123.86
82	SA	201	PEB	O2C-CGC-CBC	2.36	121.62	114.03
82	WJ	201	PEB	CMA-C2A-C1A	-2.36	107.31	112.40
85	d6	405	BCR	C16-C15-C14	-2.36	118.64	123.47
95	cL	502	DGD	O6E-C5E-C4E	-2.36	105.41	109.69
85	A2	804	BCR	C1-C6-C5	-2.36	119.29	122.61
87	L2	202	CLA	C3B-C4B-NB	-2.36	108.32	110.52
82	NF	201	PEB	CMB-C2B-C1B	2.36	128.70	125.06
87	ON	202	CLA	CHA-C4D-ND	2.36	137.44	132.50
82	HA	203	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	HB	201	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	YK	202	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	OA	202	PEB	CHC-C1D-ND	-2.36	110.74	113.72
82	hJ	202	PEB	CHA-C1B-NB	-2.36	119.99	124.93
82	KF	203	PEB	CAA-C3A-C4A	-2.36	106.61	112.67
87	D6	405	CLA	CHB-C4A-NA	2.36	127.78	124.51
82	CK	201	PEB	CAC-CBC-CGC	-2.36	108.52	113.60
82	CD	202	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
87	4N	605	CLA	O1A-CGA-CBA	2.36	130.67	123.08
82	DQ	203	PEB	CHC-C4C-NC	2.36	124.34	121.15
82	EQ	201	PEB	CMC-C3C-C4C	2.36	129.56	127.06
82	XB	202	PEB	CHB-C1C-C2C	-2.36	121.82	127.15
82	FA	201	PEB	CAC-CBC-CGC	-2.36	108.52	113.60
82	mM	202	PEB	C2A-C1A-NA	2.36	110.31	108.27
87	CL	506	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
87	C6	511	CLA	CHB-C4A-NA	2.36	127.78	124.51
87	d6	401	CLA	CHB-C4A-NA	2.36	127.78	124.51
82	AK	202	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	WI	201	PEB	OD-C4D-C3D	-2.36	124.11	129.46
82	VA	203	PEB	C1D-CHC-C4C	-2.36	109.78	113.26
87	AN	849	CLA	CMD-C2D-C3D	2.36	133.04	127.61
82	ZG	201	PEB	CMC-C3C-C4C	2.36	129.56	127.06
82	fH	201	PEB	CMB-C2B-C1B	2.36	128.70	125.06
85	Z6	101	BCR	C20-C19-C18	-2.36	119.79	126.42
82	AG	304	PEB	CHC-C1D-ND	-2.36	110.74	113.72
84	c3	1001	CYC	CAD-C3D-C4D	2.36	129.52	125.76
87	7N	609	CLA	C2A-C1A-CHA	2.36	127.98	123.86
87	CL	511	CLA	CHC-C4B-NB	2.36	126.75	124.26
82	IK	201	PEB	CHB-C4B-NB	2.36	129.49	124.58
82	A9	201	PEB	C1D-CHC-C4C	-2.36	109.78	113.26
82	LQ	203	PEB	OD-C4D-C3D	-2.36	124.11	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	BM	302	PUB	CAC-C2C-C1C	2.36	129.18	125.01
82	jF	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
82	QB	203	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	iE	202	PEB	CMB-C2B-C1B	2.36	128.70	125.06
84	p3	1001	CYC	CAB-C3B-C2B	2.36	131.56	127.53
82	kH	201	PEB	CHB-C1C-NC	-2.36	119.92	125.32
85	AN	847	BCR	C27-C26-C25	-2.36	119.31	122.73
87	BN	827	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
85	AN	804	BCR	C1-C6-C5	-2.36	119.29	122.61
82	q8	202	PEB	OD-C4D-C3D	-2.36	124.12	129.46
82	YA	303	PEB	OD-C4D-ND	-2.36	122.44	125.93
82	XF	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
82	S7	201	PEB	O2C-CGC-CBC	2.36	121.61	114.03
82	aH	202	PEB	CHC-C4C-NC	2.36	124.34	121.15
82	KP	201	PEB	CHB-C1C-C2C	-2.36	121.83	127.15
87	7N	601	CLA	C3B-C4B-NB	-2.36	108.33	110.52
82	OH	202	PEB	CMB-C2B-C1B	2.36	128.70	125.06
82	mK	202	PEB	CMB-C2B-C1B	2.36	128.70	125.06
82	GG	1002	PEB	CAC-C2C-C1C	2.36	129.52	125.76
82	kF	203	PEB	CAC-C2C-C1C	2.36	129.52	125.76
84	K3	1001	CYC	C2D-C1D-ND	2.36	110.71	107.40
82	JK	201	PEB	CAA-C3A-C4A	-2.36	106.62	112.67
85	AN	848	BCR	C24-C25-C26	-2.36	115.75	121.46
82	MM	201	PEB	CHA-C1B-NB	-2.36	120.00	124.93
82	NM	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
87	5N	602	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
84	D1	1003	CYC	CAC-C3C-C2C	-2.36	108.37	114.26
87	62	310	CLA	CHB-C4A-NA	2.36	127.77	124.51
82	VD	202	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
82	DF	202	PEB	C4C-C3C-C2C	-2.36	105.32	107.50
87	ON	202	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
82	KD	202	PEB	CHC-C4C-NC	2.36	124.34	121.15
84	v3	1001	CYC	CAD-C3D-C4D	2.36	129.52	125.76
84	M1	201	CYC	C4D-ND-C1D	-2.36	105.58	109.79
87	LN	206	CLA	C4-C3-C5	2.36	119.24	115.27
82	wK	301	PEB	CHB-C4B-NB	-2.36	119.67	124.58
82	FA	201	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
87	R2	202	CLA	CHB-C4A-NA	2.36	127.77	124.51
83	AH	304	PUB	CBB-CAB-C3B	-2.36	106.08	112.63
87	12	607	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
84	e3	1001	CYC	CAB-C3B-C2B	2.36	131.56	127.53
85	KN	104	BCR	C34-C9-C8	2.36	121.79	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	KG	202	CYC	C4D-CHA-C1A	2.36	133.57	128.28
84	DH	1003	CYC	CAC-C3C-C2C	-2.36	108.37	114.26
82	GJ	202	PEB	CHA-C1B-NB	-2.36	120.00	124.93
82	Q9	202	PEB	CHA-C1B-NB	-2.36	120.00	124.93
87	A2	803	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
87	B2	811	CLA	O2D-CGD-CBD	2.36	115.46	111.27
82	ND	202	PEB	CHB-C1C-C2C	-2.36	121.83	127.15
82	LQ	202	PEB	OD-C4D-C3D	-2.36	124.12	129.46
84	t3	1001	CYC	CAD-C3D-C4D	2.36	129.51	125.76
83	AO	303	PUB	CHC-C1D-ND	-2.36	110.74	113.72
82	cE	201	PEB	CAC-CBC-CGC	-2.36	108.53	113.60
82	WO	201	PEB	C4B-C3B-C2B	-2.36	104.17	106.78
87	AN	821	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
84	T3	1001	CYC	CAB-C3B-C2B	2.36	131.56	127.53
84	g3	1001	CYC	CAB-C3B-C2B	2.36	131.56	127.53
85	cL	518	BCR	C29-C30-C25	2.36	114.11	110.48
82	fF	202	PEB	C4C-C3C-C2C	-2.36	105.33	107.50
85	K2	105	BCR	C34-C9-C8	2.36	121.79	118.08
83	AG	302	PUB	C2C-C1C-NC	2.36	113.48	110.05
82	G7	202	PEB	CAB-C3B-C4B	2.36	129.18	125.01
87	B2	827	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
82	F5	203	PEB	C3C-C4C-NC	2.36	110.45	108.33
84	L1	1001	CYC	C2B-C1B-NB	2.36	110.44	106.99
87	A2	821	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
85	A2	848	BCR	C24-C25-C26	-2.36	115.76	121.46
87	32	307	CLA	O2A-CGA-O1A	-2.36	117.43	123.30
103	82	310	ZEX	O23-C23-C22	-2.36	104.42	109.91
87	AN	826	CLA	CMB-C2B-C3B	2.36	132.29	126.59
85	F2	204	BCR	C16-C15-C14	-2.36	118.65	123.47
82	pF	201	PEB	CAA-C3A-C2A	-2.36	108.37	114.26
87	62	306	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
82	KK	203	PEB	CAA-C3A-C4A	-2.36	106.62	112.67
82	gJ	202	PEB	OD-C4D-C3D	-2.36	124.12	129.46
87	a6	607	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
82	k1	201	PEB	CHB-C1C-NC	-2.36	119.92	125.32
82	D5	201	PEB	C4B-NB-C1B	-2.36	102.07	106.51
87	32	303	CLA	CHC-C4B-NB	-2.35	121.76	124.26
82	ZH	203	PEB	C2A-C1A-NA	2.35	110.30	108.27
82	JI	202	PEB	CAB-C3B-C4B	2.35	129.17	125.01
82	NK	201	PEB	CAB-C3B-C4B	2.35	129.17	125.01
82	OH	201	PEB	CHB-C4B-NB	-2.35	119.68	124.58
82	YJ	201	PEB	C1D-CHC-C4C	-2.35	109.78	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	827	CLA	CHB-C4A-NA	2.35	127.77	124.51
82	YG	202	PEB	C3C-C4C-NC	2.35	110.45	108.33
82	UB	302	PEB	CHA-C1B-NB	-2.35	120.01	124.93
82	YF	202	PEB	CHA-C1B-NB	-2.35	120.01	124.93
82	qK	203	PEB	C3B-C4B-NB	2.35	113.47	110.05
82	dE	203	PEB	OD-C4D-C3D	-2.35	124.13	129.46
87	B2	834	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
84	N4	1001	CYC	C1B-NB-C4B	-2.35	107.67	110.67
82	KQ	202	PEB	CHC-C4C-NC	2.35	124.33	121.15
82	OA	201	PEB	CHC-C1D-ND	-2.35	110.75	113.72
94	AL	413	PL9	C35-C34-C33	-2.35	117.64	123.68
82	D7	202	PEB	CAC-C2C-C1C	2.35	129.51	125.76
84	m3	1001	CYC	CAD-C3D-C4D	2.35	129.51	125.76
87	6N	612	CLA	C2A-C1A-CHA	2.35	127.97	123.86
87	72	602	CLA	CHD-C1D-C2D	2.35	130.42	125.48
84	C1	1001	CYC	CHB-C1B-NB	-2.35	121.00	126.06
88	BL	610	LHG	O8-C23-O10	-2.35	117.65	123.59
82	EB	501	PEB	CHA-C1B-NB	-2.35	120.01	124.93
87	cL	512	CLA	CMC-C2C-C3C	2.35	132.51	126.12
82	dO	201	PEB	C2B-C1B-NB	2.35	115.55	110.53
82	OK	203	PEB	CHC-C4C-NC	2.35	124.33	121.15
82	VD	203	PEB	C3C-C4C-NC	2.35	110.45	108.33
87	cL	511	CLA	C2A-C1A-CHA	2.35	127.97	123.86
85	b6	602	BCR	C21-C20-C19	2.35	130.56	123.22
82	G7	202	PEB	OD-C4D-ND	-2.35	122.44	125.93
87	B2	827	CLA	CHB-C4A-NA	2.35	127.77	124.51
82	k1	202	PEB	C3B-C4B-NB	2.35	113.47	110.05
87	B2	823	CLA	C3B-C4B-NB	-2.35	108.33	110.52
82	LM	202	PEB	OD-C4D-C3D	-2.35	124.13	129.46
87	cL	512	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
82	R1	202	PEB	C4B-C3B-C2B	-2.35	104.18	106.78
82	Y1	201	PEB	CHC-C4C-NC	2.35	124.33	121.15
82	cK	203	PEB	C1C-NC-C4C	-2.35	105.41	109.60
82	GA	202	PEB	OD-C4D-ND	-2.35	122.44	125.93
82	QF	203	PEB	CHB-C4B-C3B	2.35	130.76	125.32
87	AN	827	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
85	FL	101	BCR	C12-C13-C14	2.35	122.55	118.94
103	82	310	ZEX	C10-C11-C12	2.35	130.56	123.22
82	VA	203	PEB	CMC-C3C-C4C	2.35	129.55	127.06
84	K3	1001	CYC	CAD-C3D-C4D	2.35	129.51	125.76
82	i1	201	PEB	C2B-C1B-NB	2.35	115.55	110.53
87	7N	602	CLA	CHD-C1D-C2D	2.35	130.41	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HG	1002	PEB	O2B-CGB-CBB	2.35	121.59	114.03
82	X7	201	PEB	CAA-C3A-C2A	-2.35	108.38	114.26
82	h1	201	PEB	C3B-C4B-NB	2.35	113.47	110.05
84	KH	1001	CYC	CHB-C4A-NA	-2.35	120.01	124.93
82	TM	202	PEB	C4C-C3C-C2C	-2.35	105.33	107.50
82	dO	201	PEB	C4C-C3C-C2C	-2.35	105.33	107.50
84	R3	1001	CYC	CAD-C3D-C4D	2.35	129.51	125.76
82	WF	202	PEB	CAB-C3B-C4B	2.35	129.17	125.01
82	OQ	202	PEB	C2A-C1A-NA	2.35	110.30	108.27
82	ZM	201	PEB	C1D-CHC-C4C	2.35	116.72	113.26
87	42	607	CLA	OBD-CAD-C3D	2.35	134.18	128.52
82	qF	203	PEB	C3B-C4B-NB	2.35	113.47	110.05
82	rK	201	PEB	CAC-C2C-C1C	2.35	129.51	125.76
82	HM	202	PEB	OD-C4D-C3D	-2.35	124.13	129.46
84	A3	1001	CYC	CAB-C3B-C2B	2.35	131.55	127.53
82	WA	201	PEB	CAB-CBB-CGB	-2.35	108.54	113.60
82	CA	201	PEB	CAB-C3B-C4B	2.35	129.17	125.01
82	R1	202	PEB	CAB-C3B-C4B	2.35	129.17	125.01
83	QJ	201	PUB	CAC-C2C-C1C	2.35	129.17	125.01
87	72	608	CLA	O2D-CGD-CBD	2.35	115.44	111.27
82	tC	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
82	aJ	202	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
82	UF	201	PEB	C4C-C3C-C2C	-2.35	105.33	107.50
82	NQ	203	PEB	CHC-C4C-NC	2.35	124.33	121.15
82	MJ	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	AO	301	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	e1	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
87	bL	618	CLA	CMD-C2D-C3D	2.35	133.02	127.61
82	oF	203	PEB	CBA-CAA-C3A	-2.35	108.23	113.47
84	JH	1003	CYC	C1B-CHB-C4A	-2.35	122.34	128.08
82	B5	201	PEB	C2B-C1B-NB	2.35	115.55	110.53
83	YA	302	PUB	CHC-C1D-ND	-2.35	110.75	113.72
92	B6	622	LMG	O8-C28-C29	2.35	119.28	111.91
82	OD	202	PEB	C2A-C1A-NA	2.35	110.30	108.27
82	U5	201	PEB	C2C-C1C-NC	2.35	110.74	107.57
95	h6	101	DGD	O3G-C1D-C2D	2.35	111.97	108.30
87	B2	814	CLA	C3B-C4B-NB	-2.35	108.33	110.52
87	AN	839	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
83	AJ	304	PUB	CHA-C1B-NB	2.35	124.33	121.15
82	UQ	202	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
87	ON	203	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
82	rC	202	PEB	C3B-C4B-NB	2.35	113.47	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	cL	512	CLA	CMB-C2B-C3B	2.35	132.28	126.59
82	RF	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	DP	202	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	P1	202	PEB	OD-C4D-C3D	-2.35	124.14	129.46
87	DL	403	CLA	O2D-CGD-CBD	2.35	115.44	111.27
82	CF	201	PEB	CAC-CBC-CGC	-2.35	108.55	113.60
82	F9	203	PEB	CAA-C3A-C4A	-2.35	106.64	112.67
82	UG	202	PEB	CAA-C3A-C2A	-2.35	108.39	114.26
85	AN	848	BCR	C34-C9-C10	-2.35	119.63	122.92
82	HE	1002	PEB	O2B-CGB-CBB	2.35	121.58	114.03
82	L5	201	PEB	OD-C4D-ND	-2.35	122.45	125.93
82	DK	203	PEB	C4B-NB-C1B	-2.35	102.08	106.51
82	RE	201	PEB	CBB-CAB-C3B	2.35	119.15	112.63
82	jJ	202	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	HF	202	PEB	CHA-C4A-NA	-2.35	122.41	125.20
82	CA	201	PEB	C1C-CHB-C4B	2.35	133.55	128.28
82	HG	1002	PEB	C2A-C1A-NA	2.35	110.30	108.27
85	AN	804	BCR	C39-C30-C25	-2.35	106.49	110.30
82	KJ	203	PEB	C2B-C1B-NB	2.35	115.54	110.53
87	C6	516	CLA	CHB-C4A-NA	2.35	127.76	124.51
87	5N	607	CLA	C2A-C1A-CHA	2.35	127.97	123.86
82	J4	1002	PEB	CBA-CAA-C3A	-2.35	108.24	113.47
82	A7	201	PEB	C1D-CHC-C4C	2.35	116.72	113.26
83	AO	302	PUB	CMD-C2D-C3D	2.35	131.29	127.77
82	HQ	203	PEB	C4C-C3C-C2C	-2.35	105.33	107.50
96	v6	201	HEM	C1A-CHA-C4D	-2.35	120.77	126.34
84	HG	1001	CYC	CMC-C2C-C1C	-2.35	107.34	112.40
82	yC	203	PEB	CHA-C1B-NB	-2.35	120.02	124.93
87	3N	304	CLA	CHC-C4B-NB	-2.35	121.77	124.26
83	A1	304	PUB	CHB-C1C-C2C	2.35	130.75	125.32
82	AK	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
87	O2	203	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
82	C7	201	PEB	C1C-CHB-C4B	2.35	133.55	128.28
82	J9	202	PEB	CMB-C2B-C1B	2.35	128.68	125.06
84	CH	1001	CYC	CHB-C4A-C3A	2.35	130.94	124.90
82	F4	1002	PEB	C3C-C4C-NC	2.35	110.45	108.33
82	kH	201	PEB	CHC-C1D-ND	-2.35	110.75	113.72
82	L9	201	PEB	O2B-CGB-CBB	2.35	121.57	114.03
87	2N	304	CLA	C3B-C4B-NB	-2.35	108.34	110.52
85	Z6	101	BCR	C28-C27-C26	-2.35	109.89	114.08
82	iK	201	PEB	CMB-C2B-C1B	2.35	128.68	125.06
85	B6	621	BCR	C38-C26-C25	-2.35	121.89	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	4N	607	CLA	OBD-CAD-C3D	2.35	134.17	128.52
82	dK	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	L7	203	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
82	J1	1002	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
85	c6	602	BCR	C35-C13-C12	2.35	121.78	118.08
82	Q9	201	PEB	O1B-CGB-CBB	-2.35	115.54	123.08
82	uK	202	PEB	CMB-C2B-C1B	2.35	128.68	125.06
82	B5	202	PEB	C3C-C4C-NC	2.35	110.45	108.33
82	W7	201	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
87	A2	821	CLA	C3B-C4B-NB	-2.35	108.34	110.52
82	1C	203	PEB	OD-C4D-ND	-2.35	122.45	125.93
82	OD	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
82	MF	202	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	g1	202	PEB	OD-C4D-C3D	-2.35	124.14	129.46
82	hH	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
87	BN	834	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
82	CK	202	PEB	CHC-C1D-ND	-2.35	110.76	113.72
82	JJ	201	PEB	CAB-C3B-C4B	2.35	129.16	125.01
82	NF	202	PEB	C4C-C3C-C2C	-2.35	105.33	107.50
82	ZK	202	PEB	C4C-C3C-C2C	-2.35	105.33	107.50
82	UG	202	PEB	CMB-C2B-C1B	2.35	128.68	125.06
82	DM	202	PEB	CHB-C1C-NC	-2.35	119.95	125.32
84	P3	1001	CYC	CAD-C3D-C4D	2.35	129.50	125.76
87	12	609	CLA	CAA-C2A-C1A	2.35	117.33	112.14
82	QH	203	PEB	CMC-C3C-C4C	2.35	129.55	127.06
84	p3	1001	CYC	C2D-C1D-ND	2.35	110.70	107.40
84	N3	1001	CYC	CAB-C3B-C2B	2.35	131.54	127.53
82	A7	201	PEB	C2A-C1A-NA	2.35	110.30	108.27
87	O2	202	CLA	CHC-C4B-NB	2.35	126.74	124.26
82	SP	201	PEB	CAC-CBC-CGC	-2.35	108.56	113.60
82	jJ	203	PEB	CAB-CBB-CGB	-2.35	108.56	113.60
87	C6	519	CLA	CHB-C4A-NA	2.35	127.75	124.51
82	uK	202	PEB	C4C-C3C-C2C	-2.35	105.34	107.50
82	uC	201	PEB	C1D-CHC-C4C	-2.35	109.80	113.26
82	d4	201	PEB	C2B-C1B-NB	2.35	115.53	110.53
84	C3	1001	CYC	CAB-C3B-C2B	2.35	131.54	127.53
82	UB	302	PEB	CAA-C3A-C2A	-2.35	108.40	114.26
82	ZK	201	PEB	CHA-C4A-NA	2.34	127.99	125.20
82	RQ	202	PEB	CMC-C3C-C4C	2.34	129.55	127.06
82	FD	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
85	b6	601	BCR	C8-C7-C6	-2.34	120.62	127.20
87	CL	513	CLA	O2D-CGD-CBD	2.34	115.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	6N	605	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
82	AJ	301	PEB	CMB-C2B-C1B	2.34	128.67	125.06
84	HE	1001	CYC	CMC-C2C-C1C	-2.34	107.35	112.40
82	YO	201	PEB	CHA-C4A-NA	2.34	127.99	125.20
84	p3	1001	CYC	CAD-C3D-C4D	2.34	129.50	125.76
82	FB	201	PEB	CAC-CBC-CGC	-2.34	108.56	113.60
82	YJ	203	PEB	CAB-CBB-CGB	-2.34	108.56	113.60
103	8N	310	ZEX	O23-C23-C22	-2.34	104.45	109.91
82	RO	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
82	uK	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
85	bL	603	BCR	C20-C21-C22	-2.34	123.97	127.31
87	1N	607	CLA	CAA-CBA-CGA	-2.34	106.40	113.25
87	AN	825	CLA	CHB-C1B-NB	2.34	126.74	124.26
87	b6	615	CLA	CHB-C1B-NB	2.34	126.74	124.26
82	SO	202	PEB	CHA-C1B-NB	-2.34	120.03	124.93
84	K1	1001	CYC	CHB-C4A-NA	-2.34	120.03	124.93
82	fK	201	PEB	C3B-C4B-NB	2.34	113.46	110.05
82	cJ	202	PEB	O2B-CGB-CBB	2.34	121.56	114.03
82	W1	203	PEB	C3C-C4C-NC	2.34	110.44	108.33
82	lG	203	PEB	C3C-C4C-NC	2.34	110.44	108.33
82	kH	203	PEB	C3C-C4C-NC	2.34	110.44	108.33
82	W5	201	PEB	CAC-C2C-C1C	2.34	129.49	125.76
84	J3	1001	CYC	CAD-C3D-C4D	2.34	129.49	125.76
87	32	313	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
82	mJ	202	PEB	C2A-C1A-NA	2.34	110.29	108.27
82	RE	201	PEB	CHC-C4C-NC	2.34	124.32	121.15
82	AE	304	PEB	CHC-C1D-ND	-2.34	110.76	113.72
82	UO	201	PEB	OA-C1A-C2A	-2.34	124.31	126.17
82	J5	201	PEB	CHA-C1B-NB	-2.34	120.03	124.93
82	KF	203	PEB	C4C-C3C-C2C	-2.34	105.34	107.50
82	GK	203	PEB	C4C-C3C-C2C	-2.34	105.34	107.50
82	RQ	202	PEB	C4C-C3C-C2C	-2.34	105.34	107.50
82	iF	201	PEB	CMB-C2B-C1B	2.34	128.67	125.06
82	V7	202	PEB	CMC-C3C-C4C	2.34	129.54	127.06
83	xF	306	PUB	C2C-C1C-NC	2.34	113.46	110.05
82	hB	301	PEB	CBB-CAB-C3B	2.34	119.14	112.63
83	QM	201	PUB	CHB-C1C-NC	-2.34	119.70	124.58
82	qC	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
82	cF	203	PEB	OD-C4D-C3D	-2.34	124.15	129.46
82	BI	201	PEB	C4B-NB-C1B	-2.34	102.10	106.51
87	1N	609	CLA	CAA-C2A-C1A	2.34	117.33	112.14
88	iL	101	LHG	O8-C23-C24	2.34	119.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	wF	301	PEB	CHB-C4B-NB	-2.34	119.70	124.58
84	J3	1001	CYC	CAB-C3B-C2B	2.34	131.53	127.53
82	HB	203	PEB	OD-C4D-C3D	-2.34	124.15	129.46
82	LD	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
82	JF	201	PEB	CAA-C3A-C4A	-2.34	106.66	112.67
82	SI	201	PEB	CAC-CBC-CGC	-2.34	108.56	113.60
82	XD	202	PEB	C2A-C1A-NA	2.34	110.29	108.27
82	UI	201	PEB	CHB-C1C-NC	-2.34	119.95	125.32
82	GK	202	PEB	C1C-NC-C4C	-2.34	105.43	109.60
87	32	302	CLA	C2A-C1A-CHA	2.34	127.95	123.86
82	oF	203	PEB	CMA-C2A-C1A	-2.34	107.36	112.40
82	u8	201	PEB	C1D-CHC-C4C	-2.34	109.80	113.26
84	W3	1001	CYC	OC-C1C-NC	-2.34	122.11	124.94
82	VP	201	PEB	CAB-C3B-C4B	2.34	129.15	125.01
82	mK	201	PEB	CAB-C3B-C4B	2.34	129.15	125.01
87	D6	405	CLA	CHB-C1B-NB	2.34	126.74	124.26
84	K3	1001	CYC	CAB-C3B-C2B	2.34	131.53	127.53
84	A3	1001	CYC	CAD-C3D-C4D	2.34	129.49	125.76
82	WF	201	PEB	CBA-CAA-C3A	2.34	118.68	113.47
82	lK	203	PEB	CBA-CAA-C3A	-2.34	108.25	113.47
87	AN	823	CLA	C3B-C4B-NB	-2.34	108.34	110.52
82	l1	201	PEB	C3C-C4C-NC	2.34	110.44	108.33
82	UB	303	PEB	CHA-C1B-NB	-2.34	120.04	124.93
82	dM	201	PEB	CHA-C1B-NB	-2.34	120.04	124.93
85	k6	102	BCR	C10-C11-C12	2.34	130.52	123.22
82	c1	201	PEB	C2B-C1B-NB	2.34	115.53	110.53
82	YK	202	PEB	CAC-C2C-C1C	2.34	129.49	125.76
82	N4	1002	PEB	CAC-C2C-C1C	2.34	129.49	125.76
82	IM	202	PEB	CHB-C1C-C2C	-2.34	121.87	127.15
88	cL	501	LHG	O7-C7-O9	-2.34	118.05	123.70
87	M2	101	CLA	C2A-C1A-CHA	2.34	127.95	123.86
82	DF	203	PEB	C4B-NB-C1B	-2.34	102.10	106.51
82	TK	201	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
82	jK	201	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
87	8N	301	CLA	CHD-C1D-ND	-2.34	122.30	124.45
82	OD	201	PEB	CAA-C3A-C2A	-2.34	108.41	114.26
82	UB	302	PEB	CBC-CAC-C2C	2.34	119.13	112.63
87	K2	106	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
82	h1	201	PEB	CMB-C2B-C1B	2.34	128.67	125.06
82	m1	201	PEB	CHA-C1B-NB	-2.34	120.04	124.93
82	W5	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
87	72	609	CLA	C2A-C1A-CHA	2.34	127.95	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	LN	202	CLA	C3B-C4B-NB	-2.34	108.34	110.52
87	bL	615	CLA	C3B-C4B-NB	-2.34	108.34	110.52
82	KB	301	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
84	DH	1001	CYC	C1A-C2A-C3A	-2.34	104.19	106.78
85	Z6	101	BCR	C36-C18-C17	-2.34	119.64	122.92
82	jH	202	PEB	CHB-C4B-C3B	2.34	130.73	125.32
96	fL	102	HEM	C1A-CHA-C4D	-2.34	120.79	126.34
87	BN	834	CLA	O2D-CGD-CBD	2.34	115.43	111.27
82	h4	201	PEB	C2A-C1A-NA	2.34	110.29	108.27
82	PK	201	PEB	CMB-C2B-C1B	2.34	128.67	125.06
82	mF	201	PEB	CHB-C1C-C2C	-2.34	121.87	127.15
82	B5	202	PEB	C3B-C4B-NB	2.34	113.45	110.05
82	WD	201	PEB	CMD-C2D-C3D	2.34	133.36	130.06
84	IE	1001	CYC	CHA-C1A-C2A	-2.34	119.91	125.32
87	22	601	CLA	C3B-C4B-NB	-2.34	108.34	110.52
82	RQ	203	PEB	CMB-C2B-C1B	2.34	128.67	125.06
82	LD	203	PEB	OD-C4D-C3D	-2.34	124.16	129.46
82	mE	201	PEB	CAC-C2C-C1C	2.34	129.49	125.76
87	2N	304	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
82	PM	202	PEB	CHB-C1C-NC	-2.34	119.96	125.32
87	B2	822	CLA	CHA-C1A-NA	-2.34	121.04	126.40
82	FA	203	PEB	C2A-C1A-NA	2.34	110.29	108.27
82	mO	201	PEB	OD-C4D-C3D	-2.34	124.16	129.46
87	82	302	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
82	gM	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
83	xF	301	PUB	CAC-C2C-C1C	2.34	129.15	125.01
82	jM	201	PEB	C1C-CHB-C4B	-2.34	123.04	128.28
82	OM	201	PEB	CHA-C4A-NA	2.34	127.98	125.20
87	BN	824	CLA	C3B-C4B-NB	-2.34	108.35	110.52
87	1N	607	CLA	C3B-C4B-NB	-2.34	108.35	110.52
87	32	308	CLA	CHB-C4A-NA	2.34	127.75	124.51
87	A2	805	CLA	CHB-C4A-NA	2.34	127.75	124.51
87	KN	105	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
82	QP	202	PEB	C3C-C4C-NC	2.34	110.44	108.33
95	BL	613	DGD	O5D-C6D-C5D	2.34	113.37	109.05
82	XD	203	PEB	CMB-C2B-C1B	2.34	128.66	125.06
82	AA	201	PEB	C1D-CHC-C4C	2.34	116.70	113.26
82	FD	201	PEB	OD-C4D-C3D	-2.34	124.16	129.46
87	c6	614	CLA	C1-C2-C3	-2.34	122.00	126.04
84	y3	1001	CYC	OC-C1C-NC	-2.34	122.11	124.94
82	AO	301	PEB	C4C-C3C-C2C	-2.34	105.34	107.50
82	bO	201	PEB	C4C-C3C-C2C	-2.34	105.34	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eM	201	PEB	CHA-C1B-C2B	2.34	130.91	124.90
82	uC	203	PEB	C1C-CHB-C4B	2.34	133.52	128.28
82	OG	201	PEB	C4B-C3B-C2B	-2.34	104.20	106.78
82	dE	203	PEB	C4B-C3B-C2B	-2.34	104.20	106.78
82	VB	201	PEB	OD-C4D-C3D	-2.34	124.17	129.46
82	gH	202	PEB	OD-C4D-C3D	-2.34	124.17	129.46
82	HE	1002	PEB	OD-C4D-ND	-2.34	122.47	125.93
82	Z5	301	PEB	C1D-CHC-C4C	-2.34	109.81	113.26
82	XI	202	PEB	C2B-C1B-NB	2.34	115.52	110.53
82	UJ	203	PEB	C3B-C4B-NB	2.34	113.45	110.05
85	A6	401	BCR	C31-C1-C6	-2.34	106.51	110.30
82	A7	201	PEB	CBB-CAB-C3B	2.34	119.12	112.63
87	BN	825	CLA	CAA-C2A-C1A	2.34	119.63	111.97
82	u8	203	PEB	C1C-CHB-C4B	2.34	133.52	128.28
84	NE	201	CYC	C4D-CHA-C1A	2.34	133.52	128.28
82	OK	202	PEB	CHC-C4C-NC	2.34	124.31	121.15
87	AN	829	CLA	C1-C2-C3	-2.34	122.00	126.04
82	g1	201	PEB	CAC-C2C-C1C	2.34	129.48	125.76
82	eJ	202	PEB	CAC-CBC-CGC	-2.34	108.58	113.60
82	YJ	203	PEB	CMB-C2B-C1B	2.34	128.66	125.06
82	MF	203	PEB	CHA-C1B-C2B	2.34	130.91	124.90
82	l1	203	PEB	C2A-C1A-NA	2.34	110.29	108.27
85	CL	501	BCR	C15-C14-C13	-2.34	123.98	127.31
82	YK	201	PEB	CAB-CBB-CGB	-2.34	108.58	113.60
87	B2	834	CLA	O2D-CGD-CBD	2.34	115.42	111.27
82	VM	202	PEB	CAA-C3A-C2A	-2.34	108.42	114.26
82	OQ	201	PEB	CHB-C4B-C3B	-2.34	119.92	125.32
82	tC	202	PEB	C4B-C3B-C2B	-2.34	104.20	106.78
82	lF	203	PEB	CBA-CAA-C3A	-2.34	108.27	113.47
82	RG	202	PEB	CAB-CBB-CGB	-2.34	108.58	113.60
82	ZG	202	PEB	OD-C4D-C3D	-2.34	124.17	129.46
82	WI	203	PEB	C4C-C3C-C2C	-2.34	105.34	107.50
85	K6	102	BCR	C10-C11-C12	2.34	130.50	123.22
82	l1	203	PEB	CHB-C4B-C3B	2.34	130.72	125.32
82	Z9	301	PEB	C2B-C1B-NB	2.34	115.51	110.53
87	42	603	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
87	A2	826	CLA	CMB-C2B-C3B	2.34	132.24	126.59
82	UJ	203	PEB	C1C-CHB-C4B	-2.34	123.05	128.28
85	b6	601	BCR	C38-C26-C27	2.34	118.10	113.62
82	F5	202	PEB	CBA-CAA-C3A	-2.34	108.27	113.47
82	GM	201	PEB	C2A-C1A-NA	2.34	110.29	108.27
82	TF	201	PEB	CAB-CBB-CGB	-2.34	108.58	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MP	203	PEB	CAC-CBC-CGC	-2.34	108.58	113.60
82	SP	202	PEB	CAA-C3A-C4A	-2.34	106.68	112.67
87	BN	801	CLA	C2A-C1A-CHA	2.34	127.94	123.86
82	AH	305	PEB	OD-C4D-C3D	-2.34	124.17	129.46
82	E7	201	PEB	OD-C4D-C3D	-2.34	124.17	129.46
84	t3	1001	CYC	C2D-C1D-ND	2.33	110.68	107.40
82	x8	201	PEB	C4B-C3B-C2B	-2.33	104.20	106.78
82	WG	203	PEB	CAB-CBB-CGB	-2.33	108.58	113.60
82	S4	202	PEB	CHA-C1B-NB	-2.33	120.05	124.93
87	B2	824	CLA	CAA-C2A-C1A	2.33	119.62	111.97
82	hM	201	PEB	OD-C4D-ND	-2.33	122.47	125.93
82	iH	202	PEB	CAB-C3B-C4B	2.33	129.14	125.01
82	V7	203	PEB	CMC-C3C-C4C	2.33	129.53	127.06
87	AN	828	CLA	CHA-C1A-NA	-2.33	121.05	126.40
87	3N	307	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
87	3N	305	CLA	CHB-C4A-NA	2.33	127.74	124.51
95	aL	603	DGD	O1G-C1A-C2A	2.33	119.23	111.91
82	WE	203	PEB	CAB-CBB-CGB	-2.33	108.58	113.60
82	F5	202	PEB	OD-C4D-C3D	-2.33	124.17	129.46
87	AL	404	CLA	CHC-C4B-NB	2.33	126.73	124.26
82	LK	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
82	q8	203	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
82	UH	201	PEB	CHA-C1B-C2B	2.33	130.90	124.90
87	B2	826	CLA	C2D-C1D-ND	-2.33	108.38	110.10
82	JJ	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
82	s8	203	PEB	C3B-C4B-NB	2.33	113.44	110.05
82	CD	201	PEB	C4B-NB-C1B	-2.33	102.11	106.51
87	72	601	CLA	C3B-C4B-NB	-2.33	108.35	110.52
82	oF	202	PEB	CHB-C1C-NC	-2.33	119.97	125.32
96	v6	201	HEM	C4A-CHB-C1B	-2.33	120.80	126.34
87	BN	823	CLA	CHA-C1A-NA	-2.33	121.05	126.40
82	UB	303	PEB	C3C-C4C-NC	2.33	110.43	108.33
82	ZH	201	PEB	CAA-C3A-C2A	-2.33	108.43	114.26
87	MN	101	CLA	C2A-C1A-CHA	2.33	127.94	123.86
82	XP	201	PEB	CAB-C3B-C4B	2.33	129.14	125.01
82	YP	503	PEB	C4C-C3C-C2C	-2.33	105.35	107.50
82	1C	203	PEB	C4C-C3C-C2C	-2.33	105.35	107.50
82	NP	201	PEB	CAC-CBC-CGC	-2.33	108.58	113.60
87	B2	819	CLA	CHB-C1B-NB	2.33	126.73	124.26
82	OK	203	PEB	CAA-C3A-C4A	-2.33	106.68	112.67
82	ZG	203	PEB	CHA-C4A-NA	2.33	127.98	125.20
82	MA	201	PEB	CHB-C4B-NB	-2.33	119.72	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	B6	610	CLA	CHB-C4A-NA	2.33	127.74	124.51
82	uK	202	PEB	CHC-C1D-ND	-2.33	110.77	113.72
82	P7	202	PEB	OD-C4D-C3D	-2.33	124.17	129.46
82	tK	201	PEB	OD-C4D-C3D	-2.33	124.17	129.46
92	j6	101	LMG	C3-C4-C5	2.33	114.40	110.24
82	AM	302	PEB	CHA-C1B-NB	-2.33	120.05	124.93
85	fL	101	BCR	C7-C6-C5	2.33	127.11	121.46
87	22	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
82	gJ	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
82	UP	202	PEB	C1D-CHC-C4C	2.33	116.69	113.26
87	A2	836	CLA	CHB-C1B-NB	2.33	126.73	124.26
83	KA	203	PUB	C1D-CHC-C4C	-2.33	108.29	113.37
82	U5	203	PEB	OD-C4D-C3D	-2.33	124.18	129.46
82	F5	201	PEB	CHB-C4B-C3B	-2.33	119.92	125.32
82	aB	202	PEB	CAC-CBC-CGC	-2.33	108.58	113.60
82	18	201	PEB	OA-C1A-C2A	-2.33	124.32	126.17
82	YE	201	PEB	C4B-NB-C1B	-2.33	102.12	106.51
82	T7	202	PEB	C4B-NB-C1B	-2.33	102.12	106.51
82	ND	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
87	1N	609	CLA	CHA-C1A-NA	-2.33	121.06	126.40
82	bP	502	PEB	CBC-CAC-C2C	-2.33	106.15	112.63
82	iG	201	PEB	C4C-C3C-C2C	-2.33	105.35	107.50
82	F5	201	PEB	C2B-C1B-NB	2.33	115.50	110.53
82	NB	203	PEB	OD-C4D-ND	-2.33	122.48	125.93
82	HI	201	PEB	CAA-C3A-C2A	-2.33	108.44	114.26
82	f1	201	PEB	CAB-C3B-C4B	2.33	129.13	125.01
87	O2	202	CLA	CHA-C4D-ND	2.33	137.38	132.50
96	vL	201	HEM	CHB-C1B-C2B	-2.33	120.25	126.73
87	12	608	CLA	CHD-C1D-ND	-2.33	122.31	124.45
84	LH	1002	CYC	CMA-C3A-C2A	-2.33	119.79	126.12
84	G3	1001	CYC	C2D-C1D-ND	2.33	110.67	107.40
84	i3	1001	CYC	C2D-C1D-ND	2.33	110.67	107.40
83	AE	302	PUB	CHB-C1C-NC	-2.33	119.73	124.58
82	y8	203	PEB	CHA-C1B-NB	-2.33	120.06	124.93
82	UE	202	PEB	CMB-C2B-C1B	2.33	128.65	125.06
82	J5	203	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
87	4N	611	CLA	C3B-C4B-NB	-2.33	108.35	110.52
82	QD	201	PEB	CBB-CAB-C3B	2.33	119.10	112.63
87	2N	311	CLA	C2A-C1A-CHA	2.33	127.93	123.86
82	NJ	202	PEB	O1B-CGB-CBB	-2.33	115.59	123.08
82	XF	201	PEB	CAC-CBC-CGC	-2.33	108.59	113.60
82	EK	201	PEB	CMB-C2B-C3B	-2.33	119.79	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	CL	508	CLA	CHB-C1B-NB	2.33	126.72	124.26
82	ZK	201	PEB	OD-C4D-C3D	-2.33	124.18	129.46
82	lF	201	PEB	OD-C4D-C3D	-2.33	124.18	129.46
85	CL	502	BCR	C15-C16-C17	2.33	128.25	123.47
83	K7	203	PUB	C1D-CHC-C4C	-2.33	108.30	113.37
82	hF	202	PEB	CHC-C4C-NC	2.33	124.30	121.15
82	OQ	201	PEB	CAA-C3A-C2A	-2.33	108.44	114.26
82	gM	202	PEB	CHB-C1C-NC	-2.33	119.98	125.32
82	z8	202	PEB	C3B-C4B-NB	2.33	113.44	110.05
82	UQ	202	PEB	CHA-C4A-NA	-2.33	122.44	125.20
82	FP	202	PEB	OD-C4D-C3D	-2.33	124.18	129.46
82	PP	201	PEB	OD-C4D-C3D	-2.33	124.18	129.46
82	GQ	202	PEB	OD-C4D-C3D	-2.33	124.18	129.46
82	jH	201	PEB	OD-C4D-C3D	-2.33	124.18	129.46
87	A2	827	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
82	TA	202	PEB	C4B-NB-C1B	-2.33	102.12	106.51
87	BN	815	CLA	C3B-C4B-NB	-2.33	108.35	110.52
85	A6	401	BCR	C35-C13-C14	-2.33	119.66	122.92
87	B2	825	CLA	C2A-C1A-CHA	2.33	127.93	123.86
82	jF	202	PEB	OD-C4D-C3D	-2.33	124.18	129.46
87	CL	507	CLA	O2D-CGD-CBD	2.33	115.41	111.27
82	BI	202	PEB	C2B-C1B-NB	2.33	115.50	110.53
82	eF	203	PEB	CHC-C4C-NC	2.33	124.30	121.15
83	AG	303	PUB	CBA-CAA-C3A	-2.33	109.45	112.98
82	SP	203	PEB	C3B-C4B-NB	2.33	113.44	110.05
82	RE	202	PEB	CAB-CBB-CGB	-2.33	108.59	113.60
82	18	203	PEB	OD-C4D-ND	-2.33	122.48	125.93
82	TD	201	PEB	C3C-C4C-NC	2.33	110.43	108.33
82	Q5	202	PEB	C3C-C4C-NC	2.33	110.43	108.33
82	u8	202	PEB	C3C-C4C-NC	2.33	110.43	108.33
82	JI	202	PEB	C4C-C3C-C2C	-2.33	105.35	107.50
82	uF	203	PEB	OD-C4D-C3D	-2.33	124.18	129.46
82	ED	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
82	jF	202	PEB	CMC-C3C-C4C	2.33	129.53	127.06
82	QQ	201	PEB	CBB-CAB-C3B	2.33	119.10	112.63
82	BK	201	PEB	CMB-C2B-C1B	2.33	128.65	125.06
82	MM	203	PEB	CMB-C2B-C1B	2.33	128.65	125.06
82	dM	201	PEB	CMB-C2B-C1B	2.33	128.65	125.06
82	YO	202	PEB	C1C-NC-C4C	-2.33	105.45	109.60
82	NP	201	PEB	OD-C4D-C3D	-2.33	124.19	129.46
82	aE	201	PEB	CMA-C2A-C1A	-2.33	107.38	112.40
82	DK	201	PEB	CHB-C1C-C2C	-2.33	121.90	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WK	201	PEB	OD-C4D-ND	-2.33	122.48	125.93
84	l3	1001	CYC	CAD-C3D-C4D	2.33	129.47	125.76
82	eK	202	PEB	C3C-C4C-NC	2.33	110.43	108.33
84	N3	1001	CYC	C2D-C1D-ND	2.33	110.67	107.40
87	2N	303	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
82	iJ	201	PEB	C4C-C3C-C2C	-2.33	105.35	107.50
82	CP	202	PEB	CHA-C1B-C2B	2.33	130.89	124.90
82	cK	203	PEB	CMC-C3C-C4C	2.33	129.53	127.06
82	GA	202	PEB	CAB-CBB-CGB	-2.33	108.59	113.60
82	kM	201	PEB	CBC-CAC-C2C	-2.33	106.16	112.63
84	BE	1001	CYC	O2D-CGD-CBD	2.33	121.51	114.03
82	KM	202	PEB	C1D-CHC-C4C	-2.33	109.82	113.26
82	cF	203	PEB	C1D-CHC-C4C	-2.33	109.82	113.26
87	A2	828	CLA	CHC-C4B-NB	2.33	126.72	124.26
82	YJ	201	PEB	CAA-C3A-C2A	-2.33	108.44	114.26
82	CB	202	PEB	CHA-C1B-C2B	2.33	130.88	124.90
82	F1	1002	PEB	CMB-C2B-C1B	2.33	128.65	125.06
82	H9	201	PEB	CHB-C4B-C3B	-2.33	119.94	125.32
84	NH	1001	CYC	CHA-C1A-C2A	-2.33	119.94	125.32
84	N4	1001	CYC	CHA-C1A-C2A	-2.33	119.94	125.32
82	ZM	202	PEB	CAC-C2C-C1C	2.33	129.47	125.76
82	B9	202	PEB	CAB-C3B-C4B	2.33	129.12	125.01
82	Y9	201	PEB	CHA-C1B-C2B	-2.33	118.92	124.90
82	JP	201	PEB	O2B-CGB-CBB	2.33	121.51	114.03
82	AM	301	PEB	CHB-C4B-NB	-2.33	119.73	124.58
82	bH	201	PEB	C4C-C3C-C2C	-2.33	105.35	107.50
82	aK	202	PEB	OA-C1A-C2A	-2.33	124.32	126.17
82	PH	202	PEB	OD-C4D-C3D	-2.33	124.19	129.46
82	EQ	201	PEB	CMA-C2A-C1A	-2.33	107.39	112.40
85	B2	838	BCR	C37-C22-C21	-2.33	119.66	122.92
84	T3	1001	CYC	C2D-C1D-ND	2.33	110.67	107.40
82	UD	202	PEB	CHA-C4A-NA	-2.33	122.44	125.20
87	CL	518	CLA	O1D-CGD-CBD	2.33	129.24	124.48
82	FQ	201	PEB	C3B-C4B-NB	2.33	113.43	110.05
82	ZE	202	PEB	OD-C4D-C3D	-2.33	124.19	129.46
82	NO	1002	PEB	OD-C4D-C3D	-2.33	124.19	129.46
87	4N	603	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
82	YJ	201	PEB	CMB-C2B-C1B	2.33	128.65	125.06
82	z8	201	PEB	C2B-C1B-NB	2.33	115.49	110.53
82	aF	201	PEB	C2B-C1B-NB	2.33	115.49	110.53
82	U1	201	PEB	CHA-C1B-C2B	2.33	130.88	124.90
85	Z6	101	BCR	C37-C22-C21	-2.33	119.67	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	B9	201	PEB	CAC-C2C-C1C	2.33	129.47	125.76
82	SQ	201	PEB	C2A-C1A-NA	2.33	110.28	108.27
82	AF	201	PEB	OD-C4D-C3D	-2.33	124.19	129.46
82	WH	203	PEB	OD-C4D-C3D	-2.33	124.19	129.46
84	P3	1001	CYC	C2D-C1D-ND	2.33	110.67	107.40
84	R3	1001	CYC	C2D-C1D-ND	2.33	110.67	107.40
87	C6	518	CLA	CHB-C4A-NA	2.33	127.73	124.51
82	HK	202	PEB	CHA-C4A-NA	-2.33	122.44	125.20
82	HD	202	PEB	OA-C1A-C2A	-2.33	124.32	126.17
82	CM	202	PEB	CMC-C3C-C2C	2.33	130.64	125.61
82	GI	203	PEB	C2B-C1B-NB	2.33	115.49	110.53
82	W5	202	PEB	C2B-C1B-NB	2.33	115.49	110.53
82	B5	201	PEB	CHB-C1C-NC	-2.33	119.99	125.32
82	W7	201	PEB	O2C-CGC-CBC	2.33	121.50	114.03
87	IN	103	CLA	O2D-CGD-CBD	2.33	115.40	111.27
87	BN	809	CLA	C3B-C4B-NB	-2.33	108.36	110.52
84	BG	1001	CYC	O2D-CGD-CBD	2.33	121.50	114.03
82	fB	301	PEB	CBB-CAB-C3B	2.33	119.09	112.63
82	F9	203	PEB	CAA-C3A-C2A	-2.32	108.45	114.26
82	TK	202	PEB	CMC-C3C-C2C	-2.32	120.58	125.61
82	gH	203	PEB	C3B-C4B-NB	2.32	113.43	110.05
82	QJ	204	PEB	OD-C4D-C3D	-2.32	124.19	129.46
94	A6	410	PL9	C51-C49-C50	2.32	119.74	114.60
87	AN	823	CLA	CHB-C1B-NB	2.32	126.72	124.26
82	gJ	202	PEB	CAC-C2C-C1C	2.32	129.46	125.76
87	BN	834	CLA	C2D-C1D-ND	-2.32	108.39	110.10
82	ZM	202	PEB	O2B-CGB-CBB	2.32	121.50	114.03
82	HB	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	QQ	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	kM	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	gM	201	PEB	CHB-C4B-NB	-2.32	119.74	124.58
82	HI	201	PEB	CAB-CBB-CGB	2.32	118.61	113.60
85	kL	100	BCR	C33-C5-C4	2.32	118.08	113.62
82	uF	202	PEB	C3B-C4B-NB	2.32	113.43	110.05
87	3N	313	CLA	C2A-C1A-CHA	2.32	127.92	123.86
87	aL	605	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
82	VP	202	PEB	CAC-C2C-C1C	2.32	129.46	125.76
85	c6	603	BCR	C12-C13-C14	2.32	122.51	118.94
84	73	1002	CYC	C1A-C2A-C3A	-2.32	104.21	106.78
87	A2	829	CLA	C1-C2-C3	-2.32	122.02	126.04
82	T1	201	PEB	CMA-C2A-C1A	-2.32	107.39	112.40
84	LO	1001	CYC	C1B-NB-C4B	-2.32	107.71	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	L1	1001	CYC	CBA-CAA-C2A	-2.32	106.17	112.63
87	7N	608	CLA	O2D-CGD-CBD	2.32	115.40	111.27
82	EI	202	PEB	C2B-C1B-NB	2.32	115.49	110.53
82	l1	202	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
87	B6	615	CLA	CHB-C4A-NA	2.32	127.72	124.51
87	c6	605	CLA	CHB-C4A-NA	2.32	127.72	124.51
82	G7	202	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	bF	201	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	lO	201	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	KB	304	PEB	CAC-C2C-C1C	2.32	129.46	125.76
82	KA	201	PEB	CHB-C4B-C3B	-2.32	119.94	125.32
95	hL	101	DGD	O3G-C1D-C2D	2.32	111.93	108.30
82	KI	203	PEB	C2B-C1B-NB	2.32	115.49	110.53
82	vK	202	PEB	CAB-C3B-C4B	2.32	129.12	125.01
82	NA	202	PEB	CMC-C3C-C4C	2.32	129.52	127.06
82	PH	202	PEB	CMC-C3C-C4C	2.32	129.52	127.06
82	PA	202	PEB	CHA-C4A-NA	2.32	127.97	125.20
82	J7	203	PEB	CHA-C1B-NB	-2.32	120.07	124.93
85	J2	103	BCR	C2-C3-C4	2.32	116.57	111.38
82	O5	203	PEB	OD-C4D-ND	-2.32	122.49	125.93
84	e3	1001	CYC	C2D-C1D-ND	2.32	110.66	107.40
85	JN	102	BCR	C20-C21-C22	-2.32	124.00	127.31
87	A2	850	CLA	CHB-C4A-NA	2.32	127.72	124.51
82	FP	202	PEB	C1D-CHC-C4C	-2.32	109.83	113.26
82	M5	301	PEB	C1D-CHC-C4C	-2.32	109.83	113.26
91	a6	613	PHO	C4B-NB-C1B	-2.32	105.23	108.83
82	FQ	201	PEB	OD-C4D-C3D	-2.32	124.20	129.46
82	rF	201	PEB	CAC-C2C-C1C	2.32	129.46	125.76
82	WP	202	PEB	CAA-C3A-C4A	-2.32	106.71	112.67
82	a1	202	PEB	CHC-C4C-NC	2.32	124.29	121.15
82	Q5	201	PEB	CHC-C4C-NC	2.32	124.29	121.15
82	PF	202	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	l4	201	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	e1	201	PEB	CMA-C2A-C1A	-2.32	107.40	112.40
82	K7	201	PEB	CHB-C4B-C3B	-2.32	119.95	125.32
82	SK	201	PEB	C1C-NC-C4C	-2.32	105.47	109.60
82	PF	202	PEB	C1C-CHB-C4B	2.32	133.49	128.28
82	FD	202	PEB	OD-C4D-ND	-2.32	122.49	125.93
85	BN	838	BCR	C37-C22-C21	-2.32	119.67	122.92
82	wK	303	PEB	CHA-C4A-NA	2.32	127.97	125.20
87	A2	831	CLA	CHC-C1C-NC	2.32	127.73	124.20
87	B2	809	CLA	O2D-CGD-O1D	-2.32	119.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aK	202	PEB	C4B-C3B-C2B	-2.32	104.21	106.78
87	B6	606	CLA	CHB-C4A-NA	2.32	127.72	124.51
82	JO	1002	PEB	CAC-C2C-C1C	2.32	129.46	125.76
87	6N	601	CLA	C3B-C4B-NB	-2.32	108.36	110.52
82	zK	501	PEB	CHC-C1D-ND	-2.32	110.79	113.72
82	LA	203	PEB	OA-C1A-C2A	-2.32	124.33	126.17
82	O5	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
82	Q1	201	PEB	CMB-C2B-C1B	2.32	128.64	125.06
82	qC	203	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	F9	201	PEB	O2B-CGB-CBB	2.32	121.49	114.03
82	cB	403	PEB	CHB-C1C-C2C	-2.32	121.91	127.15
82	aO	203	PEB	CHB-C1C-C2C	-2.32	121.91	127.15
82	IM	201	PEB	C1C-NC-C4C	-2.32	105.47	109.60
82	BQ	201	PEB	C2A-C1A-NA	2.32	110.27	108.27
87	82	306	CLA	CHD-C1D-ND	-2.32	122.32	124.45
82	JI	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	WK	202	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	SP	201	PEB	OD-C4D-ND	-2.32	122.49	125.93
82	jO	202	PEB	OD-C4D-ND	-2.32	122.49	125.93
82	ZF	201	PEB	OD-C4D-C3D	-2.32	124.20	129.46
82	MK	202	PEB	OD-C4D-C3D	-2.32	124.20	129.46
82	pF	201	PEB	CAC-C2C-C1C	2.32	129.46	125.76
87	32	313	CLA	C2A-C1A-CHA	2.32	127.92	123.86
82	PK	202	PEB	CAC-CBC-CGC	-2.32	108.61	113.60
87	CL	512	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
82	VJ	202	PEB	CMA-C2A-C1A	-2.32	107.40	112.40
87	32	309	CLA	CHA-C1A-NA	-2.32	121.08	126.40
82	NI	202	PEB	C2B-C1B-NB	2.32	115.48	110.53
82	QA	201	PEB	CAB-C3B-C4B	2.32	129.11	125.01
82	XQ	203	PEB	CMB-C2B-C1B	2.32	128.64	125.06
84	ME	1001	CYC	CHA-C1A-C2A	-2.32	119.95	125.32
82	YM	202	PEB	C3B-C4B-NB	2.32	113.42	110.05
82	iF	203	PEB	CHA-C1B-NB	-2.32	120.08	124.93
82	m1	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	mH	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
82	A1	305	PEB	OD-C4D-C3D	-2.32	124.20	129.46
82	tF	201	PEB	OD-C4D-C3D	-2.32	124.20	129.46
82	aM	204	PEB	OD-C4D-C3D	-2.32	124.20	129.46
82	zC	201	PEB	C4B-NB-C1B	-2.32	102.14	106.51
82	HE	1002	PEB	C2A-C1A-NA	2.32	110.27	108.27
82	wK	303	PEB	C2A-C1A-NA	2.32	110.27	108.27
87	1N	608	CLA	CHD-C1D-ND	-2.32	122.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	42	611	CLA	C3B-C4B-NB	-2.32	108.36	110.52
82	H7	202	PEB	C3B-C4B-NB	2.32	113.42	110.05
84	BE	1002	CYC	C1A-C2A-C3A	-2.32	104.22	106.78
82	EM	203	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	HA	202	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	N4	1002	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	sF	203	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	bK	201	PEB	C3C-C4C-NC	2.32	110.42	108.33
82	SM	201	PEB	OD-C4D-ND	-2.32	122.50	125.93
82	MP	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
82	iH	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
82	WA	201	PEB	O2C-CGC-CBC	2.32	121.48	114.03
84	BE	1002	CYC	CAB-C3B-C2B	2.32	131.50	127.53
87	cL	515	CLA	CMB-C2B-C3B	2.32	132.20	126.59
82	wC	201	PEB	C1C-CHB-C4B	2.32	133.48	128.28
82	V7	203	PEB	C1D-CHC-C4C	-2.32	109.84	113.26
82	fF	202	PEB	CHA-C1B-NB	-2.32	120.08	124.93
82	P1	201	PEB	CMA-C2A-C1A	-2.32	107.41	112.40
82	aG	201	PEB	CMA-C2A-C1A	-2.32	107.41	112.40
82	tC	202	PEB	CAA-C3A-C2A	-2.32	108.47	114.26
85	J2	103	BCR	C3-C4-C5	-2.32	109.94	114.08
82	OA	201	PEB	CAC-C2C-C3C	2.32	132.38	127.07
87	RN	202	CLA	CHB-C4A-NA	2.32	127.72	124.51
82	II	202	PEB	C2B-C1B-NB	2.32	115.48	110.53
82	aH	202	PEB	C3B-C4B-NB	2.32	113.42	110.05
83	YA	302	PUB	C2C-C1C-NC	2.32	113.42	110.05
87	c6	613	CLA	CHB-C1B-NB	2.32	126.71	124.26
82	ZE	202	PEB	CHB-C4B-C3B	-2.32	119.96	125.32
96	V6	201	HEM	CHD-C1D-C2D	-2.32	121.36	124.98
82	O7	202	PEB	CHC-C1D-ND	-2.32	110.79	113.72
83	AE	302	PUB	CHA-C4A-NA	-2.32	110.79	113.72
82	dG	203	PEB	OD-C4D-C3D	-2.32	124.21	129.46
82	iM	201	PEB	OD-C4D-C3D	-2.32	124.21	129.46
82	cJ	202	PEB	CMA-C2A-C1A	-2.32	107.41	112.40
87	CL	504	CLA	CHB-C4A-NA	2.32	127.72	124.51
95	AL	415	DGD	O1G-C1A-C2A	2.32	119.18	111.91
82	AM	301	PEB	CAC-C2C-C1C	2.32	129.45	125.76
82	UM	201	PEB	CMB-C2B-C1B	2.32	128.63	125.06
82	mF	202	PEB	CMB-C2B-C1B	2.32	128.63	125.06
87	2N	302	CLA	C3B-C4B-NB	-2.32	108.36	110.52
82	NE	202	PEB	CAB-C3B-C4B	2.32	129.11	125.01
82	fH	201	PEB	CAB-C3B-C4B	2.32	129.11	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	V1	203	PEB	CHC-C4C-NC	2.32	124.28	121.15
84	IG	1001	CYC	CHA-C1A-C2A	-2.32	119.96	125.32
83	A4	302	PUB	CMD-C2D-C3D	2.32	131.25	127.77
87	A2	823	CLA	CHB-C1B-NB	2.32	126.71	124.26
87	B6	609	CLA	CHB-C1B-NB	2.32	126.71	124.26
82	hE	203	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	BI	202	PEB	CBD-CAD-C3D	-2.32	116.09	127.62
85	b6	602	BCR	C33-C5-C4	2.32	118.07	113.62
82	MD	202	PEB	OD-C4D-C3D	-2.32	124.21	129.46
82	HD	201	PEB	CMB-C2B-C1B	2.32	128.63	125.06
87	A2	828	CLA	CHA-C1A-NA	-2.32	121.09	126.40
87	I2	103	CLA	O2D-CGD-CBD	2.32	115.39	111.27
82	BP	201	PEB	CBC-CAC-C2C	-2.32	106.19	112.63
82	O1	201	PEB	CHB-C4B-NB	-2.32	119.76	124.58
82	M7	201	PEB	CHB-C4B-NB	-2.32	119.76	124.58
87	B6	607	CLA	CHD-C1D-ND	-2.32	122.33	124.45
82	J4	1002	PEB	CHB-C1C-NC	-2.32	120.01	125.32
82	CI	202	PEB	C2B-C1B-NB	2.32	115.47	110.53
85	c6	602	BCR	C23-C24-C25	-2.32	120.70	127.20
82	aB	202	PEB	OD-C4D-C3D	-2.32	124.21	129.46
85	J2	102	BCR	C20-C21-C22	-2.32	124.00	127.31
87	72	608	CLA	C3B-C4B-NB	-2.32	108.37	110.52
82	Q5	201	PEB	CMA-C2A-C1A	-2.32	107.41	112.40
82	lK	202	PEB	CAB-C3B-C4B	2.32	129.11	125.01
82	NJ	202	PEB	CHA-C1B-NB	-2.32	120.09	124.93
84	NO	1001	CYC	CHA-C1A-C2A	-2.32	119.96	125.32
82	RJ	201	PEB	CHB-C4B-NB	-2.32	119.76	124.58
82	F5	201	PEB	CHB-C1C-NC	-2.32	120.01	125.32
82	iM	202	PEB	CAA-C3A-C2A	-2.32	108.47	114.26
84	y3	1001	CYC	C1B-C2B-C3B	-2.32	105.45	107.87
82	cH	201	PEB	C2B-C1B-NB	2.32	115.47	110.53
82	KK	203	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	dJ	201	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
82	hM	201	PEB	C4C-C3C-C2C	-2.32	105.36	107.50
84	L4	1001	CYC	C1B-NB-C4B	-2.32	107.72	110.67
82	WE	203	PEB	CHB-C4B-C3B	-2.32	119.96	125.32
82	oK	203	PEB	CBA-CAA-C3A	-2.32	108.31	113.47
82	Q5	203	PEB	C1B-C2B-C3B	-2.32	103.85	106.51
95	a6	603	DGD	C2G-O2G-C1B	-2.32	112.09	117.79
82	HI	201	PEB	OD-C4D-C3D	-2.32	124.21	129.46
82	VI	202	PEB	C2B-C1B-NB	2.32	115.47	110.53
82	mJ	201	PEB	C1C-CHB-C4B	-2.32	123.09	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LM	202	PEB	CAB-CBB-CGB	2.32	118.59	113.60
87	32	304	CLA	CHB-C4A-NA	2.32	127.71	124.51
87	bL	605	CLA	CHB-C4A-NA	2.32	127.71	124.51
87	5N	607	CLA	CMB-C2B-C3B	2.32	132.20	126.59
87	7N	609	CLA	C3B-C4B-NB	-2.32	108.37	110.52
82	P1	202	PEB	C2A-C1A-NA	2.32	110.27	108.27
85	JN	103	BCR	C3-C4-C5	-2.32	109.94	114.08
82	kF	202	PEB	CAB-C3B-C4B	2.32	129.10	125.01
87	AN	827	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
82	Z9	303	PEB	OD-C4D-C3D	-2.32	124.22	129.46
87	2N	311	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
82	BA	203	PEB	CAC-CBC-CGC	-2.32	108.62	113.60
82	G7	202	PEB	CAB-CBB-CGB	-2.32	108.62	113.60
82	EM	201	PEB	CMB-C2B-C1B	2.31	128.63	125.06
85	L2	205	BCR	C24-C23-C22	-2.31	122.74	126.23
82	eK	202	PEB	CHA-C1B-C2B	2.31	130.85	124.90
82	iK	202	PEB	O1C-CGC-CBC	-2.31	115.64	123.08
82	NI	201	PEB	C4C-C3C-C2C	-2.31	105.36	107.50
82	g4	201	PEB	C4C-C3C-C2C	-2.31	105.36	107.50
82	fK	202	PEB	C4C-C3C-C2C	-2.31	105.36	107.50
82	lK	201	PEB	OD-C4D-C3D	-2.31	124.22	129.46
82	kE	202	PEB	CAB-C3B-C4B	2.31	129.10	125.01
82	Y7	303	PEB	CMC-C3C-C4C	-2.31	124.61	127.06
82	J4	1002	PEB	CAC-C2C-C1C	2.31	129.45	125.76
82	PG	202	PEB	CMC-C3C-C2C	2.31	130.61	125.61
84	A3	1001	CYC	C2D-C1D-ND	2.31	110.65	107.40
87	AN	838	CLA	C4-C3-C5	2.31	119.16	115.27
82	wF	303	PEB	C2A-C1A-NA	2.31	110.27	108.27
82	iJ	202	PEB	C2A-C1A-NA	2.31	110.27	108.27
82	PF	202	PEB	CAC-CBC-CGC	-2.31	108.62	113.60
87	AN	805	CLA	CHB-C4A-NA	2.31	127.71	124.51
82	eH	202	PEB	C3B-C4B-NB	2.31	113.42	110.05
84	CH	1001	CYC	C1A-C2A-C3A	-2.31	104.22	106.78
82	rC	201	PEB	CMC-C3C-C2C	2.31	130.61	125.61
82	gH	201	PEB	CAC-C2C-C1C	2.31	129.45	125.76
82	U9	202	PEB	C1C-NC-C4C	-2.31	105.48	109.60
87	72	606	CLA	CHA-C1A-NA	-2.31	121.10	126.40
82	Y1	202	PEB	C1C-CHB-C4B	2.31	133.47	128.28
82	EJ	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
84	CH	1001	CYC	CHB-C1B-NB	-2.31	121.09	126.06
82	hK	202	PEB	CHC-C4C-NC	2.31	124.28	121.15
82	AD	303	PEB	CMA-C2A-C1A	-2.31	107.42	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
96	E6	101	HEM	C4C-C3C-C2C	-2.31	104.85	106.75
82	VP	202	PEB	OD-C4D-C3D	-2.31	124.22	129.46
87	8N	303	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
87	3N	301	CLA	CHB-C4A-NA	2.31	127.71	124.51
82	kF	202	PEB	C3B-C4B-NB	2.31	113.41	110.05
83	QJ	201	PUB	CMD-C2D-C3D	2.31	131.24	127.77
82	WD	202	PEB	C2A-C1A-NA	2.31	110.27	108.27
82	JA	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
82	SP	203	PEB	CHA-C1B-NB	-2.31	120.09	124.93
87	BN	810	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
87	32	306	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
82	wC	201	PEB	CHB-C1C-C2C	-2.31	121.93	127.15
82	GK	203	PEB	O2B-CGB-CBB	2.31	121.46	114.03
82	KB	301	PEB	C3B-C4B-NB	2.31	113.41	110.05
83	AD	302	PUB	C2C-C1C-NC	2.31	113.41	110.05
87	22	611	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
82	MB	202	PEB	CHA-C1B-NB	-2.31	120.10	124.93
87	A2	838	CLA	C4-C3-C5	2.31	119.16	115.27
82	jJ	203	PEB	CAB-C3B-C4B	2.31	129.10	125.01
82	lM	201	PEB	CAB-C3B-C4B	2.31	129.10	125.01
84	E3	1001	CYC	C2D-C1D-ND	2.31	110.65	107.40
82	SO	201	PEB	C4B-C3B-C2B	-2.31	104.22	106.78
82	MM	203	PEB	CAC-C2C-C1C	2.31	129.44	125.76
84	NE	201	CYC	CHB-C1B-NB	-2.31	121.09	126.06
82	TH	201	PEB	CMA-C2A-C1A	-2.31	107.42	112.40
82	YJ	201	PEB	CMA-C2A-C1A	-2.31	107.42	112.40
82	HM	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	BP	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	k1	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	kH	202	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	EK	201	PEB	CAC-C2C-C3C	2.31	132.36	127.07
87	BN	820	CLA	CHB-C1B-NB	2.31	126.70	124.26
82	U5	202	PEB	CHA-C4A-NA	-2.31	122.46	125.20
82	Q1	203	PEB	C4B-C3B-C2B	-2.31	104.22	106.78
82	O1	201	PEB	C3C-C4C-NC	2.31	110.41	108.33
82	IB	202	PEB	CMB-C2B-C1B	2.31	128.62	125.06
87	BN	823	CLA	C2A-C1A-CHA	2.31	127.90	123.86
82	BP	201	PEB	CAB-C3B-C4B	2.31	129.10	125.01
82	PE	202	PEB	CMC-C3C-C2C	2.31	130.60	125.61
82	H7	203	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	kK	202	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
83	yK	302	PUB	C2C-C1C-NC	2.31	113.41	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	bL	616	CLA	C2A-C1A-CHA	2.31	127.90	123.86
82	YF	201	PEB	CAB-CBB-CGB	-2.31	108.63	113.60
82	mJ	201	PEB	CAB-CBB-CGB	-2.31	108.63	113.60
82	OQ	202	PEB	CMB-C2B-C1B	2.31	128.62	125.06
82	t8	202	PEB	C4B-C3B-C2B	-2.31	104.23	106.78
82	AP	201	PEB	CHB-C1C-C2C	-2.31	121.94	127.15
82	HB	203	PEB	CHA-C1B-NB	-2.31	120.10	124.93
87	CL	503	CLA	C3B-C4B-NB	-2.31	108.37	110.52
85	JN	103	BCR	C2-C3-C4	2.31	116.54	111.38
82	SH	203	PEB	CAC-CBC-CGC	-2.31	108.63	113.60
82	aK	202	PEB	CAB-CBB-CGB	-2.31	108.63	113.60
87	12	609	CLA	CHA-C1A-NA	-2.31	121.11	126.40
82	LF	201	PEB	O2B-CGB-CBB	2.31	121.45	114.03
82	T1	201	PEB	CHB-C4B-C3B	-2.31	119.97	125.32
87	AN	850	CLA	CHB-C4A-NA	2.31	127.71	124.51
82	UD	202	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
82	H9	202	PEB	C2A-C1A-NA	2.31	110.26	108.27
82	xK	304	PEB	CAC-C2C-C1C	2.31	129.44	125.76
82	NQ	202	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	VQ	201	PEB	OD-C4D-ND	-2.31	122.51	125.93
82	PA	201	PEB	CAA-C3A-C2A	-2.31	108.49	114.26
82	Z9	301	PEB	CBD-CAD-C3D	-2.31	116.13	127.62
82	iJ	201	PEB	C1C-CHB-C4B	-2.31	123.10	128.28
82	F5	203	PEB	CAC-C2C-C1C	2.31	129.44	125.76
82	tK	201	PEB	CAC-C2C-C1C	2.31	129.44	125.76
82	hM	203	PEB	CAC-C2C-C1C	2.31	129.44	125.76
82	XJ	202	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
82	gO	201	PEB	CHA-C1B-NB	-2.31	120.10	124.93
82	KF	201	PEB	C1D-CHC-C4C	-2.31	109.85	113.26
82	WE	201	PEB	C4B-C3B-C2B	-2.31	104.23	106.78
83	AQ	302	PUB	C2C-C1C-NC	2.31	113.41	110.05
87	B6	604	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
82	TJ	202	PEB	C2A-C1A-NA	2.31	110.26	108.27
82	dJ	202	PEB	C2A-C1A-NA	2.31	110.26	108.27
94	D6	408	PL9	C47-C48-C49	-2.31	119.86	127.75
82	d4	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	kH	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	kJ	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
87	A2	827	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
84	BG	1002	CYC	CAB-C3B-C2B	2.31	131.48	127.53
82	XK	201	PEB	CAC-CBC-CGC	-2.31	108.64	113.60
82	TE	201	PEB	CHB-C4B-C3B	-2.31	119.98	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	lJ	202	PEB	CAC-C2C-C3C	2.31	132.35	127.07
83	xF	305	PUB	CBA-CAA-C3A	-2.31	109.48	112.98
82	GA	202	PEB	CHB-C1C-C2C	-2.31	121.94	127.15
82	NP	202	PEB	CHA-C1B-C2B	2.31	130.84	124.90
96	VL	201	HEM	CHB-C1B-C2B	-2.31	120.32	126.73
87	22	604	CLA	C3B-C4B-NB	-2.31	108.37	110.52
82	g4	201	PEB	CHA-C1B-NB	-2.31	120.11	124.93
82	q8	203	PEB	CAC-CBC-CGC	-2.31	108.64	113.60
82	WJ	201	PEB	C4B-C3B-C2B	-2.31	104.23	106.78
82	XM	202	PEB	CHC-C1D-ND	-2.31	110.81	113.72
82	iF	202	PEB	O1C-CGC-CBC	-2.31	115.67	123.08
82	XF	203	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
84	m3	1001	CYC	C2D-C1D-ND	2.31	110.64	107.40
87	B2	817	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
83	yK	303	PUB	CMD-C2D-C3D	2.31	131.23	127.77
82	DF	201	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
82	OM	203	PEB	CMC-C3C-C4C	2.31	129.51	127.06
85	fL	101	BCR	C12-C13-C14	2.31	122.48	118.94
82	CF	202	PEB	CHC-C1D-ND	-2.31	110.81	113.72
87	6N	607	CLA	O2D-CGD-CBD	2.31	115.37	111.27
82	dH	202	PEB	OA-C1A-C2A	-2.31	124.34	126.17
82	PD	202	PEB	CMA-C2A-C1A	-2.31	107.43	112.40
82	B9	202	PEB	CMB-C2B-C1B	2.31	128.62	125.06
82	MP	201	PEB	C1D-CHC-C4C	-2.31	109.86	113.26
87	B2	822	CLA	C2A-C1A-CHA	2.31	127.89	123.86
82	BQ	201	PEB	CHA-C1B-C2B	2.31	130.83	124.90
87	aL	606	CLA	CBA-CAA-C2A	-2.31	107.06	113.86
83	Y7	302	PUB	C2C-C1C-NC	2.31	113.40	110.05
82	XB	201	PEB	CBC-CAC-C2C	-2.31	106.22	112.63
82	RB	201	PEB	CHA-C1B-NB	-2.31	120.11	124.93
82	RG	201	PEB	CHC-C4C-NC	2.31	124.27	121.15
82	LF	202	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
82	iK	203	PEB	CAB-C3B-C4B	2.31	129.09	125.01
96	v6	201	HEM	C4B-C3B-C2B	-2.31	105.28	107.11
87	B2	823	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
82	NM	202	PEB	OD-C4D-C3D	-2.31	124.24	129.46
82	OM	203	PEB	OD-C4D-C3D	-2.31	124.24	129.46
87	LN	202	CLA	C2A-C1A-CHA	2.31	127.89	123.86
87	7N	602	CLA	C2A-C1A-CHA	2.31	127.89	123.86
82	hG	202	PEB	C1D-CHC-C4C	-2.31	109.86	113.26
82	U7	202	PEB	CHB-C1C-C2C	-2.31	121.95	127.15
84	D1	1001	CYC	C2A-C1A-NA	2.31	113.40	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BL	608	CLA	C3B-C4B-NB	-2.31	108.38	110.52
82	fM	202	PEB	C3C-C4C-NC	2.31	110.41	108.33
82	GJ	201	PEB	CHA-C1B-C2B	2.31	130.83	124.90
82	mF	201	PEB	CAB-C3B-C4B	2.31	129.09	125.01
82	AD	301	PEB	CHC-C4C-NC	2.31	124.27	121.15
82	QF	203	PEB	OD-C4D-C3D	-2.31	124.24	129.46
82	MQ	202	PEB	OD-C4D-C3D	-2.31	124.24	129.46
82	s8	203	PEB	OD-C4D-C3D	-2.31	124.24	129.46
82	VQ	201	PEB	OA-C1A-C2A	-2.31	124.34	126.17
82	B9	202	PEB	C1C-CHB-C4B	2.31	133.45	128.28
82	NQ	202	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
82	R4	203	PEB	CMB-C2B-C1B	2.31	128.61	125.06
82	OM	203	PEB	CMA-C2A-C1A	-2.31	107.43	112.40
83	AM	303	PUB	CMD-C2D-C3D	2.31	131.23	127.77
85	BL	616	BCR	C28-C27-C26	-2.31	109.96	114.08
82	WE	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	EI	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	ZK	201	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
82	pK	202	PEB	C4C-C3C-C2C	-2.31	105.37	107.50
87	O2	201	CLA	O2D-CGD-CBD	2.31	115.36	111.27
82	pC	202	PEB	OD-C4D-C3D	-2.31	124.24	129.46
82	M9	304	PEB	OD-C4D-C3D	-2.31	124.24	129.46
82	B5	202	PEB	CAB-C3B-C4B	2.31	129.09	125.01
82	a1	202	PEB	C3B-C4B-NB	2.31	113.40	110.05
82	L7	203	PEB	CAC-CBC-CGC	-2.30	108.64	113.60
87	52	607	CLA	CMB-C2B-C3B	2.30	132.17	126.59
82	TF	202	PEB	CMC-C3C-C2C	-2.30	120.62	125.61
92	J6	102	LMG	C3-C4-C5	2.30	114.35	110.24
82	W9	201	PEB	CHB-C4B-C3B	-2.30	119.99	125.32
82	dG	203	PEB	C1D-CHC-C4C	-2.30	109.86	113.26
82	D5	203	PEB	C1B-C2B-C3B	-2.30	103.86	106.51
85	A6	401	BCR	C37-C22-C21	-2.30	119.69	122.92
82	XM	202	PEB	O2B-CGB-CBB	2.30	121.43	114.03
96	fL	102	HEM	C4D-ND-C1D	2.30	107.45	105.07
87	bL	607	CLA	C2D-C1D-ND	-2.30	108.41	110.10
82	BA	203	PEB	C4C-C3C-C2C	-2.30	105.37	107.50
82	gB	203	PEB	C4C-C3C-C2C	-2.30	105.37	107.50
82	lM	202	PEB	CHB-C1C-C2C	-2.30	121.95	127.15
82	gH	203	PEB	CAB-CBB-CGB	-2.30	108.64	113.60
84	HE	1001	CYC	C4D-ND-C1D	-2.30	105.68	109.79
84	JH	1003	CYC	C4D-ND-C1D	-2.30	105.68	109.79
82	OK	201	PEB	CAB-C3B-C4B	2.30	129.08	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	BN	840	BCR	C15-C14-C13	-2.30	124.02	127.31
82	r8	201	PEB	C2A-C1A-NA	2.30	110.26	108.27
84	MG	1001	CYC	CHA-C1A-C2A	-2.30	119.99	125.32
82	FQ	202	PEB	OD-C4D-C3D	-2.30	124.24	129.46
82	eO	202	PEB	CHC-C1D-ND	-2.30	110.81	113.72
82	XF	203	PEB	C4B-NB-C1B	-2.30	102.17	106.51
87	7N	602	CLA	C3B-C4B-NB	-2.30	108.38	110.52
82	YE	201	PEB	CBC-CAC-C2C	2.30	119.03	112.63
82	aF	202	PEB	CAB-CBB-CGB	-2.30	108.65	113.60
82	eF	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
82	CK	203	PEB	C3C-C4C-NC	2.30	110.41	108.33
82	1C	202	PEB	CHA-C1B-NB	-2.30	120.11	124.93
82	DM	201	PEB	CAC-C2C-C1C	2.30	129.43	125.76
82	DA	202	PEB	C1C-NC-C4C	-2.30	105.50	109.60
87	BN	818	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
87	32	306	CLA	CHB-C1B-NB	2.30	126.69	124.26
82	JK	202	PEB	CHA-C4A-NA	2.30	127.94	125.20
82	UP	202	PEB	CMC-C3C-C2C	2.30	130.59	125.61
82	ID	202	PEB	CBB-CAB-C3B	2.30	119.03	112.63
82	a4	203	PEB	CHB-C1C-C2C	-2.30	121.95	127.15
87	52	601	CLA	O2A-CGA-O1A	-2.30	117.56	123.30
87	B2	834	CLA	CHB-C4A-NA	2.30	127.70	124.51
92	aL	611	LMG	C6-C5-C4	-2.30	107.61	113.00
82	QM	202	PEB	CHA-C1B-NB	-2.30	120.12	124.93
82	iK	203	PEB	CHA-C1B-NB	-2.30	120.12	124.93
82	J7	203	PEB	OD-C4D-C3D	-2.30	124.24	129.46
82	oK	202	PEB	CHB-C1C-NC	-2.30	120.05	125.32
87	ON	201	CLA	O2D-CGD-CBD	2.30	115.36	111.27
82	qC	203	PEB	CAC-CBC-CGC	-2.30	108.65	113.60
82	hF	202	PEB	CHC-C1D-ND	-2.30	110.81	113.72
82	aG	202	PEB	CHC-C1D-ND	-2.30	110.81	113.72
87	A2	850	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
82	dG	203	PEB	CAC-C2C-C1C	2.30	129.43	125.76
82	HP	201	PEB	OD-C4D-C3D	-2.30	124.25	129.46
82	eJ	202	PEB	OD-C4D-C3D	-2.30	124.25	129.46
82	PO	203	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
82	M9	301	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
83	AG	302	PUB	CHB-C1C-NC	-2.30	119.79	124.58
82	JO	1002	PEB	CHB-C1C-NC	-2.30	120.05	125.32
82	B5	203	PEB	C1B-C2B-C3B	-2.30	103.86	106.51
87	a6	607	CLA	CHB-C4A-NA	2.30	127.69	124.51
82	QO	201	PEB	CAB-C3B-C4B	2.30	129.08	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PP	202	PEB	CAB-C3B-C4B	2.30	129.08	125.01
82	ZG	202	PEB	CHB-C4B-C3B	-2.30	119.99	125.32
82	PI	202	PEB	C2B-C1B-NB	2.30	115.44	110.53
82	RI	202	PEB	C2B-C1B-NB	2.30	115.44	110.53
82	TP	202	PEB	OD-C4D-C3D	-2.30	124.25	129.46
82	S5	203	PEB	C2A-C1A-NA	2.30	110.26	108.27
82	Z1	201	PEB	CAA-C3A-C2A	-2.30	108.51	114.26
82	M9	302	PEB	CBD-CAD-C3D	-2.30	116.17	127.62
82	D5	201	PEB	CAC-C2C-C1C	2.30	129.43	125.76
87	BN	824	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
94	d6	408	PL9	C51-C49-C50	2.30	119.69	114.60
87	A6	404	CLA	O2D-CGD-CBD	2.30	115.36	111.27
82	N4	1002	PEB	OD-C4D-C3D	-2.30	124.25	129.46
103	82	309	ZEX	C31-C32-C33	-2.30	119.95	126.42
82	GI	202	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
96	v6	201	HEM	CHD-C1D-C2D	-2.30	121.39	124.98
82	Q7	201	PEB	CAB-C3B-C4B	2.30	129.08	125.01
82	OE	201	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
82	qC	201	PEB	CHA-C4A-NA	2.30	127.94	125.20
82	KB	302	PEB	C3B-C4B-NB	2.30	113.39	110.05
83	AE	303	PUB	CBA-CAA-C3A	-2.30	109.49	112.98
82	OK	201	PEB	C3C-C4C-NC	2.30	110.40	108.33
82	HP	202	PEB	C3C-C4C-NC	2.30	110.40	108.33
87	A2	832	CLA	C2D-C1D-ND	-2.30	108.41	110.10
84	W3	1001	CYC	C1B-C2B-C3B	-2.30	105.47	107.87
83	wF	304	PUB	CAB-CBB-CGB	-2.30	108.65	113.60
94	DL	401	PL9	C16-C17-C18	-2.30	104.32	111.88
82	j1	201	PEB	OD-C4D-C3D	-2.30	124.25	129.46
82	GF	203	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
82	TQ	203	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
87	72	602	CLA	C2A-C1A-CHA	2.30	127.88	123.86
82	BA	203	PEB	CHC-C4C-NC	2.30	124.26	121.15
82	18	202	PEB	CHA-C1B-NB	-2.30	120.12	124.93
95	b6	621	DGD	C6D-C5D-C4D	-2.30	107.29	112.09
82	YA	301	PEB	CHA-C4A-NA	2.30	127.94	125.20
85	CL	501	BCR	C35-C13-C12	2.30	121.70	118.08
82	NI	203	PEB	CHB-C4B-NB	-2.30	119.79	124.58
82	iG	201	PEB	OD-C4D-ND	-2.30	122.52	125.93
82	GF	203	PEB	O2B-CGB-CBB	2.30	121.42	114.03
82	JA	203	PEB	CHA-C1B-NB	-2.30	120.12	124.93
82	YM	201	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
82	oF	203	PEB	CHB-C4B-NB	-2.30	119.79	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	oK	203	PEB	CHB-C4B-NB	-2.30	119.79	124.58
82	CA	201	PEB	C3C-C4C-NC	2.30	110.40	108.33
82	KB	301	PEB	CHC-C1D-ND	-2.30	110.82	113.72
82	IM	203	PEB	OD-C4D-C3D	-2.30	124.25	129.46
87	62	308	CLA	O2D-CGD-CBD	2.30	115.35	111.27
82	pK	201	PEB	CAC-C2C-C1C	2.30	129.42	125.76
87	bL	606	CLA	C4-C3-C5	2.30	119.14	115.27
87	A6	402	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
82	DQ	202	PEB	CMA-C2A-C1A	-2.30	107.45	112.40
82	kH	203	PEB	OD-C4D-ND	-2.30	122.53	125.93
82	TD	203	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
83	QM	201	PUB	C1B-C2B-C3B	-2.30	105.38	107.50
82	eA	301	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
82	dK	202	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
82	HE	1002	PEB	CHB-C4B-NB	-2.30	119.79	124.58
82	QJ	203	PEB	CHB-C4B-NB	-2.30	119.79	124.58
82	T1	201	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
82	w8	201	PEB	CHB-C1C-C2C	-2.30	121.97	127.15
82	MM	201	PEB	CAB-C3B-C4B	2.30	129.07	125.01
87	AN	840	CLA	CHB-C1B-NB	2.30	126.69	124.26
87	4N	609	CLA	CHC-C4B-NB	2.30	126.69	124.26
82	WQ	201	PEB	CMD-C2D-C3D	2.30	133.31	130.06
82	MJ	201	PEB	CMB-C2B-C1B	2.30	128.60	125.06
82	OF	202	PEB	CHC-C4C-NC	2.30	124.26	121.15
82	QH	203	PEB	CHC-C1D-ND	-2.30	110.82	113.72
88	I6	101	LHG	O8-C23-C24	2.30	119.12	111.91
82	YB	201	PEB	CHA-C1B-C2B	2.30	130.81	124.90
82	D5	202	PEB	C2B-C1B-NB	2.30	115.43	110.53
82	P7	201	PEB	CAA-C3A-C2A	-2.30	108.52	114.26
82	QP	201	PEB	CMA-C2A-C1A	-2.30	107.45	112.40
82	eH	201	PEB	CMA-C2A-C1A	-2.30	107.45	112.40
82	BI	201	PEB	CHA-C1B-NB	-2.30	120.13	124.93
85	AN	804	BCR	C20-C21-C22	-2.30	124.03	127.31
82	R4	201	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
82	jE	202	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
82	OM	202	PEB	OD-C4D-C3D	-2.30	124.25	129.46
82	lF	203	PEB	C3B-C4B-NB	2.30	113.39	110.05
82	RB	201	PEB	CAC-CBC-CGC	-2.30	108.66	113.60
82	c1	201	PEB	CHC-C4C-NC	2.30	124.26	121.15
87	42	609	CLA	CHC-C4B-NB	2.30	126.69	124.26
82	jK	202	PEB	CAB-C3B-C4B	2.30	129.07	125.01
82	O7	201	PEB	CAC-C2C-C3C	2.30	132.33	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	eE	203	PEB	CAC-C2C-C3C	2.30	132.33	127.07
82	EA	201	PEB	OD-C4D-C3D	-2.30	124.26	129.46
87	62	304	CLA	C3B-C4B-NB	-2.30	108.38	110.52
82	fE	203	PEB	C1D-CHC-C4C	2.30	116.64	113.26
87	H6	102	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
82	CQ	201	PEB	C1C-CHB-C4B	2.30	133.43	128.28
82	fF	201	PEB	C3B-C4B-NB	2.30	113.39	110.05
87	H6	102	CLA	CHB-C4A-NA	2.30	127.69	124.51
82	GD	202	PEB	OD-C4D-C3D	-2.30	124.26	129.46
82	VG	202	PEB	CMC-C3C-C4C	-2.30	124.63	127.06
82	WK	202	PEB	CAB-C3B-C4B	2.30	129.07	125.01
82	AI	202	PEB	C2B-C1B-NB	2.30	115.43	110.53
87	cL	515	CLA	CHA-C1A-NA	-2.30	121.14	126.40
82	AA	202	PEB	CHB-C1C-NC	-2.30	120.06	125.32
92	ML	101	LMG	O7-C10-O9	-2.30	118.15	123.70
84	L1	1001	CYC	CHA-C1A-NA	2.30	129.36	124.58
82	xC	201	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
82	Y9	203	PEB	OD-C4D-C3D	-2.30	124.26	129.46
88	dL	405	LHG	O8-C23-C24	2.30	119.11	111.91
82	S5	203	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
82	hK	202	PEB	CHC-C1D-ND	-2.30	110.82	113.72
82	N7	202	PEB	C1D-CHC-C4C	-2.30	109.87	113.26
82	O5	203	PEB	C3C-C4C-NC	2.30	110.40	108.33
82	ZJ	201	PEB	CAB-CBB-CGB	-2.30	108.66	113.60
82	II	201	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
82	SO	202	PEB	C4C-C3C-C2C	-2.30	105.38	107.50
87	aL	606	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
82	W1	203	PEB	OD-C4D-C3D	-2.30	124.26	129.46
82	S9	201	PEB	OD-C4D-C3D	-2.30	124.26	129.46
85	HL	103	BCR	C39-C30-C25	-2.30	106.58	110.30
82	hH	201	PEB	OA-C1A-C2A	-2.30	124.35	126.17
82	CK	202	PEB	CHA-C1B-NB	-2.30	120.13	124.93
87	6N	608	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
82	QH	201	PEB	CAB-C3B-C4B	2.29	129.07	125.01
85	KL	100	BCR	C33-C5-C4	2.29	118.02	113.62
82	OF	203	PEB	CAA-C3A-C4A	-2.29	106.78	112.67
87	c6	611	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
87	CL	512	CLA	CHC-C4B-NB	2.29	126.69	124.26
92	BL	612	LMG	C6-C5-C4	-2.29	107.63	113.00
82	J4	1002	PEB	C1D-CHC-C4C	2.29	116.64	113.26
82	CD	202	PEB	CAB-C3B-C4B	2.29	129.07	125.01
82	C7	201	PEB	CAB-C3B-C4B	2.29	129.07	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iG	202	PEB	CAC-CBC-CGC	-2.29	108.67	113.60
82	HG	1002	PEB	CHB-C4B-NB	-2.29	119.80	124.58
84	LH	1001	CYC	CMC-C2C-C1C	-2.29	107.46	112.40
82	O4	202	PEB	C4B-C3B-C2B	-2.29	104.24	106.78
82	PA	203	PEB	OD-C4D-ND	-2.29	122.53	125.93
87	K2	101	CLA	C3B-C4B-NB	-2.29	108.39	110.52
82	mH	201	PEB	CHA-C1B-NB	-2.29	120.14	124.93
82	B7	203	PEB	CAC-CBC-CGC	-2.29	108.67	113.60
91	DL	405	PHO	CGD-CBD-CAD	-2.29	103.31	110.73
85	BN	803	BCR	C28-C29-C30	-2.29	106.40	114.60
87	CL	506	CLA	CHB-C1B-NB	2.29	126.69	124.26
87	3N	311	CLA	CHB-C1B-NB	2.29	126.69	124.26
87	3N	309	CLA	CHA-C1A-NA	-2.29	121.15	126.40
84	JO	1001	CYC	C4D-ND-C1D	-2.29	105.70	109.79
82	Z1	201	PEB	C4C-C3C-C2C	-2.29	105.38	107.50
82	J9	201	PEB	C4C-C3C-C2C	-2.29	105.38	107.50
82	cB	402	PEB	C4C-C3C-C2C	-2.29	105.38	107.50
82	eK	201	PEB	C2B-C1B-NB	2.29	115.42	110.53
84	l3	1001	CYC	C2D-C1D-ND	2.29	110.62	107.40
82	zC	202	PEB	C3B-C4B-NB	2.29	113.38	110.05
87	A2	821	CLA	CHB-C1B-NB	2.29	126.68	124.26
87	bL	622	CLA	CHB-C1B-NB	2.29	126.68	124.26
82	tF	201	PEB	CAC-C2C-C1C	2.29	129.41	125.76
82	H5	203	PEB	CHA-C1B-NB	-2.29	120.14	124.93
82	zK	501	PEB	CHA-C1B-NB	-2.29	120.14	124.93
82	iE	202	PEB	CAC-CBC-CGC	-2.29	108.67	113.60
96	V6	201	HEM	C4A-CHB-C1B	-2.29	120.90	126.34
82	Z5	301	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	W9	203	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	DF	201	PEB	CHB-C1C-C2C	-2.29	121.98	127.15
82	OQ	202	PEB	CAA-C3A-C4A	2.29	118.56	112.67
87	A2	816	CLA	C3B-C4B-NB	-2.29	108.39	110.52
94	aL	601	PL9	C42-C43-C44	-2.29	122.14	127.66
82	PF	201	PEB	CMB-C2B-C1B	2.29	128.59	125.06
82	UA	202	PEB	CHB-C1C-C2C	-2.29	121.98	127.15
95	CL	517	DGD	O1G-C1A-C2A	2.29	119.10	111.91
87	L2	202	CLA	C2A-C1A-CHA	2.29	127.87	123.86
88	DL	407	LHG	O8-C23-O10	-2.29	117.81	123.59
82	W9	201	PEB	CAA-C3A-C2A	-2.29	108.53	114.26
82	pF	202	PEB	OD-C4D-C3D	-2.29	124.27	129.46
92	dL	407	LMG	O6-C1-O1	-2.29	104.55	109.97
82	H7	202	PEB	C3C-C4C-NC	2.29	110.40	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	mF	202	PEB	C3C-C4C-NC	2.29	110.40	108.33
82	SI	202	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	cG	201	PEB	CAC-CBC-CGC	-2.29	108.67	113.60
82	R4	202	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	L9	203	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	W9	201	PEB	C4B-NB-C1B	-2.29	102.19	106.51
82	NB	203	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
82	DD	202	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
82	TI	203	PEB	C2B-C1B-NB	2.29	115.42	110.53
87	B2	812	CLA	C2D-C1D-ND	-2.29	108.42	110.10
82	zF	501	PEB	CHA-C1B-NB	-2.29	120.14	124.93
82	U5	202	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	DI	201	PEB	CAB-CBB-CGB	-2.29	108.67	113.60
82	GB	202	PEB	CAB-C3B-C4B	2.29	129.06	125.01
82	jK	201	PEB	CMB-C2B-C1B	2.29	128.59	125.06
87	cL	509	CLA	CMC-C2C-C3C	2.29	132.33	126.12
82	LA	203	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	PA	202	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	HB	202	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	TJ	201	PEB	OD-C4D-C3D	-2.29	124.27	129.46
82	IB	201	PEB	CAB-CBB-CGB	-2.29	108.67	113.60
82	BM	301	PEB	CAB-CBB-CGB	-2.29	108.67	113.60
82	E7	202	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
84	NH	1001	CYC	C1B-NB-C4B	-2.29	107.75	110.67
85	A2	804	BCR	C20-C21-C22	-2.29	124.04	127.31
82	hK	202	PEB	CAB-C3B-C4B	2.29	129.06	125.01
82	HQ	201	PEB	CMB-C2B-C1B	2.29	128.59	125.06
82	QB	204	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
82	rF	202	PEB	C4B-C3B-C2B	-2.29	104.25	106.78
82	KK	201	PEB	C1D-CHC-C4C	-2.29	109.88	113.26
82	QP	201	PEB	C1D-CHC-C4C	-2.29	109.88	113.26
82	gM	201	PEB	C1D-CHC-C4C	2.29	116.63	113.26
87	A2	823	CLA	C3B-C4B-NB	-2.29	108.39	110.52
82	IQ	202	PEB	CBB-CAB-C3B	2.29	118.99	112.63
87	7N	606	CLA	CHA-C1A-NA	-2.29	121.16	126.40
85	B2	802	BCR	C28-C29-C30	-2.29	106.42	114.60
82	lO	202	PEB	O2B-CGB-CBB	2.29	121.39	114.03
82	eK	203	PEB	CHC-C4C-NC	2.29	124.25	121.15
82	W1	203	PEB	CMC-C3C-C4C	2.29	129.49	127.06
87	d6	406	CLA	C1-C2-C3	-2.29	122.08	126.04
82	jF	201	PEB	CMB-C2B-C1B	2.29	128.59	125.06
87	AN	829	CLA	CMB-C2B-C3B	2.29	132.13	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JQ	202	PEB	C2B-C1B-NB	2.29	115.41	110.53
82	AI	201	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	BI	202	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	18	203	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	JM	202	PEB	CAC-C2C-C1C	2.29	129.41	125.76
84	I4	1001	CYC	CMB-C2B-C1B	2.29	127.02	124.17
82	XP	201	PEB	OD-C4D-C3D	-2.29	124.28	129.46
82	Q4	201	PEB	CAB-C3B-C4B	2.29	129.06	125.01
87	22	602	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
87	72	602	CLA	C3B-C4B-NB	-2.29	108.39	110.52
82	t8	202	PEB	CAA-C3A-C2A	-2.29	108.54	114.26
82	dE	203	PEB	C1D-CHC-C4C	-2.29	109.88	113.26
82	HJ	201	PEB	CAB-CBB-CGB	-2.29	108.68	113.60
82	YJ	202	PEB	CHA-C1B-C2B	2.29	130.78	124.90
82	u8	202	PEB	CHA-C1B-NB	-2.29	120.15	124.93
88	M6	101	LHG	O8-C23-C24	2.29	119.09	111.91
82	AJ	301	PEB	C1C-CHB-C4B	-2.29	123.15	128.28
82	kF	202	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	iK	203	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	DD	203	PEB	CHC-C4C-NC	2.29	124.25	121.15
82	MK	203	PEB	CHA-C1B-C2B	2.29	130.78	124.90
82	QG	202	PEB	CAC-C2C-C1C	2.29	129.41	125.76
82	fM	202	PEB	CAC-C2C-C1C	2.29	129.41	125.76
82	CJ	203	PEB	CAB-C3B-C4B	2.29	129.06	125.01
82	SJ	201	PEB	CAB-C3B-C4B	2.29	129.06	125.01
82	WI	202	PEB	CBA-CAA-C3A	-2.29	108.37	113.47
82	L7	203	PEB	CHB-C1C-NC	-2.29	120.08	125.32
82	LP	201	PEB	OD-C4D-C3D	-2.29	124.28	129.46
82	EA	202	PEB	OD-C4D-ND	-2.29	122.54	125.93
82	E7	202	PEB	OD-C4D-ND	-2.29	122.54	125.93
82	pK	202	PEB	CHB-C1C-C2C	-2.29	121.99	127.15
82	LQ	201	PEB	C3B-C4B-NB	2.29	113.38	110.05
96	E6	101	HEM	CHC-C4B-NB	2.29	126.90	124.42
82	r8	201	PEB	CMC-C3C-C2C	2.29	130.55	125.61
82	qC	203	PEB	CMB-C2B-C1B	2.29	128.59	125.06
85	B2	840	BCR	C15-C14-C13	-2.29	124.05	127.31
82	UG	203	PEB	CAB-C3B-C4B	2.29	129.05	125.01
82	OD	202	PEB	CAA-C3A-C4A	2.29	118.55	112.67
82	BI	201	PEB	CAA-C3A-C4A	-2.29	106.80	112.67
87	BN	823	CLA	CAC-C3C-C4C	2.29	127.78	124.81
82	NA	201	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	zC	202	PEB	CHB-C1C-C2C	2.29	132.31	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YG	201	PEB	CBC-CAC-C2C	2.29	118.98	112.63
85	AN	847	BCR	C34-C9-C10	-2.29	119.72	122.92
82	tK	201	PEB	C3B-C4B-NB	2.29	113.38	110.05
82	VB	201	PEB	C1D-CHC-C4C	2.29	116.63	113.26
87	B2	815	CLA	C3A-C2A-C1A	2.29	104.76	101.34
87	bL	608	CLA	CHB-C1B-NB	2.29	126.68	124.26
87	c6	611	CLA	O2D-CGD-CBD	2.29	115.33	111.27
82	NB	202	PEB	OD-C4D-ND	-2.29	122.54	125.93
82	KM	202	PEB	OD-C4D-ND	-2.29	122.54	125.93
87	d6	406	CLA	O1D-CGD-CBD	2.29	129.16	124.48
82	B9	202	PEB	C2B-C1B-NB	2.29	115.41	110.53
82	GJ	202	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	NP	201	PEB	C4C-C3C-C2C	-2.29	105.39	107.50
82	QG	201	PEB	OD-C4D-C3D	-2.29	124.28	129.46
82	bH	202	PEB	CHC-C4C-NC	2.29	124.24	121.15
82	O9	202	PEB	CMC-C3C-C4C	-2.29	124.64	127.06
87	BN	808	CLA	C2A-C1A-CHA	2.29	127.86	123.86
82	Q1	201	PEB	CAB-C3B-C4B	2.29	129.05	125.01
82	vK	201	PEB	CHA-C1B-NB	-2.29	120.15	124.93
82	QJ	202	PEB	OD-C4D-C3D	-2.29	124.28	129.46
82	p8	202	PEB	OD-C4D-C3D	-2.29	124.28	129.46
82	q8	201	PEB	CHA-C4A-NA	2.29	127.92	125.20
82	wK	303	PEB	CBB-CAB-C3B	2.29	118.98	112.63
82	aF	201	PEB	CMB-C2B-C1B	2.29	128.58	125.06
82	WI	201	PEB	CAC-C2C-C1C	2.28	129.40	125.76
85	LN	205	BCR	C35-C13-C12	2.28	121.68	118.08
82	qC	202	PEB	C1D-CHC-C4C	-2.28	109.89	113.26
83	A1	304	PUB	CMA-C2A-C1A	2.28	126.77	121.39
85	C6	508	BCR	C33-C5-C4	2.28	118.00	113.62
82	jF	202	PEB	CAB-C3B-C4B	2.28	129.05	125.01
82	g1	201	PEB	CHC-C1D-ND	-2.28	110.83	113.72
82	b4	202	PEB	C4C-C3C-C2C	-2.28	105.39	107.50
82	bP	502	PEB	C4C-C3C-C2C	-2.28	105.39	107.50
83	xK	305	PUB	C1B-C2B-C3B	-2.28	105.39	107.50
82	ZB	201	PEB	C3C-C4C-NC	2.28	110.39	108.33
82	RG	202	PEB	C3C-C4C-NC	2.28	110.39	108.33
82	lG	201	PEB	C3C-C4C-NC	2.28	110.39	108.33
85	L2	201	BCR	C29-C28-C27	-2.28	106.27	111.38
84	c3	1001	CYC	C2D-C1D-ND	2.28	110.61	107.40
82	lG	202	PEB	OD-C4D-ND	-2.28	122.55	125.93
87	BL	604	CLA	CHB-C4A-NA	2.28	127.67	124.51
82	F9	202	PEB	CAB-CBB-CGB	-2.28	108.69	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	j1	202	PEB	CHB-C4B-C3B	2.28	130.60	125.32
82	MM	203	PEB	CHA-C1B-NB	-2.28	120.16	124.93
85	FL	101	BCR	C38-C26-C25	-2.28	121.96	124.53
94	D6	408	PL9	C17-C18-C19	-2.28	122.16	127.66
82	PA	201	PEB	C4B-C3B-C2B	-2.28	104.25	106.78
82	PE	202	PEB	CHC-C1D-ND	-2.28	110.83	113.72
103	8N	309	ZEX	C31-C32-C33	-2.28	120.00	126.42
82	GA	202	PEB	CAB-C3B-C4B	2.28	129.05	125.01
82	vF	202	PEB	CAB-C3B-C4B	2.28	129.05	125.01
82	JB	202	PEB	CAB-CBB-CGB	-2.28	108.69	113.60
82	KI	202	PEB	C4C-C3C-C2C	-2.28	105.39	107.50
82	ND	202	PEB	CMC-C3C-C4C	2.28	129.48	127.06
82	yK	301	PEB	OD-C4D-C3D	-2.28	124.29	129.46
82	mK	202	PEB	C3C-C4C-NC	2.28	110.39	108.33
82	YM	203	PEB	CHA-C1B-NB	-2.28	120.16	124.93
82	gG	201	PEB	C2B-C1B-NB	2.28	115.40	110.53
87	42	609	CLA	C2A-C1A-CHA	2.28	127.84	123.85
87	4N	609	CLA	C2A-C1A-CHA	2.28	127.84	123.85
87	AN	821	CLA	CHB-C1B-NB	2.28	126.67	124.26
87	d6	406	CLA	CHB-C1B-NB	2.28	126.67	124.26
87	CL	512	CLA	CHB-C4A-NA	2.28	127.67	124.51
87	B2	805	CLA	C2A-C1A-CHA	2.28	127.85	123.86
82	B5	203	PEB	C2A-C1A-NA	2.28	110.24	108.27
82	IQ	202	PEB	CHB-C1C-C2C	-2.28	122.00	127.15
94	d6	408	PL9	C40-C39-C41	2.28	119.11	115.27
82	QQ	201	PEB	CAA-C3A-C2A	-2.28	108.56	114.26
85	cL	518	BCR	C4-C5-C6	-2.28	119.42	122.73
82	NQ	202	PEB	CMB-C2B-C1B	2.28	128.58	125.06
82	KB	302	PEB	OD-C4D-ND	-2.28	122.55	125.93
87	BN	813	CLA	C2D-C1D-ND	-2.28	108.42	110.10
84	IO	1001	CYC	CMB-C2B-C1B	2.28	127.02	124.17
82	VI	203	PEB	CHC-C1D-ND	-2.28	110.84	113.72
87	62	306	CLA	CHB-C1B-NB	2.28	126.67	124.26
87	62	313	CLA	CHC-C4B-NB	2.28	126.67	124.26
103	8N	309	ZEX	C11-C12-C13	-2.28	120.00	126.42
82	M5	301	PEB	OD-C4D-C3D	-2.28	124.29	129.46
82	IB	203	PEB	CAC-C2C-C1C	2.28	129.40	125.76
82	QE	202	PEB	CAC-C2C-C1C	2.28	129.40	125.76
82	bH	202	PEB	CAC-C2C-C1C	2.28	129.40	125.76
82	CQ	202	PEB	CAB-C3B-C4B	2.28	129.04	125.01
82	V4	201	PEB	CHC-C4C-NC	2.28	124.24	121.15
82	kO	202	PEB	C1C-NC-C4C	-2.28	105.54	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	f1	203	PEB	OD-C4D-ND	-2.28	122.55	125.93
87	2N	310	CLA	CMD-C2D-C3D	2.28	132.86	127.61
82	rC	201	PEB	C2A-C1A-NA	2.28	110.24	108.27
82	CD	201	PEB	C1C-CHB-C4B	2.28	133.40	128.28
82	lH	202	PEB	C3B-C4B-NB	2.28	113.37	110.05
84	C3	1001	CYC	C2D-C1D-ND	2.28	110.61	107.40
82	oK	203	PEB	CMA-C2A-C1A	-2.28	107.48	112.40
85	F2	203	BCR	C11-C10-C9	-2.28	124.05	127.31
103	82	309	ZEX	C11-C12-C13	-2.28	120.01	126.42
96	FL	102	HEM	C4C-CHD-C1D	-2.28	121.14	126.06
82	w8	201	PEB	C4C-C3C-C2C	-2.28	105.39	107.50
87	BN	819	CLA	CHC-C4B-NB	2.28	126.67	124.26
87	bL	618	CLA	CHC-C4B-NB	2.28	126.67	124.26
82	H9	201	PEB	C3C-C4C-NC	2.28	110.39	108.33
82	DD	201	PEB	OD-C4D-ND	-2.28	122.55	125.93
82	QD	201	PEB	CAA-C3A-C2A	-2.28	108.56	114.26
82	kH	202	PEB	C3B-C4B-NB	2.28	113.37	110.05
84	J3	1001	CYC	C2D-C1D-ND	2.28	110.61	107.40
84	v3	1001	CYC	C2D-C1D-ND	2.28	110.61	107.40
84	HH	1001	CYC	OB-C4B-NB	-2.28	119.78	125.08
95	lL	101	DGD	O6D-C1D-C2D	2.28	115.18	110.35
87	b6	616	CLA	O2D-CGD-CBD	2.28	115.32	111.27
82	CJ	202	PEB	CAC-C2C-C1C	2.28	129.39	125.76
82	lE	203	PEB	CMB-C2B-C1B	2.28	128.58	125.06
82	IP	201	PEB	C4B-C3B-C2B	-2.28	104.26	106.78
82	AP	201	PEB	C2B-C1B-NB	2.28	115.40	110.53
94	aL	601	PL9	C15-C14-C16	2.28	119.11	115.27
82	WE	202	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
85	aL	604	BCR	C19-C18-C17	2.28	122.44	118.94
87	AN	821	CLA	C2A-C1A-CHA	2.28	127.85	123.86
87	bL	608	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
87	b6	604	CLA	CHB-C4A-NA	2.28	127.67	124.51
82	J7	202	PEB	CHA-C4A-NA	2.28	127.92	125.20
84	LH	1002	CYC	CBA-CAA-C2A	-2.28	106.29	112.63
82	xK	304	PEB	CHB-C1C-NC	-2.28	120.10	125.32
87	A2	809	CLA	CMB-C2B-C3B	2.28	132.11	126.59
82	tC	201	PEB	OD-C4D-C3D	-2.28	124.30	129.46
82	CB	202	PEB	CAC-CBC-CGC	-2.28	108.70	113.60
82	WQ	201	PEB	CAB-CBB-CGB	-2.28	108.70	113.60
82	eE	202	PEB	CAC-CBC-CGC	-2.28	108.70	113.60
85	CL	501	BCR	C16-C15-C14	-2.28	118.80	123.47
82	z8	201	PEB	C4B-C3B-C2B	-2.28	104.26	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	P4	202	PEB	C1C-NC-C4C	-2.28	105.54	109.60
82	tK	203	PEB	CAC-C2C-C1C	2.28	129.39	125.76
82	FD	201	PEB	CHA-C4A-NA	2.28	127.92	125.20
82	Z9	301	PEB	CHB-C4B-NB	-2.28	119.83	124.58
82	lK	203	PEB	CHB-C1C-NC	2.28	130.54	125.32
82	CI	201	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
82	kF	201	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
88	AL	406	LHG	O8-C23-O10	-2.28	117.84	123.59
82	uC	202	PEB	CHA-C1B-NB	-2.28	120.17	124.93
82	TB	202	PEB	CAB-CBB-CGB	-2.28	108.70	113.60
82	RD	201	PEB	CAC-CBC-CGC	-2.28	108.70	113.60
87	BL	603	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
82	E5	202	PEB	CHB-C4B-C3B	-2.28	120.05	125.32
82	w8	201	PEB	C1C-CHB-C4B	2.28	133.39	128.28
85	B6	602	BCR	C33-C5-C4	2.28	117.99	113.62
82	cM	202	PEB	CAB-CBB-CGB	2.28	118.51	113.60
84	JH	1003	CYC	CAD-CBD-CGD	-2.28	108.70	113.60
82	BD	201	PEB	C2A-C1A-NA	2.28	110.24	108.27
84	HG	1001	CYC	C4D-ND-C1D	-2.28	105.72	109.79
82	OE	201	PEB	OD-C4D-C3D	-2.28	124.30	129.46
82	HI	203	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
82	RD	203	PEB	CMB-C2B-C1B	2.28	128.57	125.06
82	lM	203	PEB	CMB-C2B-C1B	2.28	128.57	125.06
82	FQ	201	PEB	C1C-NC-C4C	-2.28	105.54	109.60
82	hF	202	PEB	CAB-C3B-C4B	2.28	129.04	125.01
87	4N	602	CLA	C3B-C4B-NB	-2.28	108.40	110.52
95	C6	504	DGD	C3G-C2G-C1G	-2.28	106.40	111.79
84	FE	1001	CYC	C4D-ND-C1D	-2.28	105.73	109.79
82	YG	201	PEB	C4B-NB-C1B	-2.28	102.22	106.51
82	JF	202	PEB	CHB-C1C-NC	-2.28	120.10	125.32
82	f1	203	PEB	CAB-C3B-C4B	2.28	129.04	125.01
92	k6	101	LMG	O1-C7-C8	-2.28	105.40	110.90
84	JH	1001	CYC	C2C-C1C-NC	2.28	110.24	108.27
84	S3	1001	CYC	C2C-C1C-NC	2.28	110.24	108.27
84	CG	1001	CYC	C4D-ND-C1D	-2.28	105.73	109.79
82	lE	201	PEB	CAC-CBC-CGC	-2.28	108.70	113.60
87	6N	602	CLA	C2D-C1D-ND	-2.28	108.43	110.10
82	Y4	203	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
82	P5	202	PEB	CHB-C4B-C3B	-2.28	120.05	125.32
85	LN	201	BCR	C29-C28-C27	-2.28	106.29	111.38
87	AN	850	CLA	CAA-CBA-CGA	-2.28	106.60	113.25
82	mG	201	PEB	CAA-C3A-C2A	-2.28	108.57	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	kJ	201	PEB	C1C-CHB-C4B	-2.28	123.18	128.28
83	xK	305	PUB	CAB-C3B-C4B	2.28	129.39	125.76
87	42	608	CLA	CMB-C2B-C3B	2.28	132.10	126.59
87	AN	831	CLA	C4-C3-C5	2.28	119.10	115.27
82	HA	202	PEB	C3B-C4B-NB	2.28	113.36	110.05
82	SM	201	PEB	C3B-C4B-NB	2.28	113.36	110.05
82	WG	203	PEB	CHB-C4B-C3B	-2.28	120.05	125.32
82	ZK	201	PEB	CHA-C1B-C2B	2.28	130.75	124.90
82	TH	201	PEB	CBD-CAD-C3D	-2.28	116.30	127.62
87	B2	822	CLA	CAC-C3C-C4C	2.28	127.76	124.81
84	g3	1001	CYC	C2D-C1D-ND	2.28	110.60	107.40
84	O3	1001	CYC	C2C-C1C-NC	2.28	110.23	108.27
82	GF	203	PEB	O2C-CGC-CBC	2.28	121.34	114.03
82	SD	201	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
82	OM	202	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
82	kF	203	PEB	C4C-C3C-C2C	-2.28	105.40	107.50
87	DL	403	CLA	CMB-C2B-C3B	2.28	132.10	126.59
87	12	607	CLA	O2D-CGD-CBD	2.28	115.31	111.27
87	b6	609	CLA	CHB-C4A-NA	2.28	127.66	124.51
87	b6	612	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
87	B2	824	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
82	QP	202	PEB	CAC-C2C-C3C	2.28	132.28	127.07
82	k1	202	PEB	CHB-C4B-C3B	-2.28	120.05	125.32
87	AL	403	CLA	CHB-C1B-NB	2.28	126.67	124.26
87	2N	311	CLA	C3B-C4B-NB	-2.28	108.40	110.52
82	dF	201	PEB	OD-C4D-C3D	-2.28	124.31	129.46
82	RF	201	PEB	CAA-C3A-C2A	-2.28	108.57	114.26
82	NA	202	PEB	C1D-CHC-C4C	-2.28	109.90	113.26
84	H1	1001	CYC	OB-C4B-NB	-2.28	119.79	125.08
84	J1	1001	CYC	OC-C1C-C2C	-2.28	124.36	126.17
85	C6	507	BCR	C21-C20-C19	-2.28	116.12	123.22
82	ND	203	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
82	RO	201	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
82	YO	203	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
82	Z9	303	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
82	T1	201	PEB	CBD-CAD-C3D	-2.27	116.30	127.62
82	TH	201	PEB	CHB-C4B-C3B	-2.27	120.06	125.32
82	NJ	202	PEB	C2A-C1A-NA	2.27	110.23	108.27
82	aJ	203	PEB	CBC-CAC-C2C	-2.27	106.31	112.63
87	d6	401	CLA	CHB-C1B-NB	2.27	126.67	124.26
82	OG	201	PEB	OD-C4D-C3D	-2.27	124.31	129.46
82	YF	201	PEB	C1C-CHB-C4B	2.27	133.38	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ND	203	PEB	CHC-C4C-NC	2.27	124.23	121.15
87	b6	607	CLA	CHD-C1D-ND	-2.27	122.36	124.45
85	BN	841	BCR	C29-C30-C25	2.27	113.98	110.48
91	D6	404	PHO	C4A-C3A-C2A	-2.27	100.67	102.84
82	WF	201	PEB	CAA-C3A-C2A	2.27	119.94	114.26
87	3N	313	CLA	O2A-CGA-O1A	-2.27	117.63	123.30
84	KG	202	CYC	CHB-C1B-NB	-2.27	121.18	126.06
82	D7	202	PEB	C1C-NC-C4C	-2.27	105.55	109.60
87	BN	832	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
82	cK	203	PEB	C1D-CHC-C4C	-2.27	109.90	113.26
85	I2	101	BCR	C11-C10-C9	-2.27	124.06	127.31
82	VH	202	PEB	CHC-C4C-NC	2.27	124.23	121.15
82	U9	201	PEB	OD-C4D-C3D	-2.27	124.31	129.46
82	Y9	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
87	A6	404	CLA	CHB-C1B-NB	2.27	126.66	124.26
82	XB	202	PEB	CMA-C2A-C1A	-2.27	107.50	112.40
84	GO	1001	CYC	CBD-CAD-C3D	-2.27	106.31	112.63
87	c6	613	CLA	CHB-C4A-NA	2.27	127.66	124.51
82	sK	203	PEB	C3B-C4B-NB	2.27	113.36	110.05
87	KN	105	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
87	12	608	CLA	C3B-C4B-NB	-2.27	108.41	110.52
84	M1	201	CYC	CAD-CBD-CGD	-2.27	108.71	113.60
82	UB	301	PEB	CAC-C2C-C3C	2.27	132.28	127.07
82	O5	202	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
82	VE	202	PEB	CMC-C3C-C4C	-2.27	124.65	127.06
87	12	611	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
82	s8	203	PEB	CHB-C1C-C2C	-2.27	122.02	127.15
82	z8	202	PEB	CHB-C1C-C2C	2.27	132.28	127.15
87	BN	834	CLA	CHB-C4A-NA	2.27	127.66	124.51
87	B6	609	CLA	CHB-C4A-NA	2.27	127.66	124.51
82	UJ	203	PEB	CAC-CBC-CGC	-2.27	108.71	113.60
82	SP	202	PEB	OA-C1A-C2A	-2.27	124.37	126.17
82	cM	202	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
85	BN	839	BCR	C1-C6-C7	2.27	122.21	115.78
82	JI	201	PEB	CAC-C2C-C1C	2.27	129.38	125.76
82	AD	301	PEB	C3C-C4C-NC	2.27	110.38	108.33
87	12	607	CLA	C3B-C4B-NB	-2.27	108.41	110.52
82	YG	202	PEB	CMA-C2A-C1A	-2.27	107.50	112.40
82	pK	201	PEB	CAB-C3B-C4B	2.27	129.03	125.01
85	FL	101	BCR	C33-C5-C4	2.27	117.98	113.62
82	TH	201	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
82	W1	203	PEB	C3B-C4B-NB	2.27	113.35	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BB	201	PEB	CHC-C1D-ND	-2.27	110.85	113.72
82	VD	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
82	S4	201	PEB	CMD-C2D-C3D	2.27	133.27	130.06
82	MB	202	PEB	CAB-CBB-CGB	-2.27	108.71	113.60
82	YQ	201	PEB	CAC-CBC-CGC	-2.27	108.71	113.60
82	ED	201	PEB	CMA-C2A-C1A	-2.27	107.51	112.40
82	YA	303	PEB	CHA-C1B-C2B	2.27	130.74	124.90
82	Y7	303	PEB	CHA-C1B-C2B	2.27	130.74	124.90
87	6N	605	CLA	CHB-C1B-NB	2.27	126.66	124.26
87	6N	612	CLA	CHC-C4B-NB	2.27	126.66	124.26
82	B9	202	PEB	C1C-NC-C4C	-2.27	105.56	109.60
82	WP	202	PEB	C2B-C1B-NB	2.27	115.38	110.53
82	PI	201	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
82	iM	201	PEB	C4C-C3C-C2C	-2.27	105.40	107.50
87	A2	812	CLA	C2A-C1A-CHA	2.27	127.83	123.86
82	eJ	202	PEB	O2B-CGB-CBB	2.27	121.33	114.03
82	YK	201	PEB	C1C-CHB-C4B	2.27	133.38	128.28
87	A2	849	CLA	CHB-C4A-NA	2.27	127.65	124.51
82	UD	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
84	M3	1001	CYC	C2C-C1C-NC	2.27	110.23	108.27
82	l4	202	PEB	O2B-CGB-CBB	2.27	121.33	114.03
82	HM	201	PEB	CMD-C2D-C3D	2.27	133.27	130.06
87	62	302	CLA	C3B-C4B-NB	-2.27	108.41	110.52
82	kK	202	PEB	CAB-C3B-C4B	2.27	129.03	125.01
94	AL	413	PL9	C30-C29-C28	-2.27	117.85	123.68
82	V5	202	PEB	CHB-C4B-C3B	-2.27	120.06	125.32
85	L2	205	BCR	C35-C13-C12	2.27	121.66	118.08
87	b6	608	CLA	CAA-CBA-CGA	-2.27	106.62	113.25
95	c6	618	DGD	O2G-C1B-O1B	-2.27	118.21	123.70
85	FL	101	BCR	C37-C22-C21	-2.27	119.74	122.92
85	A2	846	BCR	C33-C5-C6	-2.27	121.98	124.53
82	ND	202	PEB	CMB-C2B-C1B	2.27	128.56	125.06
87	32	311	CLA	CHB-C1B-NB	2.27	126.66	124.26
87	b6	612	CLA	CHB-C4A-NA	2.27	127.65	124.51
82	VA	203	PEB	C3B-C4B-NB	2.27	113.35	110.05
82	L7	203	PEB	OD-C4D-C3D	-2.27	124.32	129.46
82	WM	201	PEB	C4B-C3B-C2B	-2.27	104.27	106.78
82	eJ	202	PEB	CAC-C2C-C1C	2.27	129.38	125.76
82	O7	202	PEB	C1D-CHC-C4C	-2.27	109.91	113.26
87	BL	602	CLA	CAC-C3C-C4C	2.27	127.76	124.81
82	ZF	201	PEB	C4C-C3C-C2C	-2.27	105.41	107.50
87	AN	830	CLA	CMB-C2B-C3B	2.27	132.09	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	812	CLA	C2A-C1A-CHA	2.27	127.83	123.86
82	CP	203	PEB	CHA-C1B-NB	-2.27	120.18	124.93
87	B6	616	CLA	CAA-C2A-C1A	-2.27	104.53	111.97
82	QE	201	PEB	OD-C4D-C3D	-2.27	124.32	129.46
87	7N	602	CLA	O2D-CGD-CBD	2.27	115.30	111.27
84	d3	1001	CYC	C2C-C1C-NC	2.27	110.23	108.27
82	cH	201	PEB	CHC-C4C-NC	2.27	124.22	121.15
82	kJ	202	PEB	CHB-C1C-NC	-2.27	120.12	125.32
87	AN	820	CLA	CHC-C4B-NB	2.27	126.66	124.26
87	1N	607	CLA	O2D-CGD-CBD	2.27	115.30	111.27
82	IB	202	PEB	C4C-C3C-C2C	-2.27	105.41	107.50
82	EK	202	PEB	C4C-C3C-C2C	-2.27	105.41	107.50
82	QM	202	PEB	C4C-C3C-C2C	-2.27	105.41	107.50
87	BN	816	CLA	C3A-C2A-C1A	2.27	104.74	101.34
83	AH	303	PUB	CHA-C1B-NB	2.27	124.22	121.15
87	bL	615	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
87	4N	608	CLA	CMB-C2B-C3B	2.27	132.08	126.59
85	b6	603	BCR	C38-C26-C27	2.27	117.97	113.62
82	hF	201	PEB	CHA-C1B-C2B	2.27	130.74	124.90
82	l4	201	PEB	C3C-C4C-NC	2.27	110.38	108.33
87	5N	601	CLA	O2A-CGA-O1A	-2.27	117.64	123.30
82	ZM	201	PEB	CHC-C1D-ND	2.27	116.60	113.72
87	BN	806	CLA	C2A-C1A-CHA	2.27	127.83	123.86
82	lK	203	PEB	CHB-C4B-NB	-2.27	119.86	124.58
82	M9	302	PEB	CHB-C4B-NB	-2.27	119.86	124.58
82	VO	201	PEB	CHC-C4C-NC	2.27	124.22	121.15
82	dG	201	PEB	CHC-C4C-NC	2.27	124.22	121.15
87	C6	510	CLA	CHB-C4A-NA	2.27	127.65	124.51
87	A2	821	CLA	CMB-C2B-C3B	2.27	132.08	126.59
82	ZE	203	PEB	CHA-C4A-NA	2.27	127.90	125.20
87	6N	612	CLA	CHA-C4D-ND	2.27	137.24	132.50
82	LH	1003	PEB	OD-C4D-ND	-2.27	122.57	125.93
82	GJ	201	PEB	CHB-C1C-C2C	-2.27	122.03	127.15
87	2N	305	CLA	C3B-C4B-NB	-2.27	108.41	110.52
82	WQ	201	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
82	eG	203	PEB	CAC-C2C-C3C	2.27	132.26	127.07
82	AQ	301	PEB	CHC-C4C-NC	2.27	124.22	121.15
84	H3	1001	CYC	C2C-C1C-NC	2.27	110.23	108.27
82	lG	201	PEB	CAC-CBC-CGC	-2.27	108.72	113.60
87	52	605	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
87	5N	605	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
82	L7	203	PEB	OA-C1A-C2A	-2.27	124.37	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	aL	611	LMG	O6-C5-C4	2.27	113.81	109.69
87	A2	830	CLA	CMB-C2B-C3B	2.27	132.08	126.59
82	m1	201	PEB	OD-C4D-C3D	-2.27	124.32	129.46
87	dL	401	CLA	O2D-CGD-CBD	2.27	115.30	111.27
85	LN	205	BCR	C24-C23-C22	-2.27	122.81	126.23
82	S4	202	PEB	C4C-C3C-C2C	-2.27	105.41	107.50
82	WD	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
83	wK	304	PUB	CAB-CBB-CGB	-2.27	108.72	113.60
85	K6	102	BCR	C8-C9-C10	2.27	122.42	118.94
82	kG	202	PEB	CAB-C3B-C4B	2.27	129.02	125.01
82	YE	202	PEB	CMA-C2A-C1A	-2.27	107.52	112.40
87	C6	509	CLA	C1-C2-C3	-2.27	122.12	126.04
82	B9	203	PEB	CHC-C4C-NC	2.27	124.22	121.15
82	EJ	201	PEB	CAA-C3A-C4A	-2.27	106.85	112.67
82	TJ	201	PEB	CHB-C4B-NB	-2.27	119.86	124.58
82	QB	204	PEB	CHB-C1C-C2C	-2.27	122.04	127.15
82	WE	202	PEB	OD-C4D-C3D	-2.27	124.33	129.46
82	O9	203	PEB	OD-C4D-C3D	-2.27	124.33	129.46
87	BN	825	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
85	h6	102	BCR	C16-C15-C14	-2.27	118.83	123.47
82	T5	202	PEB	CHB-C4B-C3B	-2.27	120.08	125.32
82	qF	201	PEB	C3B-C4B-NB	2.27	113.35	110.05
87	22	602	CLA	CMB-C2B-C3B	2.27	132.08	126.59
82	LM	201	PEB	CAC-CBC-CGC	-2.27	108.73	113.60
82	AQ	303	PEB	CMA-C2A-C1A	-2.27	107.52	112.40
82	XI	201	PEB	C4C-C3C-C2C	-2.27	105.41	107.50
87	B2	818	CLA	CHC-C4B-NB	2.27	126.66	124.26
82	dG	203	PEB	C4B-C3B-C2B	-2.27	104.28	106.78
82	wF	303	PEB	CBB-CAB-C3B	2.27	118.92	112.63
85	k6	102	BCR	C8-C9-C10	2.27	122.42	118.94
82	JA	202	PEB	CHA-C4A-NA	2.27	127.90	125.20
87	22	603	CLA	C3B-C4B-NB	-2.27	108.41	110.52
82	fG	203	PEB	C1D-CHC-C4C	2.27	116.60	113.26
82	WJ	203	PEB	CAA-C3A-C2A	-2.27	108.60	114.26
82	PH	201	PEB	CMA-C2A-C1A	-2.27	107.52	112.40
82	IJ	202	PEB	C3C-C4C-NC	2.27	110.37	108.33
84	B3	1001	CYC	C2C-C1C-NC	2.27	110.23	108.27
82	XK	203	PEB	C4B-NB-C1B	-2.27	102.24	106.51
85	B2	843	BCR	C19-C18-C17	2.27	122.42	118.94
83	AH	304	PUB	CMA-C2A-C1A	2.27	126.72	121.39
87	2N	305	CLA	CHB-C1B-NB	2.27	126.66	124.26
82	V7	202	PEB	CMB-C2B-C1B	2.26	128.55	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FD	201	PEB	C1C-NC-C4C	-2.26	105.57	109.60
82	YD	201	PEB	CAC-CBC-CGC	-2.26	108.73	113.60
87	A2	831	CLA	C4-C3-C5	2.26	119.08	115.27
82	SH	203	PEB	OD-C4D-C3D	-2.26	124.33	129.46
82	mH	201	PEB	OD-C4D-C3D	-2.26	124.33	129.46
87	BN	826	CLA	C2D-C1D-ND	-2.26	108.44	110.10
87	AN	837	CLA	C3B-C4B-NB	-2.26	108.41	110.52
87	72	609	CLA	C3B-C4B-NB	-2.26	108.41	110.52
82	sF	203	PEB	C3B-C4B-NB	2.26	113.34	110.05
82	mM	201	PEB	CHB-C4B-NB	-2.26	119.86	124.58
82	yC	202	PEB	CMB-C2B-C1B	2.26	128.55	125.06
82	RM	202	PEB	CAC-C2C-C1C	2.26	129.37	125.76
84	N1	1001	CYC	CHA-C1A-C2A	-2.26	120.08	125.32
82	OB	201	PEB	CAC-CBC-CGC	-2.26	108.73	113.60
82	P4	201	PEB	CAB-CBB-CGB	-2.26	108.73	113.60
87	AN	809	CLA	CMB-C2B-C3B	2.26	132.07	126.59
85	B2	841	BCR	C29-C30-C25	2.26	113.97	110.48
82	V7	203	PEB	C3B-C4B-NB	2.26	113.34	110.05
82	q8	202	PEB	C1D-CHC-C4C	-2.26	109.92	113.26
82	JD	202	PEB	C2B-C1B-NB	2.26	115.36	110.53
82	t8	201	PEB	OD-C4D-C3D	-2.26	124.33	129.46
87	dL	402	CLA	CHB-C4A-NA	2.26	127.64	124.51
82	lF	201	PEB	CHB-C4B-NB	-2.26	119.87	124.58
82	OF	203	PEB	CHC-C4C-NC	2.26	124.21	121.15
82	M9	305	PEB	C3C-C4C-NC	2.26	110.37	108.33
82	LG	1002	PEB	C3C-C4C-NC	-2.26	106.30	108.33
87	62	309	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
82	Q5	201	PEB	C2B-C1B-NB	2.26	115.36	110.53
82	GB	203	PEB	C4C-C3C-C2C	-2.26	105.41	107.50
82	PE	202	PEB	C4C-C3C-C2C	-2.26	105.41	107.50
95	L6	102	DGD	O5D-C6D-C5D	-2.26	104.86	109.05
82	UJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
82	Y5	203	PEB	OD-C4D-C3D	-2.26	124.33	129.46
82	OF	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
87	5N	608	CLA	CMA-C3A-C2A	-2.26	110.82	116.10
82	YO	203	PEB	CAC-CBC-CGC	-2.26	108.73	113.60
82	lF	203	PEB	CHB-C1C-NC	2.26	130.50	125.32
82	V1	201	PEB	CHA-C1B-C2B	2.26	130.72	124.90
82	OQ	202	PEB	CHA-C4A-NA	-2.26	122.52	125.20
82	T7	202	PEB	CHB-C4B-NB	-2.26	119.87	124.58
87	dL	404	CLA	C2A-C1A-CHA	2.26	127.81	123.86
82	fK	202	PEB	CHA-C1B-NB	-2.26	120.20	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LB	201	PEB	OD-C4D-C3D	-2.26	124.33	129.46
82	iE	201	PEB	OD-C4D-ND	-2.26	122.58	125.93
82	RQ	201	PEB	CAC-CBC-CGC	-2.26	108.73	113.60
92	jL	101	LMG	C4-C3-C2	2.26	114.77	110.82
82	lK	201	PEB	CHB-C4B-NB	-2.26	119.87	124.58
87	AN	805	CLA	C4-C3-C5	2.26	119.08	115.27
82	FK	201	PEB	C4C-C3C-C2C	-2.26	105.41	107.50
82	kK	201	PEB	C4C-C3C-C2C	-2.26	105.41	107.50
87	22	610	CLA	CMD-C2D-C3D	2.26	132.82	127.61
92	B6	622	LMG	O7-C10-O9	-2.26	118.24	123.70
87	52	608	CLA	CMA-C3A-C2A	-2.26	110.82	116.10
82	NJ	202	PEB	CAB-CBB-CGB	2.26	118.47	113.60
82	zC	201	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
87	ON	202	CLA	CHA-C1A-NA	-2.26	121.22	126.40
82	K5	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
82	b1	201	PEB	CBB-CAB-C3B	-2.26	106.34	112.63
82	JM	201	PEB	CHB-C1C-NC	-2.26	120.14	125.32
82	GM	202	PEB	CMB-C2B-C1B	2.26	128.55	125.06
82	OA	202	PEB	C1D-CHC-C4C	-2.26	109.92	113.26
82	P4	202	PEB	C1D-CHC-C4C	-2.26	109.92	113.26
87	K2	106	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
82	Y1	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
82	MB	202	PEB	CMC-C3C-C4C	2.26	129.46	127.06
82	q8	203	PEB	C4C-C3C-C2C	-2.26	105.41	107.50
82	fM	202	PEB	C4C-C3C-C2C	-2.26	105.41	107.50
82	WM	201	PEB	CMA-C2A-C1A	-2.26	107.53	112.40
82	WQ	202	PEB	CMA-C2A-C1A	-2.26	107.53	112.40
82	KB	302	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
84	BG	1002	CYC	C1A-C2A-C3A	-2.26	104.28	106.78
82	z8	201	PEB	C4B-NB-C1B	-2.26	102.25	106.51
82	JJ	201	PEB	CHB-C4B-NB	-2.26	119.87	124.58
82	TM	202	PEB	CAC-C2C-C1C	2.26	129.36	125.76
82	A5	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
82	R5	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
82	eF	202	PEB	CHA-C1B-C2B	2.26	130.71	124.90
82	WP	201	PEB	C1C-NC-C4C	2.26	113.62	109.60
82	QE	201	PEB	CMB-C2B-C1B	2.26	128.54	125.06
87	AN	836	CLA	C3B-C4B-NB	-2.26	108.42	110.52
87	BL	601	CLA	C2A-C1A-CHA	2.26	127.81	123.86
82	I5	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
85	F2	203	BCR	C8-C9-C10	-2.26	115.47	118.94
82	dE	203	PEB	CAC-C2C-C1C	2.26	129.36	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	AJ	302	PEB	C1C-CHB-C4B	-2.26	123.21	128.28
82	QP	202	PEB	O1C-CGC-CBC	-2.26	115.82	123.08
82	GJ	203	PEB	CAA-C3A-C2A	-2.26	108.61	114.26
84	F3	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
84	j3	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
82	RD	202	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	EF	202	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
85	bL	602	BCR	C1-C6-C5	-2.26	119.43	122.61
87	bL	619	CLA	CHC-C4B-NB	2.26	126.65	124.26
87	bL	620	CLA	O2D-CGD-CBD	2.26	115.28	111.27
85	BN	843	BCR	C19-C18-C17	2.26	122.41	118.94
94	AL	413	PL9	C25-C24-C23	-2.26	117.88	123.68
87	BN	811	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
85	B6	602	BCR	C15-C16-C17	-2.26	118.85	123.47
85	B2	839	BCR	C1-C6-C7	2.26	122.17	115.78
82	CF	202	PEB	CHA-C1B-NB	-2.26	120.21	124.93
82	MF	202	PEB	CHA-C1B-NB	-2.26	120.21	124.93
87	KN	103	CLA	O2D-CGD-CBD	2.26	115.28	111.27
84	D1	1001	CYC	C1A-C2A-C3A	-2.26	104.28	106.78
82	W1	202	PEB	OA-C1A-C2A	-2.26	124.38	126.17
82	q8	203	PEB	OD-C4D-C3D	-2.26	124.34	129.46
82	sC	203	PEB	OD-C4D-C3D	-2.26	124.34	129.46
82	lF	202	PEB	CAB-C3B-C4B	2.26	129.00	125.01
87	52	611	CLA	C3A-C2A-C1A	2.26	104.72	101.34
82	EA	202	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	F5	203	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	lM	203	PEB	CHC-C1D-ND	2.26	116.58	113.72
82	MJ	202	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
82	PJ	202	PEB	CHA-C1B-NB	-2.26	120.21	124.93
87	B2	806	CLA	CHB-C4A-NA	2.26	127.64	124.51
85	B2	842	BCR	C38-C26-C25	-2.26	121.99	124.53
82	kH	202	PEB	OA-C1A-NA	2.26	127.68	124.94
82	JP	202	PEB	OD-C4D-C3D	-2.26	124.34	129.46
82	sC	201	PEB	OD-C4D-C3D	-2.26	124.34	129.46
82	R7	203	PEB	O1B-CGB-CBB	-2.26	115.83	123.08
82	WF	201	PEB	OD-C4D-ND	-2.26	122.58	125.93
87	b6	610	CLA	C1-C2-C3	-2.26	122.14	126.04
87	A2	821	CLA	C2A-C1A-CHA	2.26	127.81	123.86
82	WH	202	PEB	OD-C4D-C3D	-2.26	124.34	129.46
82	RE	202	PEB	C3C-C4C-NC	2.26	110.37	108.33
82	NO	1002	PEB	C3C-C4C-NC	2.26	110.37	108.33
87	5N	608	CLA	O2D-CGD-CBD	2.26	115.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
94	D6	408	PL9	C25-C24-C26	2.26	119.07	115.27
82	dK	201	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	X5	202	PEB	CHB-C4B-C3B	-2.26	120.10	125.32
84	L3	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
82	LI	201	PEB	CAA-C3A-C2A	-2.26	108.62	114.26
82	Y5	201	PEB	CAB-C3B-C2B	2.26	132.08	127.88
87	B2	807	CLA	C2A-C1A-CHA	2.26	127.81	123.86
82	iM	202	PEB	O2B-CGB-CBB	2.26	121.28	114.03
87	2N	303	CLA	CMB-C2B-C3B	2.26	132.06	126.59
87	c6	616	CLA	C3B-C4B-NB	-2.26	108.42	110.52
82	1C	203	PEB	C1D-CHC-C4C	2.26	116.58	113.26
87	B2	801	CLA	CHB-C4A-NA	2.26	127.63	124.51
82	mE	201	PEB	CAA-C3A-C2A	-2.26	108.62	114.26
82	NE	202	PEB	CHB-C1C-NC	-2.26	120.15	125.32
85	b6	602	BCR	C15-C16-C17	-2.26	118.85	123.47
87	A2	829	CLA	CMB-C2B-C3B	2.26	132.05	126.59
87	1N	611	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
82	XA	203	PEB	CHA-C1B-NB	-2.26	120.21	124.93
85	C6	508	BCR	C20-C19-C18	2.26	132.75	126.42
82	ZE	203	PEB	CAB-C3B-C4B	2.26	129.00	125.01
82	OG	202	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	j4	203	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	F9	201	PEB	C1C-CHB-C4B	-2.26	123.22	128.28
84	k3	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
88	bL	612	LHG	O8-C23-O10	-2.26	117.90	123.59
87	AN	812	CLA	C3B-C4B-NB	-2.26	108.42	110.52
82	FO	1002	PEB	CAC-CBC-CGC	-2.26	108.75	113.60
82	GQ	201	PEB	CMC-C3C-C4C	2.26	129.45	127.06
82	dH	202	PEB	OD-C4D-C3D	-2.26	124.35	129.46
82	XM	201	PEB	CHC-C4C-NC	2.26	124.20	121.15
82	FQ	203	PEB	C4B-NB-C1B	2.26	110.76	106.51
82	KM	203	PEB	C2B-C1B-NB	2.26	115.34	110.53
87	B2	822	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
87	bL	619	CLA	CMB-C2B-C3B	2.26	132.05	126.59
87	AN	849	CLA	CHB-C4A-NA	2.26	127.63	124.51
82	dF	201	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
82	vK	201	PEB	C4C-C3C-C2C	-2.26	105.42	107.50
92	a6	614	LMG	C7-O1-C1	-2.26	109.33	113.74
82	eK	202	PEB	CHC-C4C-NC	2.26	124.20	121.15
82	bH	201	PEB	CBB-CAB-C3B	-2.26	106.36	112.63
82	kO	201	PEB	CMB-C2B-C1B	2.26	128.54	125.06
83	xK	305	PUB	CBA-CAA-C3A	-2.26	109.56	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	52	608	CLA	O2D-CGD-CBD	2.25	115.28	111.27
82	ZM	201	PEB	CAC-C2C-C1C	2.25	129.35	125.76
82	sC	203	PEB	CHB-C1C-C2C	-2.25	122.06	127.15
82	OA	201	PEB	O2C-CGC-CBC	2.25	121.27	114.03
82	PJ	201	PEB	CAB-C3B-C4B	2.25	129.00	125.01
82	gJ	202	PEB	CHB-C1C-NC	-2.25	120.16	125.32
84	N1	1001	CYC	CMC-C2C-C1C	-2.25	107.54	112.40
87	cL	506	CLA	C2A-C1A-CHA	2.25	127.80	123.86
87	32	313	CLA	O2A-CGA-O1A	-2.25	117.68	123.30
82	yF	301	PEB	OD-C4D-C3D	-2.25	124.35	129.46
82	QK	202	PEB	C4C-C3C-C2C	-2.25	105.42	107.50
82	SE	201	PEB	CAC-C2C-C1C	2.25	129.35	125.76
82	YJ	203	PEB	CAC-C2C-C1C	2.25	129.35	125.76
82	cK	202	PEB	CAC-C2C-C1C	2.25	129.35	125.76
94	AL	413	PL9	C32-C31-C29	2.25	120.39	112.98
83	yK	302	PUB	CAC-C2C-C1C	2.25	129.00	125.01
82	lK	203	PEB	C3B-C4B-NB	2.25	113.33	110.05
82	xF	303	PEB	OD-C4D-ND	-2.25	122.59	125.93
87	BL	609	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
82	IP	201	PEB	CHB-C1C-C2C	-2.25	122.06	127.15
84	u3	1001	CYC	C2C-C1C-NC	2.25	110.22	108.27
84	73	1001	CYC	C2C-C1C-NC	2.25	110.22	108.27
87	C6	516	CLA	O2D-CGD-CBD	2.25	115.27	111.27
87	cL	512	CLA	O2D-CGD-CBD	2.25	115.27	111.27
82	O7	201	PEB	O2C-CGC-CBC	2.25	121.27	114.03
82	gE	201	PEB	C2B-C1B-NB	2.25	115.34	110.53
82	TA	202	PEB	CHB-C4B-NB	-2.25	119.89	124.58
82	Y4	202	PEB	C1C-NC-C4C	-2.25	105.59	109.60
85	A2	847	BCR	C34-C9-C10	-2.25	119.77	122.92
92	mL	101	LMG	O7-C10-O9	-2.25	118.26	123.70
87	3N	306	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
82	DG	1002	PEB	OD-C4D-ND	-2.25	122.59	125.93
82	eB	202	PEB	C3C-C4C-NC	2.25	110.36	108.33
84	LH	1002	CYC	CHA-C1A-NA	2.25	129.27	124.58
82	U5	201	PEB	CMB-C2B-C1B	2.25	128.53	125.06
82	eF	201	PEB	CMC-C3C-C4C	2.25	129.45	127.06
82	M9	304	PEB	C4C-C3C-C2C	-2.25	105.42	107.50
85	cL	504	BCR	C37-C22-C21	-2.25	119.77	122.92
82	SK	201	PEB	CHB-C1C-NC	2.25	130.48	125.32
82	V1	202	PEB	CAC-CBC-CGC	-2.25	108.75	113.60
82	Y7	303	PEB	OD-C4D-ND	-2.25	122.59	125.93
82	C5	202	PEB	CHB-C4B-C3B	-2.25	120.11	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	Q3	1001	CYC	C2C-C1C-NC	2.25	110.22	108.27
92	DL	402	LMG	O8-C28-C29	2.25	118.98	111.91
82	SO	201	PEB	CHB-C1C-C2C	-2.25	122.07	127.15
87	AN	832	CLA	C2D-C1D-ND	-2.25	108.44	110.10
82	s8	201	PEB	OD-C4D-C3D	-2.25	124.36	129.46
82	LO	1002	PEB	CAB-C3B-C4B	2.25	128.99	125.01
95	a6	604	DGD	O6D-C5D-C6D	2.25	111.21	106.67
82	Y9	202	PEB	CMA-C2A-C1A	-2.25	107.55	112.40
82	HB	202	PEB	C3C-C4C-NC	2.25	110.36	108.33
82	jO	201	PEB	C3C-C4C-NC	2.25	110.36	108.33
82	GG	1002	PEB	C1D-CHC-C4C	2.25	116.58	113.26
82	P1	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
85	L2	201	BCR	C33-C5-C6	-2.25	122.00	124.53
82	KJ	201	PEB	OD-C4D-C3D	-2.25	124.36	129.46
82	iE	201	PEB	C4C-C3C-C2C	-2.25	105.42	107.50
82	sC	202	PEB	OD-C4D-ND	-2.25	122.59	125.93
85	b6	601	BCR	C10-C11-C12	-2.25	116.19	123.22
82	y8	202	PEB	CMB-C2B-C1B	2.25	128.53	125.06
82	G5	202	PEB	CHB-C4B-C3B	-2.25	120.11	125.32
87	A2	836	CLA	C3B-C4B-NB	-2.25	108.43	110.52
82	X7	203	PEB	CHA-C1B-NB	-2.25	120.22	124.93
82	jK	201	PEB	CAA-C3A-C2A	-2.25	108.63	114.26
82	BD	201	PEB	CHA-C1B-C2B	2.25	130.69	124.90
82	YH	202	PEB	CHC-C4C-NC	2.25	124.20	121.15
84	h3	1001	CYC	C2C-C1C-NC	2.25	110.21	108.27
82	d4	201	PEB	C4B-NB-C1B	-2.25	102.27	106.51
85	BN	841	BCR	C19-C18-C17	-2.25	115.49	118.94
82	EF	201	PEB	CMB-C2B-C3B	-2.25	120.00	126.12
82	j4	203	PEB	C1C-NC-C4C	-2.25	105.59	109.60
82	N5	202	PEB	CHB-C4B-C3B	-2.25	120.11	125.32
87	bL	615	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
82	AK	202	PEB	CMC-C3C-C4C	2.25	129.45	127.06
82	RJ	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
82	nF	201	PEB	CHB-C1C-C2C	-2.25	122.07	127.15
82	VQ	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
87	cL	509	CLA	C2D-C1D-ND	-2.25	108.44	110.10
82	VH	201	PEB	CHA-C1B-C2B	2.25	130.69	124.90
82	AO	304	PEB	CAC-C2C-C1C	2.25	129.35	125.76
87	AN	821	CLA	CMB-C2B-C3B	2.25	132.04	126.59
82	bG	201	PEB	CHB-C4B-C3B	-2.25	120.11	125.32
82	jE	201	PEB	C4C-C3C-C2C	-2.25	105.42	107.50
82	h1	201	PEB	CAB-CBB-CGB	-2.25	108.76	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	RK	201	PEB	CAA-C3A-C2A	-2.25	108.64	114.26
82	QK	202	PEB	C1C-CHB-C4B	2.25	133.33	128.28
82	sK	201	PEB	CAC-C2C-C3C	2.25	132.22	127.07
82	UE	203	PEB	CAB-C3B-C4B	2.25	128.99	125.01
82	x8	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
82	VB	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
82	fJ	203	PEB	CMB-C2B-C1B	2.25	128.53	125.06
83	QM	201	PUB	CMD-C2D-C3D	2.25	131.15	127.77
87	AN	820	CLA	CHA-C1A-NA	-2.25	121.24	126.40
82	GP	203	PEB	CAB-CBB-CGB	-2.25	108.76	113.60
82	cB	401	PEB	CAC-C2C-C1C	2.25	129.35	125.76
87	c6	610	CLA	CHB-C4A-NA	2.25	127.62	124.51
84	I1	1001	CYC	CMC-C2C-C1C	-2.25	107.55	112.40
82	pF	202	PEB	CHB-C1C-C2C	-2.25	122.07	127.15
82	JK	202	PEB	CHB-C1C-NC	-2.25	120.17	125.32
82	j1	203	PEB	OD-C4D-C3D	-2.25	124.36	129.46
82	fJ	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
85	FN	202	BCR	C10-C11-C12	-2.25	116.19	123.22
82	vC	202	PEB	C3B-C4B-NB	2.25	113.32	110.05
82	fJ	202	PEB	CHA-C1B-NB	-2.25	120.23	124.93
92	qL	301	LMG	O8-C28-C29	2.25	118.97	111.91
82	R7	201	PEB	CMC-C3C-C4C	2.25	129.44	127.06
82	WI	203	PEB	OD-C4D-C3D	-2.25	124.36	129.46
82	GQ	201	PEB	CAA-C3A-C4A	-2.25	106.90	112.67
87	2N	305	CLA	C2A-C1A-CHA	2.25	127.79	123.86
82	XK	203	PEB	C2B-C1B-NB	2.25	115.33	110.53
82	mE	202	PEB	CAB-CBB-CGB	-2.25	108.76	113.60
87	A6	402	CLA	CHB-C1B-NB	2.25	126.64	124.26
82	YF	202	PEB	CHC-C1D-ND	-2.25	110.88	113.72
82	VF	202	PEB	CHA-C4A-NA	2.25	127.88	125.20
85	B2	841	BCR	C19-C18-C17	-2.25	115.49	118.94
82	LA	202	PEB	CHA-C1B-NB	-2.25	120.23	124.93
82	WO	201	PEB	C4C-C3C-C2C	-2.25	105.42	107.50
82	DM	202	PEB	CHB-C4B-NB	-2.25	119.90	124.58
85	FN	202	BCR	C11-C10-C9	-2.25	124.10	127.31
84	G4	1001	CYC	CHB-C1B-NB	-2.25	121.23	126.06
87	BN	802	CLA	CHB-C4A-NA	2.25	127.62	124.51
82	OD	202	PEB	CHC-C1D-ND	-2.25	110.88	113.72
87	ON	202	CLA	CHB-C1B-C2B	-2.25	120.89	127.24
87	B2	832	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
82	PJ	201	PEB	CHB-C1C-NC	-2.25	120.17	125.32
88	CL	522	LHG	C9-C8-C7	-2.25	105.44	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	tC	201	PEB	C4B-C3B-C2B	-2.25	104.30	106.78
82	iM	202	PEB	C3B-C4B-NB	2.25	113.32	110.05
82	TO	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
87	BN	823	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
82	FA	201	PEB	C1C-CHB-C4B	2.25	133.32	128.28
82	wF	303	PEB	C4C-C3C-C2C	-2.25	105.43	107.50
82	lO	201	PEB	C4C-C3C-C2C	-2.25	105.43	107.50
82	WF	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
82	OK	203	PEB	CMC-C3C-C4C	2.25	129.44	127.06
82	FJ	202	PEB	C1D-CHC-C4C	-2.25	109.94	113.26
87	bL	621	CLA	C3B-C4B-NB	-2.25	108.43	110.52
87	3N	310	CLA	C3B-C4B-NB	-2.25	108.43	110.52
84	K4	1001	CYC	CHB-C1B-NB	-2.25	121.23	126.06
82	LK	201	PEB	OD-C4D-C3D	-2.25	124.37	129.46
87	BL	603	CLA	CHC-C4B-NB	2.25	126.64	124.26
87	B2	820	CLA	CHB-C1B-NB	2.25	126.64	124.26
84	NH	1001	CYC	CMC-C2C-C1C	-2.25	107.56	112.40
88	cL	501	LHG	C9-C8-C7	-2.25	105.45	113.62
87	B2	818	CLA	O1D-CGD-CBD	2.25	129.08	124.48
87	AL	405	CLA	C2D-C1D-ND	-2.25	108.45	110.10
87	cL	512	CLA	C2D-C1D-ND	-2.25	108.45	110.10
82	LA	203	PEB	CHC-C4C-NC	2.25	124.19	121.15
82	U9	203	PEB	CHB-C4B-NB	-2.25	119.90	124.58
87	C6	516	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
87	a6	608	CLA	CHB-C4A-NA	2.25	127.62	124.51
82	YH	201	PEB	CAB-C3B-C4B	2.25	128.98	125.01
82	gF	201	PEB	CAB-C3B-C4B	2.25	128.98	125.01
82	q8	203	PEB	CMB-C2B-C1B	2.25	128.52	125.06
82	lG	203	PEB	CMB-C2B-C1B	2.25	128.52	125.06
82	PM	202	PEB	CAC-C2C-C1C	2.25	129.34	125.76
82	SO	202	PEB	C3C-C4C-NC	2.25	110.36	108.33
82	pF	202	PEB	C4C-C3C-C2C	-2.25	105.43	107.50
82	jG	201	PEB	C4C-C3C-C2C	-2.25	105.43	107.50
82	FK	201	PEB	O2B-CGB-CBB	2.25	121.25	114.03
85	F2	203	BCR	C10-C11-C12	-2.25	116.21	123.22
87	AN	821	CLA	C3B-C4B-NB	-2.25	108.43	110.52
82	LA	203	PEB	CAC-CBC-CGC	-2.25	108.77	113.60
82	YI	202	PEB	CAC-CBC-CGC	-2.25	108.77	113.60
82	FA	201	PEB	C1D-CHC-C4C	2.25	116.57	113.26
82	m4	203	PEB	CHB-C4B-NB	-2.25	119.90	124.58
82	NB	201	PEB	C1B-C2B-C3B	-2.25	103.93	106.51
82	a1	202	PEB	C1B-C2B-C3B	-2.25	103.93	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	fM	202	PEB	CHA-C1B-NB	-2.25	120.23	124.93
87	C6	510	CLA	CHD-C1D-ND	-2.25	122.39	124.45
82	ID	202	PEB	CHB-C1C-C2C	-2.25	122.08	127.15
82	Q1	203	PEB	CHC-C1D-ND	-2.25	110.88	113.72
82	gO	203	PEB	CHC-C1D-ND	-2.25	110.88	113.72
82	mO	202	PEB	C1C-NC-C4C	-2.25	105.60	109.60
82	mG	202	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
96	v6	201	HEM	CAD-CBD-CGD	-2.25	108.77	113.60
82	UH	202	PEB	CAB-C3B-C4B	2.25	128.98	125.01
82	N5	201	PEB	CHC-C4C-NC	2.25	124.19	121.15
82	YD	202	PEB	C3C-C4C-NC	2.25	110.36	108.33
82	OF	202	PEB	C3C-C4C-NC	2.25	110.36	108.33
82	uC	203	PEB	C4C-C3C-C2C	-2.25	105.43	107.50
82	U5	203	PEB	CHA-C1B-NB	-2.25	120.24	124.93
82	yC	203	PEB	CHB-C1C-NC	-2.25	120.18	125.32
82	AA	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
87	AN	819	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
82	s8	202	PEB	OD-C4D-ND	-2.25	122.60	125.93
87	O2	202	CLA	CHA-C1A-NA	-2.25	121.26	126.40
82	l1	203	PEB	C3B-C4B-NB	2.25	113.31	110.05
82	gM	201	PEB	CAB-C3B-C4B	2.25	128.98	125.01
85	FL	101	BCR	C11-C12-C13	-2.25	120.11	126.42
82	SO	201	PEB	CMD-C2D-C3D	2.24	133.23	130.06
82	aK	201	PEB	CMB-C2B-C1B	2.24	128.52	125.06
82	m4	202	PEB	C1C-NC-C4C	-2.24	105.60	109.60
82	j1	202	PEB	C1C-CHB-C4B	-2.24	123.25	128.28
87	32	305	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
87	A2	805	CLA	C4-C3-C5	2.24	119.05	115.27
82	LA	203	PEB	CHB-C1C-NC	-2.24	120.18	125.32
82	FD	203	PEB	C4B-NB-C1B	2.24	110.74	106.51
82	l1	201	PEB	OD-C4D-ND	-2.24	122.61	125.93
82	AB	501	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	aF	202	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
84	H4	1001	CYC	CAB-C3B-C2B	2.24	131.37	127.53
95	c6	601	DGD	O6D-C5D-C6D	-2.24	102.13	106.67
82	VK	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
82	S7	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
82	jK	201	PEB	C1B-C2B-C3B	-2.24	103.93	106.51
87	5N	607	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
82	mO	203	PEB	CHB-C4B-NB	-2.24	119.91	124.58
82	O5	202	PEB	OD-C4D-C3D	-2.24	124.38	129.46
82	BI	201	PEB	CAC-CBC-CGC	-2.24	108.77	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	HI	201	PEB	CAC-CBC-CGC	-2.24	108.77	113.60
87	BN	827	CLA	CHA-C4D-ND	2.24	137.19	132.50
87	B2	827	CLA	CHA-C4D-ND	2.24	137.19	132.50
82	NQ	204	PEB	CBA-CAA-C3A	-2.24	108.47	113.47
83	xF	306	PUB	CMD-C2D-C3D	2.24	131.13	127.77
82	DJ	202	PEB	O2B-CGB-CBB	2.24	121.24	114.03
82	AD	303	PEB	CBC-CAC-C2C	-2.24	106.39	112.63
82	JD	202	PEB	CHB-C1C-C2C	-2.24	122.09	127.15
82	jH	203	PEB	OD-C4D-C3D	-2.24	124.38	129.46
87	a6	609	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
87	7N	602	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
82	RI	201	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	bG	201	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	jH	202	PEB	C1C-CHB-C4B	-2.24	123.25	128.28
82	DM	202	PEB	O2B-CGB-CBB	2.24	121.24	114.03
87	MN	101	CLA	CMB-C2B-C3B	2.24	132.02	126.59
82	18	202	PEB	C3B-C4B-NB	2.24	113.31	110.05
87	72	602	CLA	O2D-CGD-CBD	2.24	115.25	111.27
82	KP	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
83	xF	305	PUB	CAB-C3B-C4B	2.24	129.33	125.76
82	wC	203	PEB	CAB-C3B-C4B	2.24	128.98	125.01
82	HA	203	PEB	CHB-C1C-C2C	-2.24	122.09	127.15
87	BN	823	CLA	CMB-C2B-C3B	2.24	132.02	126.59
83	yF	302	PUB	CHA-C4A-NA	-2.24	110.89	113.72
87	A2	841	CLA	C11-C12-C13	-2.24	108.67	115.92
82	S5	202	PEB	C1B-C2B-C3B	-2.24	103.93	106.51
82	XM	202	PEB	CAA-C3A-C2A	-2.24	108.66	114.26
82	b1	202	PEB	C3B-C4B-NB	2.24	113.31	110.05
82	YI	202	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	pF	201	PEB	CAB-C3B-C4B	2.24	128.97	125.01
87	72	602	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
82	FJ	202	PEB	CHA-C1B-NB	-2.24	120.24	124.93
87	32	310	CLA	C3B-C4B-NB	-2.24	108.44	110.52
87	K2	104	CLA	O2D-CGD-CBD	2.24	115.25	111.27
82	YK	202	PEB	CHC-C1D-ND	-2.24	110.89	113.72
87	M2	101	CLA	CMB-C2B-C3B	2.24	132.02	126.59
85	FN	204	BCR	C20-C19-C18	-2.24	120.12	126.42
82	HK	202	PEB	CHB-C4B-NB	2.24	129.24	124.58
82	ZG	203	PEB	CAB-C3B-C4B	2.24	128.97	125.01
82	gM	202	PEB	CBA-CAA-C3A	-2.24	108.48	113.47
96	f6	101	HEM	O2A-CGA-CBA	2.24	121.23	114.03
87	BN	809	CLA	CMB-C2B-C1B	-2.24	121.95	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	A2	840	CLA	CHB-C1B-NB	2.24	126.63	124.26
85	BN	842	BCR	C38-C26-C25	-2.24	122.01	124.53
82	GM	201	PEB	CAA-C3A-C2A	-2.24	108.66	114.26
82	WG	202	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	MK	202	PEB	CHA-C1B-NB	-2.24	120.25	124.93
82	vF	201	PEB	CHA-C1B-NB	-2.24	120.25	124.93
82	G5	201	PEB	CHC-C4C-NC	2.24	124.18	121.15
82	PO	201	PEB	CAB-CBB-CGB	-2.24	108.78	113.60
82	L9	201	PEB	OA-C1A-C2A	-2.24	124.39	126.17
82	QP	203	PEB	CAB-C3B-C4B	2.24	128.97	125.01
82	VQ	201	PEB	CAB-C3B-C4B	2.24	128.97	125.01
82	KK	203	PEB	C2B-C1B-NB	2.24	115.31	110.53
87	B2	822	CLA	CMB-C2B-C3B	2.24	132.02	126.59
82	U9	202	PEB	C2A-C1A-NA	2.24	110.20	108.27
82	UI	201	PEB	OD-C4D-C3D	-2.24	124.38	129.46
82	dJ	202	PEB	OD-C4D-C3D	-2.24	124.38	129.46
82	BF	201	PEB	CMB-C2B-C1B	2.24	128.51	125.06
82	D5	202	PEB	CMB-C2B-C1B	2.24	128.51	125.06
84	GO	1001	CYC	CHB-C1B-NB	-2.24	121.25	126.06
82	KJ	201	PEB	CAA-C3A-C2A	-2.24	108.66	114.26
82	WK	201	PEB	CAA-C3A-C2A	2.24	119.86	114.26
82	AE	301	PEB	CAB-CBB-CGB	-2.24	108.78	113.60
82	PJ	202	PEB	C1D-CHC-C4C	-2.24	109.95	113.26
82	HM	202	PEB	CHA-C1B-C2B	2.24	130.66	124.90
82	uC	203	PEB	CHB-C1C-C2C	-2.24	122.09	127.15
82	PJ	201	PEB	CHB-C4B-NB	-2.24	119.92	124.58
82	UM	203	PEB	CHB-C4B-NB	-2.24	119.92	124.58
87	BN	807	CLA	CHB-C4A-NA	2.24	127.61	124.51
84	EO	1001	CYC	CHA-C1A-C2A	-2.24	120.14	125.32
85	BN	843	BCR	C29-C28-C27	-2.24	106.37	111.38
82	eG	202	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	J9	203	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	H7	203	PEB	CHB-C1C-C2C	-2.24	122.10	127.15
82	vC	202	PEB	C3C-C4C-NC	2.24	110.35	108.33
82	WD	201	PEB	C1B-C2B-C3B	-2.24	103.94	106.51
82	ZO	201	PEB	C2A-C1A-NA	-2.24	106.34	108.27
85	A2	847	BCR	C38-C26-C27	2.24	117.92	113.62
82	KB	301	PEB	CAB-CBB-CGB	-2.24	108.78	113.60
82	H9	203	PEB	CAC-C2C-C1C	2.24	129.33	125.76
82	LI	201	PEB	CHC-C4C-NC	2.24	124.18	121.15
83	A1	303	PUB	CHA-C1B-NB	2.24	124.18	121.15
82	LF	201	PEB	OD-C4D-C3D	-2.24	124.39	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WJ	202	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	QK	203	PEB	OD-C4D-C3D	-2.24	124.39	129.46
87	52	608	CLA	CHB-C4A-NA	2.24	127.61	124.51
82	YA	301	PEB	CBA-CAA-C3A	2.24	118.45	113.47
82	W9	202	PEB	CBB-CAB-C3B	2.24	118.85	112.63
82	PO	202	PEB	C1D-CHC-C4C	-2.24	109.95	113.26
82	bE	201	PEB	CHB-C4B-C3B	-2.24	120.14	125.32
84	D3	1001	CYC	C2C-C3C-C4C	2.24	104.69	101.34
87	AN	841	CLA	C11-C12-C13	-2.24	108.68	115.92
87	A2	818	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
82	PH	202	PEB	C1B-C2B-C3B	-2.24	103.94	106.51
82	VI	201	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	SJ	203	PEB	C4C-C3C-C2C	-2.24	105.43	107.50
82	bH	202	PEB	C3B-C4B-NB	2.24	113.31	110.05
82	Q5	201	PEB	C3C-C4C-NC	2.24	110.35	108.33
83	yF	302	PUB	CAC-C2C-C1C	2.24	128.97	125.01
87	A6	402	CLA	CHB-C4A-NA	2.24	127.61	124.51
82	GD	201	PEB	CAA-C3A-C4A	-2.24	106.92	112.67
82	MB	201	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	OK	203	PEB	OD-C4D-C3D	-2.24	124.39	129.46
84	o3	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
82	GK	202	PEB	CMA-C2A-C3A	-2.24	104.80	113.83
85	c6	603	BCR	C11-C12-C13	-2.24	120.13	126.42
82	JO	1002	PEB	C1D-CHC-C4C	2.24	116.56	113.26
82	z8	201	PEB	CAC-C2C-C1C	2.24	129.33	125.76
82	qC	201	PEB	CAC-C2C-C1C	2.24	129.33	125.76
82	c1	201	PEB	CAB-CBB-CGB	-2.24	108.79	113.60
82	FI	202	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	dM	202	PEB	CMB-C2B-C1B	2.24	128.51	125.06
82	XF	203	PEB	C2B-C1B-NB	2.24	115.31	110.53
82	XJ	201	PEB	CHA-C1B-C2B	2.24	130.66	124.90
82	YB	201	PEB	C3B-C4B-NB	2.24	113.31	110.05
82	R5	201	PEB	CHC-C4C-NC	2.24	124.18	121.15
82	WI	201	PEB	CHB-C1C-NC	-2.24	120.19	125.32
82	bE	201	PEB	C4C-C3C-C2C	-2.24	105.44	107.50
82	R7	203	PEB	CHA-C1B-NB	-2.24	120.25	124.93
87	AN	809	CLA	C2A-C1A-CHA	2.24	127.77	123.86
82	eK	201	PEB	CAB-C3B-C4B	2.24	128.97	125.01
87	C6	514	CLA	CHB-C1B-NB	2.24	126.63	124.26
82	RA	203	PEB	O1B-CGB-CBB	-2.24	115.89	123.08
87	AN	815	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
84	n3	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U9	202	PEB	OD-C4D-C3D	-2.24	124.39	129.46
87	AN	841	CLA	O2D-CGD-CBD	2.24	115.24	111.27
85	fL	101	BCR	C23-C24-C25	2.24	133.49	127.20
82	zC	201	PEB	CAC-C2C-C1C	2.24	129.32	125.76
82	cK	201	PEB	CAC-C2C-C3C	2.24	132.19	127.07
87	5N	611	CLA	C3A-C2A-C1A	2.24	104.69	101.34
82	Q9	201	PEB	CHC-C1D-ND	-2.24	110.89	113.72
82	DF	203	PEB	CMC-C3C-C4C	2.24	129.43	127.06
82	aF	203	PEB	CHB-C4B-C3B	-2.24	120.14	125.32
82	W9	202	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	NK	201	PEB	CMA-C2A-C1A	-2.24	107.58	112.40
82	RA	203	PEB	CHA-C1B-NB	-2.24	120.25	124.93
82	SB	202	PEB	C4C-C3C-C2C	-2.24	105.44	107.50
82	N7	201	PEB	C4C-C3C-C2C	-2.24	105.44	107.50
85	AN	847	BCR	C38-C26-C27	2.24	117.91	113.62
82	II	203	PEB	CHB-C1C-NC	2.24	130.44	125.32
82	Y7	303	PEB	CHB-C4B-C3B	2.24	130.49	125.32
87	AN	809	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
82	cH	201	PEB	C3C-C4C-NC	2.24	110.35	108.33
87	7N	610	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
82	JQ	202	PEB	CHB-C1C-C2C	-2.24	122.10	127.15
83	xK	306	PUB	CMD-C2D-C3D	2.24	131.12	127.77
82	aH	202	PEB	C1B-C2B-C3B	-2.24	103.94	106.51
84	D3	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
82	k4	201	PEB	CMB-C2B-C1B	2.24	128.51	125.06
82	P7	202	PEB	CHA-C4A-NA	2.24	127.86	125.20
82	fH	202	PEB	CHB-C1C-NC	-2.24	120.20	125.32
82	SH	201	PEB	C1C-CHB-C4B	2.24	133.30	128.28
82	qC	203	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	gK	201	PEB	OD-C4D-C3D	-2.24	124.39	129.46
82	S4	201	PEB	CHB-C1C-C2C	-2.24	122.11	127.15
84	W3	1001	CYC	CHA-C4D-C3D	-2.24	122.11	127.15
82	FM	201	PEB	CAB-CBB-CGB	-2.24	108.79	113.60
82	hK	201	PEB	CHA-C1B-C2B	2.24	130.65	124.90
82	DB	203	PEB	C1D-CHC-C4C	2.24	116.55	113.26
82	NG	201	PEB	CHB-C1C-NC	-2.24	120.20	125.32
84	I3	1001	CYC	C2C-C3C-C4C	2.24	104.69	101.34
82	TI	202	PEB	C4C-C3C-C2C	-2.24	105.44	107.50
82	ZI	401	PEB	O1C-CGC-CBC	-2.24	115.90	123.08
82	gE	202	PEB	CAC-CBC-CGC	-2.24	108.79	113.60
82	cH	202	PEB	C1B-C2B-C3B	-2.24	103.94	106.51
82	KM	203	PEB	CMA-C2A-C1A	-2.24	107.58	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Z9	304	PEB	C3C-C4C-NC	2.24	110.35	108.33
87	CL	505	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
82	UP	201	PEB	CAC-C2C-C1C	2.24	129.32	125.76
82	A4	304	PEB	CAC-C2C-C1C	2.24	129.32	125.76
87	bL	605	CLA	CMB-C2B-C3B	2.24	132.00	126.59
82	IB	201	PEB	OD-C4D-C3D	-2.24	124.40	129.46
84	U3	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
87	72	610	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
82	PM	201	PEB	CAB-CBB-CGB	-2.24	108.79	113.60
82	WH	202	PEB	OA-C1A-C2A	-2.23	124.40	126.17
82	HA	201	PEB	C3B-C4B-NB	2.23	113.30	110.05
82	V1	202	PEB	OD-C4D-C3D	-2.23	124.40	129.46
82	XB	202	PEB	CMC-C3C-C2C	-2.23	120.77	125.61
82	FI	201	PEB	CAC-C2C-C1C	2.23	129.32	125.76
84	G4	1001	CYC	CBD-CAD-C3D	-2.23	106.42	112.63
82	gG	202	PEB	CAC-CBC-CGC	-2.23	108.79	113.60
82	SA	202	PEB	C2B-C1B-NB	2.23	115.30	110.53
82	D1	1002	PEB	C1D-CHC-C4C	-2.23	109.96	113.26
82	T7	202	PEB	C1D-CHC-C4C	-2.23	109.96	113.26
82	C5	201	PEB	CHC-C4C-NC	2.23	124.17	121.15
82	jJ	201	PEB	CAA-C3A-C2A	-2.23	108.68	114.26
82	S1	202	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	QG	201	PEB	CMB-C2B-C1B	2.23	128.50	125.06
82	hM	203	PEB	CMB-C2B-C1B	2.23	128.50	125.06
82	fH	203	PEB	CAB-C3B-C4B	2.23	128.96	125.01
87	b6	609	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
82	KB	304	PEB	CAC-CBC-CGC	-2.23	108.80	113.60
82	HM	202	PEB	C2A-C1A-NA	2.23	110.20	108.27
82	WQ	202	PEB	C2A-C1A-NA	2.23	110.20	108.27
82	bP	501	PEB	CAC-C2C-C1C	2.23	129.32	125.76
87	D6	405	CLA	O2D-CGD-CBD	2.23	115.24	111.27
82	R5	201	PEB	CBB-CAB-C3B	-2.23	106.42	112.63
87	A2	819	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
82	A5	201	PEB	CHC-C4C-NC	2.23	124.17	121.15
82	W5	202	PEB	CAB-C3B-C4B	2.23	128.96	125.01
87	AN	805	CLA	C2A-C1A-CHA	2.23	127.77	123.86
85	B2	839	BCR	C21-C20-C19	-2.23	116.25	123.22
82	GM	202	PEB	C4C-C3C-C2C	-2.23	105.44	107.50
82	UI	201	PEB	CHA-C1B-NB	-2.23	120.26	124.93
85	cL	518	BCR	C1-C6-C7	2.23	122.10	115.78
82	pK	202	PEB	OD-C4D-C3D	-2.23	124.40	129.46
82	WI	203	PEB	C3C-C4C-NC	2.23	110.34	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	v8	202	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	yF	301	PEB	CAB-C3B-C4B	2.23	128.96	125.01
83	ND	201	PUB	CAC-C2C-C1C	2.23	128.96	125.01
87	A2	824	CLA	C2A-C1A-CHA	2.23	127.76	123.86
82	TB	202	PEB	C2B-C1B-NB	2.23	115.30	110.53
82	ZB	201	PEB	CHA-C1B-NB	-2.23	120.26	124.93
87	c6	612	CLA	CHB-C4A-NA	2.23	127.60	124.51
85	F2	204	BCR	C32-C1-C6	-2.23	106.68	110.30
82	a1	202	PEB	C2A-C1A-NA	2.23	110.20	108.27
87	62	313	CLA	CHA-C4D-ND	2.23	137.17	132.50
82	xF	304	PEB	CHB-C1C-NC	-2.23	120.20	125.32
82	gG	201	PEB	CHB-C4B-C3B	-2.23	120.15	125.32
87	62	306	CLA	C2A-C1A-CHA	2.23	127.76	123.86
82	EM	203	PEB	CHA-C1B-NB	-2.23	120.26	124.93
82	KM	202	PEB	C4C-C3C-C2C	-2.23	105.44	107.50
82	IA	202	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	jM	202	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	RA	203	PEB	C1C-CHB-C4B	2.23	133.29	128.28
85	a6	605	BCR	C37-C22-C23	2.23	121.59	118.08
82	HB	201	PEB	CHA-C1B-NB	-2.23	120.26	124.93
82	kK	202	PEB	C3B-C4B-NB	2.23	113.30	110.05
87	B2	815	CLA	C2A-C1A-CHA	2.23	127.76	123.86
87	A2	820	CLA	CHC-C4B-NB	2.23	126.62	124.26
87	2N	308	CLA	CHB-C1B-NB	2.23	126.62	124.26
82	DB	203	PEB	OD-C4D-ND	-2.23	122.62	125.93
82	gB	203	PEB	CBA-CAA-C3A	2.23	118.44	113.47
87	CL	513	CLA	CHA-C1A-NA	-2.23	121.29	126.40
84	73	1002	CYC	C1D-C2D-C3D	-2.23	104.95	107.79
82	N7	202	PEB	CMC-C3C-C4C	2.23	129.43	127.06
87	62	307	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
82	cE	201	PEB	C4C-C3C-C2C	-2.23	105.44	107.50
83	AO	303	PUB	CBA-CAA-C3A	-2.23	109.59	112.98
82	WJ	201	PEB	CHB-C1C-C2C	-2.23	122.12	127.15
82	L7	202	PEB	CHA-C1B-NB	-2.23	120.27	124.93
82	WE	203	PEB	C1D-CHC-C4C	-2.23	109.97	113.26
82	fH	203	PEB	OD-C4D-ND	-2.23	122.62	125.93
87	dL	409	CLA	CHB-C1B-NB	2.23	126.62	124.26
82	UH	203	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	U1	203	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	j1	201	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	jJ	202	PEB	CHC-C1D-ND	2.23	116.55	113.72
82	kH	201	PEB	CHC-C4C-NC	2.23	124.17	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U5	202	PEB	C2B-C1B-NB	2.23	115.29	110.53
85	B2	843	BCR	C29-C28-C27	-2.23	106.39	111.38
82	TQ	202	PEB	CHB-C4B-C3B	-2.23	120.16	125.32
83	AD	302	PUB	CHB-C4B-NB	-2.23	120.21	125.32
85	A2	845	BCR	C39-C30-C25	-2.23	106.68	110.30
82	Y4	203	PEB	CAC-CBC-CGC	-2.23	108.80	113.60
87	cL	505	CLA	O2A-C1-C2	2.23	114.50	108.64
87	B2	808	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
82	Q9	202	PEB	CBA-CAA-C3A	-2.23	108.50	113.47
82	LF	201	PEB	C4C-C3C-C2C	-2.23	105.44	107.50
82	T4	202	PEB	CAB-C3B-C4B	2.23	128.95	125.01
82	lJ	201	PEB	C2B-C1B-NB	2.23	115.29	110.53
82	xF	304	PEB	CAC-C2C-C1C	2.23	129.31	125.76
82	TD	202	PEB	CHB-C4B-C3B	-2.23	120.16	125.32
84	KO	1001	CYC	CHB-C1B-NB	-2.23	121.27	126.06
82	UM	203	PEB	CMC-C3C-C2C	2.23	130.43	125.61
82	ZF	201	PEB	CHA-C1B-C2B	2.23	130.63	124.90
82	QI	201	PEB	OD-C4D-C3D	-2.23	124.41	129.46
82	KF	203	PEB	C2B-C1B-NB	2.23	115.29	110.53
87	22	604	CLA	C2A-C1A-CHA	2.23	127.76	123.86
87	A2	805	CLA	C2A-C1A-CHA	2.23	127.76	123.86
82	L1	1002	PEB	OD-C4D-ND	-2.23	122.63	125.93
82	F4	1002	PEB	CAC-CBC-CGC	-2.23	108.81	113.60
82	ND	203	PEB	OD-C4D-C3D	-2.23	124.41	129.46
87	A2	809	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
82	NI	203	PEB	C2B-C1B-NB	2.23	115.29	110.53
82	cF	201	PEB	C2B-C1B-NB	2.23	115.29	110.53
87	6N	613	CLA	C3B-C4B-NB	-2.23	108.45	110.52
82	FO	1002	PEB	OD-C4D-C3D	-2.23	124.41	129.46
82	MB	202	PEB	C1C-CHB-C4B	-2.23	123.28	128.28
82	b1	202	PEB	CHA-C1B-C2B	2.23	130.63	124.90
82	O1	201	PEB	C2B-C1B-NB	2.23	115.29	110.53
85	BN	839	BCR	C21-C20-C19	-2.23	116.26	123.22
84	d3	1001	CYC	C2C-C3C-C4C	2.23	104.68	101.34
82	18	203	PEB	C1D-CHC-C4C	2.23	116.54	113.26
82	wF	301	PEB	C2A-C1A-NA	2.23	110.19	108.27
84	I3	1001	CYC	C2C-C1C-NC	2.23	110.19	108.27
84	q3	1001	CYC	C2C-C1C-NC	2.23	110.19	108.27
82	MK	201	PEB	CHA-C1B-NB	-2.23	120.27	124.93
87	AN	827	CLA	CHB-C1B-NB	2.23	126.62	124.26
87	c6	607	CLA	CHB-C1B-NB	2.23	126.62	124.26
82	kJ	201	PEB	OD-C4D-C3D	-2.23	124.41	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U1	202	PEB	CAB-C3B-C4B	2.23	128.95	125.01
82	O9	203	PEB	CAB-C3B-C4B	2.23	128.95	125.01
85	FN	202	BCR	C8-C9-C10	-2.23	115.52	118.94
82	TJ	201	PEB	CHB-C1C-NC	-2.23	120.22	125.32
87	O2	202	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
84	Q3	1001	CYC	C2C-C3C-C4C	2.23	104.68	101.34
82	UB	301	PEB	CHA-C1B-C2B	2.23	130.63	124.90
82	TP	201	PEB	OD-C4D-C3D	-2.23	124.41	129.46
87	7N	602	CLA	CBA-CAA-C2A	2.23	120.44	113.86
82	c1	202	PEB	C1B-C2B-C3B	-2.23	103.95	106.51
82	KJ	202	PEB	OD-C4D-ND	-2.23	122.63	125.93
82	EJ	202	PEB	CHB-C1C-C2C	-2.23	122.12	127.15
82	aK	203	PEB	CHB-C4B-C3B	-2.23	120.17	125.32
84	73	1002	CYC	CMA-C3A-C2A	-2.23	120.07	126.12
82	V5	201	PEB	CBB-CAB-C3B	-2.23	106.44	112.63
82	I7	202	PEB	CHA-C1B-NB	-2.23	120.27	124.93
82	uC	201	PEB	OD-C4D-C3D	-2.23	124.41	129.46
87	22	605	CLA	CHC-C4B-NB	2.23	126.61	124.26
82	dF	202	PEB	CMA-C2A-C1A	-2.23	107.60	112.40
82	ZK	202	PEB	CAC-C2C-C1C	2.23	129.31	125.76
82	bF	202	PEB	CAC-C2C-C1C	2.23	129.31	125.76
82	XK	203	PEB	C4C-C3C-C2C	-2.23	105.44	107.50
92	b6	620	LMG	O7-C10-O9	-2.23	118.32	123.70
82	ZB	202	PEB	CHC-C1D-ND	-2.23	110.91	113.72
87	bL	614	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
87	7N	601	CLA	O2A-CGA-O1A	-2.23	117.75	123.30
94	DL	401	PL9	C11-C9-C8	-2.23	116.61	121.12
82	Q1	203	PEB	C3C-C4C-NC	2.23	110.34	108.33
82	HA	202	PEB	OD-C4D-C3D	-2.23	124.42	129.46
82	PP	202	PEB	OD-C4D-C3D	-2.23	124.42	129.46
82	gK	201	PEB	CAB-C3B-C4B	2.23	128.95	125.01
87	A2	834	CLA	CHB-C1B-NB	2.23	126.61	124.26
82	CM	203	PEB	CAA-C3A-C4A	-2.23	106.96	112.67
87	42	601	CLA	C2A-C1A-CHA	2.23	127.75	123.86
82	GF	202	PEB	CMA-C2A-C3A	-2.23	104.85	113.83
96	E6	101	HEM	CHD-C1D-C2D	-2.23	121.50	124.98
82	H5	202	PEB	CHA-C4A-NA	-2.23	122.56	125.20
94	D6	408	PL9	C40-C39-C41	2.23	119.02	115.27
82	DQ	201	PEB	CHC-C1D-ND	-2.23	110.91	113.72
82	cG	201	PEB	C4C-C3C-C2C	-2.23	105.45	107.50
82	wK	303	PEB	C4C-C3C-C2C	-2.23	105.45	107.50
85	IN	101	BCR	C11-C10-C9	-2.23	124.13	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	818	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
87	B6	611	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
82	WF	202	PEB	C2A-C1A-NA	2.23	110.19	108.27
82	BI	202	PEB	CAC-C2C-C1C	2.23	129.31	125.76
82	VD	203	PEB	CBD-CAD-C3D	-2.23	116.55	127.62
87	A2	812	CLA	C3B-C4B-NB	-2.23	108.45	110.52
87	b6	611	CLA	CHB-C4A-NA	2.23	127.59	124.51
87	5N	608	CLA	CHB-C4A-NA	2.23	127.59	124.51
82	N5	201	PEB	CBB-CAB-C3B	-2.23	106.44	112.63
85	AN	845	BCR	C39-C30-C25	-2.23	106.69	110.30
82	J7	202	PEB	C3C-C4C-NC	2.23	110.34	108.33
85	cL	504	BCR	C33-C5-C6	-2.23	122.03	124.53
82	KG	201	PEB	CAB-C3B-C4B	2.23	128.94	125.01
82	PH	201	PEB	C2B-C1B-NB	2.23	115.28	110.53
87	A2	809	CLA	C2A-C1A-CHA	2.23	127.75	123.86
82	bP	501	PEB	C4C-C3C-C2C	-2.23	105.45	107.50
82	X5	201	PEB	CBB-CAB-C3B	-2.23	106.44	112.63
82	V5	201	PEB	CHC-C4C-NC	2.22	124.16	121.15
82	MJ	202	PEB	CAB-CBB-CGB	-2.22	108.81	113.60
82	cH	201	PEB	CAB-CBB-CGB	-2.22	108.81	113.60
83	AE	303	PUB	CAC-CBC-CGC	-2.22	108.81	113.60
87	6N	602	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
84	w3	1001	CYC	C2C-C1C-NC	2.22	110.19	108.27
87	CL	513	CLA	C3B-C4B-NB	-2.22	108.45	110.52
87	A2	832	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
82	g1	202	PEB	CAB-C3B-C4B	2.22	128.94	125.01
87	BN	831	CLA	CHA-C1A-NA	-2.22	121.30	126.40
87	72	602	CLA	CBA-CAA-C2A	2.22	120.43	113.86
82	u8	201	PEB	OD-C4D-C3D	-2.22	124.42	129.46
82	ID	201	PEB	CBB-CAB-C3B	2.22	118.81	112.63
82	Q5	203	PEB	CHA-C4A-NA	-2.22	122.56	125.20
85	AN	847	BCR	C2-C3-C4	-2.22	106.41	111.38
82	rK	202	PEB	C4B-C3B-C2B	-2.22	104.32	106.78
82	CM	201	PEB	CHA-C1B-C2B	2.22	130.62	124.90
82	VF	202	PEB	C2B-C1B-NB	2.22	115.28	110.53
87	3N	301	CLA	CMD-C2D-C1D	-2.22	120.79	124.71
82	Y1	202	PEB	CHC-C4C-NC	2.22	124.16	121.15
87	BN	824	CLA	CHD-C1D-ND	-2.22	122.41	124.45
85	Z6	101	BCR	C28-C29-C30	-2.22	106.65	114.60
82	q8	201	PEB	CAC-C2C-C1C	2.22	129.30	125.76
92	A6	408	LMG	O7-C10-O9	-2.22	118.33	123.70
82	QF	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	XF	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	IQ	201	PEB	CBB-CAB-C3B	2.22	118.81	112.63
84	h3	1001	CYC	C2C-C3C-C4C	2.22	104.67	101.34
87	62	303	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
82	WG	202	PEB	OD-C4D-C3D	-2.22	124.42	129.46
83	AG	302	PUB	CHA-C4A-NA	-2.22	110.91	113.72
82	pK	202	PEB	CHB-C4B-C3B	-2.22	120.17	125.32
82	bB	201	PEB	CHB-C1C-C2C	-2.22	122.13	127.15
87	42	602	CLA	C3B-C4B-NB	-2.22	108.45	110.52
87	A2	837	CLA	C3B-C4B-NB	-2.22	108.45	110.52
87	b6	607	CLA	CHB-C4A-NA	2.22	127.59	124.51
82	xC	201	PEB	CAB-C3B-C4B	2.22	128.94	125.01
82	E5	201	PEB	CBB-CAB-C3B	-2.22	106.45	112.63
82	UQ	201	PEB	CAB-CBB-CGB	-2.22	108.82	113.60
87	A2	826	CLA	CHA-C1A-NA	-2.22	121.31	126.40
82	pK	202	PEB	C1B-C2B-C3B	-2.22	103.95	106.51
82	W1	202	PEB	OD-C4D-C3D	-2.22	124.42	129.46
82	vK	201	PEB	OD-C4D-C3D	-2.22	124.42	129.46
82	JB	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
82	A7	202	PEB	CHB-C1C-NC	-2.22	120.23	125.32
91	D6	404	PHO	O2A-CGA-O1A	-2.22	117.98	123.59
84	k3	1001	CYC	C2C-C3C-C4C	2.22	104.67	101.34
82	C5	201	PEB	CBB-CAB-C3B	-2.22	106.45	112.63
82	G5	201	PEB	CBB-CAB-C3B	-2.22	106.45	112.63
82	UH	201	PEB	C3B-C4B-NB	2.22	113.28	110.05
82	O9	203	PEB	CAC-CBC-CGC	-2.22	108.82	113.60
82	YK	203	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
85	F2	204	BCR	C20-C19-C18	-2.22	120.17	126.42
82	TB	201	PEB	CHB-C4B-C3B	-2.22	120.18	125.32
82	eE	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	VM	202	PEB	CHB-C1C-NC	-2.22	120.23	125.32
82	eH	202	PEB	CHA-C1B-C2B	2.22	130.62	124.90
94	aL	601	PL9	C30-C29-C28	-2.22	117.98	123.68
82	WB	402	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
82	WD	202	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
82	U7	201	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
95	B6	620	DGD	C6D-C5D-C4D	-2.22	107.45	112.09
82	qC	201	PEB	CHC-C1D-ND	-2.22	110.91	113.72
83	xK	306	PUB	CHC-C1D-ND	-2.22	110.91	113.72
82	TI	201	PEB	CMC-C3C-C4C	2.22	129.42	127.06
82	YI	201	PEB	OD-C4D-C3D	-2.22	124.43	129.46
82	dE	201	PEB	CHC-C4C-NC	2.22	124.16	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cF	201	PEB	CAC-C2C-C3C	2.22	132.16	127.07
82	P4	201	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	J7	203	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	aK	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
87	7N	607	CLA	O2D-CGD-CBD	2.22	115.22	111.27
82	HD	202	PEB	CAB-CBB-CGB	-2.22	108.82	113.60
82	qF	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
87	1N	608	CLA	C3B-C4B-NB	-2.22	108.45	110.52
85	B6	621	BCR	C29-C30-C25	2.22	113.90	110.48
82	nK	201	PEB	CHB-C1C-C2C	-2.22	122.14	127.15
82	FA	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
82	Y7	301	PEB	CBA-CAA-C3A	2.22	118.41	113.47
82	P5	201	PEB	CBB-CAB-C3B	-2.22	106.45	112.63
82	T5	201	PEB	CBB-CAB-C3B	-2.22	106.45	112.63
82	QK	203	PEB	CHC-C1D-ND	-2.22	110.91	113.72
82	XJ	202	PEB	CAA-C3A-C2A	-2.22	108.71	114.26
87	B6	612	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
87	BN	811	CLA	C2A-C1A-CHA	2.22	127.74	123.86
82	tK	201	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
82	c1	201	PEB	CAC-CBC-CGC	-2.22	108.82	113.60
82	m4	203	PEB	CAB-CBB-CGB	2.22	118.38	113.60
82	O5	202	PEB	CMC-C3C-C4C	2.22	129.41	127.06
82	hE	203	PEB	CMC-C3C-C4C	2.22	129.41	127.06
82	P1	201	PEB	C2B-C1B-NB	2.22	115.27	110.53
82	SM	202	PEB	OD-C4D-ND	-2.22	122.64	125.93
85	B2	842	BCR	C19-C18-C17	-2.22	115.53	118.94
82	Z5	304	PEB	CMD-C2D-C3D	2.22	133.20	130.06
82	OM	202	PEB	CAB-C3B-C4B	2.22	128.94	125.01
82	w8	203	PEB	CAB-C3B-C4B	2.22	128.94	125.01
87	A2	820	CLA	CHA-C1A-NA	-2.22	121.31	126.40
82	TF	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	aO	203	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
87	B2	810	CLA	C2A-C1A-CHA	2.22	127.74	123.86
82	lF	203	PEB	CHB-C4B-NB	-2.22	119.96	124.58
84	w3	1001	CYC	C2C-C3C-C4C	2.22	104.67	101.34
82	jF	201	PEB	CAA-C3A-C2A	-2.22	108.71	114.26
87	C6	512	CLA	C3B-C4B-NB	-2.22	108.45	110.52
87	BN	833	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
87	B6	608	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
82	hE	202	PEB	C1D-CHC-C4C	-2.22	109.98	113.26
82	IB	202	PEB	OD-C4D-ND	-2.22	122.64	125.93
82	LP	201	PEB	CAC-C2C-C1C	2.22	129.30	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	dG	204	PEB	CAC-C2C-C1C	2.22	129.30	125.76
82	A7	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
82	XA	203	PEB	C2A-C1A-NA	2.22	110.19	108.27
87	6N	606	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
82	HF	202	PEB	CHB-C4B-NB	2.22	129.20	124.58
87	c6	611	CLA	CAA-C2A-C1A	-2.22	104.70	111.97
82	L5	201	PEB	C4B-C3B-C2B	-2.22	104.33	106.78
87	A2	814	CLA	C2D-C1D-ND	-2.22	108.47	110.10
82	QD	201	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
82	GF	203	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
84	U3	1001	CYC	C2C-C3C-C4C	2.22	104.66	101.34
82	VM	202	PEB	O2B-CGB-CBB	2.22	121.16	114.03
82	LQ	202	PEB	CHC-C1D-ND	-2.22	110.92	113.72
82	VB	202	PEB	CAC-CBC-CGC	-2.22	108.83	113.60
87	BN	821	CLA	CHB-C1B-NB	2.22	126.61	124.26
96	VL	201	HEM	C1A-CHA-C4D	-2.22	121.07	126.34
87	32	308	CLA	CMD-C2D-C1D	-2.22	120.80	124.71
82	P7	203	PEB	OD-C4D-ND	-2.22	122.64	125.93
87	4N	601	CLA	C2A-C1A-CHA	2.22	127.74	123.86
82	OG	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
85	kL	100	BCR	C1-C6-C7	2.22	122.06	115.78
84	u3	1001	CYC	C2C-C3C-C4C	2.22	104.66	101.34
91	d6	404	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
84	63	901	CYC	CAA-C2A-C1A	2.22	128.93	125.01
82	xK	303	PEB	OD-C4D-ND	-2.22	122.64	125.93
87	3N	308	CLA	C3D-C4D-ND	2.22	113.83	110.24
87	A2	841	CLA	O2D-CGD-CBD	2.22	115.21	111.27
82	AG	301	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
96	V6	201	HEM	CAD-CBD-CGD	-2.22	108.83	113.60
82	UM	203	PEB	CHB-C1C-NC	-2.22	120.24	125.32
82	MM	201	PEB	C1C-NC-C4C	-2.22	105.65	109.60
82	F4	1002	PEB	CHA-C1B-NB	-2.22	120.29	124.93
82	VK	202	PEB	CHA-C4A-NA	2.22	127.84	125.20
87	AN	850	CLA	C2D-C1D-ND	-2.22	108.47	110.10
82	g4	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	tC	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
87	BL	623	CLA	CMB-C2B-C3B	2.22	131.96	126.59
82	S1	201	PEB	C1C-CHB-C4B	2.22	133.26	128.28
82	I7	202	PEB	CHB-C1C-C2C	-2.22	122.15	127.15
87	CL	506	CLA	CHC-C4B-NB	2.22	126.61	124.26
87	22	608	CLA	CHB-C1B-NB	2.22	126.61	124.26
87	D6	403	CLA	CHB-C4A-NA	2.22	127.58	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	H5	203	PEB	C2A-C1A-NA	2.22	110.19	108.27
87	2N	307	CLA	O2A-CGA-O1A	-2.22	117.77	123.30
87	6N	605	CLA	C2A-C1A-CHA	2.22	127.74	123.86
87	FN	205	CLA	CHA-C1A-NA	-2.22	121.32	126.40
87	3N	312	CLA	CHA-C1A-NA	-2.22	121.32	126.40
82	fG	201	PEB	C2B-C1B-NB	2.22	115.26	110.53
85	BN	838	BCR	C12-C13-C14	-2.22	115.54	118.94
82	GI	201	PEB	CHB-C1C-NC	2.22	130.40	125.32
82	NP	201	PEB	CMB-C2B-C1B	2.22	128.48	125.06
82	u8	203	PEB	CHB-C1C-C2C	-2.22	122.15	127.15
92	B6	618	LMG	O7-C10-O9	-2.22	118.34	123.70
82	DB	202	PEB	C4C-C3C-C2C	-2.22	105.45	107.50
82	LQ	203	PEB	CMC-C3C-C4C	2.22	129.41	127.06
82	UQ	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
84	M3	1001	CYC	C2C-C3C-C4C	2.22	104.66	101.34
82	LA	203	PEB	CAC-C2C-C1C	2.22	129.29	125.76
82	GK	203	PEB	O2C-CGC-CBC	2.22	121.15	114.03
83	AG	303	PUB	CAC-CBC-CGC	-2.22	108.83	113.60
82	BB	201	PEB	CHA-C1B-C2B	2.22	130.60	124.90
82	VA	202	PEB	CMB-C2B-C1B	2.22	128.48	125.06
82	wK	301	PEB	CHA-C1B-NB	-2.22	120.30	124.93
82	T7	202	PEB	CHB-C1C-NC	2.22	130.40	125.32
82	JD	203	PEB	CBD-CAD-C3D	-2.22	116.59	127.62
82	GA	202	PEB	C3C-C4C-NC	2.22	110.33	108.33
82	OH	201	PEB	C3C-C4C-NC	2.22	110.33	108.33
82	QF	202	PEB	C1C-CHB-C4B	2.22	133.25	128.28
82	LM	201	PEB	CAC-C2C-C1C	2.22	129.29	125.76
84	B3	1001	CYC	C2C-C3C-C4C	2.22	104.66	101.34
82	QG	203	PEB	CHB-C4B-C3B	-2.22	120.19	125.32
82	KQ	201	PEB	CHA-C1B-NB	-2.22	120.30	124.93
82	PJ	202	PEB	CAB-C3B-C4B	2.22	128.93	125.01
82	TA	202	PEB	CHB-C1C-NC	2.22	130.40	125.32
82	OI	201	PEB	CHB-C1C-NC	-2.22	120.24	125.32
87	A2	852	CLA	O2A-CGA-O1A	-2.22	117.78	123.30
92	J6	102	LMG	O7-C10-O9	-2.22	118.35	123.70
82	M5	305	PEB	CHA-C4A-NA	-2.22	122.57	125.20
83	wF	304	PUB	CAC-CBC-CGC	-2.22	108.83	113.60
82	J7	201	PEB	CHC-C4C-NC	2.22	124.15	121.15
87	4N	604	CLA	CHB-C1B-NB	2.22	126.60	124.26
82	SF	201	PEB	CHB-C1C-NC	2.22	130.40	125.32
87	B2	810	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
82	CP	202	PEB	CAC-CBC-CGC	-2.22	108.83	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	V7	203	PEB	CMB-C2B-C1B	2.22	128.48	125.06
82	DQ	201	PEB	OD-C4D-ND	-2.22	122.65	125.93
82	WH	203	PEB	C3C-C4C-NC	2.22	110.33	108.33
82	DK	203	PEB	CMC-C3C-C4C	2.22	129.41	127.06
82	B5	203	PEB	CHA-C4A-NA	-2.22	122.57	125.20
82	I5	201	PEB	CBB-CAB-C3B	-2.22	106.47	112.63
82	CB	202	PEB	C4C-C3C-C2C	-2.22	105.46	107.50
82	NB	202	PEB	C4C-C3C-C2C	-2.22	105.46	107.50
82	S9	203	PEB	C4C-C3C-C2C	-2.22	105.46	107.50
82	vK	202	PEB	C4C-C3C-C2C	-2.22	105.46	107.50
82	LP	201	PEB	CAB-C3B-C4B	2.22	128.93	125.01
85	FN	204	BCR	C32-C1-C6	-2.22	106.71	110.30
94	AL	413	PL9	C26-C27-C28	2.22	119.16	111.88
87	AL	404	CLA	CHB-C1B-NB	2.22	126.60	124.26
82	CQ	201	PEB	OD-C4D-C3D	-2.22	124.44	129.46
82	TD	203	PEB	CMB-C2B-C1B	2.21	128.47	125.06
82	dJ	201	PEB	CHA-C1B-NB	-2.21	120.30	124.93
82	IK	203	PEB	C2B-C1B-NB	2.21	115.26	110.53
87	B2	833	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
82	fM	203	PEB	CAA-C3A-C4A	-2.21	106.99	112.67
82	FI	202	PEB	CAC-CBC-CGC	-2.21	108.84	113.60
87	A2	815	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
82	B7	203	PEB	CHC-C4C-NC	2.21	124.15	121.15
82	UD	202	PEB	OD-C4D-C3D	-2.21	124.44	129.46
82	RK	202	PEB	C2B-C1B-NB	2.21	115.25	110.53
84	J1	1001	CYC	C2C-C1C-NC	2.21	110.18	108.27
82	R7	203	PEB	C1C-CHB-C4B	2.21	133.25	128.28
82	w8	202	PEB	CHC-C1D-ND	-2.21	110.92	113.72
87	AN	852	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
82	AA	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
87	A2	827	CLA	CHB-C1B-NB	2.21	126.60	124.26
82	dK	201	PEB	CAA-C3A-C2A	-2.21	108.73	114.26
87	a6	608	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
91	a6	613	PHO	O2A-CGA-CBA	2.21	118.86	111.91
82	OH	203	PEB	OD-C4D-C3D	-2.21	124.44	129.46
82	PG	202	PEB	CAA-C3A-C4A	-2.21	106.99	112.67
82	dO	201	PEB	C4B-NB-C1B	-2.21	102.34	106.51
82	cB	402	PEB	OD-C4D-C3D	-2.21	124.45	129.46
83	AD	302	PUB	CMD-C2D-C3D	2.21	131.09	127.77
84	j3	1001	CYC	C2C-C3C-C4C	2.21	104.65	101.34
82	E5	201	PEB	CHC-C4C-NC	2.21	124.14	121.15
82	A5	201	PEB	CBB-CAB-C3B	-2.21	106.48	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WF	201	PEB	C2B-C1B-NB	2.21	115.25	110.53
82	RF	202	PEB	OD-C4D-ND	-2.21	122.65	125.93
82	WH	203	PEB	C3B-C4B-NB	2.21	113.27	110.05
82	KG	201	PEB	CAC-CBC-CGC	-2.21	108.84	113.60
87	52	607	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
82	pF	202	PEB	CHB-C4B-C3B	-2.21	120.20	125.32
82	X5	201	PEB	CHC-C4C-NC	2.21	124.14	121.15
87	72	602	CLA	CMD-C2D-C1D	-2.21	120.81	124.71
82	WP	202	PEB	OA-C1A-C2A	-2.21	124.41	126.17
82	RK	202	PEB	C4B-NB-C1B	-2.21	102.34	106.51
87	22	607	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
87	2N	301	CLA	CHC-C4B-NB	2.21	126.60	124.26
84	f3	1001	CYC	C2C-C1C-NC	2.21	110.18	108.27
82	F5	201	PEB	OD-C4D-C3D	-2.21	124.45	129.46
82	eG	202	PEB	CAC-CBC-CGC	-2.21	108.84	113.60
84	n3	1001	CYC	C2C-C3C-C4C	2.21	104.65	101.34
82	eM	201	PEB	C1C-CHB-C4B	-2.21	123.32	128.28
82	F7	201	PEB	C1D-CHC-C4C	2.21	116.52	113.26
87	AN	832	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
82	RH	201	PEB	CAB-C3B-C4B	2.21	128.92	125.01
82	gH	202	PEB	CAB-C3B-C4B	2.21	128.92	125.01
87	22	602	CLA	CHA-C1A-NA	-2.21	121.33	126.40
82	aE	202	PEB	CHC-C1D-ND	-2.21	110.93	113.72
82	YP	503	PEB	C3C-C4C-NC	2.21	110.32	108.33
82	BP	201	PEB	OD-C4D-C3D	-2.21	124.45	129.46
82	18	201	PEB	CHB-C1C-NC	-2.21	120.25	125.32
82	dG	204	PEB	CHB-C4B-NB	-2.21	119.98	124.58
82	dK	202	PEB	CMA-C2A-C1A	-2.21	107.64	112.40
82	QD	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	PG	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	oF	203	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
87	bL	619	CLA	C2A-C1A-CHA	2.21	127.72	123.86
82	P5	201	PEB	CHC-C4C-NC	2.21	124.14	121.15
82	gF	201	PEB	CHC-C4C-NC	2.21	124.14	121.15
84	63	901	CYC	C2A-C1A-NA	2.21	113.27	110.05
82	OH	201	PEB	C2B-C1B-NB	2.21	115.25	110.53
94	D6	408	PL9	C22-C21-C19	-2.21	105.70	112.98
87	C6	513	CLA	CHB-C4A-NA	2.21	127.57	124.51
82	hE	202	PEB	CHA-C1B-NB	-2.21	120.31	124.93
87	6N	608	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
82	kJ	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
82	VI	202	PEB	CHB-C4B-NB	-2.21	119.98	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	a4	202	PEB	CHB-C4B-NB	-2.21	119.98	124.58
87	AN	801	CLA	C3A-C2A-C1A	2.21	104.65	101.34
85	B6	601	BCR	C29-C30-C25	2.21	113.88	110.48
87	B6	615	CLA	CHB-C1B-NB	2.21	126.60	124.26
82	F7	201	PEB	C1C-CHB-C4B	2.21	133.24	128.28
82	q8	201	PEB	CHC-C1D-ND	-2.21	110.93	113.72
82	mO	202	PEB	CAC-C2C-C1C	2.21	129.28	125.76
82	W9	203	PEB	OD-C4D-C3D	-2.21	124.45	129.46
83	AQ	302	PUB	CHB-C4B-NB	-2.21	120.26	125.32
82	cB	403	PEB	C3C-C4C-NC	2.21	110.32	108.33
82	lE	203	PEB	C3C-C4C-NC	2.21	110.32	108.33
84	H3	1001	CYC	C2C-C3C-C4C	2.21	104.65	101.34
82	AD	301	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	LK	201	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	L9	203	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	JQ	203	PEB	CBD-CAD-C3D	-2.21	116.62	127.62
96	V6	201	HEM	CHA-C4D-C3D	-2.21	121.18	125.33
87	bL	617	CLA	C3B-C4B-NB	-2.21	108.47	110.52
82	J7	203	PEB	CHB-C1C-NC	-2.21	120.26	125.32
96	vL	201	HEM	C1A-CHA-C4D	-2.21	121.10	126.34
82	CD	201	PEB	CMA-C2A-C1A	-2.21	107.64	112.40
82	WM	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
82	yK	301	PEB	CAB-C3B-C4B	2.21	128.92	125.01
96	VL	201	HEM	C4C-CHD-C1D	-2.21	121.29	126.06
82	U9	204	PEB	CHB-C4B-C3B	2.21	130.43	125.32
82	JO	1002	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
87	72	601	CLA	O2A-CGA-O1A	-2.21	117.79	123.30
82	U1	201	PEB	C3B-C4B-NB	2.21	113.26	110.05
82	PO	202	PEB	C1C-NC-C4C	-2.21	105.67	109.60
82	mJ	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
84	q3	1001	CYC	C2C-C3C-C4C	2.21	104.65	101.34
82	XA	203	PEB	CBC-CAC-C2C	2.21	118.77	112.63
82	KD	202	PEB	CHA-C1B-C2B	2.21	130.58	124.90
82	MD	201	PEB	C4B-C3B-C2B	-2.21	104.34	106.78
82	JB	201	PEB	CHB-C4B-C3B	-2.21	120.21	125.32
84	E4	1001	CYC	CHA-C1A-C2A	-2.21	120.21	125.32
82	cE	202	PEB	CAB-C3B-C4B	2.21	128.92	125.01
87	BL	622	CLA	CHD-C1D-ND	-2.21	122.42	124.45
87	AN	827	CLA	CHD-C1D-ND	-2.21	122.42	124.45
82	KB	304	PEB	C3C-C4C-NC	2.21	110.32	108.33
82	gF	202	PEB	CMC-C3C-C4C	2.21	129.40	127.06
82	DH	1002	PEB	C1D-CHC-C4C	-2.21	110.00	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UK	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	HP	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	bF	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	aM	204	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	dF	202	PEB	C2A-C1A-NA	2.21	110.18	108.27
82	hK	201	PEB	C2A-C1A-NA	2.21	110.18	108.27
82	GK	203	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
87	A2	801	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
87	3N	310	CLA	CHA-C4D-ND	2.21	137.12	132.50
84	o3	1001	CYC	C2C-C3C-C4C	2.21	104.65	101.34
82	vF	201	PEB	OD-C4D-C3D	-2.21	124.46	129.46
82	ZM	202	PEB	CHA-C1B-NB	-2.21	120.31	124.93
82	V1	202	PEB	CHA-C1B-NB	-2.21	120.31	124.93
82	P7	201	PEB	C4B-C3B-C2B	-2.21	104.34	106.78
82	NF	201	PEB	CMA-C2A-C1A	-2.21	107.64	112.40
82	VJ	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
82	M5	304	PEB	CMD-C2D-C3D	2.21	133.18	130.06
82	b1	202	PEB	CHC-C4C-NC	2.21	124.14	121.15
82	gK	202	PEB	CHC-C4C-NC	2.21	124.14	121.15
84	S3	1001	CYC	C2C-C3C-C4C	2.21	104.65	101.34
82	v8	201	PEB	CAB-C3B-C4B	2.21	128.91	125.01
95	C6	502	DGD	O6D-C5D-C6D	-2.21	102.21	106.67
82	zC	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
82	HB	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	UJ	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	w8	203	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
82	KD	202	PEB	C1C-CHB-C4B	-2.21	123.33	128.28
82	h4	201	PEB	CBA-CAA-C3A	-2.21	108.55	113.47
95	BN	844	DGD	O6D-C5D-C6D	2.21	111.12	106.67
85	b6	603	BCR	C2-C1-C6	2.21	113.88	110.48
82	FD	201	PEB	C1C-CHB-C4B	2.21	133.23	128.28
82	ZI	401	PEB	C2A-C3A-C4A	2.21	104.64	101.34
84	f3	1001	CYC	C2C-C3C-C4C	2.21	104.64	101.34
82	II	203	PEB	CHC-C1D-ND	2.21	116.52	113.72
87	b6	612	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
82	DM	202	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
82	ED	201	PEB	OD-C4D-ND	-2.21	122.66	125.93
82	eH	201	PEB	CAB-C3B-C4B	2.21	128.91	125.01
82	lO	202	PEB	C3B-C4B-NB	2.21	113.26	110.05
82	IJ	203	PEB	C3C-C4C-NC	2.21	110.32	108.33
82	VJ	202	PEB	C4C-C3C-C2C	-2.21	105.46	107.50
85	a6	605	BCR	C38-C26-C27	2.21	117.86	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	AL	415	DGD	O3G-C1D-C2D	2.21	111.75	108.30
87	A2	850	CLA	C2D-C1D-ND	-2.21	108.48	110.10
82	ID	201	PEB	CAC-CBC-CGC	-2.21	108.86	113.60
85	A2	847	BCR	C2-C3-C4	-2.21	106.45	111.38
82	S4	201	PEB	CAB-C3B-C4B	2.21	128.91	125.01
82	VQ	202	PEB	CMC-C3C-C4C	2.21	129.40	127.06
82	qK	203	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
82	CQ	201	PEB	CMA-C2A-C1A	-2.21	107.65	112.40
82	SG	201	PEB	CAC-C2C-C1C	2.21	129.28	125.76
82	w8	204	PEB	CMB-C2B-C1B	2.21	128.46	125.06
82	WE	201	PEB	CAC-CBC-CGC	-2.21	108.86	113.60
85	AN	846	BCR	C33-C5-C6	-2.21	122.05	124.53
82	L7	203	PEB	CHC-C4C-NC	2.21	124.13	121.15
87	22	608	CLA	CAA-C2A-C1A	2.21	119.20	111.97
82	B7	203	PEB	C4C-C3C-C2C	-2.21	105.47	107.50
82	hJ	202	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
82	SA	202	PEB	CHA-C1B-NB	-2.21	120.32	124.93
82	S7	202	PEB	CHA-C1B-NB	-2.21	120.32	124.93
82	VA	203	PEB	CMB-C2B-C1B	2.21	128.46	125.06
82	FH	1002	PEB	CMB-C2B-C1B	2.21	128.46	125.06
82	TF	201	PEB	C1B-C2B-C3B	-2.21	103.98	106.51
87	F2	205	CLA	CHA-C1A-NA	-2.21	121.35	126.40
82	WI	203	PEB	CAB-C3B-C4B	2.21	128.91	125.01
82	hG	202	PEB	CHA-C1B-NB	-2.20	120.32	124.93
82	OE	202	PEB	OD-C4D-C3D	-2.20	124.47	129.46
84	KO	1001	CYC	CBD-CAD-C3D	-2.20	106.50	112.63
87	42	602	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
83	xF	301	PUB	CHB-C1C-NC	-2.20	119.99	124.58
82	gE	201	PEB	CHB-C4B-C3B	-2.20	120.22	125.32
82	d1	202	PEB	OA-C1A-C2A	-2.20	124.42	126.17
87	B2	831	CLA	CHA-C1A-NA	-2.20	121.35	126.40
82	jM	203	PEB	CAA-C3A-C4A	-2.20	107.01	112.67
85	A2	804	BCR	C16-C15-C14	-2.20	118.96	123.47
82	AQ	301	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	dQ	401	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	HB	202	PEB	CHA-C1B-NB	-2.20	120.32	124.93
87	22	611	CLA	C3B-C4B-NB	-2.20	108.47	110.52
82	JA	201	PEB	CHC-C4C-NC	2.20	124.13	121.15
82	eO	202	PEB	C1C-NC-C4C	-2.20	105.67	109.60
87	62	309	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
82	FQ	201	PEB	C1C-CHB-C4B	2.20	133.22	128.28
87	32	307	CLA	C3D-C4D-ND	2.20	113.80	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	824	CLA	C2A-C1A-CHA	2.20	127.71	123.86
85	LN	201	BCR	C33-C5-C6	-2.20	122.05	124.53
83	wF	304	PUB	CAB-C3B-C4B	2.20	129.27	125.76
82	CD	201	PEB	OD-C4D-C3D	-2.20	124.47	129.46
82	GJ	202	PEB	CMB-C2B-C1B	2.20	128.46	125.06
85	KL	100	BCR	C1-C6-C7	2.20	122.01	115.78
82	bF	202	PEB	CHB-C1C-C2C	-2.20	122.18	127.15
87	AN	802	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
87	AN	828	CLA	C2D-C1D-ND	-2.20	108.48	110.10
82	OF	203	PEB	C2B-C1B-NB	2.20	115.23	110.53
83	wK	304	PUB	C4B-CHB-C1C	2.20	133.22	128.28
85	h6	102	BCR	C23-C24-C25	-2.20	121.01	127.20
82	jM	201	PEB	CHA-C4A-NA	2.20	127.83	125.20
82	YO	201	PEB	CHC-C4C-NC	2.20	124.13	121.15
82	K5	201	PEB	CHC-C4C-NC	2.20	124.13	121.15
82	T5	201	PEB	CHC-C4C-NC	2.20	124.13	121.15
84	MO	1001	CYC	CBC-CAC-C3C	-2.20	108.56	113.47
82	PO	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	Y4	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	L5	202	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	hG	203	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	j4	201	PEB	C3C-C4C-NC	2.20	110.32	108.33
82	D5	203	PEB	C3C-C4C-NC	2.20	110.32	108.33
82	lJ	203	PEB	C3C-C4C-NC	2.20	110.32	108.33
82	KQ	202	PEB	CHA-C1B-C2B	2.20	130.57	124.90
82	cG	202	PEB	CAB-C3B-C4B	2.20	128.91	125.01
87	A2	815	CLA	C3B-C4B-NB	-2.20	108.47	110.52
82	IF	203	PEB	C2B-C1B-NB	2.20	115.23	110.53
82	WK	203	PEB	CMC-C3C-C4C	2.20	129.40	127.06
82	VD	203	PEB	C1C-CHB-C4B	2.20	133.22	128.28
83	YA	302	PUB	C4B-CHB-C1C	2.20	133.22	128.28
85	B6	621	BCR	C16-C15-C14	-2.20	118.96	123.47
95	cL	502	DGD	C3G-O3G-C1D	-2.20	109.44	113.74
87	62	313	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
82	QE	203	PEB	CHB-C4B-C3B	-2.20	120.22	125.32
87	AN	829	CLA	C2A-C1A-CHA	2.20	127.71	123.86
84	JH	1001	CYC	CBB-CAB-C3B	-2.20	106.36	112.43
82	WK	202	PEB	C2A-C1A-NA	2.20	110.17	108.27
87	C6	515	CLA	CHB-C1B-NB	2.20	126.59	124.26
82	QB	201	PEB	CHC-C4C-NC	-2.20	118.17	121.15
82	F7	202	PEB	C2B-C1B-NB	2.20	115.23	110.53
82	vC	201	PEB	CAB-C3B-C4B	2.20	128.91	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	819	CLA	O1D-CGD-CBD	2.20	128.99	124.48
82	fG	201	PEB	CAA-C3A-C4A	-2.20	107.02	112.67
82	TQ	203	PEB	CMB-C2B-C1B	2.20	128.46	125.06
82	LD	201	PEB	CAB-CBB-CGB	-2.20	108.86	113.60
82	WG	201	PEB	CAC-CBC-CGC	-2.20	108.86	113.60
87	I2	103	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
85	AN	804	BCR	C16-C15-C14	-2.20	118.96	123.47
82	wC	202	PEB	CHC-C1D-ND	-2.20	110.94	113.72
82	AQ	303	PEB	CBC-CAC-C2C	-2.20	106.51	112.63
82	kO	202	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	KA	201	PEB	CMC-C3C-C4C	2.20	129.40	127.06
82	I5	201	PEB	CHC-C4C-NC	2.20	124.13	121.15
82	U9	202	PEB	CMB-C2B-C1B	2.20	128.46	125.06
84	N1	1001	CYC	C1B-NB-C4B	-2.20	107.86	110.67
87	8N	306	CLA	O1A-CGA-CBA	2.20	130.16	123.08
82	VM	201	PEB	CHB-C1C-NC	-2.20	120.28	125.32
82	V7	202	PEB	OD-C4D-C3D	-2.20	124.47	129.46
87	BL	623	CLA	C2A-C1A-CHA	2.20	127.71	123.86
87	8N	305	CLA	C2A-C1A-CHA	2.20	127.71	123.86
82	NA	203	PEB	CMA-C2A-C1A	-2.20	107.66	112.40
82	OO	201	PEB	CHC-C1D-ND	-2.20	110.94	113.72
82	e1	201	PEB	CAB-C3B-C4B	2.20	128.90	125.01
82	V1	201	PEB	CBB-CAB-C3B	2.20	118.74	112.63
85	A6	401	BCR	C36-C18-C17	-2.20	119.84	122.92
82	fK	201	PEB	CAC-C2C-C1C	2.20	129.27	125.76
82	FJ	202	PEB	CHB-C4B-NB	-2.20	120.00	124.58
82	RF	202	PEB	C2B-C1B-NB	2.20	115.23	110.53
82	gK	202	PEB	CMC-C3C-C4C	2.20	129.39	127.06
82	BI	203	PEB	CAC-CBC-CGC	-2.20	108.87	113.60
82	t8	202	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
87	4N	608	CLA	C2A-C1A-CHA	2.20	127.71	123.86
87	AL	405	CLA	C3A-C2A-C1A	2.20	104.64	101.34
82	LE	1002	PEB	C3C-C4C-NC	-2.20	106.36	108.33
95	BL	614	DGD	C3G-O3G-C1D	-2.20	109.44	113.74
82	sF	201	PEB	CAC-C2C-C3C	2.20	132.11	127.07
82	e1	202	PEB	CHA-C1B-C2B	2.20	130.56	124.90
87	12	607	CLA	CHB-C1B-NB	2.20	126.59	124.26
87	A2	802	CLA	CHB-C1B-NB	2.20	126.59	124.26
87	B6	606	CLA	CHC-C4B-NB	2.20	126.59	124.26
85	c6	602	BCR	C38-C26-C27	2.20	117.84	113.62
82	xC	201	PEB	CHC-C1D-ND	-2.20	110.94	113.72
82	JA	201	PEB	CAB-CBB-CGB	-2.20	108.87	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	M5	305	PEB	CAC-CBC-CGC	-2.20	108.87	113.60
95	BL	607	DGD	O1G-C1A-C2A	2.20	118.81	111.91
82	TA	202	PEB	C1D-CHC-C4C	-2.20	110.01	113.26
92	ML	101	LMG	O8-C28-O10	-2.20	118.04	123.59
84	HO	1001	CYC	CAB-C3B-C2B	2.20	131.29	127.53
84	F3	1001	CYC	C2C-C3C-C4C	2.20	104.64	101.34
82	BB	202	PEB	CAB-C3B-C4B	2.20	128.90	125.01
82	F4	1002	PEB	OD-C4D-C3D	-2.20	124.47	129.46
82	WJ	203	PEB	C2B-C1B-NB	2.20	115.22	110.53
82	GI	201	PEB	CBA-CAA-C3A	-2.20	108.57	113.47
87	BL	619	CLA	CMB-C2B-C3B	2.20	131.92	126.59
82	KJ	201	PEB	CHA-C1B-C2B	2.20	130.56	124.90
82	K5	201	PEB	CBB-CAB-C3B	-2.20	106.51	112.63
85	C6	508	BCR	C35-C13-C14	-2.20	119.84	122.92
85	k6	102	BCR	C29-C30-C25	2.20	113.87	110.48
82	FF	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	OG	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	uF	203	PEB	CMB-C2B-C1B	2.20	128.45	125.06
82	NQ	203	PEB	OD-C4D-C3D	-2.20	124.48	129.46
87	82	305	CLA	O1A-CGA-CBA	2.20	130.15	123.08
82	OG	201	PEB	C3C-C4C-NC	2.20	110.31	108.33
82	K7	201	PEB	C1D-CHC-C4C	2.20	116.50	113.26
82	DJ	202	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
82	JM	202	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
87	32	312	CLA	CHA-C1A-NA	-2.20	121.36	126.40
82	VO	201	PEB	CAC-CBC-CGC	-2.20	108.87	113.60
82	MB	201	PEB	CHA-C1B-C2B	2.20	130.56	124.90
82	NM	201	PEB	CMC-C3C-C2C	-2.20	120.85	125.61
82	IA	202	PEB	CHA-C1B-NB	-2.20	120.33	124.93
87	CL	510	CLA	CMC-C2C-C3C	2.20	132.09	126.12
85	CL	502	BCR	C2-C1-C6	2.20	113.87	110.48
87	5N	604	CLA	C2A-C1A-CHA	2.20	127.70	123.86
82	N7	203	PEB	CMA-C2A-C1A	-2.20	107.66	112.40
82	HM	202	PEB	CMB-C2B-C1B	2.20	128.45	125.06
82	KE	201	PEB	CAC-CBC-CGC	-2.20	108.87	113.60
82	H7	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
98	A2	842	PQN	C11-C12-C13	-2.20	123.13	126.79
82	oK	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	bO	202	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
87	6N	602	CLA	CHB-C1B-NB	2.20	126.58	124.26
84	y3	1001	CYC	CHA-C4D-C3D	-2.20	122.19	127.15
87	3N	307	CLA	C2A-C1A-CHA	2.20	127.70	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	yF	301	PEB	CAB-CBB-CGB	-2.20	108.87	113.60
82	YF	203	PEB	C3C-C4C-NC	2.20	110.31	108.33
85	K6	102	BCR	C29-C30-C25	2.20	113.87	110.48
87	A6	402	CLA	O1D-CGD-CBD	2.20	128.98	124.48
82	BI	201	PEB	OD-C4D-C3D	-2.20	124.48	129.46
82	JP	201	PEB	CHA-C4A-NA	2.20	127.82	125.20
98	AN	842	PQN	C11-C12-C13	-2.20	123.13	126.79
82	mO	203	PEB	CAB-CBB-CGB	2.20	118.33	113.60
82	LQ	202	PEB	OA-C1A-C2A	-2.20	124.42	126.17
92	m6	103	LMG	O7-C10-O9	-2.20	118.39	123.70
82	WJ	202	PEB	CHB-C1C-NC	-2.20	120.28	125.32
85	B6	601	BCR	C23-C24-C25	-2.20	121.03	127.20
82	GJ	203	PEB	C2B-C1B-NB	2.20	115.22	110.53
82	OK	203	PEB	C2B-C1B-NB	2.20	115.22	110.53
82	cK	201	PEB	C2B-C1B-NB	2.20	115.22	110.53
87	5N	602	CLA	CHC-C4B-NB	2.20	126.58	124.26
82	OH	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	y8	203	PEB	CHB-C1C-NC	-2.20	120.28	125.32
84	L3	1001	CYC	C2C-C3C-C4C	2.20	104.63	101.34
84	O3	1001	CYC	C2C-C3C-C4C	2.20	104.63	101.34
82	JA	202	PEB	C3C-C4C-NC	2.20	110.31	108.33
82	PG	202	PEB	CHC-C1D-ND	-2.20	110.94	113.72
82	BA	201	PEB	CHA-C4A-NA	2.20	127.82	125.20
82	F5	203	PEB	CHA-C4A-NA	-2.20	122.59	125.20
82	CM	201	PEB	CHB-C1C-C2C	-2.20	122.19	127.15
82	UJ	201	PEB	C2B-C1B-NB	2.20	115.22	110.53
82	PJ	202	PEB	CHB-C4B-NB	-2.20	120.00	124.58
82	ZH	201	PEB	C1C-NC-C4C	-2.20	105.69	109.60
82	YQ	201	PEB	OD-C4D-ND	-2.20	122.67	125.93
82	KF	202	PEB	OA-C1A-C2A	-2.20	124.43	126.17
82	WK	201	PEB	C2B-C1B-NB	2.20	115.22	110.53
82	PP	201	PEB	C2B-C1B-NB	2.20	115.22	110.53
82	qF	201	PEB	CAB-C3B-C4B	2.20	128.90	125.01
82	AI	203	PEB	C1C-CHB-C4B	2.20	133.21	128.28
82	rC	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
82	Q1	201	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	fE	201	PEB	CAA-C3A-C4A	-2.20	107.03	112.67
82	gH	202	PEB	CMB-C2B-C1B	2.20	128.45	125.06
82	MJ	202	PEB	C3C-C4C-NC	2.20	110.31	108.33
82	M9	302	PEB	C3C-C4C-NC	2.20	110.31	108.33
82	J9	201	PEB	CHB-C1C-NC	-2.20	120.29	125.32
82	eK	201	PEB	CMC-C3C-C4C	2.20	129.39	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	z8	201	PEB	CAB-CBB-CGB	-2.20	108.88	113.60
87	c6	605	CLA	C1-C2-C3	-2.20	122.24	126.04
82	V9	201	PEB	CAB-C3B-C4B	2.20	128.89	125.01
82	KQ	202	PEB	C1C-CHB-C4B	-2.20	123.36	128.28
82	GJ	201	PEB	OD-C4D-C3D	-2.20	124.48	129.46
82	WJ	203	PEB	OD-C4D-C3D	-2.20	124.48	129.46
82	b1	202	PEB	CAC-C2C-C1C	2.20	129.26	125.76
82	ND	204	PEB	CBA-CAA-C3A	-2.20	108.58	113.47
87	F2	201	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
87	K6	101	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
85	b6	602	BCR	C2-C1-C6	2.20	113.86	110.48
87	52	602	CLA	CHC-C4B-NB	2.20	126.58	124.26
87	A2	834	CLA	CHC-C4B-NB	2.20	126.58	124.26
82	DD	201	PEB	CHC-C1D-ND	-2.20	110.95	113.72
87	AN	837	CLA	CMB-C2B-C3B	2.20	131.91	126.59
87	nL	101	CLA	CMB-C2B-C3B	2.20	131.91	126.59
82	W1	203	PEB	CAB-C3B-C4B	2.20	128.89	125.01
87	B2	821	CLA	CAA-C2A-C1A	2.20	119.17	111.97
82	X7	203	PEB	C2A-C1A-NA	2.20	110.17	108.27
82	a4	203	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
82	d4	202	PEB	C4C-C3C-C2C	-2.20	105.47	107.50
87	B2	832	CLA	CMB-C2B-C3B	2.20	131.91	126.59
82	LD	201	PEB	C3B-C4B-NB	2.20	113.24	110.05
85	C6	507	BCR	C38-C26-C27	2.20	117.83	113.62
87	CL	503	CLA	C2D-C1D-ND	-2.20	108.49	110.10
82	mK	201	PEB	C3C-C4C-NC	2.20	110.31	108.33
82	KJ	203	PEB	CAB-C3B-C4B	2.20	128.89	125.01
82	NP	201	PEB	CAB-C3B-C4B	2.20	128.89	125.01
87	7N	602	CLA	CMD-C2D-C1D	-2.20	120.84	124.71
85	b6	603	BCR	C16-C15-C14	-2.20	118.98	123.47
82	J9	203	PEB	CAA-C3A-C4A	2.20	118.31	112.67
87	AN	801	CLA	CHB-C1B-NB	2.20	126.58	124.26
87	a6	609	CLA	CHB-C1B-NB	2.20	126.58	124.26
82	GI	203	PEB	CHB-C4B-NB	-2.20	120.01	124.58
82	UP	202	PEB	C3B-C4B-NB	2.20	113.24	110.05
82	LJ	202	PEB	CHA-C1B-NB	-2.19	120.34	124.93
85	BN	843	BCR	C33-C5-C4	2.19	117.83	113.62
83	AM	304	PUB	CBA-CAA-C3A	-2.19	109.65	112.98
87	BN	832	CLA	CMB-C2B-C3B	2.19	131.90	126.59
82	v8	202	PEB	C3B-C4B-NB	2.19	113.24	110.05
82	CM	203	PEB	OD-C4D-C3D	-2.19	124.49	129.46
87	A2	828	CLA	C2D-C1D-ND	-2.19	108.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	c6	614	CLA	C2D-C1D-ND	-2.19	108.49	110.10
85	KN	104	BCR	C30-C25-C26	-2.19	119.52	122.61
82	VQ	203	PEB	CBD-CAD-C3D	-2.19	116.70	127.62
82	U1	202	PEB	C2B-C1B-NB	2.19	115.21	110.53
82	Y5	201	PEB	C2B-C1B-NB	2.19	115.21	110.53
82	BF	201	PEB	CMA-C2A-C1A	-2.19	107.67	112.40
82	yC	202	PEB	OD-C4D-C3D	-2.19	124.49	129.46
82	cG	201	PEB	CAB-CBB-CGB	-2.19	108.88	113.60
82	gJ	201	PEB	CMC-C3C-C4C	2.19	129.39	127.06
87	52	604	CLA	C2A-C1A-CHA	2.19	127.69	123.86
82	N9	201	PEB	CAB-C3B-C4B	2.19	128.89	125.01
83	A1	303	PUB	CAC-C2C-C1C	2.19	128.89	125.01
82	X7	203	PEB	CBC-CAC-C2C	2.19	118.72	112.63
87	a6	607	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
87	1N	607	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
87	A2	819	CLA	C2C-C1C-NC	-2.19	107.92	109.97
82	U1	202	PEB	CMB-C2B-C1B	2.19	128.44	125.06
82	F9	202	PEB	C2B-C1B-NB	2.19	115.21	110.53
82	NI	202	PEB	CHB-C4B-NB	-2.19	120.01	124.58
87	82	304	CLA	C2A-C1A-CHA	2.19	127.69	123.86
82	WK	201	PEB	C1C-NC-C4C	-2.19	105.69	109.60
84	IO	1001	CYC	CHB-C1B-NB	-2.19	121.35	126.06
82	WI	203	PEB	CHC-C1D-ND	-2.19	110.95	113.72
82	KF	203	PEB	C1C-CHB-C4B	2.19	133.20	128.28
87	42	603	CLA	C2D-C1D-ND	-2.19	108.49	110.10
87	2N	308	CLA	CAA-C2A-C1A	2.19	119.16	111.97
82	rK	202	PEB	CMC-C3C-C2C	-2.19	120.86	125.61
82	IA	202	PEB	CHB-C1C-C2C	-2.19	122.20	127.15
82	CP	201	PEB	CAC-C2C-C1C	2.19	129.25	125.76
82	DQ	202	PEB	CHB-C1C-NC	2.19	130.34	125.32
82	JI	202	PEB	CHB-C4B-C3B	-2.19	120.25	125.32
82	QK	202	PEB	CAA-C3A-C4A	-2.19	107.04	112.67
82	EM	201	PEB	C2B-C1B-NB	2.19	115.21	110.53
82	NJ	201	PEB	CMA-C2A-C1A	-2.19	107.68	112.40
82	rF	202	PEB	CMC-C3C-C2C	-2.19	120.86	125.61
82	RI	202	PEB	CHB-C4B-NB	-2.19	120.02	124.58
87	BN	802	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
82	WM	201	PEB	C3B-C4B-NB	2.19	113.24	110.05
82	SH	202	PEB	C3C-C4C-NC	2.19	110.31	108.33
82	KK	202	PEB	OA-C1A-C2A	-2.19	124.43	126.17
85	K2	105	BCR	C30-C25-C26	-2.19	119.53	122.61
82	FM	201	PEB	CHA-C1B-NB	-2.19	120.35	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WJ	201	PEB	CAB-CBB-CGB	-2.19	108.89	113.60
96	VL	201	HEM	C4D-ND-C1D	2.19	107.34	105.07
82	VB	201	PEB	CHB-C1C-C2C	-2.19	122.20	127.15
87	A2	802	CLA	C3A-C2A-C1A	2.19	104.62	101.34
82	gM	202	PEB	CAA-C3A-C4A	2.19	118.30	112.67
82	E7	201	PEB	C1C-CHB-C4B	2.19	133.20	128.28
87	BN	822	CLA	CAA-C2A-C1A	2.19	119.16	111.97
87	B2	823	CLA	CHD-C1D-ND	-2.19	122.44	124.45
87	IN	103	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
87	B6	611	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
82	CQ	201	PEB	C2B-C1B-NB	2.19	115.21	110.53
87	aL	605	CLA	C2D-C1D-ND	-2.19	108.49	110.10
82	AP	201	PEB	CAC-CBC-CGC	-2.19	108.89	113.60
82	V4	201	PEB	CAC-CBC-CGC	-2.19	108.89	113.60
82	F4	1002	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
82	ZF	202	PEB	CAC-C2C-C1C	2.19	129.25	125.76
95	B2	844	DGD	O6D-C5D-C6D	2.19	111.09	106.67
82	k1	202	PEB	OA-C1A-NA	2.19	127.60	124.94
82	MK	202	PEB	CHC-C1D-ND	-2.19	110.95	113.72
82	dM	201	PEB	C1C-NC-C4C	-2.19	105.70	109.60
84	73	1001	CYC	C2C-C3C-C4C	2.19	104.62	101.34
82	UO	201	PEB	CMA-C2A-C3A	-2.19	104.99	113.83
87	A2	838	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
82	Z5	305	PEB	CAC-CBC-CGC	-2.19	108.89	113.60
85	B2	843	BCR	C33-C5-C4	2.19	117.83	113.62
82	KK	203	PEB	O2C-CGC-CBC	2.19	121.07	114.03
83	xF	301	PUB	CBD-CAD-C3D	-2.19	106.39	112.43
82	XI	202	PEB	CHB-C4B-NB	-2.19	120.02	124.58
82	L7	203	PEB	CAC-C2C-C1C	2.19	129.25	125.76
84	K4	1001	CYC	CBD-CAD-C3D	-2.19	106.54	112.63
87	A2	837	CLA	CMB-C2B-C3B	2.19	131.89	126.59
87	BL	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
82	iF	202	PEB	O2C-CGC-CBC	2.19	121.07	114.03
82	U7	202	PEB	CHA-C1B-NB	-2.19	120.35	124.93
87	AN	806	CLA	CHD-C1D-ND	-2.19	122.44	124.45
82	OE	201	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
87	BN	816	CLA	C2A-C1A-CHA	2.19	127.69	123.86
82	J4	1002	PEB	C1B-C2B-C3B	-2.19	103.99	106.51
87	AN	826	CLA	CHA-C1A-NA	-2.19	121.38	126.40
87	42	610	CLA	CHA-C1A-NA	-2.19	121.38	126.40
82	m4	202	PEB	CAC-C2C-C1C	2.19	129.25	125.76
82	dE	204	PEB	CAC-C2C-C1C	2.19	129.25	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UE	201	PEB	CAB-CBB-CGB	-2.19	108.89	113.60
84	j3	1001	CYC	CHD-C1D-C2D	2.19	132.87	127.49
82	DE	1002	PEB	OD-C4D-ND	-2.19	122.69	125.93
82	QM	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
82	SJ	201	PEB	C1C-CHB-C4B	-2.19	123.37	128.28
82	fM	201	PEB	C1D-CHC-C4C	-2.19	110.03	113.26
85	bL	601	BCR	C33-C5-C6	-2.19	122.07	124.53
87	32	306	CLA	C2A-C1A-CHA	2.19	127.69	123.86
82	SH	201	PEB	CAB-C3B-C4B	2.19	128.88	125.01
82	PG	201	PEB	CMA-C2A-C1A	-2.19	107.68	112.40
87	bL	615	CLA	C7-C6-C5	-2.19	107.41	113.36
82	EP	202	PEB	CHA-C1B-NB	-2.19	120.35	124.93
82	DB	203	PEB	CAC-CBC-CGC	-2.19	108.89	113.60
87	KN	102	CLA	CHB-C1B-NB	2.19	126.58	124.26
87	A2	822	CLA	CHC-C4B-NB	2.19	126.58	124.26
82	GB	201	PEB	CAC-C2C-C1C	2.19	129.25	125.76
82	VQ	203	PEB	C1C-CHB-C4B	2.19	133.19	128.28
87	2N	303	CLA	CHA-C1A-NA	-2.19	121.38	126.40
82	XJ	202	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
82	PM	201	PEB	CHA-C4A-NA	2.19	127.81	125.20
82	OF	202	PEB	CAC-C2C-C3C	2.19	132.08	127.07
84	d3	1001	CYC	CHD-C1D-C2D	2.19	132.86	127.49
82	FP	201	PEB	CAB-C3B-C4B	2.19	128.88	125.01
82	HD	201	PEB	C2B-C1B-NB	2.19	115.20	110.53
82	OD	201	PEB	C2B-C1B-NB	2.19	115.20	110.53
87	AN	838	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
84	LG	1001	CYC	C4D-ND-C1D	-2.19	105.88	109.79
87	A2	810	CLA	CMD-C2D-C1D	-2.19	120.86	124.71
82	OQ	202	PEB	CHC-C1D-ND	-2.19	110.95	113.72
82	bK	202	PEB	CAC-C2C-C1C	2.19	129.25	125.76
82	bB	201	PEB	C1C-CHB-C4B	2.19	133.19	128.28
87	AN	852	CLA	CHA-C1A-NA	-2.19	121.39	126.40
82	tK	202	PEB	CHB-C4B-NB	2.19	129.13	124.58
82	RB	201	PEB	C3B-C4B-NB	2.19	113.23	110.05
87	AL	405	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
82	SB	203	PEB	CAB-CBB-CGB	-2.19	108.89	113.60
82	iO	202	PEB	OD-C4D-ND	-2.19	122.69	125.93
87	82	306	CLA	CHA-C1A-NA	-2.19	121.39	126.40
82	WG	203	PEB	C1D-CHC-C4C	-2.19	110.03	113.26
82	MJ	202	PEB	CAC-C2C-C3C	2.19	132.08	127.07
82	YF	203	PEB	CMA-C2A-C1A	-2.19	107.69	112.40
95	L6	102	DGD	C3G-O3G-C1D	-2.19	109.46	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	CD	201	PEB	C2B-C1B-NB	2.19	115.20	110.53
82	wF	301	PEB	CHA-C1B-NB	-2.19	120.36	124.93
82	r8	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
82	SD	201	PEB	CHC-C4C-NC	2.19	124.11	121.15
87	BN	813	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
82	aO	202	PEB	CHB-C1C-NC	2.19	130.33	125.32
82	RF	202	PEB	C4B-NB-C1B	-2.19	102.39	106.51
82	PE	201	PEB	CMA-C2A-C1A	-2.19	107.69	112.40
82	fE	201	PEB	C2B-C1B-NB	2.19	115.20	110.53
82	h1	201	PEB	C3C-C4C-NC	2.19	110.30	108.33
82	gE	201	PEB	CAB-CBB-CGB	-2.19	108.89	113.60
92	CL	519	LMG	O1-C7-C8	-2.19	105.62	110.90
82	XF	201	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
82	UE	203	PEB	CAC-C2C-C1C	2.19	129.25	125.76
82	qK	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
82	HH	1002	PEB	CHB-C4B-NB	-2.19	120.03	124.58
82	EI	202	PEB	CHB-C4B-NB	-2.19	120.03	124.58
87	cL	509	CLA	C2A-C1A-CHA	2.19	127.68	123.86
82	DB	202	PEB	CHC-C1D-ND	-2.19	110.96	113.72
82	LD	202	PEB	CHC-C1D-ND	-2.19	110.96	113.72
82	bK	202	PEB	CHB-C1C-C2C	-2.19	122.22	127.15
85	FL	101	BCR	C38-C26-C27	2.19	117.82	113.62
82	KB	302	PEB	CMA-C2A-C1A	-2.19	107.69	112.40
82	iF	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
82	OE	202	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
82	O5	203	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
82	hK	202	PEB	C1D-CHC-C4C	2.19	116.48	113.26
87	CL	512	CLA	C3B-C4B-NB	-2.19	108.49	110.52
82	AA	201	PEB	OD-C4D-C3D	-2.19	124.51	129.46
82	Z5	305	PEB	CHA-C4A-NA	-2.19	122.61	125.20
87	AN	833	CLA	CHC-C4B-NB	2.19	126.57	124.26
87	4N	602	CLA	CHB-C1B-NB	2.19	126.57	124.26
84	BE	1002	CYC	C4D-CHA-C1A	2.19	133.19	128.28
82	A1	302	PEB	C3C-C4C-NC	2.19	110.30	108.33
82	S4	202	PEB	C3C-C4C-NC	2.19	110.30	108.33
82	C7	201	PEB	C3C-C4C-NC	2.19	110.30	108.33
82	XM	201	PEB	CHA-C1B-C2B	2.19	130.52	124.90
82	rF	202	PEB	C2A-C1A-NA	2.19	110.16	108.27
82	RD	201	PEB	CAC-C2C-C1C	2.19	129.24	125.76
82	L4	1002	PEB	CAB-C3B-C4B	2.19	128.88	125.01
82	X9	201	PEB	CAB-C3B-C4B	2.19	128.88	125.01
85	B2	838	BCR	C12-C13-C14	-2.19	115.59	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	L5	202	PEB	OD-C4D-C3D	-2.19	124.51	129.46
87	72	604	CLA	C2A-C1A-CHA	2.19	127.68	123.86
82	OF	203	PEB	CMC-C3C-C4C	2.19	129.38	127.06
82	cB	401	PEB	CMC-C3C-C4C	2.19	129.38	127.06
82	KD	202	PEB	CHB-C1C-NC	-2.19	120.31	125.32
82	FM	201	PEB	CHB-C1C-NC	-2.19	120.31	125.32
82	BB	201	PEB	C3B-C4B-NB	2.19	113.23	110.05
82	UF	202	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
82	U5	203	PEB	C4C-C3C-C2C	-2.19	105.48	107.50
82	TI	203	PEB	CHB-C4B-NB	-2.19	120.03	124.58
82	pF	202	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
82	mM	202	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
82	cE	201	PEB	CAB-CBB-CGB	-2.19	108.90	113.60
87	CL	509	CLA	CHA-C1A-NA	-2.19	121.39	126.40
82	UB	303	PEB	C1D-CHC-C4C	-2.19	110.03	113.26
82	t8	201	PEB	C4B-C3B-C2B	-2.19	104.36	106.78
82	aH	201	PEB	C3C-C4C-NC	2.19	110.30	108.33
82	Z9	301	PEB	C3C-C4C-NC	2.19	110.30	108.33
87	B2	801	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
84	I4	1001	CYC	CHB-C1B-NB	-2.19	121.37	126.06
82	bH	202	PEB	CHA-C1B-C2B	2.19	130.52	124.90
87	8N	301	CLA	CHA-C1A-NA	-2.19	121.39	126.40
87	B2	812	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
82	IM	203	PEB	CAC-C2C-C1C	2.19	129.24	125.76
82	JP	201	PEB	CMB-C2B-C1B	2.19	128.43	125.06
82	H9	201	PEB	CMB-C2B-C1B	2.19	128.43	125.06
82	MB	202	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
82	Y4	203	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
84	W3	1001	CYC	C4A-C3A-C2A	-2.19	104.00	106.51
82	FQ	201	PEB	CHC-C1D-ND	-2.19	110.96	113.72
85	BN	842	BCR	C19-C18-C17	-2.19	115.59	118.94
95	AL	414	DGD	O6E-C5E-C4E	-2.18	105.73	109.69
82	FO	1002	PEB	C4C-C3C-C2C	-2.18	105.48	107.50
87	B2	827	CLA	C3B-C4B-NB	-2.18	108.49	110.52
83	Y7	302	PUB	C4B-CHB-C1C	2.18	133.18	128.28
84	DE	1001	CYC	C1B-CHB-C4A	-2.18	122.74	128.08
87	22	604	CLA	CHB-C1B-NB	2.18	126.57	124.26
87	22	607	CLA	CHB-C1B-NB	2.18	126.57	124.26
87	dL	401	CLA	CHC-C4B-NB	2.18	126.57	124.26
82	HJ	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	RQ	203	PEB	OD-C4D-ND	-2.18	122.69	125.93
95	AL	416	DGD	C1D-O6D-C5D	2.18	117.98	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	R2	201	CLA	CHA-C1A-NA	-2.18	121.39	126.40
85	B6	621	BCR	C15-C16-C17	-2.18	119.00	123.47
82	HQ	202	PEB	CAB-CBB-CGB	-2.18	108.90	113.60
82	qF	201	PEB	CAC-CBC-CGC	-2.18	108.90	113.60
85	b6	603	BCR	C35-C13-C14	-2.18	119.86	122.92
82	BB	203	PEB	C3C-C4C-NC	2.18	110.30	108.33
87	D6	403	CLA	C1-C2-C3	-2.18	122.27	126.04
87	b6	608	CLA	C1-C2-C3	-2.18	122.27	126.04
87	AN	822	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
84	U3	1001	CYC	CHD-C1D-C2D	2.18	132.85	127.49
82	AO	305	PEB	CHC-C1D-ND	-2.18	110.96	113.72
82	MM	202	PEB	C1B-C2B-C3B	-2.18	104.00	106.51
82	OD	202	PEB	CHA-C4A-NA	-2.18	122.61	125.20
82	SB	201	PEB	OD-C4D-C3D	-2.18	124.51	129.46
82	k1	202	PEB	OD-C4D-C3D	-2.18	124.51	129.46
87	22	608	CLA	CHA-C1A-NA	-2.18	121.40	126.40
82	eM	202	PEB	CAA-C3A-C2A	-2.18	108.80	114.26
82	UA	201	PEB	CMA-C2A-C1A	-2.18	107.69	112.40
82	IB	201	PEB	C4C-C3C-C2C	-2.18	105.48	107.50
82	LI	202	PEB	C4C-C3C-C2C	-2.18	105.48	107.50
82	O9	203	PEB	C4C-C3C-C2C	-2.18	105.48	107.50
82	PH	202	PEB	CHA-C1B-NB	-2.18	120.36	124.93
82	P1	202	PEB	CHA-C1B-NB	-2.18	120.36	124.93
82	AQ	301	PEB	CMB-C2B-C1B	2.18	128.43	125.06
82	hO	201	PEB	CBA-CAA-C3A	-2.18	108.61	113.47
82	LJ	201	PEB	OD-C4D-C3D	-2.18	124.51	129.46
82	CI	202	PEB	CHB-C4B-NB	-2.18	120.03	124.58
87	c6	606	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
85	JN	103	BCR	C16-C15-C14	-2.18	119.00	123.47
82	QJ	202	PEB	CAA-C3A-C4A	-2.18	107.07	112.67
82	C9	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	ZF	202	PEB	CHB-C1C-NC	-2.18	120.32	125.32
82	1C	201	PEB	CHB-C1C-NC	-2.18	120.32	125.32
82	O9	201	PEB	O1B-CGB-CBB	-2.18	116.07	123.08
87	B6	614	CLA	O2D-CGD-CBD	2.18	115.15	111.27
82	YI	202	PEB	CHB-C1C-C2C	-2.18	122.22	127.15
82	AQ	301	PEB	C3C-C4C-NC	2.18	110.30	108.33
82	TJ	201	PEB	CMD-C2D-C3D	2.18	133.14	130.06
87	K2	101	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
82	BK	201	PEB	CMA-C2A-C1A	-2.18	107.70	112.40
82	QK	201	PEB	CAC-CBC-CGC	2.18	118.30	113.60
82	BA	201	PEB	CAC-CBC-CGC	-2.18	108.91	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	LQ	201	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
87	K2	103	CLA	CHB-C1B-NB	2.18	126.57	124.26
87	2N	307	CLA	CHB-C1B-NB	2.18	126.57	124.26
85	FN	202	BCR	C21-C20-C19	-2.18	116.41	123.22
82	ED	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
82	A7	201	PEB	OD-C4D-C3D	-2.18	124.52	129.46
82	CP	203	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
82	QF	202	PEB	CAA-C3A-C4A	-2.18	107.07	112.67
87	C6	516	CLA	C1-C2-C3	-2.18	122.27	126.04
98	B2	837	PQN	C21-C20-C18	-2.18	108.86	115.92
82	L9	202	PEB	CMB-C2B-C1B	2.18	128.43	125.06
82	CF	202	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	WH	203	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	DK	203	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	R1	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	dF	202	PEB	CAB-C3B-C4B	2.18	128.87	125.01
84	IG	1001	CYC	CMC-C2C-C1C	-2.18	107.70	112.40
82	BF	201	PEB	O2B-CGB-CBB	2.18	121.04	114.03
87	32	302	CLA	CHB-C1B-NB	2.18	126.57	124.26
92	CL	519	LMG	C1-O6-C5	2.18	117.97	113.69
82	qF	202	PEB	C2A-C1A-NA	2.18	110.15	108.27
82	QK	201	PEB	CMB-C2B-C3B	-2.18	120.19	126.12
84	EG	1001	CYC	CMC-C2C-C1C	-2.18	107.70	112.40
85	CL	501	BCR	C38-C26-C25	-2.18	122.08	124.53
82	u8	203	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
85	J2	103	BCR	C16-C15-C14	-2.18	119.00	123.47
82	ZG	203	PEB	CHA-C1B-C2B	2.18	130.51	124.90
85	BL	616	BCR	C10-C11-C12	-2.18	116.41	123.22
82	LD	203	PEB	CMC-C3C-C4C	2.18	129.37	127.06
82	hG	203	PEB	CMC-C3C-C4C	2.18	129.37	127.06
82	P9	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	H7	201	PEB	C3B-C4B-NB	2.18	113.22	110.05
87	AN	827	CLA	CMB-C2B-C3B	2.18	131.87	126.59
87	BN	833	CLA	CMB-C2B-C3B	2.18	131.87	126.59
82	J7	201	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
82	qK	201	PEB	CAC-CBC-CGC	-2.18	108.91	113.60
82	AI	202	PEB	CHB-C4B-NB	-2.18	120.04	124.58
82	II	202	PEB	CHB-C4B-NB	-2.18	120.04	124.58
82	wC	204	PEB	CMB-C2B-C1B	2.18	128.42	125.06
82	fE	203	PEB	OD-C4D-ND	-2.18	122.70	125.93
82	VI	203	PEB	CAD-C3D-C2D	-2.18	121.42	128.60
87	CL	513	CLA	CMB-C2B-C3B	2.18	131.87	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	JH	1001	CYC	OC-C1C-C2C	-2.18	124.44	126.17
82	dK	202	PEB	C2A-C1A-NA	2.18	110.15	108.27
82	lJ	202	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
82	uF	201	PEB	CAC-C2C-C1C	2.18	129.24	125.76
82	dE	204	PEB	CHB-C4B-NB	-2.18	120.04	124.58
82	V1	203	PEB	CAB-C3B-C4B	2.18	128.87	125.01
82	KJ	203	PEB	OD-C4D-C3D	-2.18	124.52	129.46
82	AP	202	PEB	CBA-CAA-C3A	-2.18	108.61	113.47
87	4N	602	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
82	TH	202	PEB	OD-C4D-ND	-2.18	122.70	125.93
82	Z5	301	PEB	CHB-C1C-NC	-2.18	120.33	125.32
82	DD	201	PEB	C1D-CHC-C4C	-2.18	110.04	113.26
82	Y4	203	PEB	CHB-C1C-C2C	-2.18	122.23	127.15
82	TA	202	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
84	f3	1001	CYC	CHD-C1D-C2D	2.18	132.84	127.49
85	cL	518	BCR	C16-C15-C14	-2.18	119.01	123.47
82	CJ	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
84	M4	1001	CYC	CBC-CAC-C3C	-2.18	108.61	113.47
82	KF	203	PEB	CHB-C4B-C3B	-2.18	120.28	125.32
82	CF	203	PEB	CHA-C1B-NB	-2.18	120.37	124.93
87	dL	404	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
82	S5	203	PEB	C3C-C4C-NC	2.18	110.30	108.33
82	L7	201	PEB	C3B-C4B-NB	2.18	113.22	110.05
82	WF	201	PEB	CAC-CBC-CGC	-2.18	108.91	113.60
84	o3	1001	CYC	CHD-C1D-C2D	2.18	132.84	127.49
94	aL	601	PL9	C25-C24-C23	-2.18	118.09	123.68
87	6N	612	CLA	O2A-CGA-O1A	-2.18	117.87	123.30
82	YJ	201	PEB	OD-C4D-C3D	-2.18	124.52	129.46
82	NQ	202	PEB	CMC-C3C-C4C	2.18	129.37	127.06
82	CJ	201	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
82	q8	202	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
87	AN	815	CLA	C3B-C4B-NB	-2.18	108.49	110.52
85	CL	502	BCR	C38-C26-C27	2.18	117.80	113.62
82	g4	203	PEB	CHC-C1D-ND	-2.18	110.97	113.72
83	yK	302	PUB	CHA-C4A-NA	-2.18	110.97	113.72
82	PE	201	PEB	C2B-C1B-NB	2.18	115.18	110.53
87	AN	835	CLA	CMB-C2B-C3B	2.18	131.87	126.59
82	QB	201	PEB	OD-C4D-ND	-2.18	122.70	125.93
82	XJ	201	PEB	CHB-C1C-NC	-2.18	120.33	125.32
82	VA	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
82	MP	201	PEB	C4B-NB-C1B	-2.18	102.41	106.51
87	2N	309	CLA	CMC-C2C-C1C	-2.18	121.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	A4	303	PUB	CBA-CAA-C3A	-2.18	109.67	112.98
85	Z6	101	BCR	C8-C7-C6	-2.18	121.08	127.20
84	D3	1001	CYC	CHD-C1D-C2D	2.18	132.84	127.49
87	bL	622	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
82	I9	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
82	SQ	201	PEB	CHC-C4C-NC	2.18	124.10	121.15
82	YQ	202	PEB	C2B-C1B-NB	2.18	115.18	110.53
82	GM	201	PEB	OD-C4D-C3D	-2.18	124.53	129.46
87	LN	204	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
87	B2	833	CLA	CMB-C2B-C3B	2.18	131.86	126.59
82	hJ	201	PEB	CAC-C2C-C1C	2.18	129.23	125.76
87	AN	822	CLA	CHC-C4B-NB	2.18	126.56	124.26
85	F2	203	BCR	C35-C13-C14	-2.18	119.87	122.92
82	B7	201	PEB	CAC-CBC-CGC	-2.18	108.92	113.60
82	cH	201	PEB	CAC-CBC-CGC	-2.18	108.92	113.60
82	WA	202	PEB	OD-C4D-C3D	-2.18	124.53	129.46
87	CL	510	CLA	C2D-C1D-ND	-2.18	108.50	110.10
82	VH	201	PEB	CBB-CAB-C3B	2.18	118.68	112.63
82	FI	201	PEB	CBC-CAC-C2C	-2.18	106.58	112.63
82	TD	202	PEB	C1C-CHB-C4B	2.18	133.17	128.28
82	OK	202	PEB	C3C-C4C-NC	2.18	110.29	108.33
82	a1	201	PEB	C3C-C4C-NC	2.18	110.29	108.33
82	WF	203	PEB	CMC-C3C-C4C	2.18	129.37	127.06
82	S4	201	PEB	C4B-C3B-C2B	-2.18	104.37	106.78
84	63	901	CYC	CBD-CAD-C3D	-2.18	106.58	112.63
82	sF	202	PEB	CHA-C4A-NA	2.18	127.79	125.20
87	bL	619	CLA	C3B-C4B-NB	-2.18	108.50	110.52
82	TP	202	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
82	w8	204	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
98	BN	837	PQN	C21-C20-C18	-2.18	108.88	115.92
82	FM	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
83	AQ	302	PUB	CMD-C2D-C3D	2.18	131.03	127.77
87	12	611	CLA	C2A-C1A-CHA	2.18	127.67	123.86
82	OF	203	PEB	OD-C4D-C3D	-2.18	124.53	129.46
82	Z9	301	PEB	OA-C1A-C2A	-2.18	124.44	126.17
82	WM	202	PEB	CBA-CAA-C3A	-2.18	108.62	113.47
82	cJ	202	PEB	CAA-C3A-C4A	2.18	118.26	112.67
82	FF	201	PEB	O2B-CGB-CBB	2.18	121.02	114.03
82	fG	201	PEB	CHA-C1B-NB	-2.18	120.38	124.93
84	DG	1001	CYC	C1B-CHB-C4A	-2.18	122.76	128.08
85	FN	202	BCR	C35-C13-C14	-2.18	119.87	122.92
87	FN	203	CLA	CMB-C2B-C1B	-2.18	122.05	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	B3	1001	CYC	CHD-C1D-C2D	2.18	132.83	127.49
87	32	310	CLA	CHA-C4D-ND	2.18	137.05	132.50
82	dF	201	PEB	CAA-C3A-C2A	-2.18	108.82	114.26
82	EQ	201	PEB	OD-C4D-ND	-2.18	122.71	125.93
87	B6	615	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
82	UE	203	PEB	C1C-CHB-C4B	-2.18	123.40	128.28
87	DL	403	CLA	CHB-C1B-NB	2.18	126.56	124.26
82	PK	202	PEB	C4C-C3C-C2C	-2.18	105.49	107.50
82	F5	203	PEB	C1D-CHC-C4C	-2.18	110.05	113.26
87	82	301	CLA	C1D-ND-C4D	-2.18	104.79	106.33
95	BL	614	DGD	O5D-C6D-C5D	2.18	113.07	109.05
82	k1	201	PEB	CHC-C4C-NC	2.18	124.09	121.15
82	aB	202	PEB	CAB-CBB-CGB	-2.18	108.92	113.60
95	CL	520	DGD	C4D-C3D-C2D	2.18	114.62	110.82
87	BN	802	CLA	CMC-C2C-C1C	-2.18	121.72	125.04
91	DL	405	PHO	O2A-CGA-CBA	2.18	118.74	111.91
87	A2	808	CLA	C16-C15-C13	-2.18	108.89	115.92
84	h3	1001	CYC	CHD-C1D-C2D	2.18	132.83	127.49
82	T7	201	PEB	C3B-C4B-NB	2.18	113.21	110.05
82	WB	402	PEB	OD-C4D-C3D	-2.18	124.53	129.46
85	A2	847	BCR	C40-C30-C25	-2.18	106.77	110.30
85	B2	841	BCR	C39-C30-C25	-2.18	106.77	110.30
84	L4	1001	CYC	C4D-ND-C1D	-2.18	105.91	109.79
82	XD	202	PEB	CAB-C3B-C4B	2.18	128.86	125.01
82	E9	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
82	YP	502	PEB	C3C-C4C-NC	2.18	110.29	108.33
82	dK	201	PEB	C1B-C2B-C3B	-2.18	104.01	106.51
82	eG	203	PEB	O2C-CGC-CBC	2.18	121.02	114.03
87	AN	836	CLA	O2A-CGA-O1A	-2.18	117.88	123.30
87	AN	815	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
82	WK	201	PEB	CAC-CBC-CGC	-2.18	108.92	113.60
85	F2	203	BCR	C21-C20-C19	-2.18	116.43	123.22
82	qK	202	PEB	C3B-C4B-NB	2.18	113.21	110.05
82	eE	203	PEB	O2C-CGC-CBC	2.18	121.02	114.03
82	aB	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
82	zF	501	PEB	CAB-C3B-C4B	2.18	128.86	125.01
82	aH	202	PEB	C2A-C1A-NA	2.17	110.15	108.27
84	H3	1001	CYC	CHD-C1D-C2D	2.17	132.83	127.49
87	2N	308	CLA	CHA-C1A-NA	-2.17	121.42	126.40
82	IP	201	PEB	C1D-CHC-C4C	-2.17	110.05	113.26
82	XA	201	PEB	C4B-C3B-C2B	-2.17	104.38	106.78
82	e4	202	PEB	CHC-C1D-ND	-2.17	110.97	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	DL	407	LHG	C5-O7-C7	-2.17	112.44	117.79
84	H4	1001	CYC	C1B-CHB-C4A	-2.17	122.77	128.08
87	A2	835	CLA	CMB-C2B-C3B	2.17	131.85	126.59
82	VF	201	PEB	C1B-C2B-C3B	-2.17	104.01	106.51
82	R9	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
87	4N	607	CLA	C3A-C2A-C1A	2.17	104.60	101.34
87	HL	102	CLA	CHC-C4B-NB	2.17	126.56	124.26
87	B6	610	CLA	CHB-C1B-NB	2.17	126.56	124.26
87	b6	607	CLA	CHB-C1B-NB	2.17	126.56	124.26
82	KF	203	PEB	O2C-CGC-CBC	2.17	121.02	114.03
82	iK	202	PEB	O2C-CGC-CBC	2.17	121.02	114.03
82	QH	203	PEB	C3C-C4C-NC	2.17	110.29	108.33
82	FP	202	PEB	C3C-C4C-NC	2.17	110.29	108.33
82	Z9	303	PEB	C3C-C4C-NC	2.17	110.29	108.33
82	1C	202	PEB	C3B-C4B-NB	2.17	113.21	110.05
84	j3	1001	CYC	CAB-C3B-C2B	2.17	131.25	127.53
82	Q5	202	PEB	C1D-CHC-C4C	-2.17	110.05	113.26
82	EF	202	PEB	C2B-C1B-NB	2.17	115.17	110.53
82	MA	201	PEB	O1C-CGC-CBC	-2.17	116.10	123.08
87	62	301	CLA	C3B-C4B-NB	-2.17	108.50	110.52
82	EJ	203	PEB	C4C-C3C-C2C	-2.17	105.49	107.50
82	wC	201	PEB	C4C-C3C-C2C	-2.17	105.49	107.50
84	Q3	1001	CYC	CHD-C1D-C2D	2.17	132.83	127.49
84	n3	1001	CYC	CHD-C1D-C2D	2.17	132.83	127.49
82	WH	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
85	C6	508	BCR	C23-C22-C21	-2.17	115.61	118.94
87	cL	511	CLA	O2D-CGD-CBD	2.17	115.13	111.27
82	V1	202	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
87	4N	608	CLA	C3C-C4C-NC	-2.17	108.13	110.57
82	B9	202	PEB	CAB-CBB-CGB	-2.17	108.92	113.60
82	WF	202	PEB	C1C-CHB-C4B	2.17	133.16	128.28
87	B2	804	CLA	C2A-C1A-CHA	2.17	127.66	123.86
82	A9	202	PEB	C3B-C4B-NB	2.17	113.21	110.05
87	FN	205	CLA	CHA-C4D-ND	2.17	137.05	132.50
82	AJ	302	PEB	CHB-C4B-NB	-2.17	120.05	124.58
83	NQ	201	PUB	CAC-C2C-C1C	2.17	128.85	125.01
82	CP	201	PEB	CAC-CBC-CGC	-2.17	108.93	113.60
87	3N	308	CLA	CHA-C1A-NA	-2.17	121.42	126.40
84	LO	1001	CYC	O2A-CGA-CBA	2.17	121.01	114.03
87	nL	101	CLA	CHC-C1C-NC	2.17	127.50	124.20
82	W5	201	PEB	OD-C4D-C3D	-2.17	124.54	129.46
82	aK	203	PEB	OD-C4D-ND	-2.17	122.71	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DK	202	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	D9	203	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	lO	202	PEB	CBA-CAA-C3A	-2.17	108.63	113.47
82	NJ	201	PEB	CMC-C3C-C2C	-2.17	120.91	125.61
84	G3	1001	CYC	C1B-NB-C4B	-2.17	107.90	110.67
82	UG	201	PEB	CAB-CBB-CGB	-2.17	108.93	113.60
82	GE	1002	PEB	C1D-CHC-C4C	2.17	116.46	113.26
82	IB	201	PEB	CHB-C1C-C2C	-2.17	122.25	127.15
82	DQ	202	PEB	C2A-C1A-NA	2.17	110.15	108.27
82	DQ	202	PEB	CMD-C2D-C3D	2.17	133.13	130.06
82	IQ	201	PEB	CAC-CBC-CGC	-2.17	108.93	113.60
82	gO	201	PEB	CAB-CBB-CGB	-2.17	108.93	113.60
92	JL	103	LMG	C7-O1-C1	-2.17	109.50	113.74
82	OF	203	PEB	CHB-C4B-C3B	-2.17	120.29	125.32
84	NE	201	CYC	C4D-ND-C1D	-2.17	105.91	109.79
82	cM	202	PEB	CAA-C3A-C4A	2.17	118.25	112.67
82	b4	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
87	72	607	CLA	O2D-CGD-CBD	2.17	115.13	111.27
95	lL	101	DGD	O1G-C1A-O1A	-2.17	118.11	123.59
82	PI	202	PEB	CHB-C4B-NB	-2.17	120.06	124.58
84	k3	1001	CYC	CHD-C1D-C2D	2.17	132.82	127.49
82	CJ	201	PEB	CAA-C3A-C2A	-2.17	108.83	114.26
87	7N	604	CLA	C2A-C1A-CHA	2.17	127.66	123.86
84	IE	1001	CYC	CMC-C2C-C1C	-2.17	107.72	112.40
82	XK	201	PEB	C1B-C2B-C3B	-2.17	104.01	106.51
82	dE	201	PEB	C1C-CHB-C4B	-2.17	123.41	128.28
82	dD	401	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
87	A2	827	CLA	CHD-C1D-ND	-2.17	122.46	124.45
82	XP	201	PEB	C2B-C1B-NB	2.17	115.16	110.53
87	2N	303	CLA	C3A-C2A-C1A	2.17	104.59	101.34
82	jJ	202	PEB	CHB-C1C-NC	-2.17	120.34	125.32
87	42	601	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
87	82	307	CLA	CHB-C1B-NB	2.17	126.56	124.26
87	c6	606	CLA	CHB-C1B-NB	2.17	126.56	124.26
82	S7	201	PEB	CHA-C4A-NA	2.17	127.79	125.20
82	sF	202	PEB	CHB-C1C-C2C	-2.17	122.25	127.15
87	BN	827	CLA	CHB-C1B-C2B	-2.17	121.10	127.24
84	KG	202	CYC	C4D-ND-C1D	-2.17	105.92	109.79
87	6N	607	CLA	C2D-C1D-ND	-2.17	108.50	110.10
82	K9	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
82	T9	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
82	CJ	201	PEB	C3C-C4C-NC	2.17	110.29	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QK	202	PEB	C3C-C4C-NC	2.17	110.29	108.33
95	L6	102	DGD	C3G-C2G-C1G	-2.17	106.65	111.79
82	SH	203	PEB	CHA-C1B-NB	-2.17	120.39	124.93
82	k1	202	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
87	A2	829	CLA	C2A-C1A-CHA	2.17	127.66	123.86
82	JA	203	PEB	CHB-C1C-NC	-2.17	120.35	125.32
82	GJ	201	PEB	CHC-C1D-ND	-2.17	110.98	113.72
82	GK	202	PEB	CHA-C4A-NA	-2.17	122.62	125.20
82	OJ	203	PEB	CAC-C2C-C1C	2.17	129.22	125.76
82	R1	201	PEB	CAC-C2C-C1C	2.17	129.22	125.76
82	Y5	202	PEB	C1C-CHB-C4B	2.17	133.15	128.28
84	EH	1001	CYC	CMC-C2C-C1C	-2.17	107.72	112.40
84	j3	1001	CYC	C1B-NB-C4B	-2.17	107.91	110.67
91	dL	403	PHO	O1D-CGD-CBD	-2.17	121.12	124.74
96	v6	201	HEM	CHA-C4D-C3D	-2.17	121.25	125.33
84	BE	1002	CYC	OB-C4B-NB	-2.17	120.03	125.08
82	UJ	201	PEB	CAA-C3A-C4A	-2.17	107.10	112.67
82	gJ	201	PEB	C1B-C2B-C3B	-2.17	104.02	106.51
87	A2	822	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
82	PB	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
87	RN	201	CLA	CHA-C1A-NA	-2.17	121.43	126.40
84	S3	1001	CYC	CHD-C1D-C2D	2.17	132.82	127.49
82	TM	202	PEB	C3C-C4C-NC	2.17	110.29	108.33
82	c1	201	PEB	C3C-C4C-NC	2.17	110.29	108.33
87	A2	827	CLA	CAA-CBA-CGA	-2.17	106.91	113.25
84	J1	1001	CYC	CBB-CAB-C3B	-2.17	106.45	112.43
82	TB	202	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
87	a6	607	CLA	CHB-C1B-NB	2.17	126.55	124.26
84	IO	1001	CYC	CHA-C1A-C2A	-2.17	120.30	125.32
91	a6	613	PHO	O2D-CGD-O1D	-2.17	119.60	123.84
87	B2	827	CLA	CHB-C1B-C2B	-2.17	121.11	127.24
82	l4	202	PEB	C3B-C4B-NB	2.17	113.20	110.05
82	P7	201	PEB	CAC-C2C-C1C	2.17	129.22	125.76
92	j6	101	LMG	O7-C10-O9	-2.17	118.46	123.70
82	e4	202	PEB	C1C-NC-C4C	-2.17	105.74	109.60
82	DI	201	PEB	C1B-C2B-C3B	-2.17	104.02	106.51
82	eF	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
84	C1	1001	CYC	C1A-C2A-C3A	-2.17	104.38	106.78
87	b6	613	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
87	C6	519	CLA	C1-C2-C3	-2.17	122.29	126.04
87	b6	616	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
96	f6	101	HEM	CHA-C4D-C3D	-2.17	121.25	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	MF	201	PEB	CHB-C4B-C3B	-2.17	120.30	125.32
82	rK	202	PEB	C2A-C1A-NA	2.17	110.14	108.27
82	UE	203	PEB	OD-C4D-C3D	-2.17	124.55	129.46
82	RB	202	PEB	CHA-C1B-NB	-2.17	120.40	124.93
82	OP	203	PEB	C2B-C1B-NB	2.17	115.16	110.53
82	fG	203	PEB	OD-C4D-ND	-2.17	122.72	125.93
95	AL	416	DGD	O2G-C1B-O1B	-2.17	118.46	123.70
84	p3	1001	CYC	C1B-NB-C4B	-2.17	107.91	110.67
82	AD	301	PEB	CMB-C2B-C1B	2.17	128.40	125.06
82	PQ	201	PEB	CHB-C4B-C3B	-2.17	120.30	125.32
83	AM	303	PUB	CAB-C3B-C4B	2.17	129.22	125.76
82	D7	202	PEB	CAB-C3B-C4B	2.17	128.84	125.01
87	4N	610	CLA	CHA-C1A-NA	-2.17	121.43	126.40
82	UG	203	PEB	C1D-CHC-C4C	-2.17	110.06	113.26
82	FH	1002	PEB	C1D-CHC-C4C	-2.17	110.06	113.26
87	62	303	CLA	CHB-C1B-NB	2.17	126.55	124.26
85	c6	603	BCR	C19-C18-C17	2.17	122.27	118.94
82	O1	201	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	vF	201	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
84	L1	1001	CYC	CAA-CBA-CGA	2.17	118.27	113.60
82	kH	202	PEB	OD-C4D-C3D	-2.17	124.55	129.46
82	VO	202	PEB	CHB-C1C-NC	2.17	130.29	125.32
82	gB	202	PEB	CHC-C1D-ND	-2.17	110.98	113.72
84	LE	1001	CYC	C4D-ND-C1D	-2.17	105.92	109.79
82	y8	202	PEB	OD-C4D-C3D	-2.17	124.55	129.46
82	QF	201	PEB	CMB-C2B-C3B	-2.17	120.23	126.12
82	jJ	202	PEB	CAC-C2C-C1C	2.17	129.22	125.76
82	JF	201	PEB	C3B-C4B-NB	2.17	113.20	110.05
84	e3	1001	CYC	C1B-NB-C4B	-2.17	107.91	110.67
87	c6	609	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
82	B5	203	PEB	C1D-CHC-C4C	-2.17	110.06	113.26
82	aJ	203	PEB	CHA-C1B-NB	-2.17	120.40	124.93
82	AH	301	PEB	CHC-C4C-NC	2.17	124.08	121.15
82	eF	202	PEB	CHC-C4C-NC	2.17	124.08	121.15
82	FQ	202	PEB	CBA-CAA-C3A	-2.17	108.64	113.47
82	WD	202	PEB	CAC-CBC-CGC	-2.17	108.94	113.60
82	M9	304	PEB	C3C-C4C-NC	2.17	110.28	108.33
82	RD	203	PEB	OD-C4D-ND	-2.17	122.72	125.93
82	s8	203	PEB	CHC-C1D-ND	-2.17	110.98	113.72
84	I3	1001	CYC	CHD-C1D-C2D	2.17	132.81	127.49
82	MP	201	PEB	CAC-C2C-C1C	2.17	129.21	125.76
82	YA	303	PEB	CHB-C4B-C3B	2.17	130.33	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TA	201	PEB	C3B-C4B-NB	2.17	113.20	110.05
82	hJ	203	PEB	CHA-C4A-NA	-2.17	122.63	125.20
82	PQ	203	PEB	OD-C4D-C3D	-2.17	124.55	129.46
82	d1	202	PEB	OD-C4D-C3D	-2.17	124.55	129.46
82	JI	202	PEB	CAC-CBC-CGC	-2.17	108.94	113.60
82	HM	202	PEB	O2B-CGB-CBB	2.17	120.99	114.03
85	c6	617	BCR	C1-C6-C5	-2.17	119.56	122.61
82	RP	202	PEB	CAB-C3B-C4B	2.17	128.84	125.01
82	m1	201	PEB	CAB-C3B-C4B	2.17	128.84	125.01
82	G9	201	PEB	CAB-C3B-C4B	2.17	128.84	125.01
87	CL	503	CLA	CHA-C1A-NA	-2.17	121.44	126.40
87	c6	613	CLA	C2D-C1D-ND	-2.17	108.51	110.10
94	A6	410	PL9	C25-C24-C23	-2.17	118.12	123.68
96	f6	101	HEM	C4C-NC-C1C	2.17	107.47	105.35
87	AN	834	CLA	CHB-C1B-NB	2.17	126.55	124.26
82	qK	201	PEB	C3B-C4B-NB	2.17	113.20	110.05
82	RD	203	PEB	CAA-C3A-C4A	-2.17	107.11	112.67
82	eK	202	PEB	CMB-C2B-C3B	-2.17	120.23	126.12
82	QM	204	PEB	CHA-C1B-NB	-2.17	120.40	124.93
82	l4	202	PEB	CBA-CAA-C3A	-2.17	108.64	113.47
82	RP	201	PEB	CAB-C3B-C4B	2.17	128.84	125.01
82	hJ	202	PEB	CHB-C1C-C2C	-2.17	122.26	127.15
82	JA	203	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	NB	201	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	AF	202	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	D5	201	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	DE	1002	PEB	CAA-C3A-C2A	-2.17	108.85	114.26
85	BN	841	BCR	C39-C30-C25	-2.17	106.78	110.30
84	u3	1001	CYC	CHD-C1D-C2D	2.17	132.81	127.49
82	VP	202	PEB	CAB-CBB-CGB	-2.17	108.94	113.60
82	BK	201	PEB	O2B-CGB-CBB	2.17	120.99	114.03
87	K2	106	CLA	C2A-C1A-CHA	2.17	127.65	123.86
82	aB	202	PEB	CHA-C1B-NB	-2.17	120.40	124.93
82	dD	401	PEB	CMA-C2A-C1A	-2.17	107.73	112.40
85	L2	205	BCR	C23-C24-C25	-2.17	121.12	127.20
87	CL	513	CLA	C3C-C4C-NC	-2.17	108.14	110.57
87	b6	610	CLA	CHB-C4A-NA	2.17	127.51	124.51
84	v3	1001	CYC	C1B-NB-C4B	-2.17	107.91	110.67
87	bL	613	CLA	C2A-C1A-CHA	2.17	127.65	123.86
82	PH	202	PEB	C2A-C1A-NA	2.17	110.14	108.27
82	NI	201	PEB	C2A-C1A-NA	2.17	110.14	108.27
82	hK	202	PEB	CHB-C1C-C2C	-2.17	122.26	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	HO	1001	CYC	C1B-CHB-C4A	-2.17	122.79	128.08
82	KQ	202	PEB	CHB-C1C-NC	-2.17	120.36	125.32
82	I7	202	PEB	C3C-C4C-NC	2.17	110.28	108.33
82	OJ	201	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	R1	202	PEB	C4C-C3C-C2C	-2.17	105.50	107.50
82	gO	202	PEB	C1C-NC-C4C	-2.17	105.74	109.60
82	PA	202	PEB	CMC-C3C-C4C	2.17	129.36	127.06
96	vL	201	HEM	C4C-CHD-C1D	-2.17	121.39	126.06
82	SO	201	PEB	CAB-C3B-C4B	2.17	128.84	125.01
82	zK	501	PEB	CAB-C3B-C4B	2.17	128.84	125.01
82	YF	203	PEB	CAC-CBC-CGC	-2.17	108.94	113.60
82	kJ	202	PEB	CHB-C4B-NB	-2.17	120.07	124.58
83	xK	301	PUB	CHB-C1C-NC	-2.17	120.07	124.58
87	RN	201	CLA	O2A-CGA-O1A	-2.17	117.90	123.30
82	PE	202	PEB	CAA-C3A-C4A	-2.17	107.11	112.67
82	iG	202	PEB	CHB-C1C-NC	-2.17	120.36	125.32
87	42	608	CLA	C2A-C1A-CHA	2.17	127.64	123.86
84	q3	1001	CYC	CHD-C1D-C2D	2.17	132.81	127.49
82	QK	201	PEB	OD-C4D-C3D	-2.17	124.56	129.46
87	42	607	CLA	C3A-C2A-C1A	2.17	104.58	101.34
87	AN	827	CLA	CAA-CBA-CGA	-2.17	106.93	113.25
91	D6	404	PHO	O1D-CGD-CBD	-2.17	121.13	124.74
84	T3	1001	CYC	C1B-NB-C4B	-2.17	107.91	110.67
87	C6	516	CLA	CHB-C1B-NB	2.17	126.55	124.26
82	OJ	202	PEB	CMB-C2B-C1B	2.16	128.40	125.06
87	A2	852	CLA	CHA-C1A-NA	-2.16	121.44	126.40
82	cB	403	PEB	CBC-CAC-C2C	2.16	118.64	112.63
82	wF	303	PEB	CHA-C4A-NA	2.16	127.78	125.20
82	S9	203	PEB	C1C-CHB-C4B	-2.16	123.43	128.28
82	RP	202	PEB	CHB-C1C-C2C	-2.16	122.27	127.15
82	YM	202	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
87	7N	610	CLA	C2A-C1A-CHA	2.16	127.64	123.86
82	NK	202	PEB	C2A-C1A-NA	2.16	110.14	108.27
82	kM	202	PEB	CAA-C3A-C2A	-2.16	108.85	114.26
87	7N	607	CLA	C3B-C4B-NB	-2.16	108.51	110.52
82	VJ	202	PEB	C3C-C4C-NC	2.16	110.28	108.33
82	KI	203	PEB	CHB-C4B-NB	-2.16	120.07	124.58
82	aO	202	PEB	CHB-C4B-NB	-2.16	120.07	124.58
83	xK	301	PUB	CBD-CAD-C3D	-2.16	106.46	112.43
85	FN	204	BCR	C15-C14-C13	-2.16	124.22	127.31
82	O9	201	PEB	C4C-C3C-C2C	-2.16	105.50	107.50
84	LG	1001	CYC	CHB-C1B-NB	-2.16	121.41	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	W3	1001	CYC	C2A-C1A-NA	2.16	113.20	110.05
82	MP	202	PEB	CAB-CBB-CGB	-2.16	108.95	113.60
87	R2	202	CLA	C2A-C1A-CHA	2.16	127.64	123.86
82	fM	203	PEB	C2B-C1B-NB	2.16	115.15	110.53
82	a4	202	PEB	CHB-C1C-NC	2.16	130.28	125.32
82	UA	202	PEB	CHA-C1B-NB	-2.16	120.41	124.93
82	MF	201	PEB	CHA-C1B-NB	-2.16	120.41	124.93
87	AN	808	CLA	C16-C15-C13	-2.16	108.92	115.92
87	AN	819	CLA	C2C-C1C-NC	-2.16	107.94	109.97
82	tF	201	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
82	Y7	301	PEB	OD-C4D-ND	-2.16	122.72	125.93
87	32	307	CLA	CHA-C1A-NA	-2.16	121.44	126.40
82	JJ	201	PEB	C1C-CHB-C4B	-2.16	123.43	128.28
84	R3	1001	CYC	C1B-NB-C4B	-2.16	107.91	110.67
84	c3	1001	CYC	C1B-NB-C4B	-2.16	107.91	110.67
87	12	607	CLA	C2A-C1A-CHA	2.16	127.64	123.86
82	hG	203	PEB	OD-C4D-C3D	-2.16	124.56	129.46
82	PJ	202	PEB	C2A-C1A-NA	2.16	110.14	108.27
82	JB	202	PEB	C4C-C3C-C2C	-2.16	105.50	107.50
82	j4	202	PEB	C4C-C3C-C2C	-2.16	105.50	107.50
82	L9	202	PEB	C4C-C3C-C2C	-2.16	105.50	107.50
82	gG	202	PEB	C4C-C3C-C2C	-2.16	105.50	107.50
82	dO	202	PEB	C4C-C3C-C2C	-2.16	105.50	107.50
87	K6	101	CLA	CHD-C1D-ND	-2.16	122.47	124.45
85	BN	843	BCR	C11-C12-C13	-2.16	120.34	126.42
82	gJ	201	PEB	CAC-C2C-C1C	2.16	129.21	125.76
82	FP	202	PEB	CAC-CBC-CGC	-2.16	108.95	113.60
87	AN	834	CLA	CHC-C4B-NB	2.16	126.55	124.26
87	8N	307	CLA	CHB-C1B-NB	2.16	126.55	124.26
82	QE	202	PEB	C4B-C3B-C2B	-2.16	104.39	106.78
82	L5	203	PEB	OD-C4D-ND	-2.16	122.73	125.93
82	UI	201	PEB	CAA-C3A-C2A	-2.16	108.86	114.26
82	QB	204	PEB	CHA-C1B-NB	-2.16	120.41	124.93
87	2N	301	CLA	CMA-C3A-C2A	-2.16	105.10	113.83
83	AM	304	PUB	CMD-C2D-C3D	2.16	131.01	127.77
84	L4	1001	CYC	O2A-CGA-CBA	2.16	120.98	114.03
82	VH	202	PEB	CAC-C2C-C1C	2.16	129.21	125.76
82	KM	202	PEB	CHB-C1C-NC	-2.16	120.37	125.32
82	YD	202	PEB	C2B-C1B-NB	2.16	115.14	110.53
82	DG	1002	PEB	CAA-C3A-C2A	-2.16	108.86	114.26
84	O3	1001	CYC	CHD-C1D-C2D	2.16	132.80	127.49
92	m6	101	LMG	O8-C28-O10	-2.16	118.14	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hE	202	PEB	C3C-C4C-NC	2.16	110.28	108.33
82	AM	301	PEB	CAC-CBC-CGC	-2.16	108.95	113.60
82	VB	201	PEB	C1C-CHB-C4B	2.16	133.13	128.28
87	8N	302	CLA	C1D-ND-C4D	-2.16	104.80	106.33
87	c6	609	CLA	CHD-C1D-ND	-2.16	122.47	124.45
82	S7	202	PEB	CHB-C1C-C2C	-2.16	122.27	127.15
94	D6	408	PL9	C12-C13-C14	-2.16	122.45	127.66
82	PG	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
82	UD	202	PEB	CAC-C2C-C1C	2.16	129.21	125.76
84	GE	1001	CYC	CHA-C1A-C2A	-2.16	120.32	125.32
82	KP	202	PEB	C4B-NB-C1B	-2.16	102.44	106.51
82	TE	201	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
87	RN	202	CLA	C2A-C1A-CHA	2.16	127.64	123.86
84	BG	1002	CYC	OB-C4B-NB	-2.16	120.05	125.08
82	TH	202	PEB	CAB-CBB-CGB	-2.16	108.95	113.60
82	DK	203	PEB	CAC-CBC-CGC	-2.16	108.95	113.60
82	kO	202	PEB	CAC-CBC-CGC	-2.16	108.95	113.60
82	J9	201	PEB	CAA-C3A-C2A	-2.16	108.86	114.26
82	FP	202	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
82	A9	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
82	eG	203	PEB	CAB-C3B-C4B	2.16	128.83	125.01
87	A2	827	CLA	CMB-C2B-C3B	2.16	131.82	126.59
82	KD	201	PEB	CHA-C1B-NB	-2.16	120.41	124.93
82	HO	1002	PEB	CHA-C1B-NB	-2.16	120.41	124.93
82	CJ	203	PEB	CAA-C3A-C4A	-2.16	107.12	112.67
82	WJ	202	PEB	CAC-C2C-C1C	2.16	129.20	125.76
82	OK	202	PEB	CAC-C2C-C3C	2.16	132.02	127.07
82	TQ	202	PEB	C1C-CHB-C4B	2.16	133.13	128.28
82	YH	202	PEB	CAC-CBC-CGC	-2.16	108.95	113.60
82	R1	201	PEB	CHB-C1C-NC	-2.16	120.37	125.32
82	f1	202	PEB	CHB-C1C-NC	-2.16	120.37	125.32
87	42	604	CLA	CHB-C1B-NB	2.16	126.55	124.26
87	B6	603	CLA	CHB-C1B-NB	2.16	126.55	124.26
87	c6	610	CLA	CHB-C1B-NB	2.16	126.55	124.26
82	B9	203	PEB	C4C-C3C-C2C	-2.16	105.51	107.50
82	iO	202	PEB	C4C-C3C-C2C	-2.16	105.51	107.50
83	AJ	303	PUB	CMC-C3C-C4C	2.16	132.85	126.37
82	PD	203	PEB	OD-C4D-C3D	-2.16	124.56	129.46
82	YP	502	PEB	CAC-C2C-C1C	2.16	129.20	125.76
82	O9	201	PEB	CAC-C2C-C1C	2.16	129.20	125.76
98	B2	837	PQN	C5-C4-C3	2.16	122.38	118.42
82	UJ	202	PEB	CAC-C2C-C3C	2.16	132.02	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W1	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
85	bL	603	BCR	C21-C20-C19	-2.16	116.47	123.22
82	DD	202	PEB	CHB-C1C-NC	2.16	130.27	125.32
82	AO	304	PEB	CHB-C1C-NC	-2.16	120.37	125.32
83	AH	303	PUB	CAC-C2C-C1C	2.16	128.83	125.01
87	6N	608	CLA	CHA-C4D-ND	2.16	137.02	132.50
87	4N	603	CLA	C2D-C1D-ND	-2.16	108.51	110.10
87	B2	823	CLA	O1D-CGD-CBD	2.16	128.90	124.48
87	4N	601	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
87	a6	608	CLA	CHD-C1D-ND	-2.16	122.47	124.45
82	h1	202	PEB	C3C-C4C-NC	2.16	110.28	108.33
82	VF	202	PEB	CHB-C1C-NC	-2.16	120.37	125.32
82	M5	301	PEB	CHB-C1C-NC	-2.16	120.37	125.32
82	R9	202	PEB	C3B-C4B-NB	2.16	113.19	110.05
84	CH	1001	CYC	CHD-C1D-C2D	2.16	132.79	127.49
82	MD	202	PEB	CAB-CBB-CGB	-2.16	108.95	113.60
82	M9	301	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
87	BN	821	CLA	O2D-CGD-CBD	2.16	115.11	111.27
82	L4	1002	PEB	CHA-C4A-NA	2.16	127.77	125.20
82	FD	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
82	aJ	202	PEB	CAA-C3A-C2A	-2.16	108.86	114.26
82	EM	203	PEB	OD-C4D-ND	-2.16	122.73	125.93
87	BN	805	CLA	CMD-C2D-C3D	2.16	132.58	127.61
87	B6	610	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
82	WQ	202	PEB	CAC-CBC-CGC	-2.16	108.96	113.60
87	L2	204	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
82	U7	202	PEB	C2B-C1B-NB	2.16	115.14	110.53
87	82	306	CLA	C3A-C2A-C1A	2.16	104.57	101.34
82	TO	203	PEB	CMB-C2B-C1B	2.16	128.39	125.06
87	BL	605	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
82	YD	201	PEB	OD-C4D-ND	-2.16	122.73	125.93
87	62	308	CLA	C2D-C1D-ND	-2.16	108.51	110.10
82	kH	202	PEB	CHB-C4B-C3B	-2.16	120.32	125.32
82	OI	202	PEB	C3C-C4C-NC	2.16	110.28	108.33
82	NA	201	PEB	CAC-C2C-C1C	2.16	129.20	125.76
82	UD	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
82	DF	203	PEB	CAB-C3B-C4B	2.16	128.83	125.01
85	B2	843	BCR	C11-C12-C13	-2.16	120.35	126.42
82	Y1	202	PEB	CAC-CBC-CGC	-2.16	108.96	113.60
87	22	602	CLA	C3A-C2A-C1A	2.16	104.57	101.34
88	C6	505	LHG	C5-O7-C7	-2.16	112.48	117.79
85	AN	847	BCR	C40-C30-C25	-2.16	106.80	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	72	605	CLA	C2A-C1A-CHA	2.16	127.63	123.86
82	BK	202	PEB	C2B-C1B-NB	2.16	115.14	110.53
82	Q5	203	PEB	OA-C1A-C2A	-2.16	124.46	126.17
82	W7	202	PEB	OD-C4D-C3D	-2.16	124.57	129.46
87	cL	510	CLA	CHC-C1C-NC	2.16	127.48	124.20
82	MJ	202	PEB	C1D-CHC-C4C	-2.16	110.07	113.26
82	RA	201	PEB	CMC-C3C-C4C	2.16	129.35	127.06
82	RH	202	PEB	C4C-C3C-C2C	-2.16	105.51	107.50
82	EP	201	PEB	C4C-C3C-C2C	-2.16	105.51	107.50
82	m1	202	PEB	C4C-C3C-C2C	-2.16	105.51	107.50
82	W9	202	PEB	C3B-C4B-NB	2.16	113.19	110.05
87	62	303	CLA	C2A-C1A-CHA	2.16	127.63	123.86
82	A1	301	PEB	CHC-C4C-NC	2.16	124.07	121.15
82	VJ	202	PEB	CAA-C3A-C2A	-2.16	108.87	114.26
82	EQ	202	PEB	OD-C4D-C3D	-2.16	124.57	129.46
82	iK	202	PEB	OD-C4D-C3D	-2.16	124.57	129.46
82	QO	201	PEB	C1C-NC-C4C	-2.16	105.76	109.60
82	dM	202	PEB	CHA-C1B-NB	-2.16	120.42	124.93
82	U1	201	PEB	CAC-C2C-C1C	2.16	129.20	125.76
84	w3	1001	CYC	CHD-C1D-C2D	2.16	132.79	127.49
82	wK	301	PEB	C2B-C1B-NB	2.16	115.13	110.53
82	YJ	203	PEB	CBC-CAC-C2C	-2.16	106.63	112.63
82	AE	301	PEB	CHA-C4A-NA	-2.16	122.64	125.20
82	OK	203	PEB	CHB-C4B-C3B	-2.16	120.33	125.32
84	t3	1001	CYC	C1B-NB-C4B	-2.16	107.92	110.67
82	MQ	202	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
82	a4	201	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
82	Z1	201	PEB	C1C-NC-C4C	-2.16	105.76	109.60
96	vL	201	HEM	C4D-ND-C1D	2.16	107.30	105.07
82	kJ	202	PEB	O2B-CGB-CBB	2.16	120.96	114.03
87	42	608	CLA	C3C-C4C-NC	-2.16	108.15	110.57
82	OQ	201	PEB	OD-C4D-ND	-2.16	122.73	125.93
82	kM	202	PEB	C4C-C3C-C2C	-2.16	105.51	107.50
82	UG	203	PEB	C1C-CHB-C4B	-2.16	123.44	128.28
82	CF	202	PEB	C1C-CHB-C4B	2.16	133.12	128.28
82	YG	202	PEB	CHB-C1C-C2C	-2.16	122.28	127.15
84	L3	1001	CYC	CAB-C3B-C2B	2.16	131.22	127.53
82	J9	201	PEB	O1B-CGB-CBB	-2.16	116.15	123.08
82	lM	202	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
82	QF	203	PEB	CHC-C1D-ND	-2.16	111.00	113.72
82	TQ	201	PEB	C3B-C4B-NB	2.16	113.19	110.05
82	aB	202	PEB	CHA-C4A-NA	-2.16	122.64	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	OK	201	PEB	C2B-C1B-NB	2.16	115.13	110.53
84	d3	1001	CYC	C1B-NB-C4B	-2.16	107.92	110.67
82	tF	202	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
82	tK	202	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
84	L3	1001	CYC	CHD-C1D-C2D	2.16	132.78	127.49
84	73	1001	CYC	CHD-C1D-C2D	2.16	132.78	127.49
84	I3	1001	CYC	CAB-C3B-C2B	2.16	131.22	127.53
82	UB	301	PEB	CAC-CBC-CGC	-2.16	108.96	113.60
82	T7	202	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
83	AD	302	PUB	C1D-CHC-C4C	-2.16	108.68	113.37
84	I1	1001	CYC	CAC-C3C-C2C	2.16	119.65	114.26
82	HF	202	PEB	C4B-NB-C1B	-2.16	102.45	106.51
82	BF	202	PEB	C2B-C1B-NB	2.16	115.13	110.53
82	AJ	301	PEB	C2B-C1B-NB	2.16	115.13	110.53
82	OQ	201	PEB	C2B-C1B-NB	2.16	115.13	110.53
82	Q4	201	PEB	C1C-NC-C4C	-2.16	105.76	109.60
85	b6	601	BCR	C37-C22-C21	-2.16	119.90	122.92
82	FP	201	PEB	CHC-C1D-ND	-2.16	111.00	113.72
87	8N	302	CLA	CHA-C1A-NA	-2.16	121.46	126.40
82	MB	202	PEB	CAC-CBC-CGC	-2.16	108.96	113.60
82	UH	201	PEB	CAC-C2C-C1C	2.16	129.19	125.76
82	V1	203	PEB	CAC-C2C-C1C	2.16	129.19	125.76
82	JB	201	PEB	OA-C1A-C2A	-2.16	124.46	126.17
82	SA	201	PEB	CHA-C4A-NA	2.16	127.77	125.20
87	42	602	CLA	CHB-C1B-NB	2.16	126.54	124.26
82	BM	301	PEB	CHC-C4C-NC	2.16	124.07	121.15
82	X7	201	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
82	LK	202	PEB	C2B-C1B-NB	2.16	115.13	110.53
82	KK	203	PEB	CHB-C4B-C3B	-2.16	120.33	125.32
87	BN	805	CLA	C2A-C1A-CHA	2.16	127.63	123.86
85	IN	101	BCR	C36-C18-C19	2.16	121.47	118.08
82	F1	1002	PEB	C1D-CHC-C4C	-2.16	110.08	113.26
83	wK	304	PUB	CAB-C3B-C4B	2.16	129.19	125.76
82	H9	201	PEB	O1B-CGB-CBB	-2.15	116.16	123.08
87	DL	406	CLA	C2A-C1A-CHA	2.15	127.63	123.86
82	i4	202	PEB	OD-C4D-ND	-2.15	122.74	125.93
95	J6	101	DGD	O6D-C5D-C6D	2.15	111.02	106.67
84	LE	1001	CYC	CHB-C1B-NB	-2.15	121.43	126.06
82	W5	202	PEB	CAC-CBC-CGC	-2.15	108.97	113.60
82	DA	202	PEB	CAB-C3B-C4B	2.15	128.82	125.01
83	A4	303	PUB	CAC-C2C-C1C	2.15	128.82	125.01
83	AQ	302	PUB	C1D-CHC-C4C	-2.15	108.68	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	EA	201	PEB	C1C-CHB-C4B	2.15	133.11	128.28
82	gF	201	PEB	OD-C4D-C3D	-2.15	124.58	129.46
82	hF	202	PEB	C1D-CHC-C4C	2.15	116.43	113.26
87	R2	201	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
82	WB	402	PEB	CMC-C3C-C2C	2.15	130.27	125.61
82	H1	1002	PEB	CHB-C4B-NB	-2.15	120.09	124.58
87	22	605	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
82	UF	201	PEB	O2C-CGC-CBC	2.15	120.95	114.03
82	LO	1002	PEB	CHB-C4B-C3B	-2.15	120.33	125.32
82	JM	202	PEB	CAA-C3A-C2A	-2.15	108.88	114.26
84	J3	1001	CYC	C1B-NB-C4B	-2.15	107.93	110.67
84	i3	1001	CYC	C1B-NB-C4B	-2.15	107.93	110.67
82	AJ	301	PEB	CHB-C4B-NB	-2.15	120.09	124.58
84	73	1001	CYC	CAB-C3B-C2B	2.15	131.21	127.53
82	UQ	202	PEB	CAC-C2C-C1C	2.15	129.19	125.76
82	yC	202	PEB	CAC-C2C-C1C	2.15	129.19	125.76
82	P4	201	PEB	CHB-C4B-C3B	-2.15	120.34	125.32
87	6N	606	CLA	C3B-C4B-NB	-2.15	108.52	110.52
82	KE	201	PEB	CAB-C3B-C4B	2.15	128.82	125.01
82	O1	201	PEB	CAB-C3B-C4B	2.15	128.82	125.01
87	c6	611	CLA	CHD-C1D-ND	-2.15	122.47	124.45
82	UQ	201	PEB	CHC-C1D-ND	-2.15	111.00	113.72
82	FK	201	PEB	CAA-C3A-C2A	-2.15	108.88	114.26
84	C3	1001	CYC	C1B-NB-C4B	-2.15	107.93	110.67
84	E3	1001	CYC	C1B-NB-C4B	-2.15	107.93	110.67
84	DG	1001	CYC	C4D-ND-C1D	-2.15	105.95	109.79
84	EH	1001	CYC	C4D-ND-C1D	-2.15	105.95	109.79
82	eA	301	PEB	CAC-C2C-C1C	2.15	129.19	125.76
82	M9	302	PEB	OA-C1A-C2A	-2.15	124.46	126.17
82	XQ	201	PEB	C2B-C1B-NB	2.15	115.12	110.53
82	jG	201	PEB	CAB-C3B-C4B	2.15	128.82	125.01
84	EE	1001	CYC	CMC-C2C-C1C	-2.15	107.76	112.40
87	2N	308	CLA	CHB-C1B-C2B	-2.15	121.16	127.24
84	M3	1001	CYC	CHD-C1D-C2D	2.15	132.78	127.49
82	EI	201	PEB	C2A-C1A-NA	2.15	110.13	108.27
82	WI	201	PEB	CAC-CBC-CGC	-2.15	108.97	113.60
82	iF	203	PEB	CAB-CBB-CGB	-2.15	108.97	113.60
87	72	607	CLA	O1D-CGD-CBD	2.15	128.89	124.48
84	D3	1001	CYC	CAB-C3B-C2B	2.15	131.21	127.53
82	V4	201	PEB	C4C-C3C-C2C	-2.15	105.51	107.50
82	Y9	201	PEB	C4C-C3C-C2C	-2.15	105.51	107.50
82	fO	202	PEB	CBA-CAA-C3A	-2.15	108.67	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KJ	202	PEB	CMC-C3C-C4C	-2.15	124.78	127.06
82	T4	201	PEB	CHA-C4A-NA	2.15	127.76	125.20
82	TG	201	PEB	CMA-C2A-C1A	-2.15	107.76	112.40
95	C6	503	DGD	C1E-C2E-C3E	2.15	114.48	110.00
84	BE	1002	CYC	CMA-C3A-C2A	-2.15	120.28	126.12
82	N7	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
82	gG	201	PEB	CAB-CBB-CGB	-2.15	108.97	113.60
82	CK	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
82	j1	203	PEB	CAB-C3B-C4B	2.15	128.81	125.01
87	LN	202	CLA	CMA-C3A-C4A	2.15	117.56	111.77
84	LO	1001	CYC	C4D-ND-C1D	-2.15	105.95	109.79
82	DF	203	PEB	CAC-CBC-CGC	-2.15	108.97	113.60
82	UG	203	PEB	OD-C4D-C3D	-2.15	124.59	129.46
82	S9	202	PEB	C1C-NC-C4C	-2.15	105.77	109.60
82	WG	201	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	ZM	201	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
92	b6	619	LMG	O7-C10-O9	-2.15	118.50	123.70
82	QM	202	PEB	CHB-C4B-C3B	-2.15	120.34	125.32
82	F4	1002	PEB	CHB-C4B-C3B	-2.15	120.34	125.32
82	mE	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
82	DB	202	PEB	C3C-C4C-NC	2.15	110.27	108.33
82	jH	201	PEB	C3C-C4C-NC	2.15	110.27	108.33
83	ND	201	PUB	CHA-C1B-NB	2.15	124.06	121.15
96	VL	201	HEM	C4A-CHB-C1B	-2.15	121.24	126.34
82	PO	203	PEB	CAB-CBB-CGB	2.15	118.23	113.60
85	KN	101	BCR	C32-C1-C6	-2.15	106.81	110.30
82	V9	202	PEB	C3B-C4B-NB	2.15	113.18	110.05
84	H3	1001	CYC	C1B-NB-C4B	-2.15	107.93	110.67
84	I1	1001	CYC	CHB-C4A-C3A	2.15	130.43	124.90
82	U1	201	PEB	OD-C4D-ND	-2.15	122.74	125.93
82	KD	201	PEB	CAB-C3B-C4B	2.15	128.81	125.01
82	VH	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
87	aL	605	CLA	C11-C12-C13	-2.15	108.97	115.92
82	TO	201	PEB	CHA-C4A-NA	2.15	127.76	125.20
82	qF	201	PEB	C1D-CHC-C4C	-2.15	110.08	113.26
87	82	301	CLA	CHA-C1A-NA	-2.15	121.47	126.40
82	RQ	203	PEB	CAA-C3A-C4A	-2.15	107.15	112.67
82	A7	202	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
84	S3	1001	CYC	CAB-C3B-C2B	2.15	131.21	127.53
84	k3	1001	CYC	CAB-C3B-C2B	2.15	131.21	127.53
87	7N	605	CLA	C2A-C1A-CHA	2.15	127.62	123.86
82	PD	201	PEB	CHB-C4B-C3B	-2.15	120.34	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	VD	201	PEB	CAB-C3B-C4B	2.15	128.81	125.01
103	82	309	ZEX	C39-C29-C30	-2.15	119.91	122.92
87	L2	202	CLA	CMA-C3A-C4A	2.15	117.55	111.77
94	a6	601	PL9	C35-C34-C36	2.15	118.89	115.27
84	L3	1001	CYC	C1B-NB-C4B	-2.15	107.93	110.67
82	ZJ	202	PEB	CAA-C3A-C2A	-2.15	108.89	114.26
82	GK	202	PEB	CHA-C1B-NB	-2.15	120.44	124.93
87	A2	851	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
87	A2	833	CLA	CHC-C4B-NB	2.15	126.53	124.26
87	A2	831	CLA	CMC-C2C-C1C	-2.15	121.77	125.04
82	x8	202	PEB	CHB-C4B-C3B	2.15	130.29	125.32
87	1N	607	CLA	C2A-C1A-CHA	2.15	127.62	123.86
82	LO	1002	PEB	CHA-C4A-NA	2.15	127.76	125.20
87	BL	619	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
84	F3	1001	CYC	CHD-C1D-C2D	2.15	132.77	127.49
82	JI	201	PEB	CAB-CBB-CGB	2.15	118.23	113.60
87	F2	205	CLA	C6-C7-C8	-2.15	108.97	115.92
82	GF	202	PEB	CHA-C1B-NB	-2.15	120.44	124.93
82	P7	202	PEB	CMC-C3C-C4C	2.15	129.34	127.06
82	Q9	202	PEB	CAC-C2C-C1C	2.15	129.19	125.76
82	WB	402	PEB	CAC-C2C-C1C	-2.15	122.34	125.76
84	y3	1001	CYC	C4A-C3A-C2A	-2.15	104.04	106.51
82	OJ	203	PEB	C2B-C1B-NB	2.15	115.12	110.53
87	82	307	CLA	C3B-C4B-NB	-2.15	108.52	110.52
82	rC	201	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	RK	201	PEB	C1C-CHB-C4B	2.15	133.10	128.28
85	CL	501	BCR	C19-C18-C17	-2.15	115.64	118.94
82	IB	203	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
85	B6	601	BCR	C10-C11-C12	-2.15	116.51	123.22
88	m6	102	LHG	C6-C5-C4	-2.15	106.70	111.79
82	QI	201	PEB	CAB-C3B-C4B	2.15	128.81	125.01
82	OF	201	PEB	CHB-C1C-NC	2.15	130.24	125.32
87	8N	308	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
82	W1	202	PEB	CHA-C1B-C2B	2.15	130.43	124.90
84	C1	1001	CYC	CHD-C1D-C2D	2.15	132.76	127.49
82	cH	202	PEB	C3C-C4C-NC	2.15	110.27	108.33
82	ZB	203	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
85	FL	101	BCR	C29-C30-C25	2.15	113.79	110.48
84	U3	1001	CYC	CAB-C3B-C2B	2.15	131.20	127.53
84	f3	1001	CYC	CAB-C3B-C2B	2.15	131.20	127.53
82	ZH	201	PEB	CHB-C4B-NB	2.15	129.05	124.58
82	QG	203	PEB	OD-C4D-C3D	-2.15	124.59	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	dL	405	LHG	C5-O7-C7	-2.15	112.50	117.79
87	AN	810	CLA	CMD-C2D-C1D	-2.15	120.93	124.71
82	SB	201	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	KF	202	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	XK	202	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	RK	202	PEB	OD-C4D-ND	-2.15	122.75	125.93
82	T1	202	PEB	OD-C4D-ND	-2.15	122.75	125.93
82	EP	201	PEB	CHB-C4B-C3B	-2.15	120.35	125.32
87	bL	607	CLA	CHC-C1C-NC	2.15	127.46	124.20
82	UK	202	PEB	CHB-C4B-NB	-2.15	120.11	124.58
82	M7	201	PEB	O1C-CGC-CBC	-2.15	116.18	123.08
87	A2	830	CLA	C2A-C1A-CHA	2.15	127.61	123.86
87	MN	101	CLA	CHB-C1B-NB	2.15	126.53	124.26
82	HQ	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
82	x8	201	PEB	CHC-C1D-ND	-2.15	111.01	113.72
82	ZK	202	PEB	CHB-C1C-NC	-2.15	120.40	125.32
82	JK	201	PEB	C3B-C4B-NB	2.15	113.17	110.05
82	eG	203	PEB	CMC-C3C-C2C	2.15	130.25	125.61
87	72	610	CLA	C2A-C1A-CHA	2.15	127.61	123.86
87	B2	804	CLA	CMD-C2D-C3D	2.15	132.55	127.61
82	GQ	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
85	K2	102	BCR	C32-C1-C6	-2.15	106.82	110.30
87	52	607	CLA	CAA-CBA-CGA	-2.15	106.98	113.25
82	YK	203	PEB	CAC-CBC-CGC	-2.15	108.98	113.60
94	D6	408	PL9	C8-C7-C3	-2.15	105.90	111.98
83	AM	304	PUB	CHB-C4B-NB	-2.15	120.40	125.32
87	72	606	CLA	O2A-CGA-O1A	-2.15	117.95	123.30
91	AL	410	PHO	O2D-CGD-O1D	-2.15	119.64	123.84
82	UO	201	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	qC	202	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	AM	301	PEB	C1C-CHB-C4B	-2.15	123.47	128.28
82	IM	203	PEB	C1C-CHB-C4B	-2.15	123.47	128.28
84	P3	1001	CYC	C1B-NB-C4B	-2.15	107.94	110.67
87	F2	205	CLA	CHA-C4D-ND	2.15	136.99	132.50
82	RQ	201	PEB	C3B-C4B-NB	2.15	113.17	110.05
87	B2	814	CLA	CAA-C2A-C3A	-2.15	108.89	114.26
82	OP	202	PEB	C4B-C3B-C2B	-2.15	104.41	106.78
82	Q9	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
82	jH	203	PEB	CAB-C3B-C4B	2.15	128.81	125.01
82	O1	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
82	IB	202	PEB	C3C-C4C-NC	2.15	110.27	108.33
82	NA	201	PEB	OD-C4D-C3D	-2.15	124.60	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	831	CLA	CMC-C2C-C1C	-2.15	121.77	125.04
87	B2	801	CLA	CMC-C2C-C1C	-2.15	121.77	125.04
82	A4	304	PEB	CHB-C1C-NC	-2.15	120.40	125.32
84	FO	1001	CYC	C1B-CHB-C4A	-2.15	122.84	128.08
82	SK	201	PEB	CAC-CBC-CGC	-2.15	108.98	113.60
82	HO	1002	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
87	b6	614	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
84	O3	1001	CYC	CAB-C3B-C2B	2.15	131.20	127.53
82	D9	203	PEB	OD-C4D-C3D	-2.15	124.60	129.46
82	hF	202	PEB	CHB-C1C-C2C	-2.15	122.31	127.15
82	XM	201	PEB	C1C-CHB-C4B	-2.15	123.47	128.28
82	OH	201	PEB	C1C-CHB-C4B	2.15	133.09	128.28
83	wF	304	PUB	C4B-CHB-C1C	2.15	133.09	128.28
84	LH	1001	CYC	CAC-C3C-C2C	2.15	119.62	114.26
87	A2	815	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
87	RN	204	CLA	O2A-CGA-O1A	-2.15	117.95	123.30
82	S1	202	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	wC	204	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	dE	203	PEB	C4C-C3C-C2C	-2.15	105.52	107.50
82	f4	202	PEB	CBA-CAA-C3A	-2.15	108.69	113.47
82	XA	201	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
87	AN	811	CLA	O2D-CGD-CBD	2.15	115.08	111.27
82	OH	201	PEB	C1D-CHC-C4C	2.15	116.42	113.26
82	RA	203	PEB	CBD-CAD-C3D	-2.15	116.94	127.62
82	R7	203	PEB	CBD-CAD-C3D	-2.15	116.94	127.62
87	1N	611	CLA	C2A-C1A-CHA	2.15	127.61	123.86
82	S1	201	PEB	CAB-C3B-C4B	2.15	128.80	125.01
82	XD	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
82	RQ	201	PEB	CAC-C2C-C1C	2.15	129.18	125.76
87	BN	824	CLA	O1D-CGD-CBD	2.15	128.87	124.48
82	QQ	201	PEB	CAB-CBB-CGB	-2.15	108.99	113.60
84	n3	1001	CYC	C1B-NB-C4B	-2.15	107.94	110.67
82	FJ	201	PEB	CAA-C3A-C4A	-2.15	107.16	112.67
82	gJ	202	PEB	CAA-C3A-C4A	-2.15	107.16	112.67
82	fJ	201	PEB	CHB-C4B-NB	-2.15	120.11	124.58
87	c6	615	CLA	CHB-C1B-NB	2.15	126.53	124.26
82	UP	202	PEB	CHA-C1B-NB	-2.15	120.45	124.93
82	UQ	201	PEB	CAB-C3B-C4B	2.15	128.80	125.01
82	uC	203	PEB	CAB-C3B-C4B	2.15	128.80	125.01
87	8N	301	CLA	C3A-C2A-C1A	2.15	104.55	101.34
82	kH	202	PEB	C1B-C2B-C3B	-2.15	104.05	106.51
83	yF	303	PUB	CAB-CBB-CGB	-2.15	108.99	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bF	201	PEB	OD-C4D-C3D	-2.14	124.60	129.46
82	YE	202	PEB	CHB-C1C-C2C	-2.14	122.31	127.15
82	jF	201	PEB	CHB-C1C-C2C	-2.14	122.31	127.15
82	OJ	201	PEB	C2A-C1A-NA	2.14	110.12	108.27
82	tC	201	PEB	C3B-C4B-NB	2.14	113.17	110.05
85	CL	501	BCR	C16-C17-C18	-2.14	124.25	127.31
82	B5	202	PEB	CMC-C3C-C4C	2.14	129.33	127.06
82	UH	202	PEB	C2B-C1B-NB	2.14	115.11	110.53
82	O1	203	PEB	C1C-NC-C4C	-2.14	105.78	109.60
82	bK	201	PEB	CHA-C4A-NA	2.14	127.75	125.20
85	I2	101	BCR	C36-C18-C19	2.14	121.46	118.08
82	vK	202	PEB	OD-C4D-C3D	-2.14	124.60	129.46
82	SB	202	PEB	C3C-C4C-NC	2.14	110.26	108.33
82	EP	202	PEB	CAC-C2C-C1C	2.14	129.18	125.76
82	TB	201	PEB	OA-C1A-C2A	-2.14	124.47	126.17
82	O1	201	PEB	C1C-CHB-C4B	2.14	133.09	128.28
87	B2	824	CLA	CHC-C4B-NB	2.14	126.53	124.26
87	5N	601	CLA	CHB-C1B-NB	2.14	126.53	124.26
82	T7	203	PEB	CHA-C1B-NB	-2.14	120.45	124.93
82	WA	202	PEB	CBA-CAA-C3A	-2.14	108.69	113.47
82	XD	202	PEB	C3B-C4B-NB	2.14	113.17	110.05
82	aJ	204	PEB	C1C-NC-C4C	-2.14	105.78	109.60
87	BL	604	CLA	CMB-C2B-C3B	2.14	131.78	126.59
82	j1	202	PEB	CAB-C3B-C4B	2.14	128.80	125.01
87	BN	827	CLA	C3B-C4B-NB	-2.14	108.53	110.52
87	72	607	CLA	C3B-C4B-NB	-2.14	108.53	110.52
82	WG	202	PEB	CHB-C1C-C2C	-2.14	122.31	127.15
87	42	606	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
84	g3	1001	CYC	C1B-NB-C4B	-2.14	107.94	110.67
82	CF	203	PEB	CHB-C4B-C3B	-2.14	120.36	125.32
82	WF	202	PEB	C1D-CHC-C4C	-2.14	110.09	113.26
82	O9	202	PEB	CMB-C2B-C1B	2.14	128.37	125.06
87	B2	820	CLA	O2D-CGD-CBD	2.14	115.08	111.27
85	fL	101	BCR	C33-C5-C6	2.14	126.94	124.53
82	XJ	202	PEB	C3C-C4C-NC	2.14	110.26	108.33
82	jF	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
87	AN	813	CLA	CHB-C1B-NB	2.14	126.53	124.26
87	B6	611	CLA	CHB-C1B-NB	2.14	126.53	124.26
82	MQ	201	PEB	C4B-C3B-C2B	-2.14	104.41	106.78
82	sC	203	PEB	CHC-C1D-ND	-2.14	111.01	113.72
82	WK	202	PEB	OD-C4D-C3D	-2.14	124.61	129.46
82	EP	201	PEB	CBB-CAB-C3B	-2.14	106.67	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iE	202	PEB	CHB-C1C-NC	-2.14	120.41	125.32
82	xC	202	PEB	CHB-C4B-C3B	2.14	130.28	125.32
82	mH	201	PEB	CAB-C3B-C4B	2.14	128.80	125.01
82	kE	201	PEB	CMC-C3C-C4C	2.14	129.33	127.06
82	eF	202	PEB	CMB-C2B-C3B	-2.14	120.30	126.12
82	JP	201	PEB	CMA-C2A-C1A	-2.14	107.78	112.40
82	X9	202	PEB	C3B-C4B-NB	2.14	113.17	110.05
94	D6	408	PL9	C11-C12-C13	-2.14	104.84	111.88
82	U4	201	PEB	CMA-C2A-C3A	-2.14	105.19	113.83
82	RH	201	PEB	CHB-C1C-NC	-2.14	120.41	125.32
82	cG	201	PEB	CHB-C4B-C3B	-2.14	120.36	125.32
87	b6	609	CLA	CMB-C2B-C3B	2.14	131.78	126.59
82	RG	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
82	SP	202	PEB	C2B-C1B-NB	2.14	115.10	110.53
82	a1	202	PEB	CHA-C1B-C2B	2.14	130.41	124.90
84	A3	1001	CYC	C1B-NB-C4B	-2.14	107.94	110.67
82	bF	202	PEB	CHC-C4C-NC	-2.14	118.25	121.15
87	4N	604	CLA	CAA-C2A-C1A	2.14	116.88	112.14
87	R2	204	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
87	dL	402	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
82	OG	203	PEB	C2B-C1B-NB	2.14	115.10	110.53
82	JM	201	PEB	CMC-C3C-C4C	2.14	129.33	127.06
82	P4	201	PEB	CMA-C2A-C1A	-2.14	107.79	112.40
82	PG	202	PEB	CBC-CAC-C2C	2.14	118.58	112.63
87	12	607	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
82	M9	301	PEB	CAB-CBB-CGB	2.14	118.21	113.60
87	A2	836	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
85	F2	204	BCR	C28-C27-C26	-2.14	110.25	114.08
98	BN	837	PQN	C5-C4-C3	2.14	122.35	118.42
82	P7	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
82	vF	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
82	lK	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
84	q3	1001	CYC	C1B-NB-C4B	-2.14	107.94	110.67
82	UA	202	PEB	C2B-C1B-NB	2.14	115.10	110.53
82	wF	301	PEB	C2B-C1B-NB	2.14	115.10	110.53
87	C6	519	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
82	F5	202	PEB	CHB-C4B-C3B	-2.14	120.36	125.32
82	gK	203	PEB	CAB-C3B-C4B	2.14	128.80	125.01
82	YQ	202	PEB	C3C-C4C-NC	2.14	110.26	108.33
82	m4	201	PEB	C1D-CHC-C4C	-2.14	110.10	113.26
85	k6	102	BCR	C1-C6-C5	-2.14	119.60	122.61
82	HE	1002	PEB	CHB-C1C-C2C	-2.14	122.32	127.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hE	201	PEB	CHA-C1B-NB	-2.14	120.45	124.93
84	D4	1001	CYC	CHA-C1A-C2A	-2.14	120.37	125.32
82	AQ	303	PEB	CAA-C3A-C4A	2.14	118.17	112.67
84	F3	1001	CYC	C1B-NB-C4B	-2.14	107.94	110.67
82	I5	201	PEB	CAC-C2C-C1C	2.14	129.17	125.76
82	PE	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51
82	PG	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51
87	H6	103	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
87	AN	832	CLA	CHB-C1B-NB	2.14	126.52	124.26
87	7N	606	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
87	DL	403	CLA	CHD-C1D-ND	-2.14	122.49	124.45
82	Z1	201	PEB	CHB-C4B-NB	2.14	129.03	124.58
82	dG	201	PEB	C1C-CHB-C4B	-2.14	123.48	128.28
82	g4	202	PEB	C1C-NC-C4C	-2.14	105.79	109.60
82	F9	202	PEB	C1C-NC-C4C	-2.14	105.79	109.60
82	PE	202	PEB	CBC-CAC-C2C	2.14	118.57	112.63
82	cH	202	PEB	OD-C4D-ND	-2.14	122.76	125.93
87	K2	106	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
82	K9	202	PEB	C3B-C4B-NB	2.14	113.16	110.05
82	IM	201	PEB	CAC-C2C-C1C	2.14	129.17	125.76
85	FN	204	BCR	C28-C27-C26	-2.14	110.26	114.08
82	SF	201	PEB	CAC-CBC-CGC	-2.14	109.00	113.60
85	F2	204	BCR	C15-C14-C13	-2.14	124.26	127.31
87	22	608	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
82	eJ	202	PEB	CBA-CAA-C3A	-2.14	108.70	113.47
87	7N	606	CLA	C3B-C4B-NB	-2.14	108.53	110.52
83	QM	201	PUB	C1D-CHC-C4C	-2.14	108.71	113.37
82	O7	201	PEB	C4C-C3C-C2C	-2.14	105.53	107.50
87	4N	606	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
82	zK	501	PEB	C1C-CHB-C4B	2.14	133.08	128.28
87	32	308	CLA	C2A-C1A-CHA	2.14	127.60	123.86
82	LI	201	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
82	m1	201	PEB	OA-C1A-C2A	-2.14	124.47	126.17
83	NQ	201	PUB	CHA-C1B-NB	2.14	124.04	121.15
82	UD	201	PEB	CHC-C1D-ND	-2.14	111.02	113.72
82	W5	202	PEB	CAA-C3A-C4A	-2.14	107.18	112.67
87	BN	812	CLA	CMA-C3A-C2A	-2.14	105.20	113.83
82	LF	202	PEB	C2B-C1B-NB	2.14	115.09	110.53
82	TI	202	PEB	C2A-C1A-NA	2.14	110.12	108.27
82	BF	201	PEB	C1C-CHB-C4B	2.14	133.08	128.28
82	CK	202	PEB	C1C-CHB-C4B	2.14	133.08	128.28
82	H4	1002	PEB	CAB-CBB-CGB	-2.14	109.00	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y5	202	PEB	C3C-C4C-NC	2.14	110.26	108.33
87	CL	511	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
82	GB	203	PEB	CHA-C4A-NA	-2.14	122.66	125.20
82	hE	203	PEB	OD-C4D-C3D	-2.14	124.61	129.46
82	UK	201	PEB	O2C-CGC-CBC	2.14	120.90	114.03
84	F3	1001	CYC	CAB-C3B-C2B	2.14	131.19	127.53
82	RE	201	PEB	CMA-C2A-C1A	-2.14	107.79	112.40
82	CM	202	PEB	CBC-CAC-C2C	-2.14	106.69	112.63
82	IM	203	PEB	CHB-C1C-NC	-2.14	120.42	125.32
82	VG	201	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
87	6N	602	CLA	C2A-C1A-CHA	2.14	127.60	123.86
87	BN	802	CLA	CHD-C1D-ND	2.14	126.42	124.45
82	HG	1002	PEB	CHB-C1C-C2C	-2.14	122.33	127.15
82	WK	202	PEB	C1C-CHB-C4B	2.14	133.08	128.28
84	B3	1001	CYC	CAB-C3B-C2B	2.14	131.19	127.53
88	CL	521	LHG	O8-C23-O10	-2.14	118.20	123.59
82	VP	201	PEB	O2B-CGB-CBB	2.14	120.90	114.03
92	x6	601	LMG	O7-C10-O9	-2.14	118.53	123.70
87	2N	305	CLA	CAC-C3C-C4C	2.14	127.58	124.81
82	B5	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51
82	eG	203	PEB	C3B-C4B-NB	2.14	113.16	110.05
82	WF	201	PEB	C1C-NC-C4C	-2.14	105.79	109.60
82	HF	201	PEB	CBA-CAA-C3A	2.14	118.23	113.47
87	DL	406	CLA	O2D-CGD-CBD	2.14	115.07	111.27
82	EF	202	PEB	OD-C4D-C3D	-2.14	124.62	129.46
84	x3	1001	CYC	C1A-C2A-C3A	-2.14	104.42	106.78
82	YJ	202	PEB	C3C-C4C-NC	2.14	110.26	108.33
82	hG	202	PEB	C3C-C4C-NC	2.14	110.26	108.33
82	AG	304	PEB	CHB-C1C-NC	-2.14	120.42	125.32
92	B6	619	LMG	C1-C2-C3	2.14	114.45	110.00
87	32	302	CLA	CHC-C4B-NB	2.14	126.52	124.26
82	UB	302	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
82	ND	204	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
87	AN	806	CLA	C3B-C4B-NB	-2.14	108.53	110.52
87	cL	516	CLA	C3B-C4B-NB	-2.14	108.53	110.52
82	T5	201	PEB	CAC-C2C-C1C	2.14	129.17	125.76
82	L9	202	PEB	OD-C4D-C3D	-2.14	124.62	129.46
103	8N	309	ZEX	C39-C29-C30	-2.14	119.93	122.92
87	22	607	CLA	O2D-CGD-CBD	2.14	115.07	111.27
84	I4	1001	CYC	CHA-C1A-C2A	-2.14	120.37	125.32
87	82	308	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
87	BN	815	CLA	CAA-C2A-C3A	-2.14	108.92	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	UJ	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
82	aJ	204	PEB	CAB-C3B-C4B	2.14	128.79	125.01
87	B2	801	CLA	CHD-C1D-ND	2.14	126.42	124.45
87	B2	811	CLA	CMA-C3A-C2A	-2.14	105.21	113.83
82	JP	202	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
87	1N	611	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
82	O5	202	PEB	CHC-C1D-ND	-2.14	111.02	113.72
94	dL	406	PL9	C32-C31-C29	-2.14	105.95	112.98
82	Y4	201	PEB	CHB-C1C-NC	-2.14	120.42	125.32
82	dQ	401	PEB	CMA-C2A-C1A	-2.14	107.80	112.40
84	O3	1001	CYC	C1B-NB-C4B	-2.14	107.95	110.67
82	SD	201	PEB	C2A-C1A-NA	2.14	110.11	108.27
82	Z4	201	PEB	C2A-C1A-NA	-2.14	106.43	108.27
87	R2	202	CLA	CHC-C4B-NB	2.14	126.52	124.26
82	GD	202	PEB	CAB-C3B-C4B	2.14	128.79	125.01
82	UI	202	PEB	CAC-CBC-CGC	-2.14	109.00	113.60
82	E9	202	PEB	C3B-C4B-NB	2.14	113.16	110.05
82	FO	1002	PEB	CHA-C1B-NB	-2.14	120.46	124.93
87	8N	307	CLA	C3B-C4B-NB	-2.14	108.53	110.52
82	eG	202	PEB	CHB-C1C-NC	2.14	130.21	125.32
82	cJ	201	PEB	C1B-C2B-C3B	-2.14	104.06	106.51
83	xF	305	PUB	C4B-CHB-C1C	-2.14	123.49	128.28
84	q3	1001	CYC	CAB-C3B-C2B	2.14	131.18	127.53
82	R1	201	PEB	C4C-C3C-C2C	-2.14	105.53	107.50
87	CL	515	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
84	NH	1001	CYC	CBC-CAC-C3C	2.14	118.22	113.47
82	MF	202	PEB	CHC-C1D-ND	-2.14	111.02	113.72
82	cB	403	PEB	OD-C4D-C3D	-2.14	124.62	129.46
82	X7	201	PEB	C4B-C3B-C2B	-2.14	104.42	106.78
87	IN	103	CLA	CHC-C4B-NB	2.14	126.52	124.26
82	XA	202	PEB	CAA-C3A-C2A	-2.14	108.92	114.26
82	Q5	203	PEB	CAC-C2C-C1C	2.14	129.16	125.76
82	PO	201	PEB	CHB-C4B-C3B	-2.14	120.38	125.32
82	SH	203	PEB	CMA-C2A-C1A	-2.14	107.80	112.40
82	LF	201	PEB	CHA-C1B-C2B	2.14	130.39	124.90
82	aH	202	PEB	CHA-C1B-C2B	2.14	130.39	124.90
82	P9	202	PEB	C3B-C4B-NB	2.14	113.16	110.05
82	T9	202	PEB	C3B-C4B-NB	2.14	113.16	110.05
95	b6	622	DGD	C6D-C5D-C4D	-2.14	107.64	112.09
82	FA	203	PEB	C4C-C3C-C2C	-2.14	105.53	107.50
82	lG	202	PEB	C4C-C3C-C2C	-2.14	105.53	107.50
84	K3	1001	CYC	C1B-NB-C4B	-2.14	107.95	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	o3	1001	CYC	CAB-C3B-C2B	2.14	131.18	127.53
82	CK	203	PEB	CHB-C4B-C3B	-2.14	120.38	125.32
82	UP	202	PEB	CHB-C1C-NC	-2.14	120.43	125.32
84	V3	1001	CYC	O1A-CGA-CBA	-2.13	116.22	123.08
82	fH	201	PEB	CAC-C2C-C1C	2.13	129.16	125.76
82	bO	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
87	B6	605	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
87	BN	807	CLA	CHC-C4B-NB	2.13	126.52	124.26
87	B6	615	CLA	CHC-C4B-NB	2.13	126.52	124.26
82	M5	301	PEB	CAC-CBC-CGC	-2.13	109.01	113.60
87	H6	103	CLA	CHB-C4A-NA	2.13	127.46	124.51
82	kF	202	PEB	CHA-C1B-NB	-2.13	120.47	124.93
82	V4	202	PEB	CHB-C1C-NC	2.13	130.21	125.32
82	iM	202	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
82	GM	203	PEB	C1C-NC-C4C	-2.13	105.80	109.60
87	4N	608	CLA	CHB-C1B-C2B	-2.13	121.21	127.24
84	LH	1001	CYC	CHB-C4A-C3A	2.13	130.39	124.90
82	OF	203	PEB	CMB-C2B-C1B	2.13	128.35	125.06
82	nK	202	PEB	CMC-C3C-C4C	2.13	129.32	127.06
87	KN	105	CLA	C2A-C1A-CHA	2.13	127.59	123.86
84	GG	1001	CYC	CHA-C1A-C2A	-2.13	120.38	125.32
82	dG	203	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
82	KK	203	PEB	C1C-CHB-C4B	2.13	133.07	128.28
82	HF	201	PEB	C2B-C1B-NB	2.13	115.08	110.53
87	3N	305	CLA	CHA-C1A-NA	-2.13	121.51	126.40
82	HK	201	PEB	CBA-CAA-C3A	2.13	118.22	113.47
82	T1	202	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
82	fH	203	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
84	BG	1001	CYC	CAA-C2A-C3A	2.13	131.85	127.88
82	XI	201	PEB	CAC-C2C-C1C	2.13	129.16	125.76
82	f1	201	PEB	CAC-C2C-C1C	2.13	129.16	125.76
82	yC	203	PEB	CAC-C2C-C1C	2.13	129.16	125.76
85	B2	840	BCR	C23-C22-C21	2.13	122.22	118.94
82	EK	202	PEB	OD-C4D-C3D	-2.13	124.63	129.46
82	RO	201	PEB	OD-C4D-C3D	-2.13	124.63	129.46
83	AG	302	PUB	CAB-CBB-CGB	-2.13	109.01	113.60
87	5N	607	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
82	Y5	202	PEB	CAB-C3B-C4B	2.13	128.78	125.01
82	qK	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
87	A2	807	CLA	C6-C7-C8	-2.13	109.02	115.92
82	U4	201	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
82	gJ	201	PEB	C4C-C3C-C2C	-2.13	105.53	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	W7	202	PEB	CBA-CAA-C3A	-2.13	108.72	113.47
82	mM	201	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
82	NA	203	PEB	CHA-C4A-NA	-2.13	122.67	125.20
82	MM	203	PEB	CHC-C1D-ND	2.13	116.42	113.72
87	H6	102	CLA	CHB-C1B-NB	2.13	126.52	124.26
87	C6	510	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
87	A2	831	CLA	CMC-C2C-C3C	2.13	131.91	126.12
87	LN	203	CLA	C3C-C4C-NC	-2.13	108.18	110.57
91	DL	405	PHO	O2D-CGD-O1D	-2.13	119.67	123.84
84	d3	1001	CYC	CAB-C3B-C2B	2.13	131.18	127.53
82	h1	201	PEB	OD-C4D-C3D	-2.13	124.63	129.46
82	Z5	305	PEB	CHB-C1C-NC	-2.13	120.44	125.32
91	D6	404	PHO	O2D-CGD-O1D	-2.13	119.67	123.84
82	iO	201	PEB	CHA-C1B-NB	-2.13	120.47	124.93
82	tF	202	PEB	CHB-C4B-NB	2.13	129.02	124.58
84	L1	1001	CYC	CBD-CAD-C3D	2.13	118.55	112.63
82	OJ	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
82	Z1	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
82	GI	202	PEB	C2A-C1A-NA	2.13	110.11	108.27
82	iK	202	PEB	C2B-C1B-NB	2.13	115.08	110.53
84	D3	1001	CYC	C1B-NB-C4B	-2.13	107.95	110.67
82	YB	202	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
82	GM	201	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
87	7N	608	CLA	CHB-C4A-NA	2.13	127.46	124.51
82	kJ	202	PEB	CAC-C2C-C1C	2.13	129.16	125.76
87	12	611	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
82	fE	201	PEB	CHA-C1B-NB	-2.13	120.47	124.93
82	C9	202	PEB	C3B-C4B-NB	2.13	113.15	110.05
87	42	608	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
94	AL	413	PL9	O1-C4-C5	-2.13	114.45	120.73
82	jJ	201	PEB	OD-C4D-C3D	-2.13	124.63	129.46
82	WF	202	PEB	CAC-CBC-CGC	2.13	118.19	113.60
82	VD	202	PEB	CMC-C3C-C4C	2.13	129.32	127.06
82	F7	201	PEB	CAA-C3A-C4A	-2.13	107.20	112.67
84	Q3	1001	CYC	C1B-NB-C4B	-2.13	107.95	110.67
84	73	1001	CYC	C1B-NB-C4B	-2.13	107.95	110.67
82	c1	202	PEB	OD-C4D-ND	-2.13	122.77	125.93
84	E1	1001	CYC	CMC-C2C-C1C	-2.13	107.81	112.40
82	UI	201	PEB	C2B-C1B-NB	2.13	115.08	110.53
82	JF	202	PEB	C4B-NB-C1B	-2.13	102.50	106.51
82	RH	202	PEB	C2A-C1A-NA	2.13	110.11	108.27
84	F4	1001	CYC	C1B-CHB-C4A	-2.13	122.88	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BB	202	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
82	FH	1002	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
82	C7	201	PEB	CBA-CAA-C3A	-2.13	108.72	113.47
84	N1	1001	CYC	CBC-CAC-C3C	2.13	118.21	113.47
87	B2	836	CLA	CHD-C1D-ND	-2.13	122.50	124.45
84	H3	1001	CYC	CAB-C3B-C2B	2.13	131.17	127.53
82	I9	202	PEB	C3B-C4B-NB	2.13	113.15	110.05
84	LH	1002	CYC	CBD-CAD-C3D	2.13	118.55	112.63
87	3N	301	CLA	C2A-C1A-CHA	2.13	127.58	123.86
85	B6	602	BCR	C23-C24-C25	-2.13	121.22	127.20
87	RN	202	CLA	CHC-C4B-NB	2.13	126.51	124.26
87	c6	614	CLA	CHB-C1B-NB	2.13	126.51	124.26
85	K2	105	BCR	C2-C1-C6	2.13	113.76	110.48
85	aL	604	BCR	C2-C1-C6	2.13	113.76	110.48
82	V5	201	PEB	CAC-C2C-C1C	2.13	129.15	125.76
84	BG	1002	CYC	CMA-C3A-C2A	-2.13	120.33	126.12
82	AJ	301	PEB	CBA-CAA-C3A	-2.13	108.72	113.47
82	IM	201	PEB	CMA-C2A-C1A	-2.13	107.81	112.40
82	QH	201	PEB	C4C-C3C-C2C	-2.13	105.53	107.50
82	O4	201	PEB	CHC-C1D-ND	-2.13	111.03	113.72
84	M3	1001	CYC	C1B-NB-C4B	-2.13	107.96	110.67
82	YM	201	PEB	CAA-C3A-C2A	-2.13	108.94	114.26
82	zF	501	PEB	C1C-CHB-C4B	2.13	133.06	128.28
95	AL	415	DGD	C1E-O6E-C5E	2.13	117.87	113.69
95	C6	502	DGD	C6D-O5D-C1E	2.13	117.90	113.74
82	y8	202	PEB	CAC-C2C-C1C	2.13	129.15	125.76
84	Q3	1001	CYC	CAB-C3B-C2B	2.13	131.17	127.53
82	OJ	203	PEB	CAC-CBC-CGC	-2.13	109.02	113.60
82	EF	202	PEB	C1C-CHB-C4B	2.13	133.06	128.28
87	B2	817	CLA	C2A-C1A-CHA	2.13	127.58	123.86
96	vL	201	HEM	C4A-CHB-C1B	-2.13	121.29	126.34
87	62	309	CLA	CHC-C4B-NB	-2.13	122.00	124.26
87	32	304	CLA	CHA-C1A-NA	-2.13	121.52	126.40
84	DH	1003	CYC	CHA-C1A-C2A	-2.13	120.39	125.32
82	M5	305	PEB	CHB-C1C-NC	-2.13	120.44	125.32
87	AN	851	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
87	A2	823	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
84	I3	1001	CYC	C1B-NB-C4B	-2.13	107.96	110.67
82	MM	203	PEB	C1D-CHC-C4C	-2.13	110.12	113.26
87	62	309	CLA	CHA-C4D-ND	2.13	136.95	132.50
82	XF	201	PEB	C1C-CHB-C4B	2.13	133.06	128.28
82	lM	201	PEB	CAB-CBB-CGB	-2.13	109.02	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	wC	203	PEB	C4C-C3C-C2C	-2.13	105.54	107.50
87	4N	605	CLA	CHA-C1A-NA	-2.13	121.52	126.40
82	LD	203	PEB	CHB-C4B-C3B	-2.13	120.39	125.32
82	UH	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
82	MQ	201	PEB	C2A-C1A-NA	2.13	110.11	108.27
87	AN	815	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
82	Y5	203	PEB	CHA-C1B-NB	-2.13	120.48	124.93
87	2N	309	CLA	CHA-C1A-NA	-2.13	121.52	126.40
82	uC	201	PEB	CBC-CAC-C2C	-2.13	106.71	112.63
87	3N	303	CLA	CHB-C1B-NB	2.13	126.51	124.26
84	M3	1001	CYC	CAB-C3B-C2B	2.13	131.17	127.53
84	m3	1001	CYC	C1B-NB-C4B	-2.13	107.96	110.67
82	N7	201	PEB	OD-C4D-C3D	-2.13	124.64	129.46
82	C5	201	PEB	CAC-C2C-C1C	2.13	129.15	125.76
85	k6	102	BCR	C21-C20-C19	2.13	129.86	123.22
82	MM	201	PEB	CMA-C2A-C1A	-2.13	107.82	112.40
82	gB	203	PEB	CHA-C1B-C2B	2.13	130.37	124.90
82	Z9	301	PEB	OD-C4D-ND	-2.13	122.78	125.93
82	VA	203	PEB	CHA-C4A-NA	-2.13	122.67	125.20
84	V3	1001	CYC	C1A-C2A-C3A	-2.13	104.43	106.78
82	OF	201	PEB	C2B-C1B-NB	2.13	115.07	110.53
82	oK	201	PEB	C2B-C1B-NB	2.13	115.07	110.53
82	ID	202	PEB	CBC-CAC-C2C	-2.13	106.72	112.63
82	g4	202	PEB	CAC-CBC-CGC	-2.13	109.02	113.60
82	eM	201	PEB	CAB-CBB-CGB	-2.13	109.02	113.60
83	yF	302	PUB	CAB-CBB-CGB	-2.13	109.02	113.60
82	cO	202	PEB	C3B-C4B-NB	2.13	113.14	110.05
82	VQ	201	PEB	C4C-C3C-C2C	-2.13	105.54	107.50
82	S4	201	PEB	C4C-C3C-C2C	-2.13	105.54	107.50
82	u8	203	PEB	CAB-C3B-C4B	2.13	128.77	125.01
82	fF	201	PEB	CAC-C2C-C1C	2.13	129.15	125.76
84	h3	1001	CYC	C1B-NB-C4B	-2.13	107.96	110.67
87	BN	825	CLA	CHC-C4B-NB	2.13	126.51	124.26
87	12	610	CLA	CHB-C1B-NB	2.13	126.51	124.26
87	A2	811	CLA	O2D-CGD-CBD	2.13	115.05	111.27
91	d6	404	PHO	CMA-C3A-C4A	-2.13	109.72	114.38
82	HA	202	PEB	C2B-C1B-NB	2.13	115.07	110.53
87	72	606	CLA	C3B-C4B-NB	-2.13	108.54	110.52
84	B3	1001	CYC	C1B-NB-C4B	-2.13	107.96	110.67
87	A2	808	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
82	PD	203	PEB	C4C-C3C-C2C	-2.13	105.54	107.50
82	C5	201	PEB	C4C-C3C-C2C	-2.13	105.54	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	K5	201	PEB	C4C-C3C-C2C	-2.13	105.54	107.50
82	V5	201	PEB	C4C-C3C-C2C	-2.13	105.54	107.50
82	dK	202	PEB	CAB-C3B-C4B	2.13	128.77	125.01
82	gH	203	PEB	OD-C4D-C3D	-2.13	124.64	129.46
95	BL	614	DGD	C3D-C4D-C5D	2.13	114.03	110.24
87	FN	205	CLA	C6-C7-C8	-2.13	109.05	115.92
82	DP	202	PEB	CAA-C3A-C4A	-2.13	107.21	112.67
82	gJ	201	PEB	CAA-C3A-C4A	-2.13	107.21	112.67
87	AN	814	CLA	C2A-C1A-CHA	2.13	127.58	123.86
82	S5	203	PEB	CHA-C4A-NA	-2.13	122.68	125.20
82	HQ	202	PEB	CMA-C2A-C1A	-2.13	107.82	112.40
82	QG	202	PEB	C4B-C3B-C2B	-2.13	104.43	106.78
82	kK	202	PEB	CHA-C1B-NB	-2.13	120.49	124.93
92	mL	101	LMG	O1-C7-C8	-2.13	105.77	110.90
82	HB	203	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
82	g4	201	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
82	L9	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
82	UH	201	PEB	OD-C4D-ND	-2.13	122.78	125.93
82	GD	201	PEB	CMC-C3C-C4C	2.13	129.31	127.06
82	BM	301	PEB	CMC-C3C-C4C	2.13	129.31	127.06
87	cL	517	CLA	C2A-C1A-CHA	2.13	127.58	123.86
87	1N	610	CLA	C2A-C1A-CHA	2.13	127.58	123.86
82	IQ	202	PEB	CBC-CAC-C2C	-2.13	106.72	112.63
87	3N	311	CLA	CAA-C2A-C3A	-2.13	108.95	114.26
82	mO	202	PEB	CMA-C2A-C1A	-2.13	107.82	112.40
82	qF	202	PEB	C3B-C4B-NB	2.13	113.14	110.05
82	E5	201	PEB	CAC-C2C-C1C	2.13	129.15	125.76
82	y8	203	PEB	CAC-C2C-C1C	2.13	129.15	125.76
84	KH	1001	CYC	C3A-C4A-NA	2.13	115.06	110.53
82	FA	203	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
82	Z5	301	PEB	CAC-CBC-CGC	-2.13	109.03	113.60
87	AN	823	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
82	tC	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
87	I2	103	CLA	CHC-C4B-NB	2.13	126.51	124.26
82	RB	202	PEB	CHB-C4B-C3B	-2.13	120.40	125.32
82	MM	201	PEB	OD-C4D-C3D	-2.13	124.65	129.46
87	BN	832	CLA	C2D-C1D-ND	-2.13	108.54	110.10
84	S3	1001	CYC	C1B-NB-C4B	-2.12	107.96	110.67
84	f3	1001	CYC	C1B-NB-C4B	-2.12	107.96	110.67
84	w3	1001	CYC	C1B-NB-C4B	-2.12	107.96	110.67
82	WE	201	PEB	CAC-C2C-C1C	2.12	129.15	125.76
82	c1	202	PEB	CMC-C3C-C4C	2.12	129.31	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	uF	201	PEB	CBA-CAA-C3A	-2.12	108.74	113.47
84	73	1002	CYC	CHB-C1B-C2B	-2.12	122.74	126.95
84	IG	1001	CYC	C4D-ND-C1D	-2.12	106.00	109.79
84	u3	1001	CYC	CAB-C3B-C2B	2.12	131.16	127.53
82	X7	202	PEB	CHA-C1B-NB	-2.12	120.49	124.93
87	cL	515	CLA	C3B-C4B-NB	-2.12	108.54	110.52
82	IB	203	PEB	OD-C4D-C3D	-2.12	124.65	129.46
87	AN	808	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
82	f1	203	PEB	CAB-CBB-CGB	-2.12	109.03	113.60
82	B7	201	PEB	CHA-C4A-NA	2.12	127.73	125.20
82	sK	202	PEB	CHA-C4A-NA	2.12	127.73	125.20
82	OH	203	PEB	C1C-NC-C4C	-2.12	105.82	109.60
82	q8	202	PEB	C1C-NC-C4C	-2.12	105.82	109.60
87	A2	813	CLA	CHB-C1B-NB	2.12	126.51	124.26
87	c6	609	CLA	CHB-C1B-NB	2.12	126.51	124.26
82	QG	202	PEB	CHA-C1B-C2B	2.12	130.36	124.90
82	WH	202	PEB	CHA-C1B-C2B	2.12	130.36	124.90
82	VD	201	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	VP	201	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	P9	201	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
84	N3	1001	CYC	C1B-NB-C4B	-2.12	107.96	110.67
84	o3	1001	CYC	C1B-NB-C4B	-2.12	107.96	110.67
87	42	604	CLA	CAA-C2A-C1A	2.12	116.84	112.14
84	w3	1001	CYC	CAB-C3B-C2B	2.12	131.16	127.53
82	UM	201	PEB	C1C-NC-C4C	-2.12	105.82	109.60
91	d6	404	PHO	C6-C5-C3	-2.12	107.89	113.45
82	MP	201	PEB	OA-C1A-NA	2.12	127.51	124.94
82	IQ	201	PEB	OD-C4D-C3D	-2.12	124.65	129.46
82	c1	202	PEB	CHA-C4A-NA	2.12	127.73	125.20
82	S9	203	PEB	CAB-C3B-C4B	2.12	128.76	125.01
82	gF	203	PEB	CAB-C3B-C4B	2.12	128.76	125.01
82	H7	202	PEB	C2B-C1B-NB	2.12	115.06	110.53
82	PM	202	PEB	CHB-C4B-NB	-2.12	120.16	124.58
87	1N	610	CLA	CHB-C1B-NB	2.12	126.50	124.26
82	UJ	201	PEB	C1C-NC-C4C	-2.12	105.82	109.60
82	IM	203	PEB	C3C-C4C-NC	2.12	110.25	108.33
82	b1	203	PEB	C3C-C4C-NC	2.12	110.25	108.33
82	RB	202	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	WK	202	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	YM	203	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	UP	201	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	XQ	202	PEB	C4C-C3C-C2C	-2.12	105.54	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	fO	202	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
85	BN	840	BCR	C23-C22-C21	2.12	122.20	118.94
82	W9	202	PEB	CAB-C3B-C2B	-2.12	123.92	127.88
87	bL	605	CLA	CHD-C1D-ND	-2.12	122.50	124.45
87	5N	611	CLA	CHA-C1A-NA	-2.12	121.54	126.40
85	BL	618	BCR	C21-C20-C19	-2.12	116.59	123.22
87	AN	830	CLA	C2A-C1A-CHA	2.12	127.57	123.86
96	v6	201	HEM	C4C-CHD-C1D	-2.12	121.48	126.06
82	XQ	202	PEB	C2A-C1A-NA	2.12	110.10	108.27
82	TA	203	PEB	CHA-C1B-NB	-2.12	120.49	124.93
82	AO	305	PEB	CAC-CBC-CGC	-2.12	109.03	113.60
82	DP	202	PEB	CHC-C1D-ND	-2.12	111.04	113.72
92	qL	301	LMG	O1-C1-C2	2.12	111.62	108.30
87	BN	818	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
88	AN	843	LHG	O8-C23-O10	-2.12	118.23	123.59
87	22	612	CLA	CHA-C1A-NA	-2.12	121.54	126.40
87	52	611	CLA	CHA-C1A-NA	-2.12	121.54	126.40
82	OH	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
82	F9	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
82	L9	202	PEB	CAC-C2C-C1C	2.12	129.14	125.76
82	cB	403	PEB	CAC-C2C-C1C	-2.12	122.38	125.76
82	lJ	201	PEB	CAC-C2C-C1C	2.12	129.14	125.76
82	YO	203	PEB	C1B-C2B-C3B	-2.12	104.07	106.51
82	p8	202	PEB	C1B-C2B-C3B	-2.12	104.07	106.51
87	62	310	CLA	C2D-C1D-ND	-2.12	108.54	110.10
82	CM	203	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	CA	201	PEB	CBA-CAA-C3A	-2.12	108.74	113.47
82	OF	201	PEB	C3C-C4C-NC	2.12	110.24	108.33
87	L2	203	CLA	C3C-C4C-NC	-2.12	108.19	110.57
82	G9	202	PEB	C3B-C4B-NB	2.12	113.14	110.05
82	O1	203	PEB	OD-C4D-C3D	-2.12	124.65	129.46
82	wF	301	PEB	OD-C4D-C3D	-2.12	124.65	129.46
84	l3	1001	CYC	C1B-NB-C4B	-2.12	107.97	110.67
82	gM	202	PEB	CHC-C1D-ND	-2.12	111.04	113.72
82	QF	201	PEB	CAC-CBC-CGC	2.12	118.17	113.60
83	yK	303	PUB	CAB-CBB-CGB	-2.12	109.04	113.60
82	nK	202	PEB	C2B-C1B-NB	2.12	115.06	110.53
82	LE	1002	PEB	CHA-C1B-NB	-2.12	120.50	124.93
82	FO	1002	PEB	CHB-C4B-C3B	-2.12	120.41	125.32
82	FF	201	PEB	CAA-C3A-C2A	-2.12	108.96	114.26
85	A2	804	BCR	C21-C20-C19	-2.12	116.60	123.22
82	A7	201	PEB	C1C-CHB-C4B	2.12	133.04	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Z1	203	PEB	OD-C4D-C3D	-2.12	124.65	129.46
82	P7	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
82	wF	301	PEB	CAC-C2C-C1C	2.12	129.14	125.76
87	J2	101	CLA	C2A-C1A-CHA	2.12	127.57	123.86
82	dG	204	PEB	OD-C4D-ND	-2.12	122.79	125.93
82	sK	201	PEB	OD-C4D-ND	-2.12	122.79	125.93
82	j4	201	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	r8	202	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
85	bL	601	BCR	C15-C16-C17	-2.12	119.13	123.47
82	SP	202	PEB	C3C-C4C-NC	2.12	110.24	108.33
82	D5	201	PEB	C3C-C4C-NC	2.12	110.24	108.33
87	AN	807	CLA	C6-C7-C8	-2.12	109.06	115.92
82	k4	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
87	KN	105	CLA	CHD-C1D-ND	-2.12	122.50	124.45
82	UB	301	PEB	CHC-C4C-NC	2.12	124.02	121.15
82	LG	1002	PEB	CHA-C1B-NB	-2.12	120.50	124.93
82	t8	201	PEB	C3B-C4B-NB	2.12	113.13	110.05
82	qF	203	PEB	C1B-C2B-C3B	-2.12	104.07	106.51
82	TA	203	PEB	O1B-CGB-CBB	-2.12	116.27	123.08
82	IP	202	PEB	OD-C4D-C3D	-2.12	124.66	129.46
82	xF	302	PEB	OD-C4D-C3D	-2.12	124.66	129.46
87	CL	511	CLA	C2A-C1A-CHA	2.12	127.57	123.86
87	72	607	CLA	C2A-C1A-CHA	2.12	127.57	123.86
82	HJ	201	PEB	CMA-C2A-C1A	-2.12	107.83	112.40
84	n3	1001	CYC	CAB-C3B-C2B	2.12	131.16	127.53
87	B2	822	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
85	B6	601	BCR	C38-C26-C25	-2.12	122.15	124.53
82	i4	201	PEB	CHA-C1B-NB	-2.12	120.50	124.93
82	u8	201	PEB	CBC-CAC-C2C	-2.12	106.74	112.63
87	22	604	CLA	CAC-C3C-C4C	2.12	127.56	124.81
87	B2	810	CLA	CAC-C3C-C4C	2.12	127.56	124.81
82	eE	203	PEB	CMC-C3C-C2C	2.12	130.19	125.61
82	nF	202	PEB	CMC-C3C-C4C	2.12	129.31	127.06
82	g1	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
82	r8	201	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
82	gB	202	PEB	C4C-C3C-C2C	-2.12	105.54	107.50
85	LN	205	BCR	C23-C24-C25	-2.12	121.25	127.20
82	aJ	202	PEB	CAB-CBB-CGB	-2.12	109.04	113.60
82	GF	201	PEB	C2B-C1B-NB	2.12	115.05	110.53
82	P5	201	PEB	CAC-C2C-C1C	2.12	129.14	125.76
87	dL	402	CLA	CHD-C1D-ND	-2.12	122.51	124.45
87	B6	606	CLA	CHB-C1B-NB	2.12	126.50	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	4N	608	CLA	CHC-C4B-NB	2.12	126.50	124.26
87	32	303	CLA	C2B-C1B-NB	2.12	111.65	110.23
96	V6	201	HEM	C4C-CHD-C1D	-2.12	121.48	126.06
87	C6	515	CLA	CHB-C4A-NA	2.12	127.44	124.51
82	PA	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
82	dM	201	PEB	C2B-C1B-NB	2.12	115.05	110.53
84	CO	1001	CYC	CHB-C1B-NB	-2.12	121.51	126.06
82	eE	202	PEB	CHB-C1C-NC	2.12	130.18	125.32
82	UH	202	PEB	CHA-C1B-NB	-2.12	120.50	124.93
82	wK	301	PEB	C2A-C1A-NA	2.12	110.10	108.27
82	kK	202	PEB	CAC-C2C-C1C	2.12	129.14	125.76
82	DJ	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
82	eM	202	PEB	O2B-CGB-CBB	2.12	120.84	114.03
87	A2	810	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
82	A4	305	PEB	CAC-CBC-CGC	-2.12	109.04	113.60
85	F6	101	BCR	C1-C6-C5	-2.12	119.63	122.61
82	ZE	203	PEB	CHA-C1B-C2B	2.12	130.35	124.90
96	E6	101	HEM	CHA-C4D-C3D	-2.12	121.35	125.33
87	A2	815	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
82	lJ	203	PEB	CAB-C3B-C4B	2.12	128.76	125.01
82	QD	201	PEB	CAB-CBB-CGB	-2.12	109.04	113.60
82	HP	202	PEB	CAC-CBC-CGC	-2.12	109.04	113.60
82	XA	202	PEB	CHA-C1B-NB	-2.12	120.50	124.93
85	BN	841	BCR	C30-C25-C24	2.12	121.77	115.78
87	B2	806	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
87	32	305	CLA	C3B-C4B-NB	-2.12	108.55	110.52
82	R5	201	PEB	CAC-CBC-CGC	-2.12	109.05	113.60
82	X5	201	PEB	CAC-CBC-CGC	-2.12	109.05	113.60
83	wK	304	PUB	CAC-CBC-CGC	-2.12	109.05	113.60
82	XQ	202	PEB	C3B-C4B-NB	2.12	113.13	110.05
82	HB	201	PEB	CAC-C2C-C1C	2.12	129.13	125.76
82	hG	201	PEB	CHA-C1B-NB	-2.12	120.50	124.93
92	J6	102	LMG	C1-O6-C5	-2.12	109.53	113.69
82	QF	202	PEB	C3C-C4C-NC	2.12	110.24	108.33
87	b6	608	CLA	C2A-C1A-CHA	2.12	127.56	123.86
87	22	609	CLA	CMC-C2C-C1C	-2.12	121.81	125.04
87	AN	828	CLA	O2D-CGD-CBD	2.12	115.03	111.27
84	L4	1001	CYC	CAB-C3B-C2B	2.12	131.15	127.53
82	yK	301	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
84	C4	1001	CYC	C4D-ND-C1D	-2.12	106.01	109.79
87	A2	808	CLA	C1-C2-C3	-2.12	122.38	126.04
82	LA	201	PEB	C3B-C4B-NB	2.12	113.13	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	tK	203	PEB	C3B-C4B-NB	2.12	113.13	110.05
82	i4	203	PEB	CAB-C3B-C2B	2.12	131.82	127.88
82	VE	201	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
82	OP	201	PEB	CAC-CBC-CGC	-2.12	109.05	113.60
82	dM	203	PEB	CHA-C4A-NA	-2.12	122.69	125.20
85	B2	841	BCR	C30-C25-C24	2.12	121.77	115.78
95	C6	521	DGD	O2G-C1B-O1B	-2.12	118.59	123.70
82	VA	203	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	SO	201	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	A1	302	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	J9	202	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	lM	201	PEB	CAC-C2C-C1C	2.12	129.13	125.76
84	BG	1002	CYC	C4D-CHA-C1A	2.12	133.03	128.28
82	TF	202	PEB	CAC-CBC-CGC	-2.12	109.05	113.60
82	YP	502	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
87	BN	823	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
82	Y4	201	PEB	CHC-C4C-NC	2.12	124.01	121.15
82	FD	202	PEB	CBA-CAA-C3A	-2.12	108.75	113.47
96	fL	102	HEM	O2D-CGD-CBD	2.12	120.83	114.03
82	h4	201	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
82	TA	202	PEB	CAC-C2C-C1C	2.12	129.13	125.76
82	A5	201	PEB	CAC-C2C-C1C	2.12	129.13	125.76
87	BN	818	CLA	C2A-C1A-CHA	2.12	127.56	123.86
85	B6	601	BCR	C39-C30-C25	-2.12	106.87	110.30
87	AN	801	CLA	CHC-C4B-NB	2.12	126.50	124.26
84	LG	1001	CYC	CMD-C2D-C1D	2.12	128.66	125.56
87	A2	825	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
82	ZJ	201	PEB	CAB-C3B-C4B	2.12	128.75	125.01
82	AQ	301	PEB	OD-C4D-ND	-2.12	122.80	125.93
82	DD	201	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	NO	1002	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	VO	201	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
82	R5	201	PEB	C4C-C3C-C2C	-2.12	105.55	107.50
84	J1	1001	CYC	CHA-C1A-C2A	-2.12	120.42	125.32
92	B6	619	LMG	O7-C10-O9	-2.12	118.59	123.70
87	CL	508	CLA	CMC-C2C-C3C	2.12	131.86	126.12
84	BE	1001	CYC	CAA-C2A-C3A	2.12	131.82	127.88
82	VJ	202	PEB	OA-C1A-NA	2.12	127.50	124.94
82	XA	201	PEB	CHB-C1C-NC	-2.12	120.47	125.32
82	UF	202	PEB	CHB-C4B-NB	-2.12	120.17	124.58
82	OF	202	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
82	UJ	202	PEB	CAB-CBB-CGB	-2.12	109.05	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SQ	202	PEB	CHA-C4A-NA	-2.12	122.69	125.20
82	DQ	201	PEB	C1D-CHC-C4C	-2.12	110.14	113.26
82	O1	201	PEB	C1D-CHC-C4C	2.12	116.38	113.26
82	WI	201	PEB	C2B-C1B-NB	2.12	115.04	110.53
82	IJ	201	PEB	C2B-C1B-NB	2.12	115.04	110.53
82	cJ	201	PEB	CAB-C3B-C4B	2.12	128.75	125.01
82	M9	302	PEB	OD-C4D-ND	-2.12	122.80	125.93
85	B6	621	BCR	C8-C7-C6	-2.11	121.26	127.20
87	I2	102	CLA	CHB-C1B-NB	2.11	126.50	124.26
87	B6	604	CLA	CHB-C1B-NB	2.11	126.50	124.26
82	L4	1002	PEB	CHB-C4B-C3B	-2.11	120.43	125.32
83	xK	306	PUB	O2B-CGB-CBB	2.11	120.82	114.03
85	K6	102	BCR	C21-C20-C19	2.11	129.82	123.22
103	8N	309	ZEX	C19-C9-C10	-2.11	119.96	122.92
87	AN	802	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
82	dH	203	PEB	C3C-C4C-NC	2.11	110.24	108.33
82	dE	204	PEB	OD-C4D-ND	-2.11	122.80	125.93
82	qC	202	PEB	C1C-NC-C4C	-2.11	105.83	109.60
82	RM	202	PEB	CAB-CBB-CGB	2.11	118.15	113.60
82	G5	201	PEB	CAC-CBC-CGC	-2.11	109.05	113.60
82	18	203	PEB	CMB-C2B-C1B	2.11	128.32	125.06
87	42	605	CLA	CHA-C1A-NA	-2.11	121.56	126.40
82	y8	203	PEB	CHC-C4C-NC	2.11	124.01	121.15
87	3N	303	CLA	CHC-C4B-NB	2.11	126.50	124.26
87	52	610	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
82	HI	202	PEB	CHC-C1D-ND	2.11	116.40	113.72
82	CM	202	PEB	C1D-CHC-C4C	-2.11	110.14	113.26
82	lH	202	PEB	CAC-CBC-CGC	-2.11	109.05	113.60
82	hO	201	PEB	CAB-CBB-CGB	-2.11	109.05	113.60
87	AN	810	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
82	AD	303	PEB	CAA-C3A-C4A	2.11	118.10	112.67
82	fJ	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
87	62	307	CLA	C3B-C4B-NB	-2.11	108.55	110.52
82	OD	201	PEB	OD-C4D-ND	-2.11	122.80	125.93
82	mF	201	PEB	C1B-C2B-C3B	-2.11	104.08	106.51
82	RH	201	PEB	CAC-C2C-C1C	2.11	129.13	125.76
82	m4	202	PEB	CMA-C2A-C1A	-2.11	107.85	112.40
87	A2	822	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
82	CP	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	i1	201	PEB	C4B-NB-C1B	-2.11	102.53	106.51
82	QE	202	PEB	CHA-C1B-C2B	2.11	130.34	124.90
82	AG	301	PEB	CHB-C4B-NB	-2.11	120.18	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BN	835	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
82	KP	202	PEB	CBB-CAB-C3B	-2.11	106.75	112.63
82	PP	201	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
82	WH	201	PEB	C2B-C1B-NB	2.11	115.04	110.53
84	LH	1001	CYC	CHB-C1B-NB	-2.11	121.52	126.06
87	A2	826	CLA	CHD-C1D-ND	-2.11	122.51	124.45
82	UE	203	PEB	C1D-CHC-C4C	-2.11	110.14	113.26
87	2N	307	CLA	O2D-CGD-CBD	2.11	115.02	111.27
82	lJ	202	PEB	OA-C1A-NA	2.11	127.50	124.94
82	Q9	203	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
82	iK	203	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
84	h3	1001	CYC	CAB-C3B-C2B	2.11	131.14	127.53
82	KQ	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
82	j1	201	PEB	C2B-C1B-NB	2.11	115.04	110.53
87	32	311	CLA	CAA-C2A-C3A	-2.11	108.98	114.26
82	OI	202	PEB	CMC-C3C-C2C	-2.11	121.03	125.61
87	CL	505	CLA	C1-C2-C3	-2.11	122.39	126.04
87	K6	101	CLA	C1-C2-C3	-2.11	122.39	126.04
87	AN	827	CLA	C4-C3-C5	2.11	118.83	115.27
84	JH	1001	CYC	CHA-C1A-C2A	-2.11	120.43	125.32
87	AN	817	CLA	C2A-C1A-CHA	2.11	127.55	123.86
82	KA	201	PEB	C1D-CHC-C4C	2.11	116.37	113.26
82	KB	304	PEB	C1D-CHC-C4C	-2.11	110.14	113.26
82	H7	202	PEB	C1D-CHC-C4C	-2.11	110.14	113.26
82	V7	201	PEB	C3B-C4B-NB	2.11	113.12	110.05
82	PM	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	W4	201	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	vF	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	F7	203	PEB	CHB-C1C-NC	-2.11	120.48	125.32
82	EM	203	PEB	CMB-C2B-C1B	2.11	128.32	125.06
82	eH	201	PEB	CAC-C2C-C1C	2.11	129.13	125.76
103	82	309	ZEX	C40-C33-C34	-2.11	119.96	122.92
85	C6	508	BCR	C38-C26-C25	-2.11	122.16	124.53
84	x3	1001	CYC	O1A-CGA-CBA	-2.11	116.30	123.08
82	Q1	202	PEB	C3C-C4C-NC	2.11	110.23	108.33
82	b4	201	PEB	C3C-C4C-NC	2.11	110.23	108.33
94	dL	406	PL9	C45-C44-C46	2.11	118.82	115.27
82	WE	202	PEB	CHB-C1C-C2C	-2.11	122.39	127.15
82	F7	203	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
87	cL	513	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
87	AN	831	CLA	CMC-C2C-C3C	2.11	131.85	126.12
82	eE	203	PEB	C3B-C4B-NB	2.11	113.12	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	y3	1001	CYC	C2A-C1A-NA	2.11	113.12	110.05
82	RF	201	PEB	C1C-CHB-C4B	2.11	133.02	128.28
82	Q9	203	PEB	OD-C4D-C3D	-2.11	124.68	129.46
87	BN	811	CLA	CAC-C3C-C4C	2.11	127.55	124.81
87	22	612	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
82	AF	202	PEB	CMC-C3C-C4C	2.11	129.30	127.06
85	d6	405	BCR	C34-C9-C10	-2.11	119.97	122.92
87	2N	312	CLA	CHA-C1A-NA	-2.11	121.56	126.40
83	xF	306	PUB	O2B-CGB-CBB	2.11	120.81	114.03
88	A2	843	LHG	O8-C23-O10	-2.11	118.26	123.59
87	AN	814	CLA	C2D-C1D-ND	-2.11	108.55	110.10
87	12	610	CLA	C2A-C1A-CHA	2.11	127.55	123.86
87	A6	402	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
82	QQ	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	O4	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	mH	201	PEB	CAA-C3A-C2A	-2.11	108.98	114.26
82	A7	201	PEB	CAB-C3B-C2B	-2.11	123.95	127.88
82	O5	201	PEB	CHA-C1B-NB	-2.11	120.52	124.93
82	EQ	202	PEB	CHC-C4C-NC	2.11	124.01	121.15
82	I5	201	PEB	CAC-CBC-CGC	-2.11	109.06	113.60
82	S9	202	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
82	YI	201	PEB	C2B-C1B-NB	2.11	115.03	110.53
82	cB	403	PEB	CMC-C3C-C2C	2.11	130.17	125.61
85	B6	601	BCR	C36-C18-C19	2.11	121.40	118.08
82	DO	1002	PEB	C1C-CHB-C4B	2.11	133.02	128.28
87	AL	405	CLA	C2A-C1A-CHA	2.11	127.55	123.86
87	7N	607	CLA	C2A-C1A-CHA	2.11	127.55	123.86
84	U3	1001	CYC	C1B-NB-C4B	-2.11	107.98	110.67
84	k3	1001	CYC	C1B-NB-C4B	-2.11	107.98	110.67
82	yF	301	PEB	CHC-C1D-ND	-2.11	111.05	113.72
85	c6	603	BCR	C23-C24-C25	-2.11	121.27	127.20
82	DG	1002	PEB	O1B-CGB-CBB	-2.11	116.30	123.08
82	GP	203	PEB	CAC-C2C-C1C	2.11	129.12	125.76
83	AG	302	PUB	CAB-C3B-C4B	2.11	129.12	125.76
82	m1	201	PEB	CAA-C3A-C2A	-2.11	108.99	114.26
84	x3	1001	CYC	OC-C1C-C2C	-2.11	124.50	126.17
96	f6	101	HEM	CHC-C4B-NB	2.11	126.71	124.42
82	HD	202	PEB	CMA-C2A-C1A	-2.11	107.85	112.40
82	KQ	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	aH	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
87	A2	814	CLA	C2A-C1A-CHA	2.11	127.55	123.86
82	QF	201	PEB	CAC-C2C-C3C	2.11	131.90	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	6N	608	CLA	CHC-C4B-NB	-2.11	122.02	124.26
82	V7	203	PEB	CHA-C4A-NA	-2.11	122.70	125.20
82	tC	201	PEB	CHB-C1C-NC	-2.11	120.49	125.32
83	xK	305	PUB	C4B-CHB-C1C	-2.11	123.55	128.28
84	I1	1001	CYC	CAB-C3B-C2B	2.11	131.14	127.53
82	LH	1003	PEB	C3C-C4C-NC	2.11	110.23	108.33
82	dG	201	PEB	C3C-C4C-NC	2.11	110.23	108.33
87	BL	606	CLA	CHA-C1A-NA	-2.11	121.57	126.40
85	IN	101	BCR	C2-C1-C6	2.11	113.73	110.48
82	T4	203	PEB	CAC-C2C-C1C	2.11	129.12	125.76
87	7N	607	CLA	O1D-CGD-CBD	2.11	128.80	124.48
82	hE	201	PEB	C4B-C3B-C2B	-2.11	104.45	106.78
82	PM	202	PEB	CHA-C1B-NB	-2.11	120.52	124.93
82	c4	202	PEB	C3B-C4B-NB	2.11	113.12	110.05
87	C6	513	CLA	O2D-CGD-CBD	2.11	115.02	111.27
82	T1	202	PEB	CHC-C4C-NC	2.11	124.00	121.15
84	LH	1002	CYC	CAA-CBA-CGA	2.11	118.14	113.60
82	QP	201	PEB	CHB-C4B-C3B	-2.11	120.44	125.32
82	LK	201	PEB	CHA-C1B-C2B	2.11	130.32	124.90
95	C6	503	DGD	O6D-C5D-C4D	2.11	113.53	109.69
87	AN	809	CLA	CBA-CAA-C2A	2.11	120.09	113.86
87	bL	621	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
87	nL	101	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
87	22	609	CLA	CHA-C1A-NA	-2.11	121.57	126.40
82	BI	203	PEB	CHB-C1C-C2C	-2.11	122.39	127.15
87	4N	608	CLA	CED-O2D-CGD	2.11	120.71	115.94
82	NA	203	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
82	UG	202	PEB	CHA-C1B-NB	-2.11	120.52	124.93
82	U1	202	PEB	CHA-C1B-NB	-2.11	120.52	124.93
87	H6	103	CLA	CHC-C4B-NB	2.11	126.49	124.26
82	AI	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	RP	202	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	BQ	201	PEB	C4C-C3C-C2C	-2.11	105.55	107.50
82	tK	203	PEB	CBA-CAA-C3A	-2.11	108.77	113.47
82	RD	201	PEB	C3B-C4B-NB	2.11	113.12	110.05
87	12	611	CLA	CHA-C1A-NA	-2.11	121.57	126.40
87	32	313	CLA	CHA-C1A-NA	-2.11	121.57	126.40
82	II	201	PEB	C2A-C1A-NA	2.11	110.09	108.27
82	H4	1002	PEB	CHA-C1B-NB	-2.11	120.52	124.93
87	AN	825	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
82	cM	202	PEB	O2B-CGB-CBB	2.11	120.81	114.03
87	3N	312	CLA	O2A-CGA-O1A	-2.11	118.04	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	J2	103	BCR	C38-C26-C25	-2.11	122.16	124.53
82	ZH	203	PEB	OD-C4D-C3D	-2.11	124.68	129.46
87	42	604	CLA	O2D-CGD-CBD	2.11	115.02	111.27
82	SP	202	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	m1	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	Y5	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
85	KN	104	BCR	C2-C1-C6	2.11	113.73	110.48
85	b6	603	BCR	C28-C27-C26	-2.11	110.31	114.08
82	DK	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
82	OK	203	PEB	CMB-C2B-C1B	2.11	128.31	125.06
82	YP	501	PEB	CMB-C2B-C1B	2.11	128.31	125.06
82	W9	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
82	aH	202	PEB	CAA-C3A-C4A	2.11	118.09	112.67
82	UG	202	PEB	CAC-CBC-CGC	-2.11	109.07	113.60
83	AE	302	PUB	CAB-CBB-CGB	-2.11	109.07	113.60
82	MQ	201	PEB	C1C-CHB-C4B	2.11	133.01	128.28
82	CD	202	PEB	C4C-C3C-C2C	-2.11	105.56	107.50
82	eE	201	PEB	C4C-C3C-C2C	-2.11	105.56	107.50
87	FN	205	CLA	C1-O2A-CGA	2.11	121.97	116.44
82	cM	202	PEB	CAA-C3A-C2A	-2.11	108.99	114.26
82	K5	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
87	A2	827	CLA	C4-C3-C5	2.11	118.82	115.27
85	CL	501	BCR	C2-C1-C6	2.11	113.73	110.48
85	cL	518	BCR	C38-C26-C25	-2.11	122.16	124.53
82	OK	202	PEB	CAB-CBB-CGB	-2.11	109.07	113.60
82	OQ	202	PEB	CHB-C1C-NC	-2.11	120.49	125.32
82	RG	201	PEB	CMA-C2A-C1A	-2.11	107.86	112.40
87	CL	515	CLA	C2A-C1A-CHA	2.11	127.54	123.86
82	FQ	201	PEB	CAB-C3B-C4B	2.11	128.74	125.01
82	EK	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
85	AN	804	BCR	C21-C20-C19	-2.11	116.64	123.22
82	OB	201	PEB	CHB-C1C-C2C	-2.11	122.40	127.15
82	AH	302	PEB	C1D-CHC-C4C	-2.11	110.15	113.26
82	R1	202	PEB	OD-C4D-ND	-2.11	122.81	125.93
82	DE	1002	PEB	O1B-CGB-CBB	-2.11	116.31	123.08
82	aH	201	PEB	OD-C4D-C3D	-2.11	124.69	129.46
82	i4	202	PEB	CAC-CBC-CGC	-2.11	109.07	113.60
83	yK	302	PUB	CAB-CBB-CGB	-2.11	109.07	113.60
82	I7	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
82	EQ	202	PEB	CHB-C1C-C2C	-2.11	122.40	127.15
87	32	312	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
87	3N	306	CLA	CAA-CBA-CGA	-2.11	106.92	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WG	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	CP	202	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	G5	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	lJ	202	PEB	CAB-C3B-C4B	2.11	128.74	125.01
82	gH	203	PEB	C3C-C4C-NC	2.11	110.23	108.33
82	WJ	201	PEB	C3B-C4B-NB	2.11	113.11	110.05
82	QK	201	PEB	CAC-C2C-C3C	2.11	131.89	127.07
85	b6	602	BCR	C38-C26-C27	2.11	117.66	113.62
96	fL	102	HEM	C4C-CHD-C1D	-2.11	121.51	126.06
82	N5	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	dM	202	PEB	CHC-C1D-ND	-2.11	111.06	113.72
82	NM	201	PEB	CHA-C4A-NA	2.11	127.71	125.20
82	RH	201	PEB	C4C-C3C-C2C	-2.11	105.56	107.50
82	N7	201	PEB	CAC-CBC-CGC	-2.11	109.07	113.60
82	J9	202	PEB	CAC-CBC-CGC	-2.11	109.07	113.60
96	FL	102	HEM	CHA-C4D-C3D	-2.11	121.37	125.33
82	DF	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
82	sF	203	PEB	CMB-C2B-C1B	2.11	128.31	125.06
82	RE	201	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
82	VK	201	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
82	k1	202	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
82	hG	201	PEB	C1D-CHC-C4C	2.11	116.36	113.26
87	BL	608	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
82	bK	201	PEB	OD-C4D-C3D	-2.11	124.69	129.46
82	I5	202	PEB	C1C-CHB-C4B	2.11	133.00	128.28
87	A2	802	CLA	CHC-C4B-NB	2.11	126.49	124.26
87	B2	814	CLA	CHC-C4B-NB	2.11	126.49	124.26
82	GB	203	PEB	CHA-C1B-NB	-2.11	120.53	124.93
82	R5	201	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	kF	202	PEB	CAC-C2C-C1C	2.11	129.12	125.76
82	SA	202	PEB	CHB-C1C-C2C	-2.11	122.40	127.15
84	G4	1001	CYC	CMB-C2B-C1B	2.11	126.80	124.17
84	E1	1001	CYC	CHD-C1D-C2D	2.11	132.66	127.49
87	B2	804	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
94	DL	401	PL9	C16-C14-C13	-2.11	116.86	121.12
87	52	601	CLA	C2A-C1A-CHA	2.11	127.54	123.86
82	fO	201	PEB	CMC-C3C-C4C	2.11	129.29	127.06
82	XA	201	PEB	CAB-CBB-CGB	-2.11	109.07	113.60
82	V5	201	PEB	CAC-CBC-CGC	-2.11	109.07	113.60
82	l4	201	PEB	CAB-C3B-C4B	2.11	128.73	125.01
87	AL	403	CLA	CAA-C2A-C1A	-2.10	105.08	111.97
82	T5	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	F9	202	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	pC	201	PEB	CHB-C4B-C3B	-2.10	120.45	125.32
82	UG	203	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	EI	201	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	II	201	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	YB	202	PEB	CBB-CAB-C3B	-2.10	106.78	112.63
87	B2	832	CLA	C2D-C1D-ND	-2.10	108.55	110.10
82	A5	201	PEB	CAC-CBC-CGC	-2.10	109.07	113.60
82	yC	203	PEB	CHC-C4C-NC	2.10	124.00	121.15
82	mM	201	PEB	CHA-C1B-NB	-2.10	120.53	124.93
87	B2	817	CLA	CHD-C1D-ND	-2.10	122.52	124.45
82	SB	203	PEB	CHC-C1D-ND	-2.10	111.06	113.72
82	hF	201	PEB	CHC-C1D-ND	-2.10	111.06	113.72
82	eH	201	PEB	C1D-CHC-C4C	-2.10	110.15	113.26
87	AN	822	CLA	O2A-CGA-O1A	-2.10	118.05	123.30
82	PJ	201	PEB	OD-C4D-C3D	-2.10	124.69	129.46
82	OF	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
82	VI	201	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	JJ	202	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	Y1	202	PEB	CAC-C2C-C1C	2.10	129.11	125.76
83	AE	302	PUB	CAB-C3B-C4B	2.10	129.11	125.76
85	B2	843	BCR	C28-C27-C26	-2.10	110.32	114.08
82	LQ	203	PEB	CHB-C4B-C3B	-2.10	120.45	125.32
87	5N	601	CLA	C2A-C1A-CHA	2.10	127.54	123.86
87	BN	805	CLA	CMD-C2D-C1D	-2.10	121.00	124.71
82	z8	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
82	WK	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
82	bH	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
82	xK	302	PEB	CAB-C3B-C4B	2.10	128.73	125.01
82	S5	202	PEB	OD-C4D-C3D	-2.10	124.69	129.46
82	RO	203	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	I5	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
103	8N	309	ZEX	C40-C33-C34	-2.10	119.98	122.92
82	FD	201	PEB	CHC-C1D-ND	-2.10	111.06	113.72
82	C5	201	PEB	CAC-CBC-CGC	-2.10	109.08	113.60
82	iO	202	PEB	CAC-CBC-CGC	-2.10	109.08	113.60
87	CL	510	CLA	O2D-CGD-CBD	2.10	115.01	111.27
87	BL	608	CLA	C2A-C1A-CHA	2.10	127.54	123.86
82	dG	204	PEB	CAA-C3A-C4A	-2.10	107.27	112.67
87	3N	313	CLA	CHA-C1A-NA	-2.10	121.58	126.40
82	TP	202	PEB	C3C-C4C-NC	2.10	110.23	108.33
82	Y1	201	PEB	C3C-C4C-NC	2.10	110.23	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	BL	608	CLA	CHC-C1C-NC	2.10	127.39	124.20
87	82	303	CLA	C2B-C1B-NB	2.10	111.64	110.23
82	IJ	202	PEB	C1B-C2B-C3B	-2.10	104.09	106.51
82	F5	202	PEB	C1B-C2B-C3B	-2.10	104.09	106.51
87	B2	816	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
82	kK	203	PEB	C1C-NC-C4C	-2.10	105.86	109.60
82	PI	201	PEB	C2A-C1A-NA	2.10	110.09	108.27
84	DG	1001	CYC	C3A-C4A-NA	2.10	115.02	110.53
87	A2	809	CLA	C3B-C4B-NB	-2.10	108.56	110.52
87	A2	828	CLA	O2D-CGD-CBD	2.10	115.00	111.27
82	RI	201	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	AE	301	PEB	CHB-C4B-NB	-2.10	120.20	124.58
82	dO	202	PEB	CHB-C1C-NC	-2.10	120.50	125.32
83	AO	303	PUB	CAC-C2C-C1C	2.10	128.73	125.01
82	A5	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	X9	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	A5	202	PEB	C1C-CHB-C4B	2.10	133.00	128.28
82	WK	202	PEB	C1D-CHC-C4C	-2.10	110.16	113.26
82	uF	201	PEB	C1D-CHC-C4C	2.10	116.36	113.26
87	b6	604	CLA	C1-C2-C3	-2.10	122.41	126.04
96	f6	101	HEM	CMB-C2B-C3B	-2.10	123.15	128.30
84	GG	1001	CYC	C4D-ND-C1D	-2.10	106.04	109.79
82	m4	203	PEB	CAC-CBC-CGC	-2.10	109.08	113.60
82	T5	201	PEB	CAC-CBC-CGC	-2.10	109.08	113.60
82	AA	201	PEB	C3B-C4B-NB	2.10	113.11	110.05
82	OH	203	PEB	C2B-C1B-NB	2.10	115.02	110.53
82	B7	203	PEB	OD-C4D-C3D	-2.10	124.70	129.46
82	M5	305	PEB	CBA-CAA-C3A	2.10	118.15	113.47
82	OA	202	PEB	CBB-CAB-C3B	-2.10	106.79	112.63
82	TK	202	PEB	CAC-CBC-CGC	-2.10	109.08	113.60
87	BN	815	CLA	CHC-C4B-NB	2.10	126.48	124.26
87	B2	806	CLA	CHC-C4B-NB	2.10	126.48	124.26
87	1N	607	CLA	CHB-C1B-NB	2.10	126.48	124.26
87	B2	835	CLA	C2A-C1A-CHA	2.10	127.53	123.86
82	N7	201	PEB	CAC-C2C-C1C	2.10	129.11	125.76
82	HA	202	PEB	C1D-CHC-C4C	-2.10	110.16	113.26
82	AQ	303	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	i4	202	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	jO	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	OE	203	PEB	C2B-C1B-NB	2.10	115.01	110.53
87	BN	807	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
82	G5	202	PEB	C1C-CHB-C4B	2.10	133.00	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	2N	312	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
82	XM	202	PEB	C1B-C2B-C3B	-2.10	104.09	106.51
87	32	309	CLA	CBA-CAA-C2A	2.10	120.07	113.86
87	aL	605	CLA	C6-C7-C8	-2.10	109.13	115.92
87	BN	813	CLA	C1-C2-C3	-2.10	122.41	126.04
82	FA	203	PEB	CHB-C1C-NC	-2.10	120.51	125.32
82	RD	203	PEB	CHB-C4B-NB	-2.10	120.20	124.58
82	WK	203	PEB	CHB-C1C-C2C	-2.10	122.41	127.15
87	3N	306	CLA	C3B-C4B-NB	-2.10	108.57	110.52
87	3N	309	CLA	CBA-CAA-C2A	2.10	120.06	113.86
82	J7	201	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
82	H9	202	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
82	d4	202	PEB	CHB-C1C-NC	-2.10	120.51	125.32
82	aG	201	PEB	CHB-C1C-NC	-2.10	120.51	125.32
82	d1	203	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	UE	202	PEB	CHA-C1B-NB	-2.10	120.54	124.93
82	lF	201	PEB	CHA-C1B-NB	-2.10	120.54	124.93
82	a1	202	PEB	CAA-C3A-C4A	2.10	118.07	112.67
82	aF	203	PEB	OD-C4D-ND	-2.10	122.82	125.93
82	RK	201	PEB	CMA-C2A-C1A	-2.10	107.88	112.40
82	sK	202	PEB	CHB-C1C-C2C	-2.10	122.41	127.15
82	aJ	203	PEB	CMB-C2B-C1B	2.10	128.30	125.06
87	BN	817	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
87	7N	603	CLA	C2A-C1A-CHA	2.10	127.53	123.86
82	FA	201	PEB	CAA-C3A-C4A	-2.10	107.28	112.67
82	ZG	201	PEB	C2B-C1B-NB	2.10	115.01	110.53
95	O6	301	DGD	O1G-C1A-C2A	2.10	118.50	111.91
87	CL	513	CLA	CHD-C1D-C2D	2.10	129.88	125.48
82	A1	302	PEB	C1D-CHC-C4C	-2.10	110.16	113.26
82	AI	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
82	ZG	203	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	G5	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	cJ	202	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	HA	201	PEB	CAB-CBB-CGB	-2.10	109.08	113.60
82	gF	202	PEB	CHC-C4C-NC	2.10	123.99	121.15
85	B2	842	BCR	C33-C5-C4	2.10	117.65	113.62
82	mO	203	PEB	CHA-C1B-NB	-2.10	120.54	124.93
82	J5	202	PEB	CHA-C4A-NA	-2.10	122.71	125.20
82	BI	201	PEB	CAA-C3A-C2A	-2.10	109.01	114.26
87	AN	806	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
82	DE	1002	PEB	CAC-C2C-C1C	2.10	129.10	125.76
82	KI	202	PEB	CAC-C2C-C1C	2.10	129.10	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	kM	202	PEB	O2B-CGB-CBB	2.10	120.77	114.03
84	GO	1001	CYC	CMB-C2B-C1B	2.10	126.79	124.17
82	AA	201	PEB	C1C-CHB-C4B	2.10	132.99	128.28
82	hJ	203	PEB	OD-C4D-ND	-2.10	122.82	125.93
82	KJ	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
82	b1	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
82	BB	203	PEB	CMA-C2A-C1A	-2.10	107.88	112.40
82	QF	201	PEB	OD-C4D-C3D	-2.10	124.71	129.46
82	a4	202	PEB	CMC-C3C-C4C	2.10	129.28	127.06
82	X7	202	PEB	CAA-C3A-C2A	-2.10	109.02	114.26
82	C5	202	PEB	C1C-CHB-C4B	2.10	132.99	128.28
87	A2	803	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
82	HM	202	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	E9	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	p8	201	PEB	OA-C1A-NA	2.10	127.48	124.94
82	oK	203	PEB	CAC-CBC-CGC	-2.10	109.09	113.60
82	JA	201	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
82	XK	201	PEB	C1C-CHB-C4B	2.10	132.99	128.28
82	K5	202	PEB	C1C-CHB-C4B	2.10	132.99	128.28
82	VK	202	PEB	CBC-CAC-C2C	2.10	118.46	112.63
87	CL	513	CLA	CHB-C1B-NB	2.10	126.48	124.26
87	6N	610	CLA	O2D-CGD-CBD	2.10	115.00	111.27
82	T7	202	PEB	CAC-C2C-C1C	2.10	129.10	125.76
82	ED	202	PEB	CHB-C1C-C2C	-2.10	122.42	127.15
95	a6	604	DGD	O5D-C6D-C5D	-2.10	105.17	109.05
87	BN	805	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
82	D5	201	PEB	CHA-C1B-NB	-2.10	120.55	124.93
87	F2	205	CLA	C1-O2A-CGA	2.10	121.95	116.44
84	CO	1001	CYC	C4D-ND-C1D	-2.10	106.05	109.79
85	c6	617	BCR	C12-C13-C14	2.10	122.16	118.94
82	XA	201	PEB	OD-C4D-C3D	-2.10	124.71	129.46
82	ID	201	PEB	OD-C4D-C3D	-2.10	124.71	129.46
87	72	603	CLA	C3B-C4B-NB	-2.10	108.57	110.52
87	KN	105	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
82	AG	301	PEB	CHA-C4A-NA	-2.10	122.71	125.20
82	eB	201	PEB	CHA-C4A-NA	2.10	127.70	125.20
82	OD	202	PEB	CHB-C1C-NC	-2.10	120.52	125.32
84	D1	1003	CYC	CHA-C1A-C2A	-2.10	120.47	125.32
103	82	309	ZEX	C19-C9-C10	-2.10	119.98	122.92
82	RO	201	PEB	CMA-C2A-C1A	-2.10	107.88	112.40
82	OA	201	PEB	C4C-C3C-C2C	-2.10	105.56	107.50
82	bK	202	PEB	C4C-C3C-C2C	-2.10	105.56	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DM	202	PEB	CAC-C2C-C1C	2.10	129.10	125.76
82	mH	202	PEB	CAC-C2C-C1C	2.10	129.10	125.76
82	BA	203	PEB	OD-C4D-C3D	-2.10	124.71	129.46
82	vF	202	PEB	OD-C4D-C3D	-2.10	124.71	129.46
87	C6	512	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
85	AL	401	BCR	C33-C5-C6	-2.10	122.17	124.53
85	AN	845	BCR	C33-C5-C6	-2.10	122.17	124.53
82	eJ	201	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
87	42	608	CLA	CAC-C3C-C4C	2.10	127.53	124.81
87	AN	808	CLA	C1-C2-C3	-2.10	122.42	126.04
85	cL	503	BCR	C35-C13-C12	2.10	121.38	118.08
82	SF	201	PEB	C2B-C1B-NB	2.10	115.00	110.53
82	JM	202	PEB	O2B-CGB-CBB	2.10	120.77	114.03
82	tK	203	PEB	C1D-CHC-C4C	2.10	116.35	113.26
82	LJ	201	PEB	CHA-C1B-C2B	2.10	130.29	124.90
82	cH	202	PEB	CHA-C4A-NA	2.10	127.70	125.20
87	B2	824	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
84	I4	1001	CYC	C4D-ND-C1D	-2.10	106.05	109.79
82	U5	201	PEB	CAC-C2C-C1C	2.10	129.10	125.76
82	dM	201	PEB	CAC-C2C-C1C	2.10	129.10	125.76
82	cE	201	PEB	CHB-C4B-C3B	-2.10	120.47	125.32
88	M6	101	LHG	O7-C7-O9	-2.10	118.64	123.70
82	OI	203	PEB	C3C-C4C-NC	2.10	110.22	108.33
82	f4	201	PEB	C3C-C4C-NC	2.10	110.22	108.33
82	jE	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
82	W9	201	PEB	CHA-C1B-C2B	-2.10	119.51	124.90
87	B2	808	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
87	82	303	CLA	O1A-CGA-CBA	2.10	129.82	123.08
85	BN	842	BCR	C33-C5-C4	2.10	117.64	113.62
82	HJ	201	PEB	C4C-C3C-C2C	-2.10	105.57	107.50
82	gO	202	PEB	C4C-C3C-C2C	-2.10	105.57	107.50
84	EG	1001	CYC	CHA-C1A-C2A	-2.10	120.47	125.32
87	A2	832	CLA	CHB-C1B-NB	2.10	126.48	124.26
82	VG	201	PEB	C2B-C1B-NB	2.10	115.00	110.53
87	B2	812	CLA	C1-C2-C3	-2.10	122.42	126.04
87	c6	609	CLA	C1-C2-C3	-2.10	122.42	126.04
82	YJ	203	PEB	CHA-C1B-NB	-2.10	120.55	124.93
84	u3	1001	CYC	C1B-NB-C4B	-2.10	108.00	110.67
82	WD	201	PEB	OD-C4D-C3D	-2.10	124.71	129.46
82	TG	201	PEB	CHA-C4A-NA	2.10	127.70	125.20
84	K1	1001	CYC	CHD-C4C-NC	2.10	127.70	125.20
82	O5	202	PEB	C1C-NC-C4C	-2.10	105.87	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	304	CLA	C2B-C1B-NB	2.10	111.64	110.23
82	CP	203	PEB	CHB-C1C-NC	-2.10	120.52	125.32
82	B5	203	PEB	CHC-C1D-ND	-2.10	111.07	113.72
87	BN	809	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
87	BN	825	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
82	c1	202	PEB	C3C-C4C-NC	2.10	110.22	108.33
82	iM	201	PEB	CBC-CAC-C2C	-2.10	106.81	112.63
82	PO	203	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
92	AL	411	LMG	C4-C3-C2	2.10	114.48	110.82
82	t8	201	PEB	CHB-C1C-NC	-2.10	120.52	125.32
84	GE	1001	CYC	CAD-CBD-CGD	-2.10	109.09	113.60
82	LP	202	PEB	C4C-C3C-C2C	-2.10	105.57	107.50
82	Z5	305	PEB	C4C-C3C-C2C	-2.10	105.57	107.50
82	K9	201	PEB	C4C-C3C-C2C	-2.10	105.57	107.50
82	kJ	202	PEB	C4C-C3C-C2C	-2.10	105.57	107.50
87	K6	101	CLA	O2D-CGD-CBD	2.10	114.99	111.27
82	SP	203	PEB	O2C-CGC-CBC	2.10	120.76	114.03
82	W1	201	PEB	C2B-C1B-NB	2.10	115.00	110.53
84	IE	1001	CYC	C4D-ND-C1D	-2.10	106.05	109.79
82	KI	202	PEB	C2A-C1A-NA	2.09	110.08	108.27
82	QE	202	PEB	CAC-CBC-CGC	-2.09	109.09	113.60
85	K6	102	BCR	C1-C6-C5	-2.09	119.66	122.61
84	I1	1001	CYC	CHB-C1B-NB	-2.09	121.56	126.06
82	G7	202	PEB	C2B-C1B-NB	2.09	115.00	110.53
87	B2	805	CLA	O2D-CGD-CBD	2.09	114.99	111.27
82	YO	201	PEB	CHB-C1C-NC	-2.09	120.52	125.32
82	LM	202	PEB	CAA-C3A-C2A	-2.09	109.03	114.26
84	E1	1001	CYC	C4D-ND-C1D	-2.09	106.05	109.79
82	SP	202	PEB	C1C-CHB-C4B	2.09	132.98	128.28
82	N5	202	PEB	C1C-CHB-C4B	2.09	132.98	128.28
82	UJ	203	PEB	C3C-C4C-NC	2.09	110.22	108.33
84	63	901	CYC	CBA-CAA-C2A	-2.09	106.81	112.63
82	hK	201	PEB	CHC-C1D-ND	-2.09	111.08	113.72
82	QB	203	PEB	OD-C4D-C3D	-2.09	124.72	129.46
82	X7	201	PEB	OD-C4D-C3D	-2.09	124.72	129.46
87	DL	403	CLA	O1A-CGA-CBA	2.09	131.90	123.73
82	N5	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
82	eG	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
82	m4	203	PEB	CHA-C1B-NB	-2.09	120.55	124.93
87	4N	604	CLA	O2D-CGD-CBD	2.09	114.99	111.27
87	5N	608	CLA	CHD-C1D-C2D	2.09	129.87	125.48
82	k1	201	PEB	CAC-CBC-CGC	-2.09	109.10	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gO	202	PEB	CAC-CBC-CGC	-2.09	109.10	113.60
87	ON	202	CLA	C1-C2-C3	-2.09	123.36	126.75
87	bL	606	CLA	C2D-C1D-ND	-2.09	108.56	110.10
82	K7	201	PEB	CMC-C3C-C4C	2.09	129.28	127.06
87	BN	835	CLA	C2A-C1A-CHA	2.09	127.52	123.86
82	QH	201	PEB	C2B-C1B-NB	2.09	115.00	110.53
82	AE	304	PEB	CMA-C2A-C1A	-2.09	107.89	112.40
82	XA	202	PEB	CHB-C1C-NC	2.09	130.12	125.32
82	j4	203	PEB	CAC-CBC-CGC	-2.09	109.10	113.60
82	jH	201	PEB	CHC-C1D-ND	-2.09	111.08	113.72
82	HI	203	PEB	C3C-C4C-NC	2.09	110.22	108.33
87	C6	520	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
82	LE	1002	PEB	CAA-C3A-C4A	-2.09	107.30	112.67
87	BN	802	CLA	O1D-CGD-CBD	2.09	128.77	124.48
87	12	608	CLA	C2A-C1A-CHA	2.09	127.51	123.85
82	E5	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
84	HG	1001	CYC	CBB-CAB-C3B	-2.09	106.66	112.43
82	NQ	204	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
82	GI	202	PEB	CAC-C2C-C1C	2.09	129.09	125.76
82	mO	201	PEB	C1D-CHC-C4C	-2.09	110.17	113.26
82	HK	202	PEB	C4B-NB-C1B	-2.09	102.57	106.51
82	f4	201	PEB	CMC-C3C-C4C	2.09	129.28	127.06
82	WQ	201	PEB	OD-C4D-C3D	-2.09	124.72	129.46
82	VE	201	PEB	C2B-C1B-NB	2.09	115.00	110.53
82	GK	201	PEB	C2B-C1B-NB	2.09	115.00	110.53
87	CL	508	CLA	CHC-C1C-NC	2.09	127.38	124.20
82	eM	202	PEB	CHB-C1C-NC	-2.09	120.53	125.32
84	EH	1001	CYC	CHD-C1D-C2D	2.09	132.63	127.49
82	W4	201	PEB	CHC-C1D-ND	-2.09	111.08	113.72
82	UP	203	PEB	CAB-C3B-C4B	2.09	128.71	125.01
82	E5	201	PEB	CAC-CBC-CGC	-2.09	109.10	113.60
87	82	302	CLA	CHD-C4C-NC	-2.09	120.91	124.20
82	oK	201	PEB	CMA-C2A-C1A	-2.09	107.89	112.40
87	7N	603	CLA	C3B-C4B-NB	-2.09	108.57	110.52
82	RD	202	PEB	CHB-C1C-C2C	-2.09	122.43	127.15
87	B2	816	CLA	C7-C6-C5	-2.09	107.68	113.36
87	32	305	CLA	CAA-CBA-CGA	-2.09	106.95	112.51
84	GG	1001	CYC	CAD-CBD-CGD	-2.09	109.10	113.60
82	B5	201	PEB	CAB-C3B-C2B	2.09	131.77	127.88
82	WF	202	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
87	2N	306	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
82	eH	201	PEB	C2B-C1B-NB	2.09	114.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	PA	201	PEB	CAC-C2C-C1C	2.09	129.09	125.76
82	OA	202	PEB	CAC-CBC-CGC	-2.09	109.10	113.60
82	WI	203	PEB	OA-C1A-C2A	-2.09	124.51	126.17
82	QE	203	PEB	OD-C4D-C3D	-2.09	124.72	129.46
82	KK	202	PEB	CBB-CAB-C3B	-2.09	106.82	112.63
88	i6	101	LHG	O8-C23-C24	2.09	118.47	111.91
82	YA	301	PEB	OD-C4D-ND	-2.09	122.83	125.93
87	AN	826	CLA	CHD-C1D-ND	-2.09	122.53	124.45
82	QE	201	PEB	C2B-C1B-NB	2.09	114.99	110.53
87	AN	805	CLA	C4-C3-C2	-2.09	118.31	123.68
87	c6	612	CLA	C1-C2-C3	-2.09	122.43	126.04
85	B2	840	BCR	C7-C6-C5	-2.09	116.40	121.46
82	N9	202	PEB	C3B-C4B-NB	2.09	113.09	110.05
82	W5	201	PEB	CMD-C2D-C3D	2.09	133.01	130.06
82	YH	201	PEB	C3C-C4C-NC	2.09	110.22	108.33
82	L1	1002	PEB	C3C-C4C-NC	2.09	110.22	108.33
82	fH	202	PEB	OD-C4D-C3D	-2.09	124.72	129.46
82	MK	201	PEB	CHB-C4B-C3B	-2.09	120.48	125.32
82	HM	202	PEB	CAC-C2C-C1C	2.09	129.09	125.76
85	I2	101	BCR	C2-C1-C6	2.09	113.70	110.48
82	cH	202	PEB	CMC-C3C-C4C	2.09	129.28	127.06
87	A6	402	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
82	P9	201	PEB	C2B-C1B-NB	2.09	114.99	110.53
82	fF	202	PEB	C2B-C1B-NB	2.09	114.99	110.53
82	gK	202	PEB	C2B-C1B-NB	2.09	114.99	110.53
82	f4	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
82	oF	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
84	LH	1001	CYC	CAB-C3B-C2B	2.09	131.10	127.53
96	f6	101	HEM	C3B-C2B-C1B	2.09	108.04	106.49
82	K5	201	PEB	CAC-CBC-CGC	-2.09	109.10	113.60
82	qK	203	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
87	DL	404	CLA	CHB-C4A-NA	2.09	127.40	124.51
85	bL	601	BCR	C37-C22-C23	2.09	121.37	118.08
82	KF	202	PEB	CBB-CAB-C3B	-2.09	106.82	112.63
82	YO	202	PEB	CAC-C2C-C1C	2.09	129.09	125.76
82	JI	202	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
82	lF	201	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
87	A2	805	CLA	C4-C3-C2	-2.09	118.32	123.68
87	cL	510	CLA	CMC-C2C-C3C	2.09	131.79	126.12
82	bP	501	PEB	C3C-C4C-NC	2.09	110.22	108.33
82	CI	201	PEB	CAC-C2C-C1C	2.09	129.09	125.76
82	XQ	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	P7	201	PEB	OD-C4D-C3D	-2.09	124.73	129.46
87	BN	823	CLA	C2D-C1D-ND	-2.09	108.56	110.10
82	aO	201	PEB	CAB-CBB-CGB	-2.09	109.11	113.60
82	Y9	203	PEB	CHB-C1C-NC	-2.09	120.53	125.32
82	aE	201	PEB	CHB-C1C-NC	-2.09	120.53	125.32
82	T4	202	PEB	C1C-NC-C4C	-2.09	105.88	109.60
82	u8	202	PEB	C2B-C1B-NB	2.09	114.99	110.53
82	nF	202	PEB	C2B-C1B-NB	2.09	114.99	110.53
82	dJ	201	PEB	C2B-C1B-NB	2.09	114.99	110.53
87	42	608	CLA	CED-O2D-CGD	2.09	120.66	115.94
87	AN	809	CLA	CHC-C4B-NB	2.09	126.47	124.26
87	52	601	CLA	CHB-C1B-NB	2.09	126.47	124.26
85	hL	102	BCR	C39-C30-C25	-2.09	106.91	110.30
87	C6	514	CLA	CHD-C1D-ND	-2.09	122.53	124.45
83	AJ	304	PUB	CAB-CBB-CGB	-2.09	109.11	113.60
82	dE	203	PEB	CHB-C1C-NC	-2.09	120.53	125.32
87	BN	833	CLA	C2A-C1A-CHA	2.09	127.51	123.86
82	NI	203	PEB	C1C-CHB-C4B	2.09	132.97	128.28
82	R5	202	PEB	C1C-CHB-C4B	2.09	132.97	128.28
82	p8	201	PEB	CHC-C4C-NC	2.09	123.98	121.15
82	YE	201	PEB	C2B-C1B-NB	2.09	114.99	110.53
87	B2	835	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
82	VK	202	PEB	CHB-C1C-NC	-2.09	120.53	125.32
82	QG	202	PEB	CAC-CBC-CGC	-2.09	109.11	113.60
82	R9	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
82	dH	203	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
82	T5	202	PEB	C1C-CHB-C4B	2.09	132.97	128.28
87	BN	820	CLA	C2A-C1A-CHA	2.09	127.51	123.86
82	A9	201	PEB	C2B-C1B-NB	2.09	114.99	110.53
95	cL	502	DGD	O6D-C5D-C6D	2.09	110.88	106.67
87	d6	403	CLA	O2D-CGD-CBD	2.09	114.98	111.27
82	X7	201	PEB	CHB-C1C-NC	-2.09	120.54	125.32
82	UH	203	PEB	CHA-C4A-NA	-2.09	122.72	125.20
82	VP	201	PEB	CHA-C4A-NA	2.09	127.69	125.20
87	B2	817	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
87	5N	610	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
82	VA	202	PEB	OA-C1A-NA	2.09	127.47	124.94
82	P5	202	PEB	C1C-CHB-C4B	2.09	132.97	128.28
87	AL	405	CLA	CHA-C4D-ND	2.09	136.87	132.50
82	fK	202	PEB	C2B-C1B-NB	2.09	114.98	110.53
82	i4	201	PEB	CHB-C4B-C3B	-2.09	120.49	125.32
87	B2	833	CLA	C2A-C1A-CHA	2.09	127.51	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	BP	201	PEB	O2B-CGB-CBB	2.09	120.74	114.03
82	ZI	401	PEB	CBC-CAC-C2C	-2.09	106.83	112.63
82	c4	203	PEB	CHC-C1D-ND	-2.09	111.08	113.72
82	U9	201	PEB	CHC-C1D-ND	-2.09	111.08	113.72
82	H7	201	PEB	CAB-CBB-CGB	-2.09	109.11	113.60
82	mO	203	PEB	CAC-CBC-CGC	-2.09	109.11	113.60
82	H5	203	PEB	OA-C1A-C2A	-2.09	124.51	126.17
82	WB	402	PEB	C3C-C4C-NC	2.09	110.21	108.33
82	PE	202	PEB	C3C-C4C-NC	2.09	110.21	108.33
82	w8	203	PEB	C3C-C4C-NC	2.09	110.21	108.33
87	A2	806	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
82	p8	201	PEB	CHB-C4B-C3B	-2.09	120.49	125.32
82	UM	201	PEB	C4C-C3C-C2C	-2.09	105.57	107.50
87	c6	604	CLA	CHB-C1B-NB	2.09	126.47	124.26
82	N7	203	PEB	CHA-C4A-NA	-2.09	122.72	125.20
82	RA	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
82	tK	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
82	Q9	203	PEB	CHB-C1C-NC	-2.09	120.54	125.32
82	dD	401	PEB	C1D-CHC-C4C	2.09	116.33	113.26
87	dL	409	CLA	C2A-C1A-CHA	2.09	127.51	123.86
85	BL	617	BCR	C35-C13-C14	-2.09	120.00	122.92
82	UJ	201	PEB	CAC-C2C-C1C	2.09	129.09	125.76
87	5N	609	CLA	CHA-C1A-NA	-2.09	121.62	126.40
82	R4	201	PEB	OD-C4D-C3D	-2.09	124.73	129.46
87	A2	806	CLA	CHD-C1D-ND	-2.09	122.54	124.45
87	B6	603	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
82	eO	202	PEB	CAB-CBB-CGB	-2.09	109.11	113.60
87	B2	801	CLA	O1D-CGD-CBD	2.09	128.75	124.48
87	AN	809	CLA	C3B-C4B-NB	-2.09	108.58	110.52
87	7N	604	CLA	C3B-C4B-NB	-2.09	108.58	110.52
82	LI	201	PEB	CHA-C1B-NB	-2.09	120.57	124.93
87	72	603	CLA	C2A-C1A-CHA	2.09	127.51	123.86
82	M5	301	PEB	CHC-C4C-NC	2.09	123.97	121.15
87	2N	306	CLA	O2D-CGD-CBD	2.09	114.98	111.27
82	gK	201	PEB	CHA-C4A-NA	2.09	127.69	125.20
82	f1	202	PEB	OD-C4D-C3D	-2.09	124.73	129.46
82	UM	201	PEB	CAC-C2C-C1C	2.09	129.09	125.76
83	YA	302	PUB	CAB-C3B-C4B	2.09	129.09	125.76
87	M2	101	CLA	CHB-C1B-NB	2.09	126.47	124.26
82	RG	201	PEB	C3C-C4C-NC	2.09	110.21	108.33
87	CL	509	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
82	SQ	201	PEB	C4C-C3C-C2C	-2.09	105.58	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	iO	203	PEB	C4C-C3C-C2C	-2.09	105.58	107.50
82	N5	201	PEB	CAC-CBC-CGC	-2.09	109.11	113.60
82	EM	202	PEB	O1C-CGC-CBC	-2.09	116.38	123.08
82	fM	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
82	kJ	202	PEB	CHA-C1B-NB	-2.09	120.57	124.93
85	BN	840	BCR	C7-C6-C5	-2.09	116.41	121.46
87	4N	608	CLA	CAC-C3C-C4C	2.09	127.52	124.81
82	MP	201	PEB	C4B-C3B-C2B	-2.09	104.47	106.78
82	YJ	202	PEB	CAC-C2C-C3C	2.09	131.85	127.07
82	a4	201	PEB	CMA-C2A-C1A	-2.09	107.91	112.40
82	CJ	203	PEB	C2B-C1B-NB	2.09	114.98	110.53
84	K1	1001	CYC	C3A-C4A-NA	2.09	114.98	110.53
82	L9	201	PEB	CHC-C4C-NC	2.09	123.97	121.15
84	HE	1001	CYC	CBB-CAB-C3B	-2.09	106.68	112.43
82	Y1	202	PEB	CHB-C1C-C2C	-2.09	122.44	127.15
87	22	606	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
82	m4	201	PEB	CHB-C4B-C3B	-2.09	120.49	125.32
82	T7	203	PEB	O1B-CGB-CBB	-2.09	116.38	123.08
82	b1	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
87	IN	102	CLA	CHB-C1B-NB	2.09	126.47	124.26
82	LI	202	PEB	CAB-CBB-CGB	-2.09	109.11	113.60
82	L9	201	PEB	CAA-C3A-C4A	-2.09	107.32	112.67
82	PD	201	PEB	C4C-C3C-C2C	-2.09	105.58	107.50
82	SQ	202	PEB	C4C-C3C-C2C	-2.09	105.58	107.50
82	R4	203	PEB	C4C-C3C-C2C	-2.09	105.58	107.50
82	rC	202	PEB	C4C-C3C-C2C	-2.09	105.58	107.50
82	iM	202	PEB	C4C-C3C-C2C	-2.09	105.58	107.50
82	IQ	202	PEB	CAC-C2C-C1C	2.09	129.08	125.76
95	b6	621	DGD	C1E-C2E-C3E	2.09	114.34	110.00
82	DD	202	PEB	OD-C4D-C3D	-2.09	124.74	129.46
82	CB	202	PEB	OA-C1A-C2A	-2.09	124.52	126.17
82	t8	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
82	FA	201	PEB	CHA-C4A-NA	2.08	127.68	125.20
87	AN	803	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
87	7N	604	CLA	CAC-C3C-C4C	2.08	127.52	124.81
82	LM	202	PEB	CAC-C2C-C1C	2.08	129.08	125.76
82	e1	201	PEB	C1D-CHC-C4C	-2.08	110.18	113.26
87	BN	802	CLA	CMC-C2C-C3C	2.08	131.78	126.12
84	F4	1001	CYC	CMB-C2B-C1B	2.08	126.77	124.17
84	DO	1001	CYC	CHA-C1A-C2A	-2.08	120.50	125.32
82	DD	202	PEB	C2A-C1A-NA	2.08	110.07	108.27
82	CK	203	PEB	CHA-C1B-NB	-2.08	120.57	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GB	202	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	JK	202	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	N4	1002	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	mH	201	PEB	CMC-C3C-C4C	2.08	129.27	127.06
82	QB	202	PEB	C3B-C4B-NB	2.08	113.08	110.05
85	b6	603	BCR	C11-C12-C13	-2.08	120.56	126.42
87	b6	611	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
82	UI	202	PEB	CHB-C1C-C2C	-2.08	122.45	127.15
87	F2	201	CLA	CHA-C1A-NA	-2.08	121.62	126.40
87	1N	611	CLA	CHA-C1A-NA	-2.08	121.62	126.40
82	YO	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
82	KM	203	PEB	CAA-C3A-C2A	-2.08	109.05	114.26
84	F1	1001	CYC	CBC-CAC-C3C	2.08	118.11	113.47
82	U9	203	PEB	CAA-C3A-C4A	-2.08	107.32	112.67
87	62	311	CLA	O2D-CGD-CBD	2.08	114.97	111.27
82	OH	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
82	X5	202	PEB	C1C-CHB-C4B	2.08	132.96	128.28
82	WM	201	PEB	CBA-CAA-C3A	2.08	118.11	113.47
82	NI	201	PEB	CAC-C2C-C1C	2.08	129.08	125.76
83	A1	304	PUB	CMB-C2B-C1B	-2.08	124.85	127.06
82	M7	201	PEB	C1D-CHC-C4C	2.08	116.33	113.26
95	c6	601	DGD	C6D-O5D-C1E	2.08	117.81	113.74
82	eK	202	PEB	CHA-C4A-NA	-2.08	122.73	125.20
82	YB	202	PEB	C3C-C4C-NC	2.08	110.21	108.33
82	V5	202	PEB	C1C-CHB-C4B	2.08	132.95	128.28
87	52	609	CLA	CHA-C1A-NA	-2.08	121.63	126.40
85	BN	839	BCR	C10-C11-C12	-2.08	116.72	123.22
82	dG	203	PEB	CHB-C1C-NC	-2.08	120.55	125.32
85	CL	516	BCR	C16-C15-C14	-2.08	119.21	123.47
82	AB	501	PEB	CAC-C2C-C1C	2.08	129.08	125.76
85	B2	839	BCR	C10-C11-C12	-2.08	116.72	123.22
82	M9	305	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
87	AN	824	CLA	CHD-C1D-ND	-2.08	122.54	124.45
82	AE	304	PEB	CHB-C1C-NC	-2.08	120.55	125.32
82	U4	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
82	ZG	202	PEB	OA-C1A-NA	2.08	127.46	124.94
87	A2	809	CLA	CBA-CAA-C2A	2.08	120.01	113.86
82	RQ	202	PEB	CHB-C1C-C2C	-2.08	122.45	127.15
82	UQ	202	PEB	CHB-C1C-C2C	-2.08	122.45	127.15
82	WI	201	PEB	C1B-C2B-C3B	-2.08	104.12	106.51
82	LG	1002	PEB	CAA-C3A-C4A	-2.08	107.33	112.67
82	X5	201	PEB	CAC-C2C-C1C	2.08	129.08	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	ZE	203	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	AO	305	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	CQ	202	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	X5	201	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	hM	203	PEB	C3C-C4C-NC	2.08	110.21	108.33
87	cL	505	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
82	GF	203	PEB	CAA-C3A-C2A	-2.08	109.06	114.26
82	qK	201	PEB	C1D-CHC-C4C	-2.08	110.19	113.26
84	DE	1001	CYC	C3A-C4A-NA	2.08	114.97	110.53
87	42	608	CLA	CHC-C4B-NB	2.08	126.46	124.26
87	B2	804	CLA	CMD-C2D-C1D	-2.08	121.04	124.71
82	lO	202	PEB	C4B-C3B-C2B	-2.08	104.48	106.78
87	6N	602	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
82	VF	202	PEB	CBC-CAC-C2C	2.08	118.41	112.63
87	BN	817	CLA	C7-C6-C5	-2.08	107.70	113.36
82	O9	202	PEB	CHA-C1B-C2B	2.08	130.25	124.90
82	IA	202	PEB	C2B-C1B-NB	2.08	114.97	110.53
82	E5	202	PEB	C1C-CHB-C4B	2.08	132.95	128.28
82	NF	201	PEB	C1B-C2B-C3B	-2.08	104.12	106.51
82	HI	203	PEB	CAC-CBC-CGC	-2.08	109.12	113.60
83	AE	303	PUB	CAB-CBB-CGB	-2.08	109.12	113.60
82	hJ	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
87	HL	101	CLA	C2A-C1A-CHA	2.08	127.50	123.86
87	nL	101	CLA	C2A-C1A-CHA	2.08	127.50	123.86
82	WA	201	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	GQ	202	PEB	C3C-C4C-NC	2.08	110.21	108.33
82	gO	201	PEB	C3C-C4C-NC	2.08	110.21	108.33
82	MM	201	PEB	CAC-C2C-C1C	2.08	129.08	125.76
82	GD	201	PEB	CHB-C1C-C2C	-2.08	122.46	127.15
82	NA	201	PEB	CAC-CBC-CGC	-2.08	109.13	113.60
87	A2	822	CLA	C3B-C4B-NB	-2.08	108.58	110.52
82	PI	201	PEB	CAC-C2C-C1C	2.08	129.07	125.76
82	SF	202	PEB	OA-C1A-C2A	-2.08	124.52	126.17
82	A7	201	PEB	C3B-C4B-NB	2.08	113.08	110.05
87	c6	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
92	A6	408	LMG	O8-C28-O10	-2.08	118.34	123.59
82	ED	202	PEB	CHC-C4C-NC	2.08	123.96	121.15
82	gK	201	PEB	CHC-C4C-NC	2.08	123.96	121.15
82	HK	201	PEB	C2B-C1B-NB	2.08	114.97	110.53
87	BN	826	CLA	CHB-C1B-NB	2.08	126.46	124.26
87	c6	608	CLA	CHB-C1B-NB	2.08	126.46	124.26
87	JN	101	CLA	C2A-C1A-CHA	2.08	127.50	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	A4	305	PEB	CHC-C1D-ND	-2.08	111.09	113.72
82	GK	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60
82	P5	201	PEB	CAC-CBC-CGC	-2.08	109.13	113.60
82	O7	202	PEB	CAC-CBC-CGC	-2.08	109.13	113.60
82	PO	201	PEB	CMA-C2A-C1A	-2.08	107.92	112.40
82	FM	202	PEB	CHB-C1C-NC	-2.08	120.56	125.32
87	8N	301	CLA	CHA-C4D-ND	2.08	136.85	132.50
87	bL	615	CLA	C2A-C1A-CHA	2.08	127.50	123.86
85	A2	845	BCR	C33-C5-C6	-2.08	122.19	124.53
87	FN	203	CLA	CHA-C1A-NA	-2.08	121.64	126.40
87	1N	608	CLA	C2A-C1A-CHA	2.08	127.48	123.85
82	KA	201	PEB	CAC-C2C-C3C	-2.08	122.31	127.07
85	BL	618	BCR	C1-C6-C5	-2.08	119.69	122.61
82	IP	201	PEB	C2B-C1B-NB	2.08	114.97	110.53
82	U9	202	PEB	CHC-C1D-ND	-2.08	111.09	113.72
87	A2	835	CLA	CHB-C1B-NB	2.08	126.46	124.26
92	D6	409	LMG	O8-C28-C29	2.08	118.43	111.91
82	XM	202	PEB	CAC-CBC-CGC	-2.08	109.13	113.60
82	kF	201	PEB	OA-C1A-C2A	-2.08	124.52	126.17
84	I1	1001	CYC	CHA-C1A-C2A	-2.08	120.51	125.32
82	P5	201	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	W7	201	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
84	HH	1001	CYC	CBA-CAA-C2A	-2.08	106.85	112.63
87	bL	616	CLA	CHA-C1A-NA	-2.08	121.64	126.40
82	ZM	202	PEB	C1B-C2B-C3B	-2.08	104.12	106.51
82	eH	203	PEB	C3C-C4C-NC	2.08	110.20	108.33
82	YO	203	PEB	CHB-C1C-C2C	-2.08	122.46	127.15
82	sK	203	PEB	CMA-C2A-C1A	-2.08	107.92	112.40
82	HI	201	PEB	CHB-C1C-NC	-2.08	120.56	125.32
82	fE	202	PEB	C2A-C1A-NA	2.08	110.06	108.27
82	bK	202	PEB	CHC-C4C-NC	-2.08	118.33	121.15
82	a4	203	PEB	C1D-CHC-C4C	-2.08	110.19	113.26
82	Z9	304	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
82	JK	202	PEB	C4B-NB-C1B	-2.08	102.59	106.51
82	KM	203	PEB	CAC-C2C-C1C	2.08	129.07	125.76
82	SM	203	PEB	CAC-C2C-C1C	2.08	129.07	125.76
82	WO	201	PEB	CHC-C1D-ND	-2.08	111.09	113.72
87	B2	813	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
82	R9	201	PEB	C2B-C1B-NB	2.08	114.96	110.53
87	CL	507	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
87	BN	833	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
85	BN	842	BCR	C1-C6-C7	2.08	121.66	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	8N	304	CLA	O1A-CGA-CBA	2.08	129.76	123.08
82	JM	201	PEB	C1B-C2B-C3B	-2.08	104.12	106.51
82	NP	202	PEB	CAB-C3B-C4B	2.08	128.68	125.01
82	GP	201	PEB	CBD-CAD-C3D	-2.08	117.28	127.62
82	Z1	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
82	hE	203	PEB	C2B-C1B-NB	2.08	114.96	110.53
85	cL	518	BCR	C10-C11-C12	-2.08	116.73	123.22
82	D5	202	PEB	C3C-C4C-NC	2.08	110.20	108.33
87	bL	617	CLA	O2D-CGD-CBD	2.08	114.96	111.27
82	mO	201	PEB	CHB-C4B-C3B	-2.08	120.51	125.32
82	Q5	203	PEB	CAC-CBC-CGC	-2.08	109.13	113.60
82	A9	201	PEB	CHC-C1D-ND	-2.08	111.10	113.72
87	KN	102	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
82	lF	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
87	6N	611	CLA	CHD-C1D-ND	-2.08	122.55	124.45
82	VQ	201	PEB	C1D-CHC-C4C	-2.08	110.19	113.26
88	iL	101	LHG	C5-O7-C7	2.08	122.91	117.79
87	F2	205	CLA	CAC-C3C-C4C	2.08	127.50	124.81
96	V6	201	HEM	CHA-C1A-NA	2.08	127.67	123.85
82	QP	203	PEB	CAA-C3A-C4A	-2.08	107.34	112.67
91	a6	613	PHO	CMC-C2C-C1C	2.08	128.65	124.73
82	PQ	202	PEB	CHC-C1D-ND	-2.08	111.10	113.72
82	WF	201	PEB	CAB-C3B-C4B	2.08	128.68	125.01
82	YQ	201	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	h4	202	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	TO	202	PEB	C1C-NC-C4C	-2.08	105.90	109.60
85	KN	104	BCR	C16-C15-C14	-2.08	119.22	123.47
82	lK	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
87	c6	615	CLA	O2D-CGD-CBD	2.08	114.96	111.27
87	12	604	CLA	C2A-C1A-CHA	2.08	127.49	123.86
87	B2	819	CLA	C2A-C1A-CHA	2.08	127.49	123.86
87	dL	401	CLA	C2A-C1A-CHA	2.08	127.49	123.86
84	IO	1001	CYC	C4D-ND-C1D	-2.08	106.08	109.79
82	j1	203	PEB	CHB-C4B-NB	-2.08	120.26	124.58
85	hL	102	BCR	C21-C20-C19	-2.08	116.74	123.22
84	V3	1001	CYC	OC-C1C-C2C	-2.08	124.52	126.17
82	l4	202	PEB	CBB-CAB-C3B	-2.08	106.86	112.63
87	C6	512	CLA	CHD-C1D-ND	-2.08	122.55	124.45
87	A2	801	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
84	J4	1001	CYC	O2A-CGA-CBA	2.08	120.70	114.03
82	jH	203	PEB	CHB-C4B-NB	-2.08	120.26	124.58
82	R4	201	PEB	CMA-C2A-C1A	-2.08	107.93	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FA	203	PEB	CHC-C1D-ND	-2.08	111.10	113.72
82	W1	203	PEB	CHC-C1D-ND	-2.08	111.10	113.72
82	BI	202	PEB	CBA-CAA-C3A	-2.08	108.84	113.47
82	oF	202	PEB	CAC-CBC-CGC	-2.08	109.14	113.60
82	qF	203	PEB	CAB-CBB-CGB	-2.08	109.14	113.60
82	RP	201	PEB	CHA-C4A-NA	2.08	127.67	125.20
82	L5	203	PEB	CHA-C4A-NA	-2.08	122.74	125.20
82	O9	203	PEB	CAA-C3A-C4A	2.08	118.00	112.67
82	EB	501	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	JF	202	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	VJ	201	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	x8	202	PEB	C4C-C3C-C2C	-2.08	105.58	107.50
82	DP	202	PEB	CAB-C3B-C4B	2.08	128.68	125.01
83	M9	303	PUB	CBD-CAD-C3D	-2.08	106.71	112.43
88	l6	101	LHG	O7-C7-O9	-2.08	118.69	123.70
82	SK	201	PEB	C2B-C1B-NB	2.08	114.96	110.53
87	1N	604	CLA	C2A-C1A-CHA	2.08	127.49	123.86
87	52	608	CLA	CHD-C1D-C2D	2.08	129.83	125.48
87	8N	303	CLA	CHD-C4C-NC	-2.08	120.94	124.20
82	WP	201	PEB	CHB-C1C-C2C	-2.08	122.47	127.15
82	RI	201	PEB	C2A-C1A-NA	2.08	110.06	108.27
82	XI	201	PEB	C2A-C1A-NA	2.08	110.06	108.27
87	A2	826	CLA	C3B-C4B-NB	-2.08	108.59	110.52
87	nL	101	CLA	C3B-C4B-NB	-2.08	108.59	110.52
85	B2	839	BCR	C33-C5-C4	2.07	117.60	113.62
85	JN	103	BCR	C38-C26-C25	-2.07	122.20	124.53
82	a1	201	PEB	CHA-C1B-NB	-2.07	120.59	124.93
82	Z1	201	PEB	CAC-CBC-CGC	-2.07	109.14	113.60
82	PF	201	PEB	CHB-C1C-C2C	-2.07	122.47	127.15
85	H6	101	BCR	C34-C9-C8	2.07	121.35	118.08
82	T4	203	PEB	CMB-C2B-C1B	2.07	128.26	125.06
83	Y7	302	PUB	CAB-C3B-C4B	2.07	129.07	125.76
87	BN	812	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
82	AG	304	PEB	CMA-C2A-C1A	-2.07	107.93	112.40
82	DH	1002	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	A9	201	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	fO	201	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	hE	201	PEB	C1D-CHC-C4C	2.07	116.31	113.26
87	AN	825	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
82	jH	201	PEB	C2B-C1B-NB	2.07	114.96	110.53
87	d6	403	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
82	dO	201	PEB	C2A-C1A-NA	2.07	110.06	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	U1	203	PEB	CHA-C4A-NA	-2.07	122.74	125.20
82	AD	301	PEB	OD-C4D-ND	-2.07	122.86	125.93
87	A2	827	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
82	nF	201	PEB	CHA-C1B-C2B	2.07	130.23	124.90
82	PP	201	PEB	CHB-C4B-C3B	-2.07	120.52	125.32
82	HD	201	PEB	CAA-C3A-C4A	-2.07	107.35	112.67
82	AD	303	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	C9	201	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	TI	202	PEB	CAC-C2C-C1C	2.07	129.06	125.76
87	H6	102	CLA	C1-C2-C3	-2.07	122.46	126.04
82	NA	201	PEB	CAB-C3B-C4B	2.07	128.68	125.01
82	ZH	201	PEB	CAB-C3B-C4B	2.07	128.68	125.01
82	QH	202	PEB	C3C-C4C-NC	2.07	110.20	108.33
82	Z5	305	PEB	CBA-CAA-C3A	2.07	118.08	113.47
85	BN	843	BCR	C33-C5-C6	-2.07	122.20	124.53
82	L9	202	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
92	DL	402	LMG	O6-C1-O1	-2.07	105.06	109.97
82	j1	201	PEB	CHC-C1D-ND	-2.07	111.10	113.72
85	AL	401	BCR	C11-C12-C13	-2.07	120.59	126.42
82	GQ	201	PEB	CHC-C4C-NC	2.07	123.95	121.15
82	zC	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
82	PA	201	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
82	dF	201	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
84	JO	1001	CYC	O2A-CGA-CBA	2.07	120.69	114.03
87	72	608	CLA	CHB-C4A-NA	2.07	127.38	124.51
82	RA	203	PEB	OD-C4D-ND	-2.07	122.86	125.93
82	SQ	202	PEB	OD-C4D-ND	-2.07	122.86	125.93
82	PJ	202	PEB	CAC-CBC-CGC	-2.07	109.14	113.60
82	X7	201	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
82	aH	201	PEB	CHA-C1B-NB	-2.07	120.60	124.93
87	AN	803	CLA	CHB-C1B-NB	2.07	126.45	124.26
82	VF	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	g4	203	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	aB	201	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
84	L1	1001	CYC	O1D-CGD-CBD	-2.07	116.42	123.08
82	JJ	202	PEB	CHA-C4A-NA	-2.07	122.74	125.20
82	WK	201	PEB	CHA-C1B-C2B	2.07	130.23	124.90
87	3N	301	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
82	JA	203	PEB	CAC-C2C-C1C	2.07	129.06	125.76
82	GD	202	PEB	C3C-C4C-NC	2.07	110.20	108.33
82	DF	202	PEB	C2B-C1B-NB	2.07	114.95	110.53
82	cK	202	PEB	OD-C4D-C3D	-2.07	124.77	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GK	202	PEB	CMC-C3C-C4C	2.07	129.26	127.06
82	oK	202	PEB	CAC-CBC-CGC	-2.07	109.14	113.60
82	SE	201	PEB	CHB-C4B-C3B	-2.07	120.53	125.32
82	u8	203	PEB	C3B-C4B-NB	2.07	113.06	110.05
87	62	313	CLA	CHA-C1A-NA	-2.07	121.65	126.40
87	AN	827	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
87	BL	604	CLA	C3B-C4B-NB	-2.07	108.59	110.52
87	3N	311	CLA	C3B-C4B-NB	-2.07	108.59	110.52
82	D9	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
82	kO	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
87	O2	202	CLA	C1-C2-C3	-2.07	123.40	126.75
82	TH	202	PEB	CHC-C4C-NC	2.07	123.95	121.15
82	pC	201	PEB	CHC-C4C-NC	2.07	123.95	121.15
82	MJ	203	PEB	CMC-C3C-C2C	2.07	130.09	125.61
82	PA	201	PEB	OD-C4D-C3D	-2.07	124.77	129.46
82	tF	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
82	WB	401	PEB	C3C-C4C-NC	2.07	110.20	108.33
85	BN	843	BCR	C28-C27-C26	-2.07	110.38	114.08
87	CL	507	CLA	C2A-C1A-CHA	2.07	127.48	123.86
85	K2	105	BCR	C16-C15-C14	-2.07	119.23	123.47
87	c6	604	CLA	CHD-C1D-ND	-2.07	122.55	124.45
82	X9	201	PEB	CHC-C1D-ND	-2.07	111.11	113.72
87	82	306	CLA	CHA-C4D-ND	2.07	136.83	132.50
87	AN	837	CLA	O2D-CGD-CBD	2.07	114.95	111.27
87	62	303	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
94	d6	408	PL9	C20-C19-C18	-2.07	118.37	123.68
82	KB	304	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	MD	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	LM	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	G9	201	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	e4	202	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
87	FN	205	CLA	CAC-C3C-C4C	2.07	127.50	124.81
82	pC	202	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
82	PG	202	PEB	C3C-C4C-NC	2.07	110.20	108.33
82	LM	202	PEB	O1B-CGB-CBB	-2.07	116.43	123.08
87	A2	825	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
82	IB	202	PEB	CBC-CAC-C2C	-2.07	106.88	112.63
82	vF	201	PEB	CAA-C3A-C4A	-2.07	107.36	112.67
82	Z5	301	PEB	CHC-C4C-NC	2.07	123.95	121.15
82	uC	202	PEB	C2B-C1B-NB	2.07	114.95	110.53
82	yK	301	PEB	CHC-C1D-ND	-2.07	111.11	113.72
87	62	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	K2	106	CLA	CHD-C1D-ND	-2.07	122.55	124.45
87	K2	103	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
82	MD	201	PEB	C2A-C1A-NA	2.07	110.06	108.27
82	lE	203	PEB	CAB-C3B-C4B	2.07	128.67	125.01
82	X9	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
84	N1	1001	CYC	CAA-CBA-CGA	2.07	118.06	113.60
82	F9	203	PEB	CAC-CBC-CGC	-2.07	109.15	113.60
82	NM	201	PEB	CHA-C1B-C2B	2.07	130.22	124.90
87	b6	610	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
82	VF	202	PEB	CHC-C4C-NC	2.07	123.95	121.15
82	aO	201	PEB	CMA-C2A-C1A	-2.07	107.94	112.40
82	PO	203	PEB	CAC-C2C-C1C	2.07	129.06	125.76
82	e1	201	PEB	CAC-C2C-C1C	2.07	129.06	125.76
82	E9	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
87	22	609	CLA	CHD-C4C-C3C	2.07	127.88	124.84
82	XA	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
82	g1	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
82	GK	203	PEB	CAA-C3A-C2A	-2.07	109.09	114.26
82	J1	1002	PEB	CAA-C3A-C4A	-2.07	107.36	112.67
87	3N	307	CLA	CHC-C4B-NB	2.07	126.45	124.26
87	32	303	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
82	wK	301	PEB	OD-C4D-C3D	-2.07	124.77	129.46
82	VG	202	PEB	C1C-CHB-C4B	-2.07	123.64	128.28
82	II	203	PEB	OD-C4D-ND	-2.07	122.87	125.93
82	mG	203	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
82	N9	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
82	MB	202	PEB	CHB-C4B-NB	-2.07	120.27	124.58
83	AM	303	PUB	CAC-C2C-C1C	2.07	128.67	125.01
82	i4	202	PEB	C1C-NC-C4C	-2.07	105.92	109.60
87	22	606	CLA	O2D-CGD-CBD	2.07	114.94	111.27
82	RA	203	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	QB	204	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	CJ	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	D9	201	PEB	C4B-NB-C1B	-2.07	102.61	106.51
87	A2	840	CLA	CAC-C3C-C4C	2.07	127.49	124.81
82	TD	201	PEB	C3B-C4B-NB	2.07	113.06	110.05
82	jH	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
82	JJ	202	PEB	O2B-CGB-CBB	2.07	120.67	114.03
82	RM	201	PEB	CMA-C2A-C1A	-2.07	107.95	112.40
82	KJ	201	PEB	OA-C1A-NA	2.07	127.45	124.94
93	A6	409	BCT	O3-C-O1	-2.07	114.18	119.55
87	52	602	CLA	CHD-C1D-ND	-2.07	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	e1	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
87	BL	619	CLA	C3B-C4B-NB	-2.07	108.60	110.52
87	A2	806	CLA	C3B-C4B-NB	-2.07	108.60	110.52
82	AQ	301	PEB	CHA-C4A-NA	-2.07	122.75	125.20
82	DQ	202	PEB	OD-C4D-C3D	-2.07	124.78	129.46
82	eJ	202	PEB	CMA-C2A-C1A	-2.07	107.95	112.40
82	p8	201	PEB	CAC-C2C-C1C	2.07	129.05	125.76
82	wK	301	PEB	CAC-C2C-C1C	2.07	129.05	125.76
87	bL	613	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
82	CI	201	PEB	C2A-C1A-NA	2.07	110.06	108.27
85	JN	103	BCR	C28-C27-C26	-2.07	110.39	114.08
82	OJ	201	PEB	C1D-CHC-C4C	-2.07	110.21	113.26
87	32	311	CLA	CHA-C1A-NA	-2.07	121.66	126.40
82	AP	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	hO	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	V9	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
95	AL	414	DGD	C6D-O5D-C1E	-2.07	109.70	113.74
82	RQ	203	PEB	CHB-C4B-NB	-2.07	120.28	124.58
82	gO	203	PEB	CHB-C4B-NB	-2.07	120.28	124.58
87	B6	605	CLA	CHB-C1B-NB	2.07	126.44	124.26
92	m6	103	LMG	O8-C28-O10	-2.07	118.38	123.59
82	KB	301	PEB	CMC-C3C-C2C	2.07	130.08	125.61
82	R7	202	PEB	CAB-C3B-C4B	2.07	128.66	125.01
82	CM	203	PEB	C2B-C1B-NB	2.07	114.94	110.53
82	aM	201	PEB	C1D-CHC-C4C	-2.07	110.21	113.26
92	j6	101	LMG	C1-O6-C5	-2.07	109.63	113.69
82	JH	1002	PEB	CAA-C3A-C4A	-2.07	107.37	112.67
87	A2	825	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
82	WK	202	PEB	O1C-CGC-CBC	-2.07	116.44	123.08
82	ZE	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
82	G9	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
82	X7	202	PEB	CAB-C3B-C4B	2.07	128.66	125.01
82	GQ	201	PEB	CHB-C1C-C2C	-2.07	122.49	127.15
82	hF	201	PEB	C2A-C1A-NA	2.07	110.05	108.27
82	kJ	202	PEB	C2A-C1A-NA	2.07	110.05	108.27
82	UJ	202	PEB	OA-C1A-NA	2.07	127.44	124.94
82	SD	202	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	OM	201	PEB	C4C-C3C-C2C	-2.07	105.59	107.50
82	AI	203	PEB	CHB-C4B-NB	-2.07	120.28	124.58
82	iH	201	PEB	C4B-NB-C1B	-2.07	102.62	106.51
82	OK	201	PEB	CHB-C1C-NC	2.07	130.05	125.32
82	J9	202	PEB	CAA-C3A-C2A	-2.07	109.10	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	cL	503	BCR	C4-C5-C6	-2.07	119.73	122.73
82	g4	201	PEB	C3C-C4C-NC	2.07	110.19	108.33
82	W9	202	PEB	C3C-C4C-NC	2.07	110.19	108.33
82	VO	201	PEB	CMA-C2A-C1A	-2.07	107.95	112.40
87	B2	811	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
87	d6	406	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
82	I9	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
82	hG	203	PEB	C2B-C1B-NB	2.07	114.94	110.53
87	B2	812	CLA	C2A-C1A-CHA	2.07	127.47	123.86
82	UB	302	PEB	C1D-CHC-C4C	2.07	116.30	113.26
87	1N	606	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
83	xF	306	PUB	CHC-C1D-ND	-2.06	111.11	113.72
82	DA	202	PEB	CBD-CAD-C3D	-2.06	117.35	127.62
82	DP	201	PEB	CAB-C3B-C4B	2.06	128.66	125.01
87	22	608	CLA	CHC-C4B-NB	2.06	126.44	124.26
87	b6	613	CLA	CHC-C4B-NB	2.06	126.44	124.26
82	i4	201	PEB	C4C-C3C-C2C	-2.06	105.59	107.50
82	T9	201	PEB	C4C-C3C-C2C	-2.06	105.59	107.50
82	gO	203	PEB	C4C-C3C-C2C	-2.06	105.59	107.50
82	bF	201	PEB	CHA-C4A-NA	2.06	127.66	125.20
82	m1	202	PEB	CAC-C2C-C1C	2.06	129.05	125.76
82	mH	201	PEB	CAC-C2C-C1C	2.06	129.05	125.76
82	EJ	203	PEB	C2B-C1B-NB	2.06	114.94	110.53
82	O1	203	PEB	C2B-C1B-NB	2.06	114.94	110.53
82	a1	201	PEB	OD-C4D-C3D	-2.06	124.78	129.46
84	BE	1001	CYC	OB-C4B-NB	-2.06	120.28	125.08
82	RF	201	PEB	CMA-C2A-C1A	-2.06	107.95	112.40
82	EB	501	PEB	C3C-C4C-NC	2.06	110.19	108.33
82	CP	202	PEB	C3C-C4C-NC	2.06	110.19	108.33
82	xK	304	PEB	CMB-C2B-C1B	2.06	128.24	125.06
84	G4	1001	CYC	OC-C1C-NC	2.06	127.44	124.94
87	B6	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
87	12	606	CLA	O2A-CGA-O1A	-2.06	118.15	123.30
82	PK	201	PEB	CHB-C1C-C2C	-2.06	122.49	127.15
82	BK	201	PEB	C1C-CHB-C4B	2.06	132.91	128.28
82	D4	1002	PEB	C1C-CHB-C4B	2.06	132.91	128.28
82	YO	201	PEB	CAC-C2C-C1C	2.06	129.05	125.76
84	C4	1001	CYC	CHB-C1B-NB	-2.06	121.63	126.06
82	F7	203	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	I9	201	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	V9	201	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	U7	202	PEB	C1D-CHC-C4C	-2.06	110.21	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	A2	841	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
82	YO	202	PEB	CMC-C3C-C4C	2.06	129.25	127.06
87	bL	608	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
82	M9	304	PEB	OA-C1A-NA	2.06	127.44	124.94
82	XF	203	PEB	CHA-C1B-NB	-2.06	120.62	124.93
82	QP	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
82	WM	201	PEB	CHC-C1D-ND	-2.06	111.11	113.72
82	xC	202	PEB	O2B-CGB-CBB	2.06	120.66	114.03
82	UD	202	PEB	CHB-C1C-C2C	-2.06	122.50	127.15
82	GJ	201	PEB	C3C-C4C-NC	2.06	110.19	108.33
82	DF	201	PEB	OD-C4D-C3D	-2.06	124.79	129.46
82	OH	202	PEB	OD-C4D-C3D	-2.06	124.79	129.46
82	iF	202	PEB	C2B-C1B-NB	2.06	114.93	110.53
84	LE	1001	CYC	CMD-C2D-C1D	2.06	128.58	125.56
87	B2	833	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
87	cL	506	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
87	5N	610	CLA	CHD-C1D-ND	-2.06	122.56	124.45
82	iG	202	PEB	CHA-C4A-NA	-2.06	122.75	125.20
87	42	604	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
82	UA	202	PEB	C1D-CHC-C4C	-2.06	110.21	113.26
87	32	308	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
82	WF	203	PEB	CHB-C1C-C2C	-2.06	122.50	127.15
82	jO	202	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	DB	201	PEB	CAB-C3B-C4B	2.06	128.66	125.01
85	C6	507	BCR	C23-C24-C25	-2.06	121.41	127.20
82	SK	202	PEB	OA-C1A-C2A	-2.06	124.53	126.17
87	CL	506	CLA	C6-C7-C8	-2.06	109.25	115.92
82	KJ	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
82	OP	202	PEB	C2A-C1A-NA	2.06	110.05	108.27
82	MD	201	PEB	C1C-CHB-C4B	2.06	132.91	128.28
87	BN	813	CLA	C2A-C1A-CHA	2.06	127.47	123.86
82	eJ	202	PEB	CHB-C1C-NC	-2.06	120.60	125.32
82	NJ	202	PEB	CAC-C2C-C1C	2.06	129.05	125.76
82	Y9	203	PEB	CAC-C2C-C1C	2.06	129.05	125.76
87	2N	307	CLA	CBC-CAC-C3C	2.06	118.12	112.43
87	BN	836	CLA	CHD-C1D-ND	-2.06	122.56	124.45
84	EG	1001	CYC	OB-C4B-NB	-2.06	120.29	125.08
87	BN	806	CLA	O2D-CGD-CBD	2.06	114.93	111.27
82	HM	202	PEB	CAB-CBB-CGB	2.06	118.04	113.60
82	TM	202	PEB	O2B-CGB-CBB	2.06	120.65	114.03
87	b6	605	CLA	CHC-C4B-C3B	-2.06	118.54	127.71
82	uC	203	PEB	C3B-C4B-NB	2.06	113.05	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	hB	301	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
87	ON	201	CLA	C2A-C1A-CHA	2.06	127.45	123.85
82	UO	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
82	W7	201	PEB	C1C-NC-C4C	-2.06	105.93	109.60
82	CP	201	PEB	CAB-C3B-C4B	2.06	128.66	125.01
82	PJ	202	PEB	C1B-C2B-C3B	-2.06	104.14	106.51
87	BN	814	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
82	jH	202	PEB	CHA-C1B-C2B	2.06	130.20	124.90
82	DA	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
82	x8	201	PEB	C2A-C1A-NA	2.06	110.05	108.27
82	CQ	201	PEB	CBC-CAC-C2C	2.06	118.35	112.63
82	SG	201	PEB	CHB-C4B-C3B	-2.06	120.55	125.32
84	FH	1001	CYC	CBC-CAC-C3C	2.06	118.06	113.47
82	RF	202	PEB	CHC-C1D-ND	-2.06	111.12	113.72
82	TP	202	PEB	CHC-C1D-ND	-2.06	111.12	113.72
92	BL	612	LMG	O6-C5-C6	2.06	111.56	106.44
82	AM	301	PEB	C1D-CHC-C4C	-2.06	110.22	113.26
82	aO	203	PEB	C1D-CHC-C4C	-2.06	110.22	113.26
82	fF	202	PEB	CHC-C4C-NC	-2.06	118.36	121.15
82	GJ	203	PEB	C1C-NC-C4C	-2.06	105.93	109.60
82	YJ	202	PEB	CAB-C3B-C4B	2.06	128.65	125.01
82	OI	201	PEB	C2B-C1B-NB	2.06	114.93	110.53
82	TB	201	PEB	CAA-C3A-C4A	-2.06	107.38	112.67
82	RA	203	PEB	CAB-C3B-C2B	2.06	131.72	127.88
82	WH	203	PEB	CMC-C3C-C4C	2.06	129.25	127.06
82	iE	202	PEB	CMA-C2A-C1A	-2.06	107.96	112.40
82	KB	301	PEB	CHB-C1C-C2C	-2.06	122.50	127.15
82	UA	201	PEB	CHB-C4B-NB	-2.06	120.29	124.58
82	iE	202	PEB	CHA-C4A-NA	-2.06	122.75	125.20
82	YB	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
85	c6	602	BCR	C16-C15-C14	-2.06	119.25	123.47
82	AG	304	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	pC	202	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
87	6N	608	CLA	O1D-CGD-CBD	2.06	128.70	124.48
82	QJ	202	PEB	C2B-C1B-NB	2.06	114.93	110.53
82	ZB	201	PEB	CAC-C2C-C1C	2.06	129.04	125.76
82	KI	202	PEB	CHC-C4C-NC	2.06	123.94	121.15
87	4N	604	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
87	cL	508	CLA	C6-C7-C8	-2.06	109.26	115.92
82	EK	202	PEB	C1C-CHB-C4B	2.06	132.90	128.28
82	vC	202	PEB	C1C-CHB-C4B	2.06	132.90	128.28
82	d1	203	PEB	C3C-C4C-NC	2.06	110.19	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	SD	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
87	CL	506	CLA	CHC-C1C-NC	2.06	127.33	124.20
82	UB	301	PEB	CBA-CAA-C3A	2.06	118.05	113.47
82	lK	203	PEB	CHA-C4A-NA	2.06	127.65	125.20
87	AN	802	CLA	CHD-C1D-C2D	2.06	129.80	125.48
87	32	310	CLA	CHA-C1A-NA	-2.06	121.68	126.40
82	eF	201	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
87	b6	617	CLA	CHC-C4B-NB	2.06	126.44	124.26
87	CL	511	CLA	CHA-C1A-NA	-2.06	121.68	126.40
87	cL	506	CLA	CHA-C1A-NA	-2.06	121.68	126.40
82	MM	202	PEB	CAC-C2C-C3C	2.06	131.78	127.07
82	f4	202	PEB	CHB-C1C-NC	-2.06	120.60	125.32
87	3N	309	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
82	l1	203	PEB	CAC-CBC-CGC	-2.06	109.17	113.60
87	8N	308	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
82	aM	201	PEB	CBA-CAA-C3A	-2.06	108.88	113.47
82	OA	202	PEB	OD-C4D-C3D	-2.06	124.80	129.46
82	LM	201	PEB	C1B-C2B-C3B	-2.06	104.14	106.51
87	BN	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
87	c6	612	CLA	CHD-C1D-ND	-2.06	122.56	124.45
82	tC	201	PEB	CHB-C4B-C3B	-2.06	120.56	125.32
82	iO	201	PEB	CHB-C4B-C3B	-2.06	120.56	125.32
82	PD	202	PEB	CHC-C1D-ND	-2.06	111.12	113.72
82	K9	201	PEB	C2B-C1B-NB	2.06	114.92	110.53
84	LO	1001	CYC	CAB-C3B-C2B	2.06	131.05	127.53
82	1C	203	PEB	CMB-C2B-C1B	2.06	128.23	125.06
82	FI	202	PEB	CHB-C1C-C2C	-2.06	122.51	127.15
87	A2	805	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
82	MJ	201	PEB	CMA-C2A-C1A	-2.06	107.97	112.40
82	TJ	201	PEB	CMA-C2A-C1A	-2.06	107.97	112.40
82	O5	201	PEB	C4B-NB-C1B	-2.06	102.63	106.51
85	A6	401	BCR	C38-C26-C27	2.06	117.57	113.62
85	BN	840	BCR	C21-C20-C19	-2.06	116.79	123.22
82	gH	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
82	Y4	201	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
82	CB	202	PEB	CHC-C4C-NC	2.06	123.93	121.15
82	bP	502	PEB	C1C-CHB-C4B	2.06	132.90	128.28
82	F7	203	PEB	CHC-C1D-ND	-2.06	111.12	113.72
82	Z5	305	PEB	C3C-C4C-NC	2.06	110.19	108.33
82	dE	201	PEB	C3C-C4C-NC	2.06	110.19	108.33
87	b6	609	CLA	CHD-C1D-ND	-2.06	122.56	124.45
82	O7	202	PEB	CBB-CAB-C3B	-2.06	106.91	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	JF	202	PEB	C2B-C1B-NB	2.06	114.92	110.53
82	oF	201	PEB	C2B-C1B-NB	2.06	114.92	110.53
87	AN	825	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
82	W7	202	PEB	C1D-CHC-C4C	-2.06	110.22	113.26
82	OI	203	PEB	CAB-C3B-C4B	2.06	128.65	125.01
82	IB	202	PEB	CHB-C1C-C2C	-2.06	122.51	127.15
87	O2	201	CLA	C2A-C1A-CHA	2.06	127.44	123.85
96	v6	201	HEM	CHA-C1A-NA	2.06	127.63	123.85
87	AN	805	CLA	C16-C15-C13	-2.06	109.27	115.92
82	KB	301	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	xC	202	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	fJ	203	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
87	A2	801	CLA	CHD-C1D-C2D	2.06	129.79	125.48
85	BN	839	BCR	C33-C5-C4	2.06	117.57	113.62
82	HF	201	PEB	CAC-CBC-CGC	-2.06	109.18	113.60
82	ZH	201	PEB	CAC-CBC-CGC	-2.06	109.18	113.60
82	EM	202	PEB	CAB-CBB-CGB	-2.06	109.18	113.60
82	T9	201	PEB	C2B-C1B-NB	2.06	114.92	110.53
82	VP	202	PEB	CHA-C1B-C2B	2.06	130.19	124.90
82	BI	201	PEB	CAC-C2C-C1C	2.06	129.04	125.76
82	CM	203	PEB	CAC-C2C-C1C	2.06	129.04	125.76
82	Y4	201	PEB	CAC-C2C-C1C	2.06	129.04	125.76
87	AN	841	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
87	A2	817	CLA	C2A-C1A-CHA	2.06	127.46	123.86
82	PK	201	PEB	C1B-C2B-C3B	-2.06	104.15	106.51
85	BN	842	BCR	C28-C27-C26	-2.06	110.40	114.08
82	EM	201	PEB	CAA-C3A-C4A	-2.06	107.39	112.67
82	K7	202	PEB	CAA-C3A-C4A	-2.06	107.39	112.67
82	eE	203	PEB	CAB-C3B-C4B	2.06	128.65	125.01
82	S9	201	PEB	CAC-C2C-C3C	2.06	131.78	127.07
83	A1	303	PUB	CAB-C3B-C2B	-2.06	122.36	127.07
85	B2	840	BCR	C21-C20-C19	-2.06	116.80	123.22
82	O5	201	PEB	CHB-C4B-C3B	-2.06	120.56	125.32
82	pC	201	PEB	OA-C1A-NA	2.06	127.43	124.94
82	JM	201	PEB	CHB-C4B-NB	-2.06	120.30	124.58
87	A2	805	CLA	C16-C15-C13	-2.06	109.27	115.92
83	Z9	302	PUB	CBD-CAD-C3D	-2.06	106.76	112.43
82	sK	203	PEB	CMB-C2B-C1B	2.06	128.23	125.06
87	22	609	CLA	C2A-C1A-CHA	2.06	127.45	123.86
84	GG	1001	CYC	CHB-C1B-NB	-2.06	121.64	126.06
82	XP	202	PEB	CAB-C3B-C4B	2.06	128.65	125.01
87	32	306	CLA	CHC-C4B-NB	2.06	126.43	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	GF	202	PEB	CHA-C4A-NA	-2.06	122.76	125.20
82	J9	201	PEB	CHB-C4B-NB	-2.06	120.30	124.58
82	AB	501	PEB	CAB-CBB-CGB	-2.06	109.18	113.60
82	GD	202	PEB	CHB-C1C-C2C	-2.06	122.51	127.15
82	SH	202	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	HF	201	PEB	CHB-C1C-NC	2.06	130.03	125.32
82	x8	202	PEB	C1C-CHB-C4B	2.06	132.89	128.28
82	xC	202	PEB	C1C-CHB-C4B	2.06	132.89	128.28
82	NJ	202	PEB	CAA-C3A-C2A	-2.06	109.12	114.26
87	B2	801	CLA	CMC-C2C-C3C	2.06	131.70	126.12
82	bH	201	PEB	CMB-C2B-C1B	2.06	128.23	125.06
82	SI	201	PEB	CAC-C2C-C1C	2.06	129.04	125.76
82	rC	202	PEB	CAC-C2C-C1C	2.06	129.04	125.76
82	FF	202	PEB	CHB-C4B-NB	2.06	128.86	124.58
84	GE	1001	CYC	C4D-ND-C1D	-2.06	106.12	109.79
82	sF	201	PEB	OD-C4D-ND	-2.06	122.89	125.93
82	OM	203	PEB	C2A-C1A-NA	2.06	110.05	108.27
82	RM	202	PEB	C2A-C1A-NA	2.06	110.05	108.27
82	NB	203	PEB	C3C-C4C-NC	2.06	110.18	108.33
87	B6	608	CLA	C1-C2-C3	-2.06	122.49	126.04
87	3N	304	CLA	O2A-CGA-O1A	-2.06	118.18	123.30
85	J2	103	BCR	C28-C27-C26	-2.06	110.41	114.08
82	AE	304	PEB	CAB-C3B-C4B	2.06	128.64	125.01
103	82	309	ZEX	C20-C13-C14	-2.06	120.04	122.92
84	KH	1001	CYC	C4D-ND-C1D	-2.06	106.12	109.79
82	gE	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
87	c6	613	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
87	22	612	CLA	CAA-C2A-C1A	2.06	118.71	111.97
82	q8	201	PEB	C1C-CHB-C4B	2.06	132.89	128.28
82	U1	203	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
82	M5	305	PEB	C4C-C3C-C2C	-2.06	105.60	107.50
96	fL	102	HEM	CHB-C1B-C2B	-2.06	121.02	126.73
94	DL	401	PL9	C45-C44-C46	2.06	118.73	115.27
82	sK	202	PEB	C2A-C3A-C4A	2.05	104.42	101.34
87	72	603	CLA	C3A-C2A-C1A	2.05	104.42	101.34
82	W9	203	PEB	CAB-C3B-C4B	2.05	128.64	125.01
82	O5	202	PEB	CHA-C4A-NA	-2.05	122.76	125.20
82	aF	203	PEB	CHA-C4A-NA	2.05	127.65	125.20
82	kG	201	PEB	CHC-C1D-ND	-2.05	111.12	113.72
87	A2	834	CLA	CMC-C2C-C1C	-2.05	121.91	125.04
87	32	305	CLA	CMB-C2B-C3B	2.05	131.56	126.59
87	2N	301	CLA	CHA-C1A-NA	-2.05	121.69	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	IB	202	PEB	CAC-CBC-CGC	-2.05	109.18	113.60
82	wC	201	PEB	CAB-CBB-CGB	-2.05	109.18	113.60
82	kM	202	PEB	CAC-CBC-CGC	-2.05	109.18	113.60
82	VI	201	PEB	C2A-C1A-NA	2.05	110.04	108.27
87	RN	204	CLA	C2A-C1A-CHA	2.05	127.45	123.86
82	dQ	401	PEB	C1D-CHC-C4C	2.05	116.28	113.26
82	m1	201	PEB	CMC-C3C-C4C	2.05	129.24	127.06
87	B2	831	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
82	Y9	201	PEB	O1B-CGB-CBB	-2.05	116.48	123.08
82	cF	201	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
85	B2	842	BCR	C1-C6-C7	2.05	121.59	115.78
82	DG	1002	PEB	CAC-C2C-C1C	2.05	129.03	125.76
82	1C	201	PEB	CMB-C2B-C1B	2.05	128.23	125.06
82	B7	202	PEB	CBA-CAA-C3A	-2.05	108.89	113.47
82	HD	202	PEB	CAC-CBC-CGC	-2.05	109.18	113.60
82	J9	202	PEB	CAB-CBB-CGB	-2.05	109.18	113.60
82	CF	203	PEB	C2B-C1B-NB	2.05	114.91	110.53
82	W5	203	PEB	CHA-C4A-NA	-2.05	122.76	125.20
82	fB	301	PEB	OA-C1A-C2A	-2.05	124.54	126.17
82	iO	203	PEB	CAB-C3B-C2B	2.05	131.70	127.88
82	CD	201	PEB	CBC-CAC-C2C	2.05	118.33	112.63
82	D7	202	PEB	CBD-CAD-C3D	-2.05	117.40	127.62
82	IA	201	PEB	OD-C4D-ND	-2.05	122.89	125.93
87	7N	603	CLA	C3A-C2A-C1A	2.05	104.42	101.34
82	B5	202	PEB	C1D-CHC-C4C	-2.05	110.23	113.26
82	MB	202	PEB	CBD-CAD-C3D	-2.05	117.40	127.62
87	AN	822	CLA	C3B-C4B-NB	-2.05	108.61	110.52
82	DK	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
82	O1	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
82	C9	201	PEB	C2B-C1B-NB	2.05	114.91	110.53
82	w8	203	PEB	CAC-C2C-C1C	2.05	129.03	125.76
82	HA	202	PEB	CMB-C2B-C1B	2.05	128.23	125.06
95	O6	301	DGD	C6D-O5D-C1E	-2.05	109.73	113.74
87	A2	815	CLA	CHA-C1A-NA	-2.05	121.70	126.40
87	R2	204	CLA	C2A-C1A-CHA	2.05	127.45	123.86
87	2N	309	CLA	C2A-C1A-CHA	2.05	127.45	123.86
82	xC	202	PEB	CAB-C3B-C4B	2.05	128.64	125.01
87	2N	301	CLA	CHB-C4A-NA	2.05	127.35	124.51
84	DE	1001	CYC	C4D-ND-C1D	-2.05	106.13	109.79
82	GI	201	PEB	OD-C4D-ND	-2.05	122.89	125.93
82	H5	201	PEB	OD-C4D-ND	-2.05	122.89	125.93
82	lO	202	PEB	CBB-CAB-C3B	-2.05	106.92	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aJ	204	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	XJ	202	PEB	O2B-CGB-CBB	2.05	120.62	114.03
82	AD	304	PEB	OD-C4D-C3D	-2.05	124.81	129.46
82	H7	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
84	L1	1001	CYC	CBC-CAC-C3C	2.05	118.04	113.47
96	FL	102	HEM	CAA-CBA-CGA	-2.05	109.19	113.60
82	iO	202	PEB	C1C-NC-C4C	-2.05	105.94	109.60
87	CL	508	CLA	C2A-C1A-CHA	2.05	127.45	123.86
82	qC	201	PEB	C1C-CHB-C4B	2.05	132.88	128.28
82	S9	202	PEB	CAB-C3B-C4B	2.05	128.64	125.01
82	N9	201	PEB	CHC-C1D-ND	-2.05	111.13	113.72
87	RN	202	CLA	CHA-C1A-NA	-2.05	121.70	126.40
87	3N	311	CLA	CHA-C1A-NA	-2.05	121.70	126.40
82	OP	202	PEB	CHB-C1C-C2C	-2.05	122.52	127.15
82	eF	202	PEB	CHA-C4A-NA	-2.05	122.77	125.20
82	1C	201	PEB	CMD-C2D-C3D	2.05	132.96	130.06
82	wC	203	PEB	CAC-C2C-C1C	2.05	129.03	125.76
82	AD	301	PEB	C2B-C1B-NB	2.05	114.91	110.53
92	D6	407	LMG	O7-C10-O9	-2.05	118.74	123.70
82	KA	202	PEB	CAA-C3A-C4A	-2.05	107.40	112.67
82	fJ	203	PEB	CAB-C3B-C4B	2.05	128.64	125.01
82	OD	202	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
87	cL	515	CLA	CHA-C4D-ND	2.05	136.79	132.50
82	AK	202	PEB	OD-C4D-C3D	-2.05	124.81	129.46
87	bL	604	CLA	O2D-CGD-CBD	2.05	114.91	111.27
87	BL	622	CLA	C2D-C1D-ND	-2.05	108.59	110.10
82	B5	203	PEB	CHB-C1C-NC	-2.05	120.62	125.32
85	B6	602	BCR	C37-C22-C21	-2.05	120.05	122.92
82	EQ	201	PEB	CBD-CAD-C3D	-2.05	117.41	127.62
87	RN	201	CLA	CHB-C1B-NB	2.05	126.43	124.26
88	m6	102	LHG	C5-O7-C7	-2.05	112.74	117.79
82	Y1	201	PEB	CBB-CAB-C3B	2.05	118.33	112.63
82	E9	201	PEB	CHC-C1D-ND	-2.05	111.13	113.72
82	NH	1002	PEB	CHA-C1B-NB	-2.05	120.64	124.93
87	bL	620	CLA	C4-C3-C5	2.05	118.72	115.27
87	cL	505	CLA	CHA-C1A-NA	-2.05	121.70	126.40
82	KP	202	PEB	CHB-C1C-C2C	-2.05	122.52	127.15
82	vK	201	PEB	CHB-C1C-C2C	-2.05	122.52	127.15
82	kH	201	PEB	CAC-CBC-CGC	-2.05	109.19	113.60
83	AG	303	PUB	CAB-CBB-CGB	-2.05	109.19	113.60
95	cL	502	DGD	O1G-C1A-O1A	-2.05	118.42	123.59
83	AH	303	PUB	CAB-C3B-C2B	-2.05	122.37	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bB	201	PEB	CHB-C4B-C3B	-2.05	120.57	125.32
82	XD	202	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	J9	203	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	N9	201	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
85	B6	602	BCR	C11-C12-C13	-2.05	120.66	126.42
82	v8	202	PEB	C1C-CHB-C4B	2.05	132.88	128.28
82	XB	201	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
82	L9	203	PEB	CAC-CBC-CGC	-2.05	109.19	113.60
87	1N	601	CLA	O1A-CGA-CBA	2.05	129.67	123.08
82	GA	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
82	HF	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
87	6N	612	CLA	CHA-C1A-NA	-2.05	121.70	126.40
85	a6	605	BCR	C33-C5-C4	2.05	117.56	113.62
82	R7	203	PEB	OD-C4D-ND	-2.05	122.89	125.93
103	8N	309	ZEX	C20-C13-C14	-2.05	120.05	122.92
82	M9	301	PEB	CAC-C2C-C1C	2.05	129.03	125.76
82	EB	501	PEB	CAC-CBC-CGC	-2.05	109.19	113.60
82	TM	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
87	62	307	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
82	AQ	301	PEB	C2B-C1B-NB	2.05	114.90	110.53
82	aJ	204	PEB	CHA-C1B-C2B	2.05	130.17	124.90
87	c6	607	CLA	CHD-C1D-ND	-2.05	122.57	124.45
87	1N	602	CLA	CHA-C1A-NA	-2.05	121.70	126.40
84	C4	1001	CYC	CMC-C2C-C1C	-2.05	107.98	112.40
82	MM	201	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
84	GE	1001	CYC	CHB-C1B-NB	-2.05	121.66	126.06
82	gJ	202	PEB	O2B-CGB-CBB	2.05	120.62	114.03
87	8N	304	CLA	C3C-C4C-NC	-2.05	108.27	110.57
82	CP	203	PEB	C3C-C4C-NC	2.05	110.18	108.33
82	jF	201	PEB	CHC-C1D-ND	-2.05	111.13	113.72
82	YJ	203	PEB	CBA-CAA-C3A	-2.05	108.90	113.47
87	BL	601	CLA	CHB-C1B-NB	2.05	126.43	124.26
87	AN	823	CLA	CHC-C4B-NB	2.05	126.43	124.26
87	A2	803	CLA	CHB-C1B-NB	2.05	126.43	124.26
87	82	308	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
82	WK	202	PEB	CAC-CBC-CGC	2.05	118.01	113.60
82	HJ	202	PEB	C2A-C1A-NA	2.05	110.04	108.27
82	XP	202	PEB	C2A-C1A-NA	2.05	110.04	108.27
82	LA	202	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	YA	304	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	A4	305	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	i4	203	PEB	C4C-C3C-C2C	-2.05	105.61	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	KN	101	BCR	C20-C19-C18	-2.05	120.66	126.42
82	SH	203	PEB	CAB-C3B-C4B	2.05	128.63	125.01
82	LP	202	PEB	CAB-C3B-C4B	2.05	128.63	125.01
87	8N	305	CLA	CHA-C1A-NA	-2.05	121.70	126.40
82	HQ	201	PEB	CAA-C3A-C4A	-2.05	107.41	112.67
82	g4	203	PEB	CHB-C4B-NB	-2.05	120.31	124.58
82	HB	202	PEB	CAC-C2C-C1C	2.05	129.03	125.76
82	DP	202	PEB	CAC-C2C-C1C	2.05	129.03	125.76
84	EE	1001	CYC	CHA-C1A-C2A	-2.05	120.58	125.32
83	AO	302	PUB	CBA-CAA-C3A	-2.05	109.87	112.98
85	AL	401	BCR	C2-C1-C6	2.05	113.64	110.48
82	GF	203	PEB	O1B-CGB-CBB	-2.05	116.50	123.08
87	5N	611	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
87	AN	802	CLA	CHC-C1C-NC	2.05	127.31	124.20
82	fK	202	PEB	CHC-C4C-NC	-2.05	118.37	121.15
82	GK	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
87	dL	404	CLA	O2D-CGD-CBD	2.05	114.91	111.27
82	pC	201	PEB	CAC-C2C-C1C	2.05	129.03	125.76
82	SD	202	PEB	OD-C4D-ND	-2.05	122.89	125.93
82	FD	203	PEB	CAC-CBC-CGC	-2.05	109.19	113.60
82	gJ	201	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
87	12	601	CLA	O1A-CGA-CBA	2.05	129.66	123.08
82	j1	202	PEB	CHA-C1B-C2B	2.05	130.17	124.90
82	q8	202	PEB	CBA-CAA-C3A	-2.05	108.91	113.47
82	lK	202	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
82	P9	201	PEB	CHC-C1D-ND	-2.05	111.13	113.72
82	PD	201	PEB	CAC-C2C-C1C	2.05	129.02	125.76
82	gF	202	PEB	C2B-C1B-NB	2.05	114.90	110.53
82	MB	202	PEB	CHB-C1C-NC	-2.05	120.63	125.32
82	KP	202	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
87	6N	606	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
87	82	303	CLA	C3C-C4C-NC	-2.05	108.27	110.57
82	AF	201	PEB	CMB-C2B-C3B	-2.05	120.56	126.12
85	BL	616	BCR	C29-C30-C25	2.05	113.63	110.48
82	sC	203	PEB	CHA-C1B-NB	-2.05	120.65	124.93
82	dG	204	PEB	CAC-CBC-CGC	-2.05	109.20	113.60
82	MF	202	PEB	C2B-C1B-NB	2.05	114.90	110.53
82	QG	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
82	O9	202	PEB	CHB-C1C-NC	2.05	130.01	125.32
87	62	313	CLA	O1D-CGD-CBD	2.05	128.67	124.48
82	J9	203	PEB	CHC-C4C-NC	2.05	123.92	121.15
87	CL	510	CLA	C3A-C2A-C1A	2.05	104.41	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	R9	201	PEB	CHC-C1D-ND	-2.05	111.13	113.72
82	TG	201	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	R7	203	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	Y7	304	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	FD	201	PEB	CAC-CBC-CGC	-2.05	109.20	113.60
82	D9	201	PEB	CHA-C1B-C2B	-2.05	119.64	124.90
87	B6	604	CLA	C1-C2-C3	-2.05	122.50	126.04
82	O1	202	PEB	OD-C4D-C3D	-2.05	124.82	129.46
84	J3	1001	CYC	CAA-C2A-C1A	2.05	128.63	125.01
82	eB	202	PEB	CHB-C1C-C2C	-2.05	122.53	127.15
82	jK	201	PEB	CHB-C1C-C2C	-2.05	122.53	127.15
82	TH	201	PEB	CAC-C2C-C1C	2.05	129.02	125.76
82	EJ	201	PEB	CAC-C2C-C1C	2.05	129.02	125.76
82	JP	202	PEB	CAC-C2C-C1C	2.05	129.02	125.76
87	A2	809	CLA	C3A-C2A-C1A	2.05	104.41	101.34
85	CL	516	BCR	C8-C7-C6	-2.05	121.45	127.20
82	GF	203	PEB	CAB-CBB-CGB	2.05	118.01	113.60
82	O7	202	PEB	OD-C4D-C3D	-2.05	124.82	129.46
87	A6	403	CLA	CHB-C1B-NB	2.05	126.42	124.26
87	cL	505	CLA	CHB-C1B-NB	2.05	126.42	124.26
82	OJ	202	PEB	C2B-C1B-NB	2.05	114.90	110.53
87	b6	612	CLA	CHD-C1D-ND	-2.05	122.57	124.45
82	AF	202	PEB	CAB-C3B-C4B	2.05	128.63	125.01
82	18	201	PEB	CMB-C2B-C1B	2.05	128.22	125.06
82	B5	202	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
87	K6	101	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
87	a6	609	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
82	EP	201	PEB	C3C-C4C-NC	2.05	110.18	108.33
83	YA	302	PUB	C2B-C1B-NB	2.05	110.18	108.33
95	O6	301	DGD	O2G-C1B-O1B	-2.05	118.76	123.70
87	82	304	CLA	CHA-C1A-NA	-2.05	121.71	126.40
87	d6	403	CLA	CHB-C4A-NA	2.05	127.34	124.51
82	B5	201	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
87	bL	616	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
82	gK	203	PEB	CAC-CBC-CGC	-2.05	109.20	113.60
82	Q5	201	PEB	CBC-CAC-C2C	-2.05	106.94	112.63
82	f4	202	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	tK	201	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	eO	203	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	QJ	202	PEB	CAC-C2C-C1C	2.05	129.02	125.76
95	cL	519	DGD	O6D-C5D-C6D	2.05	110.80	106.67
87	6N	612	CLA	O1D-CGD-CBD	2.05	128.67	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gF	201	PEB	CHA-C4A-NA	2.05	127.64	125.20
82	ID	201	PEB	C1C-CHB-C4B	2.05	132.87	128.28
82	mM	202	PEB	C1D-CHC-C4C	-2.05	110.24	113.26
82	eB	201	PEB	CAB-CBB-CGB	-2.05	109.20	113.60
82	RM	202	PEB	CHB-C1C-NC	-2.05	120.63	125.32
87	cL	517	CLA	CHB-C1B-NB	2.05	126.42	124.26
82	jK	201	PEB	CHC-C1D-ND	-2.05	111.14	113.72
82	WG	201	PEB	C2B-C1B-NB	2.05	114.89	110.53
82	sF	203	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
82	TP	202	PEB	CAC-C2C-C1C	2.05	129.02	125.76
87	6N	607	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
82	JA	203	PEB	C1B-C2B-C3B	-2.05	104.16	106.51
95	c6	601	DGD	O2G-C1B-O1B	-2.05	118.76	123.70
84	G3	1001	CYC	CAA-C2A-C1A	2.05	128.63	125.01
87	3N	310	CLA	CHA-C1A-NA	-2.05	121.71	126.40
82	AF	202	PEB	OD-C4D-C3D	-2.05	124.83	129.46
82	M5	305	PEB	C3C-C4C-NC	2.05	110.17	108.33
82	fO	201	PEB	C3C-C4C-NC	2.05	110.17	108.33
82	ZG	202	PEB	CBB-CAB-C3B	-2.05	106.94	112.63
82	YP	502	PEB	C4C-C3C-C2C	-2.05	105.61	107.50
82	B5	203	PEB	C1C-CHB-C4B	-2.05	123.69	128.28
94	dL	406	PL9	C16-C14-C13	-2.05	116.98	121.12
87	A2	801	CLA	CHC-C1C-NC	2.05	127.31	124.20
82	QE	201	PEB	CHB-C4B-NB	-2.05	120.32	124.58
82	uK	202	PEB	CHB-C1C-NC	-2.05	120.64	125.32
82	x8	202	PEB	CAB-C3B-C4B	2.05	128.63	125.01
87	A2	839	CLA	C2A-C1A-CHA	2.05	127.44	123.86
87	B2	822	CLA	C2D-C1D-ND	-2.04	108.60	110.10
82	gG	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
87	62	309	CLA	O1D-CGD-CBD	2.04	128.67	124.48
87	BN	829	CLA	C3B-C4B-NB	-2.04	108.62	110.52
87	R2	202	CLA	CHA-C1A-NA	-2.04	121.72	126.40
82	HA	202	PEB	CHA-C1B-NB	-2.04	120.66	124.93
82	GA	202	PEB	C1D-CHC-C4C	2.04	116.27	113.26
87	D6	405	CLA	CHD-C1D-ND	-2.04	122.58	124.45
87	5N	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
82	OE	202	PEB	CHA-C4A-NA	2.04	127.64	125.20
82	O4	202	PEB	CAC-C2C-C1C	2.04	129.02	125.76
87	I2	102	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
82	ZH	202	PEB	C2B-C1B-NB	2.04	114.89	110.53
82	NP	201	PEB	C2B-C1B-NB	2.04	114.89	110.53
82	SG	201	PEB	CBA-CAA-C3A	-2.04	108.92	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	301	CLA	O2D-CGD-CBD	2.04	114.90	111.27
82	M5	304	PEB	C1C-CHB-C4B	-2.04	123.70	128.28
82	iJ	202	PEB	CAA-C3A-C2A	-2.04	109.15	114.26
82	VK	201	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	U5	202	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	L5	201	PEB	CHB-C4B-C3B	-2.04	120.59	125.32
82	V9	202	PEB	C4C-C3C-C2C	-2.04	105.61	107.50
82	QD	202	PEB	CHB-C1C-NC	-2.04	120.64	125.32
87	3N	306	CLA	CMB-C2B-C3B	2.04	131.54	126.59
92	j6	102	LMG	O8-C28-O10	-2.04	118.43	123.59
82	R7	203	PEB	CAB-C3B-C2B	2.04	131.69	127.88
82	UK	201	PEB	CAB-C3B-C4B	2.04	128.62	125.01
82	O9	202	PEB	CAB-C3B-C4B	2.04	128.62	125.01
82	mO	203	PEB	CAC-C2C-C1C	2.04	129.02	125.76
82	UD	202	PEB	CHB-C4B-C3B	-2.04	120.59	125.32
84	NE	201	CYC	CHA-C1A-C2A	-2.04	120.59	125.32
82	lF	203	PEB	CHA-C4A-NA	2.04	127.64	125.20
87	32	311	CLA	C3B-C4B-NB	-2.04	108.62	110.52
87	AN	805	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
87	22	609	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
84	NH	1001	CYC	CAA-CBA-CGA	2.04	118.00	113.60
82	gH	202	PEB	CAB-CBB-CGB	-2.04	109.20	113.60
82	TK	202	PEB	CBD-CAD-C3D	-2.04	117.45	127.62
87	2N	312	CLA	CAA-C2A-C1A	2.04	118.67	111.97
82	DB	201	PEB	CBB-CAB-C3B	-2.04	106.95	112.63
82	RH	202	PEB	OD-C4D-ND	-2.04	122.90	125.93
95	CL	520	DGD	O1G-C1A-C2A	2.04	118.32	111.91
82	IK	201	PEB	O2C-CGC-O1C	-2.04	118.21	123.30
82	R5	201	PEB	C1D-CHC-C4C	-2.04	110.24	113.26
83	AJ	304	PUB	C4A-CHA-C1B	2.04	116.27	113.26
82	AO	305	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	HQ	202	PEB	CAC-CBC-CGC	-2.04	109.21	113.60
82	JF	202	PEB	CHC-C4C-NC	-2.04	118.38	121.15
82	ZH	203	PEB	C4C-C3C-C2C	-2.04	105.61	107.50
82	aF	201	PEB	C4C-C3C-C2C	-2.04	105.61	107.50
87	bL	607	CLA	C6-C7-C8	-2.04	109.31	115.92
91	dL	403	PHO	C7-C6-C5	-2.04	107.81	113.36
87	6N	610	CLA	CHA-C1A-NA	-2.04	121.72	126.40
82	LK	202	PEB	CAC-C2C-C3C	2.04	131.75	127.07
87	22	605	CLA	CHB-C4A-NA	2.04	127.34	124.51
82	N7	201	PEB	CAB-C3B-C4B	2.04	128.62	125.01
82	JQ	203	PEB	OD-C4D-ND	-2.04	122.90	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	A2	837	CLA	O2D-CGD-CBD	2.04	114.90	111.27
82	UE	202	PEB	CAC-CBC-CGC	-2.04	109.21	113.60
82	J7	203	PEB	CAC-CBC-CGC	-2.04	109.21	113.60
94	d6	408	PL9	C47-C48-C49	-2.04	120.77	127.75
82	Z5	305	PEB	C1D-CHC-C4C	-2.04	110.24	113.26
82	SJ	203	PEB	C2B-C1B-NB	2.04	114.89	110.53
92	ML	101	LMG	O7-C8-C7	2.04	115.80	108.40
82	oF	201	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
94	aL	601	PL9	C53-C6-C1	2.04	119.17	114.99
87	42	602	CLA	CMB-C2B-C3B	2.04	131.53	126.59
87	b6	617	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
82	LE	1002	PEB	CAB-C3B-C2B	2.04	131.68	127.88
82	VI	201	PEB	CHC-C4C-NC	2.04	123.91	121.15
85	B2	842	BCR	C28-C27-C26	-2.04	110.43	114.08
82	HI	202	PEB	CBD-CAD-C3D	-2.04	117.46	127.62
82	Z5	305	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
82	S9	203	PEB	CHB-C4B-NB	-2.04	120.33	124.58
82	oF	203	PEB	CAC-CBC-CGC	-2.04	109.21	113.60
82	eJ	201	PEB	CAB-CBB-CGB	-2.04	109.21	113.60
85	A2	845	BCR	C30-C25-C26	-2.04	119.74	122.61
82	O9	203	PEB	C1B-C2B-C3B	-2.04	104.16	106.51
87	bL	617	CLA	C1-C2-C3	-2.04	122.51	126.04
82	O9	201	PEB	CBB-CAB-C3B	2.04	118.30	112.63
82	cO	203	PEB	CBB-CAB-C3B	2.04	118.30	112.63
84	H1	1001	CYC	CBA-CAA-C2A	-2.04	106.95	112.63
87	3N	309	CLA	CMC-C2C-C1C	2.04	128.15	125.04
82	OD	201	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	RP	202	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	eH	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	uF	203	PEB	CHB-C1C-NC	-2.04	120.64	125.32
87	8N	304	CLA	C2B-C1B-NB	2.04	111.60	110.23
82	l4	202	PEB	C4B-C3B-C2B	-2.04	104.52	106.78
82	KM	201	PEB	CHB-C1C-C2C	-2.04	122.54	127.15
82	SP	202	PEB	CHC-C1D-ND	-2.04	111.14	113.72
82	S9	203	PEB	CHA-C1B-C2B	2.04	130.15	124.90
82	F9	201	PEB	C4B-NB-C1B	-2.04	102.66	106.51
82	II	203	PEB	CMC-C3C-C4C	2.04	129.22	127.06
82	UH	203	PEB	C2B-C1B-NB	2.04	114.89	110.53
82	Q1	201	PEB	C2B-C1B-NB	2.04	114.89	110.53
103	82	310	ZEX	C20-C13-C14	-2.04	120.06	122.92
87	2N	308	CLA	C2A-C1A-CHA	2.04	127.43	123.86
95	a6	604	DGD	O2G-C1B-O1B	-2.04	118.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	KA	201	PEB	C2A-C1A-NA	2.04	110.03	108.27
82	fB	301	PEB	C2A-C1A-NA	2.04	110.03	108.27
82	QJ	203	PEB	CHB-C1C-C2C	-2.04	122.54	127.15
82	i4	201	PEB	CHB-C1C-C2C	-2.04	122.54	127.15
82	I7	201	PEB	OD-C4D-ND	-2.04	122.91	125.93
82	lK	201	PEB	CHA-C1B-NB	-2.04	120.66	124.93
82	HQ	202	PEB	CAC-C2C-C1C	2.04	129.01	125.76
82	J7	203	PEB	CAC-C2C-C1C	2.04	129.01	125.76
87	HL	101	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
87	C6	511	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
87	A2	815	CLA	C4-C3-C5	2.04	118.70	115.27
87	DL	403	CLA	CHC-C4B-NB	2.04	126.42	124.26
82	YG	201	PEB	C2B-C1B-NB	2.04	114.89	110.53
84	KH	1001	CYC	CHD-C4C-NC	2.04	127.63	125.20
82	aM	201	PEB	CHC-C1D-ND	-2.04	111.14	113.72
82	NO	1002	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
82	SI	202	PEB	CHB-C1C-C2C	-2.04	122.55	127.15
82	LA	203	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	ZG	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	j1	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	WJ	201	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	BI	203	PEB	C3B-C4B-NB	2.04	113.02	110.05
87	AN	809	CLA	C3A-C2A-C1A	2.04	104.40	101.34
94	a6	601	PL9	C47-C48-C49	-2.04	120.77	127.75
82	PB	201	PEB	CAB-CBB-CGB	-2.04	109.21	113.60
87	A2	816	CLA	C2D-C1D-ND	-2.04	108.60	110.10
91	AL	410	PHO	O1D-CGD-CBD	-2.04	121.34	124.74
82	BQ	201	PEB	C1C-NC-C4C	-2.04	105.97	109.60
82	JB	201	PEB	CHB-C1C-C2C	-2.04	122.55	127.15
95	O6	301	DGD	C2G-O2G-C1B	-2.04	112.77	117.79
87	4N	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
87	I2	103	CLA	C2A-C1A-CHA	2.04	127.43	123.86
82	l4	201	PEB	CHA-C1B-NB	-2.04	120.67	124.93
84	EE	1001	CYC	OB-C4B-NB	-2.04	120.34	125.08
82	QG	201	PEB	CHB-C4B-NB	-2.04	120.33	124.58
82	kE	201	PEB	CHC-C1D-ND	-2.04	111.14	113.72
82	fO	202	PEB	CHB-C1C-NC	-2.04	120.65	125.32
87	B2	833	CLA	CHC-C4B-NB	2.04	126.42	124.26
82	EI	201	PEB	CHC-C4C-NC	2.04	123.91	121.15
103	8N	310	ZEX	C20-C13-C14	-2.04	120.06	122.92
82	JB	201	PEB	CAA-C3A-C4A	-2.04	107.43	112.67
82	PQ	201	PEB	CAC-C2C-C1C	2.04	129.01	125.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
95	AL	414	DGD	O5D-C6D-C5D	-2.04	105.27	109.05
82	AK	201	PEB	CMB-C2B-C3B	-2.04	120.58	126.12
87	52	602	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
82	KF	203	PEB	CMC-C3C-C4C	2.04	129.22	127.06
87	AN	820	CLA	O2D-CGD-CBD	2.04	114.89	111.27
82	WH	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	D1	1002	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	g4	202	PEB	C1D-CHC-C4C	-2.04	110.25	113.26
82	I5	201	PEB	C1D-CHC-C4C	-2.04	110.25	113.26
82	JI	202	PEB	C3C-C4C-NC	2.04	110.17	108.33
82	KA	201	PEB	C2B-C1B-NB	2.04	114.88	110.53
82	AA	201	PEB	CAB-C3B-C2B	-2.04	124.08	127.88
87	52	611	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
82	PF	201	PEB	CHA-C1B-C2B	2.04	130.15	124.90
82	BD	201	PEB	C1C-NC-C4C	-2.04	105.97	109.60
82	IJ	201	PEB	C1C-NC-C4C	-2.04	105.97	109.60
87	M2	101	CLA	CHA-C1A-NA	-2.04	121.73	126.40
82	TO	203	PEB	CAC-C2C-C1C	2.04	129.01	125.76
82	Y4	202	PEB	CAC-C2C-C1C	2.04	129.01	125.76
82	wK	303	PEB	CAC-C2C-C1C	2.04	129.01	125.76
92	D6	407	LMG	O8-C28-C29	2.04	118.31	111.91
82	Z9	303	PEB	OA-C1A-NA	2.04	127.41	124.94
87	b6	613	CLA	C2D-C1D-ND	-2.04	108.60	110.10
87	B6	614	CLA	CHB-C1B-NB	2.04	126.42	124.26
87	42	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
87	22	607	CLA	CBC-CAC-C3C	2.04	118.05	112.43
82	E5	201	PEB	C1D-CHC-C4C	-2.04	110.25	113.26
85	bL	601	BCR	C10-C11-C12	-2.04	116.85	123.22
87	1N	607	CLA	CMB-C2B-C3B	2.04	131.53	126.59
82	a4	202	PEB	CHA-C1B-C2B	2.04	130.14	124.90
82	eB	201	PEB	CHA-C1B-C2B	2.04	130.14	124.90
85	AN	847	BCR	C36-C18-C19	2.04	121.29	118.08
87	52	610	CLA	CHD-C1D-ND	-2.04	122.58	124.45
87	82	303	CLA	CBA-CAA-C2A	-2.04	107.84	113.86
82	FQ	203	PEB	CAC-CBC-CGC	-2.04	109.22	113.60
82	YH	202	PEB	CAC-C2C-C1C	2.04	129.01	125.76
82	KK	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	MQ	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	S5	203	PEB	CHC-C1D-ND	-2.04	111.14	113.72
87	bL	614	CLA	C2A-C1A-CHA	2.04	127.42	123.86
82	V5	201	PEB	C1D-CHC-C4C	-2.04	110.25	113.26
82	CJ	201	PEB	CAB-CBB-CGB	-2.04	109.22	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	aJ	202	PEB	CHB-C4B-NB	-2.04	120.33	124.58
87	C6	519	CLA	CHB-C1B-NB	2.04	126.42	124.26
82	fM	202	PEB	C2B-C1B-NB	2.04	114.88	110.53
87	4N	605	CLA	C3B-C4B-NB	-2.04	108.62	110.52
82	aF	202	PEB	CAB-C3B-C4B	2.04	128.61	125.01
84	C1	1001	CYC	CHA-C1A-C2A	-2.04	120.60	125.32
87	22	608	CLA	C2A-C1A-CHA	2.04	127.42	123.86
87	B6	609	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
82	WF	202	PEB	O1C-CGC-CBC	-2.04	116.53	123.08
82	GK	203	PEB	O1B-CGB-CBB	-2.04	116.53	123.08
87	6N	609	CLA	C2D-C1D-ND	-2.04	108.60	110.10
87	1N	603	CLA	CHD-C1D-ND	-2.04	122.58	124.45
82	NF	202	PEB	C2A-C1A-NA	2.04	110.03	108.27
82	aO	202	PEB	CHA-C1B-C2B	2.04	130.14	124.90
82	PA	202	PEB	C2B-C1B-NB	2.04	114.88	110.53
82	MA	201	PEB	C1D-CHC-C4C	2.04	116.26	113.26
84	LH	1002	CYC	O1D-CGD-CBD	-2.04	116.53	123.08
87	22	605	CLA	CHA-C1A-NA	-2.04	121.73	126.40
82	hJ	203	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
87	AN	834	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
82	YG	201	PEB	CBA-CAA-C3A	-2.04	108.93	113.47
82	aG	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
82	h4	202	PEB	CAC-CBC-CGC	-2.04	109.22	113.60
85	A2	804	BCR	C11-C12-C13	-2.04	120.69	126.42
85	B2	843	BCR	C33-C5-C6	-2.04	122.24	124.53
82	WE	201	PEB	C2B-C1B-NB	2.04	114.88	110.53
87	A2	809	CLA	CHC-C4B-NB	2.04	126.41	124.26
82	b1	201	PEB	OD-C4D-ND	-2.04	122.91	125.93
82	cO	203	PEB	CHC-C1D-ND	-2.04	111.15	113.72
82	H7	201	PEB	OD-C4D-C3D	-2.04	124.84	129.46
82	DQ	202	PEB	CAB-C3B-C4B	2.04	128.61	125.01
82	V1	202	PEB	CAB-C3B-C4B	2.04	128.61	125.01
84	v3	1001	CYC	CAA-C2A-C1A	2.04	128.61	125.01
82	w8	201	PEB	CAB-CBB-CGB	-2.04	109.22	113.60
87	FN	203	CLA	O2D-CGD-CBD	2.04	114.89	111.27
82	iJ	201	PEB	CMC-C3C-C4C	2.04	129.22	127.06
82	DB	201	PEB	C1B-C2B-C3B	-2.04	104.17	106.51
87	c6	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
87	c6	615	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
87	8N	306	CLA	CHA-C4D-ND	2.04	136.76	132.50
83	AG	302	PUB	CBA-CAA-C3A	-2.04	109.89	112.98
82	S9	201	PEB	CHB-C1C-NC	-2.04	120.65	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	FK	201	PEB	OD-C4D-C3D	-2.04	124.85	129.46
82	WJ	202	PEB	CAB-CBB-CGB	-2.04	109.22	113.60
82	AE	304	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	ZJ	201	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	U9	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	eG	201	PEB	CAB-C3B-C4B	2.04	128.61	125.01
82	NI	201	PEB	CHC-C4C-NC	2.04	123.91	121.15
82	N5	201	PEB	C1D-CHC-C4C	-2.04	110.25	113.26
82	gJ	201	PEB	CMD-C2D-C3D	2.04	132.94	130.06
82	KB	304	PEB	CHC-C1D-ND	-2.04	111.15	113.72
82	C9	201	PEB	CHC-C1D-ND	-2.04	111.15	113.72
82	IQ	201	PEB	C1C-CHB-C4B	2.04	132.85	128.28
82	TM	201	PEB	CHB-C1C-NC	-2.04	120.66	125.32
82	UG	202	PEB	CAC-C2C-C1C	2.04	129.00	125.76
82	fK	202	PEB	CHB-C1C-C2C	-2.04	122.56	127.15
82	NB	201	PEB	CAC-CBC-CGC	-2.04	109.22	113.60
82	eG	201	PEB	CAB-CBB-CGB	-2.04	109.22	113.60
82	SH	203	PEB	OA-C1A-NA	2.04	127.41	124.94
87	b6	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
82	L5	202	PEB	CMC-C3C-C4C	2.04	129.22	127.06
82	F7	201	PEB	CHA-C4A-NA	2.04	127.63	125.20
82	N4	1002	PEB	CAA-C3A-C2A	-2.04	109.17	114.26
82	PG	202	PEB	CHB-C1C-C2C	-2.04	122.56	127.15
82	WH	201	PEB	CHB-C4B-NB	-2.04	120.34	124.58
82	wK	302	PEB	CHB-C4B-NB	-2.04	120.34	124.58
87	B2	833	CLA	CHA-C1A-NA	-2.04	121.74	126.40
82	BP	202	PEB	C4C-C3C-C2C	-2.04	105.62	107.50
82	SM	202	PEB	C2B-C1B-NB	2.04	114.87	110.53
87	B2	811	CLA	CHB-C1B-NB	2.04	126.41	124.26
87	32	309	CLA	CMC-C2C-C1C	2.04	128.14	125.04
82	QQ	202	PEB	CHB-C1C-NC	-2.04	120.66	125.32
82	Q9	203	PEB	CAB-C3B-C4B	2.04	128.61	125.01
82	qC	202	PEB	CBA-CAA-C3A	-2.04	108.94	113.47
82	DK	201	PEB	OD-C4D-C3D	-2.04	124.85	129.46
87	bL	621	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
87	B2	826	CLA	C2A-C1A-CHA	2.04	127.42	123.86
82	MJ	203	PEB	CBC-CAC-C2C	-2.04	106.97	112.63
82	PJ	202	PEB	O2B-CGB-CBB	2.04	120.57	114.03
82	i4	203	PEB	C1B-C2B-C3B	-2.04	104.17	106.51
82	eF	202	PEB	CHB-C4B-C3B	-2.04	120.61	125.32
82	CK	203	PEB	C2B-C1B-NB	2.04	114.87	110.53
85	fL	101	BCR	C32-C1-C6	-2.04	107.00	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y9	201	PEB	CHC-C4C-NC	2.04	123.90	121.15
87	IN	102	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
82	SQ	201	PEB	CAB-C3B-C4B	2.03	128.61	125.01
87	1N	602	CLA	CHB-C4A-NA	2.03	127.33	124.51
82	cJ	202	PEB	CAC-CBC-CGC	-2.03	109.22	113.60
94	aL	601	PL9	C45-C44-C46	2.03	118.69	115.27
87	32	309	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
87	8N	306	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
87	CL	518	CLA	CHB-C1B-NB	2.03	126.41	124.26
82	W4	201	PEB	OA-C1A-NA	2.03	127.41	124.94
82	PQ	202	PEB	C4C-C3C-C2C	-2.03	105.62	107.50
82	H5	203	PEB	C4C-C3C-C2C	-2.03	105.62	107.50
83	xF	306	PUB	C1B-C2B-C3B	-2.03	105.62	107.50
82	QB	201	PEB	CAC-C2C-C1C	2.03	129.00	125.76
82	ZF	202	PEB	C4B-NB-C1B	-2.03	102.68	106.51
82	QB	201	PEB	CAB-CBB-CGB	-2.03	109.22	113.60
82	AP	202	PEB	C3C-C4C-NC	2.03	110.17	108.33
87	62	311	CLA	CHA-C1A-NA	-2.03	121.74	126.40
82	OO	201	PEB	CBB-CAB-C3B	-2.03	106.97	112.63
82	GP	203	PEB	CHB-C1C-NC	-2.03	120.66	125.32
82	MK	202	PEB	C2B-C1B-NB	2.03	114.87	110.53
82	ED	201	PEB	CBD-CAD-C3D	-2.03	117.50	127.62
85	b6	603	BCR	C21-C20-C19	-2.03	116.87	123.22
87	B2	828	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
82	FB	201	PEB	CHC-C1D-ND	-2.03	111.15	113.72
87	M2	101	CLA	C2D-C1D-ND	-2.03	108.61	110.10
82	B7	203	PEB	CAC-C2C-C1C	2.03	129.00	125.76
84	C3	1001	CYC	CAA-C2A-C1A	2.03	128.61	125.01
82	z8	201	PEB	CHB-C1C-NC	-2.03	120.66	125.32
87	b6	612	CLA	O2D-CGD-CBD	2.03	114.88	111.27
82	hK	202	PEB	C2B-C1B-NB	2.03	114.87	110.53
87	7N	603	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
87	J2	101	CLA	CHC-C4B-NB	2.03	126.41	124.26
82	fF	202	PEB	CHB-C1C-C2C	-2.03	122.56	127.15
84	LH	1001	CYC	CHA-C1A-C2A	-2.03	120.61	125.32
82	c4	203	PEB	CBB-CAB-C3B	2.03	118.28	112.63
82	SF	202	PEB	CBC-CAC-C2C	-2.03	106.98	112.63
87	BL	609	CLA	C16-C15-C13	-2.03	109.35	115.92
92	D6	407	LMG	C6-C5-C4	-2.03	108.24	113.00
85	bL	602	BCR	C28-C27-C26	-2.03	110.45	114.08
82	IP	203	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
82	gJ	202	PEB	C2A-C1A-NA	2.03	110.03	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Y4	202	PEB	C4C-C3C-C2C	-2.03	105.62	107.50
87	AN	815	CLA	CHA-C1A-NA	-2.03	121.74	126.40
88	L6	101	LHG	O7-C7-O9	-2.03	118.79	123.70
82	H7	202	PEB	CHA-C1B-NB	-2.03	120.68	124.93
82	VJ	201	PEB	CAC-C2C-C1C	2.03	129.00	125.76
82	x8	202	PEB	CAC-C2C-C1C	2.03	129.00	125.76
82	fM	203	PEB	CAC-C2C-C1C	2.03	129.00	125.76
82	jK	202	PEB	CHB-C4B-NB	2.03	128.81	124.58
82	JM	201	PEB	CAB-C3B-C4B	2.03	128.60	125.01
82	PM	202	PEB	C3C-C4C-NC	2.03	110.16	108.33
82	BQ	202	PEB	C3C-C4C-NC	2.03	110.16	108.33
84	73	1002	CYC	CBB-CAB-C3B	-2.03	106.83	112.43
82	X7	202	PEB	CHB-C1C-NC	2.03	129.98	125.32
87	AN	816	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
82	TI	202	PEB	CHC-C4C-NC	2.03	123.90	121.15
82	RH	201	PEB	C4B-NB-C1B	-2.03	102.68	106.51
82	B5	201	PEB	OD-C4D-ND	-2.03	122.92	125.93
87	BN	817	CLA	C2D-C1D-ND	-2.03	108.61	110.10
82	UF	201	PEB	CAB-C3B-C4B	2.03	128.60	125.01
87	12	603	CLA	CHD-C1D-ND	-2.03	122.59	124.45
95	C6	523	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
82	dB	202	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
87	R2	202	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
82	ZK	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
82	hB	301	PEB	OA-C1A-C2A	-2.03	124.56	126.17
87	62	305	CLA	CAA-C2A-C3A	-2.03	109.18	114.26
82	A1	305	PEB	C4C-C3C-C2C	-2.03	105.62	107.50
83	AG	302	PUB	C1B-C2B-C3B	-2.03	105.62	107.50
82	s8	203	PEB	CHA-C1B-NB	-2.03	120.68	124.93
82	JI	201	PEB	C2B-C1B-NB	2.03	114.87	110.53
82	lK	203	PEB	C1C-NC-C4C	-2.03	105.98	109.60
82	18	201	PEB	CMD-C2D-C3D	2.03	132.93	130.06
85	K2	102	BCR	C20-C19-C18	-2.03	120.71	126.42
82	OE	201	PEB	C3C-C4C-NC	2.03	110.16	108.33
87	BN	828	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
87	22	608	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
82	K7	201	PEB	CAC-C2C-C3C	-2.03	122.41	127.07
82	T4	203	PEB	CAA-C3A-C4A	-2.03	107.45	112.67
82	YM	201	PEB	CAC-C2C-C1C	2.03	129.00	125.76
95	BL	613	DGD	O6D-C5D-C6D	2.03	110.77	106.67
82	LE	1002	PEB	CMC-C3C-C2C	-2.03	121.21	125.61
85	KN	101	BCR	C11-C12-C13	2.03	132.12	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	cB	402	PEB	CBC-CAC-C2C	-2.03	106.98	112.63
82	WA	201	PEB	C1C-NC-C4C	-2.03	105.98	109.60
82	dE	204	PEB	CAA-C3A-C4A	-2.03	107.46	112.67
87	A2	834	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
82	VP	201	PEB	C2B-C1B-NB	2.03	114.86	110.53
82	wC	201	PEB	C2B-C1B-NB	2.03	114.86	110.53
94	dL	406	PL9	C51-C49-C50	2.03	119.09	114.60
87	c6	608	CLA	C2D-C1D-ND	-2.03	108.61	110.10
82	KD	202	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	dG	201	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	iO	201	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	x8	202	PEB	O2B-CGB-CBB	2.03	120.56	114.03
85	c6	602	BCR	C33-C5-C6	-2.03	122.25	124.53
82	Q7	201	PEB	OA-C1A-C2A	-2.03	124.56	126.17
82	hE	202	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
87	B2	822	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
85	cL	518	BCR	C30-C25-C24	2.03	121.52	115.78
87	dL	404	CLA	CHB-C1B-NB	2.03	126.41	124.26
87	BN	826	CLA	C2A-C1A-CHA	2.03	127.41	123.86
82	OO	202	PEB	CAC-C2C-C1C	2.03	129.00	125.76
82	SA	201	PEB	CHB-C1C-NC	2.03	129.97	125.32
84	J4	1001	CYC	CAA-CBA-CGA	2.03	117.97	113.60
82	fG	201	PEB	CAC-CBC-CGC	-2.03	109.23	113.60
85	JN	103	BCR	C10-C11-C12	-2.03	116.88	123.22
84	NH	1001	CYC	CBB-CAB-C3B	-2.03	106.83	112.43
82	u8	201	PEB	CHA-C1B-NB	-2.03	120.69	124.93
87	6N	604	CLA	CAA-C2A-C3A	-2.03	109.19	114.26
82	L5	202	PEB	CHA-C4A-NA	-2.03	122.79	125.20
82	DJ	201	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
82	eE	201	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
82	YO	201	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	V7	203	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	K9	202	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
87	C6	514	CLA	O1D-CGD-CBD	2.03	128.64	124.48
82	QI	201	PEB	CAC-C2C-C1C	2.03	129.00	125.76
87	72	604	CLA	CAC-C3C-C4C	2.03	127.44	124.81
87	AN	812	CLA	CHB-C1B-NB	2.03	126.41	124.26
87	C6	509	CLA	CHC-C4B-NB	2.03	126.41	124.26
82	SK	202	PEB	CBC-CAC-C2C	-2.03	106.99	112.63
82	bO	201	PEB	C3C-C4C-NC	2.03	110.16	108.33
82	LF	202	PEB	CAC-C2C-C3C	2.03	131.72	127.07
82	zC	201	PEB	CHB-C1C-NC	-2.03	120.67	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	YO	201	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
82	D7	203	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
87	A6	402	CLA	CMB-C2B-C3B	2.03	131.50	126.59
82	TO	203	PEB	CAA-C3A-C4A	-2.03	107.46	112.67
82	WM	201	PEB	CHB-C1C-C2C	-2.03	122.57	127.15
82	U1	203	PEB	C2B-C1B-NB	2.03	114.86	110.53
82	AK	202	PEB	CAB-C3B-C4B	2.03	128.60	125.01
82	JK	202	PEB	CHC-C4C-NC	-2.03	118.40	121.15
82	D5	203	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
83	xK	306	PUB	C1B-C2B-C3B	-2.03	105.63	107.50
87	AN	835	CLA	CHB-C1B-NB	2.03	126.41	124.26
87	52	607	CLA	CHB-C1B-NB	2.03	126.41	124.26
87	b6	606	CLA	CHC-C4B-NB	2.03	126.41	124.26
87	cL	509	CLA	C3A-C2A-C1A	2.03	104.38	101.34
82	U7	201	PEB	CHB-C4B-NB	-2.03	120.36	124.58
82	Z5	304	PEB	C1C-CHB-C4B	-2.03	123.73	128.28
82	NB	202	PEB	C3C-C4C-NC	2.03	110.16	108.33
82	F1	1002	PEB	C3C-C4C-NC	2.03	110.16	108.33
82	Y4	201	PEB	CAB-C3B-C4B	2.03	128.60	125.01
83	AJ	304	PUB	CAC-C2C-C1C	2.03	128.60	125.01
82	R4	201	PEB	CMD-C2D-C3D	2.03	132.93	130.06
82	Y4	202	PEB	CMC-C3C-C4C	2.03	129.21	127.06
82	K7	201	PEB	C2B-C1B-NB	2.03	114.86	110.53
82	T9	201	PEB	CHC-C1D-ND	-2.03	111.16	113.72
82	fM	202	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
82	KJ	202	PEB	CHB-C4B-C3B	-2.03	120.63	125.32
87	C6	517	CLA	CHD-C1D-ND	-2.03	122.59	124.45
87	BN	823	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
91	A6	407	PHO	C1A-C2A-C3A	-2.03	100.91	102.84
87	dL	402	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
95	cL	502	DGD	C3E-C4E-C5E	2.03	113.86	110.24
82	CM	203	PEB	CAB-C3B-C4B	2.03	128.60	125.01
82	MK	201	PEB	CBB-CAB-C3B	-2.03	106.99	112.63
82	DP	202	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	iE	202	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
87	CL	509	CLA	CHB-C1B-NB	2.03	126.40	124.26
82	dB	202	PEB	CHB-C4B-C3B	-2.03	120.63	125.32
87	8N	304	CLA	C2A-C1A-CHA	2.03	127.41	123.86
95	c6	620	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
82	TB	201	PEB	CHB-C1C-C2C	-2.03	122.58	127.15
82	I9	201	PEB	CHC-C1D-ND	-2.03	111.16	113.72
87	72	609	CLA	CHA-C1A-NA	-2.03	121.75	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DB	202	PEB	C1D-CHC-C4C	-2.03	110.27	113.26
82	VD	201	PEB	C1D-CHC-C4C	-2.03	110.27	113.26
85	b6	603	BCR	C23-C24-C25	-2.03	121.51	127.20
82	RI	201	PEB	CHC-C4C-NC	2.03	123.89	121.15
82	PM	202	PEB	C2A-C1A-NA	2.03	110.02	108.27
82	HK	202	PEB	C2B-C1B-NB	2.03	114.86	110.53
82	Y7	303	PEB	CAC-C2C-C1C	2.03	128.99	125.76
82	EM	202	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
87	42	605	CLA	C3B-C4B-NB	-2.03	108.63	110.52
82	d1	202	PEB	C1C-CHB-C4B	2.03	132.83	128.28
82	RQ	201	PEB	CHB-C4B-NB	-2.03	120.36	124.58
87	bL	606	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
82	vK	201	PEB	CAA-C3A-C4A	-2.03	107.47	112.67
87	BN	833	CLA	CHA-C1A-NA	-2.03	121.75	126.40
82	hB	301	PEB	CMB-C2B-C1B	2.03	128.19	125.06
85	K2	102	BCR	C11-C12-C13	2.03	132.11	126.42
82	b1	203	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
82	M5	305	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
82	eH	203	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
85	B6	621	BCR	C40-C30-C25	-2.03	107.01	110.30
92	d6	409	LMG	O8-C28-C29	2.03	118.27	111.91
82	PB	201	PEB	CHA-C1B-NB	-2.03	120.69	124.93
82	FQ	202	PEB	CHC-C1D-ND	-2.03	111.16	113.72
82	NF	201	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	P9	202	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
87	C6	510	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
87	d6	401	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
82	WQ	201	PEB	CMC-C3C-C4C	2.03	129.21	127.06
82	CP	201	PEB	CBD-CAD-C3D	-2.03	117.54	127.62
82	FA	203	PEB	C2B-C1B-NB	2.03	114.85	110.53
84	K1	1001	CYC	C4D-ND-C1D	-2.03	106.17	109.79
82	xK	302	PEB	OD-C4D-C3D	-2.03	124.87	129.46
82	mK	201	PEB	C1B-C2B-C3B	-2.03	104.18	106.51
82	d4	201	PEB	C2A-C1A-NA	2.03	110.02	108.27
82	I7	202	PEB	C2A-C1A-NA	2.03	110.02	108.27
95	b6	621	DGD	C2G-O2G-C1B	-2.03	112.80	117.79
82	I5	201	PEB	CHB-C1C-NC	-2.03	120.68	125.32
82	VM	201	PEB	CAC-C2C-C1C	2.03	128.99	125.76
82	RO	203	PEB	CAC-C2C-C1C	2.03	128.99	125.76
82	GD	201	PEB	CHC-C4C-NC	2.03	123.89	121.15
82	RD	201	PEB	CAA-C3A-C4A	-2.03	107.47	112.67
87	B2	832	CLA	CHB-C1B-NB	2.03	126.40	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	b6	606	CLA	CHB-C1B-NB	2.03	126.40	124.26
82	N4	1002	PEB	CHA-C1B-NB	-2.03	120.69	124.93
87	BN	820	CLA	CHD-C1D-ND	-2.03	122.59	124.45
83	AH	303	PUB	CMD-C2D-C3D	2.03	130.81	127.77
82	LJ	202	PEB	CHB-C4B-NB	-2.03	120.36	124.58
87	12	602	CLA	CHA-C1A-NA	-2.03	121.76	126.40
87	A2	839	CLA	CHA-C1A-NA	-2.03	121.76	126.40
87	A2	850	CLA	CHA-C1A-NA	-2.03	121.76	126.40
82	GF	203	PEB	O1C-CGC-CBC	-2.03	116.57	123.08
94	DL	401	PL9	C51-C49-C50	2.03	119.08	114.60
82	AK	201	PEB	CMA-C2A-C1A	-2.03	108.04	112.40
87	BN	831	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
95	CL	523	DGD	O1G-C1A-O1A	-2.03	118.48	123.59
87	c6	614	CLA	O2D-CGD-CBD	2.03	114.87	111.27
82	Z4	201	PEB	C4C-C3C-C2C	-2.03	105.63	107.50
82	T1	201	PEB	CAC-C2C-C1C	2.03	128.99	125.76
87	H6	103	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
82	HD	203	PEB	CHB-C1C-NC	-2.03	120.68	125.32
82	LG	1002	PEB	CMC-C3C-C2C	-2.03	121.22	125.61
82	WH	203	PEB	CHC-C1D-ND	-2.03	111.16	113.72
82	G9	201	PEB	CHC-C1D-ND	-2.03	111.16	113.72
82	t8	201	PEB	CHB-C4B-C3B	-2.03	120.63	125.32
82	aG	201	PEB	C2B-C1B-NB	2.03	114.85	110.53
82	EB	501	PEB	CAB-CBB-CGB	-2.03	109.25	113.60
82	T5	201	PEB	CHB-C1C-NC	-2.03	120.68	125.32
87	IN	103	CLA	C2A-C1A-CHA	2.03	127.40	123.86
92	BL	611	LMG	O7-C10-O9	-2.03	118.81	123.70
82	IM	202	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
87	B2	823	CLA	C3C-C4C-NC	-2.02	108.30	110.57
82	AD	303	PEB	OD-C4D-C3D	-2.02	124.87	129.46
82	VE	202	PEB	C1C-CHB-C4B	-2.02	123.74	128.28
82	OJ	203	PEB	CAB-C3B-C4B	2.02	128.59	125.01
84	V3	1001	CYC	OC-C1C-NC	2.02	127.39	124.94
82	WQ	202	PEB	CHC-C1D-ND	-2.02	111.16	113.72
82	XD	203	PEB	CAC-C2C-C1C	2.02	128.99	125.76
82	S9	202	PEB	CAC-C2C-C1C	2.02	128.99	125.76
84	HH	1001	CYC	CHA-C1A-C2A	-2.02	120.64	125.32
87	72	602	CLA	CMD-C2D-C3D	2.02	132.27	127.61
82	AH	302	PEB	C3C-C4C-NC	2.02	110.16	108.33
82	FH	1002	PEB	C3C-C4C-NC	2.02	110.16	108.33
82	eF	201	PEB	C3C-C4C-NC	2.02	110.16	108.33
82	lJ	202	PEB	C3C-C4C-NC	2.02	110.16	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	G7	202	PEB	C1D-CHC-C4C	2.02	116.24	113.26
82	BA	202	PEB	CBA-CAA-C3A	-2.02	108.96	113.47
87	12	606	CLA	CHC-C4B-NB	2.02	126.40	124.26
82	LG	1002	PEB	CAB-C3B-C2B	2.02	131.65	127.88
82	g1	202	PEB	CAB-CBB-CGB	-2.02	109.25	113.60
82	vK	201	PEB	C1B-C2B-C3B	-2.02	104.18	106.51
82	iO	203	PEB	C1B-C2B-C3B	-2.02	104.18	106.51
82	TF	202	PEB	CBD-CAD-C3D	-2.02	117.55	127.62
82	eG	202	PEB	CHC-C1D-ND	-2.02	111.16	113.72
85	c6	602	BCR	C8-C7-C6	-2.02	121.52	127.20
82	F1	1002	PEB	C4C-C3C-C2C	-2.02	105.63	107.50
82	e4	203	PEB	C4C-C3C-C2C	-2.02	105.63	107.50
87	62	308	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
82	WJ	203	PEB	CAB-C3B-C4B	2.02	128.59	125.01
84	e3	1001	CYC	CAA-C2A-C1A	2.02	128.59	125.01
82	WJ	201	PEB	CAA-C3A-C2A	-2.02	109.20	114.26
82	i4	203	PEB	CAA-C3A-C2A	-2.02	109.20	114.26
82	V4	202	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
87	BL	623	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
85	HL	103	BCR	C31-C1-C6	-2.02	107.02	110.30
82	aE	202	PEB	CMB-C2B-C1B	2.02	128.18	125.06
87	1N	606	CLA	CHC-C4B-NB	2.02	126.40	124.26
82	lO	201	PEB	CHA-C1B-NB	-2.02	120.70	124.93
87	AN	826	CLA	C3B-C4B-NB	-2.02	108.64	110.52
95	h6	101	DGD	C2G-O2G-C1B	-2.02	112.81	117.79
82	gB	203	PEB	CHB-C4B-NB	-2.02	120.37	124.58
82	WD	201	PEB	CHB-C4B-NB	2.02	128.79	124.58
82	FK	202	PEB	CHB-C4B-NB	2.02	128.79	124.58
87	a6	608	CLA	CMB-C2B-C3B	2.02	131.49	126.59
87	AN	834	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
82	DD	202	PEB	CMD-C2D-C3D	2.02	132.92	130.06
82	V7	202	PEB	OA-C1A-NA	2.02	127.39	124.94
87	c6	616	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
82	sF	202	PEB	C2A-C3A-C4A	2.02	104.37	101.34
87	AN	815	CLA	C4-C3-C5	2.02	118.67	115.27
82	P5	201	PEB	CHB-C1C-NC	-2.02	120.69	125.32
95	C6	521	DGD	C6E-C5E-C4E	-2.02	108.27	113.00
82	HK	201	PEB	CAC-CBC-CGC	-2.02	109.25	113.60
87	AN	822	CLA	C2A-C1A-CHA	2.02	127.40	123.86
82	AH	302	PEB	C4C-C3C-C2C	-2.02	105.63	107.50
82	CI	201	PEB	CHC-C4C-NC	2.02	123.89	121.15
87	52	611	CLA	CHB-C1B-NB	2.02	126.40	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	gO	202	PEB	C1D-CHC-C4C	-2.02	110.27	113.26
87	5N	602	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
82	aK	202	PEB	CHC-C1D-ND	-2.02	111.17	113.72
87	72	604	CLA	C3B-C4B-NB	-2.02	108.64	110.52
87	3N	303	CLA	C3B-C4B-NB	-2.02	108.64	110.52
82	F7	202	PEB	OA-C1A-NA	2.02	127.39	124.94
82	YF	202	PEB	C3C-C4C-NC	2.02	110.15	108.33
84	FO	1001	CYC	CMB-C2B-C1B	2.02	126.69	124.17
82	OH	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
82	UK	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
82	lG	203	PEB	CAB-C3B-C4B	2.02	128.59	125.01
95	C6	502	DGD	O2G-C1B-O1B	-2.02	118.82	123.70
82	P5	201	PEB	C1D-CHC-C4C	-2.02	110.28	113.26
82	SJ	203	PEB	C1C-NC-C4C	-2.02	106.00	109.60
82	PJ	202	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	F5	202	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	oK	203	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
87	B2	825	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
82	d4	201	PEB	CHC-C1D-ND	-2.02	111.17	113.72
87	b6	614	CLA	CHB-C1B-NB	2.02	126.40	124.26
87	8N	302	CLA	CHC-C4B-NB	2.02	126.40	124.26
82	MK	201	PEB	C1B-C2B-C3B	-2.02	104.19	106.51
82	xC	202	PEB	CAC-C2C-C1C	2.02	128.98	125.76
82	fJ	203	PEB	CAC-C2C-C1C	2.02	128.98	125.76
85	BN	841	BCR	C38-C26-C27	2.02	117.50	113.62
87	2N	312	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
87	4N	610	CLA	C2B-C1B-NB	2.02	111.59	110.23
82	vF	201	PEB	CHB-C1C-C2C	-2.02	122.59	127.15
87	a6	608	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
82	cB	403	PEB	CMC-C3C-C4C	-2.02	124.92	127.06
83	AH	304	PUB	CMB-C2B-C1B	-2.02	124.92	127.06
82	VK	202	PEB	CHC-C4C-NC	2.02	123.88	121.15
82	H9	203	PEB	C1D-CHC-C4C	2.02	116.24	113.26
82	TJ	201	PEB	CHA-C1B-C2B	2.02	130.10	124.90
87	72	603	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
82	VP	202	PEB	CAB-C3B-C4B	2.02	128.58	125.01
84	A3	1001	CYC	CAA-C2A-C1A	2.02	128.58	125.01
82	RQ	201	PEB	CAA-C3A-C4A	-2.02	107.48	112.67
87	HL	102	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
82	U5	201	PEB	CHB-C1C-C2C	-2.02	122.59	127.15
87	CL	512	CLA	CHD-C1D-ND	-2.02	122.60	124.45
87	B6	609	CLA	CHD-C1D-ND	-2.02	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	bP	502	PEB	CBA-CAA-C3A	-2.02	108.97	113.47
82	WE	203	PEB	C2B-C1B-NB	2.02	114.84	110.53
95	C6	521	DGD	O5D-C6D-C5D	-2.02	105.31	109.05
87	F2	202	CLA	CMC-C2C-C3C	2.02	131.60	126.12
82	FA	202	PEB	CBD-CAD-C3D	-2.02	117.57	127.62
82	VJ	202	PEB	C1B-C2B-C3B	-2.02	104.19	106.51
87	R2	201	CLA	CHB-C1B-NB	2.02	126.40	124.26
87	12	602	CLA	CHB-C4A-NA	2.02	127.31	124.51
82	SF	203	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	m4	203	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	gJ	202	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
83	A4	302	PUB	CBA-CAA-C3A	-2.02	109.91	112.98
83	xF	305	PUB	CAB-CBB-CGB	-2.02	109.25	113.60
87	DL	404	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
87	2N	309	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
82	FI	202	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
82	M5	305	PEB	C1D-CHC-C4C	-2.02	110.28	113.26
82	X5	201	PEB	C1D-CHC-C4C	-2.02	110.28	113.26
82	K7	202	PEB	CHB-C1C-NC	-2.02	120.69	125.32
82	GF	201	PEB	CAB-C3B-C4B	2.02	128.58	125.01
82	ZE	202	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
82	UI	201	PEB	CBC-CAC-C2C	-2.02	107.01	112.63
82	eJ	201	PEB	CAC-C2C-C1C	2.02	128.98	125.76
87	RN	202	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
82	NI	201	PEB	CAC-CBC-CGC	-2.02	109.26	113.60
82	gF	203	PEB	CAC-CBC-CGC	-2.02	109.26	113.60
82	AJ	301	PEB	C3C-C4C-NC	2.02	110.15	108.33
85	aL	604	BCR	C38-C26-C25	-2.02	122.26	124.53
82	b4	201	PEB	C2A-C1A-NA	2.02	110.01	108.27
87	H6	103	CLA	CHB-C1B-NB	2.02	126.39	124.26
82	Z5	305	PEB	CAC-C2C-C1C	2.02	128.98	125.76
82	iF	202	PEB	CAC-C2C-C3C	2.02	131.69	127.07
82	VO	202	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
82	YD	201	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	DK	203	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	X9	202	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
87	AN	839	CLA	C2A-C1A-CHA	2.02	127.39	123.86
82	vF	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
82	F7	202	PEB	CBD-CAD-C3D	-2.02	117.57	127.62
85	J2	103	BCR	C10-C11-C12	-2.02	116.92	123.22
82	GB	201	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
82	OM	202	PEB	C1C-CHB-C4B	-2.02	123.75	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	L2	206	CLA	CHA-C1A-NA	-2.02	121.77	126.40
82	uC	201	PEB	CHA-C1B-NB	-2.02	120.71	124.93
82	AF	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
87	B2	829	CLA	C3B-C4B-NB	-2.02	108.64	110.52
82	A5	201	PEB	C1D-CHC-C4C	-2.02	110.28	113.26
82	PI	201	PEB	CHC-C4C-NC	2.02	123.88	121.15
87	82	305	CLA	CHA-C4D-ND	2.02	136.72	132.50
87	BN	834	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
82	VO	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
85	AN	804	BCR	C11-C12-C13	-2.02	120.75	126.42
85	B2	841	BCR	C38-C26-C27	2.02	117.49	113.62
82	JA	203	PEB	CAC-CBC-CGC	-2.02	109.26	113.60
82	h1	202	PEB	C1C-CHB-C4B	2.02	132.81	128.28
87	2N	308	CLA	CHC-C4B-NB	2.02	126.39	124.26
83	AE	302	PUB	CBA-CAA-C3A	-2.02	109.92	112.98
82	P7	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
87	42	610	CLA	C2B-C1B-NB	2.02	111.58	110.23
82	JI	201	PEB	CMB-C2B-C1B	2.02	128.17	125.06
82	S9	202	PEB	CAC-CBC-CGC	-2.02	109.26	113.60
82	O9	203	PEB	CHA-C1B-NB	-2.02	120.71	124.93
82	xF	302	PEB	CAB-C3B-C4B	2.02	128.58	125.01
87	7N	605	CLA	C2D-C1D-ND	-2.02	108.62	110.10
82	sK	201	PEB	C1C-CHB-C4B	2.02	132.81	128.28
83	A4	302	PUB	C1D-CHC-C4C	-2.02	108.98	113.37
82	VF	201	PEB	C3C-C4C-NC	2.02	110.15	108.33
82	wK	301	PEB	C3C-C4C-NC	2.02	110.15	108.33
82	bF	202	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
82	lF	203	PEB	C1C-NC-C4C	-2.02	106.01	109.60
87	1N	605	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
82	Z4	202	PEB	CAC-C2C-C1C	2.02	128.97	125.76
82	D9	201	PEB	CMB-C2B-C1B	2.02	128.17	125.06
94	A6	410	PL9	C47-C48-C49	-2.02	120.85	127.75
82	K9	201	PEB	CHC-C1D-ND	-2.02	111.17	113.72
82	TB	201	PEB	CAB-C3B-C4B	2.02	128.58	125.01
87	b6	616	CLA	CHD-C1D-ND	-2.02	122.60	124.45
82	XI	201	PEB	CHC-C4C-NC	2.02	123.88	121.15
82	JK	202	PEB	C2B-C1B-NB	2.02	114.83	110.53
82	xC	202	PEB	C2B-C1B-NB	2.02	114.83	110.53
82	qF	203	PEB	CMC-C3C-C4C	2.02	129.20	127.06
82	hJ	203	PEB	CBD-CAD-C3D	-2.02	117.58	127.62
87	7N	609	CLA	CHA-C1A-NA	-2.02	121.78	126.40
82	lM	201	PEB	CAC-CBC-CGC	-2.02	109.26	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
96	f6	101	HEM	CAD-C3D-C4D	2.02	128.18	124.66
82	OP	202	PEB	CMA-C2A-C1A	-2.02	108.06	112.40
82	XK	203	PEB	CHA-C1B-NB	-2.02	120.71	124.93
82	iJ	201	PEB	CHA-C1B-C2B	2.02	130.09	124.90
87	8N	304	CLA	CBA-CAA-C2A	-2.02	107.91	113.86
82	PA	201	PEB	C3B-C4B-NB	2.02	112.98	110.05
82	xF	303	PEB	CAC-C2C-C1C	2.02	128.97	125.76
82	w8	202	PEB	CHB-C1C-NC	2.02	129.94	125.32
82	V5	201	PEB	CHB-C1C-NC	-2.02	120.70	125.32
82	TQ	202	PEB	CHB-C1C-C2C	-2.02	122.60	127.15
82	T1	201	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
82	dE	204	PEB	CAC-CBC-CGC	-2.02	109.26	113.60
83	AM	304	PUB	CAC-CBC-CGC	-2.02	109.26	113.60
87	B2	801	CLA	C2B-C1B-NB	2.02	111.58	110.23
82	DB	201	PEB	C3C-C4C-NC	2.02	110.15	108.33
82	lJ	201	PEB	C1C-NC-C4C	-2.02	106.01	109.60
82	AQ	303	PEB	OD-C4D-C3D	-2.02	124.89	129.46
82	TH	202	PEB	CBD-CAD-C3D	-2.02	117.59	127.62
82	w8	201	PEB	C2B-C1B-NB	2.02	114.83	110.53
82	aM	203	PEB	C2B-C1B-NB	2.02	114.83	110.53
84	x3	1001	CYC	OC-C1C-NC	2.02	127.38	124.94
82	AE	301	PEB	CAB-C3B-C4B	2.02	128.57	125.01
82	tK	201	PEB	CMB-C2B-C1B	2.02	128.17	125.06
82	mO	203	PEB	C4C-C3C-C2C	-2.02	105.64	107.50
82	VM	202	PEB	C2A-C1A-NA	2.02	110.01	108.27
82	Q5	201	PEB	C2A-C1A-NA	2.02	110.01	108.27
87	12	605	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
95	BL	613	DGD	O2G-C1B-O1B	-2.02	118.83	123.70
82	DQ	202	PEB	CAC-C2C-C3C	2.02	131.69	127.07
82	sF	201	PEB	C1C-CHB-C4B	2.02	132.80	128.28
87	A2	823	CLA	C2A-C1A-CHA	2.02	127.38	123.86
82	nK	201	PEB	CHA-C1B-C2B	2.02	130.08	124.90
103	8N	310	ZEX	C4-C5-C6	-2.02	116.36	120.85
91	aL	610	PHO	O2D-CGD-O1D	-2.02	119.90	123.84
82	VI	203	PEB	CAB-C3B-C2B	2.02	131.63	127.88
82	ZF	202	PEB	CMB-C2B-C1B	2.02	128.17	125.06
82	x8	202	PEB	C2B-C1B-NB	2.02	114.83	110.53
83	A1	303	PUB	CMD-C2D-C3D	2.02	130.79	127.77
95	BN	844	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
82	T7	201	PEB	C1B-C2B-C3B	-2.02	104.19	106.51
87	A2	824	CLA	CHD-C1D-ND	-2.02	122.60	124.45
87	b6	618	CLA	CHD-C1D-ND	-2.02	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	TP	202	PEB	CAB-C3B-C4B	2.02	128.57	125.01
82	V9	201	PEB	CHC-C1D-ND	-2.02	111.17	113.72
84	C4	1001	CYC	CHB-C4A-C3A	2.02	130.08	124.90
84	L1	1001	CYC	OB-C4B-NB	-2.02	120.39	125.08
82	QK	202	PEB	CAC-C2C-C1C	2.02	128.97	125.76
82	aE	201	PEB	C2B-C1B-NB	2.02	114.83	110.53
85	b6	602	BCR	C12-C13-C14	2.01	122.03	118.94
84	H1	1001	CYC	CHA-C1A-C2A	-2.01	120.66	125.32
82	EP	202	PEB	C1D-CHC-C4C	-2.01	110.28	113.26
87	12	609	CLA	CHC-C4B-NB	2.01	126.39	124.26
87	K2	103	CLA	C2A-C1A-CHA	2.01	127.38	123.86
87	AN	840	CLA	CAC-C3C-C4C	2.01	127.42	124.81
87	7N	605	CLA	C3B-C4B-NB	-2.01	108.65	110.52
82	AF	201	PEB	CAC-C2C-C3C	2.01	131.68	127.07
82	hH	201	PEB	C1C-CHB-C4B	2.01	132.80	128.28
82	PK	202	PEB	CHB-C1C-NC	-2.01	120.70	125.32
87	B2	834	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
83	A4	302	PUB	CHB-C1C-NC	-2.01	120.39	124.58
82	O9	202	PEB	CBC-CAC-C2C	2.01	118.22	112.63
82	IJ	201	PEB	CAC-CBC-CGC	-2.01	109.27	113.60
82	QD	201	PEB	CHA-C4A-NA	2.01	127.60	125.20
82	OM	201	PEB	CMA-C2A-C1A	-2.01	108.06	112.40
87	HL	101	CLA	CHD-C1D-ND	-2.01	122.60	124.45
82	vK	202	PEB	C2B-C1B-NB	2.01	114.83	110.53
82	OP	201	PEB	CAB-C3B-C4B	2.01	128.57	125.01
82	PP	201	PEB	CAB-C3B-C4B	2.01	128.57	125.01
82	bB	201	PEB	CAB-C3B-C4B	2.01	128.57	125.01
82	XJ	201	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
82	EM	201	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
82	wK	301	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
87	B6	608	CLA	CHB-C1B-NB	2.01	126.39	124.26
87	AN	809	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
87	A2	809	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
82	MP	203	PEB	OD-C4D-ND	-2.01	122.95	125.93
82	bH	201	PEB	OD-C4D-ND	-2.01	122.95	125.93
82	hK	201	PEB	CAC-C2C-C1C	2.01	128.97	125.76
87	82	305	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
82	bE	201	PEB	C2A-C1A-NA	2.01	110.01	108.27
82	iO	201	PEB	CHB-C1C-C2C	-2.01	122.61	127.15
82	X7	202	PEB	CHB-C4B-C3B	-2.01	120.66	125.32
87	BN	817	CLA	CMB-C2B-C3B	2.01	131.47	126.59
87	HL	102	CLA	C2A-C1A-CHA	2.01	127.38	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	aL	606	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
82	C5	201	PEB	C1D-CHC-C4C	-2.01	110.29	113.26
82	kE	202	PEB	C1D-CHC-C4C	2.01	116.22	113.26
87	AN	841	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
82	NQ	204	PEB	CAB-C3B-C4B	2.01	128.57	125.01
84	l3	1001	CYC	CAA-C2A-C1A	2.01	128.57	125.01
82	TJ	202	PEB	CHA-C4A-NA	-2.01	122.81	125.20
96	fL	102	HEM	CHD-C4C-NC	2.01	126.62	124.44
82	QP	202	PEB	OD-C4D-C3D	-2.01	124.90	129.46
82	PF	202	PEB	CHB-C1C-NC	-2.01	120.71	125.32
87	AL	403	CLA	C7-C6-C5	-2.01	107.89	113.36
87	2N	308	CLA	CHB-C4A-NA	2.01	127.30	124.51
82	hH	201	PEB	C3C-C4C-NC	2.01	110.15	108.33
82	WG	203	PEB	C2B-C1B-NB	2.01	114.83	110.53
82	AJ	301	PEB	CAC-CBC-CGC	-2.01	109.27	113.60
87	F2	201	CLA	O2D-CGD-CBD	2.01	114.84	111.27
87	b6	617	CLA	CHB-C1B-NB	2.01	126.39	124.26
87	AN	850	CLA	CHA-C1A-NA	-2.01	121.79	126.40
82	AG	304	PEB	CAB-C3B-C4B	2.01	128.57	125.01
82	BF	202	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
82	T9	202	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
82	gO	203	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
82	UP	201	PEB	CHA-C4A-NA	2.01	127.60	125.20
83	QM	201	PUB	CBA-CAA-C3A	2.01	116.03	112.98
82	YA	303	PEB	CAC-C2C-C1C	2.01	128.97	125.76
82	ID	202	PEB	CAC-C2C-C1C	2.01	128.97	125.76
87	2N	308	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
82	V4	201	PEB	CMA-C2A-C1A	-2.01	108.06	112.40
82	hJ	202	PEB	CAA-C3A-C2A	-2.01	109.23	114.26
95	BL	607	DGD	C1E-O6E-C5E	2.01	117.64	113.69
84	N3	1001	CYC	CAA-C2A-C1A	2.01	128.57	125.01
87	7N	602	CLA	CMD-C2D-C3D	2.01	132.24	127.61
82	VD	203	PEB	CAA-C3A-C4A	-2.01	107.51	112.67
87	c6	614	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
82	HQ	203	PEB	CHB-C1C-NC	-2.01	120.71	125.32
82	BA	202	PEB	CHB-C4B-C3B	-2.01	120.66	125.32
82	fB	301	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
82	B7	203	PEB	CHA-C1B-NB	-2.01	120.72	124.93
82	SD	202	PEB	CHA-C4A-NA	-2.01	122.81	125.20
82	lO	201	PEB	CAB-C3B-C4B	2.01	128.57	125.01
87	FN	201	CLA	CMC-C2C-C3C	2.01	131.58	126.12
82	L4	1002	PEB	CBD-CAD-C3D	-2.01	117.61	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	3N	308	CLA	CHA-C4D-ND	2.01	136.71	132.50
87	7N	604	CLA	CHA-C4D-ND	2.01	136.71	132.50
82	R1	201	PEB	C4B-NB-C1B	-2.01	102.72	106.51
94	aL	601	PL9	C51-C49-C50	2.01	119.05	114.60
82	K5	201	PEB	C1D-CHC-C4C	-2.01	110.29	113.26
82	IA	202	PEB	C2A-C1A-NA	2.01	110.01	108.27
95	D6	410	DGD	C3D-C4D-C5D	2.01	113.83	110.24
82	OJ	201	PEB	CBA-CAA-C3A	-2.01	108.99	113.47
82	dK	201	PEB	CAB-C3B-C4B	2.01	128.57	125.01
84	P3	1001	CYC	CAA-C2A-C1A	2.01	128.57	125.01
82	VA	203	PEB	OD-C4D-C3D	-2.01	124.90	129.46
87	HL	102	CLA	CHA-C1A-NA	-2.01	121.79	126.40
87	B2	813	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
84	CH	1001	CYC	CHA-C1A-C2A	-2.01	120.67	125.32
87	A2	823	CLA	CHC-C4B-NB	2.01	126.39	124.26
87	2N	309	CLA	CHD-C4C-C3C	2.01	127.80	124.84
85	CL	502	BCR	C15-C14-C13	-2.01	124.44	127.31
85	BN	840	BCR	C24-C25-C26	2.01	126.33	121.46
82	AQ	304	PEB	OD-C4D-C3D	-2.01	124.91	129.46
82	MJ	201	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
82	Z1	203	PEB	C4C-C3C-C2C	-2.01	105.64	107.50
96	FL	102	HEM	C4C-NC-C1C	2.01	107.32	105.35
85	A2	847	BCR	C36-C18-C19	2.01	121.25	118.08
83	K7	203	PUB	CBA-CAA-C3A	-2.01	109.93	112.98
82	WP	202	PEB	C4B-NB-C1B	-2.01	102.72	106.51
82	YH	202	PEB	CHB-C1C-C2C	-2.01	122.61	127.15
82	pF	201	PEB	CAC-CBC-CGC	-2.01	109.28	113.60
83	AJ	303	PUB	CAB-CBB-CGB	-2.01	109.28	113.60
82	UJ	201	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
87	BN	812	CLA	CHB-C1B-NB	2.01	126.39	124.26
87	R2	204	CLA	CHC-C4B-NB	2.01	126.39	124.26
82	NA	201	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
82	TK	201	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
82	hE	203	PEB	CAC-C2C-C1C	2.01	128.96	125.76
87	AN	807	CLA	CAC-C3C-C4C	2.01	127.42	124.81
82	AE	304	PEB	C3C-C4C-NC	2.01	110.14	108.33
82	uF	202	PEB	C3C-C4C-NC	2.01	110.14	108.33
85	LN	205	BCR	C32-C1-C6	-2.01	107.04	110.30
82	LG	1002	PEB	CMB-C2B-C1B	2.01	128.16	125.06
82	i1	202	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	Y9	202	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	kE	202	PEB	C4C-C3C-C2C	-2.01	105.65	107.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	815	CLA	C2D-C1D-ND	-2.01	108.62	110.10
87	22	612	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
87	AN	838	CLA	C2A-C1A-CHA	2.01	127.37	123.86
87	A2	820	CLA	O2D-CGD-CBD	2.01	114.84	111.27
84	g3	1001	CYC	CAA-C2A-C1A	2.01	128.56	125.01
82	WA	202	PEB	C1D-CHC-C4C	-2.01	110.29	113.26
82	CQ	201	PEB	C1D-CHC-C4C	2.01	116.22	113.26
82	fG	201	PEB	C1D-CHC-C4C	-2.01	110.29	113.26
82	hG	203	PEB	CAC-C2C-C1C	2.01	128.96	125.76
82	mE	203	PEB	CHA-C4A-NA	-2.01	122.82	125.20
87	8N	302	CLA	CHA-C4D-ND	2.01	136.70	132.50
87	BN	822	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
82	aB	201	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
87	A2	838	CLA	C2A-C1A-CHA	2.01	127.37	123.86
84	i3	1001	CYC	CAA-C2A-C1A	2.01	128.56	125.01
82	jJ	203	PEB	C2B-C1B-NB	2.01	114.82	110.53
87	BN	824	CLA	C3C-C4C-NC	-2.01	108.32	110.57
82	LO	1002	PEB	CBD-CAD-C3D	-2.01	117.62	127.62
82	BB	201	PEB	CAC-CBC-CGC	-2.01	109.28	113.60
82	FQ	201	PEB	CAC-CBC-CGC	-2.01	109.28	113.60
82	GF	202	PEB	CMC-C3C-C4C	2.01	129.19	127.06
82	HK	202	PEB	CHC-C1D-ND	-2.01	111.18	113.72
82	GQ	202	PEB	CHB-C1C-C2C	-2.01	122.62	127.15
82	EJ	203	PEB	CAC-C2C-C1C	2.01	128.96	125.76
87	L2	204	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
87	4N	602	CLA	CMB-C2B-C3B	2.01	131.45	126.59
82	hG	201	PEB	C4B-C3B-C2B	-2.01	104.56	106.78
87	dL	404	CLA	C1-C2-C3	-2.01	122.57	126.04
82	YJ	202	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	I9	202	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	WG	201	PEB	OA-C1A-C2A	-2.01	124.58	126.17
84	D1	1003	CYC	CMD-C2D-C1D	2.01	128.50	125.56
82	l4	202	PEB	CHA-C1B-NB	-2.01	120.73	124.93
82	TH	201	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
82	AA	201	PEB	CBA-CAA-C3A	2.01	117.94	113.47
82	KJ	202	PEB	CBA-CAA-C3A	-2.01	109.00	113.47
82	m4	203	PEB	C2A-C1A-NA	2.01	110.00	108.27
82	cB	401	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
84	t3	1001	CYC	CAA-C2A-C1A	2.01	128.56	125.01
84	l3	1001	CYC	CHB-C1B-C2B	-2.01	122.97	126.95
82	CD	202	PEB	C3C-C4C-NC	2.01	110.14	108.33
82	cB	402	PEB	C3C-C4C-NC	2.01	110.14	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	c6	616	CLA	CHD-C1D-ND	-2.01	122.61	124.45
87	d6	401	CLA	CHD-C1D-ND	-2.01	122.61	124.45
82	JJ	202	PEB	CAA-C3A-C4A	2.01	117.83	112.67
82	CJ	203	PEB	CAC-C2C-C1C	2.01	128.96	125.76
82	MK	201	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	L9	202	PEB	CAC-CBC-CGC	-2.01	109.28	113.60
87	L2	204	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
95	cL	520	DGD	O1G-C1A-O1A	-2.01	118.53	123.59
82	AB	501	PEB	CAA-C3A-C2A	-2.01	109.24	114.26
82	iO	203	PEB	CAA-C3A-C2A	-2.01	109.24	114.26
82	OK	202	PEB	OD-C4D-ND	-2.01	122.96	125.93
82	w8	204	PEB	C2B-C1B-NB	2.01	114.81	110.53
82	II	201	PEB	CHC-C4C-NC	2.01	123.86	121.15
82	l4	202	PEB	O1B-CGB-CBB	-2.01	116.63	123.08
82	VJ	202	PEB	CHA-C1B-NB	-2.01	120.73	124.93
82	KJ	202	PEB	CHB-C1C-C2C	-2.01	122.62	127.15
82	Q9	202	PEB	C1C-NC-C4C	-2.01	106.03	109.60
82	hG	202	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
82	hO	202	PEB	CAC-CBC-CGC	-2.01	109.28	113.60
87	AN	839	CLA	CHA-C1A-NA	-2.01	121.80	126.40
82	fG	202	PEB	C2A-C1A-NA	2.01	110.00	108.27
82	lO	202	PEB	O1B-CGB-CBB	-2.01	116.63	123.08
82	h4	201	PEB	CMD-C2D-C3D	2.01	132.89	130.06
85	c6	602	BCR	C34-C9-C10	-2.01	120.11	122.92
92	qL	301	LMG	C7-O1-C1	-2.01	109.82	113.74
82	u8	203	PEB	CAC-CBC-CGC	-2.01	109.28	113.60
82	gB	201	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
82	KF	201	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	WJ	201	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
87	LN	206	CLA	CHA-C1A-NA	-2.01	121.80	126.40
82	HA	201	PEB	OD-C4D-C3D	-2.01	124.92	129.46
82	AK	201	PEB	CAC-C2C-C3C	2.01	131.66	127.07
87	B2	835	CLA	CHC-C4B-NB	2.01	126.38	124.26
84	K3	1001	CYC	CAA-C2A-C1A	2.01	128.56	125.01
84	c3	1001	CYC	CAA-C2A-C1A	2.01	128.56	125.01
92	A6	408	LMG	C7-O1-C1	-2.01	109.82	113.74
82	TE	201	PEB	CHA-C4A-NA	2.01	127.59	125.20
82	A5	201	PEB	CHB-C1C-NC	-2.01	120.72	125.32
82	wC	202	PEB	CHB-C1C-NC	2.01	129.91	125.32
82	CP	201	PEB	OD-C4D-ND	-2.01	122.96	125.93
87	c6	616	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
82	MJ	202	PEB	OA-C1A-NA	2.01	127.37	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AN	816	CLA	C2D-C1D-ND	-2.01	108.63	110.10
82	U1	202	PEB	OD-C4D-C3D	-2.01	124.92	129.46
82	aK	203	PEB	C3C-C4C-NC	2.01	110.14	108.33
85	B2	840	BCR	C24-C25-C26	2.01	126.32	121.46
82	GK	201	PEB	CBA-CAA-C3A	2.01	117.93	113.47
87	82	301	CLA	CHB-C1B-NB	2.01	126.38	124.26
82	WK	203	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
82	gE	202	PEB	C4C-C3C-C2C	-2.01	105.65	107.50
87	22	608	CLA	CHB-C4A-NA	2.01	127.28	124.51
82	XI	201	PEB	CAC-CBC-CGC	-2.01	109.29	113.60
87	cL	514	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
82	YE	201	PEB	CBA-CAA-C3A	-2.00	109.00	113.47
87	72	604	CLA	CHA-C4D-ND	2.00	136.69	132.50
82	aB	201	PEB	CHB-C1C-C2C	-2.00	122.63	127.15
87	B2	810	CLA	C2B-C1B-NB	-2.00	108.89	110.23
82	Z4	201	PEB	C1C-NC-C4C	-2.00	106.03	109.60
82	dH	201	PEB	C2B-C1B-NB	2.00	114.81	110.53
82	CD	201	PEB	C1D-CHC-C4C	2.00	116.21	113.26
82	CP	203	PEB	CAB-CBB-CGB	-2.00	109.29	113.60
82	R5	201	PEB	CHB-C1C-NC	-2.00	120.73	125.32
87	AN	823	CLA	C2A-C1A-CHA	2.00	127.36	123.86
87	K2	106	CLA	C3C-C4C-NC	-2.00	108.32	110.57
82	i4	203	PEB	C2A-C1A-NA	2.00	110.00	108.27
82	mO	203	PEB	C2A-C1A-NA	2.00	110.00	108.27
82	LF	201	PEB	CHB-C1C-C2C	-2.00	122.63	127.15
82	FI	201	PEB	C2B-C1B-NB	2.00	114.81	110.53
82	KM	202	PEB	C2B-C1B-NB	2.00	114.81	110.53
87	B2	807	CLA	CHA-C1A-NA	-2.00	121.81	126.40
82	BP	201	PEB	CMA-C2A-C1A	-2.00	108.08	112.40
96	E6	101	HEM	CMC-C2C-C1C	2.00	128.25	124.71
82	DJ	201	PEB	C1B-C2B-C3B	-2.00	104.21	106.51
82	JB	201	PEB	CAB-C3B-C4B	2.00	128.55	125.01
87	BN	806	CLA	C3B-C4B-NB	-2.00	108.66	110.52
82	oK	202	PEB	OD-C4D-C3D	-2.00	124.92	129.46
82	IF	201	PEB	O2C-CGC-O1C	-2.00	118.31	123.30
87	A2	831	CLA	C3C-C4C-NC	-2.00	108.32	110.57
95	J6	101	DGD	O2G-C1B-O1B	-2.00	118.86	123.70
82	DF	203	PEB	CHA-C1B-C2B	-2.00	119.75	124.90
87	BL	621	CLA	O2D-CGD-CBD	2.00	114.83	111.27
82	AI	201	PEB	CHC-C4C-NC	2.00	123.86	121.15
87	5N	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
87	MN	101	CLA	CHA-C1A-NA	-2.00	121.81	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	M9	303	PUB	CAB-CBB-CGB	-2.00	109.29	113.60
85	AN	845	BCR	C30-C25-C26	-2.00	119.79	122.61
82	OQ	201	PEB	C3C-C4C-NC	2.00	110.14	108.33
82	PQ	201	PEB	C4C-C3C-C2C	-2.00	105.65	107.50
82	oF	203	PEB	CAC-C2C-C1C	2.00	128.95	125.76
83	AO	303	PUB	CAB-C3B-C4B	2.00	128.95	125.76
82	WF	201	PEB	CHA-C1B-C2B	2.00	130.05	124.90
82	PE	202	PEB	CHB-C1C-C2C	-2.00	122.63	127.15
83	AO	302	PUB	C1D-CHC-C4C	-2.00	109.01	113.37
82	W1	201	PEB	CHB-C4B-NB	-2.00	120.41	124.58
87	D6	402	CLA	O2D-CGD-CBD	2.00	114.83	111.27
83	BM	302	PUB	CHB-C4B-NB	-2.00	120.73	125.32
82	IP	202	PEB	CHA-C1B-NB	-2.00	120.74	124.93
82	dH	202	PEB	C1C-CHB-C4B	2.00	132.77	128.28
87	A2	841	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
82	OJ	202	PEB	CHB-C4B-NB	-2.00	120.41	124.58
82	BB	201	PEB	CAC-C2C-C1C	2.00	128.95	125.76
82	HD	202	PEB	CAC-C2C-C1C	2.00	128.95	125.76
87	A2	850	CLA	CMC-C2C-C3C	2.00	131.55	126.12
94	a6	601	PL9	C37-C36-C34	-2.00	106.39	112.98
85	h6	102	BCR	C34-C9-C10	-2.00	120.12	122.92
82	uC	201	PEB	C2B-C1B-NB	2.00	114.80	110.53
82	C5	201	PEB	CHB-C1C-NC	-2.00	120.73	125.32
82	N5	201	PEB	CHB-C1C-NC	-2.00	120.73	125.32
82	DB	202	PEB	CAC-CBC-CGC	-2.00	109.29	113.60
82	DJ	201	PEB	CAC-CBC-CGC	-2.00	109.29	113.60
87	B6	609	CLA	C1-C2-C3	-2.00	122.58	126.04
82	QB	202	PEB	CBA-CAA-C3A	2.00	117.92	113.47
84	CO	1001	CYC	CMC-C2C-C1C	-2.00	108.09	112.40
82	TJ	201	PEB	C1B-C2B-C3B	-2.00	104.21	106.51
91	dL	403	PHO	CMC-C2C-C1C	2.00	128.51	124.73
82	TF	202	PEB	C2A-C1A-NA	2.00	110.00	108.27
82	s8	201	PEB	C2A-C1A-NA	2.00	110.00	108.27
87	B6	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
95	B2	844	DGD	C2G-O2G-C1B	-2.00	112.86	117.79
82	O1	203	PEB	CMB-C2B-C1B	2.00	128.15	125.06
82	F5	201	PEB	C1D-CHC-C4C	-2.00	110.30	113.26
82	i1	202	PEB	CHC-C4C-NC	2.00	123.86	121.15
82	VA	201	PEB	C3B-C4B-NB	2.00	112.96	110.05
82	EQ	201	PEB	CBA-CAA-C3A	-2.00	109.01	113.47
87	CL	508	CLA	O1D-CGD-CBD	2.00	128.58	124.48
87	62	305	CLA	C2B-C1B-NB	2.00	111.57	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	cL	511	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
84	LE	1001	CYC	CMC-C2C-C1C	-2.00	108.09	112.40
84	GG	1001	CYC	CMC-C2C-C1C	-2.00	108.09	112.40
84	BG	1001	CYC	OB-C4B-NB	-2.00	120.43	125.08
87	BN	801	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
82	DF	201	PEB	O2B-CGB-CBB	2.00	120.46	114.03
82	iE	201	PEB	CHC-C1D-ND	-2.00	111.19	113.72
82	AD	301	PEB	CHA-C4A-NA	-2.00	122.83	125.20
82	kH	203	PEB	CHA-C4A-NA	2.00	127.58	125.20
87	B2	805	CLA	C3B-C4B-NB	-2.00	108.66	110.52
84	T3	1001	CYC	CHB-C1B-C2B	-2.00	122.98	126.95
87	1N	611	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
82	aK	202	PEB	CAB-C3B-C4B	2.00	128.55	125.01
87	82	301	CLA	CHA-C4D-ND	2.00	136.69	132.50
87	bL	607	CLA	CHC-C4B-NB	2.00	126.38	124.26
87	5N	611	CLA	CHB-C1B-NB	2.00	126.38	124.26
85	L2	201	BCR	C28-C27-C26	-2.00	110.50	114.08
82	XI	201	PEB	CAB-CBB-CGB	-2.00	109.30	113.60
84	LH	1002	CYC	CBC-CAC-C3C	2.00	117.92	113.47
82	G5	201	PEB	C1D-CHC-C4C	-2.00	110.31	113.26
84	A3	1001	CYC	CHB-C1B-C2B	-2.00	122.98	126.95
87	A2	822	CLA	C2A-C1A-CHA	2.00	127.36	123.86
82	f1	201	PEB	C4C-C3C-C2C	-2.00	105.65	107.50
82	T1	201	PEB	C2B-C1B-NB	2.00	114.80	110.53
82	F9	201	PEB	OA-C1A-C2A	-2.00	124.58	126.17
84	LH	1002	CYC	C4D-ND-C1D	-2.00	106.22	109.79
87	AN	831	CLA	C3C-C4C-NC	-2.00	108.33	110.57
92	BL	612	LMG	O1-C7-C8	-2.00	106.07	110.90
82	MF	201	PEB	CBB-CAB-C3B	-2.00	107.07	112.63
87	B2	826	CLA	CHB-C1B-NB	2.00	126.38	124.26
87	62	303	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
87	72	605	CLA	C3B-C4B-NB	-2.00	108.66	110.52
82	XM	201	PEB	CHB-C4B-NB	-2.00	120.41	124.58
82	wF	302	PEB	CHB-C4B-NB	-2.00	120.41	124.58
95	BL	614	DGD	O6E-C5E-C4E	2.00	113.33	109.69
82	mH	202	PEB	C4B-C3B-C2B	-2.00	104.57	106.78
82	Y5	202	PEB	C2B-C1B-NB	2.00	114.80	110.53
82	GB	203	PEB	CAB-C3B-C4B	2.00	128.55	125.01
84	m3	1001	CYC	CAA-C2A-C1A	2.00	128.55	125.01
82	OD	202	PEB	CAC-CBC-CGC	-2.00	109.30	113.60
82	GI	202	PEB	CAC-CBC-CGC	-2.00	109.30	113.60
87	82	303	CLA	C2A-C1A-CHA	2.00	127.36	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	QP	202	PEB	O2C-CGC-CBC	2.00	120.46	114.03
96	V6	201	HEM	C4A-NA-C1A	2.00	107.31	105.35
82	YH	201	PEB	CBB-CAB-C3B	2.00	118.19	112.63
82	GJ	203	PEB	CHB-C4B-C3B	-2.00	120.69	125.32
82	E5	201	PEB	CHB-C1C-NC	-2.00	120.74	125.32
87	72	605	CLA	C2D-C1D-ND	-2.00	108.63	110.10
82	iG	201	PEB	CHC-C1D-ND	-2.00	111.19	113.72
87	12	607	CLA	CMB-C2B-C3B	2.00	131.43	126.59
83	KA	203	PUB	CBA-CAA-C3A	-2.00	109.94	112.98
82	VB	201	PEB	CMC-C3C-C2C	-2.00	121.28	125.61
82	QA	201	PEB	CBA-CAA-C3A	-2.00	109.01	113.47
87	H6	102	CLA	CHD-C1D-ND	-2.00	122.62	124.45
87	b6	615	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (28) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
87	aL	606	CLA	C8
91	AL	410	PHO	C13
91	AL	410	PHO	C2A
91	AL	410	PHO	C8
91	DL	405	PHO	C13
91	DL	405	PHO	C2A
91	DL	405	PHO	C8
91	A6	407	PHO	C13
91	A6	407	PHO	C2A
91	A6	407	PHO	C8
91	D6	404	PHO	C13
91	D6	404	PHO	C2A
91	D6	404	PHO	C8
91	a6	613	PHO	C13
91	a6	613	PHO	C2A
91	a6	613	PHO	C8
91	d6	404	PHO	C13
91	d6	404	PHO	C2A
91	d6	404	PHO	C8
91	aL	610	PHO	C13
91	aL	610	PHO	C2A
91	aL	610	PHO	C8
91	dL	403	PHO	C13
91	dL	403	PHO	C2A
91	dL	403	PHO	C8

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Mol	Chain	Res	Type	Atom
92	bL	609	LMG	C4
92	bL	609	LMG	C5
92	bL	609	LMG	C8

All (23196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	AA	201	PEB	ND-C1D-CHC-C4C
82	AA	201	PEB	C2D-C1D-CHC-C4C
82	AA	201	PEB	NB-C1B-CHA-C4A
82	AA	201	PEB	C2B-C1B-CHA-C4A
82	AA	202	PEB	ND-C1D-CHC-C4C
82	AA	202	PEB	C2D-C1D-CHC-C4C
82	AA	202	PEB	C2D-C3D-CAD-CBD
82	AA	202	PEB	C4D-C3D-CAD-CBD
82	AA	202	PEB	C2A-C3A-CAA-CBA
82	AA	202	PEB	C4A-C3A-CAA-CBA
82	AA	202	PEB	NB-C1B-CHA-C4A
82	AA	202	PEB	C2B-C1B-CHA-C4A
82	BA	201	PEB	ND-C1D-CHC-C4C
82	BA	201	PEB	C2D-C1D-CHC-C4C
82	BA	201	PEB	NB-C1B-CHA-C4A
82	BA	201	PEB	C2B-C1B-CHA-C4A
82	BA	202	PEB	C2A-C3A-CAA-CBA
82	BA	202	PEB	C4A-C3A-CAA-CBA
82	BA	202	PEB	NB-C1B-CHA-C4A
82	BA	202	PEB	C2B-C1B-CHA-C4A
82	BA	203	PEB	NC-C1C-CHB-C4B
82	BA	203	PEB	C2C-C1C-CHB-C4B
82	BA	203	PEB	C2A-C3A-CAA-CBA
82	BA	203	PEB	NB-C1B-CHA-C4A
82	BA	203	PEB	C2B-C1B-CHA-C4A
82	CA	201	PEB	ND-C1D-CHC-C4C
82	CA	201	PEB	C2D-C1D-CHC-C4C
82	CA	201	PEB	NB-C1B-CHA-C4A
82	CA	201	PEB	C2B-C1B-CHA-C4A
82	CA	202	PEB	NC-C1C-CHB-C4B
82	CA	202	PEB	C2C-C1C-CHB-C4B
82	CA	202	PEB	C2A-C3A-CAA-CBA
82	CA	202	PEB	C4A-C3A-CAA-CBA
82	CA	202	PEB	NB-C1B-CHA-C4A
82	CA	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	DA	201	PEB	ND-C1D-CHC-C4C
82	DA	201	PEB	C2D-C1D-CHC-C4C
82	DA	201	PEB	NB-C1B-CHA-C4A
82	DA	201	PEB	C2B-C1B-CHA-C4A
82	DA	202	PEB	ND-C1D-CHC-C4C
82	DA	202	PEB	C2D-C1D-CHC-C4C
82	DA	202	PEB	C4A-C3A-CAA-CBA
82	DA	202	PEB	NB-C1B-CHA-C4A
82	DA	202	PEB	C2B-C1B-CHA-C4A
82	DA	203	PEB	ND-C1D-CHC-C4C
82	DA	203	PEB	C2D-C1D-CHC-C4C
82	DA	203	PEB	NC-C1C-CHB-C4B
82	DA	203	PEB	C2C-C1C-CHB-C4B
82	DA	203	PEB	NB-C1B-CHA-C4A
82	DA	203	PEB	C2B-C1B-CHA-C4A
82	EA	201	PEB	NB-C1B-CHA-C4A
82	EA	201	PEB	C2B-C1B-CHA-C4A
82	EA	202	PEB	ND-C1D-CHC-C4C
82	EA	202	PEB	C2D-C1D-CHC-C4C
82	EA	202	PEB	C4A-C3A-CAA-CBA
82	EA	202	PEB	NB-C1B-CHA-C4A
82	EA	202	PEB	C2B-C1B-CHA-C4A
82	FA	201	PEB	NB-C1B-CHA-C4A
82	FA	201	PEB	C2B-C1B-CHA-C4A
82	FA	202	PEB	C4A-C3A-CAA-CBA
82	FA	202	PEB	NB-C1B-CHA-C4A
82	FA	202	PEB	C2B-C1B-CHA-C4A
82	FA	203	PEB	ND-C1D-CHC-C4C
82	FA	203	PEB	C2D-C1D-CHC-C4C
82	FA	203	PEB	NC-C1C-CHB-C4B
82	FA	203	PEB	C2A-C3A-CAA-CBA
82	FA	203	PEB	C4A-C3A-CAA-CBA
82	FA	203	PEB	NB-C1B-CHA-C4A
82	FA	203	PEB	C2B-C1B-CHA-C4A
82	GA	201	PEB	C2A-C3A-CAA-CBA
82	GA	201	PEB	C4A-C3A-CAA-CBA
82	GA	201	PEB	NB-C1B-CHA-C4A
82	GA	201	PEB	C2B-C1B-CHA-C4A
82	GA	202	PEB	C2A-C3A-CAA-CBA
82	GA	202	PEB	C4A-C3A-CAA-CBA
82	GA	202	PEB	NB-C1B-CHA-C4A
82	GA	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	HA	201	PEB	NB-C1B-CHA-C4A
82	HA	201	PEB	C2B-C1B-CHA-C4A
82	HA	202	PEB	ND-C1D-CHC-C4C
82	HA	202	PEB	C2D-C1D-CHC-C4C
82	HA	202	PEB	C4A-C3A-CAA-CBA
82	HA	202	PEB	NB-C1B-CHA-C4A
82	HA	202	PEB	C2B-C1B-CHA-C4A
82	HA	203	PEB	NB-C1B-CHA-C4A
82	HA	203	PEB	C2B-C1B-CHA-C4A
82	HA	203	PEB	C2B-C3B-CAB-CBB
82	IA	201	PEB	ND-C1D-CHC-C4C
82	IA	201	PEB	C2D-C1D-CHC-C4C
82	IA	201	PEB	C2A-C3A-CAA-CBA
82	IA	201	PEB	C4A-C3A-CAA-CBA
82	IA	201	PEB	NB-C1B-CHA-C4A
82	IA	201	PEB	C2B-C1B-CHA-C4A
82	IA	202	PEB	C2A-C3A-CAA-CBA
82	IA	202	PEB	C4A-C3A-CAA-CBA
82	IA	202	PEB	NB-C1B-CHA-C4A
82	IA	202	PEB	C2B-C1B-CHA-C4A
82	JA	201	PEB	ND-C1D-CHC-C4C
82	JA	201	PEB	C2D-C1D-CHC-C4C
82	JA	201	PEB	NB-C1B-CHA-C4A
82	JA	201	PEB	C2B-C1B-CHA-C4A
82	JA	202	PEB	C4A-C3A-CAA-CBA
82	JA	202	PEB	NB-C1B-CHA-C4A
82	JA	202	PEB	C2B-C1B-CHA-C4A
82	JA	203	PEB	ND-C1D-CHC-C4C
82	JA	203	PEB	C2A-C3A-CAA-CBA
82	JA	203	PEB	C4A-C3A-CAA-CBA
82	JA	203	PEB	NB-C1B-CHA-C4A
82	JA	203	PEB	C2B-C1B-CHA-C4A
82	KA	201	PEB	NB-C1B-CHA-C4A
82	KA	201	PEB	C2B-C1B-CHA-C4A
82	KA	202	PEB	C2D-C3D-CAD-CBD
82	KA	202	PEB	C4D-C3D-CAD-CBD
82	KA	202	PEB	NB-C1B-CHA-C4A
82	KA	202	PEB	C2B-C1B-CHA-C4A
82	LA	201	PEB	NB-C1B-CHA-C4A
82	LA	201	PEB	C2B-C1B-CHA-C4A
82	LA	202	PEB	C4A-C3A-CAA-CBA
82	LA	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	LA	202	PEB	C2B-C1B-CHA-C4A
82	LA	203	PEB	NC-C1C-CHB-C4B
82	LA	203	PEB	C2C-C1C-CHB-C4B
82	LA	203	PEB	NB-C1B-CHA-C4A
82	LA	203	PEB	C2B-C1B-CHA-C4A
82	MA	201	PEB	NB-C1B-CHA-C4A
82	MA	201	PEB	C2B-C1B-CHA-C4A
82	MA	202	PEB	ND-C1D-CHC-C4C
82	MA	202	PEB	C2D-C1D-CHC-C4C
82	MA	202	PEB	C4A-C3A-CAA-CBA
82	MA	202	PEB	NB-C1B-CHA-C4A
82	MA	202	PEB	C2B-C1B-CHA-C4A
82	NA	201	PEB	NB-C1B-CHA-C4A
82	NA	201	PEB	C2B-C1B-CHA-C4A
82	NA	202	PEB	C4A-C3A-CAA-CBA
82	NA	202	PEB	NB-C1B-CHA-C4A
82	NA	202	PEB	C2B-C1B-CHA-C4A
82	NA	203	PEB	NB-C1B-CHA-C4A
82	NA	203	PEB	C2B-C1B-CHA-C4A
82	OA	201	PEB	C2B-C1B-CHA-C4A
82	OA	202	PEB	C2A-C3A-CAA-CBA
82	OA	202	PEB	C4A-C3A-CAA-CBA
82	OA	202	PEB	NB-C1B-CHA-C4A
82	OA	202	PEB	C2B-C1B-CHA-C4A
82	PA	201	PEB	NB-C1B-CHA-C4A
82	PA	201	PEB	C2B-C1B-CHA-C4A
82	PA	202	PEB	C4A-C3A-CAA-CBA
82	PA	202	PEB	NB-C1B-CHA-C4A
82	PA	202	PEB	C2B-C1B-CHA-C4A
82	PA	203	PEB	NC-C1C-CHB-C4B
82	PA	203	PEB	NB-C1B-CHA-C4A
82	PA	203	PEB	C2B-C1B-CHA-C4A
82	QA	201	PEB	NB-C1B-CHA-C4A
82	QA	201	PEB	C2B-C1B-CHA-C4A
82	QA	202	PEB	C4A-C3A-CAA-CBA
82	QA	202	PEB	NB-C1B-CHA-C4A
82	QA	202	PEB	C2B-C1B-CHA-C4A
82	RA	201	PEB	NB-C1B-CHA-C4A
82	RA	201	PEB	C2B-C1B-CHA-C4A
82	RA	202	PEB	C4A-C3A-CAA-CBA
82	RA	202	PEB	NB-C1B-CHA-C4A
82	RA	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	RA	203	PEB	C2D-C3D-CAD-CBD
82	RA	203	PEB	C4D-C3D-CAD-CBD
82	RA	203	PEB	NB-C1B-CHA-C4A
82	RA	203	PEB	C2B-C1B-CHA-C4A
82	SA	202	PEB	C4A-C3A-CAA-CBA
82	SA	202	PEB	NB-C1B-CHA-C4A
82	SA	202	PEB	C2B-C1B-CHA-C4A
82	TA	201	PEB	NB-C1B-CHA-C4A
82	TA	201	PEB	C2B-C1B-CHA-C4A
82	TA	202	PEB	C4A-C3A-CAA-CBA
82	TA	202	PEB	NB-C1B-CHA-C4A
82	TA	202	PEB	C2B-C1B-CHA-C4A
82	TA	203	PEB	NB-C1B-CHA-C4A
82	TA	203	PEB	C2B-C1B-CHA-C4A
82	UA	201	PEB	NB-C1B-CHA-C4A
82	UA	202	PEB	C4A-C3A-CAA-CBA
82	UA	202	PEB	NB-C1B-CHA-C4A
82	UA	202	PEB	C2B-C1B-CHA-C4A
82	VA	201	PEB	ND-C1D-CHC-C4C
82	VA	201	PEB	C2D-C1D-CHC-C4C
82	VA	201	PEB	C2A-C3A-CAA-CBA
82	VA	201	PEB	C4A-C3A-CAA-CBA
82	VA	201	PEB	NB-C1B-CHA-C4A
82	VA	201	PEB	C2B-C1B-CHA-C4A
82	VA	202	PEB	C2A-C3A-CAA-CBA
82	VA	202	PEB	C4A-C3A-CAA-CBA
82	VA	202	PEB	NB-C1B-CHA-C4A
82	VA	202	PEB	C2B-C1B-CHA-C4A
82	VA	203	PEB	NC-C1C-CHB-C4B
82	VA	203	PEB	C2C-C1C-CHB-C4B
82	VA	203	PEB	NB-C1B-CHA-C4A
82	VA	203	PEB	C2B-C1B-CHA-C4A
82	WA	201	PEB	NB-C1B-CHA-C4A
82	WA	201	PEB	C2B-C1B-CHA-C4A
82	WA	202	PEB	C2A-C3A-CAA-CBA
82	WA	202	PEB	C4A-C3A-CAA-CBA
82	WA	202	PEB	NB-C1B-CHA-C4A
82	WA	202	PEB	C2B-C1B-CHA-C4A
82	XA	201	PEB	NB-C1B-CHA-C4A
82	XA	201	PEB	C2B-C1B-CHA-C4A
82	XA	202	PEB	C2C-CAC-CBC-CGC
82	XA	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	XA	202	PEB	NB-C1B-CHA-C4A
82	XA	202	PEB	C2B-C1B-CHA-C4A
82	XA	203	PEB	NC-C1C-CHB-C4B
82	XA	203	PEB	C1C-C2C-CAC-CBC
82	XA	203	PEB	C2A-C3A-CAA-CBA
82	XA	203	PEB	NB-C1B-CHA-C4A
82	XA	203	PEB	C2B-C1B-CHA-C4A
82	YA	301	PEB	C3C-C4C-CHC-C1D
82	YA	301	PEB	ND-C1D-CHC-C4C
82	YA	301	PEB	C2D-C1D-CHC-C4C
82	YA	301	PEB	NC-C1C-CHB-C4B
82	YA	301	PEB	C2C-C1C-CHB-C4B
82	YA	301	PEB	C2A-C3A-CAA-CBA
82	YA	301	PEB	C4A-C3A-CAA-CBA
82	YA	301	PEB	NB-C1B-CHA-C4A
82	YA	301	PEB	C2B-C1B-CHA-C4A
82	YA	303	PEB	ND-C1D-CHC-C4C
82	YA	303	PEB	C2D-C1D-CHC-C4C
82	YA	303	PEB	NC-C1C-CHB-C4B
82	YA	303	PEB	C2C-C1C-CHB-C4B
82	YA	303	PEB	C2A-C3A-CAA-CBA
82	YA	303	PEB	NB-C1B-CHA-C4A
82	YA	303	PEB	C2B-C1B-CHA-C4A
82	YA	304	PEB	ND-C1D-CHC-C4C
82	YA	304	PEB	C2D-C1D-CHC-C4C
82	YA	304	PEB	NC-C1C-CHB-C4B
82	YA	304	PEB	C2C-C1C-CHB-C4B
82	YA	304	PEB	C2A-C3A-CAA-CBA
82	YA	304	PEB	NB-C1B-CHA-C4A
82	YA	304	PEB	C2B-C1B-CHA-C4A
82	AB	501	PEB	ND-C1D-CHC-C4C
82	AB	501	PEB	C2D-C1D-CHC-C4C
82	AB	501	PEB	C2A-C3A-CAA-CBA
82	AB	501	PEB	C4A-C3A-CAA-CBA
82	AB	501	PEB	NB-C1B-CHA-C4A
82	AB	501	PEB	C2B-C1B-CHA-C4A
82	BB	201	PEB	C2D-C1D-CHC-C4C
82	BB	201	PEB	NB-C1B-CHA-C4A
82	BB	201	PEB	C2B-C1B-CHA-C4A
82	BB	202	PEB	NB-C1B-CHA-C4A
82	BB	202	PEB	C2B-C1B-CHA-C4A
82	BB	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	BB	203	PEB	C2B-C1B-CHA-C4A
82	CB	201	PEB	NB-C1B-CHA-C4A
82	CB	201	PEB	C2B-C1B-CHA-C4A
82	CB	202	PEB	C2D-C3D-CAD-CBD
82	CB	202	PEB	C4D-C3D-CAD-CBD
82	CB	202	PEB	NB-C1B-CHA-C4A
82	CB	202	PEB	C2B-C1B-CHA-C4A
82	DB	201	PEB	NB-C1B-CHA-C4A
82	DB	201	PEB	C2B-C1B-CHA-C4A
82	DB	202	PEB	C2D-C1D-CHC-C4C
82	DB	202	PEB	NB-C1B-CHA-C4A
82	DB	202	PEB	C2B-C1B-CHA-C4A
82	DB	203	PEB	ND-C1D-CHC-C4C
82	DB	203	PEB	C2D-C1D-CHC-C4C
82	DB	203	PEB	NC-C1C-CHB-C4B
82	DB	203	PEB	C2C-C1C-CHB-C4B
82	DB	203	PEB	C2D-C3D-CAD-CBD
82	DB	203	PEB	C4D-C3D-CAD-CBD
82	DB	203	PEB	NB-C1B-CHA-C4A
82	DB	203	PEB	C2B-C1B-CHA-C4A
82	EB	501	PEB	ND-C1D-CHC-C4C
82	EB	501	PEB	C2D-C1D-CHC-C4C
82	EB	501	PEB	C2A-C3A-CAA-CBA
82	EB	501	PEB	C4A-C3A-CAA-CBA
82	EB	501	PEB	NB-C1B-CHA-C4A
82	EB	501	PEB	C2B-C1B-CHA-C4A
82	FB	201	PEB	C2D-C3D-CAD-CBD
82	FB	201	PEB	C4D-C3D-CAD-CBD
82	FB	201	PEB	C2A-C3A-CAA-CBA
82	FB	201	PEB	C4A-C3A-CAA-CBA
82	FB	201	PEB	NB-C1B-CHA-C4A
82	FB	201	PEB	C2B-C1B-CHA-C4A
82	GB	201	PEB	ND-C1D-CHC-C4C
82	GB	201	PEB	C2D-C1D-CHC-C4C
82	GB	201	PEB	NB-C1B-CHA-C4A
82	GB	201	PEB	C2B-C1B-CHA-C4A
82	GB	202	PEB	C2D-C1D-CHC-C4C
82	GB	202	PEB	NB-C1B-CHA-C4A
82	GB	202	PEB	C2B-C1B-CHA-C4A
82	GB	203	PEB	NB-C1B-CHA-C4A
82	GB	203	PEB	C2B-C1B-CHA-C4A
82	HB	201	PEB	C3C-C4C-CHC-C1D

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Mol	Chain	Res	Type	Atoms
82	HB	201	PEB	ND-C1D-CHC-C4C
82	HB	201	PEB	C2D-C1D-CHC-C4C
82	HB	201	PEB	NC-C1C-CHB-C4B
82	HB	201	PEB	C2C-C1C-CHB-C4B
82	HB	201	PEB	C2D-C3D-CAD-CBD
82	HB	201	PEB	C4D-C3D-CAD-CBD
82	HB	201	PEB	NB-C1B-CHA-C4A
82	HB	201	PEB	C2B-C1B-CHA-C4A
82	HB	202	PEB	ND-C1D-CHC-C4C
82	HB	202	PEB	C2D-C1D-CHC-C4C
82	HB	202	PEB	C4A-C3A-CAA-CBA
82	HB	202	PEB	NB-C1B-CHA-C4A
82	HB	202	PEB	C2B-C1B-CHA-C4A
82	HB	203	PEB	ND-C1D-CHC-C4C
82	HB	203	PEB	C2D-C1D-CHC-C4C
82	HB	203	PEB	NC-C1C-CHB-C4B
82	HB	203	PEB	C2C-C1C-CHB-C4B
82	HB	203	PEB	NB-C1B-CHA-C4A
82	HB	203	PEB	C2B-C1B-CHA-C4A
82	IB	201	PEB	NB-C1B-CHA-C4A
82	IB	201	PEB	C2B-C1B-CHA-C4A
82	IB	202	PEB	NB-C1B-CHA-C4A
82	IB	202	PEB	C2B-C1B-CHA-C4A
82	IB	203	PEB	ND-C1D-CHC-C4C
82	IB	203	PEB	C2D-C1D-CHC-C4C
82	IB	203	PEB	NB-C1B-CHA-C4A
82	IB	203	PEB	C2B-C1B-CHA-C4A
82	JB	201	PEB	C2A-C3A-CAA-CBA
82	JB	201	PEB	C4A-C3A-CAA-CBA
82	JB	202	PEB	C3C-C4C-CHC-C1D
82	JB	202	PEB	ND-C1D-CHC-C4C
82	JB	202	PEB	NB-C1B-CHA-C4A
82	JB	202	PEB	C2B-C1B-CHA-C4A
82	KB	301	PEB	ND-C1D-CHC-C4C
82	KB	301	PEB	C2D-C1D-CHC-C4C
82	KB	301	PEB	C2D-C3D-CAD-CBD
82	KB	301	PEB	C4D-C3D-CAD-CBD
82	KB	301	PEB	NB-C1B-CHA-C4A
82	KB	301	PEB	C2B-C1B-CHA-C4A
82	KB	302	PEB	ND-C1D-CHC-C4C
82	KB	302	PEB	C2D-C1D-CHC-C4C
82	KB	302	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
82	KB	302	PEB	C4D-C3D-CAD-CBD
82	KB	302	PEB	NB-C1B-CHA-C4A
82	KB	302	PEB	C2B-C1B-CHA-C4A
82	KB	303	PEB	ND-C1D-CHC-C4C
82	KB	303	PEB	C2D-C1D-CHC-C4C
82	KB	303	PEB	C4A-C3A-CAA-CBA
82	KB	303	PEB	NB-C1B-CHA-C4A
82	KB	303	PEB	C2B-C1B-CHA-C4A
82	KB	304	PEB	C2A-C3A-CAA-CBA
82	KB	304	PEB	C4A-C3A-CAA-CBA
82	KB	304	PEB	NB-C1B-CHA-C4A
82	KB	304	PEB	C2B-C1B-CHA-C4A
82	LB	201	PEB	ND-C1D-CHC-C4C
82	LB	201	PEB	C2D-C1D-CHC-C4C
82	LB	201	PEB	NC-C1C-CHB-C4B
82	LB	201	PEB	C2C-C1C-CHB-C4B
82	LB	201	PEB	NB-C1B-CHA-C4A
82	LB	201	PEB	C2B-C1B-CHA-C4A
82	MB	201	PEB	C2D-C1D-CHC-C4C
82	MB	201	PEB	NB-C1B-CHA-C4A
82	MB	201	PEB	C2B-C1B-CHA-C4A
82	MB	202	PEB	C2D-C3D-CAD-CBD
82	MB	202	PEB	C4D-C3D-CAD-CBD
82	MB	202	PEB	NB-C1B-CHA-C4A
82	MB	202	PEB	C2B-C1B-CHA-C4A
82	NB	201	PEB	NB-C1B-CHA-C4A
82	NB	201	PEB	C2B-C1B-CHA-C4A
82	NB	202	PEB	ND-C1D-CHC-C4C
82	NB	202	PEB	C2D-C1D-CHC-C4C
82	NB	202	PEB	NB-C1B-CHA-C4A
82	NB	202	PEB	C2B-C1B-CHA-C4A
82	NB	203	PEB	ND-C1D-CHC-C4C
82	NB	203	PEB	C2D-C1D-CHC-C4C
82	NB	203	PEB	NC-C1C-CHB-C4B
82	NB	203	PEB	C2C-C1C-CHB-C4B
82	NB	203	PEB	C2D-C3D-CAD-CBD
82	NB	203	PEB	C4D-C3D-CAD-CBD
82	NB	203	PEB	NB-C1B-CHA-C4A
82	NB	203	PEB	C2B-C1B-CHA-C4A
82	OB	201	PEB	C2D-C3D-CAD-CBD
82	OB	201	PEB	NB-C1B-CHA-C4A
82	OB	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	PB	201	PEB	C2D-C1D-CHC-C4C
82	PB	201	PEB	NB-C1B-CHA-C4A
82	PB	201	PEB	C2B-C1B-CHA-C4A
82	QB	201	PEB	C3C-C4C-CHC-C1D
82	QB	201	PEB	ND-C1D-CHC-C4C
82	QB	201	PEB	C2D-C1D-CHC-C4C
82	QB	201	PEB	NC-C1C-CHB-C4B
82	QB	201	PEB	C2C-C1C-CHB-C4B
82	QB	201	PEB	C4D-C3D-CAD-CBD
82	QB	201	PEB	NB-C1B-CHA-C4A
82	QB	201	PEB	C2B-C1B-CHA-C4A
82	QB	202	PEB	ND-C1D-CHC-C4C
82	QB	202	PEB	C2D-C1D-CHC-C4C
82	QB	202	PEB	C2A-C3A-CAA-CBA
82	QB	202	PEB	C4A-C3A-CAA-CBA
82	QB	202	PEB	NB-C1B-CHA-C4A
82	QB	202	PEB	C2B-C1B-CHA-C4A
82	QB	203	PEB	C2D-C1D-CHC-C4C
82	QB	203	PEB	C4A-C3A-CAA-CBA
82	QB	203	PEB	NB-C1B-CHA-C4A
82	QB	203	PEB	C2B-C1B-CHA-C4A
82	QB	204	PEB	ND-C1D-CHC-C4C
82	QB	204	PEB	C2D-C1D-CHC-C4C
82	QB	204	PEB	NC-C1C-CHB-C4B
82	QB	204	PEB	C2C-C1C-CHB-C4B
82	QB	204	PEB	NB-C1B-CHA-C4A
82	QB	204	PEB	C2B-C1B-CHA-C4A
82	RB	201	PEB	ND-C1D-CHC-C4C
82	RB	201	PEB	C2D-C1D-CHC-C4C
82	RB	201	PEB	NB-C1B-CHA-C4A
82	RB	201	PEB	C2B-C1B-CHA-C4A
82	RB	202	PEB	ND-C1D-CHC-C4C
82	RB	202	PEB	C2D-C1D-CHC-C4C
82	RB	202	PEB	NC-C1C-CHB-C4B
82	RB	202	PEB	C2C-C1C-CHB-C4B
82	RB	202	PEB	NB-C1B-CHA-C4A
82	RB	202	PEB	C2B-C1B-CHA-C4A
82	SB	201	PEB	NB-C1B-CHA-C4A
82	SB	201	PEB	C2B-C1B-CHA-C4A
82	SB	202	PEB	C2A-C3A-CAA-CBA
82	SB	202	PEB	C4A-C3A-CAA-CBA
82	SB	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	SB	202	PEB	C2B-C1B-CHA-C4A
82	SB	203	PEB	ND-C1D-CHC-C4C
82	SB	203	PEB	C2D-C1D-CHC-C4C
82	SB	203	PEB	NB-C1B-CHA-C4A
82	SB	203	PEB	C2B-C1B-CHA-C4A
82	TB	201	PEB	C2A-C3A-CAA-CBA
82	TB	201	PEB	C4A-C3A-CAA-CBA
82	TB	202	PEB	C3C-C4C-CHC-C1D
82	TB	202	PEB	ND-C1D-CHC-C4C
82	TB	202	PEB	NB-C1B-CHA-C4A
82	TB	202	PEB	C2B-C1B-CHA-C4A
82	UB	301	PEB	ND-C1D-CHC-C4C
82	UB	301	PEB	C2D-C1D-CHC-C4C
82	UB	301	PEB	C2D-C3D-CAD-CBD
82	UB	301	PEB	C4D-C3D-CAD-CBD
82	UB	301	PEB	C2A-C3A-CAA-CBA
82	UB	301	PEB	C4A-C3A-CAA-CBA
82	UB	301	PEB	NB-C1B-CHA-C4A
82	UB	301	PEB	C2B-C1B-CHA-C4A
82	UB	302	PEB	ND-C1D-CHC-C4C
82	UB	302	PEB	C2D-C1D-CHC-C4C
82	UB	302	PEB	C1C-C2C-CAC-CBC
82	UB	302	PEB	C3C-C2C-CAC-CBC
82	UB	302	PEB	NB-C1B-CHA-C4A
82	UB	302	PEB	C2B-C1B-CHA-C4A
82	UB	303	PEB	NB-C1B-CHA-C4A
82	UB	303	PEB	C2B-C1B-CHA-C4A
82	VB	201	PEB	ND-C1D-CHC-C4C
82	VB	201	PEB	C2D-C1D-CHC-C4C
82	VB	201	PEB	NC-C1C-CHB-C4B
82	VB	201	PEB	C2C-C1C-CHB-C4B
82	VB	201	PEB	NB-C1B-CHA-C4A
82	VB	201	PEB	C2B-C1B-CHA-C4A
82	VB	202	PEB	ND-C1D-CHC-C4C
82	VB	202	PEB	C2D-C1D-CHC-C4C
82	VB	202	PEB	C2C-CAC-CBC-CGC
82	VB	202	PEB	NB-C1B-CHA-C4A
82	VB	202	PEB	C2B-C1B-CHA-C4A
82	WB	401	PEB	C2D-C1D-CHC-C4C
82	WB	401	PEB	C2A-C3A-CAA-CBA
82	WB	401	PEB	C4A-C3A-CAA-CBA
82	WB	401	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	WB	401	PEB	C2B-C1B-CHA-C4A
82	WB	402	PEB	C1C-C2C-CAC-CBC
82	WB	402	PEB	C3C-C2C-CAC-CBC
82	WB	402	PEB	NB-C1B-CHA-C4A
82	WB	402	PEB	C2B-C1B-CHA-C4A
82	XB	201	PEB	C4A-C3A-CAA-CBA
82	XB	201	PEB	NB-C1B-CHA-C4A
82	XB	201	PEB	C2B-C1B-CHA-C4A
82	XB	202	PEB	ND-C1D-CHC-C4C
82	XB	202	PEB	C2D-C1D-CHC-C4C
82	XB	202	PEB	NC-C1C-CHB-C4B
82	XB	202	PEB	C2C-C1C-CHB-C4B
82	XB	202	PEB	NB-C1B-CHA-C4A
82	XB	202	PEB	C2B-C1B-CHA-C4A
82	YB	201	PEB	C2D-C1D-CHC-C4C
82	YB	201	PEB	NB-C1B-CHA-C4A
82	YB	201	PEB	C2B-C1B-CHA-C4A
82	YB	202	PEB	NB-C1B-CHA-C4A
82	YB	202	PEB	C2B-C1B-CHA-C4A
82	ZB	201	PEB	ND-C1D-CHC-C4C
82	ZB	201	PEB	C2D-C1D-CHC-C4C
82	ZB	201	PEB	C4A-C3A-CAA-CBA
82	ZB	201	PEB	NB-C1B-CHA-C4A
82	ZB	201	PEB	C2B-C1B-CHA-C4A
82	ZB	202	PEB	ND-C1D-CHC-C4C
82	ZB	202	PEB	C2D-C1D-CHC-C4C
82	ZB	202	PEB	C2A-C3A-CAA-CBA
82	ZB	202	PEB	C4A-C3A-CAA-CBA
82	ZB	202	PEB	NB-C1B-CHA-C4A
82	ZB	202	PEB	C2B-C1B-CHA-C4A
82	ZB	203	PEB	ND-C1D-CHC-C4C
82	ZB	203	PEB	C2D-C1D-CHC-C4C
82	ZB	203	PEB	NC-C1C-CHB-C4B
82	ZB	203	PEB	C2C-C1C-CHB-C4B
82	ZB	203	PEB	C2A-C3A-CAA-CBA
82	ZB	203	PEB	NB-C1B-CHA-C4A
82	ZB	203	PEB	C2B-C1B-CHA-C4A
82	AD	301	PEB	C2C-CAC-CBC-CGC
82	AD	301	PEB	NB-C1B-CHA-C4A
82	AD	301	PEB	C2B-C1B-CHA-C4A
82	AD	303	PEB	ND-C1D-CHC-C4C
82	AD	303	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	AD	303	PEB	C2A-C3A-CAA-CBA
82	AD	303	PEB	NB-C1B-CHA-C4A
82	AD	303	PEB	C2B-C1B-CHA-C4A
82	AD	304	PEB	NC-C4C-CHC-C1D
82	AD	304	PEB	C3C-C4C-CHC-C1D
82	AD	304	PEB	NC-C1C-CHB-C4B
82	AD	304	PEB	C2C-C1C-CHB-C4B
82	AD	304	PEB	NB-C1B-CHA-C4A
82	AD	304	PEB	C2B-C1B-CHA-C4A
82	BD	201	PEB	ND-C1D-CHC-C4C
82	BD	201	PEB	C2D-C1D-CHC-C4C
82	BD	201	PEB	NB-C1B-CHA-C4A
82	BD	201	PEB	C2B-C1B-CHA-C4A
82	BD	202	PEB	NC-C1C-CHB-C4B
82	BD	202	PEB	C2C-C1C-CHB-C4B
82	BD	202	PEB	C2A-C3A-CAA-CBA
82	BD	202	PEB	C4A-C3A-CAA-CBA
82	BD	202	PEB	NB-C1B-CHA-C4A
82	BD	202	PEB	C2B-C1B-CHA-C4A
82	BD	203	PEB	C2D-C3D-CAD-CBD
82	BD	203	PEB	C4D-C3D-CAD-CBD
82	BD	203	PEB	C4A-C3A-CAA-CBA
82	BD	203	PEB	NB-C1B-CHA-C4A
82	BD	203	PEB	C2B-C1B-CHA-C4A
82	CD	201	PEB	ND-C1D-CHC-C4C
82	CD	201	PEB	C2D-C1D-CHC-C4C
82	CD	201	PEB	NB-C1B-CHA-C4A
82	CD	201	PEB	C2B-C1B-CHA-C4A
82	CD	202	PEB	NB-C1B-CHA-C4A
82	CD	202	PEB	C2B-C1B-CHA-C4A
82	DD	201	PEB	C2D-C3D-CAD-CBD
82	DD	201	PEB	C4D-C3D-CAD-CBD
82	DD	201	PEB	C4A-C3A-CAA-CBA
82	DD	201	PEB	NB-C1B-CHA-C4A
82	DD	201	PEB	C2B-C1B-CHA-C4A
82	DD	202	PEB	ND-C1D-CHC-C4C
82	DD	202	PEB	C2D-C1D-CHC-C4C
82	DD	202	PEB	C3B-CAB-CBB-CGB
82	DD	203	PEB	NC-C1C-CHB-C4B
82	DD	203	PEB	C2C-C1C-CHB-C4B
82	DD	203	PEB	C4A-C3A-CAA-CBA
82	DD	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	DD	203	PEB	C2B-C1B-CHA-C4A
82	ED	201	PEB	ND-C1D-CHC-C4C
82	ED	201	PEB	C2D-C1D-CHC-C4C
82	ED	201	PEB	C2D-C3D-CAD-CBD
82	ED	201	PEB	C4D-C3D-CAD-CBD
82	ED	201	PEB	NB-C1B-CHA-C4A
82	ED	201	PEB	C2B-C1B-CHA-C4A
82	ED	202	PEB	NB-C1B-CHA-C4A
82	ED	202	PEB	C2B-C1B-CHA-C4A
82	FD	201	PEB	ND-C1D-CHC-C4C
82	FD	201	PEB	C2D-C1D-CHC-C4C
82	FD	201	PEB	C2D-C3D-CAD-CBD
82	FD	201	PEB	C4D-C3D-CAD-CBD
82	FD	201	PEB	NB-C1B-CHA-C4A
82	FD	201	PEB	C2B-C1B-CHA-C4A
82	FD	202	PEB	NC-C1C-CHB-C4B
82	FD	202	PEB	C2C-C1C-CHB-C4B
82	FD	202	PEB	C2A-C3A-CAA-CBA
82	FD	202	PEB	C4A-C3A-CAA-CBA
82	FD	202	PEB	NB-C1B-CHA-C4A
82	FD	202	PEB	C2B-C1B-CHA-C4A
82	FD	203	PEB	C4A-C3A-CAA-CBA
82	FD	203	PEB	NB-C1B-CHA-C4A
82	FD	203	PEB	C2B-C1B-CHA-C4A
82	GD	201	PEB	NB-C1B-CHA-C4A
82	GD	201	PEB	C2B-C1B-CHA-C4A
82	GD	202	PEB	C2A-C3A-CAA-CBA
82	GD	202	PEB	C4A-C3A-CAA-CBA
82	GD	202	PEB	NB-C1B-CHA-C4A
82	GD	202	PEB	C2B-C1B-CHA-C4A
82	HD	201	PEB	C4A-C3A-CAA-CBA
82	HD	201	PEB	NB-C1B-CHA-C4A
82	HD	201	PEB	C2B-C1B-CHA-C4A
82	HD	202	PEB	ND-C1D-CHC-C4C
82	HD	202	PEB	C2D-C1D-CHC-C4C
82	HD	202	PEB	NB-C1B-CHA-C4A
82	HD	203	PEB	ND-C1D-CHC-C4C
82	HD	203	PEB	C2D-C1D-CHC-C4C
82	HD	203	PEB	NC-C1C-CHB-C4B
82	HD	203	PEB	C2C-C1C-CHB-C4B
82	HD	203	PEB	C4A-C3A-CAA-CBA
82	HD	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	HD	203	PEB	C2B-C1B-CHA-C4A
82	ID	201	PEB	C2D-C1D-CHC-C4C
82	ID	201	PEB	C1C-C2C-CAC-CBC
82	ID	201	PEB	NB-C1B-CHA-C4A
82	ID	201	PEB	C2B-C1B-CHA-C4A
82	ID	202	PEB	NB-C1B-CHA-C4A
82	ID	202	PEB	C2B-C1B-CHA-C4A
82	JD	201	PEB	ND-C1D-CHC-C4C
82	JD	201	PEB	C2D-C1D-CHC-C4C
82	JD	201	PEB	NB-C1B-CHA-C4A
82	JD	201	PEB	C2B-C1B-CHA-C4A
82	JD	202	PEB	ND-C1D-CHC-C4C
82	JD	202	PEB	C2D-C1D-CHC-C4C
82	JD	202	PEB	NC-C1C-CHB-C4B
82	JD	202	PEB	C4A-C3A-CAA-CBA
82	JD	202	PEB	NB-C1B-CHA-C4A
82	JD	202	PEB	C2B-C1B-CHA-C4A
82	JD	203	PEB	ND-C1D-CHC-C4C
82	JD	203	PEB	C2D-C1D-CHC-C4C
82	JD	203	PEB	C2D-C3D-CAD-CBD
82	JD	203	PEB	C4D-C3D-CAD-CBD
82	JD	203	PEB	C4A-C3A-CAA-CBA
82	JD	203	PEB	NB-C1B-CHA-C4A
82	JD	203	PEB	C2B-C1B-CHA-C4A
82	KD	201	PEB	ND-C1D-CHC-C4C
82	KD	201	PEB	C2D-C1D-CHC-C4C
82	KD	201	PEB	C2A-C3A-CAA-CBA
82	KD	201	PEB	C4A-C3A-CAA-CBA
82	KD	201	PEB	NB-C1B-CHA-C4A
82	KD	201	PEB	C2B-C1B-CHA-C4A
82	KD	202	PEB	ND-C1D-CHC-C4C
82	KD	202	PEB	C2D-C1D-CHC-C4C
82	KD	202	PEB	C2D-C3D-CAD-CBD
82	KD	202	PEB	C4D-C3D-CAD-CBD
82	KD	202	PEB	NB-C1B-CHA-C4A
82	KD	202	PEB	C2B-C1B-CHA-C4A
82	LD	201	PEB	C4A-C3A-CAA-CBA
82	LD	201	PEB	NB-C1B-CHA-C4A
82	LD	201	PEB	C2B-C1B-CHA-C4A
82	LD	202	PEB	ND-C1D-CHC-C4C
82	LD	202	PEB	C2D-C1D-CHC-C4C
82	LD	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	LD	202	PEB	C2B-C1B-CHA-C4A
82	LD	203	PEB	C2A-C3A-CAA-CBA
82	LD	203	PEB	C4A-C3A-CAA-CBA
82	LD	203	PEB	NB-C1B-CHA-C4A
82	LD	203	PEB	C2B-C1B-CHA-C4A
82	MD	201	PEB	C1C-C2C-CAC-CBC
82	MD	201	PEB	NB-C1B-CHA-C4A
82	MD	201	PEB	C2B-C1B-CHA-C4A
82	MD	202	PEB	NB-C1B-CHA-C4A
82	MD	202	PEB	C2B-C1B-CHA-C4A
82	ND	202	PEB	ND-C1D-CHC-C4C
82	ND	202	PEB	C2D-C1D-CHC-C4C
82	ND	202	PEB	C2A-C3A-CAA-CBA
82	ND	202	PEB	C4A-C3A-CAA-CBA
82	ND	202	PEB	NB-C1B-CHA-C4A
82	ND	202	PEB	C2B-C1B-CHA-C4A
82	ND	203	PEB	ND-C1D-CHC-C4C
82	ND	203	PEB	C2D-C1D-CHC-C4C
82	ND	203	PEB	NC-C1C-CHB-C4B
82	ND	203	PEB	C2C-C1C-CHB-C4B
82	ND	203	PEB	C4A-C3A-CAA-CBA
82	ND	203	PEB	NB-C1B-CHA-C4A
82	ND	203	PEB	C2B-C1B-CHA-C4A
82	ND	204	PEB	C4A-C3A-CAA-CBA
82	ND	204	PEB	NB-C1B-CHA-C4A
82	ND	204	PEB	C2B-C1B-CHA-C4A
82	OD	201	PEB	ND-C1D-CHC-C4C
82	OD	201	PEB	C2D-C1D-CHC-C4C
82	OD	201	PEB	NB-C1B-CHA-C4A
82	OD	201	PEB	C2B-C1B-CHA-C4A
82	OD	202	PEB	ND-C1D-CHC-C4C
82	OD	202	PEB	C2D-C1D-CHC-C4C
82	OD	202	PEB	C2D-C3D-CAD-CBD
82	OD	202	PEB	C4D-C3D-CAD-CBD
82	OD	202	PEB	NB-C1B-CHA-C4A
82	OD	202	PEB	C2B-C1B-CHA-C4A
82	PD	201	PEB	C2A-C3A-CAA-CBA
82	PD	201	PEB	C4A-C3A-CAA-CBA
82	PD	201	PEB	NB-C1B-CHA-C4A
82	PD	201	PEB	C2B-C1B-CHA-C4A
82	PD	202	PEB	ND-C1D-CHC-C4C
82	PD	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	PD	202	PEB	NB-C1B-CHA-C4A
82	PD	202	PEB	C2B-C1B-CHA-C4A
82	PD	203	PEB	ND-C1D-CHC-C4C
82	PD	203	PEB	C2D-C1D-CHC-C4C
82	PD	203	PEB	NC-C1C-CHB-C4B
82	PD	203	PEB	C2C-C1C-CHB-C4B
82	PD	203	PEB	C2A-C3A-CAA-CBA
82	PD	203	PEB	C4A-C3A-CAA-CBA
82	PD	203	PEB	NB-C1B-CHA-C4A
82	PD	203	PEB	C2B-C1B-CHA-C4A
82	QD	201	PEB	NB-C1B-CHA-C4A
82	QD	201	PEB	C2B-C1B-CHA-C4A
82	QD	202	PEB	ND-C1D-CHC-C4C
82	QD	202	PEB	C2D-C1D-CHC-C4C
82	QD	202	PEB	NB-C1B-CHA-C4A
82	QD	202	PEB	C2B-C1B-CHA-C4A
82	RD	201	PEB	ND-C1D-CHC-C4C
82	RD	201	PEB	C2D-C1D-CHC-C4C
82	RD	201	PEB	NB-C1B-CHA-C4A
82	RD	201	PEB	C2B-C1B-CHA-C4A
82	RD	202	PEB	C4A-C3A-CAA-CBA
82	RD	202	PEB	NB-C1B-CHA-C4A
82	RD	202	PEB	C2B-C1B-CHA-C4A
82	RD	203	PEB	ND-C1D-CHC-C4C
82	RD	203	PEB	C2D-C1D-CHC-C4C
82	RD	203	PEB	C2A-C3A-CAA-CBA
82	RD	203	PEB	C4A-C3A-CAA-CBA
82	RD	203	PEB	NB-C1B-CHA-C4A
82	RD	203	PEB	C2B-C1B-CHA-C4A
82	SD	201	PEB	NB-C1B-CHA-C4A
82	SD	201	PEB	C2B-C1B-CHA-C4A
82	SD	202	PEB	NB-C1B-CHA-C4A
82	SD	202	PEB	C2B-C1B-CHA-C4A
82	TD	201	PEB	C2D-C1D-CHC-C4C
82	TD	201	PEB	C2D-C3D-CAD-CBD
82	TD	201	PEB	C4D-C3D-CAD-CBD
82	TD	201	PEB	C4A-C3A-CAA-CBA
82	TD	201	PEB	NB-C1B-CHA-C4A
82	TD	201	PEB	C2B-C1B-CHA-C4A
82	TD	202	PEB	ND-C1D-CHC-C4C
82	TD	202	PEB	C2D-C1D-CHC-C4C
82	TD	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	TD	202	PEB	C4A-C3A-CAA-CBA
82	TD	202	PEB	NB-C1B-CHA-C4A
82	TD	202	PEB	C2B-C1B-CHA-C4A
82	TD	202	PEB	C3B-CAB-CBB-CGB
82	TD	203	PEB	ND-C1D-CHC-C4C
82	TD	203	PEB	C2D-C1D-CHC-C4C
82	TD	203	PEB	NC-C1C-CHB-C4B
82	TD	203	PEB	C2C-C1C-CHB-C4B
82	TD	203	PEB	C2A-C3A-CAA-CBA
82	TD	203	PEB	C4A-C3A-CAA-CBA
82	TD	203	PEB	NB-C1B-CHA-C4A
82	TD	203	PEB	C2B-C1B-CHA-C4A
82	UD	201	PEB	ND-C1D-CHC-C4C
82	UD	201	PEB	C2D-C1D-CHC-C4C
82	UD	201	PEB	NB-C1B-CHA-C4A
82	UD	201	PEB	C2B-C1B-CHA-C4A
82	UD	202	PEB	NB-C1B-CHA-C4A
82	UD	202	PEB	C2B-C1B-CHA-C4A
82	VD	201	PEB	ND-C1D-CHC-C4C
82	VD	201	PEB	C2D-C1D-CHC-C4C
82	VD	201	PEB	NC-C1C-CHB-C4B
82	VD	201	PEB	C2C-C1C-CHB-C4B
82	VD	201	PEB	C2D-C3D-CAD-CBD
82	VD	201	PEB	C4D-C3D-CAD-CBD
82	VD	201	PEB	NB-C1B-CHA-C4A
82	VD	201	PEB	C2B-C1B-CHA-C4A
82	VD	202	PEB	ND-C1D-CHC-C4C
82	VD	202	PEB	C2D-C1D-CHC-C4C
82	VD	202	PEB	NC-C1C-CHB-C4B
82	VD	202	PEB	C2C-C1C-CHB-C4B
82	VD	202	PEB	C4A-C3A-CAA-CBA
82	VD	202	PEB	NB-C1B-CHA-C4A
82	VD	202	PEB	C2B-C1B-CHA-C4A
82	VD	203	PEB	C4D-C3D-CAD-CBD
82	VD	203	PEB	C4A-C3A-CAA-CBA
82	VD	203	PEB	NB-C1B-CHA-C4A
82	VD	203	PEB	C2B-C1B-CHA-C4A
82	WD	201	PEB	NB-C1B-CHA-C4A
82	WD	201	PEB	C2B-C1B-CHA-C4A
82	WD	202	PEB	NB-C1B-CHA-C4A
82	WD	202	PEB	C2B-C1B-CHA-C4A
82	XD	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	XD	201	PEB	NB-C1B-CHA-C4A
82	XD	201	PEB	C2B-C1B-CHA-C4A
82	XD	202	PEB	ND-C1D-CHC-C4C
82	XD	202	PEB	C2D-C1D-CHC-C4C
82	XD	202	PEB	NB-C1B-CHA-C4A
82	XD	202	PEB	C2B-C1B-CHA-C4A
82	XD	203	PEB	NC-C1C-CHB-C4B
82	XD	203	PEB	C2C-C1C-CHB-C4B
82	XD	203	PEB	C4A-C3A-CAA-CBA
82	XD	203	PEB	NB-C1B-CHA-C4A
82	XD	203	PEB	C2B-C1B-CHA-C4A
82	YD	201	PEB	NB-C1B-CHA-C4A
82	YD	201	PEB	C2B-C1B-CHA-C4A
82	YD	202	PEB	NB-C1B-CHA-C4A
82	YD	202	PEB	C2B-C1B-CHA-C4A
82	AE	301	PEB	ND-C1D-CHC-C4C
82	AE	301	PEB	C2D-C1D-CHC-C4C
82	AE	301	PEB	NC-C1C-CHB-C4B
82	AE	301	PEB	C2C-C1C-CHB-C4B
82	AE	301	PEB	NB-C1B-CHA-C4A
82	AE	301	PEB	C2B-C1B-CHA-C4A
82	AE	304	PEB	NB-C1B-CHA-C4A
82	AE	304	PEB	C2B-C1B-CHA-C4A
82	DE	1002	PEB	NB-C1B-CHA-C4A
82	DE	1002	PEB	C2B-C1B-CHA-C4A
82	GE	1002	PEB	C2D-C3D-CAD-CBD
82	GE	1002	PEB	C4D-C3D-CAD-CBD
82	GE	1002	PEB	NB-C1B-CHA-C4A
82	GE	1002	PEB	C2B-C1B-CHA-C4A
82	GE	1002	PEB	C2B-C3B-CAB-CBB
82	HE	1002	PEB	NB-C1B-CHA-C4A
82	HE	1002	PEB	C2B-C1B-CHA-C4A
82	KE	201	PEB	NB-C1B-CHA-C4A
82	KE	201	PEB	C2B-C1B-CHA-C4A
82	LE	1002	PEB	ND-C1D-CHC-C4C
82	LE	1002	PEB	C2D-C1D-CHC-C4C
82	LE	1002	PEB	NB-C1B-CHA-C4A
82	LE	1002	PEB	C2B-C1B-CHA-C4A
82	NE	202	PEB	ND-C1D-CHC-C4C
82	NE	202	PEB	C2D-C1D-CHC-C4C
82	NE	202	PEB	NB-C1B-CHA-C4A
82	NE	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	OE	201	PEB	C2D-C1D-CHC-C4C
82	OE	201	PEB	C4A-C3A-CAA-CBA
82	OE	201	PEB	NB-C1B-CHA-C4A
82	OE	201	PEB	C2B-C1B-CHA-C4A
82	OE	202	PEB	C4A-C3A-CAA-CBA
82	OE	202	PEB	NB-C1B-CHA-C4A
82	OE	202	PEB	C2B-C1B-CHA-C4A
82	OE	203	PEB	C4A-C3A-CAA-CBA
82	OE	203	PEB	NB-C1B-CHA-C4A
82	OE	203	PEB	C2B-C1B-CHA-C4A
82	PE	201	PEB	NB-C1B-CHA-C4A
82	PE	201	PEB	C2B-C1B-CHA-C4A
82	PE	202	PEB	C1C-C2C-CAC-CBC
82	PE	202	PEB	C3C-C2C-CAC-CBC
82	PE	202	PEB	C2C-CAC-CBC-CGC
82	PE	202	PEB	NB-C1B-CHA-C4A
82	PE	202	PEB	C2B-C1B-CHA-C4A
82	QE	201	PEB	C4A-C3A-CAA-CBA
82	QE	201	PEB	NB-C1B-CHA-C4A
82	QE	201	PEB	C2B-C1B-CHA-C4A
82	QE	202	PEB	ND-C1D-CHC-C4C
82	QE	202	PEB	C2D-C1D-CHC-C4C
82	QE	202	PEB	C2A-C3A-CAA-CBA
82	QE	202	PEB	C4A-C3A-CAA-CBA
82	QE	202	PEB	NB-C1B-CHA-C4A
82	QE	202	PEB	C2B-C1B-CHA-C4A
82	QE	202	PEB	C3B-CAB-CBB-CGB
82	QE	203	PEB	NB-C1B-CHA-C4A
82	QE	203	PEB	C2B-C1B-CHA-C4A
82	RE	201	PEB	C2A-C3A-CAA-CBA
82	RE	201	PEB	C4A-C3A-CAA-CBA
82	RE	201	PEB	NB-C1B-CHA-C4A
82	RE	201	PEB	C2B-C1B-CHA-C4A
82	RE	202	PEB	NC-C1C-CHB-C4B
82	RE	202	PEB	C2C-C1C-CHB-C4B
82	RE	202	PEB	C2A-C3A-CAA-CBA
82	RE	202	PEB	C4A-C3A-CAA-CBA
82	RE	202	PEB	NB-C1B-CHA-C4A
82	RE	202	PEB	C2B-C1B-CHA-C4A
82	SE	201	PEB	ND-C1D-CHC-C4C
82	SE	201	PEB	C2D-C1D-CHC-C4C
82	SE	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	SE	201	PEB	NB-C1B-CHA-C4A
82	SE	201	PEB	C2B-C1B-CHA-C4A
82	SE	202	PEB	C4A-C3A-CAA-CBA
82	SE	202	PEB	NB-C1B-CHA-C4A
82	SE	202	PEB	C2B-C1B-CHA-C4A
82	TE	201	PEB	NB-C1B-CHA-C4A
82	TE	201	PEB	C2B-C1B-CHA-C4A
82	UE	201	PEB	C2A-C3A-CAA-CBA
82	UE	201	PEB	C4A-C3A-CAA-CBA
82	UE	201	PEB	NB-C1B-CHA-C4A
82	UE	201	PEB	C2B-C1B-CHA-C4A
82	UE	202	PEB	C2D-C1D-CHC-C4C
82	UE	202	PEB	NB-C1B-CHA-C4A
82	UE	202	PEB	C2B-C1B-CHA-C4A
82	UE	203	PEB	ND-C1D-CHC-C4C
82	UE	203	PEB	C2D-C1D-CHC-C4C
82	UE	203	PEB	C4A-C3A-CAA-CBA
82	UE	203	PEB	NB-C1B-CHA-C4A
82	UE	203	PEB	C2B-C1B-CHA-C4A
82	VE	201	PEB	NB-C1B-CHA-C4A
82	VE	201	PEB	C2B-C1B-CHA-C4A
82	VE	202	PEB	ND-C1D-CHC-C4C
82	VE	202	PEB	C2D-C1D-CHC-C4C
82	VE	202	PEB	NB-C1B-CHA-C4A
82	VE	202	PEB	C2B-C1B-CHA-C4A
82	WE	201	PEB	NB-C1B-CHA-C4A
82	WE	201	PEB	C2B-C1B-CHA-C4A
82	WE	202	PEB	NB-C1B-CHA-C4A
82	WE	202	PEB	C2B-C1B-CHA-C4A
82	WE	203	PEB	C2A-C3A-CAA-CBA
82	WE	203	PEB	C4A-C3A-CAA-CBA
82	WE	203	PEB	NB-C1B-CHA-C4A
82	WE	203	PEB	C2B-C1B-CHA-C4A
82	YE	201	PEB	C2A-C3A-CAA-CBA
82	YE	201	PEB	C4A-C3A-CAA-CBA
82	YE	201	PEB	NB-C1B-CHA-C4A
82	YE	201	PEB	C2B-C1B-CHA-C4A
82	YE	202	PEB	C1C-C2C-CAC-CBC
82	YE	202	PEB	C3C-C2C-CAC-CBC
82	YE	202	PEB	NB-C1B-CHA-C4A
82	YE	202	PEB	C2B-C1B-CHA-C4A
82	ZE	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	ZE	201	PEB	C4A-C3A-CAA-CBA
82	ZE	201	PEB	NB-C1B-CHA-C4A
82	ZE	201	PEB	C2B-C1B-CHA-C4A
82	ZE	202	PEB	C2A-C3A-CAA-CBA
82	ZE	202	PEB	C4A-C3A-CAA-CBA
82	ZE	202	PEB	NB-C1B-CHA-C4A
82	ZE	202	PEB	C2B-C1B-CHA-C4A
82	ZE	203	PEB	NB-C1B-CHA-C4A
82	ZE	203	PEB	C2B-C1B-CHA-C4A
82	AF	201	PEB	ND-C1D-CHC-C4C
82	AF	201	PEB	C2D-C1D-CHC-C4C
82	AF	201	PEB	NB-C1B-CHA-C4A
82	AF	201	PEB	C2B-C1B-CHA-C4A
82	AF	202	PEB	C2A-C3A-CAA-CBA
82	AF	202	PEB	C4A-C3A-CAA-CBA
82	AF	202	PEB	NB-C1B-CHA-C4A
82	AF	202	PEB	C2B-C1B-CHA-C4A
82	BF	201	PEB	ND-C1D-CHC-C4C
82	BF	201	PEB	C2D-C1D-CHC-C4C
82	BF	201	PEB	NB-C1B-CHA-C4A
82	BF	201	PEB	C2B-C1B-CHA-C4A
82	BF	202	PEB	ND-C1D-CHC-C4C
82	BF	202	PEB	C2D-C1D-CHC-C4C
82	BF	202	PEB	NC-C1C-CHB-C4B
82	BF	202	PEB	C2A-C3A-CAA-CBA
82	BF	202	PEB	C4A-C3A-CAA-CBA
82	BF	202	PEB	NB-C1B-CHA-C4A
82	BF	202	PEB	C2B-C1B-CHA-C4A
82	CF	201	PEB	NB-C1B-CHA-C4A
82	CF	201	PEB	C2B-C1B-CHA-C4A
82	CF	202	PEB	C4A-C3A-CAA-CBA
82	CF	202	PEB	NB-C1B-CHA-C4A
82	CF	202	PEB	C2B-C1B-CHA-C4A
82	CF	203	PEB	NB-C1B-CHA-C4A
82	CF	203	PEB	C2B-C1B-CHA-C4A
82	DF	201	PEB	NB-C1B-CHA-C4A
82	DF	201	PEB	C2B-C1B-CHA-C4A
82	DF	202	PEB	C2D-C3D-CAD-CBD
82	DF	202	PEB	C4D-C3D-CAD-CBD
82	DF	202	PEB	C4A-C3A-CAA-CBA
82	DF	202	PEB	NB-C1B-CHA-C4A
82	DF	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	DF	203	PEB	ND-C1D-CHC-C4C
82	DF	203	PEB	C2D-C1D-CHC-C4C
82	DF	203	PEB	NC-C1C-CHB-C4B
82	DF	203	PEB	C2C-C1C-CHB-C4B
82	DF	203	PEB	NB-C1B-CHA-C4A
82	DF	203	PEB	C2B-C1B-CHA-C4A
82	EF	201	PEB	C2D-C1D-CHC-C4C
82	EF	201	PEB	C2A-C3A-CAA-CBA
82	EF	201	PEB	C4A-C3A-CAA-CBA
82	EF	201	PEB	NB-C1B-CHA-C4A
82	EF	201	PEB	C2B-C1B-CHA-C4A
82	EF	202	PEB	NB-C1B-CHA-C4A
82	EF	202	PEB	C2B-C1B-CHA-C4A
82	FF	201	PEB	NB-C1B-CHA-C4A
82	FF	201	PEB	C2B-C1B-CHA-C4A
82	FF	202	PEB	ND-C1D-CHC-C4C
82	FF	202	PEB	C2D-C1D-CHC-C4C
82	FF	202	PEB	NC-C1C-CHB-C4B
82	FF	202	PEB	NB-C1B-CHA-C4A
82	FF	202	PEB	C2B-C1B-CHA-C4A
82	GF	201	PEB	C2A-C3A-CAA-CBA
82	GF	201	PEB	C4A-C3A-CAA-CBA
82	GF	201	PEB	NB-C1B-CHA-C4A
82	GF	201	PEB	C2B-C1B-CHA-C4A
82	GF	202	PEB	C2A-C3A-CAA-CBA
82	GF	202	PEB	C4A-C3A-CAA-CBA
82	GF	202	PEB	NB-C1B-CHA-C4A
82	GF	202	PEB	C2B-C1B-CHA-C4A
82	GF	203	PEB	C2C-CAC-CBC-CGC
82	GF	203	PEB	NB-C1B-CHA-C4A
82	GF	203	PEB	C2B-C1B-CHA-C4A
82	HF	201	PEB	C2A-C3A-CAA-CBA
82	HF	201	PEB	C4A-C3A-CAA-CBA
82	HF	201	PEB	NB-C1B-CHA-C4A
82	HF	201	PEB	C2B-C1B-CHA-C4A
82	HF	202	PEB	ND-C1D-CHC-C4C
82	HF	202	PEB	C2D-C1D-CHC-C4C
82	HF	202	PEB	NC-C1C-CHB-C4B
82	HF	202	PEB	NB-C1B-CHA-C4A
82	HF	202	PEB	C2B-C1B-CHA-C4A
82	IF	201	PEB	C4A-C3A-CAA-CBA
82	IF	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	IF	201	PEB	C2B-C1B-CHA-C4A
82	IF	202	PEB	C2A-C3A-CAA-CBA
82	IF	202	PEB	C4A-C3A-CAA-CBA
82	IF	202	PEB	C3A-C4A-CHA-C1B
82	IF	202	PEB	NB-C1B-CHA-C4A
82	IF	202	PEB	C2B-C1B-CHA-C4A
82	IF	203	PEB	C4A-C3A-CAA-CBA
82	IF	203	PEB	NB-C1B-CHA-C4A
82	IF	203	PEB	C2B-C1B-CHA-C4A
82	JF	201	PEB	C2A-C3A-CAA-CBA
82	JF	201	PEB	NB-C1B-CHA-C4A
82	JF	201	PEB	C2B-C1B-CHA-C4A
82	JF	202	PEB	C3C-C4C-CHC-C1D
82	JF	202	PEB	ND-C1D-CHC-C4C
82	JF	202	PEB	C2D-C1D-CHC-C4C
82	JF	202	PEB	C4A-C3A-CAA-CBA
82	JF	202	PEB	NB-C1B-CHA-C4A
82	JF	202	PEB	C2B-C1B-CHA-C4A
82	KF	201	PEB	C4A-C3A-CAA-CBA
82	KF	201	PEB	NB-C1B-CHA-C4A
82	KF	201	PEB	C2B-C1B-CHA-C4A
82	KF	202	PEB	NB-C1B-CHA-C4A
82	KF	202	PEB	C2B-C1B-CHA-C4A
82	KF	203	PEB	NB-C1B-CHA-C4A
82	KF	203	PEB	C2B-C1B-CHA-C4A
82	LF	201	PEB	C2A-C3A-CAA-CBA
82	LF	201	PEB	C4A-C3A-CAA-CBA
82	LF	201	PEB	NB-C1B-CHA-C4A
82	LF	201	PEB	C2B-C1B-CHA-C4A
82	LF	202	PEB	ND-C1D-CHC-C4C
82	LF	202	PEB	C2D-C1D-CHC-C4C
82	LF	202	PEB	NC-C1C-CHB-C4B
82	LF	202	PEB	NB-C1B-CHA-C4A
82	LF	202	PEB	C2B-C1B-CHA-C4A
82	MF	201	PEB	ND-C1D-CHC-C4C
82	MF	201	PEB	C2D-C1D-CHC-C4C
82	MF	201	PEB	NB-C1B-CHA-C4A
82	MF	201	PEB	C2B-C1B-CHA-C4A
82	MF	202	PEB	NB-C1B-CHA-C4A
82	MF	202	PEB	C2B-C1B-CHA-C4A
82	MF	203	PEB	C4A-C3A-CAA-CBA
82	MF	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	MF	203	PEB	C2B-C1B-CHA-C4A
82	NF	201	PEB	NB-C1B-CHA-C4A
82	NF	201	PEB	C2B-C1B-CHA-C4A
82	NF	202	PEB	C3C-C4C-CHC-C1D
82	NF	202	PEB	ND-C1D-CHC-C4C
82	NF	202	PEB	C2D-C1D-CHC-C4C
82	NF	202	PEB	NC-C1C-CHB-C4B
82	NF	202	PEB	NB-C1B-CHA-C4A
82	NF	202	PEB	C2B-C1B-CHA-C4A
82	OF	201	PEB	NB-C1B-CHA-C4A
82	OF	201	PEB	C2B-C1B-CHA-C4A
82	OF	202	PEB	ND-C1D-CHC-C4C
82	OF	202	PEB	C2D-C1D-CHC-C4C
82	OF	202	PEB	NB-C1B-CHA-C4A
82	OF	202	PEB	C2B-C1B-CHA-C4A
82	OF	203	PEB	NB-C1B-CHA-C4A
82	OF	203	PEB	C2B-C1B-CHA-C4A
82	PF	201	PEB	NB-C1B-CHA-C4A
82	PF	201	PEB	C2B-C1B-CHA-C4A
82	PF	202	PEB	C3C-C4C-CHC-C1D
82	PF	202	PEB	ND-C1D-CHC-C4C
82	PF	202	PEB	C2D-C1D-CHC-C4C
82	PF	202	PEB	NB-C1B-CHA-C4A
82	PF	202	PEB	C2B-C1B-CHA-C4A
82	QF	201	PEB	C2A-C3A-CAA-CBA
82	QF	201	PEB	C4A-C3A-CAA-CBA
82	QF	201	PEB	NB-C1B-CHA-C4A
82	QF	201	PEB	C2B-C1B-CHA-C4A
82	QF	202	PEB	C2C-CAC-CBC-CGC
82	QF	202	PEB	NB-C1B-CHA-C4A
82	QF	202	PEB	C2B-C1B-CHA-C4A
82	QF	203	PEB	NB-C1B-CHA-C4A
82	QF	203	PEB	C2B-C1B-CHA-C4A
82	RF	201	PEB	NB-C1B-CHA-C4A
82	RF	201	PEB	C2B-C1B-CHA-C4A
82	RF	202	PEB	ND-C1D-CHC-C4C
82	RF	202	PEB	C2D-C1D-CHC-C4C
82	RF	202	PEB	NC-C1C-CHB-C4B
82	RF	202	PEB	C2C-C1C-CHB-C4B
82	RF	202	PEB	C2A-C3A-CAA-CBA
82	RF	202	PEB	C4A-C3A-CAA-CBA
82	RF	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	RF	202	PEB	C2B-C1B-CHA-C4A
82	SF	201	PEB	C2A-C3A-CAA-CBA
82	SF	201	PEB	C4A-C3A-CAA-CBA
82	SF	201	PEB	NB-C1B-CHA-C4A
82	SF	201	PEB	C2B-C1B-CHA-C4A
82	SF	202	PEB	C2D-C1D-CHC-C4C
82	SF	202	PEB	NB-C1B-CHA-C4A
82	SF	203	PEB	NB-C1B-CHA-C4A
82	SF	203	PEB	C2B-C1B-CHA-C4A
82	TF	201	PEB	NB-C1B-CHA-C4A
82	TF	201	PEB	C2B-C1B-CHA-C4A
82	TF	202	PEB	C3C-C4C-CHC-C1D
82	TF	202	PEB	ND-C1D-CHC-C4C
82	TF	202	PEB	C2D-C1D-CHC-C4C
82	TF	202	PEB	NC-C1C-CHB-C4B
82	TF	202	PEB	C2D-C3D-CAD-CBD
82	TF	202	PEB	C4D-C3D-CAD-CBD
82	TF	202	PEB	C4A-C3A-CAA-CBA
82	TF	202	PEB	NB-C1B-CHA-C4A
82	TF	202	PEB	C2B-C1B-CHA-C4A
82	UF	201	PEB	C2D-C1D-CHC-C4C
82	UF	201	PEB	C4A-C3A-CAA-CBA
82	UF	201	PEB	NB-C1B-CHA-C4A
82	UF	201	PEB	C2B-C1B-CHA-C4A
82	UF	202	PEB	C2C-CAC-CBC-CGC
82	UF	202	PEB	C2A-C3A-CAA-CBA
82	UF	202	PEB	NB-C1B-CHA-C4A
82	UF	202	PEB	C2B-C1B-CHA-C4A
82	VF	201	PEB	C2A-C3A-CAA-CBA
82	VF	201	PEB	C4A-C3A-CAA-CBA
82	VF	201	PEB	NB-C1B-CHA-C4A
82	VF	201	PEB	C2B-C1B-CHA-C4A
82	VF	202	PEB	ND-C1D-CHC-C4C
82	VF	202	PEB	C2D-C1D-CHC-C4C
82	VF	202	PEB	C2C-CAC-CBC-CGC
82	VF	202	PEB	NB-C1B-CHA-C4A
82	VF	202	PEB	C2B-C1B-CHA-C4A
82	WF	201	PEB	C2D-C3D-CAD-CBD
82	WF	201	PEB	C4D-C3D-CAD-CBD
82	WF	201	PEB	NB-C1B-CHA-C4A
82	WF	201	PEB	C2B-C1B-CHA-C4A
82	WF	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	WF	202	PEB	C4A-C3A-CAA-CBA
82	WF	202	PEB	NB-C1B-CHA-C4A
82	WF	202	PEB	C2B-C1B-CHA-C4A
82	WF	203	PEB	C2A-C3A-CAA-CBA
82	WF	203	PEB	NB-C1B-CHA-C4A
82	WF	203	PEB	C2B-C1B-CHA-C4A
82	XF	201	PEB	NB-C1B-CHA-C4A
82	XF	201	PEB	C2B-C1B-CHA-C4A
82	XF	202	PEB	C2A-C3A-CAA-CBA
82	XF	202	PEB	C4A-C3A-CAA-CBA
82	XF	202	PEB	NB-C1B-CHA-C4A
82	XF	202	PEB	C2B-C1B-CHA-C4A
82	XF	203	PEB	ND-C1D-CHC-C4C
82	XF	203	PEB	C2D-C1D-CHC-C4C
82	XF	203	PEB	NC-C1C-CHB-C4B
82	XF	203	PEB	NB-C1B-CHA-C4A
82	XF	203	PEB	C2B-C1B-CHA-C4A
82	YF	201	PEB	ND-C1D-CHC-C4C
82	YF	201	PEB	C2D-C1D-CHC-C4C
82	YF	201	PEB	NB-C1B-CHA-C4A
82	YF	201	PEB	C2B-C1B-CHA-C4A
82	YF	202	PEB	NC-C1C-CHB-C4B
82	YF	202	PEB	C2C-C1C-CHB-C4B
82	YF	202	PEB	NB-C1B-CHA-C4A
82	YF	202	PEB	C2B-C1B-CHA-C4A
82	YF	203	PEB	NC-C1C-CHB-C4B
82	YF	203	PEB	C2C-C1C-CHB-C4B
82	YF	203	PEB	NB-C1B-CHA-C4A
82	YF	203	PEB	C2B-C1B-CHA-C4A
82	ZF	201	PEB	ND-C1D-CHC-C4C
82	ZF	201	PEB	C2D-C1D-CHC-C4C
82	ZF	201	PEB	NB-C1B-CHA-C4A
82	ZF	201	PEB	C2B-C1B-CHA-C4A
82	ZF	202	PEB	ND-C1D-CHC-C4C
82	ZF	202	PEB	C2D-C1D-CHC-C4C
82	ZF	202	PEB	NC-C1C-CHB-C4B
82	ZF	202	PEB	NB-C1B-CHA-C4A
82	ZF	202	PEB	C2B-C1B-CHA-C4A
82	AG	301	PEB	ND-C1D-CHC-C4C
82	AG	301	PEB	C2D-C1D-CHC-C4C
82	AG	301	PEB	NC-C1C-CHB-C4B
82	AG	301	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	AG	301	PEB	NB-C1B-CHA-C4A
82	AG	301	PEB	C2B-C1B-CHA-C4A
82	AG	304	PEB	NB-C1B-CHA-C4A
82	AG	304	PEB	C2B-C1B-CHA-C4A
82	DG	1002	PEB	NB-C1B-CHA-C4A
82	DG	1002	PEB	C2B-C1B-CHA-C4A
82	GG	1002	PEB	C2D-C3D-CAD-CBD
82	GG	1002	PEB	C4D-C3D-CAD-CBD
82	GG	1002	PEB	NB-C1B-CHA-C4A
82	GG	1002	PEB	C2B-C1B-CHA-C4A
82	GG	1002	PEB	C2B-C3B-CAB-CBB
82	HG	1002	PEB	NB-C1B-CHA-C4A
82	HG	1002	PEB	C2B-C1B-CHA-C4A
82	KG	201	PEB	NB-C1B-CHA-C4A
82	KG	201	PEB	C2B-C1B-CHA-C4A
82	LG	1002	PEB	ND-C1D-CHC-C4C
82	LG	1002	PEB	C2D-C1D-CHC-C4C
82	LG	1002	PEB	NB-C1B-CHA-C4A
82	LG	1002	PEB	C2B-C1B-CHA-C4A
82	NG	201	PEB	ND-C1D-CHC-C4C
82	NG	201	PEB	C2D-C1D-CHC-C4C
82	NG	201	PEB	NB-C1B-CHA-C4A
82	NG	201	PEB	C2B-C1B-CHA-C4A
82	OG	201	PEB	C2D-C1D-CHC-C4C
82	OG	201	PEB	C4A-C3A-CAA-CBA
82	OG	201	PEB	NB-C1B-CHA-C4A
82	OG	201	PEB	C2B-C1B-CHA-C4A
82	OG	202	PEB	C4A-C3A-CAA-CBA
82	OG	202	PEB	NB-C1B-CHA-C4A
82	OG	202	PEB	C2B-C1B-CHA-C4A
82	OG	203	PEB	C4A-C3A-CAA-CBA
82	OG	203	PEB	NB-C1B-CHA-C4A
82	OG	203	PEB	C2B-C1B-CHA-C4A
82	PG	201	PEB	NB-C1B-CHA-C4A
82	PG	201	PEB	C2B-C1B-CHA-C4A
82	PG	202	PEB	C1C-C2C-CAC-CBC
82	PG	202	PEB	C3C-C2C-CAC-CBC
82	PG	202	PEB	C2C-CAC-CBC-CGC
82	PG	202	PEB	NB-C1B-CHA-C4A
82	PG	202	PEB	C2B-C1B-CHA-C4A
82	QG	201	PEB	C4A-C3A-CAA-CBA
82	QG	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	QG	201	PEB	C2B-C1B-CHA-C4A
82	QG	202	PEB	ND-C1D-CHC-C4C
82	QG	202	PEB	C2D-C1D-CHC-C4C
82	QG	202	PEB	C2A-C3A-CAA-CBA
82	QG	202	PEB	C4A-C3A-CAA-CBA
82	QG	202	PEB	NB-C1B-CHA-C4A
82	QG	202	PEB	C2B-C1B-CHA-C4A
82	QG	202	PEB	C3B-CAB-CBB-CGB
82	QG	203	PEB	NB-C1B-CHA-C4A
82	QG	203	PEB	C2B-C1B-CHA-C4A
82	RG	201	PEB	C2A-C3A-CAA-CBA
82	RG	201	PEB	C4A-C3A-CAA-CBA
82	RG	201	PEB	NB-C1B-CHA-C4A
82	RG	201	PEB	C2B-C1B-CHA-C4A
82	RG	202	PEB	NC-C1C-CHB-C4B
82	RG	202	PEB	C2C-C1C-CHB-C4B
82	RG	202	PEB	C2A-C3A-CAA-CBA
82	RG	202	PEB	C4A-C3A-CAA-CBA
82	RG	202	PEB	NB-C1B-CHA-C4A
82	RG	202	PEB	C2B-C1B-CHA-C4A
82	SG	201	PEB	ND-C1D-CHC-C4C
82	SG	201	PEB	C2D-C1D-CHC-C4C
82	SG	201	PEB	C4A-C3A-CAA-CBA
82	SG	201	PEB	NB-C1B-CHA-C4A
82	SG	201	PEB	C2B-C1B-CHA-C4A
82	SG	202	PEB	C2D-C1D-CHC-C4C
82	SG	202	PEB	C2A-C3A-CAA-CBA
82	SG	202	PEB	C4A-C3A-CAA-CBA
82	SG	202	PEB	NB-C1B-CHA-C4A
82	SG	202	PEB	C2B-C1B-CHA-C4A
82	SG	202	PEB	C3B-CAB-CBB-CGB
82	SG	203	PEB	C4A-C3A-CAA-CBA
82	SG	203	PEB	NB-C1B-CHA-C4A
82	SG	203	PEB	C2B-C1B-CHA-C4A
82	TG	201	PEB	NB-C1B-CHA-C4A
82	TG	201	PEB	C2B-C1B-CHA-C4A
82	UG	201	PEB	C2A-C3A-CAA-CBA
82	UG	201	PEB	C4A-C3A-CAA-CBA
82	UG	201	PEB	NB-C1B-CHA-C4A
82	UG	201	PEB	C2B-C1B-CHA-C4A
82	UG	202	PEB	NB-C1B-CHA-C4A
82	UG	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	UG	203	PEB	ND-C1D-CHC-C4C
82	UG	203	PEB	C2D-C1D-CHC-C4C
82	UG	203	PEB	C4A-C3A-CAA-CBA
82	UG	203	PEB	NB-C1B-CHA-C4A
82	UG	203	PEB	C2B-C1B-CHA-C4A
82	VG	201	PEB	NB-C1B-CHA-C4A
82	VG	201	PEB	C2B-C1B-CHA-C4A
82	VG	202	PEB	ND-C1D-CHC-C4C
82	VG	202	PEB	C2D-C1D-CHC-C4C
82	VG	202	PEB	NB-C1B-CHA-C4A
82	VG	202	PEB	C2B-C1B-CHA-C4A
82	WG	201	PEB	NB-C1B-CHA-C4A
82	WG	201	PEB	C2B-C1B-CHA-C4A
82	WG	202	PEB	NB-C1B-CHA-C4A
82	WG	202	PEB	C2B-C1B-CHA-C4A
82	WG	203	PEB	C2A-C3A-CAA-CBA
82	WG	203	PEB	C4A-C3A-CAA-CBA
82	WG	203	PEB	NB-C1B-CHA-C4A
82	WG	203	PEB	C2B-C1B-CHA-C4A
82	YG	201	PEB	C2A-C3A-CAA-CBA
82	YG	201	PEB	C4A-C3A-CAA-CBA
82	YG	201	PEB	NB-C1B-CHA-C4A
82	YG	201	PEB	C2B-C1B-CHA-C4A
82	YG	202	PEB	C1C-C2C-CAC-CBC
82	YG	202	PEB	C3C-C2C-CAC-CBC
82	YG	202	PEB	NB-C1B-CHA-C4A
82	YG	202	PEB	C2B-C1B-CHA-C4A
82	ZG	201	PEB	C2A-C3A-CAA-CBA
82	ZG	201	PEB	C4A-C3A-CAA-CBA
82	ZG	201	PEB	NB-C1B-CHA-C4A
82	ZG	201	PEB	C2B-C1B-CHA-C4A
82	ZG	202	PEB	C2D-C1D-CHC-C4C
82	ZG	202	PEB	C2A-C3A-CAA-CBA
82	ZG	202	PEB	C4A-C3A-CAA-CBA
82	ZG	202	PEB	NB-C1B-CHA-C4A
82	ZG	202	PEB	C2B-C1B-CHA-C4A
82	ZG	203	PEB	NB-C1B-CHA-C4A
82	ZG	203	PEB	C2B-C1B-CHA-C4A
82	AH	301	PEB	NB-C1B-CHA-C4A
82	AH	301	PEB	C2B-C1B-CHA-C4A
82	AH	302	PEB	C2D-C1D-CHC-C4C
82	AH	302	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	AH	302	PEB	NB-C1B-CHA-C4A
82	AH	302	PEB	C2B-C1B-CHA-C4A
82	AH	305	PEB	ND-C1D-CHC-C4C
82	AH	305	PEB	C2D-C1D-CHC-C4C
82	AH	305	PEB	NC-C1C-CHB-C4B
82	AH	305	PEB	C2C-C1C-CHB-C4B
82	AH	305	PEB	C2A-C3A-CAA-CBA
82	AH	305	PEB	C4A-C3A-CAA-CBA
82	AH	305	PEB	NB-C1B-CHA-C4A
82	AH	305	PEB	C2B-C1B-CHA-C4A
82	DH	1002	PEB	ND-C1D-CHC-C4C
82	DH	1002	PEB	C2D-C1D-CHC-C4C
82	DH	1002	PEB	C2A-C3A-CAA-CBA
82	DH	1002	PEB	C4A-C3A-CAA-CBA
82	DH	1002	PEB	NB-C1B-CHA-C4A
82	DH	1002	PEB	C2B-C1B-CHA-C4A
82	FH	1002	PEB	C2C-CAC-CBC-CGC
82	FH	1002	PEB	C4A-C3A-CAA-CBA
82	FH	1002	PEB	NB-C1B-CHA-C4A
82	FH	1002	PEB	C2B-C1B-CHA-C4A
82	HH	1002	PEB	C4A-C3A-CAA-CBA
82	HH	1002	PEB	NB-C1B-CHA-C4A
82	HH	1002	PEB	C2B-C1B-CHA-C4A
82	JH	1002	PEB	NB-C1B-CHA-C4A
82	JH	1002	PEB	C2B-C1B-CHA-C4A
82	LH	1003	PEB	C2A-C3A-CAA-CBA
82	LH	1003	PEB	C4A-C3A-CAA-CBA
82	LH	1003	PEB	NB-C1B-CHA-C4A
82	LH	1003	PEB	C2B-C1B-CHA-C4A
82	LH	1003	PEB	C3B-CAB-CBB-CGB
82	NH	1002	PEB	C2A-C3A-CAA-CBA
82	NH	1002	PEB	C4A-C3A-CAA-CBA
82	NH	1002	PEB	NB-C1B-CHA-C4A
82	NH	1002	PEB	C2B-C1B-CHA-C4A
82	OH	201	PEB	ND-C1D-CHC-C4C
82	OH	201	PEB	C2D-C1D-CHC-C4C
82	OH	201	PEB	C2A-C3A-CAA-CBA
82	OH	201	PEB	C4A-C3A-CAA-CBA
82	OH	201	PEB	NB-C1B-CHA-C4A
82	OH	201	PEB	C2B-C1B-CHA-C4A
82	OH	202	PEB	NB-C1B-CHA-C4A
82	OH	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	OH	203	PEB	C2A-C3A-CAA-CBA
82	OH	203	PEB	NB-C1B-CHA-C4A
82	OH	203	PEB	C2B-C1B-CHA-C4A
82	PH	201	PEB	NB-C1B-CHA-C4A
82	PH	201	PEB	C2B-C1B-CHA-C4A
82	PH	202	PEB	NB-C1B-CHA-C4A
82	PH	202	PEB	C2B-C1B-CHA-C4A
82	QH	201	PEB	NB-C1B-CHA-C4A
82	QH	201	PEB	C2B-C1B-CHA-C4A
82	QH	202	PEB	C2D-C1D-CHC-C4C
82	QH	202	PEB	C2A-C3A-CAA-CBA
82	QH	202	PEB	C4A-C3A-CAA-CBA
82	QH	203	PEB	NB-C1B-CHA-C4A
82	QH	203	PEB	C2B-C1B-CHA-C4A
82	QH	203	PEB	C3B-CAB-CBB-CGB
82	RH	201	PEB	C2A-C3A-CAA-CBA
82	RH	201	PEB	C4A-C3A-CAA-CBA
82	RH	201	PEB	NB-C1B-CHA-C4A
82	RH	201	PEB	C2B-C1B-CHA-C4A
82	RH	202	PEB	ND-C1D-CHC-C4C
82	RH	202	PEB	C2D-C1D-CHC-C4C
82	RH	202	PEB	NB-C1B-CHA-C4A
82	RH	202	PEB	C2B-C1B-CHA-C4A
82	SH	201	PEB	NB-C1B-CHA-C4A
82	SH	201	PEB	C2B-C1B-CHA-C4A
82	SH	202	PEB	C2C-CAC-CBC-CGC
82	SH	202	PEB	NB-C1B-CHA-C4A
82	SH	202	PEB	C2B-C1B-CHA-C4A
82	SH	203	PEB	NB-C1B-CHA-C4A
82	SH	203	PEB	C2B-C1B-CHA-C4A
82	TH	201	PEB	ND-C1D-CHC-C4C
82	TH	201	PEB	C2D-C1D-CHC-C4C
82	TH	201	PEB	NB-C1B-CHA-C4A
82	TH	201	PEB	C2B-C1B-CHA-C4A
82	TH	202	PEB	ND-C1D-CHC-C4C
82	TH	202	PEB	C2D-C1D-CHC-C4C
82	TH	202	PEB	C4D-C3D-CAD-CBD
82	TH	202	PEB	NB-C1B-CHA-C4A
82	TH	202	PEB	C2B-C1B-CHA-C4A
82	UH	201	PEB	C2A-C3A-CAA-CBA
82	UH	201	PEB	C4A-C3A-CAA-CBA
82	UH	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	UH	201	PEB	C2B-C1B-CHA-C4A
82	UH	202	PEB	C4A-C3A-CAA-CBA
82	UH	202	PEB	NB-C1B-CHA-C4A
82	UH	202	PEB	C2B-C1B-CHA-C4A
82	UH	203	PEB	C2A-C3A-CAA-CBA
82	UH	203	PEB	NB-C1B-CHA-C4A
82	UH	203	PEB	C2B-C1B-CHA-C4A
82	VH	201	PEB	NB-C1B-CHA-C4A
82	VH	202	PEB	ND-C1D-CHC-C4C
82	VH	202	PEB	C2D-C1D-CHC-C4C
82	VH	202	PEB	NB-C1B-CHA-C4A
82	VH	202	PEB	C2B-C1B-CHA-C4A
82	WH	201	PEB	ND-C1D-CHC-C4C
82	WH	201	PEB	C2D-C1D-CHC-C4C
82	WH	201	PEB	C4A-C3A-CAA-CBA
82	WH	201	PEB	NB-C1B-CHA-C4A
82	WH	201	PEB	C2B-C1B-CHA-C4A
82	WH	202	PEB	NB-C1B-CHA-C4A
82	WH	202	PEB	C2B-C1B-CHA-C4A
82	WH	203	PEB	C2A-C3A-CAA-CBA
82	WH	203	PEB	NB-C1B-CHA-C4A
82	WH	203	PEB	C2B-C1B-CHA-C4A
82	YH	201	PEB	C2A-C3A-CAA-CBA
82	YH	201	PEB	C4A-C3A-CAA-CBA
82	YH	201	PEB	NB-C1B-CHA-C4A
82	YH	201	PEB	C2B-C1B-CHA-C4A
82	YH	202	PEB	NB-C1B-CHA-C4A
82	YH	202	PEB	C2B-C1B-CHA-C4A
82	ZH	201	PEB	ND-C1D-CHC-C4C
82	ZH	201	PEB	C2D-C1D-CHC-C4C
82	ZH	201	PEB	C2A-C3A-CAA-CBA
82	ZH	201	PEB	C4A-C3A-CAA-CBA
82	ZH	201	PEB	NB-C1B-CHA-C4A
82	ZH	201	PEB	C2B-C1B-CHA-C4A
82	ZH	202	PEB	ND-C1D-CHC-C4C
82	ZH	202	PEB	C2D-C1D-CHC-C4C
82	ZH	202	PEB	C2A-C3A-CAA-CBA
82	ZH	202	PEB	C4A-C3A-CAA-CBA
82	ZH	202	PEB	NB-C1B-CHA-C4A
82	ZH	202	PEB	C2B-C1B-CHA-C4A
82	ZH	203	PEB	NB-C1B-CHA-C4A
82	ZH	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	AI	201	PEB	C2D-C1D-CHC-C4C
82	AI	201	PEB	C2A-C3A-CAA-CBA
82	AI	201	PEB	C4A-C3A-CAA-CBA
82	AI	201	PEB	NB-C1B-CHA-C4A
82	AI	201	PEB	C2B-C1B-CHA-C4A
82	AI	202	PEB	ND-C1D-CHC-C4C
82	AI	202	PEB	C2D-C1D-CHC-C4C
82	AI	202	PEB	NB-C1B-CHA-C4A
82	AI	202	PEB	C2B-C1B-CHA-C4A
82	AI	203	PEB	C2A-C3A-CAA-CBA
82	AI	203	PEB	C4A-C3A-CAA-CBA
82	AI	203	PEB	NB-C1B-CHA-C4A
82	AI	203	PEB	C2B-C1B-CHA-C4A
82	BI	201	PEB	ND-C1D-CHC-C4C
82	BI	201	PEB	C2D-C1D-CHC-C4C
82	BI	201	PEB	NB-C1B-CHA-C4A
82	BI	201	PEB	C2B-C1B-CHA-C4A
82	BI	202	PEB	C2A-C3A-CAA-CBA
82	BI	202	PEB	C4A-C3A-CAA-CBA
82	BI	202	PEB	NB-C1B-CHA-C4A
82	BI	203	PEB	NB-C1B-CHA-C4A
82	BI	203	PEB	C2B-C1B-CHA-C4A
82	CI	201	PEB	C2D-C1D-CHC-C4C
82	CI	201	PEB	C2A-C3A-CAA-CBA
82	CI	201	PEB	C4A-C3A-CAA-CBA
82	CI	201	PEB	NB-C1B-CHA-C4A
82	CI	201	PEB	C2B-C1B-CHA-C4A
82	CI	202	PEB	ND-C1D-CHC-C4C
82	CI	202	PEB	C2D-C1D-CHC-C4C
82	CI	202	PEB	NB-C1B-CHA-C4A
82	CI	202	PEB	C2B-C1B-CHA-C4A
82	DI	201	PEB	ND-C1D-CHC-C4C
82	DI	201	PEB	C2D-C1D-CHC-C4C
82	DI	201	PEB	NB-C1B-CHA-C4A
82	DI	201	PEB	C2B-C1B-CHA-C4A
82	DI	202	PEB	C2D-C1D-CHC-C4C
82	DI	202	PEB	NB-C1B-CHA-C4A
82	DI	202	PEB	C2B-C1B-CHA-C4A
82	EI	201	PEB	C2D-C1D-CHC-C4C
82	EI	201	PEB	C2A-C3A-CAA-CBA
82	EI	201	PEB	C4A-C3A-CAA-CBA
82	EI	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	EI	201	PEB	C2B-C1B-CHA-C4A
82	EI	202	PEB	ND-C1D-CHC-C4C
82	EI	202	PEB	C2D-C1D-CHC-C4C
82	EI	202	PEB	NB-C1B-CHA-C4A
82	EI	202	PEB	C2B-C1B-CHA-C4A
82	FI	201	PEB	ND-C1D-CHC-C4C
82	FI	201	PEB	C2D-C1D-CHC-C4C
82	FI	201	PEB	C2A-C3A-CAA-CBA
82	FI	201	PEB	C4A-C3A-CAA-CBA
82	FI	201	PEB	NB-C1B-CHA-C4A
82	FI	201	PEB	C2B-C1B-CHA-C4A
82	FI	202	PEB	C2D-C1D-CHC-C4C
82	FI	202	PEB	NB-C1B-CHA-C4A
82	FI	202	PEB	C2B-C1B-CHA-C4A
82	GI	201	PEB	C2D-C3D-CAD-CBD
82	GI	201	PEB	C4D-C3D-CAD-CBD
82	GI	201	PEB	C2A-C3A-CAA-CBA
82	GI	201	PEB	C4A-C3A-CAA-CBA
82	GI	201	PEB	NB-C1B-CHA-C4A
82	GI	201	PEB	C2B-C1B-CHA-C4A
82	GI	202	PEB	C2D-C1D-CHC-C4C
82	GI	202	PEB	C2A-C3A-CAA-CBA
82	GI	202	PEB	C4A-C3A-CAA-CBA
82	GI	202	PEB	NB-C1B-CHA-C4A
82	GI	202	PEB	C2B-C1B-CHA-C4A
82	GI	203	PEB	ND-C1D-CHC-C4C
82	GI	203	PEB	C2D-C1D-CHC-C4C
82	GI	203	PEB	NB-C1B-CHA-C4A
82	GI	203	PEB	C2B-C1B-CHA-C4A
82	HI	201	PEB	NB-C1B-CHA-C4A
82	HI	201	PEB	C2B-C1B-CHA-C4A
82	HI	202	PEB	C2A-C3A-CAA-CBA
82	HI	202	PEB	C4A-C3A-CAA-CBA
82	HI	202	PEB	NB-C1B-CHA-C4A
82	HI	202	PEB	C2B-C1B-CHA-C4A
82	HI	203	PEB	C2D-C1D-CHC-C4C
82	HI	203	PEB	NB-C1B-CHA-C4A
82	HI	203	PEB	C2B-C1B-CHA-C4A
82	II	201	PEB	C2D-C1D-CHC-C4C
82	II	201	PEB	C2A-C3A-CAA-CBA
82	II	201	PEB	C4A-C3A-CAA-CBA
82	II	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	II	201	PEB	C2B-C1B-CHA-C4A
82	II	202	PEB	ND-C1D-CHC-C4C
82	II	202	PEB	C2D-C1D-CHC-C4C
82	II	202	PEB	NB-C1B-CHA-C4A
82	II	202	PEB	C2B-C1B-CHA-C4A
82	II	203	PEB	C4A-C3A-CAA-CBA
82	II	203	PEB	NB-C1B-CHA-C4A
82	II	203	PEB	C2B-C1B-CHA-C4A
82	JI	201	PEB	ND-C1D-CHC-C4C
82	JI	201	PEB	C2D-C1D-CHC-C4C
82	JI	201	PEB	NB-C1B-CHA-C4A
82	JI	201	PEB	C2B-C1B-CHA-C4A
82	JI	202	PEB	C2D-C1D-CHC-C4C
82	JI	202	PEB	NB-C1B-CHA-C4A
82	JI	202	PEB	C2B-C1B-CHA-C4A
82	KI	201	PEB	C4A-C3A-CAA-CBA
82	KI	201	PEB	NB-C1B-CHA-C4A
82	KI	201	PEB	C2B-C1B-CHA-C4A
82	KI	202	PEB	C2D-C1D-CHC-C4C
82	KI	202	PEB	C2A-C3A-CAA-CBA
82	KI	202	PEB	C4A-C3A-CAA-CBA
82	KI	202	PEB	NB-C1B-CHA-C4A
82	KI	202	PEB	C2B-C1B-CHA-C4A
82	KI	203	PEB	ND-C1D-CHC-C4C
82	KI	203	PEB	C2D-C1D-CHC-C4C
82	KI	203	PEB	NB-C1B-CHA-C4A
82	KI	203	PEB	C2B-C1B-CHA-C4A
82	LI	201	PEB	ND-C1D-CHC-C4C
82	LI	201	PEB	C2D-C1D-CHC-C4C
82	LI	201	PEB	C2A-C3A-CAA-CBA
82	LI	201	PEB	C4A-C3A-CAA-CBA
82	LI	201	PEB	NB-C1B-CHA-C4A
82	LI	201	PEB	C2B-C1B-CHA-C4A
82	LI	202	PEB	NB-C1B-CHA-C4A
82	LI	202	PEB	C2B-C1B-CHA-C4A
82	MI	401	PEB	C2D-C1D-CHC-C4C
82	MI	401	PEB	C2A-C3A-CAA-CBA
82	MI	401	PEB	C4A-C3A-CAA-CBA
82	MI	401	PEB	NB-C1B-CHA-C4A
82	MI	401	PEB	C2B-C1B-CHA-C4A
82	MI	401	PEB	C3B-CAB-CBB-CGB
82	NI	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	NI	201	PEB	C2A-C3A-CAA-CBA
82	NI	201	PEB	C4A-C3A-CAA-CBA
82	NI	201	PEB	NB-C1B-CHA-C4A
82	NI	201	PEB	C2B-C1B-CHA-C4A
82	NI	202	PEB	ND-C1D-CHC-C4C
82	NI	202	PEB	C2D-C1D-CHC-C4C
82	NI	202	PEB	NB-C1B-CHA-C4A
82	NI	202	PEB	C2B-C1B-CHA-C4A
82	NI	203	PEB	C2A-C3A-CAA-CBA
82	NI	203	PEB	C4A-C3A-CAA-CBA
82	NI	203	PEB	NB-C1B-CHA-C4A
82	NI	203	PEB	C2B-C1B-CHA-C4A
82	OI	201	PEB	ND-C1D-CHC-C4C
82	OI	201	PEB	C2D-C1D-CHC-C4C
82	OI	201	PEB	NB-C1B-CHA-C4A
82	OI	201	PEB	C2B-C1B-CHA-C4A
82	OI	202	PEB	C2A-C3A-CAA-CBA
82	OI	202	PEB	C4A-C3A-CAA-CBA
82	OI	202	PEB	NB-C1B-CHA-C4A
82	OI	202	PEB	C2B-C1B-CHA-C4A
82	OI	203	PEB	NB-C1B-CHA-C4A
82	OI	203	PEB	C2B-C1B-CHA-C4A
82	PI	201	PEB	C2D-C1D-CHC-C4C
82	PI	201	PEB	C2A-C3A-CAA-CBA
82	PI	201	PEB	C4A-C3A-CAA-CBA
82	PI	201	PEB	NB-C1B-CHA-C4A
82	PI	201	PEB	C2B-C1B-CHA-C4A
82	PI	202	PEB	ND-C1D-CHC-C4C
82	PI	202	PEB	C2D-C1D-CHC-C4C
82	PI	202	PEB	NB-C1B-CHA-C4A
82	PI	202	PEB	C2B-C1B-CHA-C4A
82	QI	201	PEB	C2D-C1D-CHC-C4C
82	QI	201	PEB	NB-C1B-CHA-C4A
82	QI	201	PEB	C2B-C1B-CHA-C4A
82	RI	201	PEB	C2D-C1D-CHC-C4C
82	RI	201	PEB	C2A-C3A-CAA-CBA
82	RI	201	PEB	C4A-C3A-CAA-CBA
82	RI	201	PEB	NB-C1B-CHA-C4A
82	RI	201	PEB	C2B-C1B-CHA-C4A
82	RI	202	PEB	ND-C1D-CHC-C4C
82	RI	202	PEB	C2D-C1D-CHC-C4C
82	RI	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	RI	202	PEB	C2B-C1B-CHA-C4A
82	RI	203	PEB	C2A-C3A-CAA-CBA
82	RI	203	PEB	C4A-C3A-CAA-CBA
82	RI	203	PEB	NB-C1B-CHA-C4A
82	RI	203	PEB	C2B-C1B-CHA-C4A
82	SI	201	PEB	ND-C1D-CHC-C4C
82	SI	201	PEB	C2D-C1D-CHC-C4C
82	SI	201	PEB	NB-C1B-CHA-C4A
82	SI	201	PEB	C2B-C1B-CHA-C4A
82	SI	202	PEB	NB-C1B-CHA-C4A
82	SI	202	PEB	C2B-C1B-CHA-C4A
82	TI	201	PEB	C2A-C3A-CAA-CBA
82	TI	201	PEB	C4A-C3A-CAA-CBA
82	TI	201	PEB	NB-C1B-CHA-C4A
82	TI	201	PEB	C2B-C1B-CHA-C4A
82	TI	202	PEB	C2D-C1D-CHC-C4C
82	TI	202	PEB	C2A-C3A-CAA-CBA
82	TI	202	PEB	C4A-C3A-CAA-CBA
82	TI	202	PEB	NB-C1B-CHA-C4A
82	TI	202	PEB	C2B-C1B-CHA-C4A
82	TI	203	PEB	ND-C1D-CHC-C4C
82	TI	203	PEB	C2D-C1D-CHC-C4C
82	TI	203	PEB	NB-C1B-CHA-C4A
82	TI	203	PEB	C2B-C1B-CHA-C4A
82	UI	201	PEB	C2D-C1D-CHC-C4C
82	UI	201	PEB	NB-C1B-CHA-C4A
82	UI	201	PEB	C2B-C1B-CHA-C4A
82	UI	202	PEB	C2D-C1D-CHC-C4C
82	UI	202	PEB	NB-C1B-CHA-C4A
82	UI	202	PEB	C2B-C1B-CHA-C4A
82	VI	201	PEB	C2D-C1D-CHC-C4C
82	VI	201	PEB	C2A-C3A-CAA-CBA
82	VI	201	PEB	C4A-C3A-CAA-CBA
82	VI	201	PEB	NB-C1B-CHA-C4A
82	VI	201	PEB	C2B-C1B-CHA-C4A
82	VI	202	PEB	ND-C1D-CHC-C4C
82	VI	202	PEB	C2D-C1D-CHC-C4C
82	VI	202	PEB	NB-C1B-CHA-C4A
82	VI	202	PEB	C2B-C1B-CHA-C4A
82	VI	203	PEB	C2D-C3D-CAD-CBD
82	VI	203	PEB	C4D-C3D-CAD-CBD
82	VI	203	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	VI	203	PEB	C4A-C3A-CAA-CBA
82	VI	203	PEB	NB-C1B-CHA-C4A
82	VI	203	PEB	C2B-C1B-CHA-C4A
82	WI	201	PEB	ND-C1D-CHC-C4C
82	WI	201	PEB	C2D-C1D-CHC-C4C
82	WI	201	PEB	NB-C1B-CHA-C4A
82	WI	201	PEB	C2B-C1B-CHA-C4A
82	WI	202	PEB	C4A-C3A-CAA-CBA
82	WI	202	PEB	NB-C1B-CHA-C4A
82	WI	202	PEB	C2B-C1B-CHA-C4A
82	WI	203	PEB	C2D-C1D-CHC-C4C
82	WI	203	PEB	NB-C1B-CHA-C4A
82	WI	203	PEB	C2B-C1B-CHA-C4A
82	XI	201	PEB	C2D-C1D-CHC-C4C
82	XI	201	PEB	C2A-C3A-CAA-CBA
82	XI	201	PEB	C4A-C3A-CAA-CBA
82	XI	201	PEB	NB-C1B-CHA-C4A
82	XI	201	PEB	C2B-C1B-CHA-C4A
82	XI	202	PEB	ND-C1D-CHC-C4C
82	XI	202	PEB	C2D-C1D-CHC-C4C
82	XI	202	PEB	NB-C1B-CHA-C4A
82	XI	202	PEB	C2B-C1B-CHA-C4A
82	YI	201	PEB	ND-C1D-CHC-C4C
82	YI	201	PEB	C2D-C1D-CHC-C4C
82	YI	201	PEB	C2A-C3A-CAA-CBA
82	YI	201	PEB	C4A-C3A-CAA-CBA
82	YI	201	PEB	NB-C1B-CHA-C4A
82	YI	201	PEB	C2B-C1B-CHA-C4A
82	YI	202	PEB	NB-C1B-CHA-C4A
82	YI	202	PEB	C2B-C1B-CHA-C4A
82	ZI	401	PEB	ND-C1D-CHC-C4C
82	ZI	401	PEB	C2D-C1D-CHC-C4C
82	ZI	401	PEB	NB-C1B-CHA-C4A
82	ZI	401	PEB	C2B-C1B-CHA-C4A
82	AJ	301	PEB	ND-C1D-CHC-C4C
82	AJ	301	PEB	C2D-C1D-CHC-C4C
82	AJ	301	PEB	C2A-C3A-CAA-CBA
82	AJ	301	PEB	C4A-C3A-CAA-CBA
82	AJ	301	PEB	NB-C1B-CHA-C4A
82	AJ	301	PEB	C2B-C1B-CHA-C4A
82	AJ	302	PEB	ND-C1D-CHC-C4C
82	AJ	302	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	AJ	302	PEB	NB-C1B-CHA-C4A
82	AJ	302	PEB	C2B-C1B-CHA-C4A
82	BJ	301	PEB	ND-C1D-CHC-C4C
82	BJ	301	PEB	C1C-C2C-CAC-CBC
82	BJ	301	PEB	NB-C1B-CHA-C4A
82	BJ	301	PEB	C2B-C1B-CHA-C4A
82	CJ	201	PEB	NB-C1B-CHA-C4A
82	CJ	201	PEB	C2B-C1B-CHA-C4A
82	CJ	202	PEB	C2A-C3A-CAA-CBA
82	CJ	202	PEB	C4A-C3A-CAA-CBA
82	CJ	202	PEB	NB-C1B-CHA-C4A
82	CJ	202	PEB	C2B-C1B-CHA-C4A
82	CJ	203	PEB	C2A-C3A-CAA-CBA
82	CJ	203	PEB	C4A-C3A-CAA-CBA
82	CJ	203	PEB	NB-C1B-CHA-C4A
82	CJ	203	PEB	C2B-C1B-CHA-C4A
82	DJ	201	PEB	ND-C1D-CHC-C4C
82	DJ	201	PEB	C2D-C1D-CHC-C4C
82	DJ	201	PEB	NB-C1B-CHA-C4A
82	DJ	201	PEB	C2B-C1B-CHA-C4A
82	DJ	202	PEB	ND-C1D-CHC-C4C
82	DJ	202	PEB	C2D-C1D-CHC-C4C
82	DJ	202	PEB	NB-C1B-CHA-C4A
82	DJ	202	PEB	C2B-C1B-CHA-C4A
82	EJ	201	PEB	C4A-C3A-CAA-CBA
82	EJ	201	PEB	NB-C1B-CHA-C4A
82	EJ	201	PEB	C2B-C1B-CHA-C4A
82	EJ	202	PEB	NB-C1B-CHA-C4A
82	EJ	202	PEB	C2B-C1B-CHA-C4A
82	EJ	203	PEB	ND-C1D-CHC-C4C
82	EJ	203	PEB	C2D-C1D-CHC-C4C
82	EJ	203	PEB	C4A-C3A-CAA-CBA
82	EJ	203	PEB	NB-C1B-CHA-C4A
82	EJ	203	PEB	C2B-C1B-CHA-C4A
82	FJ	201	PEB	ND-C1D-CHC-C4C
82	FJ	201	PEB	C2D-C1D-CHC-C4C
82	FJ	201	PEB	C2C-CAC-CBC-CGC
82	FJ	201	PEB	NB-C1B-CHA-C4A
82	FJ	201	PEB	C2B-C1B-CHA-C4A
82	FJ	202	PEB	NB-C1B-CHA-C4A
82	FJ	202	PEB	C2B-C1B-CHA-C4A
82	GJ	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	GJ	201	PEB	C2B-C1B-CHA-C4A
82	GJ	202	PEB	NB-C1B-CHA-C4A
82	GJ	202	PEB	C2B-C1B-CHA-C4A
82	GJ	203	PEB	C4A-C3A-CAA-CBA
82	GJ	203	PEB	NB-C1B-CHA-C4A
82	GJ	203	PEB	C2B-C1B-CHA-C4A
82	HJ	201	PEB	ND-C1D-CHC-C4C
82	HJ	201	PEB	C2D-C1D-CHC-C4C
82	HJ	201	PEB	NB-C1B-CHA-C4A
82	HJ	201	PEB	C2B-C1B-CHA-C4A
82	HJ	202	PEB	NC-C1C-CHB-C4B
82	HJ	202	PEB	C2C-C1C-CHB-C4B
82	HJ	202	PEB	NB-C1B-CHA-C4A
82	HJ	202	PEB	C2B-C1B-CHA-C4A
82	IJ	201	PEB	C4A-C3A-CAA-CBA
82	IJ	201	PEB	NB-C1B-CHA-C4A
82	IJ	201	PEB	C2B-C1B-CHA-C4A
82	IJ	202	PEB	NB-C1B-CHA-C4A
82	IJ	202	PEB	C2B-C1B-CHA-C4A
82	IJ	203	PEB	ND-C1D-CHC-C4C
82	IJ	203	PEB	C2D-C1D-CHC-C4C
82	IJ	203	PEB	NB-C1B-CHA-C4A
82	IJ	203	PEB	C2B-C1B-CHA-C4A
82	JJ	201	PEB	ND-C1D-CHC-C4C
82	JJ	201	PEB	C2D-C1D-CHC-C4C
82	JJ	201	PEB	NB-C1B-CHA-C4A
82	JJ	201	PEB	C2B-C1B-CHA-C4A
82	JJ	202	PEB	NB-C1B-CHA-C4A
82	JJ	202	PEB	C2B-C1B-CHA-C4A
82	KJ	201	PEB	NB-C1B-CHA-C4A
82	KJ	201	PEB	C2B-C1B-CHA-C4A
82	KJ	202	PEB	NC-C4C-CHC-C1D
82	KJ	202	PEB	C3C-C4C-CHC-C1D
82	KJ	202	PEB	ND-C1D-CHC-C4C
82	KJ	202	PEB	C2D-C1D-CHC-C4C
82	KJ	202	PEB	C2A-C3A-CAA-CBA
82	KJ	202	PEB	C4A-C3A-CAA-CBA
82	KJ	202	PEB	NB-C1B-CHA-C4A
82	KJ	202	PEB	C2B-C1B-CHA-C4A
82	KJ	203	PEB	C4A-C3A-CAA-CBA
82	KJ	203	PEB	NB-C1B-CHA-C4A
82	KJ	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	LJ	201	PEB	ND-C1D-CHC-C4C
82	LJ	201	PEB	C2D-C1D-CHC-C4C
82	LJ	201	PEB	NB-C1B-CHA-C4A
82	LJ	201	PEB	C2B-C1B-CHA-C4A
82	LJ	202	PEB	NB-C1B-CHA-C4A
82	LJ	202	PEB	C2B-C1B-CHA-C4A
82	MJ	201	PEB	C4A-C3A-CAA-CBA
82	MJ	201	PEB	NB-C1B-CHA-C4A
82	MJ	201	PEB	C2B-C1B-CHA-C4A
82	MJ	202	PEB	NB-C1B-CHA-C4A
82	MJ	202	PEB	C2B-C1B-CHA-C4A
82	MJ	203	PEB	C4A-C3A-CAA-CBA
82	MJ	203	PEB	NB-C1B-CHA-C4A
82	MJ	203	PEB	C2B-C1B-CHA-C4A
82	NJ	201	PEB	ND-C1D-CHC-C4C
82	NJ	201	PEB	C2D-C1D-CHC-C4C
82	NJ	201	PEB	NB-C1B-CHA-C4A
82	NJ	201	PEB	C2B-C1B-CHA-C4A
82	NJ	202	PEB	NB-C1B-CHA-C4A
82	NJ	202	PEB	C2B-C1B-CHA-C4A
82	OJ	201	PEB	C2C-CAC-CBC-CGC
82	OJ	201	PEB	NB-C1B-CHA-C4A
82	OJ	201	PEB	C2B-C1B-CHA-C4A
82	OJ	202	PEB	ND-C1D-CHC-C4C
82	OJ	202	PEB	C2D-C1D-CHC-C4C
82	OJ	202	PEB	NC-C1C-CHB-C4B
82	OJ	202	PEB	C2C-C1C-CHB-C4B
82	OJ	202	PEB	C4A-C3A-CAA-CBA
82	OJ	202	PEB	NB-C1B-CHA-C4A
82	OJ	202	PEB	C2B-C1B-CHA-C4A
82	OJ	203	PEB	C2A-C3A-CAA-CBA
82	OJ	203	PEB	C4A-C3A-CAA-CBA
82	OJ	203	PEB	NB-C1B-CHA-C4A
82	OJ	203	PEB	C2B-C1B-CHA-C4A
82	PJ	201	PEB	ND-C1D-CHC-C4C
82	PJ	201	PEB	C2D-C1D-CHC-C4C
82	PJ	201	PEB	NB-C1B-CHA-C4A
82	PJ	201	PEB	C2B-C1B-CHA-C4A
82	PJ	202	PEB	NB-C1B-CHA-C4A
82	PJ	202	PEB	C2B-C1B-CHA-C4A
82	QJ	202	PEB	C4A-C3A-CAA-CBA
82	QJ	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	QJ	202	PEB	C2B-C1B-CHA-C4A
82	QJ	203	PEB	ND-C1D-CHC-C4C
82	QJ	203	PEB	C2D-C1D-CHC-C4C
82	QJ	203	PEB	NB-C1B-CHA-C4A
82	QJ	203	PEB	C2B-C1B-CHA-C4A
82	QJ	204	PEB	C4A-C3A-CAA-CBA
82	QJ	204	PEB	NB-C1B-CHA-C4A
82	QJ	204	PEB	C2B-C1B-CHA-C4A
82	RJ	201	PEB	ND-C1D-CHC-C4C
82	RJ	201	PEB	C2D-C1D-CHC-C4C
82	RJ	201	PEB	NB-C1B-CHA-C4A
82	RJ	201	PEB	C2B-C1B-CHA-C4A
82	RJ	202	PEB	NB-C1B-CHA-C4A
82	RJ	202	PEB	C2B-C1B-CHA-C4A
82	SJ	201	PEB	ND-C1D-CHC-C4C
82	SJ	201	PEB	C2D-C1D-CHC-C4C
82	SJ	201	PEB	NB-C1B-CHA-C4A
82	SJ	201	PEB	C2B-C1B-CHA-C4A
82	SJ	202	PEB	ND-C1D-CHC-C4C
82	SJ	202	PEB	C2D-C1D-CHC-C4C
82	SJ	202	PEB	C4A-C3A-CAA-CBA
82	SJ	202	PEB	NB-C1B-CHA-C4A
82	SJ	202	PEB	C2B-C1B-CHA-C4A
82	SJ	203	PEB	C4A-C3A-CAA-CBA
82	SJ	203	PEB	NB-C1B-CHA-C4A
82	SJ	203	PEB	C2B-C1B-CHA-C4A
82	TJ	201	PEB	ND-C1D-CHC-C4C
82	TJ	201	PEB	C2D-C1D-CHC-C4C
82	TJ	201	PEB	NB-C1B-CHA-C4A
82	TJ	201	PEB	C2B-C1B-CHA-C4A
82	TJ	202	PEB	NB-C1B-CHA-C4A
82	TJ	202	PEB	C2B-C1B-CHA-C4A
82	UJ	201	PEB	C4A-C3A-CAA-CBA
82	UJ	201	PEB	NB-C1B-CHA-C4A
82	UJ	201	PEB	C2B-C1B-CHA-C4A
82	UJ	202	PEB	NB-C1B-CHA-C4A
82	UJ	202	PEB	C2B-C1B-CHA-C4A
82	UJ	203	PEB	ND-C1D-CHC-C4C
82	UJ	203	PEB	C2D-C1D-CHC-C4C
82	UJ	203	PEB	NB-C1B-CHA-C4A
82	UJ	203	PEB	C2B-C1B-CHA-C4A
82	VJ	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	VJ	201	PEB	C2D-C1D-CHC-C4C
82	VJ	201	PEB	NB-C1B-CHA-C4A
82	VJ	201	PEB	C2B-C1B-CHA-C4A
82	VJ	202	PEB	NB-C1B-CHA-C4A
82	VJ	202	PEB	C2B-C1B-CHA-C4A
82	WJ	201	PEB	NB-C1B-CHA-C4A
82	WJ	201	PEB	C2B-C1B-CHA-C4A
82	WJ	202	PEB	NC-C4C-CHC-C1D
82	WJ	202	PEB	ND-C1D-CHC-C4C
82	WJ	202	PEB	C2D-C1D-CHC-C4C
82	WJ	202	PEB	NC-C1C-CHB-C4B
82	WJ	202	PEB	C2C-C1C-CHB-C4B
82	WJ	202	PEB	C2A-C3A-CAA-CBA
82	WJ	202	PEB	C4A-C3A-CAA-CBA
82	WJ	202	PEB	NB-C1B-CHA-C4A
82	WJ	202	PEB	C2B-C1B-CHA-C4A
82	WJ	203	PEB	C4A-C3A-CAA-CBA
82	WJ	203	PEB	NB-C1B-CHA-C4A
82	WJ	203	PEB	C2B-C1B-CHA-C4A
82	XJ	201	PEB	ND-C1D-CHC-C4C
82	XJ	201	PEB	C2D-C1D-CHC-C4C
82	XJ	201	PEB	NB-C1B-CHA-C4A
82	XJ	201	PEB	C2B-C1B-CHA-C4A
82	XJ	202	PEB	NB-C1B-CHA-C4A
82	XJ	202	PEB	C2B-C1B-CHA-C4A
82	YJ	201	PEB	C4A-C3A-CAA-CBA
82	YJ	201	PEB	NB-C1B-CHA-C4A
82	YJ	201	PEB	C2B-C1B-CHA-C4A
82	YJ	202	PEB	NB-C1B-CHA-C4A
82	YJ	202	PEB	C2B-C1B-CHA-C4A
82	YJ	203	PEB	C4A-C3A-CAA-CBA
82	YJ	203	PEB	NB-C1B-CHA-C4A
82	YJ	203	PEB	C2B-C1B-CHA-C4A
82	ZJ	201	PEB	ND-C1D-CHC-C4C
82	ZJ	201	PEB	C2D-C1D-CHC-C4C
82	ZJ	201	PEB	NB-C1B-CHA-C4A
82	ZJ	201	PEB	C2B-C1B-CHA-C4A
82	ZJ	202	PEB	NB-C1B-CHA-C4A
82	ZJ	202	PEB	C2B-C1B-CHA-C4A
82	AK	201	PEB	ND-C1D-CHC-C4C
82	AK	201	PEB	C2D-C1D-CHC-C4C
82	AK	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	AK	201	PEB	C2B-C1B-CHA-C4A
82	AK	202	PEB	C2A-C3A-CAA-CBA
82	AK	202	PEB	C4A-C3A-CAA-CBA
82	AK	202	PEB	NB-C1B-CHA-C4A
82	AK	202	PEB	C2B-C1B-CHA-C4A
82	BK	201	PEB	ND-C1D-CHC-C4C
82	BK	201	PEB	C2D-C1D-CHC-C4C
82	BK	201	PEB	NB-C1B-CHA-C4A
82	BK	201	PEB	C2B-C1B-CHA-C4A
82	BK	202	PEB	ND-C1D-CHC-C4C
82	BK	202	PEB	C2D-C1D-CHC-C4C
82	BK	202	PEB	NC-C1C-CHB-C4B
82	BK	202	PEB	C2A-C3A-CAA-CBA
82	BK	202	PEB	C4A-C3A-CAA-CBA
82	BK	202	PEB	NB-C1B-CHA-C4A
82	BK	202	PEB	C2B-C1B-CHA-C4A
82	CK	201	PEB	NB-C1B-CHA-C4A
82	CK	201	PEB	C2B-C1B-CHA-C4A
82	CK	202	PEB	C4A-C3A-CAA-CBA
82	CK	202	PEB	NB-C1B-CHA-C4A
82	CK	202	PEB	C2B-C1B-CHA-C4A
82	CK	203	PEB	NB-C1B-CHA-C4A
82	CK	203	PEB	C2B-C1B-CHA-C4A
82	DK	201	PEB	NB-C1B-CHA-C4A
82	DK	201	PEB	C2B-C1B-CHA-C4A
82	DK	202	PEB	C2D-C3D-CAD-CBD
82	DK	202	PEB	C4D-C3D-CAD-CBD
82	DK	202	PEB	C4A-C3A-CAA-CBA
82	DK	202	PEB	NB-C1B-CHA-C4A
82	DK	202	PEB	C2B-C1B-CHA-C4A
82	DK	203	PEB	ND-C1D-CHC-C4C
82	DK	203	PEB	C2D-C1D-CHC-C4C
82	DK	203	PEB	NC-C1C-CHB-C4B
82	DK	203	PEB	C2C-C1C-CHB-C4B
82	DK	203	PEB	NB-C1B-CHA-C4A
82	DK	203	PEB	C2B-C1B-CHA-C4A
82	EK	201	PEB	C2D-C1D-CHC-C4C
82	EK	201	PEB	C2A-C3A-CAA-CBA
82	EK	201	PEB	C4A-C3A-CAA-CBA
82	EK	201	PEB	NB-C1B-CHA-C4A
82	EK	201	PEB	C2B-C1B-CHA-C4A
82	EK	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	EK	202	PEB	C2B-C1B-CHA-C4A
82	FK	201	PEB	NB-C1B-CHA-C4A
82	FK	201	PEB	C2B-C1B-CHA-C4A
82	FK	202	PEB	ND-C1D-CHC-C4C
82	FK	202	PEB	C2D-C1D-CHC-C4C
82	FK	202	PEB	NC-C1C-CHB-C4B
82	FK	202	PEB	NB-C1B-CHA-C4A
82	FK	202	PEB	C2B-C1B-CHA-C4A
82	GK	201	PEB	C2A-C3A-CAA-CBA
82	GK	201	PEB	C4A-C3A-CAA-CBA
82	GK	201	PEB	NB-C1B-CHA-C4A
82	GK	201	PEB	C2B-C1B-CHA-C4A
82	GK	202	PEB	C2A-C3A-CAA-CBA
82	GK	202	PEB	C4A-C3A-CAA-CBA
82	GK	202	PEB	NB-C1B-CHA-C4A
82	GK	202	PEB	C2B-C1B-CHA-C4A
82	GK	203	PEB	C2C-CAC-CBC-CGC
82	GK	203	PEB	NB-C1B-CHA-C4A
82	GK	203	PEB	C2B-C1B-CHA-C4A
82	HK	201	PEB	C2A-C3A-CAA-CBA
82	HK	201	PEB	C4A-C3A-CAA-CBA
82	HK	201	PEB	NB-C1B-CHA-C4A
82	HK	201	PEB	C2B-C1B-CHA-C4A
82	HK	202	PEB	ND-C1D-CHC-C4C
82	HK	202	PEB	C2D-C1D-CHC-C4C
82	HK	202	PEB	NC-C1C-CHB-C4B
82	HK	202	PEB	NB-C1B-CHA-C4A
82	HK	202	PEB	C2B-C1B-CHA-C4A
82	IK	201	PEB	C4A-C3A-CAA-CBA
82	IK	201	PEB	NB-C1B-CHA-C4A
82	IK	201	PEB	C2B-C1B-CHA-C4A
82	IK	202	PEB	C2A-C3A-CAA-CBA
82	IK	202	PEB	C4A-C3A-CAA-CBA
82	IK	202	PEB	C3A-C4A-CHA-C1B
82	IK	202	PEB	NB-C1B-CHA-C4A
82	IK	202	PEB	C2B-C1B-CHA-C4A
82	IK	203	PEB	C4A-C3A-CAA-CBA
82	IK	203	PEB	NB-C1B-CHA-C4A
82	IK	203	PEB	C2B-C1B-CHA-C4A
82	JK	201	PEB	C2A-C3A-CAA-CBA
82	JK	201	PEB	NB-C1B-CHA-C4A
82	JK	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	JK	202	PEB	C3C-C4C-CHC-C1D
82	JK	202	PEB	ND-C1D-CHC-C4C
82	JK	202	PEB	C2D-C1D-CHC-C4C
82	JK	202	PEB	C4A-C3A-CAA-CBA
82	JK	202	PEB	NB-C1B-CHA-C4A
82	JK	202	PEB	C2B-C1B-CHA-C4A
82	KK	201	PEB	C4A-C3A-CAA-CBA
82	KK	201	PEB	NB-C1B-CHA-C4A
82	KK	201	PEB	C2B-C1B-CHA-C4A
82	KK	202	PEB	NB-C1B-CHA-C4A
82	KK	202	PEB	C2B-C1B-CHA-C4A
82	KK	203	PEB	NB-C1B-CHA-C4A
82	KK	203	PEB	C2B-C1B-CHA-C4A
82	LK	201	PEB	C2A-C3A-CAA-CBA
82	LK	201	PEB	C4A-C3A-CAA-CBA
82	LK	201	PEB	NB-C1B-CHA-C4A
82	LK	201	PEB	C2B-C1B-CHA-C4A
82	LK	202	PEB	ND-C1D-CHC-C4C
82	LK	202	PEB	C2D-C1D-CHC-C4C
82	LK	202	PEB	NC-C1C-CHB-C4B
82	LK	202	PEB	NB-C1B-CHA-C4A
82	LK	202	PEB	C2B-C1B-CHA-C4A
82	MK	201	PEB	ND-C1D-CHC-C4C
82	MK	201	PEB	C2D-C1D-CHC-C4C
82	MK	201	PEB	NB-C1B-CHA-C4A
82	MK	201	PEB	C2B-C1B-CHA-C4A
82	MK	202	PEB	NB-C1B-CHA-C4A
82	MK	202	PEB	C2B-C1B-CHA-C4A
82	MK	203	PEB	C4A-C3A-CAA-CBA
82	MK	203	PEB	NB-C1B-CHA-C4A
82	MK	203	PEB	C2B-C1B-CHA-C4A
82	NK	201	PEB	NB-C1B-CHA-C4A
82	NK	201	PEB	C2B-C1B-CHA-C4A
82	NK	202	PEB	C3C-C4C-CHC-C1D
82	NK	202	PEB	ND-C1D-CHC-C4C
82	NK	202	PEB	C2D-C1D-CHC-C4C
82	NK	202	PEB	NC-C1C-CHB-C4B
82	NK	202	PEB	NB-C1B-CHA-C4A
82	NK	202	PEB	C2B-C1B-CHA-C4A
82	OK	201	PEB	NB-C1B-CHA-C4A
82	OK	201	PEB	C2B-C1B-CHA-C4A
82	OK	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	OK	202	PEB	C2D-C1D-CHC-C4C
82	OK	202	PEB	NB-C1B-CHA-C4A
82	OK	202	PEB	C2B-C1B-CHA-C4A
82	OK	203	PEB	NB-C1B-CHA-C4A
82	OK	203	PEB	C2B-C1B-CHA-C4A
82	PK	201	PEB	NB-C1B-CHA-C4A
82	PK	201	PEB	C2B-C1B-CHA-C4A
82	PK	202	PEB	C3C-C4C-CHC-C1D
82	PK	202	PEB	ND-C1D-CHC-C4C
82	PK	202	PEB	C2D-C1D-CHC-C4C
82	PK	202	PEB	NB-C1B-CHA-C4A
82	PK	202	PEB	C2B-C1B-CHA-C4A
82	QK	201	PEB	C2A-C3A-CAA-CBA
82	QK	201	PEB	C4A-C3A-CAA-CBA
82	QK	201	PEB	NB-C1B-CHA-C4A
82	QK	201	PEB	C2B-C1B-CHA-C4A
82	QK	202	PEB	C2C-CAC-CBC-CGC
82	QK	202	PEB	NB-C1B-CHA-C4A
82	QK	202	PEB	C2B-C1B-CHA-C4A
82	QK	203	PEB	NB-C1B-CHA-C4A
82	QK	203	PEB	C2B-C1B-CHA-C4A
82	RK	201	PEB	NB-C1B-CHA-C4A
82	RK	201	PEB	C2B-C1B-CHA-C4A
82	RK	202	PEB	ND-C1D-CHC-C4C
82	RK	202	PEB	C2D-C1D-CHC-C4C
82	RK	202	PEB	NC-C1C-CHB-C4B
82	RK	202	PEB	C2C-C1C-CHB-C4B
82	RK	202	PEB	C2A-C3A-CAA-CBA
82	RK	202	PEB	C4A-C3A-CAA-CBA
82	RK	202	PEB	NB-C1B-CHA-C4A
82	RK	202	PEB	C2B-C1B-CHA-C4A
82	SK	201	PEB	C2A-C3A-CAA-CBA
82	SK	201	PEB	C4A-C3A-CAA-CBA
82	SK	201	PEB	NB-C1B-CHA-C4A
82	SK	201	PEB	C2B-C1B-CHA-C4A
82	SK	202	PEB	C2D-C1D-CHC-C4C
82	SK	202	PEB	NB-C1B-CHA-C4A
82	SK	203	PEB	NB-C1B-CHA-C4A
82	SK	203	PEB	C2B-C1B-CHA-C4A
82	TK	201	PEB	NB-C1B-CHA-C4A
82	TK	201	PEB	C2B-C1B-CHA-C4A
82	TK	202	PEB	C3C-C4C-CHC-C1D

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Mol	Chain	Res	Type	Atoms
82	TK	202	PEB	ND-C1D-CHC-C4C
82	TK	202	PEB	C2D-C1D-CHC-C4C
82	TK	202	PEB	NC-C1C-CHB-C4B
82	TK	202	PEB	C2D-C3D-CAD-CBD
82	TK	202	PEB	C4D-C3D-CAD-CBD
82	TK	202	PEB	C4A-C3A-CAA-CBA
82	TK	202	PEB	NB-C1B-CHA-C4A
82	TK	202	PEB	C2B-C1B-CHA-C4A
82	UK	201	PEB	C2D-C1D-CHC-C4C
82	UK	201	PEB	C4A-C3A-CAA-CBA
82	UK	201	PEB	NB-C1B-CHA-C4A
82	UK	201	PEB	C2B-C1B-CHA-C4A
82	UK	202	PEB	C2C-CAC-CBC-CGC
82	UK	202	PEB	C2A-C3A-CAA-CBA
82	UK	202	PEB	NB-C1B-CHA-C4A
82	UK	202	PEB	C2B-C1B-CHA-C4A
82	VK	201	PEB	C2A-C3A-CAA-CBA
82	VK	201	PEB	C4A-C3A-CAA-CBA
82	VK	201	PEB	NB-C1B-CHA-C4A
82	VK	201	PEB	C2B-C1B-CHA-C4A
82	VK	202	PEB	ND-C1D-CHC-C4C
82	VK	202	PEB	C2D-C1D-CHC-C4C
82	VK	202	PEB	C2C-CAC-CBC-CGC
82	VK	202	PEB	NB-C1B-CHA-C4A
82	VK	202	PEB	C2B-C1B-CHA-C4A
82	WK	201	PEB	C2D-C3D-CAD-CBD
82	WK	201	PEB	C4D-C3D-CAD-CBD
82	WK	201	PEB	NB-C1B-CHA-C4A
82	WK	201	PEB	C2B-C1B-CHA-C4A
82	WK	202	PEB	C2A-C3A-CAA-CBA
82	WK	202	PEB	C4A-C3A-CAA-CBA
82	WK	202	PEB	NB-C1B-CHA-C4A
82	WK	202	PEB	C2B-C1B-CHA-C4A
82	WK	203	PEB	C2A-C3A-CAA-CBA
82	WK	203	PEB	NB-C1B-CHA-C4A
82	WK	203	PEB	C2B-C1B-CHA-C4A
82	XK	201	PEB	NB-C1B-CHA-C4A
82	XK	201	PEB	C2B-C1B-CHA-C4A
82	XK	202	PEB	C2A-C3A-CAA-CBA
82	XK	202	PEB	C4A-C3A-CAA-CBA
82	XK	202	PEB	NB-C1B-CHA-C4A
82	XK	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	XK	203	PEB	ND-C1D-CHC-C4C
82	XK	203	PEB	C2D-C1D-CHC-C4C
82	XK	203	PEB	NC-C1C-CHB-C4B
82	XK	203	PEB	NB-C1B-CHA-C4A
82	XK	203	PEB	C2B-C1B-CHA-C4A
82	YK	201	PEB	ND-C1D-CHC-C4C
82	YK	201	PEB	C2D-C1D-CHC-C4C
82	YK	201	PEB	NB-C1B-CHA-C4A
82	YK	201	PEB	C2B-C1B-CHA-C4A
82	YK	202	PEB	NC-C1C-CHB-C4B
82	YK	202	PEB	C2C-C1C-CHB-C4B
82	YK	202	PEB	NB-C1B-CHA-C4A
82	YK	202	PEB	C2B-C1B-CHA-C4A
82	YK	203	PEB	NC-C1C-CHB-C4B
82	YK	203	PEB	C2C-C1C-CHB-C4B
82	YK	203	PEB	NB-C1B-CHA-C4A
82	YK	203	PEB	C2B-C1B-CHA-C4A
82	ZK	201	PEB	ND-C1D-CHC-C4C
82	ZK	201	PEB	C2D-C1D-CHC-C4C
82	ZK	201	PEB	NB-C1B-CHA-C4A
82	ZK	201	PEB	C2B-C1B-CHA-C4A
82	ZK	202	PEB	ND-C1D-CHC-C4C
82	ZK	202	PEB	C2D-C1D-CHC-C4C
82	ZK	202	PEB	NC-C1C-CHB-C4B
82	ZK	202	PEB	NB-C1B-CHA-C4A
82	ZK	202	PEB	C2B-C1B-CHA-C4A
82	AM	301	PEB	ND-C1D-CHC-C4C
82	AM	301	PEB	C2D-C1D-CHC-C4C
82	AM	301	PEB	C2A-C3A-CAA-CBA
82	AM	301	PEB	C4A-C3A-CAA-CBA
82	AM	301	PEB	NB-C1B-CHA-C4A
82	AM	301	PEB	C2B-C1B-CHA-C4A
82	AM	301	PEB	C3B-CAB-CBB-CGB
82	AM	302	PEB	NB-C1B-CHA-C4A
82	AM	302	PEB	C2B-C1B-CHA-C4A
82	BM	301	PEB	C1C-C2C-CAC-CBC
82	BM	301	PEB	NB-C1B-CHA-C4A
82	BM	301	PEB	C2B-C1B-CHA-C4A
82	CM	201	PEB	C2A-C3A-CAA-CBA
82	CM	201	PEB	C4A-C3A-CAA-CBA
82	CM	201	PEB	NB-C1B-CHA-C4A
82	CM	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	CM	202	PEB	ND-C1D-CHC-C4C
82	CM	202	PEB	C2D-C1D-CHC-C4C
82	CM	202	PEB	C4A-C3A-CAA-CBA
82	CM	202	PEB	NB-C1B-CHA-C4A
82	CM	202	PEB	C2B-C1B-CHA-C4A
82	CM	203	PEB	C2A-C3A-CAA-CBA
82	CM	203	PEB	C4A-C3A-CAA-CBA
82	CM	203	PEB	NB-C1B-CHA-C4A
82	CM	203	PEB	C2B-C1B-CHA-C4A
82	DM	201	PEB	ND-C1D-CHC-C4C
82	DM	201	PEB	C2D-C1D-CHC-C4C
82	DM	201	PEB	NB-C1B-CHA-C4A
82	DM	201	PEB	C2B-C1B-CHA-C4A
82	DM	202	PEB	NB-C1B-CHA-C4A
82	DM	202	PEB	C2B-C1B-CHA-C4A
82	EM	201	PEB	C2A-C3A-CAA-CBA
82	EM	201	PEB	C4A-C3A-CAA-CBA
82	EM	201	PEB	NB-C1B-CHA-C4A
82	EM	201	PEB	C2B-C1B-CHA-C4A
82	EM	202	PEB	C2D-C1D-CHC-C4C
82	EM	202	PEB	NB-C1B-CHA-C4A
82	EM	202	PEB	C2B-C1B-CHA-C4A
82	EM	203	PEB	C4A-C3A-CAA-CBA
82	EM	203	PEB	NB-C1B-CHA-C4A
82	EM	203	PEB	C2B-C1B-CHA-C4A
82	FM	201	PEB	ND-C1D-CHC-C4C
82	FM	201	PEB	C2D-C1D-CHC-C4C
82	FM	201	PEB	NB-C1B-CHA-C4A
82	FM	201	PEB	C2B-C1B-CHA-C4A
82	FM	202	PEB	NB-C1B-CHA-C4A
82	FM	202	PEB	C2B-C1B-CHA-C4A
82	GM	201	PEB	C2A-C3A-CAA-CBA
82	GM	201	PEB	C4A-C3A-CAA-CBA
82	GM	201	PEB	NB-C1B-CHA-C4A
82	GM	201	PEB	C2B-C1B-CHA-C4A
82	GM	202	PEB	ND-C1D-CHC-C4C
82	GM	202	PEB	C2D-C1D-CHC-C4C
82	GM	202	PEB	C4A-C3A-CAA-CBA
82	GM	202	PEB	NB-C1B-CHA-C4A
82	GM	202	PEB	C2B-C1B-CHA-C4A
82	GM	203	PEB	C4A-C3A-CAA-CBA
82	GM	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	GM	203	PEB	C2B-C1B-CHA-C4A
82	HM	201	PEB	ND-C1D-CHC-C4C
82	HM	201	PEB	C2D-C1D-CHC-C4C
82	HM	201	PEB	NB-C1B-CHA-C4A
82	HM	201	PEB	C2B-C1B-CHA-C4A
82	HM	202	PEB	NC-C1C-CHB-C4B
82	HM	202	PEB	C2C-C1C-CHB-C4B
82	HM	202	PEB	NB-C1B-CHA-C4A
82	HM	202	PEB	C2B-C1B-CHA-C4A
82	IM	201	PEB	C4A-C3A-CAA-CBA
82	IM	201	PEB	NB-C1B-CHA-C4A
82	IM	201	PEB	C2B-C1B-CHA-C4A
82	IM	202	PEB	ND-C1D-CHC-C4C
82	IM	202	PEB	C2D-C1D-CHC-C4C
82	IM	202	PEB	NB-C1B-CHA-C4A
82	IM	202	PEB	C2B-C1B-CHA-C4A
82	IM	203	PEB	C2D-C1D-CHC-C4C
82	IM	203	PEB	NB-C1B-CHA-C4A
82	IM	203	PEB	C2B-C1B-CHA-C4A
82	JM	201	PEB	ND-C1D-CHC-C4C
82	JM	201	PEB	C2D-C1D-CHC-C4C
82	JM	201	PEB	NB-C1B-CHA-C4A
82	JM	201	PEB	C2B-C1B-CHA-C4A
82	JM	202	PEB	NB-C1B-CHA-C4A
82	JM	202	PEB	C2B-C1B-CHA-C4A
82	KM	201	PEB	C2A-C3A-CAA-CBA
82	KM	201	PEB	C4A-C3A-CAA-CBA
82	KM	201	PEB	NB-C1B-CHA-C4A
82	KM	201	PEB	C2B-C1B-CHA-C4A
82	KM	202	PEB	C2A-C3A-CAA-CBA
82	KM	202	PEB	C4A-C3A-CAA-CBA
82	KM	202	PEB	NB-C1B-CHA-C4A
82	KM	202	PEB	C2B-C1B-CHA-C4A
82	KM	203	PEB	C4A-C3A-CAA-CBA
82	KM	203	PEB	NB-C1B-CHA-C4A
82	KM	203	PEB	C2B-C1B-CHA-C4A
82	LM	201	PEB	ND-C1D-CHC-C4C
82	LM	201	PEB	C2D-C1D-CHC-C4C
82	LM	201	PEB	NB-C1B-CHA-C4A
82	LM	201	PEB	C2B-C1B-CHA-C4A
82	LM	202	PEB	NB-C1B-CHA-C4A
82	LM	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	MM	201	PEB	C4A-C3A-CAA-CBA
82	MM	201	PEB	NB-C1B-CHA-C4A
82	MM	201	PEB	C2B-C1B-CHA-C4A
82	MM	202	PEB	C2A-C3A-CAA-CBA
82	MM	202	PEB	C4A-C3A-CAA-CBA
82	MM	202	PEB	NB-C1B-CHA-C4A
82	MM	202	PEB	C2B-C1B-CHA-C4A
82	MM	203	PEB	ND-C1D-CHC-C4C
82	MM	203	PEB	C2D-C1D-CHC-C4C
82	MM	203	PEB	C4A-C3A-CAA-CBA
82	MM	203	PEB	NB-C1B-CHA-C4A
82	MM	203	PEB	C2B-C1B-CHA-C4A
82	NM	201	PEB	ND-C1D-CHC-C4C
82	NM	201	PEB	C2D-C1D-CHC-C4C
82	NM	201	PEB	NB-C1B-CHA-C4A
82	NM	201	PEB	C2B-C1B-CHA-C4A
82	NM	202	PEB	ND-C1D-CHC-C4C
82	NM	202	PEB	C2D-C1D-CHC-C4C
82	NM	202	PEB	NB-C1B-CHA-C4A
82	NM	202	PEB	C2B-C1B-CHA-C4A
82	OM	201	PEB	NB-C1B-CHA-C4A
82	OM	201	PEB	C2B-C1B-CHA-C4A
82	OM	202	PEB	NB-C1B-CHA-C4A
82	OM	202	PEB	C2B-C1B-CHA-C4A
82	OM	203	PEB	C2A-C3A-CAA-CBA
82	OM	203	PEB	NB-C1B-CHA-C4A
82	OM	203	PEB	C2B-C1B-CHA-C4A
82	PM	201	PEB	ND-C1D-CHC-C4C
82	PM	201	PEB	C2D-C1D-CHC-C4C
82	PM	201	PEB	NB-C1B-CHA-C4A
82	PM	201	PEB	C2B-C1B-CHA-C4A
82	PM	202	PEB	NB-C1B-CHA-C4A
82	PM	202	PEB	C2B-C1B-CHA-C4A
82	QM	202	PEB	C4A-C3A-CAA-CBA
82	QM	202	PEB	NB-C1B-CHA-C4A
82	QM	202	PEB	C2B-C1B-CHA-C4A
82	QM	203	PEB	ND-C1D-CHC-C4C
82	QM	203	PEB	C2D-C1D-CHC-C4C
82	QM	203	PEB	C2A-C3A-CAA-CBA
82	QM	203	PEB	C4A-C3A-CAA-CBA
82	QM	203	PEB	NB-C1B-CHA-C4A
82	QM	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	QM	204	PEB	C4A-C3A-CAA-CBA
82	QM	204	PEB	NB-C1B-CHA-C4A
82	QM	204	PEB	C2B-C1B-CHA-C4A
82	RM	201	PEB	C2D-C1D-CHC-C4C
82	RM	201	PEB	C2A-C3A-CAA-CBA
82	RM	201	PEB	C4A-C3A-CAA-CBA
82	RM	201	PEB	NB-C1B-CHA-C4A
82	RM	201	PEB	C2B-C1B-CHA-C4A
82	RM	202	PEB	NB-C1B-CHA-C4A
82	RM	202	PEB	C2B-C1B-CHA-C4A
82	SM	201	PEB	ND-C1D-CHC-C4C
82	SM	201	PEB	C2D-C1D-CHC-C4C
82	SM	201	PEB	C4A-C3A-CAA-CBA
82	SM	201	PEB	NB-C1B-CHA-C4A
82	SM	201	PEB	C2B-C1B-CHA-C4A
82	SM	202	PEB	C2C-CAC-CBC-CGC
82	SM	202	PEB	C4A-C3A-CAA-CBA
82	SM	202	PEB	NB-C1B-CHA-C4A
82	SM	202	PEB	C2B-C1B-CHA-C4A
82	SM	203	PEB	C2A-C3A-CAA-CBA
82	SM	203	PEB	C4A-C3A-CAA-CBA
82	SM	203	PEB	NB-C1B-CHA-C4A
82	SM	203	PEB	C2B-C1B-CHA-C4A
82	TM	201	PEB	ND-C1D-CHC-C4C
82	TM	201	PEB	C2D-C1D-CHC-C4C
82	TM	201	PEB	NB-C1B-CHA-C4A
82	TM	201	PEB	C2B-C1B-CHA-C4A
82	TM	202	PEB	NB-C1B-CHA-C4A
82	TM	202	PEB	C2B-C1B-CHA-C4A
82	UM	201	PEB	C4A-C3A-CAA-CBA
82	UM	201	PEB	NB-C1B-CHA-C4A
82	UM	201	PEB	C2B-C1B-CHA-C4A
82	UM	202	PEB	NB-C1B-CHA-C4A
82	UM	202	PEB	C2B-C1B-CHA-C4A
82	UM	203	PEB	ND-C1D-CHC-C4C
82	UM	203	PEB	C2D-C1D-CHC-C4C
82	UM	203	PEB	NB-C1B-CHA-C4A
82	UM	203	PEB	C2B-C1B-CHA-C4A
82	VM	201	PEB	ND-C1D-CHC-C4C
82	VM	201	PEB	C2D-C1D-CHC-C4C
82	VM	201	PEB	NB-C1B-CHA-C4A
82	VM	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	VM	202	PEB	NB-C1B-CHA-C4A
82	VM	202	PEB	C2B-C1B-CHA-C4A
82	WM	201	PEB	C2A-C3A-CAA-CBA
82	WM	201	PEB	C4A-C3A-CAA-CBA
82	WM	201	PEB	NB-C1B-CHA-C4A
82	WM	201	PEB	C2B-C1B-CHA-C4A
82	WM	202	PEB	C2A-C3A-CAA-CBA
82	WM	202	PEB	C4A-C3A-CAA-CBA
82	WM	202	PEB	NB-C1B-CHA-C4A
82	WM	202	PEB	C2B-C1B-CHA-C4A
82	WM	203	PEB	C4A-C3A-CAA-CBA
82	WM	203	PEB	NB-C1B-CHA-C4A
82	WM	203	PEB	C2B-C1B-CHA-C4A
82	XM	201	PEB	ND-C1D-CHC-C4C
82	XM	201	PEB	C2D-C1D-CHC-C4C
82	XM	201	PEB	C4A-C3A-CAA-CBA
82	XM	201	PEB	NB-C1B-CHA-C4A
82	XM	201	PEB	C2B-C1B-CHA-C4A
82	XM	202	PEB	C2D-C1D-CHC-C4C
82	XM	202	PEB	NB-C1B-CHA-C4A
82	XM	202	PEB	C2B-C1B-CHA-C4A
82	YM	201	PEB	C2A-C3A-CAA-CBA
82	YM	201	PEB	C4A-C3A-CAA-CBA
82	YM	201	PEB	NB-C1B-CHA-C4A
82	YM	201	PEB	C2B-C1B-CHA-C4A
82	YM	202	PEB	C2A-C3A-CAA-CBA
82	YM	202	PEB	C4A-C3A-CAA-CBA
82	YM	202	PEB	NB-C1B-CHA-C4A
82	YM	202	PEB	C2B-C1B-CHA-C4A
82	YM	203	PEB	ND-C1D-CHC-C4C
82	YM	203	PEB	C2D-C1D-CHC-C4C
82	YM	203	PEB	C4A-C3A-CAA-CBA
82	YM	203	PEB	NB-C1B-CHA-C4A
82	YM	203	PEB	C2B-C1B-CHA-C4A
82	ZM	201	PEB	ND-C1D-CHC-C4C
82	ZM	201	PEB	C2D-C1D-CHC-C4C
82	ZM	201	PEB	C2A-C3A-CAA-CBA
82	ZM	201	PEB	NB-C1B-CHA-C4A
82	ZM	201	PEB	C2B-C1B-CHA-C4A
82	ZM	202	PEB	NC-C1C-CHB-C4B
82	ZM	202	PEB	C2C-C1C-CHB-C4B
82	ZM	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	ZM	202	PEB	C2B-C1B-CHA-C4A
82	AO	301	PEB	NB-C1B-CHA-C4A
82	AO	301	PEB	C2B-C1B-CHA-C4A
82	AO	304	PEB	C2A-C3A-CAA-CBA
82	AO	304	PEB	C4A-C3A-CAA-CBA
82	AO	304	PEB	NB-C1B-CHA-C4A
82	AO	304	PEB	C2B-C1B-CHA-C4A
82	AO	305	PEB	C4A-C3A-CAA-CBA
82	AO	305	PEB	NB-C1B-CHA-C4A
82	AO	305	PEB	C2B-C1B-CHA-C4A
82	DO	1002	PEB	C4A-C3A-CAA-CBA
82	DO	1002	PEB	NB-C1B-CHA-C4A
82	DO	1002	PEB	C2B-C1B-CHA-C4A
82	FO	1002	PEB	C2A-C3A-CAA-CBA
82	FO	1002	PEB	C4A-C3A-CAA-CBA
82	FO	1002	PEB	NB-C1B-CHA-C4A
82	FO	1002	PEB	C2B-C1B-CHA-C4A
82	FO	1002	PEB	C3B-CAB-CBB-CGB
82	HO	1002	PEB	NB-C1B-CHA-C4A
82	HO	1002	PEB	C2B-C1B-CHA-C4A
82	JO	1002	PEB	ND-C1D-CHC-C4C
82	JO	1002	PEB	C2D-C1D-CHC-C4C
82	JO	1002	PEB	C4A-C3A-CAA-CBA
82	JO	1002	PEB	NB-C1B-CHA-C4A
82	JO	1002	PEB	C2B-C1B-CHA-C4A
82	LO	1002	PEB	ND-C1D-CHC-C4C
82	LO	1002	PEB	C2D-C1D-CHC-C4C
82	LO	1002	PEB	C2C-CAC-CBC-CGC
82	LO	1002	PEB	NB-C1B-CHA-C4A
82	LO	1002	PEB	C2B-C1B-CHA-C4A
82	NO	1002	PEB	C4A-C3A-CAA-CBA
82	NO	1002	PEB	NB-C1B-CHA-C4A
82	NO	1002	PEB	C2B-C1B-CHA-C4A
82	OO	201	PEB	C2A-C3A-CAA-CBA
82	OO	201	PEB	C4A-C3A-CAA-CBA
82	OO	201	PEB	NB-C1B-CHA-C4A
82	OO	201	PEB	C2B-C1B-CHA-C4A
82	OO	202	PEB	ND-C1D-CHC-C4C
82	OO	202	PEB	C2D-C1D-CHC-C4C
82	OO	202	PEB	NB-C1B-CHA-C4A
82	OO	202	PEB	C2B-C1B-CHA-C4A
82	PO	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	PO	201	PEB	C2B-C1B-CHA-C4A
82	PO	202	PEB	NB-C1B-CHA-C4A
82	PO	202	PEB	C2B-C1B-CHA-C4A
82	PO	203	PEB	NB-C1B-CHA-C4A
82	PO	203	PEB	C2B-C1B-CHA-C4A
82	QO	201	PEB	C4A-C3A-CAA-CBA
82	QO	201	PEB	NB-C1B-CHA-C4A
82	QO	201	PEB	C2B-C1B-CHA-C4A
82	QO	202	PEB	C2D-C1D-CHC-C4C
82	QO	202	PEB	C4A-C3A-CAA-CBA
82	QO	202	PEB	NB-C1B-CHA-C4A
82	QO	202	PEB	C2B-C1B-CHA-C4A
82	RO	201	PEB	NB-C1B-CHA-C4A
82	RO	201	PEB	C2B-C1B-CHA-C4A
82	RO	202	PEB	C2A-C3A-CAA-CBA
82	RO	202	PEB	NB-C1B-CHA-C4A
82	RO	202	PEB	C2B-C1B-CHA-C4A
82	RO	203	PEB	NB-C1B-CHA-C4A
82	RO	203	PEB	C2B-C1B-CHA-C4A
82	SO	201	PEB	C2A-C3A-CAA-CBA
82	SO	201	PEB	C4A-C3A-CAA-CBA
82	SO	201	PEB	NB-C1B-CHA-C4A
82	SO	201	PEB	C2B-C1B-CHA-C4A
82	SO	202	PEB	ND-C1D-CHC-C4C
82	SO	202	PEB	C2D-C1D-CHC-C4C
82	SO	202	PEB	C4A-C3A-CAA-CBA
82	SO	202	PEB	NB-C1B-CHA-C4A
82	SO	202	PEB	C2B-C1B-CHA-C4A
82	TO	201	PEB	NB-C1B-CHA-C4A
82	TO	201	PEB	C2B-C1B-CHA-C4A
82	TO	202	PEB	NB-C1B-CHA-C4A
82	TO	202	PEB	C2B-C1B-CHA-C4A
82	TO	203	PEB	C2A-C3A-CAA-CBA
82	TO	203	PEB	C4A-C3A-CAA-CBA
82	TO	203	PEB	NB-C1B-CHA-C4A
82	TO	203	PEB	C2B-C1B-CHA-C4A
82	UO	201	PEB	C2A-C3A-CAA-CBA
82	UO	201	PEB	C4A-C3A-CAA-CBA
82	UO	202	PEB	ND-C1D-CHC-C4C
82	UO	202	PEB	C2D-C1D-CHC-C4C
82	UO	202	PEB	C2A-C3A-CAA-CBA
82	UO	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	UO	202	PEB	NB-C1B-CHA-C4A
82	UO	202	PEB	C2B-C1B-CHA-C4A
82	VO	201	PEB	C2A-C3A-CAA-CBA
82	VO	201	PEB	C4A-C3A-CAA-CBA
82	VO	201	PEB	NB-C1B-CHA-C4A
82	VO	201	PEB	C2B-C1B-CHA-C4A
82	VO	202	PEB	ND-C1D-CHC-C4C
82	VO	202	PEB	C2D-C3D-CAD-CBD
82	VO	202	PEB	C4D-C3D-CAD-CBD
82	VO	202	PEB	C2A-C3A-CAA-CBA
82	VO	202	PEB	NB-C1B-CHA-C4A
82	VO	202	PEB	C2B-C1B-CHA-C4A
82	WO	201	PEB	C4A-C3A-CAA-CBA
82	WO	201	PEB	NB-C1B-CHA-C4A
82	WO	201	PEB	C2B-C1B-CHA-C4A
82	YO	201	PEB	NB-C1B-CHA-C4A
82	YO	201	PEB	C2B-C1B-CHA-C4A
82	YO	202	PEB	NB-C1B-CHA-C4A
82	YO	202	PEB	C2B-C1B-CHA-C4A
82	YO	203	PEB	C2A-C3A-CAA-CBA
82	YO	203	PEB	C4A-C3A-CAA-CBA
82	YO	203	PEB	NB-C1B-CHA-C4A
82	YO	203	PEB	C2B-C1B-CHA-C4A
82	ZO	201	PEB	C4A-C3A-CAA-CBA
82	ZO	201	PEB	NB-C1B-CHA-C4A
82	ZO	201	PEB	C2B-C1B-CHA-C4A
82	ZO	202	PEB	ND-C1D-CHC-C4C
82	ZO	202	PEB	C2D-C1D-CHC-C4C
82	ZO	202	PEB	NB-C1B-CHA-C4A
82	ZO	202	PEB	C2B-C1B-CHA-C4A
82	AP	201	PEB	NB-C1B-CHA-C4A
82	AP	201	PEB	C2B-C1B-CHA-C4A
82	AP	202	PEB	C2C-CAC-CBC-CGC
82	AP	202	PEB	C4A-C3A-CAA-CBA
82	AP	202	PEB	NB-C1B-CHA-C4A
82	AP	202	PEB	C2B-C1B-CHA-C4A
82	AP	203	PEB	C3C-C4C-CHC-C1D
82	AP	203	PEB	ND-C1D-CHC-C4C
82	AP	203	PEB	C2D-C1D-CHC-C4C
82	AP	203	PEB	C2A-C3A-CAA-CBA
82	AP	203	PEB	C4A-C3A-CAA-CBA
82	AP	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	AP	203	PEB	C2B-C1B-CHA-C4A
82	BP	201	PEB	NB-C1B-CHA-C4A
82	BP	201	PEB	C2B-C1B-CHA-C4A
82	BP	202	PEB	ND-C1D-CHC-C4C
82	BP	202	PEB	C2D-C1D-CHC-C4C
82	BP	202	PEB	NB-C1B-CHA-C4A
82	BP	202	PEB	C2B-C1B-CHA-C4A
82	CP	201	PEB	ND-C1D-CHC-C4C
82	CP	201	PEB	C2D-C1D-CHC-C4C
82	CP	201	PEB	NB-C1B-CHA-C4A
82	CP	201	PEB	C2B-C1B-CHA-C4A
82	CP	202	PEB	C2A-C3A-CAA-CBA
82	CP	202	PEB	C4A-C3A-CAA-CBA
82	CP	202	PEB	NB-C1B-CHA-C4A
82	CP	202	PEB	C2B-C1B-CHA-C4A
82	CP	203	PEB	C2A-C3A-CAA-CBA
82	CP	203	PEB	C4A-C3A-CAA-CBA
82	CP	203	PEB	NB-C1B-CHA-C4A
82	CP	203	PEB	C2B-C1B-CHA-C4A
82	DP	201	PEB	NB-C1B-CHA-C4A
82	DP	201	PEB	C2B-C1B-CHA-C4A
82	DP	202	PEB	ND-C1D-CHC-C4C
82	DP	202	PEB	C2D-C1D-CHC-C4C
82	DP	202	PEB	NB-C1B-CHA-C4A
82	DP	202	PEB	C2B-C1B-CHA-C4A
82	EP	201	PEB	ND-C1D-CHC-C4C
82	EP	201	PEB	C2D-C1D-CHC-C4C
82	EP	201	PEB	NB-C1B-CHA-C4A
82	EP	201	PEB	C2B-C1B-CHA-C4A
82	EP	202	PEB	C2A-C3A-CAA-CBA
82	EP	202	PEB	C4A-C3A-CAA-CBA
82	EP	202	PEB	NB-C1B-CHA-C4A
82	EP	202	PEB	C2B-C1B-CHA-C4A
82	EP	203	PEB	C3C-C4C-CHC-C1D
82	EP	203	PEB	ND-C1D-CHC-C4C
82	EP	203	PEB	C2D-C1D-CHC-C4C
82	EP	203	PEB	C2A-C3A-CAA-CBA
82	EP	203	PEB	C4A-C3A-CAA-CBA
82	EP	203	PEB	NB-C1B-CHA-C4A
82	EP	203	PEB	C2B-C1B-CHA-C4A
82	FP	201	PEB	ND-C1D-CHC-C4C
82	FP	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	FP	201	PEB	NB-C1B-CHA-C4A
82	FP	201	PEB	C2B-C1B-CHA-C4A
82	FP	202	PEB	C2D-C1D-CHC-C4C
82	FP	202	PEB	NB-C1B-CHA-C4A
82	FP	202	PEB	C2B-C1B-CHA-C4A
82	GP	201	PEB	ND-C1D-CHC-C4C
82	GP	201	PEB	C2D-C1D-CHC-C4C
82	GP	201	PEB	NB-C1B-CHA-C4A
82	GP	201	PEB	C2B-C1B-CHA-C4A
82	GP	202	PEB	NB-C1B-CHA-C4A
82	GP	202	PEB	C2B-C1B-CHA-C4A
82	GP	203	PEB	C2A-C3A-CAA-CBA
82	GP	203	PEB	C4A-C3A-CAA-CBA
82	GP	203	PEB	NB-C1B-CHA-C4A
82	GP	203	PEB	C2B-C1B-CHA-C4A
82	HP	201	PEB	C2D-C1D-CHC-C4C
82	HP	201	PEB	NB-C1B-CHA-C4A
82	HP	201	PEB	C2B-C1B-CHA-C4A
82	HP	202	PEB	ND-C1D-CHC-C4C
82	HP	202	PEB	C2D-C1D-CHC-C4C
82	HP	202	PEB	NB-C1B-CHA-C4A
82	HP	202	PEB	C2B-C1B-CHA-C4A
82	IP	201	PEB	NB-C1B-CHA-C4A
82	IP	201	PEB	C2B-C1B-CHA-C4A
82	IP	202	PEB	ND-C1D-CHC-C4C
82	IP	202	PEB	C2D-C1D-CHC-C4C
82	IP	202	PEB	C2A-C3A-CAA-CBA
82	IP	202	PEB	C4A-C3A-CAA-CBA
82	IP	202	PEB	NB-C1B-CHA-C4A
82	IP	202	PEB	C2B-C1B-CHA-C4A
82	IP	203	PEB	C3C-C4C-CHC-C1D
82	IP	203	PEB	ND-C1D-CHC-C4C
82	IP	203	PEB	C2D-C1D-CHC-C4C
82	IP	203	PEB	C2A-C3A-CAA-CBA
82	IP	203	PEB	C4A-C3A-CAA-CBA
82	IP	203	PEB	NB-C1B-CHA-C4A
82	IP	203	PEB	C2B-C1B-CHA-C4A
82	JP	201	PEB	C2D-C1D-CHC-C4C
82	JP	201	PEB	NB-C1B-CHA-C4A
82	JP	201	PEB	C2B-C1B-CHA-C4A
82	JP	202	PEB	C2D-C1D-CHC-C4C
82	JP	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	JP	202	PEB	C2B-C1B-CHA-C4A
82	KP	201	PEB	C3C-C4C-CHC-C1D
82	KP	201	PEB	C2D-C1D-CHC-C4C
82	KP	201	PEB	C2A-C3A-CAA-CBA
82	KP	201	PEB	C4A-C3A-CAA-CBA
82	KP	201	PEB	NB-C1B-CHA-C4A
82	KP	201	PEB	C2B-C1B-CHA-C4A
82	KP	202	PEB	NB-C1B-CHA-C4A
82	KP	202	PEB	C2B-C1B-CHA-C4A
82	LP	201	PEB	C2D-C1D-CHC-C4C
82	LP	201	PEB	NB-C1B-CHA-C4A
82	LP	201	PEB	C2B-C1B-CHA-C4A
82	LP	202	PEB	ND-C1D-CHC-C4C
82	LP	202	PEB	C2D-C1D-CHC-C4C
82	LP	202	PEB	NB-C1B-CHA-C4A
82	LP	202	PEB	C2B-C1B-CHA-C4A
82	MP	201	PEB	NB-C1B-CHA-C4A
82	MP	201	PEB	C2B-C1B-CHA-C4A
82	MP	202	PEB	C2A-C3A-CAA-CBA
82	MP	202	PEB	C4A-C3A-CAA-CBA
82	MP	202	PEB	NB-C1B-CHA-C4A
82	MP	202	PEB	C2B-C1B-CHA-C4A
82	MP	203	PEB	C3C-C4C-CHC-C1D
82	MP	203	PEB	ND-C1D-CHC-C4C
82	MP	203	PEB	C2D-C1D-CHC-C4C
82	MP	203	PEB	C2A-C3A-CAA-CBA
82	MP	203	PEB	C4A-C3A-CAA-CBA
82	MP	203	PEB	NB-C1B-CHA-C4A
82	MP	203	PEB	C2B-C1B-CHA-C4A
82	NP	201	PEB	NB-C1B-CHA-C4A
82	NP	201	PEB	C2B-C1B-CHA-C4A
82	NP	202	PEB	ND-C1D-CHC-C4C
82	NP	202	PEB	C2D-C1D-CHC-C4C
82	NP	202	PEB	NB-C1B-CHA-C4A
82	NP	202	PEB	C2B-C1B-CHA-C4A
82	OP	201	PEB	ND-C1D-CHC-C4C
82	OP	201	PEB	C2D-C1D-CHC-C4C
82	OP	201	PEB	NB-C1B-CHA-C4A
82	OP	201	PEB	C2B-C1B-CHA-C4A
82	OP	202	PEB	NB-C1B-CHA-C4A
82	OP	202	PEB	C2B-C1B-CHA-C4A
82	OP	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	OP	203	PEB	C2D-C1D-CHC-C4C
82	OP	203	PEB	C2A-C3A-CAA-CBA
82	OP	203	PEB	C4A-C3A-CAA-CBA
82	OP	203	PEB	NB-C1B-CHA-C4A
82	OP	203	PEB	C2B-C1B-CHA-C4A
82	PP	201	PEB	NB-C1B-CHA-C4A
82	PP	201	PEB	C2B-C1B-CHA-C4A
82	PP	202	PEB	ND-C1D-CHC-C4C
82	PP	202	PEB	C2D-C1D-CHC-C4C
82	PP	202	PEB	NB-C1B-CHA-C4A
82	PP	202	PEB	C2B-C1B-CHA-C4A
82	QP	201	PEB	C2D-C1D-CHC-C4C
82	QP	201	PEB	NB-C1B-CHA-C4A
82	QP	201	PEB	C2B-C1B-CHA-C4A
82	QP	202	PEB	ND-C1D-CHC-C4C
82	QP	202	PEB	C2D-C1D-CHC-C4C
82	QP	202	PEB	C2C-CAC-CBC-CGC
82	QP	202	PEB	C2A-C3A-CAA-CBA
82	QP	202	PEB	C4A-C3A-CAA-CBA
82	QP	202	PEB	NB-C1B-CHA-C4A
82	QP	202	PEB	C2B-C1B-CHA-C4A
82	QP	203	PEB	C3C-C4C-CHC-C1D
82	QP	203	PEB	ND-C1D-CHC-C4C
82	QP	203	PEB	C2D-C1D-CHC-C4C
82	QP	203	PEB	NB-C1B-CHA-C4A
82	QP	203	PEB	C2B-C1B-CHA-C4A
82	RP	201	PEB	ND-C1D-CHC-C4C
82	RP	201	PEB	C2D-C1D-CHC-C4C
82	RP	201	PEB	NB-C1B-CHA-C4A
82	RP	201	PEB	C2B-C1B-CHA-C4A
82	RP	202	PEB	C2D-C1D-CHC-C4C
82	RP	202	PEB	NB-C1B-CHA-C4A
82	RP	202	PEB	C2B-C1B-CHA-C4A
82	SP	201	PEB	ND-C1D-CHC-C4C
82	SP	201	PEB	C2D-C1D-CHC-C4C
82	SP	201	PEB	NB-C1B-CHA-C4A
82	SP	201	PEB	C2B-C1B-CHA-C4A
82	SP	202	PEB	NB-C1B-CHA-C4A
82	SP	202	PEB	C2B-C1B-CHA-C4A
82	SP	203	PEB	C1C-C2C-CAC-CBC
82	SP	203	PEB	C2C-CAC-CBC-CGC
82	SP	203	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	SP	203	PEB	NB-C1B-CHA-C4A
82	SP	203	PEB	C2B-C1B-CHA-C4A
82	TP	201	PEB	ND-C1D-CHC-C4C
82	TP	201	PEB	C2D-C1D-CHC-C4C
82	TP	201	PEB	NB-C1B-CHA-C4A
82	TP	201	PEB	C2B-C1B-CHA-C4A
82	TP	202	PEB	ND-C1D-CHC-C4C
82	TP	202	PEB	C2D-C1D-CHC-C4C
82	TP	202	PEB	NB-C1B-CHA-C4A
82	TP	202	PEB	C2B-C1B-CHA-C4A
82	UP	201	PEB	NB-C1B-CHA-C4A
82	UP	201	PEB	C2B-C1B-CHA-C4A
82	UP	202	PEB	C2A-C3A-CAA-CBA
82	UP	202	PEB	C4A-C3A-CAA-CBA
82	UP	202	PEB	NB-C1B-CHA-C4A
82	UP	202	PEB	C2B-C1B-CHA-C4A
82	UP	203	PEB	C3C-C4C-CHC-C1D
82	UP	203	PEB	ND-C1D-CHC-C4C
82	UP	203	PEB	C2D-C1D-CHC-C4C
82	UP	203	PEB	NB-C1B-CHA-C4A
82	UP	203	PEB	C2B-C1B-CHA-C4A
82	VP	201	PEB	C2D-C1D-CHC-C4C
82	VP	201	PEB	NB-C1B-CHA-C4A
82	VP	201	PEB	C2B-C1B-CHA-C4A
82	VP	202	PEB	ND-C1D-CHC-C4C
82	VP	202	PEB	C2D-C1D-CHC-C4C
82	VP	202	PEB	NB-C1B-CHA-C4A
82	VP	202	PEB	C2B-C1B-CHA-C4A
82	WP	201	PEB	C3C-C4C-CHC-C1D
82	WP	201	PEB	C2D-C1D-CHC-C4C
82	WP	201	PEB	C2A-C3A-CAA-CBA
82	WP	201	PEB	C4A-C3A-CAA-CBA
82	WP	201	PEB	NB-C1B-CHA-C4A
82	WP	201	PEB	C2B-C1B-CHA-C4A
82	WP	202	PEB	NB-C1B-CHA-C4A
82	WP	202	PEB	C2B-C1B-CHA-C4A
82	XP	201	PEB	NB-C1B-CHA-C4A
82	XP	201	PEB	C2B-C1B-CHA-C4A
82	XP	202	PEB	ND-C1D-CHC-C4C
82	XP	202	PEB	C2D-C1D-CHC-C4C
82	XP	202	PEB	NB-C1B-CHA-C4A
82	XP	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	YP	501	PEB	NB-C1B-CHA-C4A
82	YP	501	PEB	C2B-C1B-CHA-C4A
82	YP	502	PEB	C2D-C1D-CHC-C4C
82	YP	502	PEB	C2A-C3A-CAA-CBA
82	YP	502	PEB	C4A-C3A-CAA-CBA
82	YP	502	PEB	NB-C1B-CHA-C4A
82	YP	502	PEB	C2B-C1B-CHA-C4A
82	YP	503	PEB	NB-C1B-CHA-C4A
82	YP	503	PEB	C2B-C1B-CHA-C4A
82	AQ	301	PEB	C2C-CAC-CBC-CGC
82	AQ	301	PEB	NB-C1B-CHA-C4A
82	AQ	301	PEB	C2B-C1B-CHA-C4A
82	AQ	303	PEB	ND-C1D-CHC-C4C
82	AQ	303	PEB	C2D-C1D-CHC-C4C
82	AQ	303	PEB	C2A-C3A-CAA-CBA
82	AQ	303	PEB	NB-C1B-CHA-C4A
82	AQ	303	PEB	C2B-C1B-CHA-C4A
82	AQ	304	PEB	NC-C4C-CHC-C1D
82	AQ	304	PEB	C3C-C4C-CHC-C1D
82	AQ	304	PEB	NC-C1C-CHB-C4B
82	AQ	304	PEB	C2C-C1C-CHB-C4B
82	AQ	304	PEB	NB-C1B-CHA-C4A
82	AQ	304	PEB	C2B-C1B-CHA-C4A
82	BQ	201	PEB	ND-C1D-CHC-C4C
82	BQ	201	PEB	C2D-C1D-CHC-C4C
82	BQ	201	PEB	NB-C1B-CHA-C4A
82	BQ	201	PEB	C2B-C1B-CHA-C4A
82	BQ	202	PEB	NC-C1C-CHB-C4B
82	BQ	202	PEB	C2C-C1C-CHB-C4B
82	BQ	202	PEB	C2A-C3A-CAA-CBA
82	BQ	202	PEB	C4A-C3A-CAA-CBA
82	BQ	202	PEB	NB-C1B-CHA-C4A
82	BQ	202	PEB	C2B-C1B-CHA-C4A
82	BQ	203	PEB	C2D-C3D-CAD-CBD
82	BQ	203	PEB	C4D-C3D-CAD-CBD
82	BQ	203	PEB	C4A-C3A-CAA-CBA
82	BQ	203	PEB	NB-C1B-CHA-C4A
82	BQ	203	PEB	C2B-C1B-CHA-C4A
82	CQ	201	PEB	ND-C1D-CHC-C4C
82	CQ	201	PEB	C2D-C1D-CHC-C4C
82	CQ	201	PEB	NB-C1B-CHA-C4A
82	CQ	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	CQ	202	PEB	NB-C1B-CHA-C4A
82	CQ	202	PEB	C2B-C1B-CHA-C4A
82	DQ	201	PEB	C2D-C3D-CAD-CBD
82	DQ	201	PEB	C4D-C3D-CAD-CBD
82	DQ	201	PEB	C4A-C3A-CAA-CBA
82	DQ	201	PEB	NB-C1B-CHA-C4A
82	DQ	201	PEB	C2B-C1B-CHA-C4A
82	DQ	202	PEB	ND-C1D-CHC-C4C
82	DQ	202	PEB	C2D-C1D-CHC-C4C
82	DQ	202	PEB	C3B-CAB-CBB-CGB
82	DQ	203	PEB	NC-C1C-CHB-C4B
82	DQ	203	PEB	C2C-C1C-CHB-C4B
82	DQ	203	PEB	C4A-C3A-CAA-CBA
82	DQ	203	PEB	NB-C1B-CHA-C4A
82	DQ	203	PEB	C2B-C1B-CHA-C4A
82	EQ	201	PEB	ND-C1D-CHC-C4C
82	EQ	201	PEB	C2D-C1D-CHC-C4C
82	EQ	201	PEB	C2D-C3D-CAD-CBD
82	EQ	201	PEB	C4D-C3D-CAD-CBD
82	EQ	201	PEB	NB-C1B-CHA-C4A
82	EQ	201	PEB	C2B-C1B-CHA-C4A
82	EQ	202	PEB	NB-C1B-CHA-C4A
82	EQ	202	PEB	C2B-C1B-CHA-C4A
82	FQ	201	PEB	ND-C1D-CHC-C4C
82	FQ	201	PEB	C2D-C1D-CHC-C4C
82	FQ	201	PEB	C2D-C3D-CAD-CBD
82	FQ	201	PEB	C4D-C3D-CAD-CBD
82	FQ	201	PEB	NB-C1B-CHA-C4A
82	FQ	201	PEB	C2B-C1B-CHA-C4A
82	FQ	202	PEB	NC-C1C-CHB-C4B
82	FQ	202	PEB	C2C-C1C-CHB-C4B
82	FQ	202	PEB	C2A-C3A-CAA-CBA
82	FQ	202	PEB	C4A-C3A-CAA-CBA
82	FQ	202	PEB	NB-C1B-CHA-C4A
82	FQ	202	PEB	C2B-C1B-CHA-C4A
82	FQ	203	PEB	C4A-C3A-CAA-CBA
82	FQ	203	PEB	NB-C1B-CHA-C4A
82	FQ	203	PEB	C2B-C1B-CHA-C4A
82	GQ	201	PEB	NB-C1B-CHA-C4A
82	GQ	201	PEB	C2B-C1B-CHA-C4A
82	GQ	202	PEB	C2A-C3A-CAA-CBA
82	GQ	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	GQ	202	PEB	NB-C1B-CHA-C4A
82	GQ	202	PEB	C2B-C1B-CHA-C4A
82	HQ	201	PEB	C4A-C3A-CAA-CBA
82	HQ	201	PEB	NB-C1B-CHA-C4A
82	HQ	201	PEB	C2B-C1B-CHA-C4A
82	HQ	202	PEB	ND-C1D-CHC-C4C
82	HQ	202	PEB	C2D-C1D-CHC-C4C
82	HQ	202	PEB	NB-C1B-CHA-C4A
82	HQ	203	PEB	ND-C1D-CHC-C4C
82	HQ	203	PEB	C2D-C1D-CHC-C4C
82	HQ	203	PEB	NC-C1C-CHB-C4B
82	HQ	203	PEB	C2C-C1C-CHB-C4B
82	HQ	203	PEB	C4A-C3A-CAA-CBA
82	HQ	203	PEB	NB-C1B-CHA-C4A
82	HQ	203	PEB	C2B-C1B-CHA-C4A
82	IQ	201	PEB	C2D-C1D-CHC-C4C
82	IQ	201	PEB	C1C-C2C-CAC-CBC
82	IQ	201	PEB	NB-C1B-CHA-C4A
82	IQ	201	PEB	C2B-C1B-CHA-C4A
82	IQ	202	PEB	NB-C1B-CHA-C4A
82	IQ	202	PEB	C2B-C1B-CHA-C4A
82	JQ	201	PEB	ND-C1D-CHC-C4C
82	JQ	201	PEB	C2D-C1D-CHC-C4C
82	JQ	201	PEB	NB-C1B-CHA-C4A
82	JQ	201	PEB	C2B-C1B-CHA-C4A
82	JQ	202	PEB	ND-C1D-CHC-C4C
82	JQ	202	PEB	C2D-C1D-CHC-C4C
82	JQ	202	PEB	NC-C1C-CHB-C4B
82	JQ	202	PEB	C4A-C3A-CAA-CBA
82	JQ	202	PEB	NB-C1B-CHA-C4A
82	JQ	202	PEB	C2B-C1B-CHA-C4A
82	JQ	203	PEB	ND-C1D-CHC-C4C
82	JQ	203	PEB	C2D-C1D-CHC-C4C
82	JQ	203	PEB	C2D-C3D-CAD-CBD
82	JQ	203	PEB	C4D-C3D-CAD-CBD
82	JQ	203	PEB	C4A-C3A-CAA-CBA
82	JQ	203	PEB	NB-C1B-CHA-C4A
82	JQ	203	PEB	C2B-C1B-CHA-C4A
82	KQ	201	PEB	ND-C1D-CHC-C4C
82	KQ	201	PEB	C2D-C1D-CHC-C4C
82	KQ	201	PEB	C2A-C3A-CAA-CBA
82	KQ	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	KQ	201	PEB	NB-C1B-CHA-C4A
82	KQ	201	PEB	C2B-C1B-CHA-C4A
82	KQ	202	PEB	ND-C1D-CHC-C4C
82	KQ	202	PEB	C2D-C1D-CHC-C4C
82	KQ	202	PEB	C2D-C3D-CAD-CBD
82	KQ	202	PEB	C4D-C3D-CAD-CBD
82	KQ	202	PEB	NB-C1B-CHA-C4A
82	KQ	202	PEB	C2B-C1B-CHA-C4A
82	LQ	201	PEB	C4A-C3A-CAA-CBA
82	LQ	201	PEB	NB-C1B-CHA-C4A
82	LQ	201	PEB	C2B-C1B-CHA-C4A
82	LQ	202	PEB	ND-C1D-CHC-C4C
82	LQ	202	PEB	C2D-C1D-CHC-C4C
82	LQ	202	PEB	NB-C1B-CHA-C4A
82	LQ	202	PEB	C2B-C1B-CHA-C4A
82	LQ	203	PEB	C2A-C3A-CAA-CBA
82	LQ	203	PEB	C4A-C3A-CAA-CBA
82	LQ	203	PEB	NB-C1B-CHA-C4A
82	LQ	203	PEB	C2B-C1B-CHA-C4A
82	MQ	201	PEB	C1C-C2C-CAC-CBC
82	MQ	201	PEB	NB-C1B-CHA-C4A
82	MQ	201	PEB	C2B-C1B-CHA-C4A
82	MQ	202	PEB	NB-C1B-CHA-C4A
82	MQ	202	PEB	C2B-C1B-CHA-C4A
82	NQ	202	PEB	ND-C1D-CHC-C4C
82	NQ	202	PEB	C2D-C1D-CHC-C4C
82	NQ	202	PEB	C2A-C3A-CAA-CBA
82	NQ	202	PEB	C4A-C3A-CAA-CBA
82	NQ	202	PEB	NB-C1B-CHA-C4A
82	NQ	202	PEB	C2B-C1B-CHA-C4A
82	NQ	203	PEB	ND-C1D-CHC-C4C
82	NQ	203	PEB	C2D-C1D-CHC-C4C
82	NQ	203	PEB	NC-C1C-CHB-C4B
82	NQ	203	PEB	C2C-C1C-CHB-C4B
82	NQ	203	PEB	C4A-C3A-CAA-CBA
82	NQ	203	PEB	NB-C1B-CHA-C4A
82	NQ	203	PEB	C2B-C1B-CHA-C4A
82	NQ	204	PEB	C4A-C3A-CAA-CBA
82	NQ	204	PEB	NB-C1B-CHA-C4A
82	NQ	204	PEB	C2B-C1B-CHA-C4A
82	OQ	201	PEB	ND-C1D-CHC-C4C
82	OQ	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	OQ	201	PEB	NB-C1B-CHA-C4A
82	OQ	201	PEB	C2B-C1B-CHA-C4A
82	OQ	202	PEB	ND-C1D-CHC-C4C
82	OQ	202	PEB	C2D-C1D-CHC-C4C
82	OQ	202	PEB	C2D-C3D-CAD-CBD
82	OQ	202	PEB	C4D-C3D-CAD-CBD
82	OQ	202	PEB	NB-C1B-CHA-C4A
82	OQ	202	PEB	C2B-C1B-CHA-C4A
82	PQ	201	PEB	C2A-C3A-CAA-CBA
82	PQ	201	PEB	C4A-C3A-CAA-CBA
82	PQ	201	PEB	NB-C1B-CHA-C4A
82	PQ	201	PEB	C2B-C1B-CHA-C4A
82	PQ	202	PEB	ND-C1D-CHC-C4C
82	PQ	202	PEB	C2D-C1D-CHC-C4C
82	PQ	202	PEB	NB-C1B-CHA-C4A
82	PQ	202	PEB	C2B-C1B-CHA-C4A
82	PQ	203	PEB	ND-C1D-CHC-C4C
82	PQ	203	PEB	C2D-C1D-CHC-C4C
82	PQ	203	PEB	NC-C1C-CHB-C4B
82	PQ	203	PEB	C2C-C1C-CHB-C4B
82	PQ	203	PEB	C2A-C3A-CAA-CBA
82	PQ	203	PEB	C4A-C3A-CAA-CBA
82	PQ	203	PEB	NB-C1B-CHA-C4A
82	PQ	203	PEB	C2B-C1B-CHA-C4A
82	QQ	201	PEB	NB-C1B-CHA-C4A
82	QQ	201	PEB	C2B-C1B-CHA-C4A
82	QQ	202	PEB	ND-C1D-CHC-C4C
82	QQ	202	PEB	C2D-C1D-CHC-C4C
82	QQ	202	PEB	NB-C1B-CHA-C4A
82	QQ	202	PEB	C2B-C1B-CHA-C4A
82	RQ	201	PEB	ND-C1D-CHC-C4C
82	RQ	201	PEB	C2D-C1D-CHC-C4C
82	RQ	201	PEB	NB-C1B-CHA-C4A
82	RQ	201	PEB	C2B-C1B-CHA-C4A
82	RQ	202	PEB	C4A-C3A-CAA-CBA
82	RQ	202	PEB	NB-C1B-CHA-C4A
82	RQ	202	PEB	C2B-C1B-CHA-C4A
82	RQ	203	PEB	ND-C1D-CHC-C4C
82	RQ	203	PEB	C2D-C1D-CHC-C4C
82	RQ	203	PEB	C2A-C3A-CAA-CBA
82	RQ	203	PEB	C4A-C3A-CAA-CBA
82	RQ	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	RQ	203	PEB	C2B-C1B-CHA-C4A
82	SQ	201	PEB	NB-C1B-CHA-C4A
82	SQ	201	PEB	C2B-C1B-CHA-C4A
82	SQ	202	PEB	NB-C1B-CHA-C4A
82	SQ	202	PEB	C2B-C1B-CHA-C4A
82	TQ	201	PEB	C2D-C1D-CHC-C4C
82	TQ	201	PEB	C2D-C3D-CAD-CBD
82	TQ	201	PEB	C4D-C3D-CAD-CBD
82	TQ	201	PEB	C4A-C3A-CAA-CBA
82	TQ	201	PEB	NB-C1B-CHA-C4A
82	TQ	201	PEB	C2B-C1B-CHA-C4A
82	TQ	202	PEB	ND-C1D-CHC-C4C
82	TQ	202	PEB	C2D-C1D-CHC-C4C
82	TQ	202	PEB	C2A-C3A-CAA-CBA
82	TQ	202	PEB	C4A-C3A-CAA-CBA
82	TQ	202	PEB	NB-C1B-CHA-C4A
82	TQ	202	PEB	C2B-C1B-CHA-C4A
82	TQ	202	PEB	C3B-CAB-CBB-CGB
82	TQ	203	PEB	ND-C1D-CHC-C4C
82	TQ	203	PEB	C2D-C1D-CHC-C4C
82	TQ	203	PEB	NC-C1C-CHB-C4B
82	TQ	203	PEB	C2C-C1C-CHB-C4B
82	TQ	203	PEB	C2A-C3A-CAA-CBA
82	TQ	203	PEB	C4A-C3A-CAA-CBA
82	TQ	203	PEB	NB-C1B-CHA-C4A
82	TQ	203	PEB	C2B-C1B-CHA-C4A
82	UQ	201	PEB	ND-C1D-CHC-C4C
82	UQ	201	PEB	C2D-C1D-CHC-C4C
82	UQ	201	PEB	NB-C1B-CHA-C4A
82	UQ	201	PEB	C2B-C1B-CHA-C4A
82	UQ	202	PEB	NB-C1B-CHA-C4A
82	UQ	202	PEB	C2B-C1B-CHA-C4A
82	VQ	201	PEB	ND-C1D-CHC-C4C
82	VQ	201	PEB	C2D-C1D-CHC-C4C
82	VQ	201	PEB	NC-C1C-CHB-C4B
82	VQ	201	PEB	C2C-C1C-CHB-C4B
82	VQ	201	PEB	C2D-C3D-CAD-CBD
82	VQ	201	PEB	C4D-C3D-CAD-CBD
82	VQ	201	PEB	NB-C1B-CHA-C4A
82	VQ	201	PEB	C2B-C1B-CHA-C4A
82	VQ	202	PEB	ND-C1D-CHC-C4C
82	VQ	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	VQ	202	PEB	NC-C1C-CHB-C4B
82	VQ	202	PEB	C2C-C1C-CHB-C4B
82	VQ	202	PEB	C4A-C3A-CAA-CBA
82	VQ	202	PEB	NB-C1B-CHA-C4A
82	VQ	202	PEB	C2B-C1B-CHA-C4A
82	VQ	203	PEB	ND-C1D-CHC-C4C
82	VQ	203	PEB	C4D-C3D-CAD-CBD
82	VQ	203	PEB	C4A-C3A-CAA-CBA
82	VQ	203	PEB	NB-C1B-CHA-C4A
82	VQ	203	PEB	C2B-C1B-CHA-C4A
82	WQ	201	PEB	NB-C1B-CHA-C4A
82	WQ	201	PEB	C2B-C1B-CHA-C4A
82	WQ	202	PEB	NB-C1B-CHA-C4A
82	WQ	202	PEB	C2B-C1B-CHA-C4A
82	XQ	201	PEB	C4A-C3A-CAA-CBA
82	XQ	201	PEB	NB-C1B-CHA-C4A
82	XQ	201	PEB	C2B-C1B-CHA-C4A
82	XQ	202	PEB	ND-C1D-CHC-C4C
82	XQ	202	PEB	C2D-C1D-CHC-C4C
82	XQ	202	PEB	NB-C1B-CHA-C4A
82	XQ	202	PEB	C2B-C1B-CHA-C4A
82	XQ	203	PEB	NC-C1C-CHB-C4B
82	XQ	203	PEB	C2C-C1C-CHB-C4B
82	XQ	203	PEB	C4A-C3A-CAA-CBA
82	XQ	203	PEB	NB-C1B-CHA-C4A
82	XQ	203	PEB	C2B-C1B-CHA-C4A
82	YQ	201	PEB	NB-C1B-CHA-C4A
82	YQ	201	PEB	C2B-C1B-CHA-C4A
82	YQ	202	PEB	NB-C1B-CHA-C4A
82	YQ	202	PEB	C2B-C1B-CHA-C4A
82	L1	1002	PEB	C2A-C3A-CAA-CBA
82	L1	1002	PEB	C4A-C3A-CAA-CBA
82	L1	1002	PEB	NB-C1B-CHA-C4A
82	L1	1002	PEB	C2B-C1B-CHA-C4A
82	L1	1002	PEB	C3B-CAB-CBB-CGB
82	N1	1002	PEB	C2A-C3A-CAA-CBA
82	N1	1002	PEB	C4A-C3A-CAA-CBA
82	N1	1002	PEB	NB-C1B-CHA-C4A
82	N1	1002	PEB	C2B-C1B-CHA-C4A
82	O1	201	PEB	ND-C1D-CHC-C4C
82	O1	201	PEB	C2D-C1D-CHC-C4C
82	O1	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	O1	201	PEB	C4A-C3A-CAA-CBA
82	O1	201	PEB	NB-C1B-CHA-C4A
82	O1	201	PEB	C2B-C1B-CHA-C4A
82	O1	202	PEB	NB-C1B-CHA-C4A
82	O1	202	PEB	C2B-C1B-CHA-C4A
82	O1	203	PEB	C2A-C3A-CAA-CBA
82	O1	203	PEB	NB-C1B-CHA-C4A
82	O1	203	PEB	C2B-C1B-CHA-C4A
82	P1	201	PEB	NB-C1B-CHA-C4A
82	P1	201	PEB	C2B-C1B-CHA-C4A
82	P1	202	PEB	NB-C1B-CHA-C4A
82	P1	202	PEB	C2B-C1B-CHA-C4A
82	Q1	201	PEB	NB-C1B-CHA-C4A
82	Q1	201	PEB	C2B-C1B-CHA-C4A
82	Q1	202	PEB	C2D-C1D-CHC-C4C
82	Q1	202	PEB	C2A-C3A-CAA-CBA
82	Q1	202	PEB	C4A-C3A-CAA-CBA
82	Q1	203	PEB	NB-C1B-CHA-C4A
82	Q1	203	PEB	C2B-C1B-CHA-C4A
82	Q1	203	PEB	C3B-CAB-CBB-CGB
82	R1	201	PEB	C2A-C3A-CAA-CBA
82	R1	201	PEB	C4A-C3A-CAA-CBA
82	R1	201	PEB	NB-C1B-CHA-C4A
82	R1	201	PEB	C2B-C1B-CHA-C4A
82	R1	202	PEB	ND-C1D-CHC-C4C
82	R1	202	PEB	C2D-C1D-CHC-C4C
82	R1	202	PEB	NB-C1B-CHA-C4A
82	R1	202	PEB	C2B-C1B-CHA-C4A
82	S1	201	PEB	NB-C1B-CHA-C4A
82	S1	201	PEB	C2B-C1B-CHA-C4A
82	S1	202	PEB	C2C-CAC-CBC-CGC
82	S1	202	PEB	NB-C1B-CHA-C4A
82	S1	202	PEB	C2B-C1B-CHA-C4A
82	T1	201	PEB	ND-C1D-CHC-C4C
82	T1	201	PEB	C2D-C1D-CHC-C4C
82	T1	201	PEB	NB-C1B-CHA-C4A
82	T1	201	PEB	C2B-C1B-CHA-C4A
82	T1	202	PEB	ND-C1D-CHC-C4C
82	T1	202	PEB	C2D-C1D-CHC-C4C
82	T1	202	PEB	C4D-C3D-CAD-CBD
82	T1	202	PEB	NB-C1B-CHA-C4A
82	T1	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	U1	201	PEB	C2A-C3A-CAA-CBA
82	U1	201	PEB	C4A-C3A-CAA-CBA
82	U1	201	PEB	NB-C1B-CHA-C4A
82	U1	201	PEB	C2B-C1B-CHA-C4A
82	U1	202	PEB	C4A-C3A-CAA-CBA
82	U1	202	PEB	NB-C1B-CHA-C4A
82	U1	202	PEB	C2B-C1B-CHA-C4A
82	U1	203	PEB	C2A-C3A-CAA-CBA
82	U1	203	PEB	NB-C1B-CHA-C4A
82	U1	203	PEB	C2B-C1B-CHA-C4A
82	A1	301	PEB	NB-C1B-CHA-C4A
82	A1	301	PEB	C2B-C1B-CHA-C4A
82	A1	302	PEB	C2D-C1D-CHC-C4C
82	A1	302	PEB	C4A-C3A-CAA-CBA
82	A1	302	PEB	NB-C1B-CHA-C4A
82	A1	302	PEB	C2B-C1B-CHA-C4A
82	A1	305	PEB	ND-C1D-CHC-C4C
82	A1	305	PEB	C2D-C1D-CHC-C4C
82	A1	305	PEB	NC-C1C-CHB-C4B
82	A1	305	PEB	C2C-C1C-CHB-C4B
82	A1	305	PEB	C2A-C3A-CAA-CBA
82	A1	305	PEB	C4A-C3A-CAA-CBA
82	A1	305	PEB	NB-C1B-CHA-C4A
82	A1	305	PEB	C2B-C1B-CHA-C4A
82	D1	1002	PEB	ND-C1D-CHC-C4C
82	D1	1002	PEB	C2D-C1D-CHC-C4C
82	D1	1002	PEB	C2A-C3A-CAA-CBA
82	D1	1002	PEB	C4A-C3A-CAA-CBA
82	D1	1002	PEB	NB-C1B-CHA-C4A
82	D1	1002	PEB	C2B-C1B-CHA-C4A
82	F1	1002	PEB	C2C-CAC-CBC-CGC
82	F1	1002	PEB	C4A-C3A-CAA-CBA
82	F1	1002	PEB	NB-C1B-CHA-C4A
82	F1	1002	PEB	C2B-C1B-CHA-C4A
82	H1	1002	PEB	C4A-C3A-CAA-CBA
82	H1	1002	PEB	NB-C1B-CHA-C4A
82	H1	1002	PEB	C2B-C1B-CHA-C4A
82	J1	1002	PEB	NB-C1B-CHA-C4A
82	J1	1002	PEB	C2B-C1B-CHA-C4A
82	V1	201	PEB	NB-C1B-CHA-C4A
82	V1	202	PEB	NB-C1B-CHA-C4A
82	V1	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	V1	203	PEB	ND-C1D-CHC-C4C
82	V1	203	PEB	C2D-C1D-CHC-C4C
82	V1	203	PEB	NB-C1B-CHA-C4A
82	V1	203	PEB	C2B-C1B-CHA-C4A
82	W1	201	PEB	ND-C1D-CHC-C4C
82	W1	201	PEB	C2D-C1D-CHC-C4C
82	W1	201	PEB	C4A-C3A-CAA-CBA
82	W1	201	PEB	NB-C1B-CHA-C4A
82	W1	201	PEB	C2B-C1B-CHA-C4A
82	W1	202	PEB	NB-C1B-CHA-C4A
82	W1	202	PEB	C2B-C1B-CHA-C4A
82	W1	203	PEB	C2A-C3A-CAA-CBA
82	W1	203	PEB	NB-C1B-CHA-C4A
82	W1	203	PEB	C2B-C1B-CHA-C4A
82	Y1	201	PEB	C2A-C3A-CAA-CBA
82	Y1	201	PEB	C4A-C3A-CAA-CBA
82	Y1	201	PEB	NB-C1B-CHA-C4A
82	Y1	201	PEB	C2B-C1B-CHA-C4A
82	Y1	202	PEB	NB-C1B-CHA-C4A
82	Y1	202	PEB	C2B-C1B-CHA-C4A
82	Z1	201	PEB	ND-C1D-CHC-C4C
82	Z1	201	PEB	C2D-C1D-CHC-C4C
82	Z1	201	PEB	C2A-C3A-CAA-CBA
82	Z1	201	PEB	C4A-C3A-CAA-CBA
82	Z1	201	PEB	NB-C1B-CHA-C4A
82	Z1	201	PEB	C2B-C1B-CHA-C4A
82	Z1	202	PEB	ND-C1D-CHC-C4C
82	Z1	202	PEB	C2D-C1D-CHC-C4C
82	Z1	202	PEB	C2A-C3A-CAA-CBA
82	Z1	202	PEB	C4A-C3A-CAA-CBA
82	Z1	202	PEB	NB-C1B-CHA-C4A
82	Z1	202	PEB	C2B-C1B-CHA-C4A
82	Z1	203	PEB	NB-C1B-CHA-C4A
82	Z1	203	PEB	C2B-C1B-CHA-C4A
82	f1	201	PEB	ND-C1D-CHC-C4C
82	f1	201	PEB	C2D-C1D-CHC-C4C
82	f1	201	PEB	NB-C1B-CHA-C4A
82	f1	201	PEB	C2B-C1B-CHA-C4A
82	f1	202	PEB	C2A-C3A-CAA-CBA
82	f1	202	PEB	NB-C1B-CHA-C4A
82	f1	202	PEB	C2B-C1B-CHA-C4A
82	f1	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	f1	203	PEB	C2D-C1D-CHC-C4C
82	f1	203	PEB	NC-C1C-CHB-C4B
82	f1	203	PEB	C2A-C3A-CAA-CBA
82	f1	203	PEB	NB-C1B-CHA-C4A
82	f1	203	PEB	C2B-C1B-CHA-C4A
82	g1	201	PEB	NB-C1B-CHA-C4A
82	g1	201	PEB	C2B-C1B-CHA-C4A
82	g1	202	PEB	NB-C1B-CHA-C4A
82	g1	202	PEB	C2B-C1B-CHA-C4A
82	h1	201	PEB	NB-C1B-CHA-C4A
82	h1	201	PEB	C2B-C1B-CHA-C4A
82	h1	202	PEB	ND-C1D-CHC-C4C
82	h1	202	PEB	C2A-C3A-CAA-CBA
82	h1	202	PEB	C4A-C3A-CAA-CBA
82	h1	202	PEB	NB-C1B-CHA-C4A
82	h1	202	PEB	C2B-C1B-CHA-C4A
82	h1	202	PEB	C3B-CAB-CBB-CGB
82	h1	203	PEB	C2C-CAC-CBC-CGC
82	h1	203	PEB	NA-C4A-CHA-C1B
82	h1	203	PEB	C3A-C4A-CHA-C1B
82	h1	203	PEB	NB-C1B-CHA-C4A
82	h1	203	PEB	C2B-C1B-CHA-C4A
82	i1	201	PEB	NB-C1B-CHA-C4A
82	i1	201	PEB	C2B-C1B-CHA-C4A
82	i1	202	PEB	ND-C1D-CHC-C4C
82	i1	202	PEB	C2D-C1D-CHC-C4C
82	i1	202	PEB	NC-C1C-CHB-C4B
82	i1	202	PEB	C2C-C1C-CHB-C4B
82	i1	202	PEB	NB-C1B-CHA-C4A
82	i1	202	PEB	C2B-C1B-CHA-C4A
82	j1	201	PEB	ND-C1D-CHC-C4C
82	j1	201	PEB	C2D-C1D-CHC-C4C
82	j1	201	PEB	NB-C1B-CHA-C4A
82	j1	201	PEB	C2B-C1B-CHA-C4A
82	j1	202	PEB	NB-C1B-CHA-C4A
82	j1	202	PEB	C2B-C1B-CHA-C4A
82	j1	203	PEB	C2A-C3A-CAA-CBA
82	j1	203	PEB	NB-C1B-CHA-C4A
82	j1	203	PEB	C2B-C1B-CHA-C4A
82	k1	201	PEB	ND-C1D-CHC-C4C
82	k1	201	PEB	C2D-C1D-CHC-C4C
82	k1	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	k1	201	PEB	NB-C1B-CHA-C4A
82	k1	201	PEB	C2B-C1B-CHA-C4A
82	k1	202	PEB	NB-C1B-CHA-C4A
82	k1	202	PEB	C2B-C1B-CHA-C4A
82	l1	201	PEB	NB-C1B-CHA-C4A
82	l1	201	PEB	C2B-C1B-CHA-C4A
82	l1	202	PEB	ND-C1D-CHC-C4C
82	l1	202	PEB	C2D-C1D-CHC-C4C
82	l1	202	PEB	C2D-C3D-CAD-CBD
82	l1	202	PEB	C4D-C3D-CAD-CBD
82	l1	202	PEB	NB-C1B-CHA-C4A
82	l1	202	PEB	C2B-C1B-CHA-C4A
82	l1	203	PEB	ND-C1D-CHC-C4C
82	l1	203	PEB	C2D-C1D-CHC-C4C
82	l1	203	PEB	C2A-C3A-CAA-CBA
82	l1	203	PEB	NB-C1B-CHA-C4A
82	l1	203	PEB	C2B-C1B-CHA-C4A
82	m1	201	PEB	ND-C1D-CHC-C4C
82	m1	201	PEB	C2D-C1D-CHC-C4C
82	m1	201	PEB	NB-C1B-CHA-C4A
82	m1	201	PEB	C2B-C1B-CHA-C4A
82	m1	202	PEB	C2D-C1D-CHC-C4C
82	m1	202	PEB	NB-C1B-CHA-C4A
82	m1	202	PEB	C2B-C1B-CHA-C4A
82	m1	202	PEB	C3B-CAB-CBB-CGB
82	a1	201	PEB	NB-C1B-CHA-C4A
82	a1	201	PEB	C2B-C1B-CHA-C4A
82	a1	202	PEB	ND-C1D-CHC-C4C
82	a1	202	PEB	C2D-C1D-CHC-C4C
82	a1	202	PEB	C2C-CAC-CBC-CGC
82	a1	202	PEB	NB-C1B-CHA-C4A
82	a1	202	PEB	C2B-C1B-CHA-C4A
82	b1	201	PEB	ND-C1D-CHC-C4C
82	b1	201	PEB	C2D-C1D-CHC-C4C
82	b1	201	PEB	NB-C1B-CHA-C4A
82	b1	201	PEB	C2B-C1B-CHA-C4A
82	b1	202	PEB	NB-C1B-CHA-C4A
82	b1	202	PEB	C2B-C1B-CHA-C4A
82	b1	203	PEB	C4A-C3A-CAA-CBA
82	b1	203	PEB	NB-C1B-CHA-C4A
82	b1	203	PEB	C2B-C1B-CHA-C4A
82	c1	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	c1	201	PEB	C4A-C3A-CAA-CBA
82	c1	201	PEB	NB-C1B-CHA-C4A
82	c1	201	PEB	C2B-C1B-CHA-C4A
82	c1	202	PEB	C4A-C3A-CAA-CBA
82	c1	202	PEB	NB-C1B-CHA-C4A
82	d1	201	PEB	NB-C1B-CHA-C4A
82	d1	201	PEB	C2B-C1B-CHA-C4A
82	d1	202	PEB	ND-C1D-CHC-C4C
82	d1	202	PEB	C2D-C1D-CHC-C4C
82	d1	202	PEB	C4A-C3A-CAA-CBA
82	d1	202	PEB	NB-C1B-CHA-C4A
82	d1	202	PEB	C2B-C1B-CHA-C4A
82	d1	203	PEB	C2A-C3A-CAA-CBA
82	d1	203	PEB	NB-C1B-CHA-C4A
82	d1	203	PEB	C2B-C1B-CHA-C4A
82	e1	201	PEB	ND-C1D-CHC-C4C
82	e1	201	PEB	C2D-C1D-CHC-C4C
82	e1	201	PEB	NB-C1B-CHA-C4A
82	e1	201	PEB	C2B-C1B-CHA-C4A
82	e1	202	PEB	ND-C1D-CHC-C4C
82	e1	202	PEB	C2D-C1D-CHC-C4C
82	e1	202	PEB	NB-C1B-CHA-C4A
82	e1	202	PEB	C2B-C1B-CHA-C4A
82	F4	1002	PEB	C2A-C3A-CAA-CBA
82	F4	1002	PEB	C4A-C3A-CAA-CBA
82	F4	1002	PEB	NB-C1B-CHA-C4A
82	F4	1002	PEB	C2B-C1B-CHA-C4A
82	F4	1002	PEB	C3B-CAB-CBB-CGB
82	H4	1002	PEB	NB-C1B-CHA-C4A
82	H4	1002	PEB	C2B-C1B-CHA-C4A
82	J4	1002	PEB	ND-C1D-CHC-C4C
82	J4	1002	PEB	C2D-C1D-CHC-C4C
82	J4	1002	PEB	C4A-C3A-CAA-CBA
82	J4	1002	PEB	NB-C1B-CHA-C4A
82	J4	1002	PEB	C2B-C1B-CHA-C4A
82	L4	1002	PEB	ND-C1D-CHC-C4C
82	L4	1002	PEB	C2D-C1D-CHC-C4C
82	L4	1002	PEB	C2C-CAC-CBC-CGC
82	L4	1002	PEB	NB-C1B-CHA-C4A
82	L4	1002	PEB	C2B-C1B-CHA-C4A
82	N4	1002	PEB	C4A-C3A-CAA-CBA
82	N4	1002	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	N4	1002	PEB	C2B-C1B-CHA-C4A
82	O4	201	PEB	C2A-C3A-CAA-CBA
82	O4	201	PEB	C4A-C3A-CAA-CBA
82	O4	201	PEB	NB-C1B-CHA-C4A
82	O4	201	PEB	C2B-C1B-CHA-C4A
82	O4	202	PEB	ND-C1D-CHC-C4C
82	O4	202	PEB	C2D-C1D-CHC-C4C
82	O4	202	PEB	NB-C1B-CHA-C4A
82	O4	202	PEB	C2B-C1B-CHA-C4A
82	A4	301	PEB	NB-C1B-CHA-C4A
82	A4	301	PEB	C2B-C1B-CHA-C4A
82	A4	304	PEB	C2A-C3A-CAA-CBA
82	A4	304	PEB	C4A-C3A-CAA-CBA
82	A4	304	PEB	NB-C1B-CHA-C4A
82	A4	304	PEB	C2B-C1B-CHA-C4A
82	A4	305	PEB	C4A-C3A-CAA-CBA
82	A4	305	PEB	NB-C1B-CHA-C4A
82	A4	305	PEB	C2B-C1B-CHA-C4A
82	D4	1002	PEB	C4A-C3A-CAA-CBA
82	D4	1002	PEB	NB-C1B-CHA-C4A
82	D4	1002	PEB	C2B-C1B-CHA-C4A
82	P4	201	PEB	NB-C1B-CHA-C4A
82	P4	201	PEB	C2B-C1B-CHA-C4A
82	P4	202	PEB	NB-C1B-CHA-C4A
82	P4	202	PEB	C2B-C1B-CHA-C4A
82	Q4	201	PEB	C4A-C3A-CAA-CBA
82	Q4	201	PEB	NB-C1B-CHA-C4A
82	Q4	201	PEB	C2B-C1B-CHA-C4A
82	Q4	202	PEB	C2D-C1D-CHC-C4C
82	Q4	202	PEB	C4A-C3A-CAA-CBA
82	Q4	202	PEB	NB-C1B-CHA-C4A
82	Q4	202	PEB	C2B-C1B-CHA-C4A
82	R4	201	PEB	NB-C1B-CHA-C4A
82	R4	201	PEB	C2B-C1B-CHA-C4A
82	R4	202	PEB	C2A-C3A-CAA-CBA
82	R4	202	PEB	NB-C1B-CHA-C4A
82	R4	202	PEB	C2B-C1B-CHA-C4A
82	R4	203	PEB	NB-C1B-CHA-C4A
82	R4	203	PEB	C2B-C1B-CHA-C4A
82	S4	201	PEB	C2A-C3A-CAA-CBA
82	S4	201	PEB	C4A-C3A-CAA-CBA
82	S4	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	S4	201	PEB	C2B-C1B-CHA-C4A
82	S4	202	PEB	ND-C1D-CHC-C4C
82	S4	202	PEB	C2D-C1D-CHC-C4C
82	S4	202	PEB	C4A-C3A-CAA-CBA
82	S4	202	PEB	NB-C1B-CHA-C4A
82	S4	202	PEB	C2B-C1B-CHA-C4A
82	T4	201	PEB	NB-C1B-CHA-C4A
82	T4	201	PEB	C2B-C1B-CHA-C4A
82	T4	202	PEB	NB-C1B-CHA-C4A
82	T4	202	PEB	C2B-C1B-CHA-C4A
82	T4	203	PEB	C2A-C3A-CAA-CBA
82	T4	203	PEB	C4A-C3A-CAA-CBA
82	T4	203	PEB	NB-C1B-CHA-C4A
82	T4	203	PEB	C2B-C1B-CHA-C4A
82	U4	201	PEB	C2A-C3A-CAA-CBA
82	U4	201	PEB	C4A-C3A-CAA-CBA
82	U4	202	PEB	ND-C1D-CHC-C4C
82	U4	202	PEB	C2D-C1D-CHC-C4C
82	U4	202	PEB	C2A-C3A-CAA-CBA
82	U4	202	PEB	C4A-C3A-CAA-CBA
82	U4	202	PEB	NB-C1B-CHA-C4A
82	U4	202	PEB	C2B-C1B-CHA-C4A
82	V4	201	PEB	C2A-C3A-CAA-CBA
82	V4	201	PEB	C4A-C3A-CAA-CBA
82	V4	201	PEB	NB-C1B-CHA-C4A
82	V4	201	PEB	C2B-C1B-CHA-C4A
82	V4	202	PEB	ND-C1D-CHC-C4C
82	V4	202	PEB	C2D-C3D-CAD-CBD
82	V4	202	PEB	C4D-C3D-CAD-CBD
82	V4	202	PEB	C2A-C3A-CAA-CBA
82	V4	202	PEB	NB-C1B-CHA-C4A
82	V4	202	PEB	C2B-C1B-CHA-C4A
82	W4	201	PEB	C4A-C3A-CAA-CBA
82	W4	201	PEB	NB-C1B-CHA-C4A
82	W4	201	PEB	C2B-C1B-CHA-C4A
82	Y4	201	PEB	NB-C1B-CHA-C4A
82	Y4	201	PEB	C2B-C1B-CHA-C4A
82	Y4	202	PEB	NB-C1B-CHA-C4A
82	Y4	202	PEB	C2B-C1B-CHA-C4A
82	Y4	203	PEB	C2A-C3A-CAA-CBA
82	Y4	203	PEB	C4A-C3A-CAA-CBA
82	Y4	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	Y4	203	PEB	C2B-C1B-CHA-C4A
82	Z4	201	PEB	C4A-C3A-CAA-CBA
82	Z4	201	PEB	NB-C1B-CHA-C4A
82	Z4	201	PEB	C2B-C1B-CHA-C4A
82	Z4	202	PEB	ND-C1D-CHC-C4C
82	Z4	202	PEB	C2D-C1D-CHC-C4C
82	Z4	202	PEB	NB-C1B-CHA-C4A
82	Z4	202	PEB	C2B-C1B-CHA-C4A
82	i4	201	PEB	C2A-C3A-CAA-CBA
82	i4	201	PEB	C4A-C3A-CAA-CBA
82	i4	201	PEB	NB-C1B-CHA-C4A
82	i4	201	PEB	C2B-C1B-CHA-C4A
82	i4	202	PEB	ND-C1D-CHC-C4C
82	i4	202	PEB	C2D-C1D-CHC-C4C
82	i4	202	PEB	C2A-C3A-CAA-CBA
82	i4	202	PEB	NB-C1B-CHA-C4A
82	i4	202	PEB	C2B-C1B-CHA-C4A
82	i4	203	PEB	NB-C1B-CHA-C4A
82	i4	203	PEB	C2B-C1B-CHA-C4A
82	i4	203	PEB	C2B-C3B-CAB-CBB
82	i4	203	PEB	C4B-C3B-CAB-CBB
82	j4	201	PEB	ND-C1D-CHC-C4C
82	j4	201	PEB	C2D-C1D-CHC-C4C
82	j4	201	PEB	C4A-C3A-CAA-CBA
82	j4	201	PEB	NB-C1B-CHA-C4A
82	j4	201	PEB	C2B-C1B-CHA-C4A
82	j4	202	PEB	ND-C1D-CHC-C4C
82	j4	202	PEB	C2D-C1D-CHC-C4C
82	j4	202	PEB	NB-C1B-CHA-C4A
82	j4	202	PEB	C2B-C1B-CHA-C4A
82	j4	203	PEB	C2D-C1D-CHC-C4C
82	j4	203	PEB	C2A-C3A-CAA-CBA
82	j4	203	PEB	NB-C1B-CHA-C4A
82	j4	203	PEB	C2B-C1B-CHA-C4A
82	k4	201	PEB	C4A-C3A-CAA-CBA
82	k4	201	PEB	NB-C1B-CHA-C4A
82	k4	201	PEB	C2B-C1B-CHA-C4A
82	k4	202	PEB	C2D-C1D-CHC-C4C
82	k4	202	PEB	C2A-C3A-CAA-CBA
82	k4	202	PEB	C4A-C3A-CAA-CBA
82	k4	202	PEB	NB-C1B-CHA-C4A
82	k4	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	k4	202	PEB	C4B-C3B-CAB-CBB
82	l4	201	PEB	ND-C1D-CHC-C4C
82	l4	201	PEB	C2D-C1D-CHC-C4C
82	l4	201	PEB	C4A-C3A-CAA-CBA
82	l4	201	PEB	NB-C1B-CHA-C4A
82	l4	201	PEB	C2B-C1B-CHA-C4A
82	l4	202	PEB	ND-C1D-CHC-C4C
82	l4	202	PEB	C2D-C1D-CHC-C4C
82	l4	202	PEB	C4A-C3A-CAA-CBA
82	l4	202	PEB	NB-C1B-CHA-C4A
82	l4	202	PEB	C2B-C1B-CHA-C4A
82	m4	201	PEB	C2D-C1D-CHC-C4C
82	m4	201	PEB	C2A-C3A-CAA-CBA
82	m4	201	PEB	C4A-C3A-CAA-CBA
82	m4	201	PEB	NB-C1B-CHA-C4A
82	m4	201	PEB	C2B-C1B-CHA-C4A
82	m4	202	PEB	NB-C1B-CHA-C4A
82	m4	202	PEB	C2B-C1B-CHA-C4A
82	m4	203	PEB	NB-C1B-CHA-C4A
82	m4	203	PEB	C2B-C1B-CHA-C4A
82	m4	203	PEB	C2B-C3B-CAB-CBB
82	m4	203	PEB	C4B-C3B-CAB-CBB
82	a4	201	PEB	NB-C1B-CHA-C4A
82	a4	201	PEB	C2B-C1B-CHA-C4A
82	a4	202	PEB	NB-C1B-CHA-C4A
82	a4	202	PEB	C2B-C1B-CHA-C4A
82	a4	203	PEB	C2A-C3A-CAA-CBA
82	a4	203	PEB	C4A-C3A-CAA-CBA
82	a4	203	PEB	NB-C1B-CHA-C4A
82	a4	203	PEB	C2B-C1B-CHA-C4A
82	b4	201	PEB	C4A-C3A-CAA-CBA
82	b4	201	PEB	NB-C1B-CHA-C4A
82	b4	201	PEB	C2B-C1B-CHA-C4A
82	b4	202	PEB	ND-C1D-CHC-C4C
82	b4	202	PEB	NB-C1B-CHA-C4A
82	b4	202	PEB	C2B-C1B-CHA-C4A
82	c4	201	PEB	NB-C1B-CHA-C4A
82	c4	201	PEB	C2B-C1B-CHA-C4A
82	c4	202	PEB	ND-C1D-CHC-C4C
82	c4	202	PEB	C2D-C1D-CHC-C4C
82	c4	202	PEB	NB-C1B-CHA-C4A
82	c4	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	c4	203	PEB	ND-C1D-CHC-C4C
82	c4	203	PEB	C2D-C1D-CHC-C4C
82	c4	203	PEB	NB-C1B-CHA-C4A
82	c4	203	PEB	C2B-C1B-CHA-C4A
82	d4	201	PEB	C2A-C3A-CAA-CBA
82	d4	201	PEB	C4A-C3A-CAA-CBA
82	d4	201	PEB	NB-C1B-CHA-C4A
82	d4	201	PEB	C2B-C1B-CHA-C4A
82	d4	202	PEB	ND-C1D-CHC-C4C
82	d4	202	PEB	C2D-C1D-CHC-C4C
82	d4	202	PEB	NB-C1B-CHA-C4A
82	d4	202	PEB	C2B-C1B-CHA-C4A
82	e4	201	PEB	NB-C1B-CHA-C4A
82	e4	201	PEB	C2B-C1B-CHA-C4A
82	e4	202	PEB	C2A-C3A-CAA-CBA
82	e4	202	PEB	NB-C1B-CHA-C4A
82	e4	202	PEB	C2B-C1B-CHA-C4A
82	e4	203	PEB	NB-C1B-CHA-C4A
82	e4	203	PEB	C2B-C1B-CHA-C4A
82	f4	201	PEB	ND-C1D-CHC-C4C
82	f4	201	PEB	C2D-C1D-CHC-C4C
82	f4	201	PEB	C4A-C3A-CAA-CBA
82	f4	201	PEB	NB-C1B-CHA-C4A
82	f4	201	PEB	C2B-C1B-CHA-C4A
82	f4	202	PEB	ND-C1D-CHC-C4C
82	f4	202	PEB	C2D-C1D-CHC-C4C
82	f4	202	PEB	C4A-C3A-CAA-CBA
82	f4	202	PEB	NB-C1B-CHA-C4A
82	f4	202	PEB	C2B-C1B-CHA-C4A
82	g4	201	PEB	NB-C1B-CHA-C4A
82	g4	201	PEB	C2B-C1B-CHA-C4A
82	g4	202	PEB	ND-C1D-CHC-C4C
82	g4	202	PEB	C2D-C1D-CHC-C4C
82	g4	202	PEB	C2A-C3A-CAA-CBA
82	g4	202	PEB	NB-C1B-CHA-C4A
82	g4	202	PEB	C2B-C1B-CHA-C4A
82	g4	203	PEB	ND-C1D-CHC-C4C
82	g4	203	PEB	C2D-C1D-CHC-C4C
82	g4	203	PEB	NB-C1B-CHA-C4A
82	g4	203	PEB	C2B-C1B-CHA-C4A
82	g4	203	PEB	C2B-C3B-CAB-CBB
82	h4	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	h4	201	PEB	C2D-C1D-CHC-C4C
82	h4	201	PEB	C4A-C3A-CAA-CBA
82	h4	201	PEB	NB-C1B-CHA-C4A
82	h4	201	PEB	C2B-C1B-CHA-C4A
82	h4	202	PEB	ND-C1D-CHC-C4C
82	h4	202	PEB	NB-C1B-CHA-C4A
82	h4	202	PEB	C2B-C1B-CHA-C4A
82	A5	201	PEB	ND-C1D-CHC-C4C
82	A5	201	PEB	C2D-C1D-CHC-C4C
82	A5	201	PEB	C2A-C3A-CAA-CBA
82	A5	201	PEB	NB-C1B-CHA-C4A
82	A5	201	PEB	C2B-C1B-CHA-C4A
82	A5	202	PEB	NC-C1C-CHB-C4B
82	A5	202	PEB	C2C-C1C-CHB-C4B
82	A5	202	PEB	NB-C1B-CHA-C4A
82	A5	202	PEB	C2B-C1B-CHA-C4A
82	B5	201	PEB	ND-C1D-CHC-C4C
82	B5	201	PEB	C2D-C1D-CHC-C4C
82	B5	201	PEB	NB-C1B-CHA-C4A
82	B5	201	PEB	C2B-C1B-CHA-C4A
82	B5	202	PEB	C4A-C3A-CAA-CBA
82	B5	202	PEB	NB-C1B-CHA-C4A
82	B5	202	PEB	C2B-C1B-CHA-C4A
82	B5	203	PEB	ND-C1D-CHC-C4C
82	B5	203	PEB	C2D-C1D-CHC-C4C
82	B5	203	PEB	NB-C1B-CHA-C4A
82	B5	203	PEB	C2B-C1B-CHA-C4A
82	C5	201	PEB	ND-C1D-CHC-C4C
82	C5	201	PEB	C2D-C1D-CHC-C4C
82	C5	201	PEB	C2A-C3A-CAA-CBA
82	C5	201	PEB	NB-C1B-CHA-C4A
82	C5	201	PEB	C2B-C1B-CHA-C4A
82	C5	202	PEB	NC-C1C-CHB-C4B
82	C5	202	PEB	C2C-C1C-CHB-C4B
82	C5	202	PEB	NB-C1B-CHA-C4A
82	C5	202	PEB	C2B-C1B-CHA-C4A
82	D5	201	PEB	ND-C1D-CHC-C4C
82	D5	201	PEB	C2D-C1D-CHC-C4C
82	D5	201	PEB	NB-C1B-CHA-C4A
82	D5	201	PEB	C2B-C1B-CHA-C4A
82	D5	202	PEB	C2A-C3A-CAA-CBA
82	D5	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	D5	202	PEB	NB-C1B-CHA-C4A
82	D5	202	PEB	C2B-C1B-CHA-C4A
82	D5	203	PEB	ND-C1D-CHC-C4C
82	D5	203	PEB	C2D-C1D-CHC-C4C
82	D5	203	PEB	NB-C1B-CHA-C4A
82	D5	203	PEB	C2B-C1B-CHA-C4A
82	E5	201	PEB	ND-C1D-CHC-C4C
82	E5	201	PEB	C2D-C1D-CHC-C4C
82	E5	201	PEB	C2A-C3A-CAA-CBA
82	E5	201	PEB	NB-C1B-CHA-C4A
82	E5	201	PEB	C2B-C1B-CHA-C4A
82	E5	202	PEB	NC-C1C-CHB-C4B
82	E5	202	PEB	C2C-C1C-CHB-C4B
82	E5	202	PEB	NB-C1B-CHA-C4A
82	E5	202	PEB	C2B-C1B-CHA-C4A
82	F5	201	PEB	ND-C1D-CHC-C4C
82	F5	201	PEB	C4A-C3A-CAA-CBA
82	F5	201	PEB	NB-C1B-CHA-C4A
82	F5	201	PEB	C2B-C1B-CHA-C4A
82	F5	202	PEB	C2A-C3A-CAA-CBA
82	F5	202	PEB	C4A-C3A-CAA-CBA
82	F5	202	PEB	NB-C1B-CHA-C4A
82	F5	202	PEB	C2B-C1B-CHA-C4A
82	F5	203	PEB	ND-C1D-CHC-C4C
82	F5	203	PEB	C2D-C1D-CHC-C4C
82	F5	203	PEB	NB-C1B-CHA-C4A
82	F5	203	PEB	C2B-C1B-CHA-C4A
82	G5	201	PEB	ND-C1D-CHC-C4C
82	G5	201	PEB	C2D-C1D-CHC-C4C
82	G5	201	PEB	C2A-C3A-CAA-CBA
82	G5	201	PEB	NB-C1B-CHA-C4A
82	G5	201	PEB	C2B-C1B-CHA-C4A
82	G5	202	PEB	NC-C1C-CHB-C4B
82	G5	202	PEB	C2C-C1C-CHB-C4B
82	G5	202	PEB	NB-C1B-CHA-C4A
82	G5	202	PEB	C2B-C1B-CHA-C4A
82	H5	201	PEB	ND-C1D-CHC-C4C
82	H5	201	PEB	C2D-C1D-CHC-C4C
82	H5	201	PEB	NB-C1B-CHA-C4A
82	H5	201	PEB	C2B-C1B-CHA-C4A
82	H5	202	PEB	C4A-C3A-CAA-CBA
82	H5	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	H5	202	PEB	C2B-C1B-CHA-C4A
82	H5	203	PEB	ND-C1D-CHC-C4C
82	H5	203	PEB	C2D-C1D-CHC-C4C
82	H5	203	PEB	NB-C1B-CHA-C4A
82	H5	203	PEB	C2B-C1B-CHA-C4A
82	I5	201	PEB	ND-C1D-CHC-C4C
82	I5	201	PEB	C2D-C1D-CHC-C4C
82	I5	201	PEB	C2A-C3A-CAA-CBA
82	I5	201	PEB	NB-C1B-CHA-C4A
82	I5	201	PEB	C2B-C1B-CHA-C4A
82	I5	202	PEB	NC-C1C-CHB-C4B
82	I5	202	PEB	C2C-C1C-CHB-C4B
82	I5	202	PEB	NB-C1B-CHA-C4A
82	I5	202	PEB	C2B-C1B-CHA-C4A
82	J5	201	PEB	ND-C1D-CHC-C4C
82	J5	201	PEB	C2D-C1D-CHC-C4C
82	J5	201	PEB	C2A-C3A-CAA-CBA
82	J5	201	PEB	C4A-C3A-CAA-CBA
82	J5	201	PEB	NB-C1B-CHA-C4A
82	J5	201	PEB	C2B-C1B-CHA-C4A
82	J5	202	PEB	C4A-C3A-CAA-CBA
82	J5	202	PEB	NB-C1B-CHA-C4A
82	J5	202	PEB	C2B-C1B-CHA-C4A
82	J5	203	PEB	ND-C1D-CHC-C4C
82	J5	203	PEB	C2D-C1D-CHC-C4C
82	J5	203	PEB	NB-C1B-CHA-C4A
82	J5	203	PEB	C2B-C1B-CHA-C4A
82	K5	201	PEB	ND-C1D-CHC-C4C
82	K5	201	PEB	C2D-C1D-CHC-C4C
82	K5	201	PEB	C2A-C3A-CAA-CBA
82	K5	201	PEB	NB-C1B-CHA-C4A
82	K5	201	PEB	C2B-C1B-CHA-C4A
82	K5	202	PEB	NC-C1C-CHB-C4B
82	K5	202	PEB	C2C-C1C-CHB-C4B
82	K5	202	PEB	NB-C1B-CHA-C4A
82	K5	202	PEB	C2B-C1B-CHA-C4A
82	L5	201	PEB	ND-C1D-CHC-C4C
82	L5	201	PEB	C2D-C3D-CAD-CBD
82	L5	201	PEB	C4D-C3D-CAD-CBD
82	L5	201	PEB	NB-C1B-CHA-C4A
82	L5	201	PEB	C2B-C1B-CHA-C4A
82	L5	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	L5	202	PEB	NB-C1B-CHA-C4A
82	L5	202	PEB	C2B-C1B-CHA-C4A
82	L5	203	PEB	ND-C1D-CHC-C4C
82	L5	203	PEB	C2D-C1D-CHC-C4C
82	L5	203	PEB	NC-C1C-CHB-C4B
82	L5	203	PEB	C2C-C1C-CHB-C4B
82	L5	203	PEB	NB-C1B-CHA-C4A
82	L5	203	PEB	C2B-C1B-CHA-C4A
82	M5	301	PEB	NB-C1B-CHA-C4A
82	M5	301	PEB	C2B-C1B-CHA-C4A
82	M5	304	PEB	C2D-C1D-CHC-C4C
82	M5	304	PEB	NB-C1B-CHA-C4A
82	M5	304	PEB	C2B-C1B-CHA-C4A
82	M5	305	PEB	ND-C1D-CHC-C4C
82	M5	305	PEB	C2D-C1D-CHC-C4C
82	M5	305	PEB	NC-C1C-CHB-C4B
82	M5	305	PEB	C2C-C1C-CHB-C4B
82	M5	305	PEB	C2A-C3A-CAA-CBA
82	M5	305	PEB	C4A-C3A-CAA-CBA
82	M5	305	PEB	NB-C1B-CHA-C4A
82	M5	305	PEB	C2B-C1B-CHA-C4A
82	N5	201	PEB	ND-C1D-CHC-C4C
82	N5	201	PEB	C2D-C1D-CHC-C4C
82	N5	201	PEB	C2A-C3A-CAA-CBA
82	N5	201	PEB	NB-C1B-CHA-C4A
82	N5	201	PEB	C2B-C1B-CHA-C4A
82	N5	202	PEB	NC-C1C-CHB-C4B
82	N5	202	PEB	C2C-C1C-CHB-C4B
82	N5	202	PEB	NB-C1B-CHA-C4A
82	N5	202	PEB	C2B-C1B-CHA-C4A
82	O5	201	PEB	ND-C1D-CHC-C4C
82	O5	201	PEB	C2D-C1D-CHC-C4C
82	O5	201	PEB	NB-C1B-CHA-C4A
82	O5	201	PEB	C2B-C1B-CHA-C4A
82	O5	202	PEB	C4A-C3A-CAA-CBA
82	O5	202	PEB	NB-C1B-CHA-C4A
82	O5	202	PEB	C2B-C1B-CHA-C4A
82	O5	203	PEB	ND-C1D-CHC-C4C
82	O5	203	PEB	C2D-C1D-CHC-C4C
82	O5	203	PEB	NB-C1B-CHA-C4A
82	O5	203	PEB	C2B-C1B-CHA-C4A
82	P5	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	P5	201	PEB	C2D-C1D-CHC-C4C
82	P5	201	PEB	C2A-C3A-CAA-CBA
82	P5	201	PEB	NB-C1B-CHA-C4A
82	P5	201	PEB	C2B-C1B-CHA-C4A
82	P5	202	PEB	NC-C1C-CHB-C4B
82	P5	202	PEB	C2C-C1C-CHB-C4B
82	P5	202	PEB	NB-C1B-CHA-C4A
82	P5	202	PEB	C2B-C1B-CHA-C4A
82	Q5	201	PEB	ND-C1D-CHC-C4C
82	Q5	201	PEB	C2D-C1D-CHC-C4C
82	Q5	201	PEB	NB-C1B-CHA-C4A
82	Q5	201	PEB	C2B-C1B-CHA-C4A
82	Q5	202	PEB	C2A-C3A-CAA-CBA
82	Q5	202	PEB	C4A-C3A-CAA-CBA
82	Q5	202	PEB	NB-C1B-CHA-C4A
82	Q5	202	PEB	C2B-C1B-CHA-C4A
82	Q5	203	PEB	ND-C1D-CHC-C4C
82	Q5	203	PEB	C2D-C1D-CHC-C4C
82	Q5	203	PEB	NB-C1B-CHA-C4A
82	Q5	203	PEB	C2B-C1B-CHA-C4A
82	R5	201	PEB	ND-C1D-CHC-C4C
82	R5	201	PEB	C2D-C1D-CHC-C4C
82	R5	201	PEB	C2A-C3A-CAA-CBA
82	R5	201	PEB	NB-C1B-CHA-C4A
82	R5	201	PEB	C2B-C1B-CHA-C4A
82	R5	202	PEB	NC-C1C-CHB-C4B
82	R5	202	PEB	C2C-C1C-CHB-C4B
82	R5	202	PEB	NB-C1B-CHA-C4A
82	R5	202	PEB	C2B-C1B-CHA-C4A
82	S5	201	PEB	ND-C1D-CHC-C4C
82	S5	201	PEB	NB-C1B-CHA-C4A
82	S5	201	PEB	C2B-C1B-CHA-C4A
82	S5	202	PEB	C4A-C3A-CAA-CBA
82	S5	202	PEB	NB-C1B-CHA-C4A
82	S5	202	PEB	C2B-C1B-CHA-C4A
82	S5	203	PEB	ND-C1D-CHC-C4C
82	S5	203	PEB	C2D-C1D-CHC-C4C
82	S5	203	PEB	NB-C1B-CHA-C4A
82	S5	203	PEB	C2B-C1B-CHA-C4A
82	S5	203	PEB	C3B-CAB-CBB-CGB
82	T5	201	PEB	ND-C1D-CHC-C4C
82	T5	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	T5	201	PEB	C2A-C3A-CAA-CBA
82	T5	201	PEB	NB-C1B-CHA-C4A
82	T5	201	PEB	C2B-C1B-CHA-C4A
82	T5	202	PEB	NC-C1C-CHB-C4B
82	T5	202	PEB	C2C-C1C-CHB-C4B
82	T5	202	PEB	NB-C1B-CHA-C4A
82	T5	202	PEB	C2B-C1B-CHA-C4A
82	U5	201	PEB	ND-C1D-CHC-C4C
82	U5	201	PEB	C2D-C1D-CHC-C4C
82	U5	201	PEB	NB-C1B-CHA-C4A
82	U5	201	PEB	C2B-C1B-CHA-C4A
82	U5	202	PEB	C4A-C3A-CAA-CBA
82	U5	202	PEB	NB-C1B-CHA-C4A
82	U5	202	PEB	C2B-C1B-CHA-C4A
82	U5	203	PEB	ND-C1D-CHC-C4C
82	U5	203	PEB	C2D-C1D-CHC-C4C
82	U5	203	PEB	NB-C1B-CHA-C4A
82	U5	203	PEB	C2B-C1B-CHA-C4A
82	V5	201	PEB	ND-C1D-CHC-C4C
82	V5	201	PEB	C2D-C1D-CHC-C4C
82	V5	201	PEB	C2A-C3A-CAA-CBA
82	V5	201	PEB	NB-C1B-CHA-C4A
82	V5	201	PEB	C2B-C1B-CHA-C4A
82	V5	202	PEB	NC-C1C-CHB-C4B
82	V5	202	PEB	C2C-C1C-CHB-C4B
82	V5	202	PEB	NB-C1B-CHA-C4A
82	V5	202	PEB	C2B-C1B-CHA-C4A
82	W5	201	PEB	ND-C1D-CHC-C4C
82	W5	201	PEB	C2D-C1D-CHC-C4C
82	W5	201	PEB	NB-C1B-CHA-C4A
82	W5	201	PEB	C2B-C1B-CHA-C4A
82	W5	202	PEB	C2A-C3A-CAA-CBA
82	W5	202	PEB	C4A-C3A-CAA-CBA
82	W5	202	PEB	NB-C1B-CHA-C4A
82	W5	202	PEB	C2B-C1B-CHA-C4A
82	W5	203	PEB	ND-C1D-CHC-C4C
82	W5	203	PEB	C2D-C1D-CHC-C4C
82	W5	203	PEB	NC-C1C-CHB-C4B
82	W5	203	PEB	NB-C1B-CHA-C4A
82	W5	203	PEB	C2B-C1B-CHA-C4A
82	X5	201	PEB	ND-C1D-CHC-C4C
82	X5	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	X5	201	PEB	C2A-C3A-CAA-CBA
82	X5	201	PEB	NB-C1B-CHA-C4A
82	X5	201	PEB	C2B-C1B-CHA-C4A
82	X5	202	PEB	NC-C1C-CHB-C4B
82	X5	202	PEB	C2C-C1C-CHB-C4B
82	X5	202	PEB	NB-C1B-CHA-C4A
82	X5	202	PEB	C2B-C1B-CHA-C4A
82	Y5	201	PEB	ND-C1D-CHC-C4C
82	Y5	201	PEB	C2D-C3D-CAD-CBD
82	Y5	201	PEB	C4D-C3D-CAD-CBD
82	Y5	201	PEB	NB-C1B-CHA-C4A
82	Y5	201	PEB	C2B-C1B-CHA-C4A
82	Y5	201	PEB	C3B-CAB-CBB-CGB
82	Y5	202	PEB	C4A-C3A-CAA-CBA
82	Y5	202	PEB	NB-C1B-CHA-C4A
82	Y5	202	PEB	C2B-C1B-CHA-C4A
82	Y5	203	PEB	ND-C1D-CHC-C4C
82	Y5	203	PEB	C2D-C1D-CHC-C4C
82	Y5	203	PEB	NC-C1C-CHB-C4B
82	Y5	203	PEB	C2C-C1C-CHB-C4B
82	Y5	203	PEB	NB-C1B-CHA-C4A
82	Y5	203	PEB	C2B-C1B-CHA-C4A
82	Z5	301	PEB	NB-C1B-CHA-C4A
82	Z5	301	PEB	C2B-C1B-CHA-C4A
82	Z5	304	PEB	C2D-C1D-CHC-C4C
82	Z5	304	PEB	NB-C1B-CHA-C4A
82	Z5	304	PEB	C2B-C1B-CHA-C4A
82	Z5	305	PEB	ND-C1D-CHC-C4C
82	Z5	305	PEB	C2D-C1D-CHC-C4C
82	Z5	305	PEB	NC-C1C-CHB-C4B
82	Z5	305	PEB	C2C-C1C-CHB-C4B
82	Z5	305	PEB	C2A-C3A-CAA-CBA
82	Z5	305	PEB	C4A-C3A-CAA-CBA
82	Z5	305	PEB	NB-C1B-CHA-C4A
82	Z5	305	PEB	C2B-C1B-CHA-C4A
82	A7	201	PEB	ND-C1D-CHC-C4C
82	A7	201	PEB	C2D-C1D-CHC-C4C
82	A7	201	PEB	NB-C1B-CHA-C4A
82	A7	201	PEB	C2B-C1B-CHA-C4A
82	A7	202	PEB	ND-C1D-CHC-C4C
82	A7	202	PEB	C2D-C1D-CHC-C4C
82	A7	202	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
82	A7	202	PEB	C4D-C3D-CAD-CBD
82	A7	202	PEB	C2A-C3A-CAA-CBA
82	A7	202	PEB	C4A-C3A-CAA-CBA
82	A7	202	PEB	NB-C1B-CHA-C4A
82	A7	202	PEB	C2B-C1B-CHA-C4A
82	B7	201	PEB	ND-C1D-CHC-C4C
82	B7	201	PEB	C2D-C1D-CHC-C4C
82	B7	201	PEB	NB-C1B-CHA-C4A
82	B7	201	PEB	C2B-C1B-CHA-C4A
82	B7	202	PEB	C2A-C3A-CAA-CBA
82	B7	202	PEB	C4A-C3A-CAA-CBA
82	B7	202	PEB	NB-C1B-CHA-C4A
82	B7	202	PEB	C2B-C1B-CHA-C4A
82	B7	203	PEB	NC-C1C-CHB-C4B
82	B7	203	PEB	C2C-C1C-CHB-C4B
82	B7	203	PEB	C2A-C3A-CAA-CBA
82	B7	203	PEB	NB-C1B-CHA-C4A
82	B7	203	PEB	C2B-C1B-CHA-C4A
82	C7	201	PEB	ND-C1D-CHC-C4C
82	C7	201	PEB	C2D-C1D-CHC-C4C
82	C7	201	PEB	NB-C1B-CHA-C4A
82	C7	201	PEB	C2B-C1B-CHA-C4A
82	C7	202	PEB	NC-C1C-CHB-C4B
82	C7	202	PEB	C2C-C1C-CHB-C4B
82	C7	202	PEB	C2A-C3A-CAA-CBA
82	C7	202	PEB	C4A-C3A-CAA-CBA
82	C7	202	PEB	NB-C1B-CHA-C4A
82	C7	202	PEB	C2B-C1B-CHA-C4A
82	D7	201	PEB	ND-C1D-CHC-C4C
82	D7	201	PEB	C2D-C1D-CHC-C4C
82	D7	201	PEB	NB-C1B-CHA-C4A
82	D7	201	PEB	C2B-C1B-CHA-C4A
82	D7	202	PEB	ND-C1D-CHC-C4C
82	D7	202	PEB	C2D-C1D-CHC-C4C
82	D7	202	PEB	C4A-C3A-CAA-CBA
82	D7	202	PEB	NB-C1B-CHA-C4A
82	D7	202	PEB	C2B-C1B-CHA-C4A
82	D7	203	PEB	ND-C1D-CHC-C4C
82	D7	203	PEB	C2D-C1D-CHC-C4C
82	D7	203	PEB	NC-C1C-CHB-C4B
82	D7	203	PEB	C2C-C1C-CHB-C4B
82	D7	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	D7	203	PEB	C2B-C1B-CHA-C4A
82	E7	201	PEB	NB-C1B-CHA-C4A
82	E7	201	PEB	C2B-C1B-CHA-C4A
82	E7	202	PEB	ND-C1D-CHC-C4C
82	E7	202	PEB	C2D-C1D-CHC-C4C
82	E7	202	PEB	C4A-C3A-CAA-CBA
82	E7	202	PEB	NB-C1B-CHA-C4A
82	E7	202	PEB	C2B-C1B-CHA-C4A
82	F7	201	PEB	NB-C1B-CHA-C4A
82	F7	201	PEB	C2B-C1B-CHA-C4A
82	F7	202	PEB	C4A-C3A-CAA-CBA
82	F7	202	PEB	NB-C1B-CHA-C4A
82	F7	202	PEB	C2B-C1B-CHA-C4A
82	F7	203	PEB	ND-C1D-CHC-C4C
82	F7	203	PEB	C2D-C1D-CHC-C4C
82	F7	203	PEB	NC-C1C-CHB-C4B
82	F7	203	PEB	C2A-C3A-CAA-CBA
82	F7	203	PEB	C4A-C3A-CAA-CBA
82	F7	203	PEB	NB-C1B-CHA-C4A
82	F7	203	PEB	C2B-C1B-CHA-C4A
82	G7	201	PEB	C2A-C3A-CAA-CBA
82	G7	201	PEB	C4A-C3A-CAA-CBA
82	G7	201	PEB	NB-C1B-CHA-C4A
82	G7	201	PEB	C2B-C1B-CHA-C4A
82	G7	202	PEB	C2A-C3A-CAA-CBA
82	G7	202	PEB	C4A-C3A-CAA-CBA
82	G7	202	PEB	NB-C1B-CHA-C4A
82	G7	202	PEB	C2B-C1B-CHA-C4A
82	H7	201	PEB	NB-C1B-CHA-C4A
82	H7	201	PEB	C2B-C1B-CHA-C4A
82	H7	202	PEB	ND-C1D-CHC-C4C
82	H7	202	PEB	C2D-C1D-CHC-C4C
82	H7	202	PEB	C4A-C3A-CAA-CBA
82	H7	202	PEB	NB-C1B-CHA-C4A
82	H7	202	PEB	C2B-C1B-CHA-C4A
82	H7	203	PEB	NB-C1B-CHA-C4A
82	H7	203	PEB	C2B-C1B-CHA-C4A
82	H7	203	PEB	C2B-C3B-CAB-CBB
82	I7	201	PEB	ND-C1D-CHC-C4C
82	I7	201	PEB	C2D-C1D-CHC-C4C
82	I7	201	PEB	C2A-C3A-CAA-CBA
82	I7	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	I7	201	PEB	NB-C1B-CHA-C4A
82	I7	201	PEB	C2B-C1B-CHA-C4A
82	I7	202	PEB	C2A-C3A-CAA-CBA
82	I7	202	PEB	C4A-C3A-CAA-CBA
82	I7	202	PEB	NB-C1B-CHA-C4A
82	I7	202	PEB	C2B-C1B-CHA-C4A
82	J7	201	PEB	ND-C1D-CHC-C4C
82	J7	201	PEB	C2D-C1D-CHC-C4C
82	J7	201	PEB	NB-C1B-CHA-C4A
82	J7	201	PEB	C2B-C1B-CHA-C4A
82	J7	202	PEB	C4A-C3A-CAA-CBA
82	J7	202	PEB	NB-C1B-CHA-C4A
82	J7	202	PEB	C2B-C1B-CHA-C4A
82	J7	203	PEB	ND-C1D-CHC-C4C
82	J7	203	PEB	C2A-C3A-CAA-CBA
82	J7	203	PEB	C4A-C3A-CAA-CBA
82	J7	203	PEB	NB-C1B-CHA-C4A
82	J7	203	PEB	C2B-C1B-CHA-C4A
82	K7	201	PEB	NB-C1B-CHA-C4A
82	K7	201	PEB	C2B-C1B-CHA-C4A
82	K7	202	PEB	C2D-C3D-CAD-CBD
82	K7	202	PEB	C4D-C3D-CAD-CBD
82	K7	202	PEB	NB-C1B-CHA-C4A
82	K7	202	PEB	C2B-C1B-CHA-C4A
82	L7	201	PEB	NB-C1B-CHA-C4A
82	L7	201	PEB	C2B-C1B-CHA-C4A
82	L7	202	PEB	C4A-C3A-CAA-CBA
82	L7	202	PEB	NB-C1B-CHA-C4A
82	L7	202	PEB	C2B-C1B-CHA-C4A
82	L7	203	PEB	NC-C1C-CHB-C4B
82	L7	203	PEB	C2C-C1C-CHB-C4B
82	L7	203	PEB	NB-C1B-CHA-C4A
82	L7	203	PEB	C2B-C1B-CHA-C4A
82	M7	201	PEB	NB-C1B-CHA-C4A
82	M7	201	PEB	C2B-C1B-CHA-C4A
82	M7	202	PEB	ND-C1D-CHC-C4C
82	M7	202	PEB	C2D-C1D-CHC-C4C
82	M7	202	PEB	C4A-C3A-CAA-CBA
82	M7	202	PEB	NB-C1B-CHA-C4A
82	M7	202	PEB	C2B-C1B-CHA-C4A
82	N7	201	PEB	NB-C1B-CHA-C4A
82	N7	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	N7	202	PEB	C4A-C3A-CAA-CBA
82	N7	202	PEB	NB-C1B-CHA-C4A
82	N7	202	PEB	C2B-C1B-CHA-C4A
82	N7	203	PEB	NB-C1B-CHA-C4A
82	N7	203	PEB	C2B-C1B-CHA-C4A
82	O7	201	PEB	C2B-C1B-CHA-C4A
82	O7	202	PEB	C2A-C3A-CAA-CBA
82	O7	202	PEB	C4A-C3A-CAA-CBA
82	O7	202	PEB	NB-C1B-CHA-C4A
82	O7	202	PEB	C2B-C1B-CHA-C4A
82	P7	201	PEB	NB-C1B-CHA-C4A
82	P7	201	PEB	C2B-C1B-CHA-C4A
82	P7	202	PEB	C4A-C3A-CAA-CBA
82	P7	202	PEB	NB-C1B-CHA-C4A
82	P7	202	PEB	C2B-C1B-CHA-C4A
82	P7	203	PEB	NC-C1C-CHB-C4B
82	P7	203	PEB	NB-C1B-CHA-C4A
82	P7	203	PEB	C2B-C1B-CHA-C4A
82	Q7	201	PEB	NB-C1B-CHA-C4A
82	Q7	201	PEB	C2B-C1B-CHA-C4A
82	Q7	202	PEB	C4A-C3A-CAA-CBA
82	Q7	202	PEB	NB-C1B-CHA-C4A
82	Q7	202	PEB	C2B-C1B-CHA-C4A
82	R7	201	PEB	NB-C1B-CHA-C4A
82	R7	201	PEB	C2B-C1B-CHA-C4A
82	R7	202	PEB	C4A-C3A-CAA-CBA
82	R7	202	PEB	NB-C1B-CHA-C4A
82	R7	202	PEB	C2B-C1B-CHA-C4A
82	R7	203	PEB	C2D-C3D-CAD-CBD
82	R7	203	PEB	C4D-C3D-CAD-CBD
82	R7	203	PEB	NB-C1B-CHA-C4A
82	R7	203	PEB	C2B-C1B-CHA-C4A
82	S7	202	PEB	C4A-C3A-CAA-CBA
82	S7	202	PEB	NB-C1B-CHA-C4A
82	S7	202	PEB	C2B-C1B-CHA-C4A
82	T7	201	PEB	NB-C1B-CHA-C4A
82	T7	201	PEB	C2B-C1B-CHA-C4A
82	T7	202	PEB	C4A-C3A-CAA-CBA
82	T7	202	PEB	NB-C1B-CHA-C4A
82	T7	202	PEB	C2B-C1B-CHA-C4A
82	T7	203	PEB	NB-C1B-CHA-C4A
82	T7	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	U7	201	PEB	NB-C1B-CHA-C4A
82	U7	202	PEB	C4A-C3A-CAA-CBA
82	U7	202	PEB	NB-C1B-CHA-C4A
82	U7	202	PEB	C2B-C1B-CHA-C4A
82	V7	201	PEB	ND-C1D-CHC-C4C
82	V7	201	PEB	C2D-C1D-CHC-C4C
82	V7	201	PEB	C2A-C3A-CAA-CBA
82	V7	201	PEB	C4A-C3A-CAA-CBA
82	V7	201	PEB	NB-C1B-CHA-C4A
82	V7	201	PEB	C2B-C1B-CHA-C4A
82	V7	202	PEB	C2A-C3A-CAA-CBA
82	V7	202	PEB	C4A-C3A-CAA-CBA
82	V7	202	PEB	NB-C1B-CHA-C4A
82	V7	202	PEB	C2B-C1B-CHA-C4A
82	V7	203	PEB	NC-C1C-CHB-C4B
82	V7	203	PEB	C2C-C1C-CHB-C4B
82	V7	203	PEB	NB-C1B-CHA-C4A
82	V7	203	PEB	C2B-C1B-CHA-C4A
82	W7	201	PEB	NB-C1B-CHA-C4A
82	W7	201	PEB	C2B-C1B-CHA-C4A
82	W7	202	PEB	C2A-C3A-CAA-CBA
82	W7	202	PEB	C4A-C3A-CAA-CBA
82	W7	202	PEB	NB-C1B-CHA-C4A
82	W7	202	PEB	C2B-C1B-CHA-C4A
82	X7	201	PEB	NB-C1B-CHA-C4A
82	X7	201	PEB	C2B-C1B-CHA-C4A
82	X7	202	PEB	C2C-CAC-CBC-CGC
82	X7	202	PEB	C4A-C3A-CAA-CBA
82	X7	202	PEB	NB-C1B-CHA-C4A
82	X7	202	PEB	C2B-C1B-CHA-C4A
82	X7	203	PEB	NC-C1C-CHB-C4B
82	X7	203	PEB	C1C-C2C-CAC-CBC
82	X7	203	PEB	C2A-C3A-CAA-CBA
82	X7	203	PEB	NB-C1B-CHA-C4A
82	X7	203	PEB	C2B-C1B-CHA-C4A
82	Y7	301	PEB	C3C-C4C-CHC-C1D
82	Y7	301	PEB	ND-C1D-CHC-C4C
82	Y7	301	PEB	C2D-C1D-CHC-C4C
82	Y7	301	PEB	NC-C1C-CHB-C4B
82	Y7	301	PEB	C2C-C1C-CHB-C4B
82	Y7	301	PEB	C2A-C3A-CAA-CBA
82	Y7	301	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	Y7	301	PEB	NB-C1B-CHA-C4A
82	Y7	301	PEB	C2B-C1B-CHA-C4A
82	Y7	303	PEB	ND-C1D-CHC-C4C
82	Y7	303	PEB	C2D-C1D-CHC-C4C
82	Y7	303	PEB	NC-C1C-CHB-C4B
82	Y7	303	PEB	C2C-C1C-CHB-C4B
82	Y7	303	PEB	C2A-C3A-CAA-CBA
82	Y7	303	PEB	NB-C1B-CHA-C4A
82	Y7	303	PEB	C2B-C1B-CHA-C4A
82	Y7	304	PEB	ND-C1D-CHC-C4C
82	Y7	304	PEB	C2D-C1D-CHC-C4C
82	Y7	304	PEB	NC-C1C-CHB-C4B
82	Y7	304	PEB	C2C-C1C-CHB-C4B
82	Y7	304	PEB	C2A-C3A-CAA-CBA
82	Y7	304	PEB	NB-C1B-CHA-C4A
82	Y7	304	PEB	C2B-C1B-CHA-C4A
82	e7	301	PEB	ND-C1D-CHC-C4C
82	e7	301	PEB	C2D-C1D-CHC-C4C
82	e7	301	PEB	NB-C1B-CHA-C4A
82	e7	301	PEB	C2B-C1B-CHA-C4A
82	y8	201	PEB	ND-C1D-CHC-C4C
82	y8	201	PEB	C2A-C3A-CAA-CBA
82	y8	201	PEB	C4A-C3A-CAA-CBA
82	y8	201	PEB	C3A-C4A-CHA-C1B
82	y8	201	PEB	NB-C1B-CHA-C4A
82	y8	201	PEB	C2B-C1B-CHA-C4A
82	y8	202	PEB	C2A-C3A-CAA-CBA
82	y8	202	PEB	C4A-C3A-CAA-CBA
82	y8	202	PEB	NB-C1B-CHA-C4A
82	y8	202	PEB	C2B-C1B-CHA-C4A
82	y8	203	PEB	ND-C1D-CHC-C4C
82	y8	203	PEB	C2D-C1D-CHC-C4C
82	y8	203	PEB	NB-C1B-CHA-C4A
82	y8	203	PEB	C2B-C1B-CHA-C4A
82	z8	201	PEB	C4A-C3A-CAA-CBA
82	z8	201	PEB	NB-C1B-CHA-C4A
82	z8	201	PEB	C2B-C1B-CHA-C4A
82	z8	202	PEB	ND-C1D-CHC-C4C
82	z8	202	PEB	C2D-C1D-CHC-C4C
82	z8	202	PEB	NC-C1C-CHB-C4B
82	z8	202	PEB	C2C-C1C-CHB-C4B
82	z8	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	z8	202	PEB	C2B-C1B-CHA-C4A
82	18	201	PEB	ND-C1D-CHC-C4C
82	18	201	PEB	C2D-C1D-CHC-C4C
82	18	201	PEB	C2A-C3A-CAA-CBA
82	18	201	PEB	C4A-C3A-CAA-CBA
82	18	201	PEB	NB-C1B-CHA-C4A
82	18	201	PEB	C2B-C1B-CHA-C4A
82	18	201	PEB	C3B-CAB-CBB-CGB
82	18	202	PEB	C2A-C3A-CAA-CBA
82	18	202	PEB	C4A-C3A-CAA-CBA
82	18	202	PEB	NB-C1B-CHA-C4A
82	18	202	PEB	C2B-C1B-CHA-C4A
82	18	203	PEB	ND-C1D-CHC-C4C
82	18	203	PEB	C2D-C1D-CHC-C4C
82	18	203	PEB	NB-C1B-CHA-C4A
82	18	203	PEB	C2B-C1B-CHA-C4A
82	p8	201	PEB	ND-C1D-CHC-C4C
82	p8	201	PEB	C2D-C1D-CHC-C4C
82	p8	201	PEB	C4A-C3A-CAA-CBA
82	p8	201	PEB	NB-C1B-CHA-C4A
82	p8	201	PEB	C2B-C1B-CHA-C4A
82	p8	202	PEB	ND-C1D-CHC-C4C
82	p8	202	PEB	C2D-C1D-CHC-C4C
82	p8	202	PEB	NC-C1C-CHB-C4B
82	p8	202	PEB	C2C-C1C-CHB-C4B
82	p8	202	PEB	C2A-C3A-CAA-CBA
82	p8	202	PEB	C4A-C3A-CAA-CBA
82	p8	202	PEB	NB-C1B-CHA-C4A
82	p8	202	PEB	C2B-C1B-CHA-C4A
82	q8	201	PEB	ND-C1D-CHC-C4C
82	q8	201	PEB	NB-C1B-CHA-C4A
82	q8	201	PEB	C2B-C1B-CHA-C4A
82	q8	202	PEB	C4A-C3A-CAA-CBA
82	q8	202	PEB	NB-C1B-CHA-C4A
82	q8	202	PEB	C2B-C1B-CHA-C4A
82	q8	203	PEB	C2D-C1D-CHC-C4C
82	q8	203	PEB	NB-C1B-CHA-C4A
82	q8	203	PEB	C2B-C1B-CHA-C4A
82	r8	201	PEB	ND-C1D-CHC-C4C
82	r8	201	PEB	C2D-C1D-CHC-C4C
82	r8	201	PEB	NB-C1B-CHA-C4A
82	r8	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	r8	202	PEB	ND-C1D-CHC-C4C
82	r8	202	PEB	C2D-C1D-CHC-C4C
82	r8	202	PEB	NC-C1C-CHB-C4B
82	r8	202	PEB	C2C-C1C-CHB-C4B
82	r8	202	PEB	C4A-C3A-CAA-CBA
82	r8	202	PEB	NB-C1B-CHA-C4A
82	r8	202	PEB	C2B-C1B-CHA-C4A
82	s8	201	PEB	ND-C1D-CHC-C4C
82	s8	201	PEB	C2D-C1D-CHC-C4C
82	s8	201	PEB	NB-C1B-CHA-C4A
82	s8	201	PEB	C2B-C1B-CHA-C4A
82	s8	202	PEB	C2A-C3A-CAA-CBA
82	s8	202	PEB	C4A-C3A-CAA-CBA
82	s8	202	PEB	NB-C1B-CHA-C4A
82	s8	202	PEB	C2B-C1B-CHA-C4A
82	s8	203	PEB	NB-C1B-CHA-C4A
82	s8	203	PEB	C2B-C1B-CHA-C4A
82	t8	201	PEB	ND-C1D-CHC-C4C
82	t8	201	PEB	C2D-C1D-CHC-C4C
82	t8	201	PEB	NB-C1B-CHA-C4A
82	t8	201	PEB	C2B-C1B-CHA-C4A
82	t8	202	PEB	ND-C1D-CHC-C4C
82	t8	202	PEB	C2D-C1D-CHC-C4C
82	t8	202	PEB	NC-C1C-CHB-C4B
82	t8	202	PEB	C2C-C1C-CHB-C4B
82	t8	202	PEB	C2D-C3D-CAD-CBD
82	t8	202	PEB	C4D-C3D-CAD-CBD
82	t8	202	PEB	C2A-C3A-CAA-CBA
82	t8	202	PEB	C4A-C3A-CAA-CBA
82	t8	202	PEB	NB-C1B-CHA-C4A
82	t8	202	PEB	C2B-C1B-CHA-C4A
82	u8	201	PEB	C4A-C3A-CAA-CBA
82	u8	201	PEB	NB-C1B-CHA-C4A
82	u8	201	PEB	C2B-C1B-CHA-C4A
82	u8	202	PEB	C4A-C3A-CAA-CBA
82	u8	202	PEB	NB-C1B-CHA-C4A
82	u8	202	PEB	C2B-C1B-CHA-C4A
82	u8	203	PEB	NB-C1B-CHA-C4A
82	u8	203	PEB	C2B-C1B-CHA-C4A
82	v8	201	PEB	ND-C1D-CHC-C4C
82	v8	201	PEB	C2D-C1D-CHC-C4C
82	v8	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	v8	201	PEB	C4A-C3A-CAA-CBA
82	v8	201	PEB	NB-C1B-CHA-C4A
82	v8	201	PEB	C2B-C1B-CHA-C4A
82	v8	202	PEB	NC-C1C-CHB-C4B
82	v8	202	PEB	C2C-C1C-CHB-C4B
82	v8	202	PEB	C4A-C3A-CAA-CBA
82	v8	202	PEB	NB-C1B-CHA-C4A
82	v8	202	PEB	C2B-C1B-CHA-C4A
82	w8	201	PEB	ND-C1D-CHC-C4C
82	w8	201	PEB	C2D-C1D-CHC-C4C
82	w8	201	PEB	C2A-C3A-CAA-CBA
82	w8	201	PEB	C4A-C3A-CAA-CBA
82	w8	201	PEB	NB-C1B-CHA-C4A
82	w8	201	PEB	C2B-C1B-CHA-C4A
82	w8	202	PEB	C4A-C3A-CAA-CBA
82	w8	202	PEB	NB-C1B-CHA-C4A
82	w8	202	PEB	C2B-C1B-CHA-C4A
82	w8	202	PEB	C3B-CAB-CBB-CGB
82	w8	203	PEB	NB-C1B-CHA-C4A
82	w8	203	PEB	C2B-C1B-CHA-C4A
82	w8	204	PEB	ND-C1D-CHC-C4C
82	w8	204	PEB	C2D-C1D-CHC-C4C
82	w8	204	PEB	C2A-C3A-CAA-CBA
82	w8	204	PEB	C4A-C3A-CAA-CBA
82	w8	204	PEB	NB-C1B-CHA-C4A
82	w8	204	PEB	C2B-C1B-CHA-C4A
82	x8	201	PEB	ND-C1D-CHC-C4C
82	x8	201	PEB	C2D-C1D-CHC-C4C
82	x8	201	PEB	C4A-C3A-CAA-CBA
82	x8	201	PEB	NB-C1B-CHA-C4A
82	x8	201	PEB	C2B-C1B-CHA-C4A
82	x8	202	PEB	ND-C1D-CHC-C4C
82	x8	202	PEB	C2D-C1D-CHC-C4C
82	x8	202	PEB	NC-C1C-CHB-C4B
82	x8	202	PEB	C2C-C1C-CHB-C4B
82	x8	202	PEB	C4A-C3A-CAA-CBA
82	x8	202	PEB	NB-C1B-CHA-C4A
82	x8	202	PEB	C2B-C1B-CHA-C4A
82	A9	201	PEB	ND-C1D-CHC-C4C
82	A9	201	PEB	C2D-C1D-CHC-C4C
82	A9	201	PEB	NB-C1B-CHA-C4A
82	A9	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	A9	202	PEB	ND-C1D-CHC-C4C
82	A9	202	PEB	C2D-C1D-CHC-C4C
82	A9	202	PEB	NC-C1C-CHB-C4B
82	A9	202	PEB	C2C-C1C-CHB-C4B
82	A9	202	PEB	C4A-C3A-CAA-CBA
82	A9	202	PEB	NB-C1B-CHA-C4A
82	A9	202	PEB	C2B-C1B-CHA-C4A
82	B9	201	PEB	ND-C1D-CHC-C4C
82	B9	201	PEB	C2D-C1D-CHC-C4C
82	B9	201	PEB	NB-C1B-CHA-C4A
82	B9	201	PEB	C2B-C1B-CHA-C4A
82	B9	202	PEB	C2A-C3A-CAA-CBA
82	B9	202	PEB	C4A-C3A-CAA-CBA
82	B9	202	PEB	NB-C1B-CHA-C4A
82	B9	202	PEB	C2B-C1B-CHA-C4A
82	B9	203	PEB	ND-C1D-CHC-C4C
82	B9	203	PEB	C2D-C1D-CHC-C4C
82	B9	203	PEB	NB-C1B-CHA-C4A
82	B9	203	PEB	C2B-C1B-CHA-C4A
82	C9	201	PEB	ND-C1D-CHC-C4C
82	C9	201	PEB	C2D-C1D-CHC-C4C
82	C9	201	PEB	NB-C1B-CHA-C4A
82	C9	201	PEB	C2B-C1B-CHA-C4A
82	C9	202	PEB	ND-C1D-CHC-C4C
82	C9	202	PEB	C2D-C1D-CHC-C4C
82	C9	202	PEB	NC-C1C-CHB-C4B
82	C9	202	PEB	C2C-C1C-CHB-C4B
82	C9	202	PEB	C4A-C3A-CAA-CBA
82	C9	202	PEB	NB-C1B-CHA-C4A
82	C9	202	PEB	C2B-C1B-CHA-C4A
82	D9	201	PEB	ND-C1D-CHC-C4C
82	D9	201	PEB	C2D-C1D-CHC-C4C
82	D9	201	PEB	NB-C1B-CHA-C4A
82	D9	201	PEB	C2B-C1B-CHA-C4A
82	D9	202	PEB	C2A-C3A-CAA-CBA
82	D9	202	PEB	C4A-C3A-CAA-CBA
82	D9	202	PEB	NB-C1B-CHA-C4A
82	D9	202	PEB	C2B-C1B-CHA-C4A
82	D9	203	PEB	ND-C1D-CHC-C4C
82	D9	203	PEB	C2D-C1D-CHC-C4C
82	D9	203	PEB	NB-C1B-CHA-C4A
82	D9	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	E9	201	PEB	ND-C1D-CHC-C4C
82	E9	201	PEB	C2D-C1D-CHC-C4C
82	E9	201	PEB	NB-C1B-CHA-C4A
82	E9	201	PEB	C2B-C1B-CHA-C4A
82	E9	202	PEB	ND-C1D-CHC-C4C
82	E9	202	PEB	C2D-C1D-CHC-C4C
82	E9	202	PEB	NC-C1C-CHB-C4B
82	E9	202	PEB	C2C-C1C-CHB-C4B
82	E9	202	PEB	C4A-C3A-CAA-CBA
82	E9	202	PEB	NB-C1B-CHA-C4A
82	E9	202	PEB	C2B-C1B-CHA-C4A
82	F9	201	PEB	ND-C1D-CHC-C4C
82	F9	201	PEB	C2D-C1D-CHC-C4C
82	F9	201	PEB	NB-C1B-CHA-C4A
82	F9	201	PEB	C2B-C1B-CHA-C4A
82	F9	202	PEB	C4A-C3A-CAA-CBA
82	F9	202	PEB	NB-C1B-CHA-C4A
82	F9	202	PEB	C2B-C1B-CHA-C4A
82	F9	203	PEB	ND-C1D-CHC-C4C
82	F9	203	PEB	C2D-C1D-CHC-C4C
82	F9	203	PEB	C4A-C3A-CAA-CBA
82	F9	203	PEB	NB-C1B-CHA-C4A
82	F9	203	PEB	C2B-C1B-CHA-C4A
82	G9	201	PEB	ND-C1D-CHC-C4C
82	G9	201	PEB	C2D-C1D-CHC-C4C
82	G9	201	PEB	NB-C1B-CHA-C4A
82	G9	201	PEB	C2B-C1B-CHA-C4A
82	G9	202	PEB	ND-C1D-CHC-C4C
82	G9	202	PEB	C2D-C1D-CHC-C4C
82	G9	202	PEB	NC-C1C-CHB-C4B
82	G9	202	PEB	C2C-C1C-CHB-C4B
82	G9	202	PEB	C4A-C3A-CAA-CBA
82	G9	202	PEB	NB-C1B-CHA-C4A
82	G9	202	PEB	C2B-C1B-CHA-C4A
82	H9	201	PEB	ND-C1D-CHC-C4C
82	H9	201	PEB	C2D-C1D-CHC-C4C
82	H9	201	PEB	NB-C1B-CHA-C4A
82	H9	201	PEB	C2B-C1B-CHA-C4A
82	H9	202	PEB	C2A-C3A-CAA-CBA
82	H9	202	PEB	C4A-C3A-CAA-CBA
82	H9	202	PEB	NB-C1B-CHA-C4A
82	H9	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	H9	203	PEB	ND-C1D-CHC-C4C
82	H9	203	PEB	C2D-C1D-CHC-C4C
82	H9	203	PEB	C2A-C3A-CAA-CBA
82	H9	203	PEB	C4A-C3A-CAA-CBA
82	H9	203	PEB	NB-C1B-CHA-C4A
82	H9	203	PEB	C2B-C1B-CHA-C4A
82	I9	201	PEB	ND-C1D-CHC-C4C
82	I9	201	PEB	C2D-C1D-CHC-C4C
82	I9	201	PEB	NB-C1B-CHA-C4A
82	I9	201	PEB	C2B-C1B-CHA-C4A
82	I9	202	PEB	ND-C1D-CHC-C4C
82	I9	202	PEB	C2D-C1D-CHC-C4C
82	I9	202	PEB	NC-C1C-CHB-C4B
82	I9	202	PEB	C2C-C1C-CHB-C4B
82	I9	202	PEB	C4A-C3A-CAA-CBA
82	I9	202	PEB	NB-C1B-CHA-C4A
82	I9	202	PEB	C2B-C1B-CHA-C4A
82	J9	201	PEB	ND-C1D-CHC-C4C
82	J9	201	PEB	C2D-C1D-CHC-C4C
82	J9	201	PEB	NB-C1B-CHA-C4A
82	J9	201	PEB	C2B-C1B-CHA-C4A
82	J9	202	PEB	C2C-CAC-CBC-CGC
82	J9	202	PEB	C2A-C3A-CAA-CBA
82	J9	202	PEB	C4A-C3A-CAA-CBA
82	J9	202	PEB	NB-C1B-CHA-C4A
82	J9	202	PEB	C2B-C1B-CHA-C4A
82	J9	203	PEB	ND-C1D-CHC-C4C
82	J9	203	PEB	C2D-C1D-CHC-C4C
82	J9	203	PEB	NB-C1B-CHA-C4A
82	J9	203	PEB	C2B-C1B-CHA-C4A
82	K9	201	PEB	ND-C1D-CHC-C4C
82	K9	201	PEB	C2D-C1D-CHC-C4C
82	K9	201	PEB	NB-C1B-CHA-C4A
82	K9	201	PEB	C2B-C1B-CHA-C4A
82	K9	202	PEB	ND-C1D-CHC-C4C
82	K9	202	PEB	C2D-C1D-CHC-C4C
82	K9	202	PEB	NC-C1C-CHB-C4B
82	K9	202	PEB	C2C-C1C-CHB-C4B
82	K9	202	PEB	C4A-C3A-CAA-CBA
82	K9	202	PEB	NB-C1B-CHA-C4A
82	K9	202	PEB	C2B-C1B-CHA-C4A
82	L9	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	L9	201	PEB	C2D-C1D-CHC-C4C
82	L9	201	PEB	NB-C1B-CHA-C4A
82	L9	201	PEB	C2B-C1B-CHA-C4A
82	L9	202	PEB	C2A-C3A-CAA-CBA
82	L9	202	PEB	C4A-C3A-CAA-CBA
82	L9	202	PEB	NB-C1B-CHA-C4A
82	L9	202	PEB	C2B-C1B-CHA-C4A
82	L9	203	PEB	ND-C1D-CHC-C4C
82	L9	203	PEB	C2D-C1D-CHC-C4C
82	L9	203	PEB	NB-C1B-CHA-C4A
82	L9	203	PEB	C2B-C1B-CHA-C4A
82	N9	201	PEB	ND-C1D-CHC-C4C
82	N9	201	PEB	C2D-C1D-CHC-C4C
82	N9	201	PEB	NB-C1B-CHA-C4A
82	N9	201	PEB	C2B-C1B-CHA-C4A
82	N9	202	PEB	ND-C1D-CHC-C4C
82	N9	202	PEB	C2D-C1D-CHC-C4C
82	N9	202	PEB	NC-C1C-CHB-C4B
82	N9	202	PEB	C2C-C1C-CHB-C4B
82	N9	202	PEB	C4A-C3A-CAA-CBA
82	N9	202	PEB	NB-C1B-CHA-C4A
82	N9	202	PEB	C2B-C1B-CHA-C4A
82	O9	201	PEB	ND-C1D-CHC-C4C
82	O9	201	PEB	C2D-C1D-CHC-C4C
82	O9	201	PEB	C2A-C3A-CAA-CBA
82	O9	201	PEB	C4A-C3A-CAA-CBA
82	O9	201	PEB	NB-C1B-CHA-C4A
82	O9	201	PEB	C2B-C1B-CHA-C4A
82	O9	202	PEB	C2A-C3A-CAA-CBA
82	O9	202	PEB	C4A-C3A-CAA-CBA
82	O9	202	PEB	NB-C1B-CHA-C4A
82	O9	202	PEB	C2B-C1B-CHA-C4A
82	O9	203	PEB	ND-C1D-CHC-C4C
82	O9	203	PEB	C2D-C1D-CHC-C4C
82	O9	203	PEB	NB-C1B-CHA-C4A
82	O9	203	PEB	C2B-C1B-CHA-C4A
82	P9	201	PEB	ND-C1D-CHC-C4C
82	P9	201	PEB	C2D-C1D-CHC-C4C
82	P9	201	PEB	NB-C1B-CHA-C4A
82	P9	201	PEB	C2B-C1B-CHA-C4A
82	P9	202	PEB	ND-C1D-CHC-C4C
82	P9	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	P9	202	PEB	NC-C1C-CHB-C4B
82	P9	202	PEB	C2C-C1C-CHB-C4B
82	P9	202	PEB	C4A-C3A-CAA-CBA
82	P9	202	PEB	NB-C1B-CHA-C4A
82	P9	202	PEB	C2B-C1B-CHA-C4A
82	Q9	201	PEB	ND-C1D-CHC-C4C
82	Q9	201	PEB	C2D-C1D-CHC-C4C
82	Q9	201	PEB	NB-C1B-CHA-C4A
82	Q9	201	PEB	C2B-C1B-CHA-C4A
82	Q9	202	PEB	C2A-C3A-CAA-CBA
82	Q9	202	PEB	C4A-C3A-CAA-CBA
82	Q9	202	PEB	NB-C1B-CHA-C4A
82	Q9	202	PEB	C2B-C1B-CHA-C4A
82	Q9	203	PEB	ND-C1D-CHC-C4C
82	Q9	203	PEB	C2D-C1D-CHC-C4C
82	Q9	203	PEB	NB-C1B-CHA-C4A
82	Q9	203	PEB	C2B-C1B-CHA-C4A
82	R9	201	PEB	ND-C1D-CHC-C4C
82	R9	201	PEB	C2D-C1D-CHC-C4C
82	R9	201	PEB	NB-C1B-CHA-C4A
82	R9	201	PEB	C2B-C1B-CHA-C4A
82	R9	202	PEB	ND-C1D-CHC-C4C
82	R9	202	PEB	C2D-C1D-CHC-C4C
82	R9	202	PEB	NC-C1C-CHB-C4B
82	R9	202	PEB	C2C-C1C-CHB-C4B
82	R9	202	PEB	C4A-C3A-CAA-CBA
82	R9	202	PEB	NB-C1B-CHA-C4A
82	R9	202	PEB	C2B-C1B-CHA-C4A
82	S9	201	PEB	ND-C1D-CHC-C4C
82	S9	201	PEB	C2D-C1D-CHC-C4C
82	S9	201	PEB	NB-C1B-CHA-C4A
82	S9	201	PEB	C2B-C1B-CHA-C4A
82	S9	202	PEB	C4A-C3A-CAA-CBA
82	S9	202	PEB	NB-C1B-CHA-C4A
82	S9	202	PEB	C2B-C1B-CHA-C4A
82	S9	203	PEB	ND-C1D-CHC-C4C
82	S9	203	PEB	C2D-C1D-CHC-C4C
82	S9	203	PEB	C2A-C3A-CAA-CBA
82	S9	203	PEB	C4A-C3A-CAA-CBA
82	S9	203	PEB	NB-C1B-CHA-C4A
82	S9	203	PEB	C2B-C1B-CHA-C4A
82	T9	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	T9	201	PEB	C2D-C1D-CHC-C4C
82	T9	201	PEB	NB-C1B-CHA-C4A
82	T9	201	PEB	C2B-C1B-CHA-C4A
82	T9	202	PEB	ND-C1D-CHC-C4C
82	T9	202	PEB	C2D-C1D-CHC-C4C
82	T9	202	PEB	NC-C1C-CHB-C4B
82	T9	202	PEB	C2C-C1C-CHB-C4B
82	T9	202	PEB	C4A-C3A-CAA-CBA
82	T9	202	PEB	NB-C1B-CHA-C4A
82	T9	202	PEB	C2B-C1B-CHA-C4A
82	U9	201	PEB	ND-C1D-CHC-C4C
82	U9	201	PEB	C2D-C1D-CHC-C4C
82	U9	201	PEB	NB-C1B-CHA-C4A
82	U9	201	PEB	C2B-C1B-CHA-C4A
82	U9	202	PEB	C2A-C3A-CAA-CBA
82	U9	202	PEB	C4A-C3A-CAA-CBA
82	U9	202	PEB	NB-C1B-CHA-C4A
82	U9	202	PEB	C2B-C1B-CHA-C4A
82	U9	203	PEB	ND-C1D-CHC-C4C
82	U9	203	PEB	C2D-C1D-CHC-C4C
82	U9	203	PEB	NB-C1B-CHA-C4A
82	U9	203	PEB	C2B-C1B-CHA-C4A
82	U9	204	PEB	ND-C1D-CHC-C4C
82	U9	204	PEB	C2D-C1D-CHC-C4C
82	U9	204	PEB	C4A-C3A-CAA-CBA
82	U9	204	PEB	NB-C1B-CHA-C4A
82	U9	204	PEB	C2B-C1B-CHA-C4A
82	V9	201	PEB	ND-C1D-CHC-C4C
82	V9	201	PEB	C2D-C1D-CHC-C4C
82	V9	201	PEB	NB-C1B-CHA-C4A
82	V9	201	PEB	C2B-C1B-CHA-C4A
82	V9	202	PEB	ND-C1D-CHC-C4C
82	V9	202	PEB	C2D-C1D-CHC-C4C
82	V9	202	PEB	NC-C1C-CHB-C4B
82	V9	202	PEB	C2C-C1C-CHB-C4B
82	V9	202	PEB	C4A-C3A-CAA-CBA
82	V9	202	PEB	NB-C1B-CHA-C4A
82	V9	202	PEB	C2B-C1B-CHA-C4A
82	W9	201	PEB	ND-C1D-CHC-C4C
82	W9	201	PEB	C2D-C1D-CHC-C4C
82	W9	201	PEB	NB-C1B-CHA-C4A
82	W9	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	W9	202	PEB	C4A-C3A-CAA-CBA
82	W9	202	PEB	NB-C1B-CHA-C4A
82	W9	202	PEB	C2B-C1B-CHA-C4A
82	W9	203	PEB	C2D-C1D-CHC-C4C
82	W9	203	PEB	NB-C1B-CHA-C4A
82	W9	203	PEB	C2B-C1B-CHA-C4A
82	W9	203	PEB	C3B-CAB-CBB-CGB
82	X9	201	PEB	ND-C1D-CHC-C4C
82	X9	201	PEB	C2D-C1D-CHC-C4C
82	X9	201	PEB	NB-C1B-CHA-C4A
82	X9	201	PEB	C2B-C1B-CHA-C4A
82	X9	202	PEB	ND-C1D-CHC-C4C
82	X9	202	PEB	C2D-C1D-CHC-C4C
82	X9	202	PEB	NC-C1C-CHB-C4B
82	X9	202	PEB	C2C-C1C-CHB-C4B
82	X9	202	PEB	C4A-C3A-CAA-CBA
82	X9	202	PEB	NB-C1B-CHA-C4A
82	X9	202	PEB	C2B-C1B-CHA-C4A
82	Y9	201	PEB	ND-C1D-CHC-C4C
82	Y9	201	PEB	C2D-C1D-CHC-C4C
82	Y9	201	PEB	NB-C1B-CHA-C4A
82	Y9	201	PEB	C2B-C1B-CHA-C4A
82	Y9	202	PEB	C2A-C3A-CAA-CBA
82	Y9	202	PEB	C4A-C3A-CAA-CBA
82	Y9	202	PEB	NB-C1B-CHA-C4A
82	Y9	202	PEB	C2B-C1B-CHA-C4A
82	Y9	203	PEB	ND-C1D-CHC-C4C
82	Y9	203	PEB	C2D-C1D-CHC-C4C
82	Y9	203	PEB	NB-C1B-CHA-C4A
82	Y9	203	PEB	C2B-C1B-CHA-C4A
82	eA	301	PEB	ND-C1D-CHC-C4C
82	eA	301	PEB	C2D-C1D-CHC-C4C
82	eA	301	PEB	NB-C1B-CHA-C4A
82	eA	301	PEB	C2B-C1B-CHA-C4A
82	fB	301	PEB	C2A-C3A-CAA-CBA
82	fB	301	PEB	NB-C1B-CHA-C4A
82	fB	301	PEB	C2B-C1B-CHA-C4A
82	fB	301	PEB	C3B-CAB-CBB-CGB
82	aB	201	PEB	NB-C1B-CHA-C4A
82	aB	201	PEB	C2B-C1B-CHA-C4A
82	aB	202	PEB	NB-C1B-CHA-C4A
82	aB	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	bB	201	PEB	ND-C1D-CHC-C4C
82	bB	201	PEB	C2D-C1D-CHC-C4C
82	bB	201	PEB	NC-C1C-CHB-C4B
82	bB	201	PEB	C2C-C1C-CHB-C4B
82	bB	201	PEB	NB-C1B-CHA-C4A
82	bB	201	PEB	C2B-C1B-CHA-C4A
82	cB	401	PEB	ND-C1D-CHC-C4C
82	cB	401	PEB	C2D-C1D-CHC-C4C
82	cB	401	PEB	NB-C1B-CHA-C4A
82	cB	401	PEB	C2B-C1B-CHA-C4A
82	cB	402	PEB	C2D-C1D-CHC-C4C
82	cB	402	PEB	C2A-C3A-CAA-CBA
82	cB	402	PEB	C4A-C3A-CAA-CBA
82	cB	402	PEB	NB-C1B-CHA-C4A
82	cB	402	PEB	C2B-C1B-CHA-C4A
82	cB	403	PEB	C2D-C1D-CHC-C4C
82	cB	403	PEB	C1C-C2C-CAC-CBC
82	cB	403	PEB	C3C-C2C-CAC-CBC
82	cB	403	PEB	NB-C1B-CHA-C4A
82	cB	403	PEB	C2B-C1B-CHA-C4A
82	dB	201	PEB	C4A-C3A-CAA-CBA
82	dB	201	PEB	NB-C1B-CHA-C4A
82	dB	201	PEB	C2B-C1B-CHA-C4A
82	dB	202	PEB	ND-C1D-CHC-C4C
82	dB	202	PEB	C2D-C1D-CHC-C4C
82	dB	202	PEB	NC-C1C-CHB-C4B
82	dB	202	PEB	C2C-C1C-CHB-C4B
82	dB	202	PEB	NB-C1B-CHA-C4A
82	dB	202	PEB	C2B-C1B-CHA-C4A
82	eB	201	PEB	NB-C1B-CHA-C4A
82	eB	201	PEB	C2B-C1B-CHA-C4A
82	eB	202	PEB	NB-C1B-CHA-C4A
82	eB	202	PEB	C2B-C1B-CHA-C4A
82	gB	201	PEB	ND-C1D-CHC-C4C
82	gB	201	PEB	C2D-C1D-CHC-C4C
82	gB	201	PEB	NB-C1B-CHA-C4A
82	gB	201	PEB	C2B-C1B-CHA-C4A
82	gB	202	PEB	ND-C1D-CHC-C4C
82	gB	202	PEB	C2D-C1D-CHC-C4C
82	gB	202	PEB	NB-C1B-CHA-C4A
82	gB	202	PEB	C2B-C1B-CHA-C4A
82	gB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	gB	203	PEB	C2D-C1D-CHC-C4C
82	gB	203	PEB	NC-C1C-CHB-C4B
82	gB	203	PEB	C2C-C1C-CHB-C4B
82	gB	203	PEB	C2A-C3A-CAA-CBA
82	gB	203	PEB	C4A-C3A-CAA-CBA
82	gB	203	PEB	NB-C1B-CHA-C4A
82	gB	203	PEB	C2B-C1B-CHA-C4A
82	hB	301	PEB	C2A-C3A-CAA-CBA
82	hB	301	PEB	NB-C1B-CHA-C4A
82	hB	301	PEB	C2B-C1B-CHA-C4A
82	hB	301	PEB	C3B-CAB-CBB-CGB
82	yC	201	PEB	ND-C1D-CHC-C4C
82	yC	201	PEB	C2A-C3A-CAA-CBA
82	yC	201	PEB	C4A-C3A-CAA-CBA
82	yC	201	PEB	C3A-C4A-CHA-C1B
82	yC	201	PEB	NB-C1B-CHA-C4A
82	yC	201	PEB	C2B-C1B-CHA-C4A
82	yC	202	PEB	C2A-C3A-CAA-CBA
82	yC	202	PEB	C4A-C3A-CAA-CBA
82	yC	202	PEB	NB-C1B-CHA-C4A
82	yC	202	PEB	C2B-C1B-CHA-C4A
82	yC	203	PEB	ND-C1D-CHC-C4C
82	yC	203	PEB	C2D-C1D-CHC-C4C
82	yC	203	PEB	NB-C1B-CHA-C4A
82	yC	203	PEB	C2B-C1B-CHA-C4A
82	zC	201	PEB	C4A-C3A-CAA-CBA
82	zC	201	PEB	NB-C1B-CHA-C4A
82	zC	201	PEB	C2B-C1B-CHA-C4A
82	zC	202	PEB	ND-C1D-CHC-C4C
82	zC	202	PEB	C2D-C1D-CHC-C4C
82	zC	202	PEB	NC-C1C-CHB-C4B
82	zC	202	PEB	C2C-C1C-CHB-C4B
82	zC	202	PEB	NB-C1B-CHA-C4A
82	zC	202	PEB	C2B-C1B-CHA-C4A
82	1C	201	PEB	ND-C1D-CHC-C4C
82	1C	201	PEB	C2D-C1D-CHC-C4C
82	1C	201	PEB	C2A-C3A-CAA-CBA
82	1C	201	PEB	C4A-C3A-CAA-CBA
82	1C	201	PEB	NB-C1B-CHA-C4A
82	1C	201	PEB	C2B-C1B-CHA-C4A
82	1C	201	PEB	C3B-CAB-CBB-CGB
82	1C	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	1C	202	PEB	C4A-C3A-CAA-CBA
82	1C	202	PEB	NB-C1B-CHA-C4A
82	1C	202	PEB	C2B-C1B-CHA-C4A
82	1C	203	PEB	ND-C1D-CHC-C4C
82	1C	203	PEB	C2D-C1D-CHC-C4C
82	1C	203	PEB	NB-C1B-CHA-C4A
82	1C	203	PEB	C2B-C1B-CHA-C4A
82	pC	201	PEB	ND-C1D-CHC-C4C
82	pC	201	PEB	C2D-C1D-CHC-C4C
82	pC	201	PEB	C4A-C3A-CAA-CBA
82	pC	201	PEB	NB-C1B-CHA-C4A
82	pC	201	PEB	C2B-C1B-CHA-C4A
82	pC	202	PEB	ND-C1D-CHC-C4C
82	pC	202	PEB	C2D-C1D-CHC-C4C
82	pC	202	PEB	NC-C1C-CHB-C4B
82	pC	202	PEB	C2C-C1C-CHB-C4B
82	pC	202	PEB	C2A-C3A-CAA-CBA
82	pC	202	PEB	C4A-C3A-CAA-CBA
82	pC	202	PEB	NB-C1B-CHA-C4A
82	pC	202	PEB	C2B-C1B-CHA-C4A
82	qC	201	PEB	ND-C1D-CHC-C4C
82	qC	201	PEB	NB-C1B-CHA-C4A
82	qC	201	PEB	C2B-C1B-CHA-C4A
82	qC	202	PEB	C4A-C3A-CAA-CBA
82	qC	202	PEB	NB-C1B-CHA-C4A
82	qC	202	PEB	C2B-C1B-CHA-C4A
82	qC	203	PEB	C2D-C1D-CHC-C4C
82	qC	203	PEB	NB-C1B-CHA-C4A
82	qC	203	PEB	C2B-C1B-CHA-C4A
82	rC	201	PEB	ND-C1D-CHC-C4C
82	rC	201	PEB	C2D-C1D-CHC-C4C
82	rC	201	PEB	NB-C1B-CHA-C4A
82	rC	201	PEB	C2B-C1B-CHA-C4A
82	rC	202	PEB	ND-C1D-CHC-C4C
82	rC	202	PEB	C2D-C1D-CHC-C4C
82	rC	202	PEB	NC-C1C-CHB-C4B
82	rC	202	PEB	C2C-C1C-CHB-C4B
82	rC	202	PEB	C4A-C3A-CAA-CBA
82	rC	202	PEB	NB-C1B-CHA-C4A
82	rC	202	PEB	C2B-C1B-CHA-C4A
82	sC	201	PEB	ND-C1D-CHC-C4C
82	sC	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	sC	201	PEB	NB-C1B-CHA-C4A
82	sC	201	PEB	C2B-C1B-CHA-C4A
82	sC	202	PEB	C2A-C3A-CAA-CBA
82	sC	202	PEB	C4A-C3A-CAA-CBA
82	sC	202	PEB	NB-C1B-CHA-C4A
82	sC	202	PEB	C2B-C1B-CHA-C4A
82	sC	203	PEB	NB-C1B-CHA-C4A
82	sC	203	PEB	C2B-C1B-CHA-C4A
82	tC	201	PEB	ND-C1D-CHC-C4C
82	tC	201	PEB	C2D-C1D-CHC-C4C
82	tC	201	PEB	NB-C1B-CHA-C4A
82	tC	201	PEB	C2B-C1B-CHA-C4A
82	tC	202	PEB	ND-C1D-CHC-C4C
82	tC	202	PEB	C2D-C1D-CHC-C4C
82	tC	202	PEB	NC-C1C-CHB-C4B
82	tC	202	PEB	C2C-C1C-CHB-C4B
82	tC	202	PEB	C2D-C3D-CAD-CBD
82	tC	202	PEB	C4D-C3D-CAD-CBD
82	tC	202	PEB	C2A-C3A-CAA-CBA
82	tC	202	PEB	C4A-C3A-CAA-CBA
82	tC	202	PEB	NB-C1B-CHA-C4A
82	tC	202	PEB	C2B-C1B-CHA-C4A
82	uC	201	PEB	C4A-C3A-CAA-CBA
82	uC	201	PEB	NB-C1B-CHA-C4A
82	uC	201	PEB	C2B-C1B-CHA-C4A
82	uC	202	PEB	C4A-C3A-CAA-CBA
82	uC	202	PEB	NB-C1B-CHA-C4A
82	uC	202	PEB	C2B-C1B-CHA-C4A
82	uC	203	PEB	NB-C1B-CHA-C4A
82	uC	203	PEB	C2B-C1B-CHA-C4A
82	vC	201	PEB	ND-C1D-CHC-C4C
82	vC	201	PEB	C2D-C1D-CHC-C4C
82	vC	201	PEB	C2A-C3A-CAA-CBA
82	vC	201	PEB	C4A-C3A-CAA-CBA
82	vC	201	PEB	NB-C1B-CHA-C4A
82	vC	201	PEB	C2B-C1B-CHA-C4A
82	vC	202	PEB	NC-C1C-CHB-C4B
82	vC	202	PEB	C2C-C1C-CHB-C4B
82	vC	202	PEB	C4A-C3A-CAA-CBA
82	vC	202	PEB	NB-C1B-CHA-C4A
82	vC	202	PEB	C2B-C1B-CHA-C4A
82	wC	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	wC	201	PEB	C2D-C1D-CHC-C4C
82	wC	201	PEB	C2A-C3A-CAA-CBA
82	wC	201	PEB	C4A-C3A-CAA-CBA
82	wC	201	PEB	NB-C1B-CHA-C4A
82	wC	201	PEB	C2B-C1B-CHA-C4A
82	wC	202	PEB	C4A-C3A-CAA-CBA
82	wC	202	PEB	NB-C1B-CHA-C4A
82	wC	202	PEB	C2B-C1B-CHA-C4A
82	wC	202	PEB	C3B-CAB-CBB-CGB
82	wC	203	PEB	NB-C1B-CHA-C4A
82	wC	203	PEB	C2B-C1B-CHA-C4A
82	wC	204	PEB	ND-C1D-CHC-C4C
82	wC	204	PEB	C2D-C1D-CHC-C4C
82	wC	204	PEB	C2A-C3A-CAA-CBA
82	wC	204	PEB	C4A-C3A-CAA-CBA
82	wC	204	PEB	NB-C1B-CHA-C4A
82	wC	204	PEB	C2B-C1B-CHA-C4A
82	xC	201	PEB	ND-C1D-CHC-C4C
82	xC	201	PEB	C2D-C1D-CHC-C4C
82	xC	201	PEB	C4A-C3A-CAA-CBA
82	xC	201	PEB	NB-C1B-CHA-C4A
82	xC	201	PEB	C2B-C1B-CHA-C4A
82	xC	202	PEB	ND-C1D-CHC-C4C
82	xC	202	PEB	C2D-C1D-CHC-C4C
82	xC	202	PEB	NC-C1C-CHB-C4B
82	xC	202	PEB	C2C-C1C-CHB-C4B
82	xC	202	PEB	C4A-C3A-CAA-CBA
82	xC	202	PEB	NB-C1B-CHA-C4A
82	xC	202	PEB	C2B-C1B-CHA-C4A
82	dD	401	PEB	NB-C1B-CHA-C4A
82	dD	401	PEB	C2B-C1B-CHA-C4A
82	aE	201	PEB	C1C-C2C-CAC-CBC
82	aE	201	PEB	NB-C1B-CHA-C4A
82	aE	201	PEB	C2B-C1B-CHA-C4A
82	aE	202	PEB	C2D-C1D-CHC-C4C
82	aE	202	PEB	NB-C1B-CHA-C4A
82	aE	202	PEB	C2B-C1B-CHA-C4A
82	bE	201	PEB	NB-C1B-CHA-C4A
82	bE	201	PEB	C2B-C1B-CHA-C4A
82	bE	202	PEB	ND-C1D-CHC-C4C
82	bE	202	PEB	C2D-C1D-CHC-C4C
82	bE	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	bE	202	PEB	C4A-C3A-CAA-CBA
82	bE	202	PEB	NB-C1B-CHA-C4A
82	bE	202	PEB	C2B-C1B-CHA-C4A
82	cE	201	PEB	NB-C1B-CHA-C4A
82	cE	201	PEB	C2B-C1B-CHA-C4A
82	cE	202	PEB	ND-C1D-CHC-C4C
82	cE	202	PEB	C2D-C1D-CHC-C4C
82	cE	202	PEB	NC-C1C-CHB-C4B
82	cE	202	PEB	NB-C1B-CHA-C4A
82	cE	202	PEB	C2B-C1B-CHA-C4A
82	dE	201	PEB	ND-C1D-CHC-C4C
82	dE	201	PEB	C2D-C1D-CHC-C4C
82	dE	201	PEB	NB-C1B-CHA-C4A
82	dE	201	PEB	C2B-C1B-CHA-C4A
82	dE	202	PEB	C4A-C3A-CAA-CBA
82	dE	202	PEB	NB-C1B-CHA-C4A
82	dE	202	PEB	C2B-C1B-CHA-C4A
82	dE	203	PEB	C2D-C1D-CHC-C4C
82	dE	203	PEB	NB-C1B-CHA-C4A
82	dE	203	PEB	C2B-C1B-CHA-C4A
82	dE	204	PEB	C2A-C3A-CAA-CBA
82	dE	204	PEB	C4A-C3A-CAA-CBA
82	dE	204	PEB	NB-C1B-CHA-C4A
82	dE	204	PEB	C2B-C1B-CHA-C4A
82	eE	201	PEB	ND-C1D-CHC-C4C
82	eE	201	PEB	C2D-C1D-CHC-C4C
82	eE	201	PEB	NB-C1B-CHA-C4A
82	eE	201	PEB	C2B-C1B-CHA-C4A
82	eE	202	PEB	C2A-C3A-CAA-CBA
82	eE	202	PEB	C4A-C3A-CAA-CBA
82	eE	202	PEB	NB-C1B-CHA-C4A
82	eE	202	PEB	C2B-C1B-CHA-C4A
82	eE	203	PEB	ND-C1D-CHC-C4C
82	eE	203	PEB	C2D-C1D-CHC-C4C
82	eE	203	PEB	NC-C1C-CHB-C4B
82	eE	203	PEB	NB-C1B-CHA-C4A
82	eE	203	PEB	C2B-C1B-CHA-C4A
82	fE	201	PEB	ND-C1D-CHC-C4C
82	fE	201	PEB	C2D-C1D-CHC-C4C
82	fE	201	PEB	NB-C1B-CHA-C4A
82	fE	201	PEB	C2B-C1B-CHA-C4A
82	fE	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	fE	202	PEB	C2B-C1B-CHA-C4A
82	fE	203	PEB	ND-C1D-CHC-C4C
82	fE	203	PEB	C2D-C1D-CHC-C4C
82	fE	203	PEB	C2A-C3A-CAA-CBA
82	fE	203	PEB	C4A-C3A-CAA-CBA
82	fE	203	PEB	NB-C1B-CHA-C4A
82	fE	203	PEB	C2B-C1B-CHA-C4A
82	gE	201	PEB	NB-C1B-CHA-C4A
82	gE	201	PEB	C2B-C1B-CHA-C4A
82	gE	202	PEB	ND-C1D-CHC-C4C
82	gE	202	PEB	C2D-C1D-CHC-C4C
82	gE	202	PEB	NC-C1C-CHB-C4B
82	gE	202	PEB	C2C-C1C-CHB-C4B
82	gE	202	PEB	NB-C1B-CHA-C4A
82	gE	202	PEB	C2B-C1B-CHA-C4A
82	gE	202	PEB	C3B-CAB-CBB-CGB
82	hE	201	PEB	ND-C1D-CHC-C4C
82	hE	201	PEB	C2D-C1D-CHC-C4C
82	hE	201	PEB	C2A-C3A-CAA-CBA
82	hE	201	PEB	C4A-C3A-CAA-CBA
82	hE	201	PEB	NB-C1B-CHA-C4A
82	hE	201	PEB	C2B-C1B-CHA-C4A
82	hE	202	PEB	ND-C1D-CHC-C4C
82	hE	202	PEB	C2D-C1D-CHC-C4C
82	hE	202	PEB	C4A-C3A-CAA-CBA
82	hE	202	PEB	NB-C1B-CHA-C4A
82	hE	202	PEB	C2B-C1B-CHA-C4A
82	hE	203	PEB	NB-C1B-CHA-C4A
82	hE	203	PEB	C2B-C1B-CHA-C4A
82	iE	201	PEB	ND-C1D-CHC-C4C
82	iE	201	PEB	C2D-C1D-CHC-C4C
82	iE	201	PEB	NB-C1B-CHA-C4A
82	iE	201	PEB	C2B-C1B-CHA-C4A
82	iE	202	PEB	NC-C1C-CHB-C4B
82	iE	202	PEB	C2C-C1C-CHB-C4B
82	iE	202	PEB	NB-C1B-CHA-C4A
82	iE	202	PEB	C2B-C1B-CHA-C4A
82	jE	201	PEB	C4A-C3A-CAA-CBA
82	jE	201	PEB	NB-C1B-CHA-C4A
82	jE	201	PEB	C2B-C1B-CHA-C4A
82	jE	202	PEB	NB-C1B-CHA-C4A
82	jE	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	kE	201	PEB	C1C-C2C-CAC-CBC
82	kE	201	PEB	C3C-C2C-CAC-CBC
82	kE	201	PEB	NB-C1B-CHA-C4A
82	kE	201	PEB	C2B-C1B-CHA-C4A
82	kE	202	PEB	C2C-CAC-CBC-CGC
82	kE	202	PEB	NB-C1B-CHA-C4A
82	kE	202	PEB	C2B-C1B-CHA-C4A
82	lE	201	PEB	ND-C1D-CHC-C4C
82	lE	201	PEB	C2D-C1D-CHC-C4C
82	lE	201	PEB	C2A-C3A-CAA-CBA
82	lE	201	PEB	C4A-C3A-CAA-CBA
82	lE	201	PEB	NB-C1B-CHA-C4A
82	lE	201	PEB	C2B-C1B-CHA-C4A
82	lE	202	PEB	ND-C1D-CHC-C4C
82	lE	202	PEB	C2D-C1D-CHC-C4C
82	lE	202	PEB	C2A-C3A-CAA-CBA
82	lE	202	PEB	C4A-C3A-CAA-CBA
82	lE	202	PEB	NA-C4A-CHA-C1B
82	lE	202	PEB	C3A-C4A-CHA-C1B
82	lE	202	PEB	NB-C1B-CHA-C4A
82	lE	202	PEB	C2B-C1B-CHA-C4A
82	lE	203	PEB	NB-C1B-CHA-C4A
82	lE	203	PEB	C2B-C1B-CHA-C4A
82	mE	201	PEB	ND-C1D-CHC-C4C
82	mE	201	PEB	C2D-C1D-CHC-C4C
82	mE	201	PEB	NB-C1B-CHA-C4A
82	mE	201	PEB	C2B-C1B-CHA-C4A
82	mE	202	PEB	C2A-C3A-CAA-CBA
82	mE	202	PEB	C4A-C3A-CAA-CBA
82	mE	202	PEB	NB-C1B-CHA-C4A
82	mE	202	PEB	C2B-C1B-CHA-C4A
82	mE	203	PEB	C2D-C1D-CHC-C4C
82	mE	203	PEB	NC-C1C-CHB-C4B
82	mE	203	PEB	C2C-C1C-CHB-C4B
82	mE	203	PEB	NB-C1B-CHA-C4A
82	mE	203	PEB	C2B-C1B-CHA-C4A
82	aF	201	PEB	ND-C1D-CHC-C4C
82	aF	201	PEB	C2A-C3A-CAA-CBA
82	aF	201	PEB	C4A-C3A-CAA-CBA
82	aF	201	PEB	NB-C1B-CHA-C4A
82	aF	201	PEB	C2B-C1B-CHA-C4A
82	aF	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	aF	202	PEB	C4A-C3A-CAA-CBA
82	aF	202	PEB	NB-C1B-CHA-C4A
82	aF	202	PEB	C2B-C1B-CHA-C4A
82	aF	203	PEB	C2A-C3A-CAA-CBA
82	aF	203	PEB	NB-C1B-CHA-C4A
82	aF	203	PEB	C2B-C1B-CHA-C4A
82	bF	201	PEB	C2A-C3A-CAA-CBA
82	bF	201	PEB	C4A-C3A-CAA-CBA
82	bF	201	PEB	NB-C1B-CHA-C4A
82	bF	201	PEB	C2B-C1B-CHA-C4A
82	bF	202	PEB	C3C-C4C-CHC-C1D
82	bF	202	PEB	ND-C1D-CHC-C4C
82	bF	202	PEB	C2D-C1D-CHC-C4C
82	bF	202	PEB	NC-C1C-CHB-C4B
82	bF	202	PEB	C2C-C1C-CHB-C4B
82	bF	202	PEB	NB-C1B-CHA-C4A
82	bF	202	PEB	C2B-C1B-CHA-C4A
82	cF	201	PEB	ND-C1D-CHC-C4C
82	cF	201	PEB	C2D-C1D-CHC-C4C
82	cF	201	PEB	NB-C1B-CHA-C4A
82	cF	201	PEB	C2B-C1B-CHA-C4A
82	cF	202	PEB	C2C-CAC-CBC-CGC
82	cF	202	PEB	NB-C1B-CHA-C4A
82	cF	202	PEB	C2B-C1B-CHA-C4A
82	cF	203	PEB	C2A-C3A-CAA-CBA
82	cF	203	PEB	NB-C1B-CHA-C4A
82	cF	203	PEB	C2B-C1B-CHA-C4A
82	dF	201	PEB	ND-C1D-CHC-C4C
82	dF	201	PEB	C2D-C1D-CHC-C4C
82	dF	201	PEB	NB-C1B-CHA-C4A
82	dF	201	PEB	C2B-C1B-CHA-C4A
82	dF	202	PEB	C3C-C4C-CHC-C1D
82	dF	202	PEB	ND-C1D-CHC-C4C
82	dF	202	PEB	C2D-C1D-CHC-C4C
82	dF	202	PEB	NC-C1C-CHB-C4B
82	dF	202	PEB	NB-C1B-CHA-C4A
82	dF	202	PEB	C2B-C1B-CHA-C4A
82	eF	201	PEB	NC-C1C-CHB-C4B
82	eF	201	PEB	NB-C1B-CHA-C4A
82	eF	201	PEB	C2B-C1B-CHA-C4A
82	eF	202	PEB	ND-C1D-CHC-C4C
82	eF	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	eF	202	PEB	C4A-C3A-CAA-CBA
82	eF	202	PEB	NB-C1B-CHA-C4A
82	eF	202	PEB	C2B-C1B-CHA-C4A
82	eF	203	PEB	NB-C1B-CHA-C4A
82	eF	203	PEB	C2B-C1B-CHA-C4A
82	fF	201	PEB	C4A-C3A-CAA-CBA
82	fF	201	PEB	NB-C1B-CHA-C4A
82	fF	201	PEB	C2B-C1B-CHA-C4A
82	fF	202	PEB	C3C-C4C-CHC-C1D
82	fF	202	PEB	ND-C1D-CHC-C4C
82	fF	202	PEB	C2D-C1D-CHC-C4C
82	fF	202	PEB	NC-C1C-CHB-C4B
82	fF	202	PEB	C2C-C1C-CHB-C4B
82	fF	202	PEB	NB-C1B-CHA-C4A
82	fF	202	PEB	C2B-C1B-CHA-C4A
82	gF	201	PEB	C2D-C1D-CHC-C4C
82	gF	201	PEB	NB-C1B-CHA-C4A
82	gF	202	PEB	NB-C1B-CHA-C4A
82	gF	202	PEB	C2B-C1B-CHA-C4A
82	gF	203	PEB	C2A-C3A-CAA-CBA
82	gF	203	PEB	NB-C1B-CHA-C4A
82	gF	203	PEB	C2B-C1B-CHA-C4A
82	hF	201	PEB	NB-C1B-CHA-C4A
82	hF	201	PEB	C2B-C1B-CHA-C4A
82	hF	202	PEB	ND-C1D-CHC-C4C
82	hF	202	PEB	C2D-C1D-CHC-C4C
82	hF	202	PEB	NC-C1C-CHB-C4B
82	hF	202	PEB	NB-C1B-CHA-C4A
82	hF	202	PEB	C2B-C1B-CHA-C4A
82	iF	201	PEB	C4A-C3A-CAA-CBA
82	iF	201	PEB	NB-C1B-CHA-C4A
82	iF	201	PEB	C2B-C1B-CHA-C4A
82	iF	202	PEB	ND-C1D-CHC-C4C
82	iF	202	PEB	C2D-C1D-CHC-C4C
82	iF	202	PEB	C4A-C3A-CAA-CBA
82	iF	202	PEB	NB-C1B-CHA-C4A
82	iF	202	PEB	C2B-C1B-CHA-C4A
82	iF	203	PEB	NC-C1C-CHB-C4B
82	iF	203	PEB	C2C-C1C-CHB-C4B
82	iF	203	PEB	C4A-C3A-CAA-CBA
82	iF	203	PEB	NB-C1B-CHA-C4A
82	iF	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	jF	201	PEB	NB-C1B-CHA-C4A
82	jF	202	PEB	ND-C1D-CHC-C4C
82	jF	202	PEB	C2D-C1D-CHC-C4C
82	jF	202	PEB	NC-C1C-CHB-C4B
82	jF	202	PEB	C2C-C1C-CHB-C4B
82	jF	202	PEB	NB-C1B-CHA-C4A
82	jF	202	PEB	C2B-C1B-CHA-C4A
82	kF	201	PEB	ND-C1D-CHC-C4C
82	kF	201	PEB	C2D-C1D-CHC-C4C
82	kF	201	PEB	NC-C1C-CHB-C4B
82	kF	201	PEB	C2C-C1C-CHB-C4B
82	kF	201	PEB	C4A-C3A-CAA-CBA
82	kF	201	PEB	NB-C1B-CHA-C4A
82	kF	201	PEB	C2B-C1B-CHA-C4A
82	kF	201	PEB	C3B-CAB-CBB-CGB
82	kF	202	PEB	NC-C1C-CHB-C4B
82	kF	202	PEB	C2C-C1C-CHB-C4B
82	kF	202	PEB	C2A-C3A-CAA-CBA
82	kF	202	PEB	NB-C1B-CHA-C4A
82	kF	202	PEB	C2B-C1B-CHA-C4A
82	kF	203	PEB	ND-C1D-CHC-C4C
82	kF	203	PEB	C2D-C1D-CHC-C4C
82	kF	203	PEB	C2A-C3A-CAA-CBA
82	kF	203	PEB	C4A-C3A-CAA-CBA
82	kF	203	PEB	NB-C1B-CHA-C4A
82	kF	203	PEB	C2B-C1B-CHA-C4A
82	lF	201	PEB	C2A-C3A-CAA-CBA
82	lF	201	PEB	C4A-C3A-CAA-CBA
82	lF	201	PEB	NB-C1B-CHA-C4A
82	lF	201	PEB	C2B-C1B-CHA-C4A
82	lF	202	PEB	ND-C1D-CHC-C4C
82	lF	202	PEB	C2D-C1D-CHC-C4C
82	lF	202	PEB	NC-C1C-CHB-C4B
82	lF	202	PEB	C2C-C1C-CHB-C4B
82	lF	202	PEB	NB-C1B-CHA-C4A
82	lF	202	PEB	C2B-C1B-CHA-C4A
82	lF	203	PEB	C2A-C3A-CAA-CBA
82	lF	203	PEB	C4A-C3A-CAA-CBA
82	lF	203	PEB	NB-C1B-CHA-C4A
82	lF	203	PEB	C2B-C1B-CHA-C4A
82	mF	201	PEB	NC-C1C-CHB-C4B
82	mF	201	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	mF	201	PEB	NB-C1B-CHA-C4A
82	mF	201	PEB	C2B-C1B-CHA-C4A
82	mF	202	PEB	C2A-C3A-CAA-CBA
82	mF	202	PEB	C4A-C3A-CAA-CBA
82	mF	202	PEB	NB-C1B-CHA-C4A
82	mF	202	PEB	C2B-C1B-CHA-C4A
82	mF	202	PEB	C3B-CAB-CBB-CGB
82	nF	201	PEB	NB-C1B-CHA-C4A
82	nF	201	PEB	C2B-C1B-CHA-C4A
82	nF	202	PEB	ND-C1D-CHC-C4C
82	nF	202	PEB	C2D-C1D-CHC-C4C
82	nF	202	PEB	NC-C1C-CHB-C4B
82	nF	202	PEB	C2C-C1C-CHB-C4B
82	nF	202	PEB	NB-C1B-CHA-C4A
82	nF	202	PEB	C2B-C1B-CHA-C4A
82	oF	201	PEB	ND-C1D-CHC-C4C
82	oF	201	PEB	C2D-C1D-CHC-C4C
82	oF	201	PEB	C2A-C3A-CAA-CBA
82	oF	201	PEB	C4A-C3A-CAA-CBA
82	oF	201	PEB	NB-C1B-CHA-C4A
82	oF	201	PEB	C2B-C1B-CHA-C4A
82	oF	202	PEB	NB-C1B-CHA-C4A
82	oF	202	PEB	C2B-C1B-CHA-C4A
82	oF	203	PEB	ND-C1D-CHC-C4C
82	oF	203	PEB	C2D-C1D-CHC-C4C
82	oF	203	PEB	C2D-C3D-CAD-CBD
82	oF	203	PEB	C4D-C3D-CAD-CBD
82	oF	203	PEB	C2A-C3A-CAA-CBA
82	oF	203	PEB	C4A-C3A-CAA-CBA
82	oF	203	PEB	NB-C1B-CHA-C4A
82	oF	203	PEB	C2B-C1B-CHA-C4A
82	pF	201	PEB	C2A-C3A-CAA-CBA
82	pF	201	PEB	C4A-C3A-CAA-CBA
82	pF	201	PEB	NB-C1B-CHA-C4A
82	pF	201	PEB	C2B-C1B-CHA-C4A
82	pF	202	PEB	ND-C1D-CHC-C4C
82	pF	202	PEB	C2D-C1D-CHC-C4C
82	pF	202	PEB	NC-C1C-CHB-C4B
82	pF	202	PEB	C2C-C1C-CHB-C4B
82	pF	202	PEB	NB-C1B-CHA-C4A
82	pF	202	PEB	C2B-C1B-CHA-C4A
82	qF	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	qF	201	PEB	C4A-C3A-CAA-CBA
82	qF	201	PEB	NB-C1B-CHA-C4A
82	qF	201	PEB	C2B-C1B-CHA-C4A
82	qF	202	PEB	C4A-C3A-CAA-CBA
82	qF	202	PEB	NB-C1B-CHA-C4A
82	qF	202	PEB	C2B-C1B-CHA-C4A
82	qF	203	PEB	NC-C1C-CHB-C4B
82	qF	203	PEB	C2C-C1C-CHB-C4B
82	qF	203	PEB	C4A-C3A-CAA-CBA
82	qF	203	PEB	NB-C1B-CHA-C4A
82	qF	203	PEB	C2B-C1B-CHA-C4A
82	rF	201	PEB	ND-C1D-CHC-C4C
82	rF	201	PEB	C2D-C1D-CHC-C4C
82	rF	201	PEB	C2A-C3A-CAA-CBA
82	rF	201	PEB	C4A-C3A-CAA-CBA
82	rF	201	PEB	NB-C1B-CHA-C4A
82	rF	201	PEB	C2B-C1B-CHA-C4A
82	rF	202	PEB	ND-C1D-CHC-C4C
82	rF	202	PEB	C2D-C1D-CHC-C4C
82	rF	202	PEB	NC-C1C-CHB-C4B
82	rF	202	PEB	C2C-C1C-CHB-C4B
82	rF	202	PEB	NB-C1B-CHA-C4A
82	rF	202	PEB	C2B-C1B-CHA-C4A
82	sF	201	PEB	ND-C1D-CHC-C4C
82	sF	201	PEB	C2D-C1D-CHC-C4C
82	sF	201	PEB	C4A-C3A-CAA-CBA
82	sF	201	PEB	NB-C1B-CHA-C4A
82	sF	201	PEB	C2B-C1B-CHA-C4A
82	sF	202	PEB	NC-C1C-CHB-C4B
82	sF	202	PEB	C2C-C1C-CHB-C4B
82	sF	202	PEB	NB-C1B-CHA-C4A
82	sF	202	PEB	C2B-C1B-CHA-C4A
82	sF	203	PEB	NB-C1B-CHA-C4A
82	sF	203	PEB	C2B-C1B-CHA-C4A
82	tF	201	PEB	NB-C1B-CHA-C4A
82	tF	201	PEB	C2B-C1B-CHA-C4A
82	tF	202	PEB	ND-C1D-CHC-C4C
82	tF	202	PEB	C2D-C1D-CHC-C4C
82	tF	202	PEB	C1C-C2C-CAC-CBC
82	tF	202	PEB	C3C-C2C-CAC-CBC
82	tF	202	PEB	NB-C1B-CHA-C4A
82	tF	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	tF	202	PEB	C3B-CAB-CBB-CGB
82	uF	201	PEB	ND-C1D-CHC-C4C
82	uF	201	PEB	C2D-C1D-CHC-C4C
82	uF	201	PEB	C4A-C3A-CAA-CBA
82	uF	201	PEB	NB-C1B-CHA-C4A
82	uF	201	PEB	C2B-C1B-CHA-C4A
82	uF	202	PEB	ND-C1D-CHC-C4C
82	uF	202	PEB	C2D-C1D-CHC-C4C
82	uF	202	PEB	C2A-C3A-CAA-CBA
82	uF	202	PEB	C4A-C3A-CAA-CBA
82	uF	202	PEB	NB-C1B-CHA-C4A
82	uF	202	PEB	C2B-C1B-CHA-C4A
82	uF	203	PEB	NB-C1B-CHA-C4A
82	uF	203	PEB	C2B-C1B-CHA-C4A
82	vF	201	PEB	NB-C1B-CHA-C4A
82	vF	201	PEB	C2B-C1B-CHA-C4A
82	vF	202	PEB	ND-C1D-CHC-C4C
82	vF	202	PEB	C2D-C1D-CHC-C4C
82	vF	202	PEB	NC-C1C-CHB-C4B
82	vF	202	PEB	C2C-C1C-CHB-C4B
82	vF	202	PEB	NB-C1B-CHA-C4A
82	vF	202	PEB	C2B-C1B-CHA-C4A
82	wF	301	PEB	C2A-C3A-CAA-CBA
82	wF	301	PEB	NB-C1B-CHA-C4A
82	wF	301	PEB	C2B-C1B-CHA-C4A
82	wF	302	PEB	ND-C1D-CHC-C4C
82	wF	302	PEB	C2D-C1D-CHC-C4C
82	wF	302	PEB	C2A-C3A-CAA-CBA
82	wF	302	PEB	C4A-C3A-CAA-CBA
82	wF	302	PEB	NB-C1B-CHA-C4A
82	wF	302	PEB	C2B-C1B-CHA-C4A
82	wF	303	PEB	NB-C1B-CHA-C4A
82	wF	303	PEB	C2B-C1B-CHA-C4A
82	xF	302	PEB	ND-C1D-CHC-C4C
82	xF	302	PEB	C2D-C1D-CHC-C4C
82	xF	302	PEB	NC-C1C-CHB-C4B
82	xF	302	PEB	C2C-C1C-CHB-C4B
82	xF	302	PEB	NB-C1B-CHA-C4A
82	xF	302	PEB	C2B-C1B-CHA-C4A
82	xF	303	PEB	ND-C1D-CHC-C4C
82	xF	303	PEB	C2D-C1D-CHC-C4C
82	xF	303	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	xF	303	PEB	NB-C1B-CHA-C4A
82	xF	303	PEB	C2B-C1B-CHA-C4A
82	xF	304	PEB	C2C-CAC-CBC-CGC
82	xF	304	PEB	NB-C1B-CHA-C4A
82	xF	304	PEB	C2B-C1B-CHA-C4A
82	yF	301	PEB	C4A-C3A-CAA-CBA
82	yF	301	PEB	NB-C1B-CHA-C4A
82	yF	301	PEB	C2B-C1B-CHA-C4A
82	zF	501	PEB	C4A-C3A-CAA-CBA
82	zF	501	PEB	NB-C1B-CHA-C4A
82	zF	501	PEB	C2B-C1B-CHA-C4A
82	aG	201	PEB	C1C-C2C-CAC-CBC
82	aG	201	PEB	NB-C1B-CHA-C4A
82	aG	201	PEB	C2B-C1B-CHA-C4A
82	aG	202	PEB	C2D-C1D-CHC-C4C
82	aG	202	PEB	NB-C1B-CHA-C4A
82	aG	202	PEB	C2B-C1B-CHA-C4A
82	bG	201	PEB	NB-C1B-CHA-C4A
82	bG	201	PEB	C2B-C1B-CHA-C4A
82	cG	201	PEB	NB-C1B-CHA-C4A
82	cG	201	PEB	C2B-C1B-CHA-C4A
82	cG	202	PEB	ND-C1D-CHC-C4C
82	cG	202	PEB	C2D-C1D-CHC-C4C
82	cG	202	PEB	NC-C1C-CHB-C4B
82	cG	202	PEB	NB-C1B-CHA-C4A
82	cG	202	PEB	C2B-C1B-CHA-C4A
82	dG	201	PEB	ND-C1D-CHC-C4C
82	dG	201	PEB	C2D-C1D-CHC-C4C
82	dG	201	PEB	NB-C1B-CHA-C4A
82	dG	201	PEB	C2B-C1B-CHA-C4A
82	dG	202	PEB	C4A-C3A-CAA-CBA
82	dG	202	PEB	NB-C1B-CHA-C4A
82	dG	202	PEB	C2B-C1B-CHA-C4A
82	dG	203	PEB	C2D-C1D-CHC-C4C
82	dG	203	PEB	NB-C1B-CHA-C4A
82	dG	203	PEB	C2B-C1B-CHA-C4A
82	dG	204	PEB	C2A-C3A-CAA-CBA
82	dG	204	PEB	C4A-C3A-CAA-CBA
82	dG	204	PEB	NB-C1B-CHA-C4A
82	dG	204	PEB	C2B-C1B-CHA-C4A
82	eG	201	PEB	ND-C1D-CHC-C4C
82	eG	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	eG	201	PEB	NB-C1B-CHA-C4A
82	eG	201	PEB	C2B-C1B-CHA-C4A
82	eG	202	PEB	C2A-C3A-CAA-CBA
82	eG	202	PEB	C4A-C3A-CAA-CBA
82	eG	202	PEB	NB-C1B-CHA-C4A
82	eG	202	PEB	C2B-C1B-CHA-C4A
82	eG	203	PEB	ND-C1D-CHC-C4C
82	eG	203	PEB	C2D-C1D-CHC-C4C
82	eG	203	PEB	NC-C1C-CHB-C4B
82	eG	203	PEB	C2C-C1C-CHB-C4B
82	eG	203	PEB	NB-C1B-CHA-C4A
82	eG	203	PEB	C2B-C1B-CHA-C4A
82	fG	201	PEB	ND-C1D-CHC-C4C
82	fG	201	PEB	C2D-C1D-CHC-C4C
82	fG	201	PEB	NB-C1B-CHA-C4A
82	fG	201	PEB	C2B-C1B-CHA-C4A
82	fG	202	PEB	NB-C1B-CHA-C4A
82	fG	202	PEB	C2B-C1B-CHA-C4A
82	fG	203	PEB	ND-C1D-CHC-C4C
82	fG	203	PEB	C2D-C1D-CHC-C4C
82	fG	203	PEB	C2A-C3A-CAA-CBA
82	fG	203	PEB	C4A-C3A-CAA-CBA
82	fG	203	PEB	NB-C1B-CHA-C4A
82	fG	203	PEB	C2B-C1B-CHA-C4A
82	gG	201	PEB	NB-C1B-CHA-C4A
82	gG	201	PEB	C2B-C1B-CHA-C4A
82	gG	202	PEB	ND-C1D-CHC-C4C
82	gG	202	PEB	C2D-C1D-CHC-C4C
82	gG	202	PEB	NC-C1C-CHB-C4B
82	gG	202	PEB	C2C-C1C-CHB-C4B
82	gG	202	PEB	NB-C1B-CHA-C4A
82	gG	202	PEB	C2B-C1B-CHA-C4A
82	gG	202	PEB	C3B-CAB-CBB-CGB
82	hG	201	PEB	ND-C1D-CHC-C4C
82	hG	201	PEB	C2D-C1D-CHC-C4C
82	hG	201	PEB	C2A-C3A-CAA-CBA
82	hG	201	PEB	C4A-C3A-CAA-CBA
82	hG	201	PEB	NB-C1B-CHA-C4A
82	hG	201	PEB	C2B-C1B-CHA-C4A
82	hG	202	PEB	ND-C1D-CHC-C4C
82	hG	202	PEB	C2D-C1D-CHC-C4C
82	hG	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	hG	202	PEB	NB-C1B-CHA-C4A
82	hG	202	PEB	C2B-C1B-CHA-C4A
82	hG	203	PEB	NB-C1B-CHA-C4A
82	hG	203	PEB	C2B-C1B-CHA-C4A
82	iG	201	PEB	ND-C1D-CHC-C4C
82	iG	201	PEB	C2D-C1D-CHC-C4C
82	iG	201	PEB	NB-C1B-CHA-C4A
82	iG	201	PEB	C2B-C1B-CHA-C4A
82	iG	202	PEB	NC-C1C-CHB-C4B
82	iG	202	PEB	C2C-C1C-CHB-C4B
82	iG	202	PEB	NB-C1B-CHA-C4A
82	iG	202	PEB	C2B-C1B-CHA-C4A
82	jG	201	PEB	C4A-C3A-CAA-CBA
82	jG	201	PEB	NB-C1B-CHA-C4A
82	jG	201	PEB	C2B-C1B-CHA-C4A
82	jG	202	PEB	NB-C1B-CHA-C4A
82	jG	202	PEB	C2B-C1B-CHA-C4A
82	kG	201	PEB	C1C-C2C-CAC-CBC
82	kG	201	PEB	C3C-C2C-CAC-CBC
82	kG	201	PEB	NB-C1B-CHA-C4A
82	kG	201	PEB	C2B-C1B-CHA-C4A
82	kG	202	PEB	C2C-CAC-CBC-CGC
82	kG	202	PEB	NB-C1B-CHA-C4A
82	kG	202	PEB	C2B-C1B-CHA-C4A
82	lG	201	PEB	ND-C1D-CHC-C4C
82	lG	201	PEB	C2D-C1D-CHC-C4C
82	lG	201	PEB	C2A-C3A-CAA-CBA
82	lG	201	PEB	C4A-C3A-CAA-CBA
82	lG	201	PEB	NB-C1B-CHA-C4A
82	lG	201	PEB	C2B-C1B-CHA-C4A
82	lG	202	PEB	ND-C1D-CHC-C4C
82	lG	202	PEB	C2D-C1D-CHC-C4C
82	lG	202	PEB	C4A-C3A-CAA-CBA
82	lG	202	PEB	NB-C1B-CHA-C4A
82	lG	202	PEB	C2B-C1B-CHA-C4A
82	lG	203	PEB	NB-C1B-CHA-C4A
82	lG	203	PEB	C2B-C1B-CHA-C4A
82	mG	201	PEB	ND-C1D-CHC-C4C
82	mG	201	PEB	C2D-C1D-CHC-C4C
82	mG	201	PEB	NB-C1B-CHA-C4A
82	mG	201	PEB	C2B-C1B-CHA-C4A
82	mG	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	mG	202	PEB	C4A-C3A-CAA-CBA
82	mG	202	PEB	NB-C1B-CHA-C4A
82	mG	202	PEB	C2B-C1B-CHA-C4A
82	mG	203	PEB	C2D-C1D-CHC-C4C
82	mG	203	PEB	NC-C1C-CHB-C4B
82	mG	203	PEB	C2C-C1C-CHB-C4B
82	mG	203	PEB	NB-C1B-CHA-C4A
82	mG	203	PEB	C2B-C1B-CHA-C4A
82	fH	201	PEB	ND-C1D-CHC-C4C
82	fH	201	PEB	C2D-C1D-CHC-C4C
82	fH	201	PEB	NB-C1B-CHA-C4A
82	fH	201	PEB	C2B-C1B-CHA-C4A
82	fH	202	PEB	C2A-C3A-CAA-CBA
82	fH	202	PEB	NB-C1B-CHA-C4A
82	fH	202	PEB	C2B-C1B-CHA-C4A
82	fH	203	PEB	ND-C1D-CHC-C4C
82	fH	203	PEB	C2D-C1D-CHC-C4C
82	fH	203	PEB	NC-C1C-CHB-C4B
82	fH	203	PEB	C2A-C3A-CAA-CBA
82	fH	203	PEB	NB-C1B-CHA-C4A
82	fH	203	PEB	C2B-C1B-CHA-C4A
82	gH	201	PEB	NB-C1B-CHA-C4A
82	gH	201	PEB	C2B-C1B-CHA-C4A
82	gH	202	PEB	NB-C1B-CHA-C4A
82	gH	202	PEB	C2B-C1B-CHA-C4A
82	gH	203	PEB	NB-C1B-CHA-C4A
82	gH	203	PEB	C2B-C1B-CHA-C4A
82	hH	201	PEB	ND-C1D-CHC-C4C
82	hH	201	PEB	C2A-C3A-CAA-CBA
82	hH	201	PEB	C4A-C3A-CAA-CBA
82	hH	201	PEB	NB-C1B-CHA-C4A
82	hH	201	PEB	C2B-C1B-CHA-C4A
82	hH	201	PEB	C3B-CAB-CBB-CGB
82	hH	202	PEB	C2C-CAC-CBC-CGC
82	hH	202	PEB	NA-C4A-CHA-C1B
82	hH	202	PEB	C3A-C4A-CHA-C1B
82	hH	202	PEB	NB-C1B-CHA-C4A
82	hH	202	PEB	C2B-C1B-CHA-C4A
82	iH	201	PEB	NB-C1B-CHA-C4A
82	iH	201	PEB	C2B-C1B-CHA-C4A
82	iH	202	PEB	ND-C1D-CHC-C4C
82	iH	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	iH	202	PEB	NC-C1C-CHB-C4B
82	iH	202	PEB	C2C-C1C-CHB-C4B
82	iH	202	PEB	NB-C1B-CHA-C4A
82	iH	202	PEB	C2B-C1B-CHA-C4A
82	jH	201	PEB	ND-C1D-CHC-C4C
82	jH	201	PEB	C2D-C1D-CHC-C4C
82	jH	201	PEB	NB-C1B-CHA-C4A
82	jH	201	PEB	C2B-C1B-CHA-C4A
82	jH	202	PEB	NB-C1B-CHA-C4A
82	jH	202	PEB	C2B-C1B-CHA-C4A
82	jH	203	PEB	C2A-C3A-CAA-CBA
82	jH	203	PEB	NB-C1B-CHA-C4A
82	jH	203	PEB	C2B-C1B-CHA-C4A
82	kH	201	PEB	ND-C1D-CHC-C4C
82	kH	201	PEB	C2D-C1D-CHC-C4C
82	kH	201	PEB	C4A-C3A-CAA-CBA
82	kH	201	PEB	NB-C1B-CHA-C4A
82	kH	201	PEB	C2B-C1B-CHA-C4A
82	kH	202	PEB	NB-C1B-CHA-C4A
82	kH	202	PEB	C2B-C1B-CHA-C4A
82	kH	203	PEB	NB-C1B-CHA-C4A
82	kH	203	PEB	C2B-C1B-CHA-C4A
82	lH	201	PEB	ND-C1D-CHC-C4C
82	lH	201	PEB	C2D-C1D-CHC-C4C
82	lH	201	PEB	C2D-C3D-CAD-CBD
82	lH	201	PEB	C4D-C3D-CAD-CBD
82	lH	201	PEB	NB-C1B-CHA-C4A
82	lH	201	PEB	C2B-C1B-CHA-C4A
82	lH	202	PEB	ND-C1D-CHC-C4C
82	lH	202	PEB	C2D-C1D-CHC-C4C
82	lH	202	PEB	C2A-C3A-CAA-CBA
82	lH	202	PEB	NB-C1B-CHA-C4A
82	lH	202	PEB	C2B-C1B-CHA-C4A
82	mH	201	PEB	ND-C1D-CHC-C4C
82	mH	201	PEB	C2D-C1D-CHC-C4C
82	mH	201	PEB	NB-C1B-CHA-C4A
82	mH	201	PEB	C2B-C1B-CHA-C4A
82	mH	202	PEB	C2D-C1D-CHC-C4C
82	mH	202	PEB	NB-C1B-CHA-C4A
82	mH	202	PEB	C2B-C1B-CHA-C4A
82	mH	202	PEB	C3B-CAB-CBB-CGB
82	aH	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	aH	201	PEB	C2B-C1B-CHA-C4A
82	aH	202	PEB	ND-C1D-CHC-C4C
82	aH	202	PEB	C2D-C1D-CHC-C4C
82	aH	202	PEB	C2C-CAC-CBC-CGC
82	aH	202	PEB	NB-C1B-CHA-C4A
82	aH	202	PEB	C2B-C1B-CHA-C4A
82	bH	201	PEB	ND-C1D-CHC-C4C
82	bH	201	PEB	C2D-C1D-CHC-C4C
82	bH	201	PEB	NB-C1B-CHA-C4A
82	bH	201	PEB	C2B-C1B-CHA-C4A
82	bH	202	PEB	NB-C1B-CHA-C4A
82	bH	202	PEB	C2B-C1B-CHA-C4A
82	cH	201	PEB	C2A-C3A-CAA-CBA
82	cH	201	PEB	C4A-C3A-CAA-CBA
82	cH	201	PEB	NB-C1B-CHA-C4A
82	cH	201	PEB	C2B-C1B-CHA-C4A
82	cH	202	PEB	C4A-C3A-CAA-CBA
82	cH	202	PEB	NB-C1B-CHA-C4A
82	dH	201	PEB	NB-C1B-CHA-C4A
82	dH	201	PEB	C2B-C1B-CHA-C4A
82	dH	202	PEB	ND-C1D-CHC-C4C
82	dH	202	PEB	C2D-C1D-CHC-C4C
82	dH	202	PEB	C4A-C3A-CAA-CBA
82	dH	202	PEB	NB-C1B-CHA-C4A
82	dH	202	PEB	C2B-C1B-CHA-C4A
82	dH	203	PEB	C2A-C3A-CAA-CBA
82	dH	203	PEB	NB-C1B-CHA-C4A
82	dH	203	PEB	C2B-C1B-CHA-C4A
82	eH	201	PEB	ND-C1D-CHC-C4C
82	eH	201	PEB	C2D-C1D-CHC-C4C
82	eH	201	PEB	NB-C1B-CHA-C4A
82	eH	201	PEB	C2B-C1B-CHA-C4A
82	eH	202	PEB	ND-C1D-CHC-C4C
82	eH	202	PEB	C2D-C1D-CHC-C4C
82	eH	202	PEB	NB-C1B-CHA-C4A
82	eH	202	PEB	C2B-C1B-CHA-C4A
82	eH	203	PEB	C4A-C3A-CAA-CBA
82	eH	203	PEB	NB-C1B-CHA-C4A
82	eH	203	PEB	C2B-C1B-CHA-C4A
82	aJ	201	PEB	C2D-C1D-CHC-C4C
82	aJ	201	PEB	NB-C1B-CHA-C4A
82	aJ	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	aJ	202	PEB	NB-C1B-CHA-C4A
82	aJ	202	PEB	C2B-C1B-CHA-C4A
82	aJ	203	PEB	NC-C4C-CHC-C1D
82	aJ	203	PEB	C3C-C4C-CHC-C1D
82	aJ	203	PEB	C2A-C3A-CAA-CBA
82	aJ	203	PEB	C4A-C3A-CAA-CBA
82	aJ	203	PEB	NB-C1B-CHA-C4A
82	aJ	203	PEB	C2B-C1B-CHA-C4A
82	aJ	204	PEB	NB-C1B-CHA-C4A
82	aJ	204	PEB	C2B-C1B-CHA-C4A
82	cJ	201	PEB	ND-C1D-CHC-C4C
82	cJ	201	PEB	C2D-C1D-CHC-C4C
82	cJ	201	PEB	NB-C1B-CHA-C4A
82	cJ	201	PEB	C2B-C1B-CHA-C4A
82	cJ	202	PEB	ND-C1D-CHC-C4C
82	cJ	202	PEB	C2D-C1D-CHC-C4C
82	cJ	202	PEB	NC-C1C-CHB-C4B
82	cJ	202	PEB	C2C-C1C-CHB-C4B
82	cJ	202	PEB	NB-C1B-CHA-C4A
82	cJ	202	PEB	C2B-C1B-CHA-C4A
82	dJ	201	PEB	C4A-C3A-CAA-CBA
82	dJ	201	PEB	NB-C1B-CHA-C4A
82	dJ	201	PEB	C2B-C1B-CHA-C4A
82	dJ	202	PEB	C1C-C2C-CAC-CBC
82	dJ	202	PEB	NB-C1B-CHA-C4A
82	dJ	202	PEB	C2B-C1B-CHA-C4A
82	eJ	201	PEB	ND-C1D-CHC-C4C
82	eJ	201	PEB	C2D-C1D-CHC-C4C
82	eJ	201	PEB	NB-C1B-CHA-C4A
82	eJ	201	PEB	C2B-C1B-CHA-C4A
82	eJ	202	PEB	ND-C1D-CHC-C4C
82	eJ	202	PEB	C2D-C1D-CHC-C4C
82	eJ	202	PEB	NC-C1C-CHB-C4B
82	eJ	202	PEB	C2C-C1C-CHB-C4B
82	eJ	202	PEB	C2C-CAC-CBC-CGC
82	eJ	202	PEB	NB-C1B-CHA-C4A
82	eJ	202	PEB	C2B-C1B-CHA-C4A
82	fJ	201	PEB	NB-C1B-CHA-C4A
82	fJ	201	PEB	C2B-C1B-CHA-C4A
82	fJ	202	PEB	C2A-C3A-CAA-CBA
82	fJ	202	PEB	C4A-C3A-CAA-CBA
82	fJ	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	fJ	202	PEB	C2B-C1B-CHA-C4A
82	fJ	203	PEB	C4A-C3A-CAA-CBA
82	fJ	203	PEB	NB-C1B-CHA-C4A
82	fJ	203	PEB	C2B-C1B-CHA-C4A
82	gJ	201	PEB	ND-C1D-CHC-C4C
82	gJ	201	PEB	C2D-C1D-CHC-C4C
82	gJ	201	PEB	NB-C1B-CHA-C4A
82	gJ	201	PEB	C2B-C1B-CHA-C4A
82	gJ	202	PEB	C2D-C1D-CHC-C4C
82	gJ	202	PEB	NB-C1B-CHA-C4A
82	gJ	202	PEB	C2B-C1B-CHA-C4A
82	hJ	201	PEB	C2A-C3A-CAA-CBA
82	hJ	201	PEB	C4A-C3A-CAA-CBA
82	hJ	201	PEB	NB-C1B-CHA-C4A
82	hJ	201	PEB	C2B-C1B-CHA-C4A
82	hJ	202	PEB	NB-C1B-CHA-C4A
82	hJ	202	PEB	C2B-C1B-CHA-C4A
82	hJ	203	PEB	NC-C4C-CHC-C1D
82	hJ	203	PEB	C3C-C4C-CHC-C1D
82	hJ	203	PEB	C2D-C3D-CAD-CBD
82	hJ	203	PEB	C4D-C3D-CAD-CBD
82	hJ	203	PEB	C4A-C3A-CAA-CBA
82	hJ	203	PEB	NB-C1B-CHA-C4A
82	hJ	203	PEB	C2B-C1B-CHA-C4A
82	iJ	201	PEB	ND-C1D-CHC-C4C
82	iJ	201	PEB	C2D-C1D-CHC-C4C
82	iJ	201	PEB	NB-C1B-CHA-C4A
82	iJ	201	PEB	C2B-C1B-CHA-C4A
82	iJ	202	PEB	NB-C1B-CHA-C4A
82	iJ	202	PEB	C2B-C1B-CHA-C4A
82	jJ	201	PEB	NB-C1B-CHA-C4A
82	jJ	201	PEB	C2B-C1B-CHA-C4A
82	jJ	202	PEB	ND-C1D-CHC-C4C
82	jJ	202	PEB	C2D-C1D-CHC-C4C
82	jJ	202	PEB	C4A-C3A-CAA-CBA
82	jJ	202	PEB	NB-C1B-CHA-C4A
82	jJ	202	PEB	C2B-C1B-CHA-C4A
82	jJ	203	PEB	C4A-C3A-CAA-CBA
82	jJ	203	PEB	NB-C1B-CHA-C4A
82	jJ	203	PEB	C2B-C1B-CHA-C4A
82	kJ	201	PEB	ND-C1D-CHC-C4C
82	kJ	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	kJ	201	PEB	C4A-C3A-CAA-CBA
82	kJ	201	PEB	NB-C1B-CHA-C4A
82	kJ	201	PEB	C2B-C1B-CHA-C4A
82	kJ	202	PEB	NB-C1B-CHA-C4A
82	kJ	202	PEB	C2B-C1B-CHA-C4A
82	lJ	201	PEB	C4A-C3A-CAA-CBA
82	lJ	201	PEB	NB-C1B-CHA-C4A
82	lJ	201	PEB	C2B-C1B-CHA-C4A
82	lJ	202	PEB	ND-C1D-CHC-C4C
82	lJ	202	PEB	C2D-C1D-CHC-C4C
82	lJ	202	PEB	NB-C1B-CHA-C4A
82	lJ	202	PEB	C2B-C1B-CHA-C4A
82	lJ	203	PEB	ND-C1D-CHC-C4C
82	lJ	203	PEB	C2D-C1D-CHC-C4C
82	lJ	203	PEB	C4A-C3A-CAA-CBA
82	lJ	203	PEB	NB-C1B-CHA-C4A
82	lJ	203	PEB	C2B-C1B-CHA-C4A
82	mJ	201	PEB	ND-C1D-CHC-C4C
82	mJ	201	PEB	C2D-C1D-CHC-C4C
82	mJ	201	PEB	NB-C1B-CHA-C4A
82	mJ	201	PEB	C2B-C1B-CHA-C4A
82	mJ	202	PEB	NB-C1B-CHA-C4A
82	mJ	202	PEB	C2B-C1B-CHA-C4A
82	aK	201	PEB	ND-C1D-CHC-C4C
82	aK	201	PEB	C2A-C3A-CAA-CBA
82	aK	201	PEB	C4A-C3A-CAA-CBA
82	aK	201	PEB	NB-C1B-CHA-C4A
82	aK	201	PEB	C2B-C1B-CHA-C4A
82	aK	202	PEB	C2A-C3A-CAA-CBA
82	aK	202	PEB	C4A-C3A-CAA-CBA
82	aK	202	PEB	NB-C1B-CHA-C4A
82	aK	202	PEB	C2B-C1B-CHA-C4A
82	aK	203	PEB	C2A-C3A-CAA-CBA
82	aK	203	PEB	NB-C1B-CHA-C4A
82	aK	203	PEB	C2B-C1B-CHA-C4A
82	bK	201	PEB	C2A-C3A-CAA-CBA
82	bK	201	PEB	C4A-C3A-CAA-CBA
82	bK	201	PEB	NB-C1B-CHA-C4A
82	bK	201	PEB	C2B-C1B-CHA-C4A
82	bK	202	PEB	C3C-C4C-CHC-C1D
82	bK	202	PEB	ND-C1D-CHC-C4C
82	bK	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	bK	202	PEB	NC-C1C-CHB-C4B
82	bK	202	PEB	C2C-C1C-CHB-C4B
82	bK	202	PEB	NB-C1B-CHA-C4A
82	bK	202	PEB	C2B-C1B-CHA-C4A
82	cK	201	PEB	ND-C1D-CHC-C4C
82	cK	201	PEB	C2D-C1D-CHC-C4C
82	cK	201	PEB	NB-C1B-CHA-C4A
82	cK	201	PEB	C2B-C1B-CHA-C4A
82	cK	202	PEB	NB-C1B-CHA-C4A
82	cK	202	PEB	C2B-C1B-CHA-C4A
82	cK	203	PEB	C2A-C3A-CAA-CBA
82	cK	203	PEB	NB-C1B-CHA-C4A
82	cK	203	PEB	C2B-C1B-CHA-C4A
82	dK	201	PEB	ND-C1D-CHC-C4C
82	dK	201	PEB	C2D-C1D-CHC-C4C
82	dK	201	PEB	NB-C1B-CHA-C4A
82	dK	201	PEB	C2B-C1B-CHA-C4A
82	dK	202	PEB	C3C-C4C-CHC-C1D
82	dK	202	PEB	ND-C1D-CHC-C4C
82	dK	202	PEB	C2D-C1D-CHC-C4C
82	dK	202	PEB	NC-C1C-CHB-C4B
82	dK	202	PEB	NB-C1B-CHA-C4A
82	dK	202	PEB	C2B-C1B-CHA-C4A
82	eK	201	PEB	NC-C1C-CHB-C4B
82	eK	201	PEB	NB-C1B-CHA-C4A
82	eK	201	PEB	C2B-C1B-CHA-C4A
82	eK	202	PEB	ND-C1D-CHC-C4C
82	eK	202	PEB	C2D-C1D-CHC-C4C
82	eK	202	PEB	C4A-C3A-CAA-CBA
82	eK	202	PEB	NB-C1B-CHA-C4A
82	eK	202	PEB	C2B-C1B-CHA-C4A
82	eK	203	PEB	NB-C1B-CHA-C4A
82	eK	203	PEB	C2B-C1B-CHA-C4A
82	fK	201	PEB	C4A-C3A-CAA-CBA
82	fK	201	PEB	NB-C1B-CHA-C4A
82	fK	201	PEB	C2B-C1B-CHA-C4A
82	fK	202	PEB	C3C-C4C-CHC-C1D
82	fK	202	PEB	ND-C1D-CHC-C4C
82	fK	202	PEB	C2D-C1D-CHC-C4C
82	fK	202	PEB	NC-C1C-CHB-C4B
82	fK	202	PEB	C2C-C1C-CHB-C4B
82	fK	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	fK	202	PEB	C2B-C1B-CHA-C4A
82	gK	201	PEB	C2D-C1D-CHC-C4C
82	gK	201	PEB	NB-C1B-CHA-C4A
82	gK	202	PEB	NB-C1B-CHA-C4A
82	gK	202	PEB	C2B-C1B-CHA-C4A
82	gK	203	PEB	C2A-C3A-CAA-CBA
82	gK	203	PEB	NB-C1B-CHA-C4A
82	gK	203	PEB	C2B-C1B-CHA-C4A
82	hK	201	PEB	NB-C1B-CHA-C4A
82	hK	201	PEB	C2B-C1B-CHA-C4A
82	hK	202	PEB	ND-C1D-CHC-C4C
82	hK	202	PEB	C2D-C1D-CHC-C4C
82	hK	202	PEB	NC-C1C-CHB-C4B
82	hK	202	PEB	NB-C1B-CHA-C4A
82	hK	202	PEB	C2B-C1B-CHA-C4A
82	iK	201	PEB	C4A-C3A-CAA-CBA
82	iK	201	PEB	NB-C1B-CHA-C4A
82	iK	201	PEB	C2B-C1B-CHA-C4A
82	iK	202	PEB	ND-C1D-CHC-C4C
82	iK	202	PEB	C2D-C1D-CHC-C4C
82	iK	202	PEB	C4A-C3A-CAA-CBA
82	iK	202	PEB	NB-C1B-CHA-C4A
82	iK	202	PEB	C2B-C1B-CHA-C4A
82	iK	203	PEB	NC-C1C-CHB-C4B
82	iK	203	PEB	C2C-C1C-CHB-C4B
82	iK	203	PEB	C4A-C3A-CAA-CBA
82	iK	203	PEB	NB-C1B-CHA-C4A
82	iK	203	PEB	C2B-C1B-CHA-C4A
82	jK	201	PEB	NB-C1B-CHA-C4A
82	jK	202	PEB	ND-C1D-CHC-C4C
82	jK	202	PEB	C2D-C1D-CHC-C4C
82	jK	202	PEB	NC-C1C-CHB-C4B
82	jK	202	PEB	C2C-C1C-CHB-C4B
82	jK	202	PEB	NB-C1B-CHA-C4A
82	jK	202	PEB	C2B-C1B-CHA-C4A
82	kK	201	PEB	ND-C1D-CHC-C4C
82	kK	201	PEB	C2D-C1D-CHC-C4C
82	kK	201	PEB	NC-C1C-CHB-C4B
82	kK	201	PEB	C2C-C1C-CHB-C4B
82	kK	201	PEB	C4A-C3A-CAA-CBA
82	kK	201	PEB	NB-C1B-CHA-C4A
82	kK	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	kK	201	PEB	C3B-CAB-CBB-CGB
82	kK	202	PEB	NC-C1C-CHB-C4B
82	kK	202	PEB	C2C-C1C-CHB-C4B
82	kK	202	PEB	C2A-C3A-CAA-CBA
82	kK	202	PEB	NB-C1B-CHA-C4A
82	kK	202	PEB	C2B-C1B-CHA-C4A
82	kK	203	PEB	ND-C1D-CHC-C4C
82	kK	203	PEB	C2D-C1D-CHC-C4C
82	kK	203	PEB	C2A-C3A-CAA-CBA
82	kK	203	PEB	C4A-C3A-CAA-CBA
82	kK	203	PEB	NB-C1B-CHA-C4A
82	kK	203	PEB	C2B-C1B-CHA-C4A
82	lK	201	PEB	C2A-C3A-CAA-CBA
82	lK	201	PEB	C4A-C3A-CAA-CBA
82	lK	201	PEB	NB-C1B-CHA-C4A
82	lK	201	PEB	C2B-C1B-CHA-C4A
82	lK	202	PEB	ND-C1D-CHC-C4C
82	lK	202	PEB	C2D-C1D-CHC-C4C
82	lK	202	PEB	NC-C1C-CHB-C4B
82	lK	202	PEB	C2C-C1C-CHB-C4B
82	lK	202	PEB	NB-C1B-CHA-C4A
82	lK	202	PEB	C2B-C1B-CHA-C4A
82	lK	203	PEB	C2A-C3A-CAA-CBA
82	lK	203	PEB	C4A-C3A-CAA-CBA
82	lK	203	PEB	NB-C1B-CHA-C4A
82	lK	203	PEB	C2B-C1B-CHA-C4A
82	mK	201	PEB	NC-C1C-CHB-C4B
82	mK	201	PEB	C2C-C1C-CHB-C4B
82	mK	201	PEB	NB-C1B-CHA-C4A
82	mK	201	PEB	C2B-C1B-CHA-C4A
82	mK	202	PEB	C2A-C3A-CAA-CBA
82	mK	202	PEB	C4A-C3A-CAA-CBA
82	mK	202	PEB	NB-C1B-CHA-C4A
82	mK	202	PEB	C2B-C1B-CHA-C4A
82	mK	202	PEB	C3B-CAB-CBB-CGB
82	nK	201	PEB	NB-C1B-CHA-C4A
82	nK	201	PEB	C2B-C1B-CHA-C4A
82	nK	202	PEB	ND-C1D-CHC-C4C
82	nK	202	PEB	C2D-C1D-CHC-C4C
82	nK	202	PEB	NC-C1C-CHB-C4B
82	nK	202	PEB	C2C-C1C-CHB-C4B
82	nK	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	nK	202	PEB	C2B-C1B-CHA-C4A
82	oK	201	PEB	ND-C1D-CHC-C4C
82	oK	201	PEB	C2D-C1D-CHC-C4C
82	oK	201	PEB	C2A-C3A-CAA-CBA
82	oK	201	PEB	C4A-C3A-CAA-CBA
82	oK	201	PEB	NB-C1B-CHA-C4A
82	oK	201	PEB	C2B-C1B-CHA-C4A
82	oK	202	PEB	NB-C1B-CHA-C4A
82	oK	202	PEB	C2B-C1B-CHA-C4A
82	oK	203	PEB	ND-C1D-CHC-C4C
82	oK	203	PEB	C2D-C1D-CHC-C4C
82	oK	203	PEB	C2D-C3D-CAD-CBD
82	oK	203	PEB	C4D-C3D-CAD-CBD
82	oK	203	PEB	C2A-C3A-CAA-CBA
82	oK	203	PEB	C4A-C3A-CAA-CBA
82	oK	203	PEB	NB-C1B-CHA-C4A
82	oK	203	PEB	C2B-C1B-CHA-C4A
82	pK	201	PEB	C2A-C3A-CAA-CBA
82	pK	201	PEB	C4A-C3A-CAA-CBA
82	pK	201	PEB	NB-C1B-CHA-C4A
82	pK	201	PEB	C2B-C1B-CHA-C4A
82	pK	202	PEB	ND-C1D-CHC-C4C
82	pK	202	PEB	C2D-C1D-CHC-C4C
82	pK	202	PEB	NC-C1C-CHB-C4B
82	pK	202	PEB	C2C-C1C-CHB-C4B
82	pK	202	PEB	NB-C1B-CHA-C4A
82	pK	202	PEB	C2B-C1B-CHA-C4A
82	qK	201	PEB	C2A-C3A-CAA-CBA
82	qK	201	PEB	C4A-C3A-CAA-CBA
82	qK	201	PEB	NB-C1B-CHA-C4A
82	qK	201	PEB	C2B-C1B-CHA-C4A
82	qK	202	PEB	C4A-C3A-CAA-CBA
82	qK	202	PEB	NB-C1B-CHA-C4A
82	qK	202	PEB	C2B-C1B-CHA-C4A
82	qK	203	PEB	NC-C1C-CHB-C4B
82	qK	203	PEB	C2C-C1C-CHB-C4B
82	qK	203	PEB	C4A-C3A-CAA-CBA
82	qK	203	PEB	NB-C1B-CHA-C4A
82	qK	203	PEB	C2B-C1B-CHA-C4A
82	rK	201	PEB	ND-C1D-CHC-C4C
82	rK	201	PEB	C2D-C1D-CHC-C4C
82	rK	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	rK	201	PEB	C4A-C3A-CAA-CBA
82	rK	201	PEB	NB-C1B-CHA-C4A
82	rK	201	PEB	C2B-C1B-CHA-C4A
82	rK	202	PEB	ND-C1D-CHC-C4C
82	rK	202	PEB	C2D-C1D-CHC-C4C
82	rK	202	PEB	NC-C1C-CHB-C4B
82	rK	202	PEB	C2C-C1C-CHB-C4B
82	rK	202	PEB	NB-C1B-CHA-C4A
82	rK	202	PEB	C2B-C1B-CHA-C4A
82	sK	201	PEB	ND-C1D-CHC-C4C
82	sK	201	PEB	C2D-C1D-CHC-C4C
82	sK	201	PEB	C4A-C3A-CAA-CBA
82	sK	201	PEB	NB-C1B-CHA-C4A
82	sK	201	PEB	C2B-C1B-CHA-C4A
82	sK	202	PEB	NC-C1C-CHB-C4B
82	sK	202	PEB	C2C-C1C-CHB-C4B
82	sK	202	PEB	NB-C1B-CHA-C4A
82	sK	202	PEB	C2B-C1B-CHA-C4A
82	sK	203	PEB	NB-C1B-CHA-C4A
82	sK	203	PEB	C2B-C1B-CHA-C4A
82	tK	201	PEB	NB-C1B-CHA-C4A
82	tK	201	PEB	C2B-C1B-CHA-C4A
82	tK	202	PEB	ND-C1D-CHC-C4C
82	tK	202	PEB	C2D-C1D-CHC-C4C
82	tK	202	PEB	C1C-C2C-CAC-CBC
82	tK	202	PEB	C3C-C2C-CAC-CBC
82	tK	202	PEB	NB-C1B-CHA-C4A
82	tK	202	PEB	C2B-C1B-CHA-C4A
82	tK	202	PEB	C3B-CAB-CBB-CGB
82	tK	203	PEB	ND-C1D-CHC-C4C
82	tK	203	PEB	C2D-C1D-CHC-C4C
82	tK	203	PEB	C4A-C3A-CAA-CBA
82	tK	203	PEB	NB-C1B-CHA-C4A
82	tK	203	PEB	C2B-C1B-CHA-C4A
82	uK	201	PEB	ND-C1D-CHC-C4C
82	uK	201	PEB	C2D-C1D-CHC-C4C
82	uK	201	PEB	C2A-C3A-CAA-CBA
82	uK	201	PEB	C4A-C3A-CAA-CBA
82	uK	201	PEB	NB-C1B-CHA-C4A
82	uK	201	PEB	C2B-C1B-CHA-C4A
82	uK	202	PEB	NB-C1B-CHA-C4A
82	uK	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	vK	201	PEB	NB-C1B-CHA-C4A
82	vK	201	PEB	C2B-C1B-CHA-C4A
82	vK	202	PEB	ND-C1D-CHC-C4C
82	vK	202	PEB	C2D-C1D-CHC-C4C
82	vK	202	PEB	NC-C1C-CHB-C4B
82	vK	202	PEB	C2C-C1C-CHB-C4B
82	vK	202	PEB	NB-C1B-CHA-C4A
82	vK	202	PEB	C2B-C1B-CHA-C4A
82	wK	301	PEB	C2A-C3A-CAA-CBA
82	wK	301	PEB	NB-C1B-CHA-C4A
82	wK	301	PEB	C2B-C1B-CHA-C4A
82	wK	302	PEB	ND-C1D-CHC-C4C
82	wK	302	PEB	C2D-C1D-CHC-C4C
82	wK	302	PEB	C2A-C3A-CAA-CBA
82	wK	302	PEB	C4A-C3A-CAA-CBA
82	wK	302	PEB	NB-C1B-CHA-C4A
82	wK	302	PEB	C2B-C1B-CHA-C4A
82	wK	303	PEB	NB-C1B-CHA-C4A
82	wK	303	PEB	C2B-C1B-CHA-C4A
82	xK	302	PEB	ND-C1D-CHC-C4C
82	xK	302	PEB	C2D-C1D-CHC-C4C
82	xK	302	PEB	NC-C1C-CHB-C4B
82	xK	302	PEB	C2C-C1C-CHB-C4B
82	xK	302	PEB	NB-C1B-CHA-C4A
82	xK	302	PEB	C2B-C1B-CHA-C4A
82	xK	303	PEB	ND-C1D-CHC-C4C
82	xK	303	PEB	C2D-C1D-CHC-C4C
82	xK	303	PEB	C4A-C3A-CAA-CBA
82	xK	303	PEB	NB-C1B-CHA-C4A
82	xK	303	PEB	C2B-C1B-CHA-C4A
82	xK	304	PEB	C2C-CAC-CBC-CGC
82	xK	304	PEB	NB-C1B-CHA-C4A
82	xK	304	PEB	C2B-C1B-CHA-C4A
82	yK	301	PEB	C4A-C3A-CAA-CBA
82	yK	301	PEB	NB-C1B-CHA-C4A
82	yK	301	PEB	C2B-C1B-CHA-C4A
82	zK	501	PEB	C4A-C3A-CAA-CBA
82	zK	501	PEB	NB-C1B-CHA-C4A
82	zK	501	PEB	C2B-C1B-CHA-C4A
82	aM	201	PEB	ND-C1D-CHC-C4C
82	aM	201	PEB	C2D-C1D-CHC-C4C
82	aM	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	aM	201	PEB	C2B-C1B-CHA-C4A
82	aM	202	PEB	C2A-C3A-CAA-CBA
82	aM	202	PEB	C4A-C3A-CAA-CBA
82	aM	202	PEB	NB-C1B-CHA-C4A
82	aM	202	PEB	C2B-C1B-CHA-C4A
82	aM	203	PEB	ND-C1D-CHC-C4C
82	aM	203	PEB	NC-C1C-CHB-C4B
82	aM	203	PEB	C2C-C1C-CHB-C4B
82	aM	203	PEB	C2A-C3A-CAA-CBA
82	aM	203	PEB	C4A-C3A-CAA-CBA
82	aM	203	PEB	NB-C1B-CHA-C4A
82	aM	203	PEB	C2B-C1B-CHA-C4A
82	aM	204	PEB	C4A-C3A-CAA-CBA
82	aM	204	PEB	NB-C1B-CHA-C4A
82	aM	204	PEB	C2B-C1B-CHA-C4A
82	cM	201	PEB	ND-C1D-CHC-C4C
82	cM	201	PEB	C2D-C1D-CHC-C4C
82	cM	201	PEB	C4A-C3A-CAA-CBA
82	cM	201	PEB	NB-C1B-CHA-C4A
82	cM	201	PEB	C2B-C1B-CHA-C4A
82	cM	202	PEB	ND-C1D-CHC-C4C
82	cM	202	PEB	C2D-C1D-CHC-C4C
82	cM	202	PEB	NB-C1B-CHA-C4A
82	cM	202	PEB	C2B-C1B-CHA-C4A
82	dM	201	PEB	C4A-C3A-CAA-CBA
82	dM	201	PEB	NB-C1B-CHA-C4A
82	dM	201	PEB	C2B-C1B-CHA-C4A
82	dM	202	PEB	C2D-C1D-CHC-C4C
82	dM	202	PEB	C4A-C3A-CAA-CBA
82	dM	202	PEB	NB-C1B-CHA-C4A
82	dM	202	PEB	C2B-C1B-CHA-C4A
82	dM	203	PEB	ND-C1D-CHC-C4C
82	dM	203	PEB	NC-C1C-CHB-C4B
82	dM	203	PEB	C2C-C1C-CHB-C4B
82	dM	203	PEB	C4A-C3A-CAA-CBA
82	dM	203	PEB	NB-C1B-CHA-C4A
82	dM	203	PEB	C2B-C1B-CHA-C4A
82	eM	201	PEB	ND-C1D-CHC-C4C
82	eM	201	PEB	C2D-C1D-CHC-C4C
82	eM	201	PEB	NB-C1B-CHA-C4A
82	eM	201	PEB	C2B-C1B-CHA-C4A
82	eM	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	eM	202	PEB	C2D-C1D-CHC-C4C
82	eM	202	PEB	NB-C1B-CHA-C4A
82	eM	202	PEB	C2B-C1B-CHA-C4A
82	fM	201	PEB	NB-C1B-CHA-C4A
82	fM	201	PEB	C2B-C1B-CHA-C4A
82	fM	202	PEB	NC-C4C-CHC-C1D
82	fM	202	PEB	C3C-C4C-CHC-C1D
82	fM	202	PEB	C2D-C3D-CAD-CBD
82	fM	202	PEB	C4D-C3D-CAD-CBD
82	fM	202	PEB	NB-C1B-CHA-C4A
82	fM	202	PEB	C2B-C1B-CHA-C4A
82	fM	203	PEB	C4A-C3A-CAA-CBA
82	fM	203	PEB	NB-C1B-CHA-C4A
82	fM	203	PEB	C2B-C1B-CHA-C4A
82	gM	201	PEB	ND-C1D-CHC-C4C
82	gM	201	PEB	C2D-C1D-CHC-C4C
82	gM	201	PEB	NC-C1C-CHB-C4B
82	gM	201	PEB	NB-C1B-CHA-C4A
82	gM	201	PEB	C2B-C1B-CHA-C4A
82	gM	202	PEB	ND-C1D-CHC-C4C
82	gM	202	PEB	C2D-C1D-CHC-C4C
82	gM	202	PEB	NC-C1C-CHB-C4B
82	gM	202	PEB	C2C-C1C-CHB-C4B
82	gM	202	PEB	NB-C1B-CHA-C4A
82	gM	202	PEB	C2B-C1B-CHA-C4A
82	hM	201	PEB	C4A-C3A-CAA-CBA
82	hM	201	PEB	NB-C1B-CHA-C4A
82	hM	201	PEB	C2B-C1B-CHA-C4A
82	hM	202	PEB	ND-C1D-CHC-C4C
82	hM	202	PEB	C2D-C1D-CHC-C4C
82	hM	202	PEB	NB-C1B-CHA-C4A
82	hM	202	PEB	C2B-C1B-CHA-C4A
82	hM	202	PEB	C3B-CAB-CBB-CGB
82	hM	203	PEB	NC-C1C-CHB-C4B
82	hM	203	PEB	C2C-C1C-CHB-C4B
82	hM	203	PEB	C4A-C3A-CAA-CBA
82	hM	203	PEB	NB-C1B-CHA-C4A
82	hM	203	PEB	C2B-C1B-CHA-C4A
82	iM	201	PEB	ND-C1D-CHC-C4C
82	iM	201	PEB	C2A-C3A-CAA-CBA
82	iM	201	PEB	C4A-C3A-CAA-CBA
82	iM	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	iM	201	PEB	C2B-C1B-CHA-C4A
82	iM	202	PEB	ND-C1D-CHC-C4C
82	iM	202	PEB	C2D-C1D-CHC-C4C
82	iM	202	PEB	NB-C1B-CHA-C4A
82	iM	202	PEB	C2B-C1B-CHA-C4A
82	jM	201	PEB	ND-C1D-CHC-C4C
82	jM	201	PEB	C2D-C1D-CHC-C4C
82	jM	201	PEB	NB-C1B-CHA-C4A
82	jM	201	PEB	C2B-C1B-CHA-C4A
82	jM	202	PEB	NC-C1C-CHB-C4B
82	jM	202	PEB	C2A-C3A-CAA-CBA
82	jM	202	PEB	C4A-C3A-CAA-CBA
82	jM	202	PEB	NB-C1B-CHA-C4A
82	jM	202	PEB	C2B-C1B-CHA-C4A
82	jM	203	PEB	C4A-C3A-CAA-CBA
82	jM	203	PEB	NB-C1B-CHA-C4A
82	jM	203	PEB	C2B-C1B-CHA-C4A
82	kM	201	PEB	ND-C1D-CHC-C4C
82	kM	201	PEB	C2D-C1D-CHC-C4C
82	kM	201	PEB	NB-C1B-CHA-C4A
82	kM	201	PEB	C2B-C1B-CHA-C4A
82	kM	202	PEB	NC-C1C-CHB-C4B
82	kM	202	PEB	NB-C1B-CHA-C4A
82	kM	202	PEB	C2B-C1B-CHA-C4A
82	lM	201	PEB	C4A-C3A-CAA-CBA
82	lM	201	PEB	NB-C1B-CHA-C4A
82	lM	201	PEB	C2B-C1B-CHA-C4A
82	lM	202	PEB	ND-C1D-CHC-C4C
82	lM	202	PEB	C2D-C1D-CHC-C4C
82	lM	202	PEB	NB-C1B-CHA-C4A
82	lM	202	PEB	C2B-C1B-CHA-C4A
82	lM	203	PEB	ND-C1D-CHC-C4C
82	lM	203	PEB	C2D-C1D-CHC-C4C
82	lM	203	PEB	C4A-C3A-CAA-CBA
82	lM	203	PEB	NB-C1B-CHA-C4A
82	lM	203	PEB	C2B-C1B-CHA-C4A
82	mM	201	PEB	ND-C1D-CHC-C4C
82	mM	201	PEB	C2D-C1D-CHC-C4C
82	mM	201	PEB	NB-C1B-CHA-C4A
82	mM	201	PEB	C2B-C1B-CHA-C4A
82	mM	202	PEB	NB-C1B-CHA-C4A
82	mM	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	iO	201	PEB	C2A-C3A-CAA-CBA
82	iO	201	PEB	C4A-C3A-CAA-CBA
82	iO	201	PEB	NB-C1B-CHA-C4A
82	iO	201	PEB	C2B-C1B-CHA-C4A
82	iO	202	PEB	ND-C1D-CHC-C4C
82	iO	202	PEB	C2D-C1D-CHC-C4C
82	iO	202	PEB	C2A-C3A-CAA-CBA
82	iO	202	PEB	NB-C1B-CHA-C4A
82	iO	202	PEB	C2B-C1B-CHA-C4A
82	iO	203	PEB	NB-C1B-CHA-C4A
82	iO	203	PEB	C2B-C1B-CHA-C4A
82	iO	203	PEB	C2B-C3B-CAB-CBB
82	iO	203	PEB	C4B-C3B-CAB-CBB
82	jO	201	PEB	ND-C1D-CHC-C4C
82	jO	201	PEB	C2D-C1D-CHC-C4C
82	jO	201	PEB	C4A-C3A-CAA-CBA
82	jO	201	PEB	NB-C1B-CHA-C4A
82	jO	201	PEB	C2B-C1B-CHA-C4A
82	jO	202	PEB	ND-C1D-CHC-C4C
82	jO	202	PEB	C2D-C1D-CHC-C4C
82	jO	202	PEB	NB-C1B-CHA-C4A
82	jO	202	PEB	C2B-C1B-CHA-C4A
82	kO	201	PEB	C4A-C3A-CAA-CBA
82	kO	201	PEB	NB-C1B-CHA-C4A
82	kO	201	PEB	C2B-C1B-CHA-C4A
82	kO	202	PEB	C2D-C1D-CHC-C4C
82	kO	202	PEB	C2A-C3A-CAA-CBA
82	kO	202	PEB	NB-C1B-CHA-C4A
82	kO	202	PEB	C2B-C1B-CHA-C4A
82	kO	203	PEB	C2D-C1D-CHC-C4C
82	kO	203	PEB	C2A-C3A-CAA-CBA
82	kO	203	PEB	C4A-C3A-CAA-CBA
82	kO	203	PEB	NB-C1B-CHA-C4A
82	kO	203	PEB	C2B-C1B-CHA-C4A
82	kO	203	PEB	C4B-C3B-CAB-CBB
82	lO	201	PEB	ND-C1D-CHC-C4C
82	lO	201	PEB	C2D-C1D-CHC-C4C
82	lO	201	PEB	C4A-C3A-CAA-CBA
82	lO	201	PEB	NB-C1B-CHA-C4A
82	lO	201	PEB	C2B-C1B-CHA-C4A
82	lO	202	PEB	ND-C1D-CHC-C4C
82	lO	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	lO	202	PEB	C4A-C3A-CAA-CBA
82	lO	202	PEB	NB-C1B-CHA-C4A
82	lO	202	PEB	C2B-C1B-CHA-C4A
82	mO	201	PEB	C2D-C1D-CHC-C4C
82	mO	201	PEB	C2A-C3A-CAA-CBA
82	mO	201	PEB	C4A-C3A-CAA-CBA
82	mO	201	PEB	NB-C1B-CHA-C4A
82	mO	201	PEB	C2B-C1B-CHA-C4A
82	mO	202	PEB	NB-C1B-CHA-C4A
82	mO	202	PEB	C2B-C1B-CHA-C4A
82	mO	203	PEB	NB-C1B-CHA-C4A
82	mO	203	PEB	C2B-C1B-CHA-C4A
82	mO	203	PEB	C2B-C3B-CAB-CBB
82	mO	203	PEB	C4B-C3B-CAB-CBB
82	aO	201	PEB	NB-C1B-CHA-C4A
82	aO	201	PEB	C2B-C1B-CHA-C4A
82	aO	202	PEB	NB-C1B-CHA-C4A
82	aO	202	PEB	C2B-C1B-CHA-C4A
82	aO	203	PEB	C2A-C3A-CAA-CBA
82	aO	203	PEB	C4A-C3A-CAA-CBA
82	aO	203	PEB	NB-C1B-CHA-C4A
82	aO	203	PEB	C2B-C1B-CHA-C4A
82	bO	201	PEB	C4A-C3A-CAA-CBA
82	bO	201	PEB	NB-C1B-CHA-C4A
82	bO	201	PEB	C2B-C1B-CHA-C4A
82	bO	202	PEB	ND-C1D-CHC-C4C
82	bO	202	PEB	NB-C1B-CHA-C4A
82	bO	202	PEB	C2B-C1B-CHA-C4A
82	cO	201	PEB	NB-C1B-CHA-C4A
82	cO	201	PEB	C2B-C1B-CHA-C4A
82	cO	202	PEB	ND-C1D-CHC-C4C
82	cO	202	PEB	C2D-C1D-CHC-C4C
82	cO	202	PEB	NB-C1B-CHA-C4A
82	cO	202	PEB	C2B-C1B-CHA-C4A
82	cO	203	PEB	ND-C1D-CHC-C4C
82	cO	203	PEB	C2D-C1D-CHC-C4C
82	cO	203	PEB	NB-C1B-CHA-C4A
82	cO	203	PEB	C2B-C1B-CHA-C4A
82	dO	201	PEB	C2A-C3A-CAA-CBA
82	dO	201	PEB	C4A-C3A-CAA-CBA
82	dO	201	PEB	NB-C1B-CHA-C4A
82	dO	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
82	dO	202	PEB	ND-C1D-CHC-C4C
82	dO	202	PEB	C2D-C1D-CHC-C4C
82	dO	202	PEB	NB-C1B-CHA-C4A
82	dO	202	PEB	C2B-C1B-CHA-C4A
82	eO	201	PEB	NB-C1B-CHA-C4A
82	eO	201	PEB	C2B-C1B-CHA-C4A
82	eO	202	PEB	C2A-C3A-CAA-CBA
82	eO	202	PEB	NB-C1B-CHA-C4A
82	eO	202	PEB	C2B-C1B-CHA-C4A
82	eO	203	PEB	NB-C1B-CHA-C4A
82	eO	203	PEB	C2B-C1B-CHA-C4A
82	fO	201	PEB	ND-C1D-CHC-C4C
82	fO	201	PEB	C2D-C1D-CHC-C4C
82	fO	201	PEB	C4A-C3A-CAA-CBA
82	fO	201	PEB	NB-C1B-CHA-C4A
82	fO	201	PEB	C2B-C1B-CHA-C4A
82	fO	202	PEB	ND-C1D-CHC-C4C
82	fO	202	PEB	C2D-C1D-CHC-C4C
82	fO	202	PEB	C4A-C3A-CAA-CBA
82	fO	202	PEB	NB-C1B-CHA-C4A
82	fO	202	PEB	C2B-C1B-CHA-C4A
82	gO	201	PEB	NB-C1B-CHA-C4A
82	gO	201	PEB	C2B-C1B-CHA-C4A
82	gO	202	PEB	ND-C1D-CHC-C4C
82	gO	202	PEB	C2D-C1D-CHC-C4C
82	gO	202	PEB	C2A-C3A-CAA-CBA
82	gO	202	PEB	NB-C1B-CHA-C4A
82	gO	202	PEB	C2B-C1B-CHA-C4A
82	gO	203	PEB	ND-C1D-CHC-C4C
82	gO	203	PEB	C2D-C1D-CHC-C4C
82	gO	203	PEB	NB-C1B-CHA-C4A
82	gO	203	PEB	C2B-C1B-CHA-C4A
82	gO	203	PEB	C2B-C3B-CAB-CBB
82	hO	201	PEB	ND-C1D-CHC-C4C
82	hO	201	PEB	C2D-C1D-CHC-C4C
82	hO	201	PEB	C4A-C3A-CAA-CBA
82	hO	201	PEB	NB-C1B-CHA-C4A
82	hO	201	PEB	C2B-C1B-CHA-C4A
82	hO	202	PEB	ND-C1D-CHC-C4C
82	hO	202	PEB	NB-C1B-CHA-C4A
82	hO	202	PEB	C2B-C1B-CHA-C4A
82	bP	501	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	bP	501	PEB	NB-C1B-CHA-C4A
82	bP	501	PEB	C2B-C1B-CHA-C4A
82	bP	502	PEB	C4A-C3A-CAA-CBA
82	bP	502	PEB	NB-C1B-CHA-C4A
82	bP	502	PEB	C2B-C1B-CHA-C4A
82	dQ	401	PEB	NB-C1B-CHA-C4A
82	dQ	401	PEB	C2B-C1B-CHA-C4A
82	Z9	301	PEB	ND-C1D-CHC-C4C
82	Z9	301	PEB	C2D-C1D-CHC-C4C
82	Z9	301	PEB	C2D-C3D-CAD-CBD
82	Z9	301	PEB	C4A-C3A-CAA-CBA
82	Z9	301	PEB	NB-C1B-CHA-C4A
82	Z9	301	PEB	C2B-C1B-CHA-C4A
82	Z9	303	PEB	ND-C1D-CHC-C4C
82	Z9	303	PEB	C2D-C1D-CHC-C4C
82	Z9	303	PEB	NB-C1B-CHA-C4A
82	Z9	303	PEB	C2B-C1B-CHA-C4A
82	Z9	304	PEB	ND-C1D-CHC-C4C
82	Z9	304	PEB	C2D-C1D-CHC-C4C
82	Z9	304	PEB	C2C-CAC-CBC-CGC
82	Z9	304	PEB	NB-C1B-CHA-C4A
82	Z9	304	PEB	C2B-C1B-CHA-C4A
82	M9	301	PEB	NB-C1B-CHA-C4A
82	M9	301	PEB	C2B-C1B-CHA-C4A
82	M9	302	PEB	ND-C1D-CHC-C4C
82	M9	302	PEB	C2D-C1D-CHC-C4C
82	M9	302	PEB	C2D-C3D-CAD-CBD
82	M9	302	PEB	C4A-C3A-CAA-CBA
82	M9	302	PEB	NB-C1B-CHA-C4A
82	M9	302	PEB	C2B-C1B-CHA-C4A
82	M9	304	PEB	ND-C1D-CHC-C4C
82	M9	304	PEB	C2D-C1D-CHC-C4C
82	M9	304	PEB	NB-C1B-CHA-C4A
82	M9	304	PEB	C2B-C1B-CHA-C4A
82	M9	305	PEB	ND-C1D-CHC-C4C
82	M9	305	PEB	C2D-C1D-CHC-C4C
82	M9	305	PEB	C2C-CAC-CBC-CGC
82	M9	305	PEB	NB-C1B-CHA-C4A
82	M9	305	PEB	C2B-C1B-CHA-C4A
83	KA	203	PUB	C3C-C4C-CHC-C1D
83	KA	203	PUB	NA-C4A-CHA-C1B
83	KA	203	PUB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
83	YA	302	PUB	ND-C1D-CHC-C4C
83	AD	302	PUB	C3C-C4C-CHC-C1D
83	AD	302	PUB	ND-C1D-CHC-C4C
83	AD	302	PUB	C2D-C1D-CHC-C4C
83	AE	302	PUB	C3C-C4C-CHC-C1D
83	AE	303	PUB	NC-C4C-CHC-C1D
83	AE	303	PUB	NA-C4A-CHA-C1B
83	AG	302	PUB	C3C-C4C-CHC-C1D
83	AG	303	PUB	NC-C4C-CHC-C1D
83	AG	303	PUB	NA-C4A-CHA-C1B
83	AH	303	PUB	NA-C4A-CHA-C1B
83	AH	304	PUB	C3C-C4C-CHC-C1D
83	AH	304	PUB	ND-C1D-CHC-C4C
83	AH	304	PUB	C2A-C3A-CAA-CBA
83	AH	304	PUB	NA-C4A-CHA-C1B
83	AH	304	PUB	C3A-C4A-CHA-C1B
83	AJ	303	PUB	NC-C4C-CHC-C1D
83	AJ	303	PUB	C3C-C4C-CHC-C1D
83	AJ	303	PUB	ND-C1D-CHC-C4C
83	AJ	303	PUB	NA-C4A-CHA-C1B
83	AJ	303	PUB	C3A-C4A-CHA-C1B
83	AJ	304	PUB	NA-C4A-CHA-C1B
83	BJ	302	PUB	NC-C4C-CHC-C1D
83	BJ	302	PUB	NA-C4A-CHA-C1B
83	QJ	201	PUB	NC-C4C-CHC-C1D
83	QJ	201	PUB	NA-C4A-CHA-C1B
83	QJ	201	PUB	C3A-C4A-CHA-C1B
83	AM	303	PUB	ND-C1D-CHC-C4C
83	AM	303	PUB	NA-C4A-CHA-C1B
83	AM	303	PUB	C3A-C4A-CHA-C1B
83	AM	304	PUB	C3C-C4C-CHC-C1D
83	AM	304	PUB	NA-C4A-CHA-C1B
83	BM	302	PUB	NC-C4C-CHC-C1D
83	BM	302	PUB	NA-C4A-CHA-C1B
83	QM	201	PUB	NC-C4C-CHC-C1D
83	QM	201	PUB	NA-C4A-CHA-C1B
83	QM	201	PUB	C3A-C4A-CHA-C1B
83	AO	302	PUB	NA-C4A-CHA-C1B
83	AO	303	PUB	C3C-C4C-CHC-C1D
83	AQ	302	PUB	C3C-C4C-CHC-C1D
83	AQ	302	PUB	ND-C1D-CHC-C4C
83	AQ	302	PUB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
83	A1	303	PUB	NA-C4A-CHA-C1B
83	A1	304	PUB	C3C-C4C-CHC-C1D
83	A1	304	PUB	ND-C1D-CHC-C4C
83	A1	304	PUB	C2A-C3A-CAA-CBA
83	A1	304	PUB	NA-C4A-CHA-C1B
83	A1	304	PUB	C3A-C4A-CHA-C1B
83	A4	302	PUB	NA-C4A-CHA-C1B
83	A4	303	PUB	C3C-C4C-CHC-C1D
83	M5	302	PUB	C3C-C4C-CHC-C1D
83	M5	302	PUB	C4B-C3B-CAB-CBB
83	M5	303	PUB	NA-C4A-CHA-C1B
83	Z5	302	PUB	C3C-C4C-CHC-C1D
83	Z5	302	PUB	C4B-C3B-CAB-CBB
83	Z5	303	PUB	NA-C4A-CHA-C1B
83	K7	203	PUB	C3C-C4C-CHC-C1D
83	K7	203	PUB	NA-C4A-CHA-C1B
83	K7	203	PUB	C3A-C4A-CHA-C1B
83	Y7	302	PUB	ND-C1D-CHC-C4C
83	wF	304	PUB	C3C-C4C-CHC-C1D
83	wF	304	PUB	NA-C4A-CHA-C1B
83	xF	301	PUB	ND-C1D-CHC-C4C
83	xF	301	PUB	C2D-C1D-CHC-C4C
83	xF	305	PUB	ND-C1D-CHC-C4C
83	xF	305	PUB	C2D-C1D-CHC-C4C
83	xF	305	PUB	NA-C4A-CHA-C1B
83	xF	305	PUB	C3A-C4A-CHA-C1B
83	xF	306	PUB	ND-C1D-CHC-C4C
83	xF	306	PUB	C2D-C1D-CHC-C4C
83	yF	302	PUB	C4D-C3D-CAD-CBD
83	wK	304	PUB	C3C-C4C-CHC-C1D
83	wK	304	PUB	NA-C4A-CHA-C1B
83	xK	301	PUB	ND-C1D-CHC-C4C
83	xK	301	PUB	C2D-C1D-CHC-C4C
83	xK	305	PUB	ND-C1D-CHC-C4C
83	xK	305	PUB	C2D-C1D-CHC-C4C
83	xK	305	PUB	NA-C4A-CHA-C1B
83	xK	305	PUB	C3A-C4A-CHA-C1B
83	xK	306	PUB	ND-C1D-CHC-C4C
83	xK	306	PUB	C2D-C1D-CHC-C4C
83	yK	302	PUB	C4D-C3D-CAD-CBD
83	Z9	302	PUB	NA-C4A-CHA-C1B
83	Z9	305	PUB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
83	Z9	305	PUB	C2D-C1D-CHC-C4C
83	Z9	305	PUB	NA-C4A-CHA-C1B
83	M9	303	PUB	NA-C4A-CHA-C1B
84	BE	1001	CYC	NA-C4A-CHB-C1B
84	BE	1001	CYC	C3A-C4A-CHB-C1B
84	BE	1001	CYC	C2C-C3C-CAC-CBC
84	BE	1001	CYC	C4C-C3C-CAC-CBC
84	DE	1001	CYC	NA-C4A-CHB-C1B
84	DE	1001	CYC	C3A-C4A-CHB-C1B
84	DE	1001	CYC	C2C-C3C-CAC-CBC
84	DE	1001	CYC	C4C-C3C-CAC-CBC
84	EE	1001	CYC	NA-C4A-CHB-C1B
84	EE	1001	CYC	C3A-C4A-CHB-C1B
84	FE	1001	CYC	NA-C4A-CHB-C1B
84	FE	1001	CYC	C3A-C4A-CHB-C1B
84	FE	1002	CYC	NA-C4A-CHB-C1B
84	FE	1002	CYC	C3A-C4A-CHB-C1B
84	FE	1002	CYC	C2C-C3C-CAC-CBC
84	FE	1002	CYC	C4C-C3C-CAC-CBC
84	GE	1001	CYC	NA-C4A-CHB-C1B
84	GE	1001	CYC	C3A-C4A-CHB-C1B
84	GE	1001	CYC	C2C-C3C-CAC-CBC
84	GE	1001	CYC	C4C-C3C-CAC-CBC
84	HE	1001	CYC	NA-C4A-CHB-C1B
84	HE	1001	CYC	C3A-C4A-CHB-C1B
84	IE	1001	CYC	NA-C4A-CHB-C1B
84	IE	1001	CYC	C3A-C4A-CHB-C1B
84	IE	1001	CYC	C2C-C3C-CAC-CBC
84	IE	1001	CYC	C4C-C3C-CAC-CBC
84	LE	1001	CYC	C2C-C3C-CAC-CBC
84	LE	1001	CYC	C4C-C3C-CAC-CBC
84	LE	1001	CYC	C2D-C3D-CAD-CBD
84	LE	1001	CYC	C4D-C3D-CAD-CBD
84	ME	1001	CYC	NA-C4A-CHB-C1B
84	ME	1001	CYC	C3A-C4A-CHB-C1B
84	ME	1001	CYC	C2C-C3C-CAC-CBC
84	ME	1001	CYC	C4C-C3C-CAC-CBC
84	NE	201	CYC	NA-C4A-CHB-C1B
84	NE	201	CYC	C3A-C4A-CHB-C1B
84	BG	1001	CYC	NA-C4A-CHB-C1B
84	BG	1001	CYC	C3A-C4A-CHB-C1B
84	BG	1001	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
84	BG	1001	CYC	C4C-C3C-CAC-CBC
84	CG	1001	CYC	NA-C4A-CHB-C1B
84	CG	1001	CYC	C3A-C4A-CHB-C1B
84	DG	1001	CYC	NA-C4A-CHB-C1B
84	DG	1001	CYC	C3A-C4A-CHB-C1B
84	DG	1001	CYC	C2C-C3C-CAC-CBC
84	DG	1001	CYC	C4C-C3C-CAC-CBC
84	EG	1001	CYC	NA-C4A-CHB-C1B
84	EG	1001	CYC	C3A-C4A-CHB-C1B
84	FG	1001	CYC	NA-C4A-CHB-C1B
84	FG	1001	CYC	C3A-C4A-CHB-C1B
84	FG	1001	CYC	C2C-C3C-CAC-CBC
84	FG	1001	CYC	C4C-C3C-CAC-CBC
84	GG	1001	CYC	NA-C4A-CHB-C1B
84	GG	1001	CYC	C3A-C4A-CHB-C1B
84	GG	1001	CYC	C2C-C3C-CAC-CBC
84	GG	1001	CYC	C4C-C3C-CAC-CBC
84	HG	1001	CYC	NA-C4A-CHB-C1B
84	HG	1001	CYC	C3A-C4A-CHB-C1B
84	IG	1001	CYC	NA-C4A-CHB-C1B
84	IG	1001	CYC	C3A-C4A-CHB-C1B
84	IG	1001	CYC	C2C-C3C-CAC-CBC
84	IG	1001	CYC	C4C-C3C-CAC-CBC
84	KG	202	CYC	NA-C4A-CHB-C1B
84	KG	202	CYC	C3A-C4A-CHB-C1B
84	LG	1001	CYC	C2C-C3C-CAC-CBC
84	LG	1001	CYC	C4C-C3C-CAC-CBC
84	LG	1001	CYC	C2D-C3D-CAD-CBD
84	LG	1001	CYC	C4D-C3D-CAD-CBD
84	MG	1001	CYC	NA-C4A-CHB-C1B
84	MG	1001	CYC	C3A-C4A-CHB-C1B
84	MG	1001	CYC	C2C-C3C-CAC-CBC
84	MG	1001	CYC	C4C-C3C-CAC-CBC
84	CH	1001	CYC	NA-C4A-CHB-C1B
84	CH	1001	CYC	C3A-C4A-CHB-C1B
84	CH	1001	CYC	C2C-C3C-CAC-CBC
84	CH	1001	CYC	C4C-C3C-CAC-CBC
84	DH	1001	CYC	NA-C4A-CHB-C1B
84	DH	1001	CYC	C3A-C4A-CHB-C1B
84	DH	1003	CYC	NA-C4A-CHB-C1B
84	DH	1003	CYC	C3A-C4A-CHB-C1B
84	DH	1003	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
84	DH	1003	CYC	C4C-C3C-CAC-CBC
84	EH	1001	CYC	NA-C4A-CHB-C1B
84	EH	1001	CYC	C3A-C4A-CHB-C1B
84	FH	1001	CYC	NA-C4A-CHB-C1B
84	FH	1001	CYC	C3A-C4A-CHB-C1B
84	FH	1001	CYC	C2C-C3C-CAC-CBC
84	FH	1001	CYC	C4C-C3C-CAC-CBC
84	HH	1001	CYC	NA-C4A-CHB-C1B
84	HH	1001	CYC	C3A-C4A-CHB-C1B
84	JH	1001	CYC	NA-C4A-CHB-C1B
84	JH	1001	CYC	C3A-C4A-CHB-C1B
84	JH	1003	CYC	NA-C4A-CHB-C1B
84	JH	1003	CYC	C3A-C4A-CHB-C1B
84	KH	1001	CYC	NA-C4A-CHB-C1B
84	KH	1001	CYC	C3A-C4A-CHB-C1B
84	KH	1001	CYC	C2C-C3C-CAC-CBC
84	KH	1001	CYC	C4C-C3C-CAC-CBC
84	LH	1001	CYC	NA-C4A-CHB-C1B
84	LH	1001	CYC	C3A-C4A-CHB-C1B
84	LH	1001	CYC	C2C-C3C-CAC-CBC
84	LH	1001	CYC	C4C-C3C-CAC-CBC
84	LH	1002	CYC	NA-C4A-CHB-C1B
84	LH	1002	CYC	C3A-C4A-CHB-C1B
84	LH	1002	CYC	C2C-C3C-CAC-CBC
84	LH	1002	CYC	C4C-C3C-CAC-CBC
84	NH	1001	CYC	NA-C4A-CHB-C1B
84	NH	1001	CYC	C3A-C4A-CHB-C1B
84	NH	1001	CYC	C2C-C3C-CAC-CBC
84	NH	1001	CYC	C4C-C3C-CAC-CBC
84	CO	1001	CYC	NA-C4A-CHB-C1B
84	CO	1001	CYC	C3A-C4A-CHB-C1B
84	CO	1001	CYC	C2C-C3C-CAC-CBC
84	CO	1001	CYC	C4C-C3C-CAC-CBC
84	DO	1001	CYC	NA-C4A-CHB-C1B
84	DO	1001	CYC	C3A-C4A-CHB-C1B
84	DO	1001	CYC	C2C-C3C-CAC-CBC
84	DO	1001	CYC	C4C-C3C-CAC-CBC
84	EO	1001	CYC	NA-C4A-CHB-C1B
84	EO	1001	CYC	C3A-C4A-CHB-C1B
84	FO	1001	CYC	NA-C4A-CHB-C1B
84	FO	1001	CYC	C3A-C4A-CHB-C1B
84	FO	1001	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
84	FO	1001	CYC	C4C-C3C-CAC-CBC
84	GO	1001	CYC	NA-C4A-CHB-C1B
84	GO	1001	CYC	C3A-C4A-CHB-C1B
84	HO	1001	CYC	NA-C4A-CHB-C1B
84	HO	1001	CYC	C3A-C4A-CHB-C1B
84	HO	1001	CYC	C2C-C3C-CAC-CBC
84	HO	1001	CYC	C4C-C3C-CAC-CBC
84	IO	1001	CYC	NA-C4A-CHB-C1B
84	IO	1001	CYC	C3A-C4A-CHB-C1B
84	IO	1001	CYC	C2C-C3C-CAC-CBC
84	IO	1001	CYC	C4C-C3C-CAC-CBC
84	JO	1001	CYC	C2C-C3C-CAC-CBC
84	JO	1001	CYC	C4C-C3C-CAC-CBC
84	KO	1001	CYC	NA-C4A-CHB-C1B
84	KO	1001	CYC	C3A-C4A-CHB-C1B
84	KO	1001	CYC	C2C-C3C-CAC-CBC
84	KO	1001	CYC	C4C-C3C-CAC-CBC
84	MO	1001	CYC	NA-C4A-CHB-C1B
84	MO	1001	CYC	C3A-C4A-CHB-C1B
84	MO	1001	CYC	C2C-C3C-CAC-CBC
84	MO	1001	CYC	C4C-C3C-CAC-CBC
84	NO	1001	CYC	NA-C4A-CHB-C1B
84	NO	1001	CYC	C3A-C4A-CHB-C1B
84	NO	1001	CYC	C2C-C3C-CAC-CBC
84	NO	1001	CYC	C4C-C3C-CAC-CBC
84	L1	1001	CYC	NA-C4A-CHB-C1B
84	L1	1001	CYC	C3A-C4A-CHB-C1B
84	L1	1001	CYC	C2C-C3C-CAC-CBC
84	L1	1001	CYC	C4C-C3C-CAC-CBC
84	M1	201	CYC	NA-C4A-CHB-C1B
84	M1	201	CYC	C3A-C4A-CHB-C1B
84	N1	1001	CYC	NA-C4A-CHB-C1B
84	N1	1001	CYC	C3A-C4A-CHB-C1B
84	N1	1001	CYC	C2C-C3C-CAC-CBC
84	N1	1001	CYC	C4C-C3C-CAC-CBC
84	C1	1001	CYC	NA-C4A-CHB-C1B
84	C1	1001	CYC	C3A-C4A-CHB-C1B
84	C1	1001	CYC	C2C-C3C-CAC-CBC
84	C1	1001	CYC	C4C-C3C-CAC-CBC
84	D1	1001	CYC	NA-C4A-CHB-C1B
84	D1	1001	CYC	C3A-C4A-CHB-C1B
84	D1	1003	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
84	D1	1003	CYC	C3A-C4A-CHB-C1B
84	D1	1003	CYC	C2C-C3C-CAC-CBC
84	D1	1003	CYC	C4C-C3C-CAC-CBC
84	E1	1001	CYC	NA-C4A-CHB-C1B
84	E1	1001	CYC	C3A-C4A-CHB-C1B
84	F1	1001	CYC	NA-C4A-CHB-C1B
84	F1	1001	CYC	C3A-C4A-CHB-C1B
84	F1	1001	CYC	C2C-C3C-CAC-CBC
84	F1	1001	CYC	C4C-C3C-CAC-CBC
84	H1	1001	CYC	NA-C4A-CHB-C1B
84	H1	1001	CYC	C3A-C4A-CHB-C1B
84	I1	1001	CYC	NA-C4A-CHB-C1B
84	I1	1001	CYC	C3A-C4A-CHB-C1B
84	I1	1001	CYC	C2C-C3C-CAC-CBC
84	I1	1001	CYC	C4C-C3C-CAC-CBC
84	J1	1001	CYC	NA-C4A-CHB-C1B
84	J1	1001	CYC	C3A-C4A-CHB-C1B
84	K1	1001	CYC	NA-C4A-CHB-C1B
84	K1	1001	CYC	C3A-C4A-CHB-C1B
84	K1	1001	CYC	C2C-C3C-CAC-CBC
84	K1	1001	CYC	C4C-C3C-CAC-CBC
84	A3	1001	CYC	ND-C1D-CHD-C4C
84	A3	1001	CYC	C2D-C1D-CHD-C4C
84	C3	1001	CYC	ND-C1D-CHD-C4C
84	C3	1001	CYC	C2D-C1D-CHD-C4C
84	E3	1001	CYC	ND-C1D-CHD-C4C
84	E3	1001	CYC	C2D-C1D-CHD-C4C
84	G3	1001	CYC	ND-C1D-CHD-C4C
84	G3	1001	CYC	C2D-C1D-CHD-C4C
84	J3	1001	CYC	ND-C1D-CHD-C4C
84	J3	1001	CYC	C2D-C1D-CHD-C4C
84	K3	1001	CYC	ND-C1D-CHD-C4C
84	K3	1001	CYC	C2D-C1D-CHD-C4C
84	N3	1001	CYC	ND-C1D-CHD-C4C
84	N3	1001	CYC	C2D-C1D-CHD-C4C
84	P3	1001	CYC	ND-C1D-CHD-C4C
84	P3	1001	CYC	C2D-C1D-CHD-C4C
84	R3	1001	CYC	ND-C1D-CHD-C4C
84	R3	1001	CYC	C2D-C1D-CHD-C4C
84	T3	1001	CYC	ND-C1D-CHD-C4C
84	T3	1001	CYC	C2D-C1D-CHD-C4C
84	V3	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	V3	1001	CYC	C2D-C1D-CHD-C4C
84	c3	1001	CYC	ND-C1D-CHD-C4C
84	c3	1001	CYC	C2D-C1D-CHD-C4C
84	e3	1001	CYC	ND-C1D-CHD-C4C
84	e3	1001	CYC	C2D-C1D-CHD-C4C
84	g3	1001	CYC	ND-C1D-CHD-C4C
84	g3	1001	CYC	C2D-C1D-CHD-C4C
84	i3	1001	CYC	ND-C1D-CHD-C4C
84	i3	1001	CYC	C2D-C1D-CHD-C4C
84	l3	1001	CYC	ND-C1D-CHD-C4C
84	l3	1001	CYC	C2D-C1D-CHD-C4C
84	m3	1001	CYC	ND-C1D-CHD-C4C
84	m3	1001	CYC	C2D-C1D-CHD-C4C
84	p3	1001	CYC	ND-C1D-CHD-C4C
84	p3	1001	CYC	C2D-C1D-CHD-C4C
84	r3	1001	CYC	NA-C4A-CHB-C1B
84	r3	1001	CYC	C3A-C4A-CHB-C1B
84	r3	1001	CYC	C4B-C3B-CAB-CBB
84	r3	1001	CYC	C2C-C3C-CAC-CBC
84	r3	1001	CYC	NC-C4C-CHD-C1D
84	t3	1001	CYC	ND-C1D-CHD-C4C
84	t3	1001	CYC	C2D-C1D-CHD-C4C
84	v3	1001	CYC	ND-C1D-CHD-C4C
84	v3	1001	CYC	C2D-C1D-CHD-C4C
84	x3	1001	CYC	ND-C1D-CHD-C4C
84	x3	1001	CYC	C2D-C1D-CHD-C4C
84	y3	1001	CYC	C2D-C1D-CHD-C4C
84	63	901	CYC	C3A-C4A-CHB-C1B
84	73	1002	CYC	C3A-C4A-CHB-C1B
84	F4	1001	CYC	NA-C4A-CHB-C1B
84	F4	1001	CYC	C3A-C4A-CHB-C1B
84	F4	1001	CYC	C2C-C3C-CAC-CBC
84	F4	1001	CYC	C4C-C3C-CAC-CBC
84	G4	1001	CYC	NA-C4A-CHB-C1B
84	G4	1001	CYC	C3A-C4A-CHB-C1B
84	H4	1001	CYC	NA-C4A-CHB-C1B
84	H4	1001	CYC	C3A-C4A-CHB-C1B
84	H4	1001	CYC	C2C-C3C-CAC-CBC
84	H4	1001	CYC	C4C-C3C-CAC-CBC
84	I4	1001	CYC	NA-C4A-CHB-C1B
84	I4	1001	CYC	C3A-C4A-CHB-C1B
84	I4	1001	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
84	I4	1001	CYC	C4C-C3C-CAC-CBC
84	J4	1001	CYC	C2C-C3C-CAC-CBC
84	J4	1001	CYC	C4C-C3C-CAC-CBC
84	K4	1001	CYC	NA-C4A-CHB-C1B
84	K4	1001	CYC	C3A-C4A-CHB-C1B
84	K4	1001	CYC	C2C-C3C-CAC-CBC
84	K4	1001	CYC	C4C-C3C-CAC-CBC
84	M4	1001	CYC	NA-C4A-CHB-C1B
84	M4	1001	CYC	C3A-C4A-CHB-C1B
84	M4	1001	CYC	C2C-C3C-CAC-CBC
84	M4	1001	CYC	C4C-C3C-CAC-CBC
84	N4	1001	CYC	NA-C4A-CHB-C1B
84	N4	1001	CYC	C3A-C4A-CHB-C1B
84	N4	1001	CYC	C2C-C3C-CAC-CBC
84	N4	1001	CYC	C4C-C3C-CAC-CBC
84	C4	1001	CYC	NA-C4A-CHB-C1B
84	C4	1001	CYC	C3A-C4A-CHB-C1B
84	C4	1001	CYC	C2C-C3C-CAC-CBC
84	C4	1001	CYC	C4C-C3C-CAC-CBC
84	D4	1001	CYC	NA-C4A-CHB-C1B
84	D4	1001	CYC	C3A-C4A-CHB-C1B
84	D4	1001	CYC	C2C-C3C-CAC-CBC
84	D4	1001	CYC	C4C-C3C-CAC-CBC
84	E4	1001	CYC	NA-C4A-CHB-C1B
84	E4	1001	CYC	C3A-C4A-CHB-C1B
85	AL	401	BCR	C23-C24-C25-C30
85	CL	502	BCR	C17-C18-C19-C20
85	CL	502	BCR	C36-C18-C19-C20
85	CL	502	BCR	C19-C20-C21-C22
85	CL	516	BCR	C7-C8-C9-C34
85	FL	101	BCR	C21-C22-C23-C24
85	FL	101	BCR	C37-C22-C23-C24
85	HL	103	BCR	C7-C8-C9-C10
85	HL	103	BCR	C7-C8-C9-C34
85	KL	100	BCR	C7-C8-C9-C10
85	KL	100	BCR	C7-C8-C9-C34
85	KL	100	BCR	C37-C22-C23-C24
85	AN	845	BCR	C5-C6-C7-C8
85	AN	845	BCR	C11-C12-C13-C14
85	AN	845	BCR	C11-C12-C13-C35
85	AN	845	BCR	C21-C22-C23-C24
85	AN	845	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
85	AN	847	BCR	C1-C6-C7-C8
85	AN	847	BCR	C7-C8-C9-C10
85	AN	847	BCR	C7-C8-C9-C34
85	AN	847	BCR	C11-C12-C13-C14
85	AN	847	BCR	C11-C12-C13-C35
85	AN	848	BCR	C23-C24-C25-C26
85	BN	803	BCR	C5-C6-C7-C8
85	BN	803	BCR	C15-C16-C17-C18
85	BN	803	BCR	C21-C22-C23-C24
85	BN	803	BCR	C37-C22-C23-C24
85	BN	838	BCR	C7-C8-C9-C10
85	BN	838	BCR	C7-C8-C9-C34
85	BN	838	BCR	C21-C22-C23-C24
85	BN	838	BCR	C37-C22-C23-C24
85	BN	840	BCR	C1-C6-C7-C8
85	BN	840	BCR	C5-C6-C7-C8
85	BN	840	BCR	C37-C22-C23-C24
85	BN	842	BCR	C5-C6-C7-C8
85	BN	842	BCR	C7-C8-C9-C10
85	BN	842	BCR	C7-C8-C9-C34
85	BN	842	BCR	C17-C18-C19-C20
85	BN	842	BCR	C36-C18-C19-C20
85	BN	842	BCR	C23-C24-C25-C26
85	BN	843	BCR	C21-C22-C23-C24
85	BN	843	BCR	C37-C22-C23-C24
85	FN	202	BCR	C7-C8-C9-C10
85	FN	202	BCR	C7-C8-C9-C34
85	FN	204	BCR	C7-C8-C9-C10
85	FN	204	BCR	C7-C8-C9-C34
85	IN	101	BCR	C7-C8-C9-C34
85	IN	101	BCR	C11-C12-C13-C14
85	IN	101	BCR	C11-C12-C13-C35
85	IN	101	BCR	C13-C14-C15-C16
85	IN	101	BCR	C21-C22-C23-C24
85	IN	101	BCR	C37-C22-C23-C24
85	IN	101	BCR	C23-C24-C25-C26
85	IN	101	BCR	C23-C24-C25-C30
85	JN	102	BCR	C36-C18-C19-C20
85	JN	103	BCR	C11-C12-C13-C35
85	JN	103	BCR	C17-C18-C19-C20
85	JN	103	BCR	C36-C18-C19-C20
85	JN	103	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
85	JN	103	BCR	C23-C24-C25-C26
85	KN	101	BCR	C11-C12-C13-C14
85	KN	101	BCR	C11-C12-C13-C35
85	KN	101	BCR	C17-C18-C19-C20
85	KN	101	BCR	C36-C18-C19-C20
85	KN	101	BCR	C21-C22-C23-C24
85	KN	101	BCR	C37-C22-C23-C24
85	LN	201	BCR	C7-C8-C9-C10
85	LN	201	BCR	C7-C8-C9-C34
85	LN	201	BCR	C17-C18-C19-C20
85	LN	201	BCR	C36-C18-C19-C20
85	LN	205	BCR	C15-C16-C17-C18
85	LN	205	BCR	C21-C22-C23-C24
85	LN	205	BCR	C37-C22-C23-C24
85	A2	845	BCR	C5-C6-C7-C8
85	A2	845	BCR	C11-C12-C13-C14
85	A2	845	BCR	C11-C12-C13-C35
85	A2	845	BCR	C21-C22-C23-C24
85	A2	845	BCR	C37-C22-C23-C24
85	A2	847	BCR	C1-C6-C7-C8
85	A2	847	BCR	C7-C8-C9-C10
85	A2	847	BCR	C7-C8-C9-C34
85	A2	847	BCR	C11-C12-C13-C14
85	A2	847	BCR	C11-C12-C13-C35
85	A2	848	BCR	C23-C24-C25-C26
85	B2	802	BCR	C5-C6-C7-C8
85	B2	802	BCR	C15-C16-C17-C18
85	B2	802	BCR	C21-C22-C23-C24
85	B2	802	BCR	C37-C22-C23-C24
85	B2	838	BCR	C7-C8-C9-C10
85	B2	838	BCR	C7-C8-C9-C34
85	B2	838	BCR	C21-C22-C23-C24
85	B2	838	BCR	C37-C22-C23-C24
85	B2	840	BCR	C1-C6-C7-C8
85	B2	840	BCR	C5-C6-C7-C8
85	B2	840	BCR	C37-C22-C23-C24
85	B2	842	BCR	C5-C6-C7-C8
85	B2	842	BCR	C7-C8-C9-C10
85	B2	842	BCR	C7-C8-C9-C34
85	B2	842	BCR	C17-C18-C19-C20
85	B2	842	BCR	C36-C18-C19-C20
85	B2	842	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
85	B2	843	BCR	C21-C22-C23-C24
85	B2	843	BCR	C37-C22-C23-C24
85	F2	203	BCR	C7-C8-C9-C10
85	F2	203	BCR	C7-C8-C9-C34
85	F2	204	BCR	C7-C8-C9-C10
85	F2	204	BCR	C7-C8-C9-C34
85	I2	101	BCR	C7-C8-C9-C34
85	I2	101	BCR	C11-C12-C13-C14
85	I2	101	BCR	C11-C12-C13-C35
85	I2	101	BCR	C13-C14-C15-C16
85	I2	101	BCR	C21-C22-C23-C24
85	I2	101	BCR	C37-C22-C23-C24
85	I2	101	BCR	C23-C24-C25-C26
85	I2	101	BCR	C23-C24-C25-C30
85	J2	102	BCR	C36-C18-C19-C20
85	J2	103	BCR	C11-C12-C13-C35
85	J2	103	BCR	C17-C18-C19-C20
85	J2	103	BCR	C36-C18-C19-C20
85	J2	103	BCR	C37-C22-C23-C24
85	J2	103	BCR	C23-C24-C25-C26
85	K2	102	BCR	C11-C12-C13-C14
85	K2	102	BCR	C11-C12-C13-C35
85	K2	102	BCR	C17-C18-C19-C20
85	K2	102	BCR	C36-C18-C19-C20
85	K2	102	BCR	C21-C22-C23-C24
85	K2	102	BCR	C37-C22-C23-C24
85	L2	201	BCR	C7-C8-C9-C10
85	L2	201	BCR	C7-C8-C9-C34
85	L2	201	BCR	C17-C18-C19-C20
85	L2	201	BCR	C36-C18-C19-C20
85	L2	205	BCR	C15-C16-C17-C18
85	L2	205	BCR	C21-C22-C23-C24
85	L2	205	BCR	C37-C22-C23-C24
85	C6	508	BCR	C21-C22-C23-C24
85	C6	508	BCR	C37-C22-C23-C24
85	F6	101	BCR	C7-C8-C9-C10
85	F6	101	BCR	C7-C8-C9-C34
85	F6	101	BCR	C17-C18-C19-C20
85	F6	101	BCR	C36-C18-C19-C20
85	F6	101	BCR	C21-C22-C23-C24
85	F6	101	BCR	C37-C22-C23-C24
85	K6	102	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
85	K6	102	BCR	C17-C18-C19-C20
85	K6	102	BCR	C36-C18-C19-C20
85	K6	102	BCR	C21-C22-C23-C24
85	K6	102	BCR	C37-C22-C23-C24
85	b6	601	BCR	C23-C24-C25-C30
85	b6	603	BCR	C7-C8-C9-C10
85	b6	603	BCR	C7-C8-C9-C34
85	c6	617	BCR	C1-C6-C7-C8
85	c6	617	BCR	C23-C24-C25-C26
85	c6	617	BCR	C23-C24-C25-C30
85	d6	405	BCR	C7-C8-C9-C34
85	d6	405	BCR	C11-C12-C13-C14
85	d6	405	BCR	C11-C12-C13-C35
85	d6	405	BCR	C17-C18-C19-C20
85	d6	405	BCR	C36-C18-C19-C20
85	d6	405	BCR	C37-C22-C23-C24
85	h6	102	BCR	C7-C8-C9-C10
85	h6	102	BCR	C7-C8-C9-C34
85	k6	102	BCR	C11-C12-C13-C35
85	k6	102	BCR	C17-C18-C19-C20
85	k6	102	BCR	C36-C18-C19-C20
85	k6	102	BCR	C21-C22-C23-C24
85	k6	102	BCR	C37-C22-C23-C24
85	bL	603	BCR	C23-C24-C25-C30
85	cL	504	BCR	C17-C18-C19-C20
85	cL	504	BCR	C36-C18-C19-C20
85	cL	504	BCR	C19-C20-C21-C22
85	cL	518	BCR	C7-C8-C9-C10
85	cL	518	BCR	C7-C8-C9-C34
85	fL	101	BCR	C21-C22-C23-C24
85	fL	101	BCR	C37-C22-C23-C24
85	hL	102	BCR	C7-C8-C9-C10
85	hL	102	BCR	C7-C8-C9-C34
85	kL	100	BCR	C7-C8-C9-C10
85	kL	100	BCR	C7-C8-C9-C34
85	kL	100	BCR	C37-C22-C23-C24
87	AL	403	CLA	CBD-CGD-O2D-CED
87	AL	405	CLA	C2B-C3B-CAB-CBB
87	AL	405	CLA	C4B-C3B-CAB-CBB
87	BL	601	CLA	C2B-C3B-CAB-CBB
87	BL	601	CLA	C4B-C3B-CAB-CBB
87	BL	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	BL	602	CLA	CHA-CBD-CGD-O2D
87	BL	603	CLA	C1A-C2A-CAA-CBA
87	BL	603	CLA	C3A-C2A-CAA-CBA
87	BL	605	CLA	C2B-C3B-CAB-CBB
87	BL	605	CLA	C4B-C3B-CAB-CBB
87	BL	605	CLA	CHA-CBD-CGD-O1D
87	BL	605	CLA	CHA-CBD-CGD-O2D
87	BL	605	CLA	C4-C3-C5-C6
87	BL	609	CLA	CHA-CBD-CGD-O1D
87	BL	609	CLA	CHA-CBD-CGD-O2D
87	BL	620	CLA	C2B-C3B-CAB-CBB
87	BL	620	CLA	C4B-C3B-CAB-CBB
87	BL	621	CLA	C2-C3-C5-C6
87	BL	621	CLA	C4-C3-C5-C6
87	BL	622	CLA	C2B-C3B-CAB-CBB
87	BL	622	CLA	C4B-C3B-CAB-CBB
87	BL	622	CLA	CBD-CGD-O2D-CED
87	BL	623	CLA	C1A-C2A-CAA-CBA
87	BL	623	CLA	C3A-C2A-CAA-CBA
87	CL	504	CLA	CHA-CBD-CGD-O1D
87	CL	504	CLA	CHA-CBD-CGD-O2D
87	CL	504	CLA	CAD-CBD-CGD-O1D
87	CL	506	CLA	CHA-CBD-CGD-O1D
87	CL	506	CLA	CHA-CBD-CGD-O2D
87	CL	506	CLA	CAD-CBD-CGD-O1D
87	CL	510	CLA	CHA-CBD-CGD-O1D
87	CL	510	CLA	CHA-CBD-CGD-O2D
87	CL	513	CLA	CHA-CBD-CGD-O1D
87	CL	513	CLA	CHA-CBD-CGD-O2D
87	CL	513	CLA	CBD-CGD-O2D-CED
87	CL	513	CLA	O1D-CGD-O2D-CED
87	CL	518	CLA	C1A-C2A-CAA-CBA
87	CL	518	CLA	C3A-C2A-CAA-CBA
87	DL	403	CLA	CHA-CBD-CGD-O1D
87	DL	403	CLA	CHA-CBD-CGD-O2D
87	DL	406	CLA	C2B-C3B-CAB-CBB
87	DL	406	CLA	C4B-C3B-CAB-CBB
87	DL	406	CLA	CHA-CBD-CGD-O1D
87	DL	406	CLA	CHA-CBD-CGD-O2D
87	DL	406	CLA	CAD-CBD-CGD-O1D
87	DL	406	CLA	CAD-CBD-CGD-O2D
87	HL	101	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	HL	101	CLA	CHA-CBD-CGD-O2D
87	HL	102	CLA	CHA-CBD-CGD-O1D
87	HL	102	CLA	CHA-CBD-CGD-O2D
87	HL	102	CLA	CAD-CBD-CGD-O1D
87	AN	801	CLA	C1A-C2A-CAA-CBA
87	AN	801	CLA	C2A-CAA-CBA-CGA
87	AN	801	CLA	C2B-C3B-CAB-CBB
87	AN	801	CLA	C4B-C3B-CAB-CBB
87	AN	802	CLA	C6-C7-C8-C9
87	AN	803	CLA	C2B-C3B-CAB-CBB
87	AN	803	CLA	C4B-C3B-CAB-CBB
87	AN	803	CLA	CHA-CBD-CGD-O1D
87	AN	803	CLA	CHA-CBD-CGD-O2D
87	AN	803	CLA	C3-C5-C6-C7
87	AN	805	CLA	C4B-C3B-CAB-CBB
87	AN	806	CLA	C1A-C2A-CAA-CBA
87	AN	806	CLA	C3A-C2A-CAA-CBA
87	AN	808	CLA	C1A-C2A-CAA-CBA
87	AN	808	CLA	C2B-C3B-CAB-CBB
87	AN	808	CLA	C4B-C3B-CAB-CBB
87	AN	809	CLA	C1A-C2A-CAA-CBA
87	AN	809	CLA	C2B-C3B-CAB-CBB
87	AN	809	CLA	C4B-C3B-CAB-CBB
87	AN	809	CLA	CHA-CBD-CGD-O1D
87	AN	809	CLA	CHA-CBD-CGD-O2D
87	AN	810	CLA	C3A-C2A-CAA-CBA
87	AN	811	CLA	C1A-C2A-CAA-CBA
87	AN	811	CLA	C2B-C3B-CAB-CBB
87	AN	811	CLA	C4B-C3B-CAB-CBB
87	AN	811	CLA	CHA-CBD-CGD-O1D
87	AN	811	CLA	CHA-CBD-CGD-O2D
87	AN	812	CLA	C2A-CAA-CBA-CGA
87	AN	812	CLA	C4B-C3B-CAB-CBB
87	AN	812	CLA	CBD-CGD-O2D-CED
87	AN	813	CLA	C2B-C3B-CAB-CBB
87	AN	813	CLA	C4B-C3B-CAB-CBB
87	AN	814	CLA	CBD-CGD-O2D-CED
87	AN	815	CLA	C2-C3-C5-C6
87	AN	815	CLA	C4-C3-C5-C6
87	AN	817	CLA	C2B-C3B-CAB-CBB
87	AN	817	CLA	C4B-C3B-CAB-CBB
87	AN	817	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	AN	818	CLA	C2B-C3B-CAB-CBB
87	AN	818	CLA	C4B-C3B-CAB-CBB
87	AN	820	CLA	C1A-C2A-CAA-CBA
87	AN	820	CLA	C3A-C2A-CAA-CBA
87	AN	821	CLA	C1A-C2A-CAA-CBA
87	AN	821	CLA	C3A-C2A-CAA-CBA
87	AN	822	CLA	C2B-C3B-CAB-CBB
87	AN	822	CLA	C4B-C3B-CAB-CBB
87	AN	824	CLA	C1A-C2A-CAA-CBA
87	AN	824	CLA	C2B-C3B-CAB-CBB
87	AN	824	CLA	CHA-CBD-CGD-O1D
87	AN	824	CLA	CHA-CBD-CGD-O2D
87	AN	824	CLA	CBD-CGD-O2D-CED
87	AN	825	CLA	CHA-CBD-CGD-O1D
87	AN	825	CLA	CHA-CBD-CGD-O2D
87	AN	828	CLA	CHA-CBD-CGD-O1D
87	AN	828	CLA	CHA-CBD-CGD-O2D
87	AN	829	CLA	C1A-C2A-CAA-CBA
87	AN	829	CLA	C3A-C2A-CAA-CBA
87	AN	829	CLA	CHA-CBD-CGD-O1D
87	AN	829	CLA	CHA-CBD-CGD-O2D
87	AN	830	CLA	CBD-CGD-O2D-CED
87	AN	831	CLA	C4-C3-C5-C6
87	AN	832	CLA	C2B-C3B-CAB-CBB
87	AN	832	CLA	C4B-C3B-CAB-CBB
87	AN	832	CLA	CHA-CBD-CGD-O1D
87	AN	832	CLA	CHA-CBD-CGD-O2D
87	AN	833	CLA	C2B-C3B-CAB-CBB
87	AN	833	CLA	C4B-C3B-CAB-CBB
87	AN	834	CLA	C2B-C3B-CAB-CBB
87	AN	834	CLA	C4B-C3B-CAB-CBB
87	AN	834	CLA	C11-C10-C8-C9
87	AN	837	CLA	CBA-CGA-O2A-C1
87	AN	837	CLA	O1A-CGA-O2A-C1
87	AN	837	CLA	CHA-CBD-CGD-O1D
87	AN	837	CLA	CHA-CBD-CGD-O2D
87	AN	837	CLA	CAD-CBD-CGD-O1D
87	AN	838	CLA	C4B-C3B-CAB-CBB
87	AN	838	CLA	CHA-CBD-CGD-O1D
87	AN	838	CLA	CHA-CBD-CGD-O2D
87	AN	838	CLA	C2-C3-C5-C6
87	AN	838	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	AN	840	CLA	C2B-C3B-CAB-CBB
87	AN	840	CLA	C4B-C3B-CAB-CBB
87	AN	841	CLA	CBD-CGD-O2D-CED
87	AN	849	CLA	C14-C13-C15-C16
87	AN	850	CLA	C1A-C2A-CAA-CBA
87	AN	850	CLA	C3A-C2A-CAA-CBA
87	AN	851	CLA	CHA-CBD-CGD-O1D
87	AN	851	CLA	CHA-CBD-CGD-O2D
87	AN	852	CLA	C2B-C3B-CAB-CBB
87	AN	852	CLA	C4B-C3B-CAB-CBB
87	BN	801	CLA	C3A-C2A-CAA-CBA
87	BN	801	CLA	CHA-CBD-CGD-O1D
87	BN	802	CLA	C2B-C3B-CAB-CBB
87	BN	802	CLA	C4B-C3B-CAB-CBB
87	BN	805	CLA	CBD-CGD-O2D-CED
87	BN	805	CLA	O1D-CGD-O2D-CED
87	BN	806	CLA	C1A-C2A-CAA-CBA
87	BN	806	CLA	C11-C12-C13-C15
87	BN	807	CLA	C2B-C3B-CAB-CBB
87	BN	807	CLA	C4B-C3B-CAB-CBB
87	BN	807	CLA	CHA-CBD-CGD-O1D
87	BN	807	CLA	CHA-CBD-CGD-O2D
87	BN	808	CLA	C3A-C2A-CAA-CBA
87	BN	808	CLA	C4B-C3B-CAB-CBB
87	BN	810	CLA	C2B-C3B-CAB-CBB
87	BN	810	CLA	C4B-C3B-CAB-CBB
87	BN	812	CLA	C1A-C2A-CAA-CBA
87	BN	812	CLA	C2B-C3B-CAB-CBB
87	BN	812	CLA	C4B-C3B-CAB-CBB
87	BN	812	CLA	CBD-CGD-O2D-CED
87	BN	812	CLA	O1D-CGD-O2D-CED
87	BN	813	CLA	C1A-C2A-CAA-CBA
87	BN	814	CLA	CBD-CGD-O2D-CED
87	BN	815	CLA	C1A-C2A-CAA-CBA
87	BN	816	CLA	C1A-C2A-CAA-CBA
87	BN	816	CLA	C3A-C2A-CAA-CBA
87	BN	816	CLA	CBD-CGD-O2D-CED
87	BN	818	CLA	C1A-C2A-CAA-CBA
87	BN	818	CLA	C3A-C2A-CAA-CBA
87	BN	819	CLA	C2B-C3B-CAB-CBB
87	BN	819	CLA	C4B-C3B-CAB-CBB
87	BN	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	BN	820	CLA	C4B-C3B-CAB-CBB
87	BN	820	CLA	CHA-CBD-CGD-O1D
87	BN	820	CLA	CHA-CBD-CGD-O2D
87	BN	820	CLA	CBD-CGD-O2D-CED
87	BN	822	CLA	C1A-C2A-CAA-CBA
87	BN	822	CLA	CHA-CBD-CGD-O1D
87	BN	822	CLA	CHA-CBD-CGD-O2D
87	BN	825	CLA	C4B-C3B-CAB-CBB
87	BN	825	CLA	CHA-CBD-CGD-O1D
87	BN	826	CLA	CHA-CBD-CGD-O1D
87	BN	826	CLA	CHA-CBD-CGD-O2D
87	BN	828	CLA	C4B-C3B-CAB-CBB
87	BN	830	CLA	C2B-C3B-CAB-CBB
87	BN	830	CLA	C4B-C3B-CAB-CBB
87	BN	830	CLA	CBD-CGD-O2D-CED
87	BN	830	CLA	O1D-CGD-O2D-CED
87	BN	831	CLA	C2B-C3B-CAB-CBB
87	BN	831	CLA	C4B-C3B-CAB-CBB
87	BN	834	CLA	C2B-C3B-CAB-CBB
87	BN	834	CLA	C4B-C3B-CAB-CBB
87	BN	835	CLA	C2B-C3B-CAB-CBB
87	BN	835	CLA	C4B-C3B-CAB-CBB
87	BN	835	CLA	CHA-CBD-CGD-O1D
87	BN	835	CLA	CHA-CBD-CGD-O2D
87	BN	835	CLA	CAD-CBD-CGD-O1D
87	BN	835	CLA	CBD-CGD-O2D-CED
87	BN	836	CLA	C2B-C3B-CAB-CBB
87	BN	836	CLA	C4B-C3B-CAB-CBB
87	FN	203	CLA	CHA-CBD-CGD-O1D
87	FN	203	CLA	CHA-CBD-CGD-O2D
87	FN	205	CLA	CBD-CGD-O2D-CED
87	IN	103	CLA	C1A-C2A-CAA-CBA
87	IN	103	CLA	C2B-C3B-CAB-CBB
87	IN	103	CLA	C4B-C3B-CAB-CBB
87	IN	103	CLA	C11-C12-C13-C14
87	JN	101	CLA	C2B-C3B-CAB-CBB
87	JN	101	CLA	C4B-C3B-CAB-CBB
87	JN	101	CLA	CBD-CGD-O2D-CED
87	KN	105	CLA	C2B-C3B-CAB-CBB
87	KN	105	CLA	C4B-C3B-CAB-CBB
87	LN	202	CLA	C3A-C2A-CAA-CBA
87	LN	202	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	LN	202	CLA	C4B-C3B-CAB-CBB
87	LN	203	CLA	CHA-CBD-CGD-O1D
87	LN	203	CLA	CHA-CBD-CGD-O2D
87	LN	204	CLA	CHA-CBD-CGD-O1D
87	LN	206	CLA	C2-C3-C5-C6
87	LN	206	CLA	C4-C3-C5-C6
87	MN	101	CLA	CHA-CBD-CGD-O1D
87	MN	101	CLA	CHA-CBD-CGD-O2D
87	ON	202	CLA	C1A-C2A-CAA-CBA
87	ON	202	CLA	C2B-C3B-CAB-CBB
87	ON	202	CLA	C4B-C3B-CAB-CBB
87	ON	203	CLA	C2B-C3B-CAB-CBB
87	ON	203	CLA	C4B-C3B-CAB-CBB
87	RN	201	CLA	C4B-C3B-CAB-CBB
87	RN	203	CLA	C2B-C3B-CAB-CBB
87	RN	203	CLA	C4B-C3B-CAB-CBB
87	RN	203	CLA	CBD-CGD-O2D-CED
87	RN	204	CLA	C1A-C2A-CAA-CBA
87	RN	204	CLA	C3A-C2A-CAA-CBA
87	RN	204	CLA	CHA-CBD-CGD-O1D
87	RN	204	CLA	CHA-CBD-CGD-O2D
87	RN	204	CLA	CBD-CGD-O2D-CED
87	RN	204	CLA	O1D-CGD-O2D-CED
87	12	601	CLA	C2B-C3B-CAB-CBB
87	12	601	CLA	C4B-C3B-CAB-CBB
87	12	601	CLA	CHA-CBD-CGD-O1D
87	12	601	CLA	CHA-CBD-CGD-O2D
87	12	601	CLA	CAD-CBD-CGD-O1D
87	12	602	CLA	C4B-C3B-CAB-CBB
87	12	602	CLA	CHA-CBD-CGD-O1D
87	12	602	CLA	CHA-CBD-CGD-O2D
87	12	604	CLA	C1A-C2A-CAA-CBA
87	12	605	CLA	C4B-C3B-CAB-CBB
87	12	605	CLA	CBD-CGD-O2D-CED
87	12	606	CLA	C1A-C2A-CAA-CBA
87	12	606	CLA	C3A-C2A-CAA-CBA
87	12	606	CLA	C2B-C3B-CAB-CBB
87	12	606	CLA	C4B-C3B-CAB-CBB
87	12	606	CLA	CBD-CGD-O2D-CED
87	12	608	CLA	CHA-CBD-CGD-O1D
87	12	608	CLA	CHA-CBD-CGD-O2D
87	12	608	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	12	609	CLA	CBD-CGD-O2D-CED
87	12	609	CLA	O1D-CGD-O2D-CED
87	12	610	CLA	C3A-C2A-CAA-CBA
87	12	610	CLA	CBD-CGD-O2D-CED
87	12	610	CLA	O1D-CGD-O2D-CED
87	12	611	CLA	C2A-CAA-CBA-CGA
87	22	601	CLA	C2B-C3B-CAB-CBB
87	22	601	CLA	C4B-C3B-CAB-CBB
87	22	602	CLA	CHA-CBD-CGD-O1D
87	22	602	CLA	CHA-CBD-CGD-O2D
87	22	603	CLA	C2B-C3B-CAB-CBB
87	22	603	CLA	C4B-C3B-CAB-CBB
87	22	603	CLA	CBD-CGD-O2D-CED
87	22	604	CLA	C1A-C2A-CAA-CBA
87	22	607	CLA	C2B-C3B-CAB-CBB
87	22	607	CLA	C4B-C3B-CAB-CBB
87	22	607	CLA	CHA-CBD-CGD-O1D
87	22	607	CLA	CHA-CBD-CGD-O2D
87	22	607	CLA	CBD-CGD-O2D-CED
87	22	608	CLA	C1A-C2A-CAA-CBA
87	22	608	CLA	C4B-C3B-CAB-CBB
87	22	608	CLA	CBD-CGD-O2D-CED
87	22	609	CLA	C1A-C2A-CAA-CBA
87	22	609	CLA	C3A-C2A-CAA-CBA
87	22	610	CLA	C2B-C3B-CAB-CBB
87	22	610	CLA	C4B-C3B-CAB-CBB
87	22	611	CLA	CHA-CBD-CGD-O1D
87	22	611	CLA	CBD-CGD-O2D-CED
87	22	612	CLA	C2B-C3B-CAB-CBB
87	22	612	CLA	C4B-C3B-CAB-CBB
87	22	612	CLA	CBD-CGD-O2D-CED
87	32	302	CLA	C1A-C2A-CAA-CBA
87	32	302	CLA	C3A-C2A-CAA-CBA
87	32	302	CLA	C2B-C3B-CAB-CBB
87	32	302	CLA	C4B-C3B-CAB-CBB
87	32	303	CLA	C4B-C3B-CAB-CBB
87	32	307	CLA	C2A-CAA-CBA-CGA
87	32	307	CLA	C2B-C3B-CAB-CBB
87	32	307	CLA	C4B-C3B-CAB-CBB
87	32	308	CLA	C2B-C3B-CAB-CBB
87	32	308	CLA	C4B-C3B-CAB-CBB
87	32	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	32	309	CLA	C4B-C3B-CAB-CBB
87	32	309	CLA	CHA-CBD-CGD-O1D
87	32	309	CLA	CHA-CBD-CGD-O2D
87	32	309	CLA	CBD-CGD-O2D-CED
87	32	310	CLA	CBD-CGD-O2D-CED
87	32	311	CLA	C3A-C2A-CAA-CBA
87	32	311	CLA	C4B-C3B-CAB-CBB
87	32	311	CLA	CBD-CGD-O2D-CED
87	32	312	CLA	C1A-C2A-CAA-CBA
87	32	312	CLA	C3A-C2A-CAA-CBA
87	32	313	CLA	C4B-C3B-CAB-CBB
87	32	313	CLA	CBD-CGD-O2D-CED
87	42	601	CLA	C2B-C3B-CAB-CBB
87	42	601	CLA	C4B-C3B-CAB-CBB
87	42	601	CLA	CBD-CGD-O2D-CED
87	42	604	CLA	C1A-C2A-CAA-CBA
87	42	604	CLA	C2B-C3B-CAB-CBB
87	42	604	CLA	C4B-C3B-CAB-CBB
87	42	604	CLA	CBD-CGD-O2D-CED
87	42	605	CLA	C3A-C2A-CAA-CBA
87	42	605	CLA	C2B-C3B-CAB-CBB
87	42	605	CLA	C4B-C3B-CAB-CBB
87	42	605	CLA	CBD-CGD-O2D-CED
87	42	605	CLA	O1D-CGD-O2D-CED
87	42	606	CLA	C2B-C3B-CAB-CBB
87	42	606	CLA	C4B-C3B-CAB-CBB
87	42	606	CLA	CBD-CGD-O2D-CED
87	42	607	CLA	CBD-CGD-O2D-CED
87	42	608	CLA	C1A-C2A-CAA-CBA
87	42	608	CLA	C2B-C3B-CAB-CBB
87	42	608	CLA	C4B-C3B-CAB-CBB
87	42	609	CLA	CBD-CGD-O2D-CED
87	42	610	CLA	CBD-CGD-O2D-CED
87	42	611	CLA	CBD-CGD-O2D-CED
87	52	601	CLA	C1A-C2A-CAA-CBA
87	52	601	CLA	C4B-C3B-CAB-CBB
87	52	601	CLA	CHA-CBD-CGD-O1D
87	52	601	CLA	CHA-CBD-CGD-O2D
87	52	603	CLA	C2B-C3B-CAB-CBB
87	52	603	CLA	C4B-C3B-CAB-CBB
87	52	604	CLA	C1A-C2A-CAA-CBA
87	52	605	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	52	605	CLA	C4B-C3B-CAB-CBB
87	52	605	CLA	CHA-CBD-CGD-O1D
87	52	605	CLA	CHA-CBD-CGD-O2D
87	52	607	CLA	C1A-C2A-CAA-CBA
87	52	608	CLA	C2B-C3B-CAB-CBB
87	52	608	CLA	C4B-C3B-CAB-CBB
87	52	608	CLA	CHA-CBD-CGD-O1D
87	52	608	CLA	CHA-CBD-CGD-O2D
87	52	608	CLA	CBD-CGD-O2D-CED
87	52	609	CLA	C2B-C3B-CAB-CBB
87	52	609	CLA	C4B-C3B-CAB-CBB
87	52	609	CLA	CBD-CGD-O2D-CED
87	52	611	CLA	C2B-C3B-CAB-CBB
87	52	611	CLA	C4B-C3B-CAB-CBB
87	62	301	CLA	C1A-C2A-CAA-CBA
87	62	301	CLA	C3A-C2A-CAA-CBA
87	62	301	CLA	C2A-CAA-CBA-CGA
87	62	301	CLA	C2B-C3B-CAB-CBB
87	62	301	CLA	C4B-C3B-CAB-CBB
87	62	302	CLA	C2B-C3B-CAB-CBB
87	62	302	CLA	C4B-C3B-CAB-CBB
87	62	304	CLA	CBD-CGD-O2D-CED
87	62	305	CLA	C1A-C2A-CAA-CBA
87	62	305	CLA	CHA-CBD-CGD-O1D
87	62	305	CLA	CHA-CBD-CGD-O2D
87	62	305	CLA	CAD-CBD-CGD-O1D
87	62	305	CLA	CAD-CBD-CGD-O2D
87	62	305	CLA	CBD-CGD-O2D-CED
87	62	306	CLA	CBD-CGD-O2D-CED
87	62	306	CLA	O1D-CGD-O2D-CED
87	62	307	CLA	C1A-C2A-CAA-CBA
87	62	307	CLA	C3A-C2A-CAA-CBA
87	62	308	CLA	C2B-C3B-CAB-CBB
87	62	308	CLA	C4B-C3B-CAB-CBB
87	62	309	CLA	C1A-C2A-CAA-CBA
87	62	310	CLA	CBD-CGD-O2D-CED
87	62	311	CLA	C2B-C3B-CAB-CBB
87	62	311	CLA	C4B-C3B-CAB-CBB
87	62	311	CLA	CBD-CGD-O2D-CED
87	62	311	CLA	O1D-CGD-O2D-CED
87	62	312	CLA	C1A-C2A-CAA-CBA
87	62	312	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	62	313	CLA	C2B-C3B-CAB-CBB
87	62	313	CLA	C4B-C3B-CAB-CBB
87	72	601	CLA	C1A-C2A-CAA-CBA
87	72	601	CLA	C3A-C2A-CAA-CBA
87	72	601	CLA	CHA-CBD-CGD-O1D
87	72	601	CLA	CHA-CBD-CGD-O2D
87	72	601	CLA	CAD-CBD-CGD-O1D
87	72	601	CLA	CAD-CBD-CGD-O2D
87	72	604	CLA	C2B-C3B-CAB-CBB
87	72	604	CLA	C4B-C3B-CAB-CBB
87	72	605	CLA	C2B-C3B-CAB-CBB
87	72	605	CLA	C4B-C3B-CAB-CBB
87	72	605	CLA	CBD-CGD-O2D-CED
87	72	605	CLA	O1D-CGD-O2D-CED
87	72	606	CLA	C1A-C2A-CAA-CBA
87	72	606	CLA	C4B-C3B-CAB-CBB
87	72	607	CLA	C2B-C3B-CAB-CBB
87	72	607	CLA	C4B-C3B-CAB-CBB
87	72	607	CLA	CBD-CGD-O2D-CED
87	72	608	CLA	CHA-CBD-CGD-O1D
87	72	608	CLA	CHA-CBD-CGD-O2D
87	72	609	CLA	CHA-CBD-CGD-O1D
87	72	609	CLA	CHA-CBD-CGD-O2D
87	72	609	CLA	CBD-CGD-O2D-CED
87	72	610	CLA	C2B-C3B-CAB-CBB
87	72	610	CLA	C4B-C3B-CAB-CBB
87	72	610	CLA	CBD-CGD-O2D-CED
87	82	301	CLA	C1A-C2A-CAA-CBA
87	82	301	CLA	C3A-C2A-CAA-CBA
87	82	301	CLA	C2B-C3B-CAB-CBB
87	82	301	CLA	C4B-C3B-CAB-CBB
87	82	301	CLA	CAD-CBD-CGD-O1D
87	82	301	CLA	CAD-CBD-CGD-O2D
87	82	303	CLA	CHA-CBD-CGD-O1D
87	82	303	CLA	CHA-CBD-CGD-O2D
87	82	303	CLA	CAD-CBD-CGD-O1D
87	82	303	CLA	CAD-CBD-CGD-O2D
87	82	304	CLA	C2A-CAA-CBA-CGA
87	82	304	CLA	C2B-C3B-CAB-CBB
87	82	304	CLA	C4B-C3B-CAB-CBB
87	82	304	CLA	CBD-CGD-O2D-CED
87	82	305	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	82	305	CLA	C2A-CAA-CBA-CGA
87	82	305	CLA	CBD-CGD-O2D-CED
87	82	306	CLA	CBA-CGA-O2A-C1
87	82	307	CLA	C1A-C2A-CAA-CBA
87	82	308	CLA	C2B-C3B-CAB-CBB
87	82	308	CLA	C4B-C3B-CAB-CBB
87	A2	802	CLA	C1A-C2A-CAA-CBA
87	A2	802	CLA	C2A-CAA-CBA-CGA
87	A2	802	CLA	C2B-C3B-CAB-CBB
87	A2	802	CLA	C4B-C3B-CAB-CBB
87	A2	803	CLA	C2B-C3B-CAB-CBB
87	A2	803	CLA	C4B-C3B-CAB-CBB
87	A2	803	CLA	CHA-CBD-CGD-O1D
87	A2	803	CLA	CHA-CBD-CGD-O2D
87	A2	803	CLA	C3-C5-C6-C7
87	A2	805	CLA	C4B-C3B-CAB-CBB
87	A2	806	CLA	C1A-C2A-CAA-CBA
87	A2	806	CLA	C3A-C2A-CAA-CBA
87	A2	808	CLA	C1A-C2A-CAA-CBA
87	A2	808	CLA	C2B-C3B-CAB-CBB
87	A2	808	CLA	C4B-C3B-CAB-CBB
87	A2	809	CLA	C1A-C2A-CAA-CBA
87	A2	809	CLA	C2B-C3B-CAB-CBB
87	A2	809	CLA	C4B-C3B-CAB-CBB
87	A2	809	CLA	CHA-CBD-CGD-O1D
87	A2	809	CLA	CHA-CBD-CGD-O2D
87	A2	810	CLA	C3A-C2A-CAA-CBA
87	A2	811	CLA	C1A-C2A-CAA-CBA
87	A2	811	CLA	C2B-C3B-CAB-CBB
87	A2	811	CLA	C4B-C3B-CAB-CBB
87	A2	811	CLA	CHA-CBD-CGD-O1D
87	A2	811	CLA	CHA-CBD-CGD-O2D
87	A2	812	CLA	C2A-CAA-CBA-CGA
87	A2	812	CLA	C4B-C3B-CAB-CBB
87	A2	812	CLA	CBD-CGD-O2D-CED
87	A2	813	CLA	C2B-C3B-CAB-CBB
87	A2	813	CLA	C4B-C3B-CAB-CBB
87	A2	814	CLA	CBD-CGD-O2D-CED
87	A2	815	CLA	C2-C3-C5-C6
87	A2	815	CLA	C4-C3-C5-C6
87	A2	817	CLA	C2B-C3B-CAB-CBB
87	A2	817	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	A2	817	CLA	CBD-CGD-O2D-CED
87	A2	818	CLA	C2B-C3B-CAB-CBB
87	A2	818	CLA	C4B-C3B-CAB-CBB
87	A2	820	CLA	C1A-C2A-CAA-CBA
87	A2	820	CLA	C3A-C2A-CAA-CBA
87	A2	821	CLA	C1A-C2A-CAA-CBA
87	A2	821	CLA	C3A-C2A-CAA-CBA
87	A2	822	CLA	C2B-C3B-CAB-CBB
87	A2	822	CLA	C4B-C3B-CAB-CBB
87	A2	824	CLA	C1A-C2A-CAA-CBA
87	A2	824	CLA	C2B-C3B-CAB-CBB
87	A2	824	CLA	CHA-CBD-CGD-O1D
87	A2	824	CLA	CHA-CBD-CGD-O2D
87	A2	824	CLA	CBD-CGD-O2D-CED
87	A2	825	CLA	CHA-CBD-CGD-O1D
87	A2	825	CLA	CHA-CBD-CGD-O2D
87	A2	828	CLA	CHA-CBD-CGD-O1D
87	A2	828	CLA	CHA-CBD-CGD-O2D
87	A2	829	CLA	C1A-C2A-CAA-CBA
87	A2	829	CLA	C3A-C2A-CAA-CBA
87	A2	829	CLA	CHA-CBD-CGD-O1D
87	A2	829	CLA	CHA-CBD-CGD-O2D
87	A2	830	CLA	CBD-CGD-O2D-CED
87	A2	831	CLA	C4-C3-C5-C6
87	A2	832	CLA	C2B-C3B-CAB-CBB
87	A2	832	CLA	C4B-C3B-CAB-CBB
87	A2	832	CLA	CHA-CBD-CGD-O1D
87	A2	832	CLA	CHA-CBD-CGD-O2D
87	A2	833	CLA	C2B-C3B-CAB-CBB
87	A2	833	CLA	C4B-C3B-CAB-CBB
87	A2	834	CLA	C2B-C3B-CAB-CBB
87	A2	834	CLA	C4B-C3B-CAB-CBB
87	A2	834	CLA	C11-C10-C8-C9
87	A2	837	CLA	CBA-CGA-O2A-C1
87	A2	837	CLA	O1A-CGA-O2A-C1
87	A2	837	CLA	CHA-CBD-CGD-O1D
87	A2	837	CLA	CHA-CBD-CGD-O2D
87	A2	837	CLA	CAD-CBD-CGD-O1D
87	A2	838	CLA	C4B-C3B-CAB-CBB
87	A2	838	CLA	CHA-CBD-CGD-O1D
87	A2	838	CLA	CHA-CBD-CGD-O2D
87	A2	838	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	A2	838	CLA	C4-C3-C5-C6
87	A2	840	CLA	C2B-C3B-CAB-CBB
87	A2	840	CLA	C4B-C3B-CAB-CBB
87	A2	841	CLA	CBD-CGD-O2D-CED
87	A2	849	CLA	C14-C13-C15-C16
87	A2	850	CLA	C1A-C2A-CAA-CBA
87	A2	850	CLA	C3A-C2A-CAA-CBA
87	A2	851	CLA	CHA-CBD-CGD-O1D
87	A2	851	CLA	CHA-CBD-CGD-O2D
87	A2	852	CLA	C2B-C3B-CAB-CBB
87	A2	852	CLA	C4B-C3B-CAB-CBB
87	B2	801	CLA	C2B-C3B-CAB-CBB
87	B2	801	CLA	C4B-C3B-CAB-CBB
87	B2	804	CLA	CBD-CGD-O2D-CED
87	B2	804	CLA	O1D-CGD-O2D-CED
87	B2	805	CLA	C1A-C2A-CAA-CBA
87	B2	805	CLA	C11-C12-C13-C15
87	B2	806	CLA	C2B-C3B-CAB-CBB
87	B2	806	CLA	C4B-C3B-CAB-CBB
87	B2	806	CLA	CHA-CBD-CGD-O1D
87	B2	806	CLA	CHA-CBD-CGD-O2D
87	B2	807	CLA	C3A-C2A-CAA-CBA
87	B2	807	CLA	C4B-C3B-CAB-CBB
87	B2	809	CLA	C2B-C3B-CAB-CBB
87	B2	809	CLA	C4B-C3B-CAB-CBB
87	B2	811	CLA	C1A-C2A-CAA-CBA
87	B2	811	CLA	C2B-C3B-CAB-CBB
87	B2	811	CLA	C4B-C3B-CAB-CBB
87	B2	811	CLA	CBD-CGD-O2D-CED
87	B2	811	CLA	O1D-CGD-O2D-CED
87	B2	812	CLA	C1A-C2A-CAA-CBA
87	B2	813	CLA	CBD-CGD-O2D-CED
87	B2	814	CLA	C1A-C2A-CAA-CBA
87	B2	815	CLA	C1A-C2A-CAA-CBA
87	B2	815	CLA	C3A-C2A-CAA-CBA
87	B2	815	CLA	CBD-CGD-O2D-CED
87	B2	817	CLA	C1A-C2A-CAA-CBA
87	B2	817	CLA	C3A-C2A-CAA-CBA
87	B2	818	CLA	C2B-C3B-CAB-CBB
87	B2	818	CLA	C4B-C3B-CAB-CBB
87	B2	818	CLA	CBD-CGD-O2D-CED
87	B2	819	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	B2	819	CLA	CHA-CBD-CGD-O1D
87	B2	819	CLA	CHA-CBD-CGD-O2D
87	B2	819	CLA	CBD-CGD-O2D-CED
87	B2	821	CLA	C1A-C2A-CAA-CBA
87	B2	821	CLA	CHA-CBD-CGD-O1D
87	B2	821	CLA	CHA-CBD-CGD-O2D
87	B2	824	CLA	C4B-C3B-CAB-CBB
87	B2	824	CLA	CHA-CBD-CGD-O1D
87	B2	825	CLA	C3A-C2A-CAA-CBA
87	B2	825	CLA	CHA-CBD-CGD-O1D
87	B2	826	CLA	CHA-CBD-CGD-O1D
87	B2	826	CLA	CHA-CBD-CGD-O2D
87	B2	828	CLA	C4B-C3B-CAB-CBB
87	B2	830	CLA	C2B-C3B-CAB-CBB
87	B2	830	CLA	C4B-C3B-CAB-CBB
87	B2	830	CLA	CBD-CGD-O2D-CED
87	B2	831	CLA	C2B-C3B-CAB-CBB
87	B2	831	CLA	C4B-C3B-CAB-CBB
87	B2	834	CLA	C2B-C3B-CAB-CBB
87	B2	834	CLA	C4B-C3B-CAB-CBB
87	B2	835	CLA	C2B-C3B-CAB-CBB
87	B2	835	CLA	C4B-C3B-CAB-CBB
87	B2	835	CLA	CHA-CBD-CGD-O1D
87	B2	835	CLA	CHA-CBD-CGD-O2D
87	B2	835	CLA	CAD-CBD-CGD-O1D
87	B2	835	CLA	CBD-CGD-O2D-CED
87	B2	836	CLA	C2B-C3B-CAB-CBB
87	B2	836	CLA	C4B-C3B-CAB-CBB
87	F2	201	CLA	CHA-CBD-CGD-O1D
87	F2	201	CLA	CHA-CBD-CGD-O2D
87	F2	205	CLA	CBD-CGD-O2D-CED
87	I2	103	CLA	C1A-C2A-CAA-CBA
87	I2	103	CLA	C2B-C3B-CAB-CBB
87	I2	103	CLA	C4B-C3B-CAB-CBB
87	I2	103	CLA	C11-C12-C13-C14
87	J2	101	CLA	C2B-C3B-CAB-CBB
87	J2	101	CLA	C4B-C3B-CAB-CBB
87	J2	101	CLA	CBD-CGD-O2D-CED
87	K2	106	CLA	C2B-C3B-CAB-CBB
87	K2	106	CLA	C4B-C3B-CAB-CBB
87	L2	202	CLA	C3A-C2A-CAA-CBA
87	L2	202	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	L2	202	CLA	C4B-C3B-CAB-CBB
87	L2	203	CLA	CHA-CBD-CGD-O1D
87	L2	203	CLA	CHA-CBD-CGD-O2D
87	L2	204	CLA	CHA-CBD-CGD-O1D
87	L2	206	CLA	C2-C3-C5-C6
87	L2	206	CLA	C4-C3-C5-C6
87	M2	101	CLA	CHA-CBD-CGD-O1D
87	M2	101	CLA	CHA-CBD-CGD-O2D
87	O2	202	CLA	C1A-C2A-CAA-CBA
87	O2	202	CLA	C2B-C3B-CAB-CBB
87	O2	202	CLA	C4B-C3B-CAB-CBB
87	O2	203	CLA	C2B-C3B-CAB-CBB
87	O2	203	CLA	C4B-C3B-CAB-CBB
87	R2	201	CLA	C4B-C3B-CAB-CBB
87	R2	203	CLA	C2B-C3B-CAB-CBB
87	R2	203	CLA	C4B-C3B-CAB-CBB
87	R2	203	CLA	CBD-CGD-O2D-CED
87	R2	204	CLA	C1A-C2A-CAA-CBA
87	R2	204	CLA	C3A-C2A-CAA-CBA
87	R2	204	CLA	CHA-CBD-CGD-O1D
87	R2	204	CLA	CHA-CBD-CGD-O2D
87	R2	204	CLA	CBD-CGD-O2D-CED
87	R2	204	CLA	O1D-CGD-O2D-CED
87	A6	402	CLA	C1A-C2A-CAA-CBA
87	A6	402	CLA	C3A-C2A-CAA-CBA
87	A6	402	CLA	CBD-CGD-O2D-CED
87	A6	402	CLA	O1D-CGD-O2D-CED
87	A6	402	CLA	C2-C3-C5-C6
87	A6	402	CLA	C4-C3-C5-C6
87	A6	402	CLA	C11-C10-C8-C7
87	A6	403	CLA	CHA-CBD-CGD-O1D
87	A6	403	CLA	CHA-CBD-CGD-O2D
87	A6	403	CLA	C11-C10-C8-C9
87	B6	603	CLA	CBD-CGD-O2D-CED
87	B6	605	CLA	CHA-CBD-CGD-O1D
87	B6	605	CLA	CHA-CBD-CGD-O2D
87	B6	605	CLA	CAD-CBD-CGD-O1D
87	B6	605	CLA	C14-C13-C15-C16
87	B6	606	CLA	C2-C3-C5-C6
87	B6	606	CLA	C4-C3-C5-C6
87	B6	607	CLA	C2-C3-C5-C6
87	B6	607	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	B6	608	CLA	C1A-C2A-CAA-CBA
87	B6	608	CLA	C3A-C2A-CAA-CBA
87	B6	609	CLA	CHA-CBD-CGD-O1D
87	B6	612	CLA	CHA-CBD-CGD-O1D
87	B6	612	CLA	C4-C3-C5-C6
87	B6	613	CLA	CHA-CBD-CGD-O1D
87	B6	613	CLA	CHA-CBD-CGD-O2D
87	B6	613	CLA	CAD-CBD-CGD-O1D
87	B6	613	CLA	CAD-CBD-CGD-O2D
87	B6	615	CLA	C2B-C3B-CAB-CBB
87	B6	615	CLA	C4B-C3B-CAB-CBB
87	B6	615	CLA	CBD-CGD-O2D-CED
87	B6	615	CLA	C6-C7-C8-C9
87	B6	616	CLA	C1A-C2A-CAA-CBA
87	B6	616	CLA	C3A-C2A-CAA-CBA
87	B6	616	CLA	C4B-C3B-CAB-CBB
87	C6	509	CLA	CHA-CBD-CGD-O1D
87	C6	509	CLA	CHA-CBD-CGD-O2D
87	C6	509	CLA	CAD-CBD-CGD-O1D
87	C6	509	CLA	C2-C3-C5-C6
87	C6	509	CLA	C4-C3-C5-C6
87	C6	510	CLA	CHA-CBD-CGD-O1D
87	C6	510	CLA	CHA-CBD-CGD-O2D
87	C6	510	CLA	CAD-CBD-CGD-O1D
87	C6	511	CLA	C12-C13-C15-C16
87	C6	512	CLA	CHA-CBD-CGD-O1D
87	C6	512	CLA	CHA-CBD-CGD-O2D
87	C6	512	CLA	CAD-CBD-CGD-O1D
87	C6	512	CLA	C11-C10-C8-C9
87	C6	514	CLA	C2B-C3B-CAB-CBB
87	C6	514	CLA	C4B-C3B-CAB-CBB
87	C6	514	CLA	CHA-CBD-CGD-O1D
87	C6	516	CLA	CHA-CBD-CGD-O1D
87	C6	516	CLA	CHA-CBD-CGD-O2D
87	C6	518	CLA	C1A-C2A-CAA-CBA
87	D6	402	CLA	CHA-CBD-CGD-O1D
87	D6	402	CLA	CHA-CBD-CGD-O2D
87	D6	402	CLA	C14-C13-C15-C16
87	D6	403	CLA	C3A-C2A-CAA-CBA
87	D6	403	CLA	C11-C12-C13-C14
87	D6	405	CLA	C2-C3-C5-C6
87	D6	405	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	H6	103	CLA	C1A-C2A-CAA-CBA
87	H6	103	CLA	C3A-C2A-CAA-CBA
87	a6	607	CLA	CBD-CGD-O2D-CED
87	a6	608	CLA	C11-C10-C8-C9
87	a6	609	CLA	CHA-CBD-CGD-O1D
87	a6	609	CLA	CHA-CBD-CGD-O2D
87	b6	606	CLA	C2-C3-C5-C6
87	b6	606	CLA	C4-C3-C5-C6
87	b6	607	CLA	C2-C3-C5-C6
87	b6	607	CLA	C4-C3-C5-C6
87	b6	608	CLA	C1A-C2A-CAA-CBA
87	b6	609	CLA	C1A-C2A-CAA-CBA
87	b6	609	CLA	C3A-C2A-CAA-CBA
87	b6	609	CLA	CHA-CBD-CGD-O1D
87	b6	609	CLA	CHA-CBD-CGD-O2D
87	b6	610	CLA	C1A-C2A-CAA-CBA
87	b6	610	CLA	C3A-C2A-CAA-CBA
87	b6	610	CLA	CHA-CBD-CGD-O1D
87	b6	610	CLA	CHA-CBD-CGD-O2D
87	b6	610	CLA	CAD-CBD-CGD-O1D
87	b6	612	CLA	CHA-CBD-CGD-O1D
87	b6	612	CLA	CHA-CBD-CGD-O2D
87	b6	613	CLA	C1A-C2A-CAA-CBA
87	b6	613	CLA	C3A-C2A-CAA-CBA
87	b6	615	CLA	CHA-CBD-CGD-O1D
87	b6	615	CLA	CHA-CBD-CGD-O2D
87	b6	615	CLA	CAD-CBD-CGD-O1D
87	c6	604	CLA	CHA-CBD-CGD-O1D
87	c6	604	CLA	CHA-CBD-CGD-O2D
87	c6	604	CLA	CAD-CBD-CGD-O1D
87	c6	604	CLA	C11-C12-C13-C14
87	c6	606	CLA	CHA-CBD-CGD-O1D
87	c6	606	CLA	CHA-CBD-CGD-O2D
87	c6	607	CLA	C2A-CAA-CBA-CGA
87	c6	607	CLA	C2-C3-C5-C6
87	c6	607	CLA	C4-C3-C5-C6
87	c6	607	CLA	C11-C10-C8-C9
87	c6	607	CLA	C11-C12-C13-C14
87	c6	608	CLA	CHA-CBD-CGD-O1D
87	c6	608	CLA	CHA-CBD-CGD-O2D
87	c6	608	CLA	CAD-CBD-CGD-O1D
87	c6	608	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
87	c6	609	CLA	C1A-C2A-CAA-CBA
87	c6	609	CLA	C3A-C2A-CAA-CBA
87	c6	613	CLA	C2-C3-C5-C6
87	c6	613	CLA	C4-C3-C5-C6
87	c6	614	CLA	CHA-CBD-CGD-O1D
87	c6	614	CLA	CHA-CBD-CGD-O2D
87	d6	401	CLA	C1A-C2A-CAA-CBA
87	d6	401	CLA	C3A-C2A-CAA-CBA
87	d6	401	CLA	CHA-CBD-CGD-O1D
87	d6	401	CLA	CHA-CBD-CGD-O2D
87	d6	403	CLA	C3A-C2A-CAA-CBA
87	d6	403	CLA	C2-C3-C5-C6
87	d6	403	CLA	C4-C3-C5-C6
87	d6	406	CLA	CAD-CBD-CGD-O1D
87	d6	406	CLA	C2-C3-C5-C6
87	d6	406	CLA	C4-C3-C5-C6
87	aL	605	CLA	CBD-CGD-O2D-CED
87	aL	605	CLA	C2-C3-C5-C6
87	aL	605	CLA	C4-C3-C5-C6
87	aL	606	CLA	CHA-CBD-CGD-O1D
87	aL	606	CLA	CHA-CBD-CGD-O2D
87	bL	604	CLA	C4B-C3B-CAB-CBB
87	bL	607	CLA	C4-C3-C5-C6
87	bL	613	CLA	C1A-C2A-CAA-CBA
87	bL	613	CLA	C3A-C2A-CAA-CBA
87	bL	613	CLA	CBD-CGD-O2D-CED
87	bL	614	CLA	CHA-CBD-CGD-O1D
87	bL	614	CLA	CHA-CBD-CGD-O2D
87	bL	615	CLA	CHA-CBD-CGD-O1D
87	bL	615	CLA	CHA-CBD-CGD-O2D
87	bL	616	CLA	C2B-C3B-CAB-CBB
87	bL	616	CLA	C4B-C3B-CAB-CBB
87	bL	618	CLA	C1A-C2A-CAA-CBA
87	bL	618	CLA	C3A-C2A-CAA-CBA
87	bL	620	CLA	CBD-CGD-O2D-CED
87	bL	620	CLA	C2-C3-C5-C6
87	bL	620	CLA	C4-C3-C5-C6
87	bL	621	CLA	CHA-CBD-CGD-O1D
87	bL	621	CLA	CHA-CBD-CGD-O2D
87	bL	622	CLA	C4B-C3B-CAB-CBB
87	bL	622	CLA	CHA-CBD-CGD-O1D
87	bL	622	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	cL	505	CLA	C1A-C2A-CAA-CBA
87	cL	505	CLA	C2B-C3B-CAB-CBB
87	cL	505	CLA	C4B-C3B-CAB-CBB
87	cL	505	CLA	CHA-CBD-CGD-O1D
87	cL	505	CLA	CHA-CBD-CGD-O2D
87	cL	506	CLA	C2B-C3B-CAB-CBB
87	cL	506	CLA	CHA-CBD-CGD-O1D
87	cL	506	CLA	CHA-CBD-CGD-O2D
87	cL	506	CLA	CAD-CBD-CGD-O1D
87	cL	508	CLA	CHA-CBD-CGD-O1D
87	cL	508	CLA	CHA-CBD-CGD-O2D
87	cL	509	CLA	CHA-CBD-CGD-O1D
87	cL	509	CLA	CAD-CBD-CGD-O1D
87	cL	510	CLA	CHA-CBD-CGD-O1D
87	cL	510	CLA	CHA-CBD-CGD-O2D
87	cL	511	CLA	C2B-C3B-CAB-CBB
87	cL	511	CLA	C4B-C3B-CAB-CBB
87	cL	511	CLA	CAD-CBD-CGD-O2D
87	cL	515	CLA	CHA-CBD-CGD-O1D
87	cL	515	CLA	CHA-CBD-CGD-O2D
87	cL	515	CLA	CBD-CGD-O2D-CED
87	cL	515	CLA	C11-C10-C8-C9
87	cL	516	CLA	C1A-C2A-CAA-CBA
87	dL	401	CLA	CHA-CBD-CGD-O1D
87	dL	401	CLA	CHA-CBD-CGD-O2D
87	dL	402	CLA	C1A-C2A-CAA-CBA
87	dL	404	CLA	CHA-CBD-CGD-O1D
87	dL	404	CLA	CHA-CBD-CGD-O2D
87	dL	404	CLA	CAD-CBD-CGD-O1D
87	dL	409	CLA	C2B-C3B-CAB-CBB
87	dL	409	CLA	C4B-C3B-CAB-CBB
87	dL	409	CLA	CHA-CBD-CGD-O1D
87	dL	409	CLA	CHA-CBD-CGD-O2D
87	1N	601	CLA	C2B-C3B-CAB-CBB
87	1N	601	CLA	C4B-C3B-CAB-CBB
87	1N	601	CLA	CHA-CBD-CGD-O1D
87	1N	601	CLA	CHA-CBD-CGD-O2D
87	1N	601	CLA	CAD-CBD-CGD-O1D
87	1N	602	CLA	C4B-C3B-CAB-CBB
87	1N	602	CLA	CHA-CBD-CGD-O1D
87	1N	602	CLA	CHA-CBD-CGD-O2D
87	1N	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	1N	605	CLA	C4B-C3B-CAB-CBB
87	1N	605	CLA	CBD-CGD-O2D-CED
87	1N	606	CLA	C1A-C2A-CAA-CBA
87	1N	606	CLA	C3A-C2A-CAA-CBA
87	1N	606	CLA	C2B-C3B-CAB-CBB
87	1N	606	CLA	C4B-C3B-CAB-CBB
87	1N	606	CLA	CBD-CGD-O2D-CED
87	1N	608	CLA	CHA-CBD-CGD-O1D
87	1N	608	CLA	CHA-CBD-CGD-O2D
87	1N	608	CLA	CAD-CBD-CGD-O1D
87	1N	609	CLA	CBD-CGD-O2D-CED
87	1N	609	CLA	O1D-CGD-O2D-CED
87	1N	610	CLA	C3A-C2A-CAA-CBA
87	1N	610	CLA	CBD-CGD-O2D-CED
87	1N	610	CLA	O1D-CGD-O2D-CED
87	1N	611	CLA	C2A-CAA-CBA-CGA
87	2N	302	CLA	C2B-C3B-CAB-CBB
87	2N	302	CLA	C4B-C3B-CAB-CBB
87	2N	303	CLA	CHA-CBD-CGD-O1D
87	2N	303	CLA	CHA-CBD-CGD-O2D
87	2N	304	CLA	C2B-C3B-CAB-CBB
87	2N	304	CLA	C4B-C3B-CAB-CBB
87	2N	304	CLA	CBD-CGD-O2D-CED
87	2N	305	CLA	C1A-C2A-CAA-CBA
87	2N	306	CLA	C4B-C3B-CAB-CBB
87	2N	307	CLA	C2B-C3B-CAB-CBB
87	2N	307	CLA	C4B-C3B-CAB-CBB
87	2N	307	CLA	CHA-CBD-CGD-O1D
87	2N	307	CLA	CHA-CBD-CGD-O2D
87	2N	307	CLA	CBD-CGD-O2D-CED
87	2N	308	CLA	C1A-C2A-CAA-CBA
87	2N	308	CLA	C4B-C3B-CAB-CBB
87	2N	308	CLA	CBD-CGD-O2D-CED
87	2N	309	CLA	C1A-C2A-CAA-CBA
87	2N	309	CLA	C3A-C2A-CAA-CBA
87	2N	310	CLA	C2B-C3B-CAB-CBB
87	2N	310	CLA	C4B-C3B-CAB-CBB
87	2N	311	CLA	CBD-CGD-O2D-CED
87	2N	312	CLA	C2B-C3B-CAB-CBB
87	2N	312	CLA	C4B-C3B-CAB-CBB
87	2N	312	CLA	CBD-CGD-O2D-CED
87	3N	301	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	3N	301	CLA	C4B-C3B-CAB-CBB
87	3N	301	CLA	CBD-CGD-O2D-CED
87	3N	303	CLA	C1A-C2A-CAA-CBA
87	3N	303	CLA	C3A-C2A-CAA-CBA
87	3N	303	CLA	C2B-C3B-CAB-CBB
87	3N	303	CLA	C4B-C3B-CAB-CBB
87	3N	304	CLA	C4B-C3B-CAB-CBB
87	3N	308	CLA	C2A-CAA-CBA-CGA
87	3N	308	CLA	C2B-C3B-CAB-CBB
87	3N	308	CLA	C4B-C3B-CAB-CBB
87	3N	309	CLA	C4B-C3B-CAB-CBB
87	3N	309	CLA	CHA-CBD-CGD-O1D
87	3N	309	CLA	CHA-CBD-CGD-O2D
87	3N	309	CLA	CBD-CGD-O2D-CED
87	3N	310	CLA	CBD-CGD-O2D-CED
87	3N	311	CLA	C3A-C2A-CAA-CBA
87	3N	311	CLA	C4B-C3B-CAB-CBB
87	3N	311	CLA	CBD-CGD-O2D-CED
87	3N	312	CLA	C1A-C2A-CAA-CBA
87	3N	312	CLA	C3A-C2A-CAA-CBA
87	3N	313	CLA	C4B-C3B-CAB-CBB
87	3N	313	CLA	CBD-CGD-O2D-CED
87	4N	601	CLA	C2B-C3B-CAB-CBB
87	4N	601	CLA	C4B-C3B-CAB-CBB
87	4N	601	CLA	CBD-CGD-O2D-CED
87	4N	604	CLA	C1A-C2A-CAA-CBA
87	4N	604	CLA	C2B-C3B-CAB-CBB
87	4N	604	CLA	C4B-C3B-CAB-CBB
87	4N	604	CLA	CBD-CGD-O2D-CED
87	4N	605	CLA	C3A-C2A-CAA-CBA
87	4N	605	CLA	C2B-C3B-CAB-CBB
87	4N	605	CLA	C4B-C3B-CAB-CBB
87	4N	605	CLA	CBD-CGD-O2D-CED
87	4N	605	CLA	O1D-CGD-O2D-CED
87	4N	606	CLA	C2B-C3B-CAB-CBB
87	4N	606	CLA	C4B-C3B-CAB-CBB
87	4N	606	CLA	CBD-CGD-O2D-CED
87	4N	607	CLA	CBD-CGD-O2D-CED
87	4N	608	CLA	C1A-C2A-CAA-CBA
87	4N	608	CLA	C2B-C3B-CAB-CBB
87	4N	608	CLA	C4B-C3B-CAB-CBB
87	4N	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	4N	610	CLA	CBD-CGD-O2D-CED
87	4N	611	CLA	CBD-CGD-O2D-CED
87	5N	601	CLA	C1A-C2A-CAA-CBA
87	5N	601	CLA	C4B-C3B-CAB-CBB
87	5N	601	CLA	CHA-CBD-CGD-O1D
87	5N	601	CLA	CHA-CBD-CGD-O2D
87	5N	603	CLA	C2B-C3B-CAB-CBB
87	5N	603	CLA	C4B-C3B-CAB-CBB
87	5N	604	CLA	C1A-C2A-CAA-CBA
87	5N	605	CLA	C2B-C3B-CAB-CBB
87	5N	605	CLA	C4B-C3B-CAB-CBB
87	5N	605	CLA	CHA-CBD-CGD-O1D
87	5N	605	CLA	CHA-CBD-CGD-O2D
87	5N	607	CLA	C1A-C2A-CAA-CBA
87	5N	608	CLA	C2B-C3B-CAB-CBB
87	5N	608	CLA	C4B-C3B-CAB-CBB
87	5N	608	CLA	CHA-CBD-CGD-O1D
87	5N	608	CLA	CHA-CBD-CGD-O2D
87	5N	608	CLA	CBD-CGD-O2D-CED
87	5N	609	CLA	C2B-C3B-CAB-CBB
87	5N	609	CLA	C4B-C3B-CAB-CBB
87	5N	609	CLA	CBD-CGD-O2D-CED
87	5N	611	CLA	C2B-C3B-CAB-CBB
87	5N	611	CLA	C4B-C3B-CAB-CBB
87	6N	601	CLA	C2B-C3B-CAB-CBB
87	6N	601	CLA	C4B-C3B-CAB-CBB
87	6N	603	CLA	CBD-CGD-O2D-CED
87	6N	604	CLA	C1A-C2A-CAA-CBA
87	6N	604	CLA	CHA-CBD-CGD-O1D
87	6N	604	CLA	CHA-CBD-CGD-O2D
87	6N	604	CLA	CAD-CBD-CGD-O1D
87	6N	604	CLA	CAD-CBD-CGD-O2D
87	6N	604	CLA	CBD-CGD-O2D-CED
87	6N	605	CLA	CBD-CGD-O2D-CED
87	6N	605	CLA	O1D-CGD-O2D-CED
87	6N	606	CLA	C1A-C2A-CAA-CBA
87	6N	606	CLA	C3A-C2A-CAA-CBA
87	6N	607	CLA	C2B-C3B-CAB-CBB
87	6N	607	CLA	C4B-C3B-CAB-CBB
87	6N	608	CLA	C1A-C2A-CAA-CBA
87	6N	609	CLA	CBD-CGD-O2D-CED
87	6N	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	6N	610	CLA	C4B-C3B-CAB-CBB
87	6N	610	CLA	CBD-CGD-O2D-CED
87	6N	610	CLA	O1D-CGD-O2D-CED
87	6N	611	CLA	C1A-C2A-CAA-CBA
87	6N	611	CLA	C2A-CAA-CBA-CGA
87	6N	612	CLA	C2B-C3B-CAB-CBB
87	6N	612	CLA	C4B-C3B-CAB-CBB
87	6N	613	CLA	C1A-C2A-CAA-CBA
87	6N	613	CLA	C3A-C2A-CAA-CBA
87	6N	613	CLA	C2A-CAA-CBA-CGA
87	6N	613	CLA	C2B-C3B-CAB-CBB
87	6N	613	CLA	C4B-C3B-CAB-CBB
87	7N	601	CLA	C1A-C2A-CAA-CBA
87	7N	601	CLA	C3A-C2A-CAA-CBA
87	7N	601	CLA	CHA-CBD-CGD-O1D
87	7N	601	CLA	CHA-CBD-CGD-O2D
87	7N	601	CLA	CAD-CBD-CGD-O1D
87	7N	601	CLA	CAD-CBD-CGD-O2D
87	7N	604	CLA	C2B-C3B-CAB-CBB
87	7N	604	CLA	C4B-C3B-CAB-CBB
87	7N	605	CLA	C2B-C3B-CAB-CBB
87	7N	605	CLA	C4B-C3B-CAB-CBB
87	7N	605	CLA	CBD-CGD-O2D-CED
87	7N	605	CLA	O1D-CGD-O2D-CED
87	7N	606	CLA	C1A-C2A-CAA-CBA
87	7N	606	CLA	C4B-C3B-CAB-CBB
87	7N	607	CLA	C2B-C3B-CAB-CBB
87	7N	607	CLA	C4B-C3B-CAB-CBB
87	7N	607	CLA	CBD-CGD-O2D-CED
87	7N	608	CLA	CHA-CBD-CGD-O1D
87	7N	608	CLA	CHA-CBD-CGD-O2D
87	7N	609	CLA	CHA-CBD-CGD-O1D
87	7N	609	CLA	CHA-CBD-CGD-O2D
87	7N	609	CLA	CBD-CGD-O2D-CED
87	7N	610	CLA	C2B-C3B-CAB-CBB
87	7N	610	CLA	C4B-C3B-CAB-CBB
87	7N	610	CLA	CBD-CGD-O2D-CED
87	8N	301	CLA	CBA-CGA-O2A-C1
87	8N	302	CLA	C1A-C2A-CAA-CBA
87	8N	302	CLA	C3A-C2A-CAA-CBA
87	8N	302	CLA	C2B-C3B-CAB-CBB
87	8N	302	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	8N	302	CLA	CAD-CBD-CGD-O1D
87	8N	302	CLA	CAD-CBD-CGD-O2D
87	8N	304	CLA	CHA-CBD-CGD-O1D
87	8N	304	CLA	CHA-CBD-CGD-O2D
87	8N	304	CLA	CAD-CBD-CGD-O1D
87	8N	304	CLA	CAD-CBD-CGD-O2D
87	8N	305	CLA	C2A-CAA-CBA-CGA
87	8N	305	CLA	C2B-C3B-CAB-CBB
87	8N	305	CLA	C4B-C3B-CAB-CBB
87	8N	305	CLA	CBD-CGD-O2D-CED
87	8N	306	CLA	C1A-C2A-CAA-CBA
87	8N	306	CLA	C2A-CAA-CBA-CGA
87	8N	306	CLA	CBD-CGD-O2D-CED
87	8N	307	CLA	C1A-C2A-CAA-CBA
87	8N	308	CLA	C2B-C3B-CAB-CBB
87	8N	308	CLA	C4B-C3B-CAB-CBB
88	AL	406	LHG	C3-O3-P-O4
88	AL	406	LHG	C3-O3-P-O5
88	AL	406	LHG	C3-O3-P-O6
88	AL	406	LHG	O6-C4-C5-O7
88	AL	407	LHG	C3-O3-P-O4
88	AL	407	LHG	C4-O6-P-O4
88	BL	610	LHG	C4-O6-P-O5
88	BL	615	LHG	C3-O3-P-O4
88	BL	615	LHG	C3-O3-P-O5
88	BL	615	LHG	C3-O3-P-O6
88	BL	615	LHG	C4-O6-P-O4
88	CL	521	LHG	O1-C1-C2-C3
88	CL	521	LHG	C1-C2-C3-O3
88	CL	521	LHG	C3-O3-P-O4
88	CL	521	LHG	C4-O6-P-O3
88	CL	521	LHG	C4-O6-P-O4
88	CL	521	LHG	C4-O6-P-O5
88	CL	522	LHG	O1-C1-C2-C3
88	CL	522	LHG	C3-O3-P-O4
88	DL	407	LHG	O2-C2-C3-O3
88	DL	407	LHG	C4-O6-P-O4
88	DL	407	LHG	C4-O6-P-O5
88	ML	102	LHG	C1-C2-C3-O3
88	AN	843	LHG	C3-O3-P-O4
88	AN	843	LHG	C4-O6-P-O5
88	AN	844	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
88	AN	844	LHG	O2-C2-C3-O3
88	AN	844	LHG	C3-O3-P-O4
88	AN	844	LHG	C3-O3-P-O5
88	AN	844	LHG	C3-O3-P-O6
88	AN	844	LHG	C4-O6-P-O4
88	A2	843	LHG	C3-O3-P-O4
88	A2	843	LHG	C4-O6-P-O5
88	A2	844	LHG	C1-C2-C3-O3
88	A2	844	LHG	O2-C2-C3-O3
88	A2	844	LHG	C3-O3-P-O4
88	A2	844	LHG	C3-O3-P-O5
88	A2	844	LHG	C3-O3-P-O6
88	A2	844	LHG	C4-O6-P-O4
88	B6	617	LHG	C4-O6-P-O4
88	C6	505	LHG	C1-C2-C3-O3
88	C6	505	LHG	C3-O3-P-O4
88	C6	505	LHG	C3-O3-P-O5
88	C6	505	LHG	C3-O3-P-O6
88	C6	522	LHG	O1-C1-C2-C3
88	C6	522	LHG	C3-O3-P-O4
88	C6	522	LHG	C4-O6-P-O4
88	D6	401	LHG	C3-O3-P-O4
88	D6	401	LHG	C4-O6-P-O3
88	D6	401	LHG	C4-O6-P-O4
88	D6	401	LHG	C4-O6-P-O5
88	D6	406	LHG	C4-O6-P-O3
88	D6	406	LHG	C4-O6-P-O4
88	D6	406	LHG	C4-O6-P-O5
88	I6	101	LHG	O1-C1-C2-C3
88	I6	101	LHG	O2-C2-C3-O3
88	I6	101	LHG	C4-O6-P-O5
88	I6	101	LHG	C8-C7-O7-C5
88	L6	101	LHG	C4-O6-P-O3
88	L6	101	LHG	C4-O6-P-O4
88	L6	101	LHG	C4-O6-P-O5
88	M6	101	LHG	C4-O6-P-O3
88	M6	101	LHG	C4-O6-P-O4
88	M6	101	LHG	C4-O6-P-O5
88	a6	610	LHG	C3-O3-P-O4
88	a6	610	LHG	C4-O6-P-O3
88	a6	610	LHG	O6-C4-C5-O7
88	c6	619	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
88	c6	619	LHG	C3-O3-P-O5
88	c6	619	LHG	C4-O6-P-O4
88	c6	619	LHG	C4-O6-P-O5
88	c6	619	LHG	C8-C7-O7-C5
88	d6	402	LHG	C3-O3-P-O4
88	d6	402	LHG	C3-O3-P-O5
88	d6	402	LHG	C4-O6-P-O4
88	d6	407	LHG	O2-C2-C3-O3
88	d6	407	LHG	C4-O6-P-O3
88	d6	407	LHG	C4-O6-P-O4
88	d6	407	LHG	C4-O6-P-O5
88	l6	101	LHG	C4-O6-P-O3
88	l6	101	LHG	C4-O6-P-O4
88	l6	101	LHG	C4-O6-P-O5
88	m6	102	LHG	C4-O6-P-O4
88	aL	607	LHG	C3-O3-P-O4
88	aL	607	LHG	C4-O6-P-O4
88	bL	612	LHG	O1-C1-C2-C3
88	bL	612	LHG	C3-O3-P-O5
88	bL	612	LHG	C4-O6-P-O3
88	cL	501	LHG	O1-C1-C2-C3
88	dL	405	LHG	C1-C2-C3-O3
88	dL	405	LHG	C4-O6-P-O3
88	dL	405	LHG	C4-O6-P-O4
88	dL	405	LHG	C4-O6-P-O5
88	dL	408	LHG	C3-O3-P-O5
88	dL	408	LHG	C4-O6-P-O3
88	mL	102	LHG	C4-O6-P-O3
88	mL	102	LHG	C4-O6-P-O4
88	mL	102	LHG	C4-O6-P-O5
92	BL	611	LMG	C11-C10-O7-C8
92	CL	519	LMG	C2-C1-O1-C7
92	CL	519	LMG	O6-C1-O1-C7
92	JL	102	LMG	C11-C10-O7-C8
92	XL	601	LMG	C2-C1-O1-C7
92	XL	601	LMG	O6-C1-O1-C7
92	XL	601	LMG	C11-C10-O7-C8
92	B6	619	LMG	C11-C10-O7-C8
92	B6	622	LMG	O9-C10-O7-C8
92	C6	501	LMG	C2-C1-O1-C7
92	C6	501	LMG	O6-C1-O1-C7
92	D6	407	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
92	D6	407	LMG	O6-C1-O1-C7
92	J6	102	LMG	C11-C10-O7-C8
92	b6	620	LMG	C2-C1-O1-C7
92	b6	620	LMG	O6-C1-O1-C7
92	b6	623	LMG	C11-C10-O7-C8
92	b6	624	LMG	O1-C7-C8-O7
92	d6	409	LMG	C8-C9-O8-C28
92	j6	101	LMG	C11-C10-O7-C8
92	j6	102	LMG	C2-C1-O1-C7
92	j6	102	LMG	O6-C1-O1-C7
92	k6	101	LMG	C2-C1-O1-C7
92	k6	101	LMG	O6-C1-O1-C7
92	m6	101	LMG	O6-C1-O1-C7
92	m6	101	LMG	O1-C7-C8-O7
92	x6	601	LMG	O6-C1-O1-C7
92	aL	611	LMG	C2-C1-O1-C7
92	aL	611	LMG	O6-C1-O1-C7
92	bL	609	LMG	O6-C1-O1-C7
92	bL	609	LMG	C11-C10-O7-C8
92	bL	611	LMG	C2-C1-O1-C7
92	bL	611	LMG	O6-C1-O1-C7
92	bL	611	LMG	C11-C10-O7-C8
92	bL	623	LMG	C11-C10-O7-C8
92	yL	101	LMG	C2-C1-O1-C7
92	yL	101	LMG	O6-C1-O1-C7
94	AL	413	PL9	C2-C3-C7-C8
94	AL	413	PL9	C4-C3-C7-C8
94	AL	413	PL9	C29-C31-C32-C33
94	AL	413	PL9	C40-C39-C41-C42
94	DL	401	PL9	C14-C16-C17-C18
94	A6	410	PL9	C2-C3-C7-C8
94	A6	410	PL9	C4-C3-C7-C8
94	A6	410	PL9	C24-C26-C27-C28
94	A6	410	PL9	C33-C34-C36-C37
94	A6	410	PL9	C35-C34-C36-C37
94	A6	410	PL9	C39-C41-C42-C43
94	A6	410	PL9	C43-C44-C46-C47
94	A6	410	PL9	C45-C44-C46-C47
94	A6	410	PL9	C44-C46-C47-C48
94	D6	408	PL9	C12-C11-C9-C8
94	D6	408	PL9	C12-C11-C9-C10
94	D6	408	PL9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
94	a6	601	PL9	C19-C21-C22-C23
94	d6	408	PL9	C12-C11-C9-C8
94	d6	408	PL9	C12-C11-C9-C10
94	d6	408	PL9	C29-C31-C32-C33
94	d6	408	PL9	C34-C36-C37-C38
94	aL	601	PL9	C23-C24-C26-C27
94	aL	601	PL9	C25-C24-C26-C27
94	aL	601	PL9	C29-C31-C32-C33
94	aL	601	PL9	C38-C39-C41-C42
94	aL	601	PL9	C40-C39-C41-C42
94	dL	406	PL9	C14-C16-C17-C18
94	dL	406	PL9	C29-C31-C32-C33
95	BL	614	DGD	O6E-C1E-O5D-C6D
95	CL	520	DGD	O1G-C1G-C2G-O2G
95	CL	523	DGD	C2E-C1E-O5D-C6D
95	CL	523	DGD	O6E-C1E-O5D-C6D
95	C6	502	DGD	O6E-C1E-O5D-C6D
95	C6	503	DGD	C2E-C1E-O5D-C6D
95	C6	503	DGD	O6E-C1E-O5D-C6D
95	C6	504	DGD	C2B-C1B-O2G-C2G
95	C6	504	DGD	O6D-C1D-O3G-C3G
95	L6	102	DGD	C2D-C1D-O3G-C3G
95	L6	102	DGD	O6D-C1D-O3G-C3G
95	b6	621	DGD	O6E-C1E-O5D-C6D
95	b6	622	DGD	C2B-C1B-O2G-C2G
95	b6	622	DGD	C2D-C1D-O3G-C3G
95	c6	601	DGD	O6E-C1E-O5D-C6D
95	h6	101	DGD	C2B-C1B-O2G-C2G
95	cL	520	DGD	C2E-C1E-O5D-C6D
95	cL	520	DGD	O6E-C1E-O5D-C6D
95	hL	101	DGD	C2B-C1B-O2G-C2G
95	lL	101	DGD	O6E-C1E-O5D-C6D
96	FL	102	HEM	C2B-C3B-CAB-CBB
96	FL	102	HEM	C4B-C3B-CAB-CBB
96	VL	201	HEM	C2C-C3C-CAC-CBC
96	VL	201	HEM	C4C-C3C-CAC-CBC
96	GN	201	HEM	C2B-C3B-CAB-CBB
96	GN	201	HEM	C4B-C3B-CAB-CBB
96	GN	201	HEM	C2C-C3C-CAC-CBC
96	G2	201	HEM	C2B-C3B-CAB-CBB
96	G2	201	HEM	C4B-C3B-CAB-CBB
96	G2	201	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
96	V6	201	HEM	C2C-C3C-CAC-CBC
96	V6	201	HEM	C4C-C3C-CAC-CBC
96	v6	201	HEM	C2C-C3C-CAC-CBC
96	v6	201	HEM	C4C-C3C-CAC-CBC
96	fL	102	HEM	C2B-C3B-CAB-CBB
96	fL	102	HEM	C4B-C3B-CAB-CBB
96	fL	102	HEM	C2C-C3C-CAC-CBC
96	fL	102	HEM	C4C-C3C-CAC-CBC
96	vL	201	HEM	C2C-C3C-CAC-CBC
96	vL	201	HEM	C4C-C3C-CAC-CBC
97	WL	101	GOL	O1-C1-C2-C3
97	wL	101	GOL	O1-C1-C2-C3
100	JN	104	3XQ	C21-C22-C24-O25
103	82	309	ZEX	C25-C26-C27-C28
103	82	309	ZEX	C7-C8-C9-C19
103	82	309	ZEX	C7-C8-C9-C10
103	82	309	ZEX	C33-C34-C35-C15
103	82	310	ZEX	C25-C26-C27-C28
103	82	310	ZEX	C7-C8-C9-C19
103	82	310	ZEX	C7-C8-C9-C10
103	82	310	ZEX	C13-C14-C15-C35
103	82	310	ZEX	C29-C30-C31-C32
103	8N	309	ZEX	C25-C26-C27-C28
103	8N	309	ZEX	C7-C8-C9-C19
103	8N	309	ZEX	C7-C8-C9-C10
103	8N	309	ZEX	C33-C34-C35-C15
103	8N	310	ZEX	C25-C26-C27-C28
103	8N	310	ZEX	C7-C8-C9-C19
103	8N	310	ZEX	C7-C8-C9-C10
103	8N	310	ZEX	C13-C14-C15-C35
103	8N	310	ZEX	C29-C30-C31-C32
87	AL	403	CLA	O1D-CGD-O2D-CED
87	AN	824	CLA	O1D-CGD-O2D-CED
87	BN	816	CLA	O1D-CGD-O2D-CED
87	BN	820	CLA	O1D-CGD-O2D-CED
87	FN	201	CLA	O1D-CGD-O2D-CED
87	LN	204	CLA	O1D-CGD-O2D-CED
87	12	601	CLA	O1D-CGD-O2D-CED
87	12	606	CLA	O1D-CGD-O2D-CED
87	12	608	CLA	O1D-CGD-O2D-CED
87	22	608	CLA	O1D-CGD-O2D-CED
87	32	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	32	311	CLA	O1D-CGD-O2D-CED
87	42	602	CLA	O1D-CGD-O2D-CED
87	42	609	CLA	O1D-CGD-O2D-CED
87	42	610	CLA	O1D-CGD-O2D-CED
87	52	601	CLA	O1D-CGD-O2D-CED
87	52	609	CLA	O1D-CGD-O2D-CED
87	72	601	CLA	O1D-CGD-O2D-CED
87	72	604	CLA	O1D-CGD-O2D-CED
87	82	308	CLA	O1D-CGD-O2D-CED
87	A2	824	CLA	O1D-CGD-O2D-CED
87	B2	815	CLA	O1D-CGD-O2D-CED
87	B2	819	CLA	O1D-CGD-O2D-CED
87	B2	830	CLA	O1D-CGD-O2D-CED
87	F2	202	CLA	O1D-CGD-O2D-CED
87	K2	101	CLA	O1D-CGD-O2D-CED
87	L2	204	CLA	O1D-CGD-O2D-CED
87	B6	603	CLA	O1D-CGD-O2D-CED
87	C6	518	CLA	O1D-CGD-O2D-CED
87	aL	605	CLA	O1D-CGD-O2D-CED
87	1N	601	CLA	O1D-CGD-O2D-CED
87	1N	606	CLA	O1D-CGD-O2D-CED
87	1N	608	CLA	O1D-CGD-O2D-CED
87	2N	308	CLA	O1D-CGD-O2D-CED
87	3N	301	CLA	O1D-CGD-O2D-CED
87	3N	311	CLA	O1D-CGD-O2D-CED
87	4N	602	CLA	O1D-CGD-O2D-CED
87	4N	609	CLA	O1D-CGD-O2D-CED
87	4N	610	CLA	O1D-CGD-O2D-CED
87	5N	601	CLA	O1D-CGD-O2D-CED
87	5N	609	CLA	O1D-CGD-O2D-CED
87	7N	601	CLA	O1D-CGD-O2D-CED
87	7N	604	CLA	O1D-CGD-O2D-CED
87	8N	308	CLA	O1D-CGD-O2D-CED
87	a6	608	CLA	C5-C6-C7-C8
87	AN	817	CLA	O1D-CGD-O2D-CED
87	AN	827	CLA	O1D-CGD-O2D-CED
87	AN	829	CLA	O1D-CGD-O2D-CED
87	BN	819	CLA	O1D-CGD-O2D-CED
87	FN	205	CLA	O1D-CGD-O2D-CED
87	ON	203	CLA	O1D-CGD-O2D-CED
87	22	604	CLA	O1D-CGD-O2D-CED
87	22	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	22	612	CLA	O1D-CGD-O2D-CED
87	32	303	CLA	O1D-CGD-O2D-CED
87	32	304	CLA	O1D-CGD-O2D-CED
87	42	611	CLA	O1D-CGD-O2D-CED
87	72	610	CLA	O1D-CGD-O2D-CED
87	82	304	CLA	O1D-CGD-O2D-CED
87	82	305	CLA	O1D-CGD-O2D-CED
87	A2	817	CLA	O1D-CGD-O2D-CED
87	A2	827	CLA	O1D-CGD-O2D-CED
87	A2	829	CLA	O1D-CGD-O2D-CED
87	B2	818	CLA	O1D-CGD-O2D-CED
87	F2	205	CLA	O1D-CGD-O2D-CED
87	O2	203	CLA	O1D-CGD-O2D-CED
87	cL	515	CLA	O1D-CGD-O2D-CED
87	2N	305	CLA	O1D-CGD-O2D-CED
87	2N	307	CLA	O1D-CGD-O2D-CED
87	2N	312	CLA	O1D-CGD-O2D-CED
87	3N	304	CLA	O1D-CGD-O2D-CED
87	3N	305	CLA	O1D-CGD-O2D-CED
87	4N	611	CLA	O1D-CGD-O2D-CED
87	7N	610	CLA	O1D-CGD-O2D-CED
87	8N	305	CLA	O1D-CGD-O2D-CED
87	8N	306	CLA	O1D-CGD-O2D-CED
87	BL	602	CLA	CBD-CGD-O2D-CED
87	BL	608	CLA	CBD-CGD-O2D-CED
87	BL	623	CLA	CBD-CGD-O2D-CED
87	CL	508	CLA	CBD-CGD-O2D-CED
87	CL	509	CLA	CBD-CGD-O2D-CED
87	CL	518	CLA	CBD-CGD-O2D-CED
87	DL	406	CLA	CBD-CGD-O2D-CED
87	HL	102	CLA	CBD-CGD-O2D-CED
87	AN	801	CLA	CBD-CGD-O2D-CED
87	AN	809	CLA	CBD-CGD-O2D-CED
87	AN	811	CLA	CBD-CGD-O2D-CED
87	AN	815	CLA	CBD-CGD-O2D-CED
87	AN	818	CLA	CBD-CGD-O2D-CED
87	AN	827	CLA	CBD-CGD-O2D-CED
87	AN	829	CLA	CBD-CGD-O2D-CED
87	AN	833	CLA	CBD-CGD-O2D-CED
87	AN	834	CLA	CBD-CGD-O2D-CED
87	BN	801	CLA	CBD-CGD-O2D-CED
87	BN	806	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	BN	807	CLA	CBD-CGD-O2D-CED
87	BN	808	CLA	CBD-CGD-O2D-CED
87	BN	811	CLA	CBD-CGD-O2D-CED
87	BN	824	CLA	CBD-CGD-O2D-CED
87	FN	201	CLA	CBD-CGD-O2D-CED
87	KN	105	CLA	CBD-CGD-O2D-CED
87	LN	204	CLA	CBD-CGD-O2D-CED
87	MN	101	CLA	CBD-CGD-O2D-CED
87	ON	202	CLA	CBD-CGD-O2D-CED
87	ON	203	CLA	CBD-CGD-O2D-CED
87	RN	202	CLA	CBD-CGD-O2D-CED
87	12	601	CLA	CBD-CGD-O2D-CED
87	12	607	CLA	CBD-CGD-O2D-CED
87	12	608	CLA	CBD-CGD-O2D-CED
87	22	604	CLA	CBD-CGD-O2D-CED
87	22	605	CLA	CBD-CGD-O2D-CED
87	22	609	CLA	CBD-CGD-O2D-CED
87	32	302	CLA	CBD-CGD-O2D-CED
87	32	303	CLA	CBD-CGD-O2D-CED
87	32	304	CLA	CBD-CGD-O2D-CED
87	32	312	CLA	CBD-CGD-O2D-CED
87	42	602	CLA	CBD-CGD-O2D-CED
87	42	608	CLA	CBD-CGD-O2D-CED
87	52	601	CLA	CBD-CGD-O2D-CED
87	52	603	CLA	CBD-CGD-O2D-CED
87	52	604	CLA	CBD-CGD-O2D-CED
87	52	606	CLA	CBD-CGD-O2D-CED
87	52	611	CLA	CBD-CGD-O2D-CED
87	62	302	CLA	CBD-CGD-O2D-CED
87	62	312	CLA	CBD-CGD-O2D-CED
87	62	313	CLA	CBD-CGD-O2D-CED
87	72	601	CLA	CBD-CGD-O2D-CED
87	72	603	CLA	CBD-CGD-O2D-CED
87	72	604	CLA	CBD-CGD-O2D-CED
87	82	301	CLA	CBD-CGD-O2D-CED
87	82	303	CLA	CBD-CGD-O2D-CED
87	82	307	CLA	CBD-CGD-O2D-CED
87	82	308	CLA	CBD-CGD-O2D-CED
87	A2	802	CLA	CBD-CGD-O2D-CED
87	A2	809	CLA	CBD-CGD-O2D-CED
87	A2	811	CLA	CBD-CGD-O2D-CED
87	A2	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	A2	818	CLA	CBD-CGD-O2D-CED
87	A2	827	CLA	CBD-CGD-O2D-CED
87	A2	829	CLA	CBD-CGD-O2D-CED
87	A2	833	CLA	CBD-CGD-O2D-CED
87	A2	834	CLA	CBD-CGD-O2D-CED
87	B2	805	CLA	CBD-CGD-O2D-CED
87	B2	806	CLA	CBD-CGD-O2D-CED
87	B2	807	CLA	CBD-CGD-O2D-CED
87	B2	810	CLA	CBD-CGD-O2D-CED
87	B2	823	CLA	CBD-CGD-O2D-CED
87	B2	825	CLA	CBD-CGD-O2D-CED
87	F2	202	CLA	CBD-CGD-O2D-CED
87	K2	101	CLA	CBD-CGD-O2D-CED
87	K2	106	CLA	CBD-CGD-O2D-CED
87	L2	204	CLA	CBD-CGD-O2D-CED
87	M2	101	CLA	CBD-CGD-O2D-CED
87	O2	202	CLA	CBD-CGD-O2D-CED
87	O2	203	CLA	CBD-CGD-O2D-CED
87	R2	202	CLA	CBD-CGD-O2D-CED
87	B6	608	CLA	CBD-CGD-O2D-CED
87	B6	612	CLA	CBD-CGD-O2D-CED
87	C6	518	CLA	CBD-CGD-O2D-CED
87	H6	103	CLA	CBD-CGD-O2D-CED
87	a6	608	CLA	CBD-CGD-O2D-CED
87	c6	607	CLA	CBD-CGD-O2D-CED
87	c6	609	CLA	CBD-CGD-O2D-CED
87	c6	614	CLA	CBD-CGD-O2D-CED
87	d6	401	CLA	CBD-CGD-O2D-CED
87	bL	604	CLA	CBD-CGD-O2D-CED
87	bL	615	CLA	CBD-CGD-O2D-CED
87	cL	510	CLA	CBD-CGD-O2D-CED
87	dL	404	CLA	CBD-CGD-O2D-CED
87	1N	601	CLA	CBD-CGD-O2D-CED
87	1N	607	CLA	CBD-CGD-O2D-CED
87	1N	608	CLA	CBD-CGD-O2D-CED
87	2N	301	CLA	CBD-CGD-O2D-CED
87	2N	305	CLA	CBD-CGD-O2D-CED
87	2N	309	CLA	CBD-CGD-O2D-CED
87	3N	303	CLA	CBD-CGD-O2D-CED
87	3N	304	CLA	CBD-CGD-O2D-CED
87	3N	305	CLA	CBD-CGD-O2D-CED
87	3N	312	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	4N	602	CLA	CBD-CGD-O2D-CED
87	4N	608	CLA	CBD-CGD-O2D-CED
87	5N	601	CLA	CBD-CGD-O2D-CED
87	5N	603	CLA	CBD-CGD-O2D-CED
87	5N	604	CLA	CBD-CGD-O2D-CED
87	5N	606	CLA	CBD-CGD-O2D-CED
87	5N	611	CLA	CBD-CGD-O2D-CED
87	6N	601	CLA	CBD-CGD-O2D-CED
87	6N	611	CLA	CBD-CGD-O2D-CED
87	6N	612	CLA	CBD-CGD-O2D-CED
87	7N	601	CLA	CBD-CGD-O2D-CED
87	7N	603	CLA	CBD-CGD-O2D-CED
87	7N	604	CLA	CBD-CGD-O2D-CED
87	8N	302	CLA	CBD-CGD-O2D-CED
87	8N	304	CLA	CBD-CGD-O2D-CED
87	8N	307	CLA	CBD-CGD-O2D-CED
87	8N	308	CLA	CBD-CGD-O2D-CED
87	AN	840	CLA	O1A-CGA-O2A-C1
87	LN	202	CLA	O1A-CGA-O2A-C1
87	32	309	CLA	O1A-CGA-O2A-C1
87	A2	840	CLA	O1A-CGA-O2A-C1
87	L2	202	CLA	O1A-CGA-O2A-C1
87	3N	309	CLA	O1A-CGA-O2A-C1
92	dL	407	LMG	O10-C28-O8-C9
100	JN	104	3XQ	O19-C1-O20-C21
100	J2	104	3XQ	O19-C1-O20-C21
87	BL	623	CLA	O1D-CGD-O2D-CED
87	AN	801	CLA	O1D-CGD-O2D-CED
87	22	611	CLA	O1D-CGD-O2D-CED
87	32	310	CLA	O1D-CGD-O2D-CED
87	62	305	CLA	O1D-CGD-O2D-CED
87	72	609	CLA	O1D-CGD-O2D-CED
87	82	303	CLA	O1D-CGD-O2D-CED
87	A2	802	CLA	O1D-CGD-O2D-CED
87	B6	615	CLA	O1D-CGD-O2D-CED
87	H6	103	CLA	O1D-CGD-O2D-CED
87	2N	311	CLA	O1D-CGD-O2D-CED
87	3N	310	CLA	O1D-CGD-O2D-CED
87	6N	604	CLA	O1D-CGD-O2D-CED
87	7N	609	CLA	O1D-CGD-O2D-CED
87	8N	304	CLA	O1D-CGD-O2D-CED
92	D6	409	LMG	C8-C9-O8-C28

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Mol	Chain	Res	Type	Atoms
87	BL	622	CLA	O1D-CGD-O2D-CED
87	AN	841	CLA	O1D-CGD-O2D-CED
87	BN	814	CLA	O1D-CGD-O2D-CED
87	ON	202	CLA	O1D-CGD-O2D-CED
87	42	604	CLA	O1D-CGD-O2D-CED
87	42	608	CLA	O1D-CGD-O2D-CED
87	52	603	CLA	O1D-CGD-O2D-CED
87	52	608	CLA	O1D-CGD-O2D-CED
87	62	310	CLA	O1D-CGD-O2D-CED
87	72	603	CLA	O1D-CGD-O2D-CED
87	A2	841	CLA	O1D-CGD-O2D-CED
87	B2	813	CLA	O1D-CGD-O2D-CED
87	O2	202	CLA	O1D-CGD-O2D-CED
87	c6	609	CLA	O1D-CGD-O2D-CED
87	bL	604	CLA	O1D-CGD-O2D-CED
87	4N	604	CLA	O1D-CGD-O2D-CED
87	4N	608	CLA	O1D-CGD-O2D-CED
87	5N	603	CLA	O1D-CGD-O2D-CED
87	5N	608	CLA	O1D-CGD-O2D-CED
87	6N	609	CLA	O1D-CGD-O2D-CED
87	7N	603	CLA	O1D-CGD-O2D-CED
87	32	309	CLA	CBA-CGA-O2A-C1
87	3N	309	CLA	CBA-CGA-O2A-C1
92	DL	402	LMG	C29-C28-O8-C9
100	JN	104	3XQ	C2-C1-O20-C21
100	J2	104	3XQ	C2-C1-O20-C21
87	CL	514	CLA	CBD-CGD-O2D-CED
87	DL	403	CLA	CBD-CGD-O2D-CED
87	HL	101	CLA	CBD-CGD-O2D-CED
87	AN	805	CLA	CBD-CGD-O2D-CED
87	AN	822	CLA	CBD-CGD-O2D-CED
87	AN	832	CLA	CBD-CGD-O2D-CED
87	AN	852	CLA	CBD-CGD-O2D-CED
87	BN	802	CLA	CBD-CGD-O2D-CED
87	BN	827	CLA	CBD-CGD-O2D-CED
87	BN	832	CLA	CBD-CGD-O2D-CED
87	IN	103	CLA	CBD-CGD-O2D-CED
87	KN	102	CLA	CBD-CGD-O2D-CED
87	KN	103	CLA	CBD-CGD-O2D-CED
87	LN	203	CLA	CBD-CGD-O2D-CED
87	22	602	CLA	CBD-CGD-O2D-CED
87	22	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	42	603	CLA	CBD-CGD-O2D-CED
87	62	307	CLA	CBD-CGD-O2D-CED
87	72	608	CLA	CBD-CGD-O2D-CED
87	82	302	CLA	CBD-CGD-O2D-CED
87	A2	805	CLA	CBD-CGD-O2D-CED
87	A2	822	CLA	CBD-CGD-O2D-CED
87	A2	832	CLA	CBD-CGD-O2D-CED
87	A2	852	CLA	CBD-CGD-O2D-CED
87	B2	801	CLA	CBD-CGD-O2D-CED
87	B2	827	CLA	CBD-CGD-O2D-CED
87	B2	832	CLA	CBD-CGD-O2D-CED
87	I2	103	CLA	CBD-CGD-O2D-CED
87	K2	103	CLA	CBD-CGD-O2D-CED
87	K2	104	CLA	CBD-CGD-O2D-CED
87	L2	203	CLA	CBD-CGD-O2D-CED
87	O2	201	CLA	CBD-CGD-O2D-CED
87	B6	610	CLA	CBD-CGD-O2D-CED
87	C6	517	CLA	CBD-CGD-O2D-CED
87	b6	605	CLA	CBD-CGD-O2D-CED
87	b6	612	CLA	CBD-CGD-O2D-CED
87	c6	606	CLA	CBD-CGD-O2D-CED
87	bL	605	CLA	CBD-CGD-O2D-CED
87	bL	617	CLA	CBD-CGD-O2D-CED
87	cL	506	CLA	CBD-CGD-O2D-CED
87	2N	303	CLA	CBD-CGD-O2D-CED
87	2N	306	CLA	CBD-CGD-O2D-CED
87	4N	603	CLA	CBD-CGD-O2D-CED
87	6N	606	CLA	CBD-CGD-O2D-CED
87	7N	608	CLA	CBD-CGD-O2D-CED
87	8N	303	CLA	CBD-CGD-O2D-CED
87	CL	507	CLA	O1A-CGA-O2A-C1
87	CL	511	CLA	O1A-CGA-O2A-C1
87	AN	803	CLA	O1A-CGA-O2A-C1
87	AN	814	CLA	O1A-CGA-O2A-C1
87	BN	818	CLA	O1A-CGA-O2A-C1
87	BN	836	CLA	O1A-CGA-O2A-C1
87	32	304	CLA	O1A-CGA-O2A-C1
87	82	302	CLA	O1A-CGA-O2A-C1
87	A2	803	CLA	O1A-CGA-O2A-C1
87	A2	814	CLA	O1A-CGA-O2A-C1
87	B2	817	CLA	O1A-CGA-O2A-C1
87	B2	836	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
87	bL	620	CLA	O1A-CGA-O2A-C1
87	cL	509	CLA	O1A-CGA-O2A-C1
87	cL	513	CLA	O1A-CGA-O2A-C1
87	3N	305	CLA	O1A-CGA-O2A-C1
87	8N	303	CLA	O1A-CGA-O2A-C1
92	DL	402	LMG	O10-C28-O8-C9
92	bL	610	LMG	O10-C28-O8-C9
87	82	306	CLA	O1A-CGA-O2A-C1
87	8N	301	CLA	O1A-CGA-O2A-C1
87	AN	814	CLA	O1D-CGD-O2D-CED
87	JN	101	CLA	O1D-CGD-O2D-CED
87	RN	203	CLA	O1D-CGD-O2D-CED
87	42	601	CLA	O1D-CGD-O2D-CED
87	42	606	CLA	O1D-CGD-O2D-CED
87	62	304	CLA	O1D-CGD-O2D-CED
87	A2	814	CLA	O1D-CGD-O2D-CED
87	J2	101	CLA	O1D-CGD-O2D-CED
87	R2	203	CLA	O1D-CGD-O2D-CED
87	a6	607	CLA	O1D-CGD-O2D-CED
87	4N	601	CLA	O1D-CGD-O2D-CED
87	4N	606	CLA	O1D-CGD-O2D-CED
87	6N	603	CLA	O1D-CGD-O2D-CED
84	r3	1001	CYC	C2B-C3B-CAB-CBB
87	82	308	CLA	C2C-C3C-CAC-CBC
87	8N	308	CLA	C2C-C3C-CAC-CBC
87	AN	812	CLA	O1D-CGD-O2D-CED
87	AN	830	CLA	O1D-CGD-O2D-CED
87	BN	835	CLA	O1D-CGD-O2D-CED
87	12	605	CLA	O1D-CGD-O2D-CED
87	32	309	CLA	O1D-CGD-O2D-CED
87	32	313	CLA	O1D-CGD-O2D-CED
87	72	607	CLA	O1D-CGD-O2D-CED
87	A2	812	CLA	O1D-CGD-O2D-CED
87	A2	830	CLA	O1D-CGD-O2D-CED
87	B2	835	CLA	O1D-CGD-O2D-CED
87	bL	613	CLA	O1D-CGD-O2D-CED
87	bL	620	CLA	O1D-CGD-O2D-CED
87	1N	605	CLA	O1D-CGD-O2D-CED
87	3N	309	CLA	O1D-CGD-O2D-CED
87	3N	313	CLA	O1D-CGD-O2D-CED
87	82	308	CLA	C4C-C3C-CAC-CBC
87	8N	308	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
87	BL	605	CLA	CBD-CGD-O2D-CED
87	AN	806	CLA	CBD-CGD-O2D-CED
87	AN	835	CLA	CBD-CGD-O2D-CED
87	BN	826	CLA	CBD-CGD-O2D-CED
87	BN	829	CLA	CBD-CGD-O2D-CED
87	FN	203	CLA	CBD-CGD-O2D-CED
87	LN	202	CLA	CBD-CGD-O2D-CED
87	ON	201	CLA	CBD-CGD-O2D-CED
87	22	601	CLA	CBD-CGD-O2D-CED
87	82	306	CLA	CBD-CGD-O2D-CED
87	A2	806	CLA	CBD-CGD-O2D-CED
87	A2	835	CLA	CBD-CGD-O2D-CED
87	B2	826	CLA	CBD-CGD-O2D-CED
87	B2	829	CLA	CBD-CGD-O2D-CED
87	F2	201	CLA	CBD-CGD-O2D-CED
87	L2	202	CLA	CBD-CGD-O2D-CED
87	b6	618	CLA	CBD-CGD-O2D-CED
87	dL	402	CLA	CBD-CGD-O2D-CED
87	2N	302	CLA	CBD-CGD-O2D-CED
87	8N	301	CLA	CBD-CGD-O2D-CED
87	b6	613	CLA	C8-C10-C11-C12
87	22	603	CLA	O1D-CGD-O2D-CED
87	52	606	CLA	O1D-CGD-O2D-CED
87	62	302	CLA	O1D-CGD-O2D-CED
87	2N	304	CLA	O1D-CGD-O2D-CED
87	5N	606	CLA	O1D-CGD-O2D-CED
87	6N	601	CLA	O1D-CGD-O2D-CED
87	7N	607	CLA	O1D-CGD-O2D-CED
88	I6	101	LHG	O9-C7-O7-C5
88	c6	619	LHG	O9-C7-O7-C5
92	BL	611	LMG	O9-C10-O7-C8
92	JL	102	LMG	O9-C10-O7-C8
92	XL	601	LMG	O9-C10-O7-C8
92	B6	619	LMG	O9-C10-O7-C8
92	J6	102	LMG	O9-C10-O7-C8
92	b6	623	LMG	O9-C10-O7-C8
92	j6	101	LMG	O9-C10-O7-C8
92	bL	609	LMG	O9-C10-O7-C8
92	bL	611	LMG	O9-C10-O7-C8
92	bL	623	LMG	O9-C10-O7-C8
92	qL	301	LMG	O9-C10-O7-C8
95	C6	504	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
95	b6	622	DGD	O1B-C1B-O2G-C2G
95	h6	101	DGD	O1B-C1B-O2G-C2G
95	hL	101	DGD	O1B-C1B-O2G-C2G
83	yF	302	PUB	C2D-C3D-CAD-CBD
83	yK	302	PUB	C2D-C3D-CAD-CBD
87	42	607	CLA	O1D-CGD-O2D-CED
87	4N	607	CLA	O1D-CGD-O2D-CED
87	BL	621	CLA	C3-C5-C6-C7
87	CL	504	CLA	C3-C5-C6-C7
87	CL	507	CLA	C3-C5-C6-C7
87	CL	511	CLA	C3-C5-C6-C7
87	AN	811	CLA	C3-C5-C6-C7
87	AN	825	CLA	C3-C5-C6-C7
87	AN	834	CLA	C3-C5-C6-C7
87	AN	839	CLA	C3-C5-C6-C7
87	AN	841	CLA	C3-C5-C6-C7
87	BN	802	CLA	C3-C5-C6-C7
87	BN	809	CLA	C3-C5-C6-C7
87	BN	816	CLA	C3-C5-C6-C7
87	BN	827	CLA	C3-C5-C6-C7
87	BN	831	CLA	C3-C5-C6-C7
87	IN	103	CLA	C3-C5-C6-C7
87	52	602	CLA	C3-C5-C6-C7
87	A2	811	CLA	C3-C5-C6-C7
87	A2	825	CLA	C3-C5-C6-C7
87	A2	834	CLA	C3-C5-C6-C7
87	A2	839	CLA	C3-C5-C6-C7
87	A2	841	CLA	C3-C5-C6-C7
87	B2	801	CLA	C3-C5-C6-C7
87	B2	808	CLA	C3-C5-C6-C7
87	B2	815	CLA	C3-C5-C6-C7
87	B2	827	CLA	C3-C5-C6-C7
87	B2	831	CLA	C3-C5-C6-C7
87	I2	103	CLA	C3-C5-C6-C7
87	C6	516	CLA	C3-C5-C6-C7
87	C6	519	CLA	C3-C5-C6-C7
87	c6	606	CLA	C3-C5-C6-C7
87	c6	607	CLA	C3-C5-C6-C7
87	bL	607	CLA	C3-C5-C6-C7
87	bL	620	CLA	C3-C5-C6-C7
87	cL	509	CLA	C3-C5-C6-C7
87	dL	404	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
87	5N	602	CLA	C3-C5-C6-C7
91	dL	403	PHO	C3-C5-C6-C7
87	BL	601	CLA	CBA-CGA-O2A-C1
87	AN	803	CLA	CBA-CGA-O2A-C1
87	AN	805	CLA	CBA-CGA-O2A-C1
87	AN	814	CLA	CBA-CGA-O2A-C1
87	AN	829	CLA	CBA-CGA-O2A-C1
87	AN	840	CLA	CBA-CGA-O2A-C1
87	BN	834	CLA	CBA-CGA-O2A-C1
87	BN	836	CLA	CBA-CGA-O2A-C1
87	LN	202	CLA	CBA-CGA-O2A-C1
87	32	304	CLA	CBA-CGA-O2A-C1
87	A2	803	CLA	CBA-CGA-O2A-C1
87	A2	805	CLA	CBA-CGA-O2A-C1
87	A2	814	CLA	CBA-CGA-O2A-C1
87	A2	829	CLA	CBA-CGA-O2A-C1
87	A2	840	CLA	CBA-CGA-O2A-C1
87	B2	834	CLA	CBA-CGA-O2A-C1
87	B2	836	CLA	CBA-CGA-O2A-C1
87	L2	202	CLA	CBA-CGA-O2A-C1
87	B6	609	CLA	CBA-CGA-O2A-C1
87	bL	616	CLA	CBA-CGA-O2A-C1
87	bL	620	CLA	CBA-CGA-O2A-C1
87	3N	305	CLA	CBA-CGA-O2A-C1
92	b6	624	LMG	C29-C28-O8-C9
92	bL	610	LMG	C29-C28-O8-C9
92	dL	407	LMG	C29-C28-O8-C9
95	L6	102	DGD	C2A-C1A-O1G-C1G
95	c6	618	DGD	O6E-C5E-C6E-O5E
92	B6	622	LMG	C11-C10-O7-C8
92	qL	301	LMG	C11-C10-O7-C8
87	HL	102	CLA	O1D-CGD-O2D-CED
87	AN	834	CLA	O1D-CGD-O2D-CED
87	A2	834	CLA	O1D-CGD-O2D-CED
87	c6	614	CLA	O1D-CGD-O2D-CED
87	AL	405	CLA	CBD-CGD-O2D-CED
87	B6	607	CLA	CBD-CGD-O2D-CED
84	EE	1001	CYC	C2B-C3B-CAB-CBB
84	EG	1001	CYC	C2B-C3B-CAB-CBB
87	AN	811	CLA	O1D-CGD-O2D-CED
82	HM	202	PEB	C2B-C3B-CAB-CBB
82	k4	202	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
82	kO	203	PEB	C2B-C3B-CAB-CBB
83	Z9	305	PUB	C3C-C2C-CAC-CBC
87	RN	203	CLA	CBA-CGA-O2A-C1
87	R2	203	CLA	CBA-CGA-O2A-C1
87	BL	620	CLA	C4-C3-C5-C6
87	AN	819	CLA	C4-C3-C5-C6
87	BN	825	CLA	C4-C3-C5-C6
87	A2	819	CLA	C4-C3-C5-C6
87	B2	824	CLA	C4-C3-C5-C6
87	b6	608	CLA	C4-C3-C5-C6
87	b6	609	CLA	C4-C3-C5-C6
87	c6	606	CLA	C4-C3-C5-C6
94	DL	401	PL9	C20-C19-C21-C22
94	d6	408	PL9	C30-C29-C31-C32
92	b6	619	LMG	C4-C5-C6-O5
87	AN	831	CLA	C2-C3-C5-C6
87	A2	831	CLA	C2-C3-C5-C6
87	bL	607	CLA	C2-C3-C5-C6
94	D6	408	PL9	C18-C19-C21-C22
82	BM	301	PEB	C3C-C2C-CAC-CBC
83	M5	302	PUB	C2B-C3B-CAB-CBB
83	Z5	302	PUB	C2B-C3B-CAB-CBB
87	BL	619	CLA	CBD-CGD-O2D-CED
87	BN	817	CLA	CBD-CGD-O2D-CED
87	RN	201	CLA	CBD-CGD-O2D-CED
87	R2	201	CLA	CBD-CGD-O2D-CED
87	C6	514	CLA	CBD-CGD-O2D-CED
87	BL	609	CLA	C2A-CAA-CBA-CGA
87	CL	505	CLA	C2A-CAA-CBA-CGA
87	CL	514	CLA	C2A-CAA-CBA-CGA
87	AN	807	CLA	C2A-CAA-CBA-CGA
87	AN	815	CLA	C2A-CAA-CBA-CGA
87	AN	818	CLA	C2A-CAA-CBA-CGA
87	AN	825	CLA	C2A-CAA-CBA-CGA
87	AN	829	CLA	C2A-CAA-CBA-CGA
87	BN	806	CLA	C2A-CAA-CBA-CGA
87	BN	814	CLA	C2A-CAA-CBA-CGA
87	FN	205	CLA	C2A-CAA-CBA-CGA
87	LN	202	CLA	C2A-CAA-CBA-CGA
87	ON	203	CLA	C2A-CAA-CBA-CGA
87	RN	201	CLA	C2A-CAA-CBA-CGA
87	RN	203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	22	601	CLA	C2A-CAA-CBA-CGA
87	32	304	CLA	C2A-CAA-CBA-CGA
87	42	601	CLA	C2A-CAA-CBA-CGA
87	42	605	CLA	C2A-CAA-CBA-CGA
87	62	306	CLA	C2A-CAA-CBA-CGA
87	62	309	CLA	C2A-CAA-CBA-CGA
87	A2	807	CLA	C2A-CAA-CBA-CGA
87	A2	815	CLA	C2A-CAA-CBA-CGA
87	A2	818	CLA	C2A-CAA-CBA-CGA
87	A2	825	CLA	C2A-CAA-CBA-CGA
87	A2	829	CLA	C2A-CAA-CBA-CGA
87	B2	805	CLA	C2A-CAA-CBA-CGA
87	B2	813	CLA	C2A-CAA-CBA-CGA
87	F2	205	CLA	C2A-CAA-CBA-CGA
87	L2	202	CLA	C2A-CAA-CBA-CGA
87	O2	203	CLA	C2A-CAA-CBA-CGA
87	R2	201	CLA	C2A-CAA-CBA-CGA
87	R2	203	CLA	C2A-CAA-CBA-CGA
87	A6	402	CLA	C2A-CAA-CBA-CGA
87	B6	604	CLA	C2A-CAA-CBA-CGA
87	b6	605	CLA	C2A-CAA-CBA-CGA
87	c6	615	CLA	C2A-CAA-CBA-CGA
87	bL	622	CLA	C2A-CAA-CBA-CGA
87	cL	511	CLA	C2A-CAA-CBA-CGA
87	cL	516	CLA	C2A-CAA-CBA-CGA
87	2N	302	CLA	C2A-CAA-CBA-CGA
87	3N	305	CLA	C2A-CAA-CBA-CGA
87	4N	601	CLA	C2A-CAA-CBA-CGA
87	4N	605	CLA	C2A-CAA-CBA-CGA
87	6N	605	CLA	C2A-CAA-CBA-CGA
87	6N	608	CLA	C2A-CAA-CBA-CGA
87	CL	509	CLA	O1D-CGD-O2D-CED
87	AN	833	CLA	O1D-CGD-O2D-CED
87	62	313	CLA	O1D-CGD-O2D-CED
87	82	301	CLA	O1D-CGD-O2D-CED
87	A2	811	CLA	O1D-CGD-O2D-CED
87	A2	833	CLA	O1D-CGD-O2D-CED
87	6N	612	CLA	O1D-CGD-O2D-CED
87	8N	302	CLA	O1D-CGD-O2D-CED
87	BN	806	CLA	C3-C5-C6-C7
87	BN	822	CLA	C3-C5-C6-C7
87	72	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
87	B2	805	CLA	C3-C5-C6-C7
87	B2	821	CLA	C3-C5-C6-C7
87	B6	608	CLA	C3-C5-C6-C7
87	a6	607	CLA	C3-C5-C6-C7
87	c6	604	CLA	C3-C5-C6-C7
87	cL	513	CLA	C3-C5-C6-C7
87	7N	602	CLA	C3-C5-C6-C7
91	DL	405	PHO	C3-C5-C6-C7
87	BL	623	CLA	CBA-CGA-O2A-C1
87	CL	507	CLA	CBA-CGA-O2A-C1
87	CL	511	CLA	CBA-CGA-O2A-C1
87	DL	406	CLA	CBA-CGA-O2A-C1
87	AN	806	CLA	CBA-CGA-O2A-C1
87	AN	811	CLA	CBA-CGA-O2A-C1
87	AN	812	CLA	CBA-CGA-O2A-C1
87	AN	819	CLA	CBA-CGA-O2A-C1
87	AN	838	CLA	CBA-CGA-O2A-C1
87	BN	818	CLA	CBA-CGA-O2A-C1
87	BN	822	CLA	CBA-CGA-O2A-C1
87	KN	105	CLA	CBA-CGA-O2A-C1
87	82	302	CLA	CBA-CGA-O2A-C1
87	A2	806	CLA	CBA-CGA-O2A-C1
87	A2	811	CLA	CBA-CGA-O2A-C1
87	A2	812	CLA	CBA-CGA-O2A-C1
87	A2	819	CLA	CBA-CGA-O2A-C1
87	A2	838	CLA	CBA-CGA-O2A-C1
87	B2	817	CLA	CBA-CGA-O2A-C1
87	B2	821	CLA	CBA-CGA-O2A-C1
87	K2	106	CLA	CBA-CGA-O2A-C1
87	B6	608	CLA	CBA-CGA-O2A-C1
87	cL	509	CLA	CBA-CGA-O2A-C1
87	cL	513	CLA	CBA-CGA-O2A-C1
87	8N	303	CLA	CBA-CGA-O2A-C1
91	AL	410	PHO	CBA-CGA-O2A-C1
92	bL	609	LMG	C29-C28-O8-C9
95	b6	621	DGD	C2A-C1A-O1G-C1G
95	lL	101	DGD	C2A-C1A-O1G-C1G
95	C6	521	DGD	C4E-C5E-C6E-O5E
84	BE	1001	CYC	ND-C1D-CHD-C4C
84	FE	1002	CYC	ND-C1D-CHD-C4C
84	HE	1001	CYC	ND-C1D-CHD-C4C
84	BG	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	FG	1001	CYC	ND-C1D-CHD-C4C
84	HG	1001	CYC	ND-C1D-CHD-C4C
84	CH	1001	CYC	ND-C1D-CHD-C4C
84	FH	1001	CYC	ND-C1D-CHD-C4C
84	KH	1001	CYC	ND-C1D-CHD-C4C
84	LH	1001	CYC	ND-C1D-CHD-C4C
84	DO	1001	CYC	ND-C1D-CHD-C4C
84	EO	1001	CYC	ND-C1D-CHD-C4C
84	FO	1001	CYC	ND-C1D-CHD-C4C
84	HO	1001	CYC	ND-C1D-CHD-C4C
84	LO	1001	CYC	ND-C1D-CHD-C4C
84	C1	1001	CYC	ND-C1D-CHD-C4C
84	F1	1001	CYC	ND-C1D-CHD-C4C
84	I1	1001	CYC	ND-C1D-CHD-C4C
84	K1	1001	CYC	ND-C1D-CHD-C4C
84	B3	1001	CYC	ND-C1D-CHD-C4C
84	D3	1001	CYC	ND-C1D-CHD-C4C
84	F3	1001	CYC	ND-C1D-CHD-C4C
84	H3	1001	CYC	ND-C1D-CHD-C4C
84	I3	1001	CYC	ND-C1D-CHD-C4C
84	L3	1001	CYC	ND-C1D-CHD-C4C
84	M3	1001	CYC	ND-C1D-CHD-C4C
84	O3	1001	CYC	ND-C1D-CHD-C4C
84	Q3	1001	CYC	ND-C1D-CHD-C4C
84	S3	1001	CYC	ND-C1D-CHD-C4C
84	U3	1001	CYC	ND-C1D-CHD-C4C
84	W3	1001	CYC	ND-C1D-CHD-C4C
84	d3	1001	CYC	ND-C1D-CHD-C4C
84	f3	1001	CYC	ND-C1D-CHD-C4C
84	h3	1001	CYC	ND-C1D-CHD-C4C
84	j3	1001	CYC	ND-C1D-CHD-C4C
84	k3	1001	CYC	ND-C1D-CHD-C4C
84	n3	1001	CYC	ND-C1D-CHD-C4C
84	o3	1001	CYC	ND-C1D-CHD-C4C
84	q3	1001	CYC	ND-C1D-CHD-C4C
84	u3	1001	CYC	ND-C1D-CHD-C4C
84	w3	1001	CYC	ND-C1D-CHD-C4C
84	y3	1001	CYC	ND-C1D-CHD-C4C
84	73	1001	CYC	ND-C1D-CHD-C4C
84	F4	1001	CYC	ND-C1D-CHD-C4C
84	H4	1001	CYC	ND-C1D-CHD-C4C
84	L4	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	D4	1001	CYC	ND-C1D-CHD-C4C
84	E4	1001	CYC	ND-C1D-CHD-C4C
84	BE	1001	CYC	C2B-C3B-CAB-CBB
84	BG	1001	CYC	C2B-C3B-CAB-CBB
82	HA	203	PEB	C4B-C3B-CAB-CBB
82	GE	1002	PEB	C4B-C3B-CAB-CBB
82	GG	1002	PEB	C4B-C3B-CAB-CBB
82	HM	202	PEB	C4B-C3B-CAB-CBB
82	g4	203	PEB	C4B-C3B-CAB-CBB
82	H7	203	PEB	C4B-C3B-CAB-CBB
82	gO	203	PEB	C4B-C3B-CAB-CBB
83	Z9	305	PUB	C1C-C2C-CAC-CBC
87	CL	518	CLA	O1D-CGD-O2D-CED
87	BN	807	CLA	O1D-CGD-O2D-CED
87	BN	824	CLA	O1D-CGD-O2D-CED
87	KN	105	CLA	O1D-CGD-O2D-CED
87	82	307	CLA	O1D-CGD-O2D-CED
87	B2	806	CLA	O1D-CGD-O2D-CED
87	B2	823	CLA	O1D-CGD-O2D-CED
87	K2	106	CLA	O1D-CGD-O2D-CED
87	8N	307	CLA	O1D-CGD-O2D-CED
95	a6	602	DGD	C4D-C5D-C6D-O5D
82	FA	203	PEB	C2C-C1C-CHB-C4B
82	HF	202	PEB	C2C-C1C-CHB-C4B
82	TF	202	PEB	C2C-C1C-CHB-C4B
82	ZF	202	PEB	C2C-C1C-CHB-C4B
82	HK	202	PEB	C2C-C1C-CHB-C4B
82	TK	202	PEB	C2C-C1C-CHB-C4B
82	ZK	202	PEB	C2C-C1C-CHB-C4B
82	RM	202	PEB	C2C-C1C-CHB-C4B
82	W5	203	PEB	C2C-C1C-CHB-C4B
82	F7	203	PEB	C2C-C1C-CHB-C4B
82	eE	203	PEB	C2C-C1C-CHB-C4B
82	hF	202	PEB	C2C-C1C-CHB-C4B
82	qF	202	PEB	C2C-C1C-CHB-C4B
82	hK	202	PEB	C2C-C1C-CHB-C4B
82	qK	202	PEB	C2C-C1C-CHB-C4B
82	gM	201	PEB	C2C-C1C-CHB-C4B
82	iM	202	PEB	C2C-C1C-CHB-C4B
82	jM	202	PEB	C2C-C1C-CHB-C4B
82	kM	202	PEB	C2C-C1C-CHB-C4B
84	BE	1001	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	BE	1002	CYC	C2D-C1D-CHD-C4C
84	EE	1001	CYC	C2D-C1D-CHD-C4C
84	FE	1001	CYC	C2D-C1D-CHD-C4C
84	FE	1002	CYC	C2D-C1D-CHD-C4C
84	GE	1001	CYC	C2D-C1D-CHD-C4C
84	HE	1001	CYC	C2D-C1D-CHD-C4C
84	IE	1001	CYC	C2D-C1D-CHD-C4C
84	ME	1001	CYC	C2D-C1D-CHD-C4C
84	BG	1001	CYC	C2D-C1D-CHD-C4C
84	BG	1002	CYC	C2D-C1D-CHD-C4C
84	CG	1001	CYC	C2D-C1D-CHD-C4C
84	EG	1001	CYC	C2D-C1D-CHD-C4C
84	FG	1001	CYC	C2D-C1D-CHD-C4C
84	GG	1001	CYC	C2D-C1D-CHD-C4C
84	HG	1001	CYC	C2D-C1D-CHD-C4C
84	IG	1001	CYC	C2D-C1D-CHD-C4C
84	MG	1001	CYC	C2D-C1D-CHD-C4C
84	CH	1001	CYC	C2D-C1D-CHD-C4C
84	EH	1001	CYC	C2D-C1D-CHD-C4C
84	FH	1001	CYC	C2D-C1D-CHD-C4C
84	KH	1001	CYC	C2D-C1D-CHD-C4C
84	LH	1001	CYC	C2D-C1D-CHD-C4C
84	DO	1001	CYC	C2D-C1D-CHD-C4C
84	FO	1001	CYC	C2D-C1D-CHD-C4C
84	GO	1001	CYC	C2D-C1D-CHD-C4C
84	HO	1001	CYC	C2D-C1D-CHD-C4C
84	IO	1001	CYC	C2D-C1D-CHD-C4C
84	KO	1001	CYC	C2D-C1D-CHD-C4C
84	LO	1001	CYC	C2D-C1D-CHD-C4C
84	MO	1001	CYC	C2D-C1D-CHD-C4C
84	NO	1001	CYC	C2D-C1D-CHD-C4C
84	C1	1001	CYC	C2D-C1D-CHD-C4C
84	E1	1001	CYC	C2D-C1D-CHD-C4C
84	I1	1001	CYC	C2D-C1D-CHD-C4C
84	K1	1001	CYC	C2D-C1D-CHD-C4C
84	B3	1001	CYC	C2D-C1D-CHD-C4C
84	D3	1001	CYC	C2D-C1D-CHD-C4C
84	F3	1001	CYC	C2D-C1D-CHD-C4C
84	H3	1001	CYC	C2D-C1D-CHD-C4C
84	I3	1001	CYC	C2D-C1D-CHD-C4C
84	L3	1001	CYC	C2D-C1D-CHD-C4C
84	M3	1001	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	O3	1001	CYC	C2D-C1D-CHD-C4C
84	Q3	1001	CYC	C2D-C1D-CHD-C4C
84	S3	1001	CYC	C2D-C1D-CHD-C4C
84	U3	1001	CYC	C2D-C1D-CHD-C4C
84	W3	1001	CYC	C2D-C1D-CHD-C4C
84	d3	1001	CYC	C2D-C1D-CHD-C4C
84	f3	1001	CYC	C2D-C1D-CHD-C4C
84	h3	1001	CYC	C2D-C1D-CHD-C4C
84	j3	1001	CYC	C2D-C1D-CHD-C4C
84	k3	1001	CYC	C2D-C1D-CHD-C4C
84	n3	1001	CYC	C2D-C1D-CHD-C4C
84	o3	1001	CYC	C2D-C1D-CHD-C4C
84	q3	1001	CYC	C2D-C1D-CHD-C4C
84	u3	1001	CYC	C2D-C1D-CHD-C4C
84	w3	1001	CYC	C2D-C1D-CHD-C4C
84	73	1001	CYC	C2D-C1D-CHD-C4C
84	F4	1001	CYC	C2D-C1D-CHD-C4C
84	G4	1001	CYC	C2D-C1D-CHD-C4C
84	H4	1001	CYC	C2D-C1D-CHD-C4C
84	I4	1001	CYC	C2D-C1D-CHD-C4C
84	K4	1001	CYC	C2D-C1D-CHD-C4C
84	L4	1001	CYC	C2D-C1D-CHD-C4C
84	M4	1001	CYC	C2D-C1D-CHD-C4C
84	N4	1001	CYC	C2D-C1D-CHD-C4C
84	D4	1001	CYC	C2D-C1D-CHD-C4C
87	AN	802	CLA	CBD-CGD-O2D-CED
87	62	303	CLA	CBD-CGD-O2D-CED
87	A2	801	CLA	CBD-CGD-O2D-CED
87	B2	816	CLA	CBD-CGD-O2D-CED
87	c6	615	CLA	CBD-CGD-O2D-CED
87	nL	101	CLA	CBD-CGD-O2D-CED
87	6N	602	CLA	CBD-CGD-O2D-CED
87	6N	608	CLA	CBD-CGD-O2D-CED
87	CL	508	CLA	O1D-CGD-O2D-CED
87	DL	406	CLA	O1D-CGD-O2D-CED
87	BN	806	CLA	O1D-CGD-O2D-CED
87	12	607	CLA	O1D-CGD-O2D-CED
87	32	312	CLA	O1D-CGD-O2D-CED
87	B2	805	CLA	O1D-CGD-O2D-CED
87	B6	612	CLA	O1D-CGD-O2D-CED
87	cL	510	CLA	O1D-CGD-O2D-CED
87	1N	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	3N	312	CLA	O1D-CGD-O2D-CED
92	CL	519	LMG	O6-C5-C6-O5
92	CL	519	LMG	O9-C10-O7-C8
95	L6	102	DGD	C4E-C5E-C6E-O5E
87	BL	601	CLA	O1A-CGA-O2A-C1
87	BL	623	CLA	O1A-CGA-O2A-C1
87	DL	406	CLA	O1A-CGA-O2A-C1
87	AN	812	CLA	O1A-CGA-O2A-C1
87	AN	819	CLA	O1A-CGA-O2A-C1
87	AN	821	CLA	O1A-CGA-O2A-C1
87	AN	823	CLA	O1A-CGA-O2A-C1
87	AN	829	CLA	O1A-CGA-O2A-C1
87	AN	838	CLA	O1A-CGA-O2A-C1
87	KN	105	CLA	O1A-CGA-O2A-C1
87	A2	812	CLA	O1A-CGA-O2A-C1
87	A2	819	CLA	O1A-CGA-O2A-C1
87	A2	821	CLA	O1A-CGA-O2A-C1
87	A2	823	CLA	O1A-CGA-O2A-C1
87	A2	829	CLA	O1A-CGA-O2A-C1
87	A2	838	CLA	O1A-CGA-O2A-C1
87	K2	106	CLA	O1A-CGA-O2A-C1
87	B6	609	CLA	O1A-CGA-O2A-C1
87	bL	616	CLA	O1A-CGA-O2A-C1
91	AL	410	PHO	O1A-CGA-O2A-C1
92	D6	409	LMG	O10-C28-O8-C9
92	d6	409	LMG	O10-C28-O8-C9
95	L6	102	DGD	O1A-C1A-O1G-C1G
95	lL	101	DGD	O1A-C1A-O1G-C1G
83	AH	304	PUB	C4A-C3A-CAA-CBA
83	A1	304	PUB	C4A-C3A-CAA-CBA
87	BL	602	CLA	O1D-CGD-O2D-CED
87	BN	801	CLA	O1D-CGD-O2D-CED
87	22	609	CLA	O1D-CGD-O2D-CED
87	B2	825	CLA	O1D-CGD-O2D-CED
87	B6	608	CLA	O1D-CGD-O2D-CED
87	a6	608	CLA	O1D-CGD-O2D-CED
87	bL	615	CLA	O1D-CGD-O2D-CED
87	2N	309	CLA	O1D-CGD-O2D-CED
92	DL	402	LMG	C8-C9-O8-C28
85	FL	101	BCR	C19-C20-C21-C22
85	KL	100	BCR	C13-C14-C15-C16
85	c6	602	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
85	kL	100	BCR	C13-C14-C15-C16
103	82	309	ZEX	C13-C14-C15-C35
103	8N	309	ZEX	C13-C14-C15-C35
87	CL	506	CLA	CBD-CGD-O2D-CED
87	AN	803	CLA	CBD-CGD-O2D-CED
87	AN	810	CLA	CBD-CGD-O2D-CED
87	AN	823	CLA	CBD-CGD-O2D-CED
87	AN	836	CLA	CBD-CGD-O2D-CED
87	AN	849	CLA	CBD-CGD-O2D-CED
87	BN	813	CLA	CBD-CGD-O2D-CED
87	BN	822	CLA	CBD-CGD-O2D-CED
87	BN	833	CLA	CBD-CGD-O2D-CED
87	LN	206	CLA	CBD-CGD-O2D-CED
87	12	602	CLA	CBD-CGD-O2D-CED
87	12	603	CLA	CBD-CGD-O2D-CED
87	52	610	CLA	CBD-CGD-O2D-CED
87	62	309	CLA	CBD-CGD-O2D-CED
87	A2	803	CLA	CBD-CGD-O2D-CED
87	A2	810	CLA	CBD-CGD-O2D-CED
87	A2	820	CLA	CBD-CGD-O2D-CED
87	A2	823	CLA	CBD-CGD-O2D-CED
87	A2	836	CLA	CBD-CGD-O2D-CED
87	A2	849	CLA	CBD-CGD-O2D-CED
87	B2	812	CLA	CBD-CGD-O2D-CED
87	B2	821	CLA	CBD-CGD-O2D-CED
87	B2	833	CLA	CBD-CGD-O2D-CED
87	L2	206	CLA	CBD-CGD-O2D-CED
87	d6	403	CLA	CBD-CGD-O2D-CED
87	d6	406	CLA	CBD-CGD-O2D-CED
87	bL	616	CLA	CBD-CGD-O2D-CED
87	cL	505	CLA	CBD-CGD-O2D-CED
87	cL	516	CLA	CBD-CGD-O2D-CED
87	dL	401	CLA	CBD-CGD-O2D-CED
87	dL	409	CLA	CBD-CGD-O2D-CED
87	1N	602	CLA	CBD-CGD-O2D-CED
87	1N	603	CLA	CBD-CGD-O2D-CED
87	5N	610	CLA	CBD-CGD-O2D-CED
87	AN	815	CLA	O1D-CGD-O2D-CED
87	52	604	CLA	O1D-CGD-O2D-CED
87	A2	815	CLA	O1D-CGD-O2D-CED
87	c6	607	CLA	O1D-CGD-O2D-CED
87	dL	404	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	5N	604	CLA	O1D-CGD-O2D-CED
95	L6	102	DGD	O6D-C5D-C6D-O5D
95	a6	603	DGD	O6D-C5D-C6D-O5D
88	C6	505	LHG	O2-C2-C3-O3
88	D6	406	LHG	O2-C2-C3-O3
88	m6	102	LHG	O2-C2-C3-O3
88	dL	405	LHG	O2-C2-C3-O3
88	mL	102	LHG	O2-C2-C3-O3
87	AN	802	CLA	C3-C5-C6-C7
87	AN	808	CLA	C3-C5-C6-C7
87	AN	819	CLA	C3-C5-C6-C7
87	AN	851	CLA	C3-C5-C6-C7
87	BN	834	CLA	C3-C5-C6-C7
87	12	602	CLA	C3-C5-C6-C7
87	A2	801	CLA	C3-C5-C6-C7
87	A2	808	CLA	C3-C5-C6-C7
87	A2	819	CLA	C3-C5-C6-C7
87	A2	851	CLA	C3-C5-C6-C7
87	B2	834	CLA	C3-C5-C6-C7
87	C6	513	CLA	C3-C5-C6-C7
87	1N	602	CLA	C3-C5-C6-C7
87	AN	810	CLA	CBA-CGA-O2A-C1
87	AN	821	CLA	CBA-CGA-O2A-C1
87	AN	823	CLA	CBA-CGA-O2A-C1
87	LN	204	CLA	CBA-CGA-O2A-C1
87	A2	810	CLA	CBA-CGA-O2A-C1
87	A2	821	CLA	CBA-CGA-O2A-C1
87	A2	823	CLA	CBA-CGA-O2A-C1
87	L2	204	CLA	CBA-CGA-O2A-C1
87	b6	611	CLA	CBA-CGA-O2A-C1
87	c6	614	CLA	CBA-CGA-O2A-C1
87	c6	616	CLA	CBA-CGA-O2A-C1
87	dL	404	CLA	CBA-CGA-O2A-C1
88	I6	101	LHG	C24-C23-O8-C6
92	D6	409	LMG	C29-C28-O8-C9
92	d6	409	LMG	C29-C28-O8-C9
95	BL	613	DGD	C2A-C1A-O1G-C1G
87	AN	805	CLA	O1A-CGA-O2A-C1
87	AN	811	CLA	O1A-CGA-O2A-C1
87	BN	822	CLA	O1A-CGA-O2A-C1
87	BN	834	CLA	O1A-CGA-O2A-C1
87	A2	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
87	A2	811	CLA	O1A-CGA-O2A-C1
87	B2	821	CLA	O1A-CGA-O2A-C1
87	B2	834	CLA	O1A-CGA-O2A-C1
87	c6	616	CLA	O1A-CGA-O2A-C1
87	bL	613	CLA	O1A-CGA-O2A-C1
92	b6	624	LMG	O10-C28-O8-C9
92	bL	609	LMG	O6-C5-C6-O5
87	22	605	CLA	O1D-CGD-O2D-CED
87	62	312	CLA	O1D-CGD-O2D-CED
87	2N	301	CLA	O1D-CGD-O2D-CED
87	6N	611	CLA	O1D-CGD-O2D-CED
88	CL	522	LHG	C8-C7-O7-C5
88	cL	501	LHG	C8-C7-O7-C5
92	CL	519	LMG	C11-C10-O7-C8
92	DL	402	LMG	C11-C10-O7-C8
92	b6	620	LMG	C11-C10-O7-C8
92	m6	103	LMG	C11-C10-O7-C8
84	FE	1001	CYC	C2B-C3B-CAB-CBB
84	CG	1001	CYC	C2B-C3B-CAB-CBB
87	BL	601	CLA	CBD-CGD-O2D-CED
87	CL	504	CLA	CBD-CGD-O2D-CED
87	AN	820	CLA	CBD-CGD-O2D-CED
87	BN	831	CLA	CBD-CGD-O2D-CED
87	22	610	CLA	CBD-CGD-O2D-CED
87	B2	831	CLA	CBD-CGD-O2D-CED
87	b6	610	CLA	CBD-CGD-O2D-CED
87	cL	517	CLA	CBD-CGD-O2D-CED
87	2N	310	CLA	CBD-CGD-O2D-CED
92	aL	611	LMG	O6-C5-C6-O5
95	cL	519	DGD	O6E-C5E-C6E-O5E
92	J6	102	LMG	C34-C35-C36-C37
92	b6	623	LMG	C29-C30-C31-C32
92	j6	101	LMG	C34-C35-C36-C37
87	RN	202	CLA	O1D-CGD-O2D-CED
87	R2	202	CLA	O1D-CGD-O2D-CED
87	d6	406	CLA	C2C-C3C-CAC-CBC
88	d6	407	LHG	C11-C12-C13-C14
92	yL	101	LMG	C35-C36-C37-C38
95	C6	502	DGD	C7B-C8B-C9B-CAB
95	C6	503	DGD	C2A-C3A-C4A-C5A
95	c6	601	DGD	C7B-C8B-C9B-CAB
95	CL	523	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
95	cL	520	DGD	O6E-C5E-C6E-O5E
87	AN	818	CLA	O1D-CGD-O2D-CED
87	52	611	CLA	O1D-CGD-O2D-CED
87	A2	818	CLA	O1D-CGD-O2D-CED
87	5N	611	CLA	O1D-CGD-O2D-CED
87	b6	609	CLA	CBD-CGD-O2D-CED
87	DL	403	CLA	C3-C5-C6-C7
87	AN	805	CLA	C3-C5-C6-C7
87	A2	805	CLA	C3-C5-C6-C7
87	b6	604	CLA	C3-C5-C6-C7
87	bL	613	CLA	CBA-CGA-O2A-C1
82	B5	201	PEB	C2B-C3B-CAB-CBB
84	NO	1001	CYC	C3A-C2A-CAA-CBA
82	KA	201	PEB	C1C-C2C-CAC-CBC
82	KB	301	PEB	C1C-C2C-CAC-CBC
82	LF	202	PEB	C1C-C2C-CAC-CBC
82	LK	202	PEB	C1C-C2C-CAC-CBC
82	K7	201	PEB	C1C-C2C-CAC-CBC
82	eE	203	PEB	C1C-C2C-CAC-CBC
82	qF	202	PEB	C1C-C2C-CAC-CBC
82	eG	203	PEB	C1C-C2C-CAC-CBC
82	qK	202	PEB	C1C-C2C-CAC-CBC
83	AH	303	PUB	C4B-C3B-CAB-CBB
83	A1	303	PUB	C4B-C3B-CAB-CBB
87	BN	808	CLA	O1D-CGD-O2D-CED
87	B2	807	CLA	O1D-CGD-O2D-CED
95	AL	414	DGD	O6E-C5E-C6E-O5E
95	CL	520	DGD	O6E-C5E-C6E-O5E
92	J6	102	LMG	C4-C5-C6-O5
92	j6	101	LMG	C4-C5-C6-O5
95	c6	618	DGD	C4E-C5E-C6E-O5E
84	W3	1001	CYC	C2B-C3B-CAB-CBB
84	y3	1001	CYC	C2B-C3B-CAB-CBB
95	C6	502	DGD	CCA-CDA-CEA-CFA
95	c6	601	DGD	CCA-CDA-CEA-CFA
87	B6	608	CLA	O1A-CGA-O2A-C1
87	b6	611	CLA	O1A-CGA-O2A-C1
92	bL	609	LMG	O10-C28-O8-C9
95	b6	621	DGD	O1A-C1A-O1G-C1G
82	BA	203	PEB	C2C-CAC-CBC-CGC
82	EA	201	PEB	C3B-CAB-CBB-CGB
82	FA	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	JA	202	PEB	C2C-CAC-CBC-CGC
82	LA	202	PEB	C2C-CAC-CBC-CGC
82	MA	202	PEB	C2C-CAC-CBC-CGC
82	OA	201	PEB	C3B-CAB-CBB-CGB
82	UA	202	PEB	C2C-CAC-CBC-CGC
82	WA	202	PEB	C2C-CAC-CBC-CGC
82	YA	301	PEB	C3B-CAB-CBB-CGB
82	GB	202	PEB	C2C-CAC-CBC-CGC
82	HB	201	PEB	C2C-CAC-CBC-CGC
82	KB	303	PEB	C2C-CAC-CBC-CGC
82	KB	303	PEB	C3B-CAB-CBB-CGB
82	QB	201	PEB	C2C-CAC-CBC-CGC
82	AD	304	PEB	C3B-CAB-CBB-CGB
82	BD	203	PEB	C2C-CAC-CBC-CGC
82	HD	202	PEB	C3B-CAB-CBB-CGB
82	JD	203	PEB	C2C-CAC-CBC-CGC
82	KD	202	PEB	C2C-CAC-CBC-CGC
82	MD	202	PEB	C3B-CAB-CBB-CGB
82	ND	202	PEB	C3B-CAB-CBB-CGB
82	TD	203	PEB	C2C-CAC-CBC-CGC
82	YD	202	PEB	C2C-CAC-CBC-CGC
82	OE	202	PEB	C3B-CAB-CBB-CGB
82	PE	202	PEB	C3B-CAB-CBB-CGB
82	QE	203	PEB	C3B-CAB-CBB-CGB
82	WE	203	PEB	C3B-CAB-CBB-CGB
82	YE	202	PEB	C2C-CAC-CBC-CGC
82	ZE	201	PEB	C2C-CAC-CBC-CGC
82	BF	202	PEB	C2C-CAC-CBC-CGC
82	DF	203	PEB	C2C-CAC-CBC-CGC
82	DF	203	PEB	C3B-CAB-CBB-CGB
82	FF	202	PEB	C2C-CAC-CBC-CGC
82	GF	202	PEB	C3B-CAB-CBB-CGB
82	HF	202	PEB	C2C-CAC-CBC-CGC
82	IF	201	PEB	C3B-CAB-CBB-CGB
82	IF	202	PEB	C2C-CAC-CBC-CGC
82	KF	203	PEB	C3B-CAB-CBB-CGB
82	MF	202	PEB	C2C-CAC-CBC-CGC
82	OF	201	PEB	C3B-CAB-CBB-CGB
82	OF	203	PEB	C2C-CAC-CBC-CGC
82	PF	201	PEB	C3B-CAB-CBB-CGB
82	PF	202	PEB	C2C-CAC-CBC-CGC
82	SF	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	XF	203	PEB	C2C-CAC-CBC-CGC
82	ZF	201	PEB	C3B-CAB-CBB-CGB
82	OG	202	PEB	C3B-CAB-CBB-CGB
82	PG	202	PEB	C3B-CAB-CBB-CGB
82	QG	203	PEB	C3B-CAB-CBB-CGB
82	WG	203	PEB	C3B-CAB-CBB-CGB
82	YG	202	PEB	C2C-CAC-CBC-CGC
82	ZG	201	PEB	C2C-CAC-CBC-CGC
82	DH	1002	PEB	C3B-CAB-CBB-CGB
82	FH	1002	PEB	C3B-CAB-CBB-CGB
82	JH	1002	PEB	C3B-CAB-CBB-CGB
82	OH	202	PEB	C3B-CAB-CBB-CGB
82	QH	202	PEB	C3B-CAB-CBB-CGB
82	QH	203	PEB	C2C-CAC-CBC-CGC
82	TH	202	PEB	C2C-CAC-CBC-CGC
82	AI	202	PEB	C2C-CAC-CBC-CGC
82	CI	202	PEB	C2C-CAC-CBC-CGC
82	EI	202	PEB	C2C-CAC-CBC-CGC
82	GI	203	PEB	C2C-CAC-CBC-CGC
82	II	202	PEB	C2C-CAC-CBC-CGC
82	KI	203	PEB	C2C-CAC-CBC-CGC
82	NI	202	PEB	C2C-CAC-CBC-CGC
82	PI	202	PEB	C2C-CAC-CBC-CGC
82	RI	202	PEB	C2C-CAC-CBC-CGC
82	TI	203	PEB	C2C-CAC-CBC-CGC
82	VI	202	PEB	C2C-CAC-CBC-CGC
82	XI	202	PEB	C2C-CAC-CBC-CGC
82	AJ	301	PEB	C2C-CAC-CBC-CGC
82	AJ	301	PEB	C3B-CAB-CBB-CGB
82	EJ	203	PEB	C3B-CAB-CBB-CGB
82	RJ	202	PEB	C2C-CAC-CBC-CGC
82	SJ	201	PEB	C2C-CAC-CBC-CGC
82	UJ	203	PEB	C3B-CAB-CBB-CGB
82	YJ	202	PEB	C2C-CAC-CBC-CGC
82	BK	202	PEB	C2C-CAC-CBC-CGC
82	DK	203	PEB	C2C-CAC-CBC-CGC
82	DK	203	PEB	C3B-CAB-CBB-CGB
82	FK	202	PEB	C2C-CAC-CBC-CGC
82	GK	202	PEB	C3B-CAB-CBB-CGB
82	HK	202	PEB	C2C-CAC-CBC-CGC
82	IK	201	PEB	C3B-CAB-CBB-CGB
82	IK	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	KK	203	PEB	C3B-CAB-CBB-CGB
82	MK	202	PEB	C2C-CAC-CBC-CGC
82	OK	201	PEB	C3B-CAB-CBB-CGB
82	OK	203	PEB	C2C-CAC-CBC-CGC
82	PK	201	PEB	C3B-CAB-CBB-CGB
82	PK	202	PEB	C2C-CAC-CBC-CGC
82	SK	203	PEB	C2C-CAC-CBC-CGC
82	XK	203	PEB	C2C-CAC-CBC-CGC
82	ZK	201	PEB	C3B-CAB-CBB-CGB
82	GM	201	PEB	C2C-CAC-CBC-CGC
82	HM	202	PEB	C3B-CAB-CBB-CGB
82	JM	202	PEB	C2C-CAC-CBC-CGC
82	KM	202	PEB	C2C-CAC-CBC-CGC
82	LM	202	PEB	C2C-CAC-CBC-CGC
82	PM	202	PEB	C2C-CAC-CBC-CGC
82	SM	201	PEB	C2C-CAC-CBC-CGC
82	SM	201	PEB	C3B-CAB-CBB-CGB
82	VM	202	PEB	C2C-CAC-CBC-CGC
82	WM	202	PEB	C2C-CAC-CBC-CGC
82	ZM	202	PEB	C2C-CAC-CBC-CGC
82	AO	305	PEB	C3B-CAB-CBB-CGB
82	HO	1002	PEB	C3B-CAB-CBB-CGB
82	JO	1002	PEB	C3B-CAB-CBB-CGB
82	RO	203	PEB	C3B-CAB-CBB-CGB
82	VO	202	PEB	C2C-CAC-CBC-CGC
82	YO	203	PEB	C3B-CAB-CBB-CGB
82	NP	201	PEB	C2C-CAC-CBC-CGC
82	OP	203	PEB	C2C-CAC-CBC-CGC
82	AQ	304	PEB	C3B-CAB-CBB-CGB
82	BQ	203	PEB	C2C-CAC-CBC-CGC
82	HQ	202	PEB	C3B-CAB-CBB-CGB
82	JQ	203	PEB	C2C-CAC-CBC-CGC
82	KQ	202	PEB	C2C-CAC-CBC-CGC
82	MQ	202	PEB	C3B-CAB-CBB-CGB
82	NQ	202	PEB	C3B-CAB-CBB-CGB
82	TQ	203	PEB	C2C-CAC-CBC-CGC
82	YQ	202	PEB	C2C-CAC-CBC-CGC
82	O1	202	PEB	C3B-CAB-CBB-CGB
82	Q1	202	PEB	C3B-CAB-CBB-CGB
82	Q1	203	PEB	C2C-CAC-CBC-CGC
82	T1	202	PEB	C2C-CAC-CBC-CGC
82	D1	1002	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	F1	1002	PEB	C3B-CAB-CBB-CGB
82	J1	1002	PEB	C3B-CAB-CBB-CGB
82	f1	203	PEB	C2C-CAC-CBC-CGC
82	g1	201	PEB	C3B-CAB-CBB-CGB
82	h1	201	PEB	C2C-CAC-CBC-CGC
82	h1	201	PEB	C3B-CAB-CBB-CGB
82	i1	202	PEB	C3B-CAB-CBB-CGB
82	j1	202	PEB	C2C-CAC-CBC-CGC
82	j1	203	PEB	C2C-CAC-CBC-CGC
82	k1	202	PEB	C2C-CAC-CBC-CGC
82	l1	203	PEB	C3B-CAB-CBB-CGB
82	H4	1002	PEB	C3B-CAB-CBB-CGB
82	J4	1002	PEB	C3B-CAB-CBB-CGB
82	A4	305	PEB	C3B-CAB-CBB-CGB
82	R4	203	PEB	C3B-CAB-CBB-CGB
82	V4	202	PEB	C2C-CAC-CBC-CGC
82	Y4	203	PEB	C3B-CAB-CBB-CGB
82	i4	203	PEB	C3B-CAB-CBB-CGB
82	e4	202	PEB	C2C-CAC-CBC-CGC
82	H5	201	PEB	C2C-CAC-CBC-CGC
82	J5	201	PEB	C2C-CAC-CBC-CGC
82	L5	201	PEB	C3B-CAB-CBB-CGB
82	L5	203	PEB	C3B-CAB-CBB-CGB
82	M5	301	PEB	C3B-CAB-CBB-CGB
82	Q5	203	PEB	C3B-CAB-CBB-CGB
82	U5	201	PEB	C2C-CAC-CBC-CGC
82	U5	203	PEB	C3B-CAB-CBB-CGB
82	Y5	201	PEB	C2C-CAC-CBC-CGC
82	Z5	301	PEB	C3B-CAB-CBB-CGB
82	B7	203	PEB	C2C-CAC-CBC-CGC
82	E7	201	PEB	C3B-CAB-CBB-CGB
82	F7	201	PEB	C2C-CAC-CBC-CGC
82	J7	202	PEB	C2C-CAC-CBC-CGC
82	L7	202	PEB	C2C-CAC-CBC-CGC
82	M7	202	PEB	C2C-CAC-CBC-CGC
82	O7	201	PEB	C3B-CAB-CBB-CGB
82	U7	202	PEB	C2C-CAC-CBC-CGC
82	W7	202	PEB	C2C-CAC-CBC-CGC
82	Y7	301	PEB	C3B-CAB-CBB-CGB
82	18	202	PEB	C3B-CAB-CBB-CGB
82	r8	202	PEB	C2C-CAC-CBC-CGC
82	s8	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	s8	203	PEB	C2C-CAC-CBC-CGC
82	t8	202	PEB	C2C-CAC-CBC-CGC
82	v8	202	PEB	C2C-CAC-CBC-CGC
82	B9	201	PEB	C2C-CAC-CBC-CGC
82	B9	201	PEB	C3B-CAB-CBB-CGB
82	D9	201	PEB	C2C-CAC-CBC-CGC
82	D9	203	PEB	C3B-CAB-CBB-CGB
82	F9	203	PEB	C3B-CAB-CBB-CGB
82	H9	202	PEB	C3B-CAB-CBB-CGB
82	J9	201	PEB	C3B-CAB-CBB-CGB
82	J9	203	PEB	C3B-CAB-CBB-CGB
82	L9	203	PEB	C3B-CAB-CBB-CGB
82	O9	201	PEB	C2C-CAC-CBC-CGC
82	O9	202	PEB	C2C-CAC-CBC-CGC
82	U9	201	PEB	C2C-CAC-CBC-CGC
82	U9	203	PEB	C3B-CAB-CBB-CGB
82	W9	201	PEB	C3B-CAB-CBB-CGB
82	Y9	201	PEB	C3B-CAB-CBB-CGB
82	Y9	203	PEB	C3B-CAB-CBB-CGB
82	aB	202	PEB	C3B-CAB-CBB-CGB
82	cB	402	PEB	C2C-CAC-CBC-CGC
82	1C	202	PEB	C3B-CAB-CBB-CGB
82	rC	202	PEB	C2C-CAC-CBC-CGC
82	sC	202	PEB	C3B-CAB-CBB-CGB
82	sC	203	PEB	C2C-CAC-CBC-CGC
82	tC	202	PEB	C2C-CAC-CBC-CGC
82	vC	202	PEB	C2C-CAC-CBC-CGC
82	bE	202	PEB	C2C-CAC-CBC-CGC
82	eE	202	PEB	C2C-CAC-CBC-CGC
82	eE	203	PEB	C2C-CAC-CBC-CGC
82	fE	202	PEB	C3B-CAB-CBB-CGB
82	fE	203	PEB	C2C-CAC-CBC-CGC
82	gE	201	PEB	C2C-CAC-CBC-CGC
82	hE	202	PEB	C3B-CAB-CBB-CGB
82	lE	202	PEB	C3B-CAB-CBB-CGB
82	aF	201	PEB	C3B-CAB-CBB-CGB
82	aF	203	PEB	C2C-CAC-CBC-CGC
82	dF	202	PEB	C3B-CAB-CBB-CGB
82	eF	201	PEB	C2C-CAC-CBC-CGC
82	eF	203	PEB	C2C-CAC-CBC-CGC
82	gF	202	PEB	C2C-CAC-CBC-CGC
82	iF	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	jF	201	PEB	C3B-CAB-CBB-CGB
82	lF	201	PEB	C3B-CAB-CBB-CGB
82	lF	203	PEB	C2C-CAC-CBC-CGC
82	lF	203	PEB	C3B-CAB-CBB-CGB
82	nF	202	PEB	C2C-CAC-CBC-CGC
82	pF	202	PEB	C2C-CAC-CBC-CGC
82	qF	202	PEB	C3B-CAB-CBB-CGB
82	rF	202	PEB	C3B-CAB-CBB-CGB
82	tF	201	PEB	C2C-CAC-CBC-CGC
82	uF	203	PEB	C2C-CAC-CBC-CGC
82	wF	302	PEB	C3B-CAB-CBB-CGB
82	wF	303	PEB	C2C-CAC-CBC-CGC
82	xF	302	PEB	C2C-CAC-CBC-CGC
82	eG	202	PEB	C2C-CAC-CBC-CGC
82	eG	203	PEB	C2C-CAC-CBC-CGC
82	fG	202	PEB	C3B-CAB-CBB-CGB
82	fG	203	PEB	C2C-CAC-CBC-CGC
82	gG	201	PEB	C2C-CAC-CBC-CGC
82	hG	202	PEB	C3B-CAB-CBB-CGB
82	lG	202	PEB	C3B-CAB-CBB-CGB
82	fH	203	PEB	C2C-CAC-CBC-CGC
82	gH	201	PEB	C3B-CAB-CBB-CGB
82	gH	203	PEB	C2C-CAC-CBC-CGC
82	gH	203	PEB	C3B-CAB-CBB-CGB
82	iH	202	PEB	C3B-CAB-CBB-CGB
82	jH	202	PEB	C2C-CAC-CBC-CGC
82	jH	203	PEB	C2C-CAC-CBC-CGC
82	kH	202	PEB	C2C-CAC-CBC-CGC
82	lH	202	PEB	C3B-CAB-CBB-CGB
82	aJ	201	PEB	C3B-CAB-CBB-CGB
82	aJ	202	PEB	C3B-CAB-CBB-CGB
82	jJ	201	PEB	C2C-CAC-CBC-CGC
82	lJ	203	PEB	C3B-CAB-CBB-CGB
82	aK	201	PEB	C3B-CAB-CBB-CGB
82	aK	203	PEB	C2C-CAC-CBC-CGC
82	dK	202	PEB	C3B-CAB-CBB-CGB
82	eK	201	PEB	C2C-CAC-CBC-CGC
82	eK	203	PEB	C2C-CAC-CBC-CGC
82	gK	202	PEB	C2C-CAC-CBC-CGC
82	iK	203	PEB	C2C-CAC-CBC-CGC
82	jK	201	PEB	C3B-CAB-CBB-CGB
82	lK	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	lK	203	PEB	C2C-CAC-CBC-CGC
82	lK	203	PEB	C3B-CAB-CBB-CGB
82	nK	202	PEB	C2C-CAC-CBC-CGC
82	pK	202	PEB	C2C-CAC-CBC-CGC
82	qK	202	PEB	C3B-CAB-CBB-CGB
82	rK	202	PEB	C3B-CAB-CBB-CGB
82	tK	201	PEB	C2C-CAC-CBC-CGC
82	uK	202	PEB	C2C-CAC-CBC-CGC
82	wK	302	PEB	C3B-CAB-CBB-CGB
82	wK	303	PEB	C2C-CAC-CBC-CGC
82	xK	302	PEB	C2C-CAC-CBC-CGC
82	dM	202	PEB	C3B-CAB-CBB-CGB
82	dM	203	PEB	C2C-CAC-CBC-CGC
82	gM	202	PEB	C2C-CAC-CBC-CGC
82	jM	201	PEB	C2C-CAC-CBC-CGC
82	lM	203	PEB	C2C-CAC-CBC-CGC
82	mM	202	PEB	C2C-CAC-CBC-CGC
82	iO	203	PEB	C3B-CAB-CBB-CGB
82	eO	202	PEB	C2C-CAC-CBC-CGC
82	bP	501	PEB	C2C-CAC-CBC-CGC
83	AE	302	PUB	C2C-CAC-CBC-CGC
83	AE	302	PUB	C3B-CAB-CBB-CGB
83	AG	302	PUB	C2C-CAC-CBC-CGC
83	AG	302	PUB	C3B-CAB-CBB-CGB
83	AJ	304	PUB	C2C-CAC-CBC-CGC
83	AM	304	PUB	C2C-CAC-CBC-CGC
83	M5	302	PUB	C2C-CAC-CBC-CGC
83	Z5	302	PUB	C2C-CAC-CBC-CGC
83	wF	304	PUB	C3B-CAB-CBB-CGB
83	yF	303	PUB	C3B-CAB-CBB-CGB
83	wK	304	PUB	C3B-CAB-CBB-CGB
83	yK	303	PUB	C3B-CAB-CBB-CGB
83	Z9	305	PUB	C2C-CAC-CBC-CGC
84	LH	1002	CYC	C2A-CAA-CBA-CGA
84	L1	1001	CYC	C2A-CAA-CBA-CGA
84	L3	1001	CYC	NA-C4A-CHB-C1B
84	j3	1001	CYC	NA-C4A-CHB-C1B
84	o3	1001	CYC	NA-C4A-CHB-C1B
84	u3	1001	CYC	NA-C4A-CHB-C1B
92	b6	619	LMG	O6-C5-C6-O5
92	jL	101	LMG	O6-C5-C6-O5
95	C6	521	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
87	AN	805	CLA	C4-C3-C5-C6
87	BN	818	CLA	C4-C3-C5-C6
87	A2	805	CLA	C4-C3-C5-C6
87	B2	817	CLA	C4-C3-C5-C6
87	C6	515	CLA	C4-C3-C5-C6
87	b6	604	CLA	C4-C3-C5-C6
87	b6	617	CLA	C4-C3-C5-C6
87	c6	610	CLA	C4-C3-C5-C6
87	bL	606	CLA	C4-C3-C5-C6
94	d6	408	PL9	C20-C19-C21-C22
92	CL	519	LMG	C4-C5-C6-O5
87	BL	605	CLA	C2-C3-C5-C6
87	AN	805	CLA	C2-C3-C5-C6
87	BN	818	CLA	C2-C3-C5-C6
87	BN	825	CLA	C2-C3-C5-C6
87	A2	805	CLA	C2-C3-C5-C6
87	B2	817	CLA	C2-C3-C5-C6
87	B2	824	CLA	C2-C3-C5-C6
87	B6	612	CLA	C2-C3-C5-C6
87	C6	515	CLA	C2-C3-C5-C6
87	b6	604	CLA	C2-C3-C5-C6
87	b6	617	CLA	C2-C3-C5-C6
87	c6	610	CLA	C2-C3-C5-C6
87	bL	606	CLA	C2-C3-C5-C6
94	AL	413	PL9	C38-C39-C41-C42
94	d6	408	PL9	C18-C19-C21-C22
82	KA	201	PEB	C3C-C2C-CAC-CBC
82	K7	201	PEB	C3C-C2C-CAC-CBC
87	AN	821	CLA	CBD-CGD-O2D-CED
87	A2	821	CLA	CBD-CGD-O2D-CED
87	C6	512	CLA	CBD-CGD-O2D-CED
95	lL	101	DGD	O6D-C5D-C6D-O5D
87	BN	801	CLA	C2A-CAA-CBA-CGA
87	BN	817	CLA	C2A-CAA-CBA-CGA
87	22	602	CLA	C2A-CAA-CBA-CGA
87	32	302	CLA	C2A-CAA-CBA-CGA
87	42	608	CLA	C2A-CAA-CBA-CGA
87	B2	816	CLA	C2A-CAA-CBA-CGA
87	B2	825	CLA	C2A-CAA-CBA-CGA
87	a6	607	CLA	C2A-CAA-CBA-CGA
87	aL	605	CLA	C2A-CAA-CBA-CGA
87	cL	507	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	2N	303	CLA	C2A-CAA-CBA-CGA
87	3N	303	CLA	C2A-CAA-CBA-CGA
87	4N	608	CLA	C2A-CAA-CBA-CGA
82	VH	201	PEB	C2B-C1B-CHA-C4A
82	BI	202	PEB	C2B-C1B-CHA-C4A
82	V1	201	PEB	C2B-C1B-CHA-C4A
82	c1	202	PEB	C2B-C1B-CHA-C4A
82	gF	201	PEB	C2B-C1B-CHA-C4A
82	jF	201	PEB	C2B-C1B-CHA-C4A
82	cH	202	PEB	C2B-C1B-CHA-C4A
82	gK	201	PEB	C2B-C1B-CHA-C4A
82	jK	201	PEB	C2B-C1B-CHA-C4A
87	AN	809	CLA	O1D-CGD-O2D-CED
87	BN	811	CLA	O1D-CGD-O2D-CED
87	32	302	CLA	O1D-CGD-O2D-CED
87	A2	809	CLA	O1D-CGD-O2D-CED
87	B2	810	CLA	O1D-CGD-O2D-CED
87	3N	303	CLA	O1D-CGD-O2D-CED
95	lL	101	DGD	C4D-C5D-C6D-O5D
84	E4	1001	CYC	C2B-C3B-CAB-CBB
92	JL	103	LMG	O6-C5-C6-O5
92	J6	102	LMG	O6-C5-C6-O5
92	j6	101	LMG	O6-C5-C6-O5
95	L6	102	DGD	O6E-C5E-C6E-O5E
95	hL	101	DGD	O6E-C5E-C6E-O5E
87	AN	806	CLA	O1A-CGA-O2A-C1
87	AN	810	CLA	O1A-CGA-O2A-C1
87	LN	204	CLA	O1A-CGA-O2A-C1
87	A2	806	CLA	O1A-CGA-O2A-C1
87	A2	810	CLA	O1A-CGA-O2A-C1
87	L2	204	CLA	O1A-CGA-O2A-C1
87	c6	614	CLA	O1A-CGA-O2A-C1
87	dL	404	CLA	O1A-CGA-O2A-C1
88	I6	101	LHG	O10-C23-O8-C6
95	BL	613	DGD	O1A-C1A-O1G-C1G
92	bL	610	LMG	O6-C1-O1-C7
95	b6	622	DGD	O6D-C1D-O3G-C3G
87	d6	401	CLA	O1D-CGD-O2D-CED
94	AL	413	PL9	C39-C41-C42-C43
94	DL	401	PL9	C29-C31-C32-C33
94	DL	401	PL9	C34-C36-C37-C38
94	A6	410	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
94	A6	410	PL9	C14-C16-C17-C18
94	D6	408	PL9	C19-C21-C22-C23
94	d6	408	PL9	C19-C21-C22-C23
84	EO	1001	CYC	C2B-C3B-CAB-CBB
87	82	306	CLA	C4C-C3C-CAC-CBC
87	a6	608	CLA	C2C-C3C-CAC-CBC
87	8N	301	CLA	C4C-C3C-CAC-CBC
87	RN	203	CLA	O1A-CGA-O2A-C1
87	R2	203	CLA	O1A-CGA-O2A-C1
87	CL	513	CLA	CBA-CGA-O2A-C1
87	AN	802	CLA	CBA-CGA-O2A-C1
87	AN	841	CLA	CBA-CGA-O2A-C1
87	A2	801	CLA	CBA-CGA-O2A-C1
87	A2	841	CLA	CBA-CGA-O2A-C1
87	nL	101	CLA	CBA-CGA-O2A-C1
95	a6	602	DGD	C2A-C1A-O1G-C1G
92	m6	101	LMG	C14-C15-C16-C17
92	yL	101	LMG	C31-C32-C33-C34
87	72	602	CLA	CBD-CGD-O2D-CED
87	bL	614	CLA	CBD-CGD-O2D-CED
87	7N	602	CLA	CBD-CGD-O2D-CED
87	CL	518	CLA	CBA-CGA-O2A-C1
82	NA	203	PEB	NC-C1C-CHB-C4B
82	GB	203	PEB	NC-C1C-CHB-C4B
82	LD	203	PEB	NC-C1C-CHB-C4B
82	WD	202	PEB	NC-C1C-CHB-C4B
82	JF	202	PEB	NC-C1C-CHB-C4B
82	PF	202	PEB	NC-C1C-CHB-C4B
82	VF	202	PEB	NC-C1C-CHB-C4B
82	DJ	202	PEB	NC-C1C-CHB-C4B
82	NJ	202	PEB	NC-C1C-CHB-C4B
82	JK	202	PEB	NC-C1C-CHB-C4B
82	PK	202	PEB	NC-C1C-CHB-C4B
82	VK	202	PEB	NC-C1C-CHB-C4B
82	FM	202	PEB	NC-C1C-CHB-C4B
82	NM	202	PEB	NC-C1C-CHB-C4B
82	RM	202	PEB	NC-C1C-CHB-C4B
82	XM	202	PEB	NC-C1C-CHB-C4B
82	LQ	203	PEB	NC-C1C-CHB-C4B
82	WQ	202	PEB	NC-C1C-CHB-C4B
82	e1	202	PEB	NC-C1C-CHB-C4B
82	B5	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	F5	203	PEB	NC-C1C-CHB-C4B
82	Q5	202	PEB	NC-C1C-CHB-C4B
82	N7	203	PEB	NC-C1C-CHB-C4B
82	aE	202	PEB	NC-C1C-CHB-C4B
82	gF	202	PEB	NC-C1C-CHB-C4B
82	qF	202	PEB	NC-C1C-CHB-C4B
82	uF	201	PEB	NC-C1C-CHB-C4B
82	aG	202	PEB	NC-C1C-CHB-C4B
82	eH	202	PEB	NC-C1C-CHB-C4B
82	gJ	201	PEB	NC-C1C-CHB-C4B
82	gJ	202	PEB	NC-C1C-CHB-C4B
82	qK	202	PEB	NC-C1C-CHB-C4B
82	tK	203	PEB	NC-C1C-CHB-C4B
82	eM	202	PEB	NC-C1C-CHB-C4B
82	iM	202	PEB	NC-C1C-CHB-C4B
82	mM	202	PEB	NC-C1C-CHB-C4B
84	BE	1002	CYC	ND-C1D-CHD-C4C
84	DE	1001	CYC	ND-C1D-CHD-C4C
84	EE	1001	CYC	ND-C1D-CHD-C4C
84	FE	1001	CYC	ND-C1D-CHD-C4C
84	GE	1001	CYC	ND-C1D-CHD-C4C
84	IE	1001	CYC	ND-C1D-CHD-C4C
84	LE	1001	CYC	ND-C1D-CHD-C4C
84	ME	1001	CYC	ND-C1D-CHD-C4C
84	NE	201	CYC	ND-C1D-CHD-C4C
84	BG	1002	CYC	ND-C1D-CHD-C4C
84	CG	1001	CYC	ND-C1D-CHD-C4C
84	DG	1001	CYC	ND-C1D-CHD-C4C
84	EG	1001	CYC	ND-C1D-CHD-C4C
84	GG	1001	CYC	ND-C1D-CHD-C4C
84	IG	1001	CYC	ND-C1D-CHD-C4C
84	KG	202	CYC	ND-C1D-CHD-C4C
84	LG	1001	CYC	ND-C1D-CHD-C4C
84	MG	1001	CYC	ND-C1D-CHD-C4C
84	DH	1001	CYC	ND-C1D-CHD-C4C
84	DH	1003	CYC	ND-C1D-CHD-C4C
84	EH	1001	CYC	ND-C1D-CHD-C4C
84	HH	1001	CYC	ND-C1D-CHD-C4C
84	JH	1001	CYC	ND-C1D-CHD-C4C
84	JH	1003	CYC	ND-C1D-CHD-C4C
84	LH	1002	CYC	ND-C1D-CHD-C4C
84	NH	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	CO	1001	CYC	ND-C1D-CHD-C4C
84	GO	1001	CYC	ND-C1D-CHD-C4C
84	IO	1001	CYC	ND-C1D-CHD-C4C
84	JO	1001	CYC	ND-C1D-CHD-C4C
84	KO	1001	CYC	ND-C1D-CHD-C4C
84	MO	1001	CYC	ND-C1D-CHD-C4C
84	NO	1001	CYC	ND-C1D-CHD-C4C
84	L1	1001	CYC	ND-C1D-CHD-C4C
84	M1	201	CYC	ND-C1D-CHD-C4C
84	N1	1001	CYC	ND-C1D-CHD-C4C
84	D1	1001	CYC	ND-C1D-CHD-C4C
84	D1	1003	CYC	ND-C1D-CHD-C4C
84	E1	1001	CYC	ND-C1D-CHD-C4C
84	H1	1001	CYC	ND-C1D-CHD-C4C
84	J1	1001	CYC	ND-C1D-CHD-C4C
84	r3	1001	CYC	ND-C1D-CHD-C4C
84	G4	1001	CYC	ND-C1D-CHD-C4C
84	I4	1001	CYC	ND-C1D-CHD-C4C
84	J4	1001	CYC	ND-C1D-CHD-C4C
84	K4	1001	CYC	ND-C1D-CHD-C4C
84	M4	1001	CYC	ND-C1D-CHD-C4C
84	N4	1001	CYC	ND-C1D-CHD-C4C
84	C4	1001	CYC	ND-C1D-CHD-C4C
82	B5	201	PEB	C4B-C3B-CAB-CBB
84	NO	1001	CYC	C1A-C2A-CAA-CBA
84	N4	1001	CYC	C1A-C2A-CAA-CBA
87	BL	608	CLA	O1D-CGD-O2D-CED
87	AN	832	CLA	O1D-CGD-O2D-CED
87	MN	101	CLA	O1D-CGD-O2D-CED
87	A2	832	CLA	O1D-CGD-O2D-CED
87	M2	101	CLA	O1D-CGD-O2D-CED
87	c6	606	CLA	O1D-CGD-O2D-CED
87	bL	617	CLA	O1D-CGD-O2D-CED
87	CL	513	CLA	O1A-CGA-O2A-C1
92	dL	407	LMG	C11-C10-O7-C8
84	DE	1001	CYC	C2D-C1D-CHD-C4C
84	LE	1001	CYC	C2D-C1D-CHD-C4C
84	NE	201	CYC	C2D-C1D-CHD-C4C
84	DG	1001	CYC	C2D-C1D-CHD-C4C
84	KG	202	CYC	C2D-C1D-CHD-C4C
84	LG	1001	CYC	C2D-C1D-CHD-C4C
84	DH	1001	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
84	DH	1003	CYC	C2D-C1D-CHD-C4C
84	HH	1001	CYC	C2D-C1D-CHD-C4C
84	JH	1001	CYC	C2D-C1D-CHD-C4C
84	JH	1003	CYC	C2D-C1D-CHD-C4C
84	LH	1002	CYC	C2D-C1D-CHD-C4C
84	NH	1001	CYC	C2D-C1D-CHD-C4C
84	CO	1001	CYC	C2D-C1D-CHD-C4C
84	EO	1001	CYC	C2D-C1D-CHD-C4C
84	JO	1001	CYC	C2D-C1D-CHD-C4C
84	L1	1001	CYC	C2D-C1D-CHD-C4C
84	M1	201	CYC	C2D-C1D-CHD-C4C
84	N1	1001	CYC	C2D-C1D-CHD-C4C
84	D1	1001	CYC	C2D-C1D-CHD-C4C
84	D1	1003	CYC	C2D-C1D-CHD-C4C
84	F1	1001	CYC	C2D-C1D-CHD-C4C
84	H1	1001	CYC	C2D-C1D-CHD-C4C
84	J1	1001	CYC	C2D-C1D-CHD-C4C
84	r3	1001	CYC	C2D-C1D-CHD-C4C
84	J4	1001	CYC	C2D-C1D-CHD-C4C
84	C4	1001	CYC	C2D-C1D-CHD-C4C
84	E4	1001	CYC	C2D-C1D-CHD-C4C
92	JL	103	LMG	C4-C5-C6-O5
95	C6	502	DGD	C5B-C6B-C7B-C8B
95	c6	601	DGD	C5B-C6B-C7B-C8B
87	CL	514	CLA	O1D-CGD-O2D-CED
87	AN	805	CLA	O1D-CGD-O2D-CED
87	AN	852	CLA	O1D-CGD-O2D-CED
87	BN	802	CLA	O1D-CGD-O2D-CED
87	A2	805	CLA	O1D-CGD-O2D-CED
87	A2	852	CLA	O1D-CGD-O2D-CED
87	B2	801	CLA	O1D-CGD-O2D-CED
87	b6	605	CLA	O1D-CGD-O2D-CED
87	b6	612	CLA	O1D-CGD-O2D-CED
87	DL	404	CLA	CBD-CGD-O2D-CED
84	G4	1001	CYC	C2B-C3B-CAB-CBB
87	62	307	CLA	O1D-CGD-O2D-CED
88	CL	522	LHG	C1-C2-C3-O3
88	DL	407	LHG	C1-C2-C3-O3
88	d6	407	LHG	C1-C2-C3-O3
88	mL	102	LHG	C1-C2-C3-O3
92	DL	402	LMG	O9-C10-O7-C8
92	m6	103	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
92	A6	408	LMG	C4-C5-C6-O5
95	hL	101	DGD	C4E-C5E-C6E-O5E
87	72	602	CLA	O1A-CGA-O2A-C1
87	7N	602	CLA	O1A-CGA-O2A-C1
92	C6	501	LMG	C29-C30-C31-C32
95	h6	101	DGD	C9A-CAA-CBA-CCA
87	CL	509	CLA	C3-C5-C6-C7
87	d6	401	CLA	C3-C5-C6-C7
87	bL	619	CLA	C3-C5-C6-C7
87	cL	506	CLA	O1D-CGD-O2D-CED
87	6N	606	CLA	O1D-CGD-O2D-CED
87	CL	503	CLA	CBA-CGA-O2A-C1
87	DL	403	CLA	CBA-CGA-O2A-C1
87	AN	815	CLA	CBA-CGA-O2A-C1
87	AN	820	CLA	CBA-CGA-O2A-C1
87	AN	828	CLA	CBA-CGA-O2A-C1
87	BN	807	CLA	CBA-CGA-O2A-C1
87	FN	205	CLA	CBA-CGA-O2A-C1
87	22	602	CLA	CBA-CGA-O2A-C1
87	62	303	CLA	CBA-CGA-O2A-C1
87	72	602	CLA	CBA-CGA-O2A-C1
87	A2	815	CLA	CBA-CGA-O2A-C1
87	A2	820	CLA	CBA-CGA-O2A-C1
87	A2	828	CLA	CBA-CGA-O2A-C1
87	B2	806	CLA	CBA-CGA-O2A-C1
87	F2	205	CLA	CBA-CGA-O2A-C1
87	C6	513	CLA	CBA-CGA-O2A-C1
87	C6	514	CLA	CBA-CGA-O2A-C1
87	D6	402	CLA	CBA-CGA-O2A-C1
87	b6	610	CLA	CBA-CGA-O2A-C1
87	c6	613	CLA	CBA-CGA-O2A-C1
87	d6	401	CLA	CBA-CGA-O2A-C1
87	d6	403	CLA	CBA-CGA-O2A-C1
87	dL	401	CLA	CBA-CGA-O2A-C1
87	2N	303	CLA	CBA-CGA-O2A-C1
87	6N	602	CLA	CBA-CGA-O2A-C1
87	7N	602	CLA	CBA-CGA-O2A-C1
91	aL	610	PHO	CBA-CGA-O2A-C1
95	AL	416	DGD	C2A-C1A-O1G-C1G
95	a6	603	DGD	C2A-C1A-O1G-C1G
87	bL	606	CLA	C8-C10-C11-C12
87	AN	851	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	A2	851	CLA	CBD-CGD-O2D-CED
87	C6	510	CLA	CBD-CGD-O2D-CED
87	c6	612	CLA	CBD-CGD-O2D-CED
92	jL	101	LMG	C4-C5-C6-O5
84	IE	1001	CYC	C2B-C3B-CAB-CBB
84	GO	1001	CYC	C2B-C3B-CAB-CBB
95	C6	523	DGD	C4D-C5D-C6D-O5D
95	a6	603	DGD	C4D-C5D-C6D-O5D
92	dL	407	LMG	C8-C9-O8-C28
103	82	310	ZEX	C9-C10-C11-C12
103	8N	310	ZEX	C9-C10-C11-C12
88	L6	101	LHG	C9-C10-C11-C12
88	l6	101	LHG	C9-C10-C11-C12
92	b6	623	LMG	C31-C32-C33-C34
87	52	602	CLA	C13-C15-C16-C17
87	c6	605	CLA	C10-C11-C12-C13
87	bL	608	CLA	C5-C6-C7-C8
87	5N	602	CLA	C13-C15-C16-C17
84	N4	1001	CYC	C3A-C2A-CAA-CBA
87	KN	103	CLA	O1D-CGD-O2D-CED
88	AL	407	LHG	O6-C4-C5-O7
88	aL	607	LHG	O6-C4-C5-O7
84	IG	1001	CYC	C2B-C3B-CAB-CBB
84	KG	202	CYC	C2B-C3B-CAB-CBB
92	J6	102	LMG	C30-C31-C32-C33
92	j6	101	LMG	C30-C31-C32-C33
87	AL	403	CLA	C15-C16-C17-C18
87	CL	503	CLA	C15-C16-C17-C18
87	CL	508	CLA	C13-C15-C16-C17
87	CL	513	CLA	C8-C10-C11-C12
87	BN	823	CLA	C13-C15-C16-C17
87	BN	824	CLA	C10-C11-C12-C13
87	72	602	CLA	C5-C6-C7-C8
87	B2	822	CLA	C13-C15-C16-C17
87	B2	823	CLA	C10-C11-C12-C13
87	b6	604	CLA	C10-C11-C12-C13
87	b6	611	CLA	C15-C16-C17-C18
87	7N	602	CLA	C5-C6-C7-C8
88	CL	521	LHG	O2-C2-C3-O3
88	CL	522	LHG	O2-C2-C3-O3
88	d6	402	LHG	O2-C2-C3-O3
95	c6	620	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
88	bL	612	LHG	C23-C24-C25-C26
92	BL	611	LMG	C28-C29-C30-C31
92	m6	101	LMG	C28-C29-C30-C31
92	bL	610	LMG	C10-C11-C12-C13
95	c6	618	DGD	C1A-C2A-C3A-C4A
92	b6	623	LMG	C2-C1-O1-C7
92	bL	609	LMG	C2-C1-O1-C7
92	mL	101	LMG	C2-C1-O1-C7
95	BL	614	DGD	C2E-C1E-O5D-C6D
95	C6	504	DGD	C2D-C1D-O3G-C3G
95	lL	101	DGD	C2E-C1E-O5D-C6D
88	AN	843	LHG	O7-C5-C6-O8
88	A2	843	LHG	O7-C5-C6-O8
92	B6	622	LMG	O1-C7-C8-O7
84	NE	201	CYC	C2B-C3B-CAB-CBB
87	AN	820	CLA	O1A-CGA-O2A-C1
87	AN	828	CLA	O1A-CGA-O2A-C1
87	A2	820	CLA	O1A-CGA-O2A-C1
87	A2	828	CLA	O1A-CGA-O2A-C1
87	b6	610	CLA	O1A-CGA-O2A-C1
87	dL	401	CLA	O1A-CGA-O2A-C1
87	AN	827	CLA	C4-C3-C5-C6
87	A2	827	CLA	C4-C3-C5-C6
87	B6	608	CLA	C4-C3-C5-C6
92	aL	611	LMG	C4-C5-C6-O5
87	AN	819	CLA	C2-C3-C5-C6
87	A2	819	CLA	C2-C3-C5-C6
87	b6	609	CLA	C2-C3-C5-C6
87	c6	606	CLA	C2-C3-C5-C6
94	DL	401	PL9	C18-C19-C21-C22
82	BJ	301	PEB	C3C-C2C-CAC-CBC
82	aE	201	PEB	C3C-C2C-CAC-CBC
82	aG	201	PEB	C3C-C2C-CAC-CBC
87	BL	608	CLA	C11-C10-C8-C9
87	CL	503	CLA	C11-C12-C13-C14
87	CL	508	CLA	C14-C13-C15-C16
87	CL	509	CLA	C14-C13-C15-C16
87	CL	513	CLA	C11-C10-C8-C9
87	AN	805	CLA	C6-C7-C8-C9
87	BN	806	CLA	C11-C10-C8-C9
87	BN	810	CLA	C14-C13-C15-C16
87	BN	825	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
87	A2	801	CLA	C6-C7-C8-C9
87	A2	805	CLA	C6-C7-C8-C9
87	B2	805	CLA	C11-C10-C8-C9
87	B2	809	CLA	C14-C13-C15-C16
87	B2	824	CLA	C6-C7-C8-C9
87	B6	603	CLA	C11-C10-C8-C9
87	B6	604	CLA	C6-C7-C8-C9
87	B6	605	CLA	C11-C10-C8-C9
87	B6	606	CLA	C6-C7-C8-C9
87	B6	606	CLA	C14-C13-C15-C16
87	B6	607	CLA	C11-C10-C8-C9
87	B6	607	CLA	C14-C13-C15-C16
87	B6	609	CLA	C11-C12-C13-C14
87	B6	613	CLA	C6-C7-C8-C9
87	B6	616	CLA	C11-C10-C8-C9
87	C6	509	CLA	C11-C12-C13-C14
87	C6	510	CLA	C14-C13-C15-C16
87	C6	512	CLA	C11-C12-C13-C14
87	C6	513	CLA	C11-C12-C13-C14
87	C6	515	CLA	C11-C10-C8-C9
87	C6	515	CLA	C14-C13-C15-C16
87	C6	516	CLA	C14-C13-C15-C16
87	C6	518	CLA	C11-C10-C8-C9
87	C6	520	CLA	C6-C7-C8-C9
87	D6	405	CLA	C14-C13-C15-C16
87	H6	103	CLA	C6-C7-C8-C9
87	H6	103	CLA	C14-C13-C15-C16
87	a6	607	CLA	C14-C13-C15-C16
87	b6	604	CLA	C6-C7-C8-C9
87	b6	609	CLA	C14-C13-C15-C16
87	b6	611	CLA	C11-C12-C13-C14
87	b6	613	CLA	C11-C12-C13-C14
87	b6	616	CLA	C14-C13-C15-C16
87	b6	617	CLA	C11-C10-C8-C9
87	c6	605	CLA	C11-C10-C8-C9
87	c6	608	CLA	C11-C10-C8-C9
87	c6	610	CLA	C11-C10-C8-C9
87	c6	610	CLA	C11-C12-C13-C14
87	c6	612	CLA	C6-C7-C8-C9
87	c6	612	CLA	C11-C12-C13-C14
87	c6	614	CLA	C6-C7-C8-C9
87	c6	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
87	d6	403	CLA	C6-C7-C8-C9
87	d6	403	CLA	C11-C12-C13-C14
87	d6	406	CLA	C11-C10-C8-C9
87	bL	616	CLA	C11-C12-C13-C14
87	cL	505	CLA	C11-C12-C13-C14
87	cL	510	CLA	C14-C13-C15-C16
87	cL	513	CLA	C14-C13-C15-C16
87	nL	101	CLA	C11-C10-C8-C9
87	K2	104	CLA	O1D-CGD-O2D-CED
87	B6	610	CLA	O1D-CGD-O2D-CED
87	8N	303	CLA	O1D-CGD-O2D-CED
87	52	607	CLA	CBD-CGD-O2D-CED
87	5N	607	CLA	CBD-CGD-O2D-CED
87	AL	403	CLA	C13-C15-C16-C17
87	BL	608	CLA	C15-C16-C17-C18
87	32	304	CLA	C10-C11-C12-C13
87	3N	305	CLA	C10-C11-C12-C13
87	AN	823	CLA	C2A-CAA-CBA-CGA
87	52	607	CLA	C2A-CAA-CBA-CGA
87	62	302	CLA	C2A-CAA-CBA-CGA
87	A2	823	CLA	C2A-CAA-CBA-CGA
87	C6	519	CLA	C2A-CAA-CBA-CGA
87	b6	608	CLA	C2A-CAA-CBA-CGA
87	5N	607	CLA	C2A-CAA-CBA-CGA
87	6N	601	CLA	C2A-CAA-CBA-CGA
85	BL	616	BCR	C36-C18-C19-C20
85	BL	618	BCR	C37-C22-C23-C24
85	FL	101	BCR	C7-C8-C9-C34
85	KL	100	BCR	C36-C18-C19-C20
85	AN	845	BCR	C7-C8-C9-C34
85	AN	847	BCR	C37-C22-C23-C24
85	AN	848	BCR	C7-C8-C9-C34
85	AN	848	BCR	C37-C22-C23-C24
85	BN	803	BCR	C7-C8-C9-C34
85	BN	839	BCR	C7-C8-C9-C34
85	BN	841	BCR	C11-C12-C13-C35
85	BN	842	BCR	C37-C22-C23-C24
85	BN	843	BCR	C7-C8-C9-C34
85	KN	104	BCR	C7-C8-C9-C34
85	KN	104	BCR	C11-C12-C13-C35
85	LN	205	BCR	C11-C12-C13-C35
85	A2	845	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
85	A2	847	BCR	C37-C22-C23-C24
85	A2	848	BCR	C7-C8-C9-C34
85	A2	848	BCR	C37-C22-C23-C24
85	B2	802	BCR	C7-C8-C9-C34
85	B2	839	BCR	C7-C8-C9-C34
85	B2	841	BCR	C11-C12-C13-C35
85	B2	842	BCR	C37-C22-C23-C24
85	B2	843	BCR	C7-C8-C9-C34
85	F2	204	BCR	C37-C22-C23-C24
85	K2	105	BCR	C7-C8-C9-C34
85	K2	105	BCR	C11-C12-C13-C35
85	L2	205	BCR	C11-C12-C13-C35
85	C6	508	BCR	C7-C8-C9-C34
85	a6	605	BCR	C7-C8-C9-C34
85	c6	602	BCR	C36-C18-C19-C20
85	c6	617	BCR	C11-C12-C13-C35
85	bL	601	BCR	C37-C22-C23-C24
85	cL	518	BCR	C37-C22-C23-C24
85	fL	101	BCR	C7-C8-C9-C34
85	kL	100	BCR	C36-C18-C19-C20
85	FL	101	BCR	C7-C8-C9-C10
85	KL	100	BCR	C17-C18-C19-C20
85	KL	100	BCR	C21-C22-C23-C24
85	AN	845	BCR	C7-C8-C9-C10
85	AN	847	BCR	C21-C22-C23-C24
85	AN	848	BCR	C7-C8-C9-C10
85	AN	848	BCR	C21-C22-C23-C24
85	BN	841	BCR	C11-C12-C13-C14
85	BN	843	BCR	C7-C8-C9-C10
85	FN	204	BCR	C21-C22-C23-C24
85	IN	101	BCR	C7-C8-C9-C10
85	JN	102	BCR	C21-C22-C23-C24
85	KN	104	BCR	C7-C8-C9-C10
85	KN	104	BCR	C11-C12-C13-C14
85	LN	205	BCR	C11-C12-C13-C14
85	A2	845	BCR	C7-C8-C9-C10
85	A2	847	BCR	C21-C22-C23-C24
85	A2	848	BCR	C7-C8-C9-C10
85	A2	848	BCR	C21-C22-C23-C24
85	B2	841	BCR	C11-C12-C13-C14
85	B2	843	BCR	C7-C8-C9-C10
85	F2	204	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
85	I2	101	BCR	C7-C8-C9-C10
85	J2	102	BCR	C21-C22-C23-C24
85	K2	105	BCR	C7-C8-C9-C10
85	K2	105	BCR	C11-C12-C13-C14
85	L2	205	BCR	C11-C12-C13-C14
85	c6	617	BCR	C11-C12-C13-C14
85	d6	405	BCR	C7-C8-C9-C10
85	cL	518	BCR	C21-C22-C23-C24
85	fL	101	BCR	C7-C8-C9-C10
85	kL	100	BCR	C17-C18-C19-C20
85	kL	100	BCR	C21-C22-C23-C24
87	42	603	CLA	O1D-CGD-O2D-CED
87	82	302	CLA	O1D-CGD-O2D-CED
88	CL	522	LHG	O9-C7-O7-C5
92	dL	407	LMG	O9-C10-O7-C8
92	b6	620	LMG	C11-C12-C13-C14
92	DL	402	LMG	C28-C29-C30-C31
92	d6	409	LMG	C28-C29-C30-C31
92	m6	103	LMG	C28-C29-C30-C31
95	B6	620	DGD	C1A-C2A-C3A-C4A
95	C6	503	DGD	C1A-C2A-C3A-C4A
87	AN	815	CLA	O1A-CGA-O2A-C1
87	BN	807	CLA	O1A-CGA-O2A-C1
87	62	303	CLA	O1A-CGA-O2A-C1
87	A2	815	CLA	O1A-CGA-O2A-C1
87	B2	806	CLA	O1A-CGA-O2A-C1
87	c6	613	CLA	O1A-CGA-O2A-C1
87	d6	401	CLA	O1A-CGA-O2A-C1
87	6N	602	CLA	O1A-CGA-O2A-C1
91	aL	610	PHO	O1A-CGA-O2A-C1
95	AL	416	DGD	O1A-C1A-O1G-C1G
95	a6	603	DGD	O1A-C1A-O1G-C1G
87	AL	403	CLA	C8-C10-C11-C12
87	BL	602	CLA	C13-C15-C16-C17
87	BL	619	CLA	C15-C16-C17-C18
87	BL	622	CLA	C5-C6-C7-C8
87	AN	805	CLA	C15-C16-C17-C18
87	AN	811	CLA	C5-C6-C7-C8
87	AN	829	CLA	C15-C16-C17-C18
87	A2	805	CLA	C15-C16-C17-C18
87	A2	811	CLA	C5-C6-C7-C8
87	A2	829	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
87	C6	516	CLA	C10-C11-C12-C13
87	bL	606	CLA	C10-C11-C12-C13
87	cL	515	CLA	C8-C10-C11-C12
87	AL	405	CLA	O1D-CGD-O2D-CED
87	AN	822	CLA	O1D-CGD-O2D-CED
87	LN	203	CLA	O1D-CGD-O2D-CED
87	22	602	CLA	O1D-CGD-O2D-CED
87	A2	822	CLA	O1D-CGD-O2D-CED
87	L2	203	CLA	O1D-CGD-O2D-CED
87	2N	303	CLA	O1D-CGD-O2D-CED
87	4N	603	CLA	O1D-CGD-O2D-CED
87	bL	604	CLA	CBA-CGA-O2A-C1
95	D6	410	DGD	O6E-C5E-C6E-O5E
84	N4	1001	CYC	C2B-C3B-CAB-CBB
87	82	306	CLA	C2C-C3C-CAC-CBC
87	8N	301	CLA	C2C-C3C-CAC-CBC
87	BN	827	CLA	O1D-CGD-O2D-CED
87	B2	827	CLA	O1D-CGD-O2D-CED
87	cL	507	CLA	C3-C5-C6-C7
91	D6	404	PHO	C3-C5-C6-C7
87	CL	504	CLA	CBA-CGA-O2A-C1
87	BN	826	CLA	CBA-CGA-O2A-C1
87	BN	832	CLA	CBA-CGA-O2A-C1
87	IN	103	CLA	CBA-CGA-O2A-C1
87	B2	826	CLA	CBA-CGA-O2A-C1
87	B2	832	CLA	CBA-CGA-O2A-C1
87	I2	103	CLA	CBA-CGA-O2A-C1
87	B6	603	CLA	CBA-CGA-O2A-C1
87	C6	509	CLA	CBA-CGA-O2A-C1
87	c6	604	CLA	CBA-CGA-O2A-C1
87	bL	622	CLA	CBA-CGA-O2A-C1
87	BL	604	CLA	C8-C10-C11-C12
87	CL	503	CLA	C13-C15-C16-C17
87	AN	829	CLA	C10-C11-C12-C13
87	AN	840	CLA	C5-C6-C7-C8
87	BN	801	CLA	C5-C6-C7-C8
87	BN	801	CLA	C15-C16-C17-C18
87	BN	807	CLA	C8-C10-C11-C12
87	BN	811	CLA	C15-C16-C17-C18
87	BN	823	CLA	C15-C16-C17-C18
87	BN	834	CLA	C5-C6-C7-C8
87	FN	205	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
87	IN	103	CLA	C8-C10-C11-C12
87	52	602	CLA	C5-C6-C7-C8
87	A2	829	CLA	C10-C11-C12-C13
87	A2	840	CLA	C5-C6-C7-C8
87	B2	806	CLA	C8-C10-C11-C12
87	B2	810	CLA	C15-C16-C17-C18
87	B2	822	CLA	C15-C16-C17-C18
87	B2	825	CLA	C5-C6-C7-C8
87	B2	825	CLA	C15-C16-C17-C18
87	B2	834	CLA	C5-C6-C7-C8
87	F2	205	CLA	C13-C15-C16-C17
87	I2	103	CLA	C8-C10-C11-C12
87	K6	101	CLA	C5-C6-C7-C8
87	c6	608	CLA	C5-C6-C7-C8
87	c6	610	CLA	C5-C6-C7-C8
87	d6	401	CLA	C15-C16-C17-C18
87	d6	403	CLA	C15-C16-C17-C18
87	bL	619	CLA	C8-C10-C11-C12
87	5N	602	CLA	C5-C6-C7-C8
84	NO	1001	CYC	C2B-C3B-CAB-CBB
88	AL	407	LHG	C7-C8-C9-C10
88	BL	615	LHG	C23-C24-C25-C26
88	dL	405	LHG	C7-C8-C9-C10
92	dL	407	LMG	C10-C11-C12-C13
95	BL	613	DGD	C1A-C2A-C3A-C4A
95	a6	603	DGD	C1A-C2A-C3A-C4A
84	DE	1001	CYC	C4B-C3B-CAB-CBB
84	EE	1001	CYC	C4B-C3B-CAB-CBB
84	DG	1001	CYC	C4B-C3B-CAB-CBB
84	EG	1001	CYC	C4B-C3B-CAB-CBB
82	DM	202	PEB	NC-C1C-CHB-C4B
82	D5	203	PEB	NC-C1C-CHB-C4B
82	H5	203	PEB	NC-C1C-CHB-C4B
82	O5	203	PEB	NC-C1C-CHB-C4B
82	Q5	203	PEB	NC-C1C-CHB-C4B
82	oF	201	PEB	NC-C1C-CHB-C4B
82	uF	203	PEB	NC-C1C-CHB-C4B
82	iJ	202	PEB	NC-C1C-CHB-C4B
82	cK	202	PEB	NC-C1C-CHB-C4B
82	gK	202	PEB	NC-C1C-CHB-C4B
82	oK	201	PEB	NC-C1C-CHB-C4B
82	uK	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
87	A6	402	CLA	C2C-C3C-CAC-CBC
87	b6	609	CLA	C2C-C3C-CAC-CBC
87	d6	406	CLA	C4C-C3C-CAC-CBC
92	JL	102	LMG	C34-C35-C36-C37
95	D6	410	DGD	C9B-CAB-CBB-CCB
95	BL	614	DGD	O6D-C5D-C6D-O5D
95	C6	503	DGD	O6D-C5D-C6D-O5D
87	CL	506	CLA	C8-C10-C11-C12
87	AN	802	CLA	C5-C6-C7-C8
87	AN	811	CLA	C15-C16-C17-C18
87	AN	815	CLA	C15-C16-C17-C18
87	AN	826	CLA	C5-C6-C7-C8
87	AN	826	CLA	C10-C11-C12-C13
87	AN	826	CLA	C13-C15-C16-C17
87	AN	828	CLA	C8-C10-C11-C12
87	BN	805	CLA	C10-C11-C12-C13
87	BN	831	CLA	C10-C11-C12-C13
87	FN	205	CLA	C15-C16-C17-C18
87	LN	203	CLA	C5-C6-C7-C8
87	42	602	CLA	C5-C6-C7-C8
87	62	303	CLA	C5-C6-C7-C8
87	82	302	CLA	C8-C10-C11-C12
87	A2	801	CLA	C5-C6-C7-C8
87	A2	811	CLA	C15-C16-C17-C18
87	A2	815	CLA	C15-C16-C17-C18
87	A2	826	CLA	C5-C6-C7-C8
87	A2	826	CLA	C10-C11-C12-C13
87	A2	826	CLA	C13-C15-C16-C17
87	A2	828	CLA	C8-C10-C11-C12
87	B2	804	CLA	C10-C11-C12-C13
87	B2	831	CLA	C10-C11-C12-C13
87	K2	101	CLA	C8-C10-C11-C12
87	L2	203	CLA	C5-C6-C7-C8
87	A6	402	CLA	C8-C10-C11-C12
87	B6	604	CLA	C13-C15-C16-C17
87	B6	615	CLA	C13-C15-C16-C17
87	C6	515	CLA	C5-C6-C7-C8
87	D6	405	CLA	C10-C11-C12-C13
87	b6	608	CLA	C15-C16-C17-C18
87	c6	605	CLA	C13-C15-C16-C17
87	aL	605	CLA	C8-C10-C11-C12
87	bL	621	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
87	nL	101	CLA	C15-C16-C17-C18
87	4N	602	CLA	C5-C6-C7-C8
87	6N	602	CLA	C5-C6-C7-C8
87	8N	303	CLA	C8-C10-C11-C12
91	A6	407	PHO	C10-C11-C12-C13
91	a6	613	PHO	C10-C11-C12-C13
95	c6	601	DGD	C4D-C5D-C6D-O5D
83	BM	302	PUB	C2D-C3D-CAD-CBD
87	DL	403	CLA	O1D-CGD-O2D-CED
87	BN	832	CLA	O1D-CGD-O2D-CED
87	72	608	CLA	O1D-CGD-O2D-CED
87	B2	832	CLA	O1D-CGD-O2D-CED
82	PA	203	PEB	C2C-C1C-CHB-C4B
82	XA	203	PEB	C2C-C1C-CHB-C4B
82	JD	202	PEB	C2C-C1C-CHB-C4B
82	LD	203	PEB	C2C-C1C-CHB-C4B
82	WD	202	PEB	C2C-C1C-CHB-C4B
82	BF	202	PEB	C2C-C1C-CHB-C4B
82	FF	202	PEB	C2C-C1C-CHB-C4B
82	PF	202	PEB	C2C-C1C-CHB-C4B
82	DJ	202	PEB	C2C-C1C-CHB-C4B
82	NJ	202	PEB	C2C-C1C-CHB-C4B
82	BK	202	PEB	C2C-C1C-CHB-C4B
82	FK	202	PEB	C2C-C1C-CHB-C4B
82	PK	202	PEB	C2C-C1C-CHB-C4B
82	FM	202	PEB	C2C-C1C-CHB-C4B
82	NM	202	PEB	C2C-C1C-CHB-C4B
82	XM	202	PEB	C2C-C1C-CHB-C4B
82	JQ	202	PEB	C2C-C1C-CHB-C4B
82	LQ	203	PEB	C2C-C1C-CHB-C4B
82	WQ	202	PEB	C2C-C1C-CHB-C4B
82	e1	202	PEB	C2C-C1C-CHB-C4B
82	B5	203	PEB	C2C-C1C-CHB-C4B
82	H5	203	PEB	C2C-C1C-CHB-C4B
82	Q5	203	PEB	C2C-C1C-CHB-C4B
82	P7	203	PEB	C2C-C1C-CHB-C4B
82	X7	203	PEB	C2C-C1C-CHB-C4B
82	z8	202	PEB	C3B-C4B-CHB-C1C
82	r8	202	PEB	C3B-C4B-CHB-C1C
82	v8	202	PEB	C3B-C4B-CHB-C1C
82	A9	202	PEB	C3B-C4B-CHB-C1C
82	C9	202	PEB	C3B-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
82	E9	202	PEB	C3B-C4B-CHB-C1C
82	G9	202	PEB	C3B-C4B-CHB-C1C
82	I9	202	PEB	C3B-C4B-CHB-C1C
82	K9	202	PEB	C3B-C4B-CHB-C1C
82	N9	202	PEB	C3B-C4B-CHB-C1C
82	P9	202	PEB	C3B-C4B-CHB-C1C
82	R9	202	PEB	C3B-C4B-CHB-C1C
82	T9	202	PEB	C3B-C4B-CHB-C1C
82	V9	202	PEB	C3B-C4B-CHB-C1C
82	X9	202	PEB	C3B-C4B-CHB-C1C
82	zC	202	PEB	C3B-C4B-CHB-C1C
82	rC	202	PEB	C3B-C4B-CHB-C1C
82	vC	202	PEB	C3B-C4B-CHB-C1C
82	aE	202	PEB	C2C-C1C-CHB-C4B
82	cE	202	PEB	C2C-C1C-CHB-C4B
82	dF	202	PEB	C2C-C1C-CHB-C4B
82	eF	201	PEB	C2C-C1C-CHB-C4B
82	oF	201	PEB	C2C-C1C-CHB-C4B
82	qF	202	PEB	C3B-C4B-CHB-C1C
82	aG	202	PEB	C2C-C1C-CHB-C4B
82	cG	202	PEB	C2C-C1C-CHB-C4B
82	eH	202	PEB	C2C-C1C-CHB-C4B
82	gJ	201	PEB	C2C-C1C-CHB-C4B
82	gJ	202	PEB	C2C-C1C-CHB-C4B
82	dK	202	PEB	C2C-C1C-CHB-C4B
82	eK	201	PEB	C2C-C1C-CHB-C4B
82	oK	201	PEB	C2C-C1C-CHB-C4B
82	qK	202	PEB	C3B-C4B-CHB-C1C
82	eM	202	PEB	C2C-C1C-CHB-C4B
82	mM	202	PEB	C2C-C1C-CHB-C4B
100	JN	104	3XQ	O23-C22-C24-O25
88	AL	407	LHG	C23-C24-C25-C26
88	m6	102	LHG	C23-C24-C25-C26
88	aL	607	LHG	C7-C8-C9-C10
88	dL	405	LHG	C23-C24-C25-C26
88	iL	101	LHG	C23-C24-C25-C26
92	CL	519	LMG	C28-C29-C30-C31
92	JL	103	LMG	C10-C11-C12-C13
92	B6	622	LMG	C10-C11-C12-C13
92	D6	409	LMG	C28-C29-C30-C31
92	b6	619	LMG	C10-C11-C12-C13
95	AL	416	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
92	D6	407	LMG	O6-C5-C6-O5
95	CL	520	DGD	C4E-C5E-C6E-O5E
87	D6	403	CLA	CBD-CGD-O2D-CED
87	c6	604	CLA	CBD-CGD-O2D-CED
87	7N	608	CLA	O1D-CGD-O2D-CED
87	CL	510	CLA	C15-C16-C17-C18
87	AN	839	CLA	C15-C16-C17-C18
87	BN	806	CLA	C5-C6-C7-C8
87	A2	839	CLA	C15-C16-C17-C18
87	B2	805	CLA	C5-C6-C7-C8
87	F2	205	CLA	C15-C16-C17-C18
87	b6	614	CLA	C8-C10-C11-C12
87	cL	506	CLA	C8-C10-C11-C12
87	cL	508	CLA	C8-C10-C11-C12
87	cL	513	CLA	C5-C6-C7-C8
82	KM	202	PEB	NC-C4C-CHC-C1D
82	SM	202	PEB	NC-C4C-CHC-C1D
82	jJ	202	PEB	NC-C4C-CHC-C1D
87	cL	517	CLA	CBA-CGA-O2A-C1
82	YE	201	PEB	C1C-C2C-CAC-CBC
82	YG	201	PEB	C1C-C2C-CAC-CBC
87	HL	101	CLA	O1D-CGD-O2D-CED
87	IN	103	CLA	O1D-CGD-O2D-CED
87	KN	102	CLA	O1D-CGD-O2D-CED
87	I2	103	CLA	O1D-CGD-O2D-CED
87	K2	103	CLA	O1D-CGD-O2D-CED
87	C6	517	CLA	O1D-CGD-O2D-CED
87	CL	511	CLA	C5-C6-C7-C8
87	AN	809	CLA	C5-C6-C7-C8
87	BN	812	CLA	C5-C6-C7-C8
87	BN	819	CLA	C15-C16-C17-C18
87	A2	809	CLA	C5-C6-C7-C8
87	B2	811	CLA	C5-C6-C7-C8
87	B2	818	CLA	C15-C16-C17-C18
87	C6	511	CLA	C8-C10-C11-C12
87	c6	611	CLA	C10-C11-C12-C13
87	dL	402	CLA	C13-C15-C16-C17
95	C6	502	DGD	C4D-C5D-C6D-O5D
88	BL	615	LHG	C7-C8-C9-C10
88	B6	617	LHG	C7-C8-C9-C10
88	M6	101	LHG	C7-C8-C9-C10
92	bL	623	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
92	dL	407	LMG	C28-C29-C30-C31
95	C6	502	DGD	C1A-C2A-C3A-C4A
95	C6	502	DGD	C1B-C2B-C3B-C4B
95	c6	601	DGD	C1B-C2B-C3B-C4B
87	BL	621	CLA	CBD-CGD-O2D-CED
82	AA	201	PEB	C3B-CAB-CBB-CGB
82	AA	202	PEB	C2C-CAC-CBC-CGC
82	BA	201	PEB	C3B-CAB-CBB-CGB
82	DA	202	PEB	C2C-CAC-CBC-CGC
82	DA	202	PEB	C3B-CAB-CBB-CGB
82	DA	203	PEB	C2C-CAC-CBC-CGC
82	EA	202	PEB	C2C-CAC-CBC-CGC
82	FA	203	PEB	C2C-CAC-CBC-CGC
82	GA	202	PEB	C2C-CAC-CBC-CGC
82	KA	202	PEB	C2C-CAC-CBC-CGC
82	VA	202	PEB	C2C-CAC-CBC-CGC
82	YA	303	PEB	C3B-CAB-CBB-CGB
82	GB	202	PEB	C3B-CAB-CBB-CGB
82	MB	202	PEB	C2C-CAC-CBC-CGC
82	NB	203	PEB	C3B-CAB-CBB-CGB
82	RB	201	PEB	C3B-CAB-CBB-CGB
82	LD	202	PEB	C3B-CAB-CBB-CGB
82	SD	202	PEB	C2C-CAC-CBC-CGC
82	UD	202	PEB	C3B-CAB-CBB-CGB
82	VD	203	PEB	C2C-CAC-CBC-CGC
82	XD	201	PEB	C2C-CAC-CBC-CGC
82	YD	201	PEB	C3B-CAB-CBB-CGB
82	YD	202	PEB	C3B-CAB-CBB-CGB
82	QE	203	PEB	C2C-CAC-CBC-CGC
82	UE	203	PEB	C3B-CAB-CBB-CGB
82	WE	202	PEB	C3B-CAB-CBB-CGB
82	ZE	203	PEB	C3B-CAB-CBB-CGB
82	AF	202	PEB	C2C-CAC-CBC-CGC
82	CF	203	PEB	C2C-CAC-CBC-CGC
82	DF	202	PEB	C2C-CAC-CBC-CGC
82	EF	202	PEB	C2C-CAC-CBC-CGC
82	EF	202	PEB	C3B-CAB-CBB-CGB
82	HF	202	PEB	C3B-CAB-CBB-CGB
82	KF	203	PEB	C2C-CAC-CBC-CGC
82	LF	201	PEB	C3B-CAB-CBB-CGB
82	LF	202	PEB	C2C-CAC-CBC-CGC
82	MF	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	QF	203	PEB	C2C-CAC-CBC-CGC
82	UF	201	PEB	C3B-CAB-CBB-CGB
82	WF	201	PEB	C3B-CAB-CBB-CGB
82	WF	203	PEB	C2C-CAC-CBC-CGC
82	WF	203	PEB	C3B-CAB-CBB-CGB
82	ZF	202	PEB	C2C-CAC-CBC-CGC
82	ZF	202	PEB	C3B-CAB-CBB-CGB
82	QG	203	PEB	C2C-CAC-CBC-CGC
82	UG	203	PEB	C3B-CAB-CBB-CGB
82	WG	202	PEB	C3B-CAB-CBB-CGB
82	ZG	203	PEB	C3B-CAB-CBB-CGB
82	AH	302	PEB	C3B-CAB-CBB-CGB
82	JH	1002	PEB	C2C-CAC-CBC-CGC
82	OH	203	PEB	C2C-CAC-CBC-CGC
82	RH	202	PEB	C2C-CAC-CBC-CGC
82	RH	202	PEB	C3B-CAB-CBB-CGB
82	SH	202	PEB	C3B-CAB-CBB-CGB
82	YH	202	PEB	C3B-CAB-CBB-CGB
82	ZH	201	PEB	C2C-CAC-CBC-CGC
82	AI	202	PEB	C3B-CAB-CBB-CGB
82	CI	202	PEB	C3B-CAB-CBB-CGB
82	EI	202	PEB	C3B-CAB-CBB-CGB
82	FI	202	PEB	C2C-CAC-CBC-CGC
82	GI	203	PEB	C3B-CAB-CBB-CGB
82	II	202	PEB	C3B-CAB-CBB-CGB
82	KI	203	PEB	C3B-CAB-CBB-CGB
82	NI	202	PEB	C3B-CAB-CBB-CGB
82	PI	202	PEB	C3B-CAB-CBB-CGB
82	RI	202	PEB	C3B-CAB-CBB-CGB
82	TI	203	PEB	C3B-CAB-CBB-CGB
82	VI	202	PEB	C3B-CAB-CBB-CGB
82	XI	202	PEB	C3B-CAB-CBB-CGB
82	CJ	202	PEB	C2C-CAC-CBC-CGC
82	DJ	202	PEB	C2C-CAC-CBC-CGC
82	GJ	201	PEB	C2C-CAC-CBC-CGC
82	HJ	202	PEB	C2C-CAC-CBC-CGC
82	KJ	202	PEB	C3B-CAB-CBB-CGB
82	QJ	204	PEB	C3B-CAB-CBB-CGB
82	SJ	201	PEB	C3B-CAB-CBB-CGB
82	SJ	202	PEB	C3B-CAB-CBB-CGB
82	XJ	201	PEB	C2C-CAC-CBC-CGC
82	XJ	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	ZJ	202	PEB	C2C-CAC-CBC-CGC
82	AK	202	PEB	C2C-CAC-CBC-CGC
82	CK	203	PEB	C2C-CAC-CBC-CGC
82	DK	202	PEB	C2C-CAC-CBC-CGC
82	EK	202	PEB	C2C-CAC-CBC-CGC
82	EK	202	PEB	C3B-CAB-CBB-CGB
82	HK	202	PEB	C3B-CAB-CBB-CGB
82	KK	203	PEB	C2C-CAC-CBC-CGC
82	LK	201	PEB	C3B-CAB-CBB-CGB
82	LK	202	PEB	C2C-CAC-CBC-CGC
82	MK	202	PEB	C3B-CAB-CBB-CGB
82	QK	203	PEB	C2C-CAC-CBC-CGC
82	UK	201	PEB	C3B-CAB-CBB-CGB
82	WK	201	PEB	C3B-CAB-CBB-CGB
82	WK	203	PEB	C2C-CAC-CBC-CGC
82	WK	203	PEB	C3B-CAB-CBB-CGB
82	ZK	202	PEB	C2C-CAC-CBC-CGC
82	ZK	202	PEB	C3B-CAB-CBB-CGB
82	CM	201	PEB	C2C-CAC-CBC-CGC
82	CM	202	PEB	C3B-CAB-CBB-CGB
82	EM	203	PEB	C3B-CAB-CBB-CGB
82	FM	201	PEB	C2C-CAC-CBC-CGC
82	GM	201	PEB	C3B-CAB-CBB-CGB
82	IM	203	PEB	C3B-CAB-CBB-CGB
82	KM	202	PEB	C3B-CAB-CBB-CGB
82	NM	201	PEB	C2C-CAC-CBC-CGC
82	QM	204	PEB	C2C-CAC-CBC-CGC
82	RM	201	PEB	C2C-CAC-CBC-CGC
82	YM	203	PEB	C2C-CAC-CBC-CGC
82	HO	1002	PEB	C2C-CAC-CBC-CGC
82	LO	1002	PEB	C3B-CAB-CBB-CGB
82	CP	203	PEB	C2C-CAC-CBC-CGC
82	GP	203	PEB	C2C-CAC-CBC-CGC
82	IP	202	PEB	C2C-CAC-CBC-CGC
82	MP	202	PEB	C2C-CAC-CBC-CGC
82	UP	202	PEB	C2C-CAC-CBC-CGC
82	LQ	202	PEB	C3B-CAB-CBB-CGB
82	SQ	202	PEB	C2C-CAC-CBC-CGC
82	UQ	202	PEB	C3B-CAB-CBB-CGB
82	VQ	203	PEB	C2C-CAC-CBC-CGC
82	XQ	201	PEB	C2C-CAC-CBC-CGC
82	YQ	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	YQ	202	PEB	C3B-CAB-CBB-CGB
82	O1	203	PEB	C2C-CAC-CBC-CGC
82	R1	202	PEB	C2C-CAC-CBC-CGC
82	R1	202	PEB	C3B-CAB-CBB-CGB
82	S1	202	PEB	C3B-CAB-CBB-CGB
82	A1	302	PEB	C3B-CAB-CBB-CGB
82	J1	1002	PEB	C2C-CAC-CBC-CGC
82	Y1	202	PEB	C3B-CAB-CBB-CGB
82	Z1	201	PEB	C2C-CAC-CBC-CGC
82	f1	202	PEB	C2C-CAC-CBC-CGC
82	k1	202	PEB	C3B-CAB-CBB-CGB
82	b1	202	PEB	C3B-CAB-CBB-CGB
82	c1	202	PEB	C3B-CAB-CBB-CGB
82	d1	203	PEB	C2C-CAC-CBC-CGC
82	H4	1002	PEB	C2C-CAC-CBC-CGC
82	L4	1002	PEB	C3B-CAB-CBB-CGB
82	i4	202	PEB	C3B-CAB-CBB-CGB
82	j4	203	PEB	C3B-CAB-CBB-CGB
82	a4	203	PEB	C3B-CAB-CBB-CGB
82	c4	203	PEB	C3B-CAB-CBB-CGB
82	B5	201	PEB	C2C-CAC-CBC-CGC
82	B5	203	PEB	C2C-CAC-CBC-CGC
82	B5	203	PEB	C3B-CAB-CBB-CGB
82	D5	203	PEB	C3B-CAB-CBB-CGB
82	F5	201	PEB	C2C-CAC-CBC-CGC
82	F5	203	PEB	C3B-CAB-CBB-CGB
82	H5	203	PEB	C3B-CAB-CBB-CGB
82	J5	203	PEB	C3B-CAB-CBB-CGB
82	L5	201	PEB	C2C-CAC-CBC-CGC
82	O5	203	PEB	C3B-CAB-CBB-CGB
82	S5	201	PEB	C2C-CAC-CBC-CGC
82	W5	201	PEB	C2C-CAC-CBC-CGC
82	W5	203	PEB	C3B-CAB-CBB-CGB
82	Y5	203	PEB	C3B-CAB-CBB-CGB
82	A7	201	PEB	C3B-CAB-CBB-CGB
82	A7	202	PEB	C2C-CAC-CBC-CGC
82	B7	201	PEB	C3B-CAB-CBB-CGB
82	D7	202	PEB	C2C-CAC-CBC-CGC
82	D7	202	PEB	C3B-CAB-CBB-CGB
82	D7	203	PEB	C2C-CAC-CBC-CGC
82	E7	202	PEB	C2C-CAC-CBC-CGC
82	F7	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	G7	202	PEB	C2C-CAC-CBC-CGC
82	K7	202	PEB	C2C-CAC-CBC-CGC
82	V7	202	PEB	C2C-CAC-CBC-CGC
82	Y7	303	PEB	C3B-CAB-CBB-CGB
82	w8	203	PEB	C3B-CAB-CBB-CGB
82	x8	201	PEB	C2C-CAC-CBC-CGC
82	D9	201	PEB	C3B-CAB-CBB-CGB
82	F9	201	PEB	C2C-CAC-CBC-CGC
82	H9	201	PEB	C2C-CAC-CBC-CGC
82	H9	203	PEB	C3B-CAB-CBB-CGB
82	L9	201	PEB	C2C-CAC-CBC-CGC
82	L9	201	PEB	C3B-CAB-CBB-CGB
82	O9	201	PEB	C3B-CAB-CBB-CGB
82	Q9	201	PEB	C2C-CAC-CBC-CGC
82	Q9	201	PEB	C3B-CAB-CBB-CGB
82	S9	201	PEB	C2C-CAC-CBC-CGC
82	cB	401	PEB	C2C-CAC-CBC-CGC
82	wC	203	PEB	C3B-CAB-CBB-CGB
82	xC	201	PEB	C2C-CAC-CBC-CGC
82	aE	202	PEB	C3B-CAB-CBB-CGB
82	bE	202	PEB	C3B-CAB-CBB-CGB
82	eE	201	PEB	C2C-CAC-CBC-CGC
82	iE	201	PEB	C2C-CAC-CBC-CGC
82	iE	202	PEB	C2C-CAC-CBC-CGC
82	iE	202	PEB	C3B-CAB-CBB-CGB
82	lE	203	PEB	C3B-CAB-CBB-CGB
82	cF	201	PEB	C3B-CAB-CBB-CGB
82	eF	201	PEB	C3B-CAB-CBB-CGB
82	iF	201	PEB	C2C-CAC-CBC-CGC
82	jF	202	PEB	C3B-CAB-CBB-CGB
82	kF	202	PEB	C2C-CAC-CBC-CGC
82	nF	201	PEB	C3B-CAB-CBB-CGB
82	oF	201	PEB	C3B-CAB-CBB-CGB
82	qF	201	PEB	C3B-CAB-CBB-CGB
82	sF	201	PEB	C2C-CAC-CBC-CGC
82	sF	201	PEB	C3B-CAB-CBB-CGB
82	sF	202	PEB	C2C-CAC-CBC-CGC
82	wF	301	PEB	C3B-CAB-CBB-CGB
82	xF	303	PEB	C3B-CAB-CBB-CGB
82	aG	202	PEB	C3B-CAB-CBB-CGB
82	eG	201	PEB	C2C-CAC-CBC-CGC
82	iG	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	iG	202	PEB	C2C-CAC-CBC-CGC
82	iG	202	PEB	C3B-CAB-CBB-CGB
82	lG	203	PEB	C3B-CAB-CBB-CGB
82	fH	202	PEB	C2C-CAC-CBC-CGC
82	kH	202	PEB	C3B-CAB-CBB-CGB
82	bH	202	PEB	C3B-CAB-CBB-CGB
82	cH	202	PEB	C3B-CAB-CBB-CGB
82	dH	203	PEB	C2C-CAC-CBC-CGC
82	aJ	201	PEB	C2C-CAC-CBC-CGC
82	gJ	201	PEB	C2C-CAC-CBC-CGC
82	hJ	201	PEB	C3B-CAB-CBB-CGB
82	iJ	202	PEB	C2C-CAC-CBC-CGC
82	cK	201	PEB	C3B-CAB-CBB-CGB
82	cK	202	PEB	C2C-CAC-CBC-CGC
82	cK	202	PEB	C3B-CAB-CBB-CGB
82	eK	201	PEB	C3B-CAB-CBB-CGB
82	iK	201	PEB	C2C-CAC-CBC-CGC
82	jK	202	PEB	C3B-CAB-CBB-CGB
82	kK	202	PEB	C2C-CAC-CBC-CGC
82	nK	201	PEB	C3B-CAB-CBB-CGB
82	oK	201	PEB	C3B-CAB-CBB-CGB
82	qK	201	PEB	C3B-CAB-CBB-CGB
82	sK	201	PEB	C2C-CAC-CBC-CGC
82	sK	201	PEB	C3B-CAB-CBB-CGB
82	sK	202	PEB	C2C-CAC-CBC-CGC
82	wK	301	PEB	C3B-CAB-CBB-CGB
82	xK	303	PEB	C3B-CAB-CBB-CGB
82	hM	203	PEB	C2C-CAC-CBC-CGC
82	iO	202	PEB	C3B-CAB-CBB-CGB
82	kO	202	PEB	C3B-CAB-CBB-CGB
82	aO	203	PEB	C3B-CAB-CBB-CGB
82	cO	203	PEB	C3B-CAB-CBB-CGB
83	AM	303	PUB	C3B-CAB-CBB-CGB
83	Z9	305	PUB	C3B-CAB-CBB-CGB
84	V3	1001	CYC	C2A-CAA-CBA-CGA
84	x3	1001	CYC	C2A-CAA-CBA-CGA
92	b6	624	LMG	C11-C10-O7-C8
87	BL	621	CLA	C8-C10-C11-C12
87	CL	505	CLA	C15-C16-C17-C18
87	AN	802	CLA	C8-C10-C11-C12
87	AN	821	CLA	C13-C15-C16-C17
87	A2	801	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
87	A2	821	CLA	C13-C15-C16-C17
87	B6	611	CLA	C10-C11-C12-C13
87	b6	607	CLA	C15-C16-C17-C18
87	dL	404	CLA	C15-C16-C17-C18
87	BL	605	CLA	O1D-CGD-O2D-CED
87	22	601	CLA	O1D-CGD-O2D-CED
87	22	606	CLA	O1D-CGD-O2D-CED
87	2N	302	CLA	O1D-CGD-O2D-CED
87	2N	306	CLA	O1D-CGD-O2D-CED
87	AN	810	CLA	C12-C13-C15-C16
87	AN	819	CLA	C11-C12-C13-C15
87	AN	840	CLA	C6-C7-C8-C10
87	BN	809	CLA	C11-C10-C8-C7
87	BN	813	CLA	C6-C7-C8-C10
87	BN	834	CLA	C6-C7-C8-C10
87	A2	801	CLA	C12-C13-C15-C16
87	A2	810	CLA	C12-C13-C15-C16
87	A2	819	CLA	C11-C12-C13-C15
87	A2	840	CLA	C6-C7-C8-C10
87	B2	808	CLA	C11-C10-C8-C7
87	B2	812	CLA	C6-C7-C8-C10
87	B2	834	CLA	C6-C7-C8-C10
87	B6	606	CLA	C11-C10-C8-C7
87	B6	612	CLA	C11-C10-C8-C7
87	B6	616	CLA	C12-C13-C15-C16
87	C6	514	CLA	C11-C10-C8-C7
87	H6	103	CLA	C11-C12-C13-C15
87	K6	101	CLA	C12-C13-C15-C16
87	a6	607	CLA	C11-C10-C8-C7
87	b6	613	CLA	C6-C7-C8-C10
87	b6	615	CLA	C11-C12-C13-C15
87	c6	605	CLA	C11-C12-C13-C15
87	c6	611	CLA	C11-C10-C8-C7
87	c6	611	CLA	C12-C13-C15-C16
87	cL	505	CLA	C11-C12-C13-C15
87	cL	514	CLA	C11-C12-C13-C15
87	cL	515	CLA	C11-C10-C8-C7
91	AL	410	PHO	C11-C12-C13-C15
91	a6	613	PHO	C11-C12-C13-C15
91	aL	610	PHO	C11-C12-C13-C15
87	HL	102	CLA	C3-C5-C6-C7
87	D6	402	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
87	d6	403	CLA	O1A-CGA-O2A-C1
88	d6	402	LHG	C25-C26-C27-C28
85	AN	845	BCR	C9-C10-C11-C12
85	BN	842	BCR	C15-C16-C17-C18
85	KN	104	BCR	C9-C10-C11-C12
85	A2	845	BCR	C9-C10-C11-C12
85	B2	842	BCR	C15-C16-C17-C18
85	K2	105	BCR	C9-C10-C11-C12
95	c6	601	DGD	C1A-C2A-C3A-C4A
87	BL	623	CLA	C2A-CAA-CBA-CGA
87	AN	830	CLA	C2A-CAA-CBA-CGA
87	BN	833	CLA	C2A-CAA-CBA-CGA
87	ON	202	CLA	C2A-CAA-CBA-CGA
87	82	308	CLA	C2A-CAA-CBA-CGA
87	A2	830	CLA	C2A-CAA-CBA-CGA
87	B2	833	CLA	C2A-CAA-CBA-CGA
87	O2	202	CLA	C2A-CAA-CBA-CGA
87	b6	604	CLA	C2A-CAA-CBA-CGA
87	bL	613	CLA	C2A-CAA-CBA-CGA
87	cL	517	CLA	C2A-CAA-CBA-CGA
87	dL	401	CLA	C2A-CAA-CBA-CGA
87	8N	308	CLA	C2A-CAA-CBA-CGA
82	DD	202	PEB	C2B-C1B-CHA-C4A
82	DQ	202	PEB	C2B-C1B-CHA-C4A
87	AN	835	CLA	O1D-CGD-O2D-CED
87	BN	826	CLA	O1D-CGD-O2D-CED
87	LN	202	CLA	O1D-CGD-O2D-CED
87	ON	201	CLA	O1D-CGD-O2D-CED
87	A2	835	CLA	O1D-CGD-O2D-CED
87	B2	826	CLA	O1D-CGD-O2D-CED
87	L2	202	CLA	O1D-CGD-O2D-CED
87	O2	201	CLA	O1D-CGD-O2D-CED
87	bL	605	CLA	O1D-CGD-O2D-CED
87	BL	608	CLA	C8-C10-C11-C12
87	HL	102	CLA	C5-C6-C7-C8
87	HL	102	CLA	C15-C16-C17-C18
87	AN	805	CLA	C13-C15-C16-C17
87	AN	828	CLA	C10-C11-C12-C13
87	BN	809	CLA	C10-C11-C12-C13
87	BN	813	CLA	C15-C16-C17-C18
87	BN	818	CLA	C5-C6-C7-C8
87	72	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
87	A2	805	CLA	C13-C15-C16-C17
87	A2	828	CLA	C10-C11-C12-C13
87	B2	808	CLA	C10-C11-C12-C13
87	B2	812	CLA	C15-C16-C17-C18
87	B2	817	CLA	C5-C6-C7-C8
87	A6	402	CLA	C5-C6-C7-C8
87	B6	603	CLA	C8-C10-C11-C12
87	B6	608	CLA	C15-C16-C17-C18
87	D6	403	CLA	C15-C16-C17-C18
87	c6	613	CLA	C15-C16-C17-C18
87	7N	602	CLA	C8-C10-C11-C12
95	AL	414	DGD	C4E-C5E-C6E-O5E
87	DL	403	CLA	O1A-CGA-O2A-C1
87	AN	841	CLA	O1A-CGA-O2A-C1
87	FN	205	CLA	O1A-CGA-O2A-C1
87	22	602	CLA	O1A-CGA-O2A-C1
87	A2	841	CLA	O1A-CGA-O2A-C1
87	F2	205	CLA	O1A-CGA-O2A-C1
87	2N	303	CLA	O1A-CGA-O2A-C1
87	bL	607	CLA	CBD-CGD-O2D-CED
92	b6	623	LMG	O6-C1-O1-C7
95	C6	523	DGD	O6E-C1E-O5D-C6D
95	a6	602	DGD	O6D-C1D-O3G-C3G
95	a6	603	DGD	O6E-C1E-O5D-C6D
95	c6	620	DGD	O6E-C1E-O5D-C6D
95	h6	101	DGD	O6D-C1D-O3G-C3G
87	BL	609	CLA	C5-C6-C7-C8
87	CL	514	CLA	C5-C6-C7-C8
87	BN	819	CLA	C8-C10-C11-C12
87	B2	818	CLA	C8-C10-C11-C12
87	I2	102	CLA	C5-C6-C7-C8
87	c6	608	CLA	C13-C15-C16-C17
87	BN	829	CLA	O1D-CGD-O2D-CED
87	B2	829	CLA	O1D-CGD-O2D-CED
94	AL	413	PL9	C9-C11-C12-C13
94	DL	401	PL9	C19-C21-C22-C23
94	D6	408	PL9	C14-C16-C17-C18
94	D6	408	PL9	C29-C31-C32-C33
94	D6	408	PL9	C34-C36-C37-C38
94	d6	408	PL9	C14-C16-C17-C18
94	aL	601	PL9	C39-C41-C42-C43
94	dL	406	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
94	dL	406	PL9	C34-C36-C37-C38
84	MO	1001	CYC	C2B-C3B-CAB-CBB
84	V3	1001	CYC	C2B-C3B-CAB-CBB
84	x3	1001	CYC	C2B-C3B-CAB-CBB
84	M4	1001	CYC	C2B-C3B-CAB-CBB
95	a6	602	DGD	O6D-C5D-C6D-O5D
84	HH	1001	CYC	C2B-C3B-CAB-CBB
84	H1	1001	CYC	C2B-C3B-CAB-CBB
87	dL	402	CLA	O1D-CGD-O2D-CED
88	ML	102	LHG	O2-C2-C3-O3
88	cL	501	LHG	O9-C7-O7-C5
92	b6	620	LMG	O9-C10-O7-C8
92	b6	624	LMG	O9-C10-O7-C8
87	D6	405	CLA	C3-C5-C6-C7
87	a6	608	CLA	C3-C5-C6-C7
87	BN	829	CLA	C2A-CAA-CBA-CGA
87	B2	829	CLA	C2A-CAA-CBA-CGA
87	BL	603	CLA	C10-C11-C12-C13
87	BL	606	CLA	C15-C16-C17-C18
87	CL	515	CLA	C10-C11-C12-C13
87	AN	809	CLA	C15-C16-C17-C18
87	AN	831	CLA	C10-C11-C12-C13
87	BN	827	CLA	C13-C15-C16-C17
87	BN	830	CLA	C10-C11-C12-C13
87	IN	102	CLA	C5-C6-C7-C8
87	A2	809	CLA	C15-C16-C17-C18
87	A2	831	CLA	C10-C11-C12-C13
87	B2	827	CLA	C13-C15-C16-C17
87	B2	830	CLA	C10-C11-C12-C13
87	B6	615	CLA	C15-C16-C17-C18
87	H6	103	CLA	C15-C16-C17-C18
87	b6	615	CLA	C13-C15-C16-C17
87	b6	618	CLA	C8-C10-C11-C12
87	bL	622	CLA	C5-C6-C7-C8
87	bL	622	CLA	C13-C15-C16-C17
87	12	602	CLA	CBA-CGA-O2A-C1
87	cL	506	CLA	CBA-CGA-O2A-C1
87	cL	510	CLA	CBA-CGA-O2A-C1
87	1N	602	CLA	CBA-CGA-O2A-C1
87	CL	503	CLA	O1A-CGA-O2A-C1
87	AN	802	CLA	O1A-CGA-O2A-C1
87	A2	801	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
87	C6	513	CLA	O1A-CGA-O2A-C1
95	a6	602	DGD	O1A-C1A-O1G-C1G
88	D6	401	LHG	C27-C28-C29-C30
87	B6	607	CLA	O1D-CGD-O2D-CED
87	BL	602	CLA	C10-C11-C12-C13
87	BL	604	CLA	C5-C6-C7-C8
87	BL	620	CLA	C8-C10-C11-C12
87	CL	505	CLA	C8-C10-C11-C12
87	AN	808	CLA	C8-C10-C11-C12
87	AN	813	CLA	C10-C11-C12-C13
87	AN	834	CLA	C8-C10-C11-C12
87	AN	851	CLA	C8-C10-C11-C12
87	BN	810	CLA	C13-C15-C16-C17
87	BN	811	CLA	C5-C6-C7-C8
87	IN	103	CLA	C10-C11-C12-C13
87	A2	808	CLA	C8-C10-C11-C12
87	A2	813	CLA	C10-C11-C12-C13
87	A2	834	CLA	C8-C10-C11-C12
87	A2	851	CLA	C8-C10-C11-C12
87	B2	809	CLA	C13-C15-C16-C17
87	B2	810	CLA	C5-C6-C7-C8
87	B2	812	CLA	C10-C11-C12-C13
87	I2	103	CLA	C10-C11-C12-C13
87	B6	607	CLA	C5-C6-C7-C8
87	B6	608	CLA	C10-C11-C12-C13
87	B6	616	CLA	C5-C6-C7-C8
87	a6	608	CLA	C10-C11-C12-C13
87	b6	615	CLA	C15-C16-C17-C18
87	c6	606	CLA	C8-C10-C11-C12
87	bL	615	CLA	C13-C15-C16-C17
87	cL	505	CLA	C13-C15-C16-C17
87	cL	507	CLA	C10-C11-C12-C13
87	cL	516	CLA	C5-C6-C7-C8
98	BN	837	PQN	C20-C21-C22-C23
98	B2	837	PQN	C20-C21-C22-C23
82	RJ	202	PEB	NC-C1C-CHB-C4B
82	H5	202	PEB	NC-C1C-CHB-C4B
82	L5	202	PEB	NC-C1C-CHB-C4B
82	aF	203	PEB	NC-C1C-CHB-C4B
95	D6	410	DGD	C4A-C5A-C6A-C7A
87	FN	203	CLA	O1D-CGD-O2D-CED
87	F2	201	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	CL	511	CLA	CBD-CGD-O2D-CED
87	CL	504	CLA	O1A-CGA-O2A-C1
87	C6	514	CLA	O1A-CGA-O2A-C1
87	c6	604	CLA	O1A-CGA-O2A-C1
87	nL	101	CLA	O1A-CGA-O2A-C1
92	C6	501	LMG	C11-C10-O7-C8
87	BL	609	CLA	C8-C10-C11-C12
87	BL	620	CLA	C10-C11-C12-C13
87	CL	504	CLA	C8-C10-C11-C12
87	BN	813	CLA	C10-C11-C12-C13
87	BN	824	CLA	C13-C15-C16-C17
87	BN	831	CLA	C5-C6-C7-C8
87	BN	836	CLA	C13-C15-C16-C17
87	B2	823	CLA	C13-C15-C16-C17
87	B2	831	CLA	C5-C6-C7-C8
87	B2	836	CLA	C13-C15-C16-C17
87	B6	605	CLA	C5-C6-C7-C8
87	B6	607	CLA	C15-C16-C17-C18
87	H6	102	CLA	C13-C15-C16-C17
87	b6	605	CLA	C8-C10-C11-C12
87	bL	622	CLA	C8-C10-C11-C12
91	AL	410	PHO	C10-C11-C12-C13
88	AL	407	LHG	C3-O3-P-O6
88	AL	407	LHG	C4-O6-P-O3
88	BL	610	LHG	C3-O3-P-O6
88	BL	610	LHG	C4-O6-P-O3
88	BL	615	LHG	C4-O6-P-O3
88	CL	521	LHG	C3-O3-P-O6
88	CL	522	LHG	C3-O3-P-O6
88	DL	407	LHG	C3-O3-P-O6
88	DL	407	LHG	C4-O6-P-O3
88	ML	102	LHG	C3-O3-P-O6
88	ML	102	LHG	C4-O6-P-O3
88	AN	843	LHG	C3-O3-P-O6
88	AN	843	LHG	C4-O6-P-O3
88	AN	844	LHG	C4-O6-P-O3
88	A2	843	LHG	C3-O3-P-O6
88	A2	843	LHG	C4-O6-P-O3
88	A2	844	LHG	C4-O6-P-O3
88	B6	617	LHG	C4-O6-P-O3
88	C6	522	LHG	C3-O3-P-O6
88	C6	522	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
88	D6	401	LHG	C3-O3-P-O6
88	D6	406	LHG	C3-O3-P-O6
88	I6	101	LHG	C3-O3-P-O6
88	M6	101	LHG	C3-O3-P-O6
88	a6	610	LHG	C3-O3-P-O6
88	c6	619	LHG	C3-O3-P-O6
88	c6	619	LHG	C4-O6-P-O3
88	d6	402	LHG	C3-O3-P-O6
88	d6	402	LHG	C4-O6-P-O3
88	d6	407	LHG	C3-O3-P-O6
88	i6	101	LHG	C4-O6-P-O3
88	aL	607	LHG	C3-O3-P-O6
88	aL	607	LHG	C4-O6-P-O3
88	bL	612	LHG	C3-O3-P-O6
88	dL	405	LHG	C3-O3-P-O6
88	dL	408	LHG	C3-O3-P-O6
88	iL	101	LHG	C3-O3-P-O6
88	mL	102	LHG	C3-O3-P-O6
88	aL	607	LHG	C23-C24-C25-C26
82	GB	203	PEB	C2C-C1C-CHB-C4B
82	LM	202	PEB	C2C-C1C-CHB-C4B
82	D5	203	PEB	C2C-C1C-CHB-C4B
82	F5	203	PEB	C2C-C1C-CHB-C4B
82	Q5	202	PEB	C2C-C1C-CHB-C4B
87	bL	605	CLA	C3-C5-C6-C7
91	d6	404	PHO	C3-C5-C6-C7
87	AN	827	CLA	CBA-CGA-O2A-C1
87	AN	832	CLA	CBA-CGA-O2A-C1
87	ON	202	CLA	CBA-CGA-O2A-C1
87	A2	827	CLA	CBA-CGA-O2A-C1
87	A2	832	CLA	CBA-CGA-O2A-C1
87	O2	202	CLA	CBA-CGA-O2A-C1
87	d6	406	CLA	CBA-CGA-O2A-C1
87	cL	508	CLA	CBA-CGA-O2A-C1
87	2N	301	CLA	CBA-CGA-O2A-C1
87	nL	101	CLA	O1D-CGD-O2D-CED
87	AN	841	CLA	C5-C6-C7-C8
87	BN	836	CLA	C5-C6-C7-C8
87	A2	841	CLA	C5-C6-C7-C8
87	B2	836	CLA	C5-C6-C7-C8
87	B6	614	CLA	C15-C16-C17-C18
87	C6	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
87	C6	520	CLA	C15-C16-C17-C18
87	dL	404	CLA	C8-C10-C11-C12
87	BN	826	CLA	O1A-CGA-O2A-C1
87	B2	826	CLA	O1A-CGA-O2A-C1
87	I2	103	CLA	O1A-CGA-O2A-C1
87	AN	806	CLA	O1D-CGD-O2D-CED
87	A2	806	CLA	O1D-CGD-O2D-CED
87	b6	618	CLA	O1D-CGD-O2D-CED
95	C6	502	DGD	O6D-C5D-C6D-O5D
95	c6	601	DGD	O6D-C5D-C6D-O5D
88	DL	407	LHG	C7-C8-C9-C10
88	D6	406	LHG	C1-C2-C3-O3
88	m6	102	LHG	C1-C2-C3-O3
92	BL	611	LMG	O6-C5-C6-O5
92	C6	501	LMG	O9-C10-O7-C8
87	K6	101	CLA	C4-C3-C5-C6
94	DL	401	PL9	C12-C11-C9-C10
92	bL	609	LMG	C4-C5-C6-O5
87	CL	512	CLA	C8-C10-C11-C12
87	bL	617	CLA	C10-C11-C12-C13
82	ID	201	PEB	C3C-C2C-CAC-CBC
82	MD	201	PEB	C3C-C2C-CAC-CBC
82	IQ	201	PEB	C3C-C2C-CAC-CBC
82	MQ	201	PEB	C3C-C2C-CAC-CBC
82	eE	203	PEB	C3C-C2C-CAC-CBC
82	eG	203	PEB	C3C-C2C-CAC-CBC
82	dJ	202	PEB	C3C-C2C-CAC-CBC
87	AN	810	CLA	O1D-CGD-O2D-CED
87	A2	810	CLA	O1D-CGD-O2D-CED
87	IN	103	CLA	O1A-CGA-O2A-C1
87	A6	404	CLA	C2C-C3C-CAC-CBC
87	AN	849	CLA	C2A-CAA-CBA-CGA
87	MN	101	CLA	C2A-CAA-CBA-CGA
87	22	609	CLA	C2A-CAA-CBA-CGA
87	32	312	CLA	C2A-CAA-CBA-CGA
87	72	607	CLA	C2A-CAA-CBA-CGA
87	A2	849	CLA	C2A-CAA-CBA-CGA
87	M2	101	CLA	C2A-CAA-CBA-CGA
87	B6	613	CLA	C2A-CAA-CBA-CGA
87	C6	513	CLA	C2A-CAA-CBA-CGA
87	b6	615	CLA	C2A-CAA-CBA-CGA
87	2N	309	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	3N	312	CLA	C2A-CAA-CBA-CGA
87	7N	607	CLA	C2A-CAA-CBA-CGA
87	BN	822	CLA	C6-C7-C8-C10
87	B2	821	CLA	C6-C7-C8-C10
87	B6	607	CLA	C16-C17-C18-C20
87	c6	605	CLA	C16-C17-C18-C19
87	BN	818	CLA	C3-C5-C6-C7
87	B2	817	CLA	C3-C5-C6-C7
87	d6	406	CLA	C3-C5-C6-C7
87	AN	813	CLA	CBA-CGA-O2A-C1
87	22	605	CLA	CBA-CGA-O2A-C1
87	42	608	CLA	CBA-CGA-O2A-C1
87	62	309	CLA	CBA-CGA-O2A-C1
87	A2	813	CLA	CBA-CGA-O2A-C1
87	D6	403	CLA	CBA-CGA-O2A-C1
87	bL	614	CLA	CBA-CGA-O2A-C1
87	6N	608	CLA	CBA-CGA-O2A-C1
91	A6	407	PHO	CBA-CGA-O2A-C1
91	a6	613	PHO	CBA-CGA-O2A-C1
92	bL	611	LMG	C29-C28-O8-C9
87	BN	832	CLA	C5-C6-C7-C8
87	B2	832	CLA	C5-C6-C7-C8
87	cL	506	CLA	C15-C16-C17-C18
88	d6	402	LHG	C27-C28-C29-C30
92	C6	501	LMG	C13-C14-C15-C16
92	b6	623	LMG	C11-C12-C13-C14
82	p8	202	PEB	C3B-C4B-CHB-C1C
82	t8	202	PEB	C3B-C4B-CHB-C1C
82	x8	202	PEB	C3B-C4B-CHB-C1C
82	pC	202	PEB	C3B-C4B-CHB-C1C
82	tC	202	PEB	C3B-C4B-CHB-C1C
82	xC	202	PEB	C3B-C4B-CHB-C1C
85	IN	101	BCR	C9-C10-C11-C12
85	I2	101	BCR	C9-C10-C11-C12
103	82	309	ZEX	C29-C30-C31-C32
103	8N	309	ZEX	C29-C30-C31-C32
92	b6	624	LMG	C11-C12-C13-C14
92	yL	101	LMG	C19-C20-C21-C22
87	R2	201	CLA	O1D-CGD-O2D-CED
87	CL	505	CLA	CBD-CGD-O2D-CED
87	C6	511	CLA	CBD-CGD-O2D-CED
88	AL	406	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
92	yL	101	LMG	C11-C10-O7-C8
95	C6	503	DGD	C2B-C1B-O2G-C2G
87	cL	505	CLA	C15-C16-C17-C18
87	CL	505	CLA	C3-C5-C6-C7
87	B6	611	CLA	C3-C5-C6-C7
87	cL	506	CLA	C3-C5-C6-C7
88	AL	406	LHG	C24-C25-C26-C27
88	C6	505	LHG	C9-C10-C11-C12
88	a6	610	LHG	C32-C33-C34-C35
88	i6	101	LHG	C15-C16-C17-C18
92	m6	101	LMG	C29-C30-C31-C32
92	yL	101	LMG	C32-C33-C34-C35
92	yL	101	LMG	C37-C38-C39-C40
95	C6	502	DGD	C4A-C5A-C6A-C7A
95	c6	601	DGD	C4A-C5A-C6A-C7A
95	h6	101	DGD	CCB-CDB-CEB-CFB
95	hL	101	DGD	C5B-C6B-C7B-C8B
100	JN	104	3XQ	C12-C13-C14-C15
87	BN	817	CLA	O1D-CGD-O2D-CED
87	RN	201	CLA	O1D-CGD-O2D-CED
87	82	306	CLA	O1D-CGD-O2D-CED
87	B2	816	CLA	O1D-CGD-O2D-CED
87	C6	514	CLA	O1D-CGD-O2D-CED
87	8N	301	CLA	O1D-CGD-O2D-CED
87	BN	819	CLA	C16-C17-C18-C19
87	22	605	CLA	C6-C7-C8-C10
87	B2	818	CLA	C16-C17-C18-C19
87	b6	604	CLA	C16-C17-C18-C19
87	b6	617	CLA	C16-C17-C18-C20
87	c6	609	CLA	C16-C17-C18-C20
87	nL	101	CLA	C16-C17-C18-C20
87	2N	301	CLA	C6-C7-C8-C10
87	CL	508	CLA	CBA-CGA-O2A-C1
87	C6	511	CLA	CBA-CGA-O2A-C1
87	4N	608	CLA	CBA-CGA-O2A-C1
92	XL	601	LMG	C29-C28-O8-C9
82	AA	201	PEB	C2B-C3B-CAB-CBB
82	A7	201	PEB	C2B-C3B-CAB-CBB
95	C6	503	DGD	C4D-C5D-C6D-O5D
88	D6	401	LHG	C25-C26-C27-C28
88	L6	101	LHG	C25-C26-C27-C28
88	i6	101	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
88	l6	101	LHG	C25-C26-C27-C28
92	C6	501	LMG	C38-C39-C40-C41
92	k6	101	LMG	C29-C30-C31-C32
100	J2	104	3XQ	C7-C8-C9-C10
82	ED	201	PEB	C1C-C2C-CAC-CBC
82	OJ	202	PEB	C1C-C2C-CAC-CBC
82	EQ	201	PEB	C1C-C2C-CAC-CBC
87	62	309	CLA	O1D-CGD-O2D-CED
87	6N	608	CLA	O1D-CGD-O2D-CED
88	AL	406	LHG	O9-C7-O7-C5
88	AN	843	LHG	O9-C7-O7-C5
92	D6	409	LMG	O9-C10-O7-C8
95	C6	503	DGD	O1B-C1B-O2G-C2G
87	BL	609	CLA	C13-C15-C16-C17
87	12	602	CLA	C8-C10-C11-C12
87	B6	607	CLA	C8-C10-C11-C12
95	b6	622	DGD	C1B-C2B-C3B-C4B
88	L6	101	LHG	C17-C18-C19-C20
88	l6	101	LHG	C17-C18-C19-C20
88	dL	408	LHG	C9-C10-C11-C12
92	BL	612	LMG	C29-C30-C31-C32
95	BN	844	DGD	C6A-C7A-C8A-C9A
95	B2	844	DGD	C6A-C7A-C8A-C9A
95	C6	502	DGD	CBA-CCA-CDA-CEA
95	c6	601	DGD	CBA-CCA-CDA-CEA
87	BL	619	CLA	O1D-CGD-O2D-CED
87	BN	813	CLA	O1D-CGD-O2D-CED
87	52	610	CLA	O1D-CGD-O2D-CED
87	B2	812	CLA	O1D-CGD-O2D-CED
87	c6	615	CLA	O1D-CGD-O2D-CED
87	cL	516	CLA	O1D-CGD-O2D-CED
87	5N	610	CLA	O1D-CGD-O2D-CED
87	cL	517	CLA	O1A-CGA-O2A-C1
82	GD	202	PEB	NC-C1C-CHB-C4B
82	HD	202	PEB	NC-C1C-CHB-C4B
82	OD	202	PEB	NC-C1C-CHB-C4B
82	VE	202	PEB	NC-C1C-CHB-C4B
82	WF	203	PEB	NC-C1C-CHB-C4B
82	VG	202	PEB	NC-C1C-CHB-C4B
82	JJ	202	PEB	NC-C1C-CHB-C4B
82	KJ	202	PEB	NC-C1C-CHB-C4B
82	LJ	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	ZJ	202	PEB	NC-C1C-CHB-C4B
82	LM	202	PEB	NC-C1C-CHB-C4B
82	GQ	202	PEB	NC-C1C-CHB-C4B
82	HQ	202	PEB	NC-C1C-CHB-C4B
82	c1	202	PEB	NC-C1C-CHB-C4B
82	g4	203	PEB	NC-C1C-CHB-C4B
82	J5	203	PEB	NC-C1C-CHB-C4B
82	S5	202	PEB	NC-C1C-CHB-C4B
82	U5	202	PEB	NC-C1C-CHB-C4B
82	w8	204	PEB	NC-C1C-CHB-C4B
82	wC	204	PEB	NC-C1C-CHB-C4B
82	cF	202	PEB	NC-C1C-CHB-C4B
82	aJ	203	PEB	NC-C1C-CHB-C4B
82	aK	203	PEB	NC-C1C-CHB-C4B
82	fM	202	PEB	NC-C1C-CHB-C4B
82	gO	203	PEB	NC-C1C-CHB-C4B
82	Z9	301	PEB	NC-C1C-CHB-C4B
82	M9	302	PEB	NC-C1C-CHB-C4B
88	AL	406	LHG	C32-C33-C34-C35
88	DL	407	LHG	C15-C16-C17-C18
88	I6	101	LHG	C16-C17-C18-C19
100	J2	104	3XQ	C9-C10-C11-C12
87	B2	824	CLA	C5-C6-C7-C8
87	b6	612	CLA	C13-C15-C16-C17
87	1N	602	CLA	C8-C10-C11-C12
88	AN	843	LHG	O2-C2-C3-O3
88	A2	843	LHG	O2-C2-C3-O3
82	EA	201	PEB	C2C-CAC-CBC-CGC
82	JA	203	PEB	C2C-CAC-CBC-CGC
82	OA	201	PEB	NB-C1B-CHA-C4A
82	SA	201	PEB	NB-C1B-CHA-C4A
82	VA	203	PEB	C2C-CAC-CBC-CGC
82	YA	301	PEB	C2C-CAC-CBC-CGC
82	JB	201	PEB	NB-C1B-CHA-C4A
82	KB	302	PEB	C2C-CAC-CBC-CGC
82	TB	201	PEB	NB-C1B-CHA-C4A
82	DD	202	PEB	NB-C1B-CHA-C4A
82	ED	202	PEB	C2C-CAC-CBC-CGC
82	FD	201	PEB	C3B-CAB-CBB-CGB
82	MD	202	PEB	C2C-CAC-CBC-CGC
82	SD	201	PEB	C2C-CAC-CBC-CGC
82	TD	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	KE	201	PEB	C3B-CAB-CBB-CGB
82	LE	1002	PEB	C2C-CAC-CBC-CGC
82	NE	202	PEB	C2C-CAC-CBC-CGC
82	NE	202	PEB	C3B-CAB-CBB-CGB
82	IF	202	PEB	C3B-CAB-CBB-CGB
82	OF	202	PEB	C3B-CAB-CBB-CGB
82	QF	201	PEB	C3B-CAB-CBB-CGB
82	KG	201	PEB	C3B-CAB-CBB-CGB
82	LG	1002	PEB	C2C-CAC-CBC-CGC
82	NG	201	PEB	C2C-CAC-CBC-CGC
82	NG	201	PEB	C3B-CAB-CBB-CGB
82	QH	201	PEB	C2C-CAC-CBC-CGC
82	QH	202	PEB	NB-C1B-CHA-C4A
82	AI	201	PEB	C2C-CAC-CBC-CGC
82	CI	201	PEB	C2C-CAC-CBC-CGC
82	EI	201	PEB	C2C-CAC-CBC-CGC
82	GI	202	PEB	C2C-CAC-CBC-CGC
82	II	201	PEB	C2C-CAC-CBC-CGC
82	KI	202	PEB	C2C-CAC-CBC-CGC
82	NI	201	PEB	C2C-CAC-CBC-CGC
82	PI	201	PEB	C2C-CAC-CBC-CGC
82	RI	201	PEB	C2C-CAC-CBC-CGC
82	TI	202	PEB	C2C-CAC-CBC-CGC
82	VI	201	PEB	C2C-CAC-CBC-CGC
82	XI	201	PEB	C2C-CAC-CBC-CGC
82	GJ	201	PEB	C3B-CAB-CBB-CGB
82	UJ	202	PEB	C2C-CAC-CBC-CGC
82	IK	202	PEB	C3B-CAB-CBB-CGB
82	OK	202	PEB	C3B-CAB-CBB-CGB
82	QK	201	PEB	C3B-CAB-CBB-CGB
82	QM	203	PEB	C3B-CAB-CBB-CGB
82	YM	201	PEB	C3B-CAB-CBB-CGB
82	AO	304	PEB	C3B-CAB-CBB-CGB
82	UO	201	PEB	NB-C1B-CHA-C4A
82	EP	202	PEB	C2C-CAC-CBC-CGC
82	XP	201	PEB	C2C-CAC-CBC-CGC
82	DQ	202	PEB	NB-C1B-CHA-C4A
82	EQ	202	PEB	C2C-CAC-CBC-CGC
82	FQ	201	PEB	C3B-CAB-CBB-CGB
82	MQ	202	PEB	C2C-CAC-CBC-CGC
82	SQ	201	PEB	C2C-CAC-CBC-CGC
82	TQ	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	Q1	201	PEB	C2C-CAC-CBC-CGC
82	Q1	202	PEB	NB-C1B-CHA-C4A
82	f1	203	PEB	C3B-CAB-CBB-CGB
82	A4	304	PEB	C3B-CAB-CBB-CGB
82	U4	201	PEB	NB-C1B-CHA-C4A
82	j4	203	PEB	C2C-CAC-CBC-CGC
82	k4	202	PEB	C3B-CAB-CBB-CGB
82	e4	202	PEB	C3B-CAB-CBB-CGB
82	f4	201	PEB	C3B-CAB-CBB-CGB
82	g4	202	PEB	C3B-CAB-CBB-CGB
82	F5	203	PEB	C2C-CAC-CBC-CGC
82	L5	203	PEB	C2C-CAC-CBC-CGC
82	O5	201	PEB	C2C-CAC-CBC-CGC
82	E7	201	PEB	C2C-CAC-CBC-CGC
82	J7	203	PEB	C2C-CAC-CBC-CGC
82	O7	201	PEB	NB-C1B-CHA-C4A
82	S7	201	PEB	NB-C1B-CHA-C4A
82	V7	203	PEB	C2C-CAC-CBC-CGC
82	Y7	301	PEB	C2C-CAC-CBC-CGC
82	y8	203	PEB	C2C-CAC-CBC-CGC
82	q8	202	PEB	C2C-CAC-CBC-CGC
82	v8	202	PEB	C3B-CAB-CBB-CGB
82	yC	203	PEB	C2C-CAC-CBC-CGC
82	qC	202	PEB	C2C-CAC-CBC-CGC
82	vC	202	PEB	C3B-CAB-CBB-CGB
82	mE	203	PEB	C3B-CAB-CBB-CGB
82	uF	201	PEB	C2C-CAC-CBC-CGC
82	mG	203	PEB	C3B-CAB-CBB-CGB
82	fH	203	PEB	C3B-CAB-CBB-CGB
82	hJ	202	PEB	C3B-CAB-CBB-CGB
82	tK	203	PEB	C2C-CAC-CBC-CGC
82	jM	201	PEB	C3B-CAB-CBB-CGB
82	kO	202	PEB	C2C-CAC-CBC-CGC
82	kO	203	PEB	C3B-CAB-CBB-CGB
82	eO	202	PEB	C3B-CAB-CBB-CGB
82	fO	201	PEB	C3B-CAB-CBB-CGB
82	gO	202	PEB	C3B-CAB-CBB-CGB
82	Z9	301	PEB	C2C-CAC-CBC-CGC
82	M9	302	PEB	C2C-CAC-CBC-CGC
83	QJ	201	PUB	C3B-CAB-CBB-CGB
83	QM	201	PUB	C3B-CAB-CBB-CGB
83	M5	303	PUB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
83	Z5	303	PUB	C2C-CAC-CBC-CGC
83	xF	305	PUB	C3B-CAB-CBB-CGB
83	xK	305	PUB	C3B-CAB-CBB-CGB
84	BE	1002	CYC	NA-C4A-CHB-C1B
84	BE	1002	CYC	C2A-CAA-CBA-CGA
84	LE	1001	CYC	NA-C4A-CHB-C1B
84	BG	1002	CYC	NA-C4A-CHB-C1B
84	BG	1002	CYC	C2A-CAA-CBA-CGA
84	LG	1001	CYC	NA-C4A-CHB-C1B
84	EO	1001	CYC	C2A-CAA-CBA-CGA
84	JO	1001	CYC	NA-C4A-CHB-C1B
84	LO	1001	CYC	NA-C4A-CHB-C1B
84	A3	1001	CYC	NA-C4A-CHB-C1B
84	B3	1001	CYC	NA-C4A-CHB-C1B
84	C3	1001	CYC	NA-C4A-CHB-C1B
84	D3	1001	CYC	NA-C4A-CHB-C1B
84	E3	1001	CYC	NA-C4A-CHB-C1B
84	F3	1001	CYC	NA-C4A-CHB-C1B
84	G3	1001	CYC	NA-C4A-CHB-C1B
84	H3	1001	CYC	NA-C4A-CHB-C1B
84	I3	1001	CYC	NA-C4A-CHB-C1B
84	J3	1001	CYC	NA-C4A-CHB-C1B
84	K3	1001	CYC	NA-C4A-CHB-C1B
84	M3	1001	CYC	NA-C4A-CHB-C1B
84	N3	1001	CYC	NA-C4A-CHB-C1B
84	O3	1001	CYC	NA-C4A-CHB-C1B
84	P3	1001	CYC	NA-C4A-CHB-C1B
84	Q3	1001	CYC	NA-C4A-CHB-C1B
84	R3	1001	CYC	NA-C4A-CHB-C1B
84	S3	1001	CYC	NA-C4A-CHB-C1B
84	T3	1001	CYC	NA-C4A-CHB-C1B
84	U3	1001	CYC	NA-C4A-CHB-C1B
84	V3	1001	CYC	NA-C4A-CHB-C1B
84	W3	1001	CYC	NA-C4A-CHB-C1B
84	c3	1001	CYC	NA-C4A-CHB-C1B
84	d3	1001	CYC	NA-C4A-CHB-C1B
84	e3	1001	CYC	NA-C4A-CHB-C1B
84	f3	1001	CYC	NA-C4A-CHB-C1B
84	g3	1001	CYC	NA-C4A-CHB-C1B
84	h3	1001	CYC	NA-C4A-CHB-C1B
84	i3	1001	CYC	NA-C4A-CHB-C1B
84	k3	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
84	l3	1001	CYC	NA-C4A-CHB-C1B
84	m3	1001	CYC	NA-C4A-CHB-C1B
84	n3	1001	CYC	NA-C4A-CHB-C1B
84	p3	1001	CYC	NA-C4A-CHB-C1B
84	q3	1001	CYC	NA-C4A-CHB-C1B
84	t3	1001	CYC	NA-C4A-CHB-C1B
84	v3	1001	CYC	NA-C4A-CHB-C1B
84	w3	1001	CYC	NA-C4A-CHB-C1B
84	x3	1001	CYC	NA-C4A-CHB-C1B
84	y3	1001	CYC	NA-C4A-CHB-C1B
84	63	901	CYC	NA-C4A-CHB-C1B
84	73	1001	CYC	NA-C4A-CHB-C1B
84	73	1002	CYC	NA-C4A-CHB-C1B
84	J4	1001	CYC	NA-C4A-CHB-C1B
84	L4	1001	CYC	NA-C4A-CHB-C1B
84	E4	1001	CYC	C2A-CAA-CBA-CGA
87	cL	515	CLA	C3-C5-C6-C7
88	DL	407	LHG	C23-C24-C25-C26
87	AN	802	CLA	O1D-CGD-O2D-CED
87	62	303	CLA	O1D-CGD-O2D-CED
87	A2	801	CLA	O1D-CGD-O2D-CED
87	6N	602	CLA	O1D-CGD-O2D-CED
92	DL	402	LMG	C2-C1-O1-C7
92	dL	407	LMG	C2-C1-O1-C7
95	B6	620	DGD	C2D-C1D-O3G-C3G
95	C6	523	DGD	C2E-C1E-O5D-C6D
95	L6	102	DGD	C2E-C1E-O5D-C6D
95	c6	620	DGD	C2E-C1E-O5D-C6D
88	CL	521	LHG	C26-C27-C28-C29
92	AL	411	LMG	C34-C35-C36-C37
92	CL	519	LMG	C37-C38-C39-C40
92	bL	609	LMG	C31-C32-C33-C34
92	bL	623	LMG	C17-C18-C19-C20
95	lL	101	DGD	C4A-C5A-C6A-C7A
82	NF	202	PEB	C2C-C1C-CHB-C4B
82	NK	202	PEB	C2C-C1C-CHB-C4B
82	DM	202	PEB	C2C-C1C-CHB-C4B
87	BL	621	CLA	C13-C15-C16-C17
87	DL	404	CLA	C15-C16-C17-C18
87	AN	849	CLA	C13-C15-C16-C17
87	BN	825	CLA	C5-C6-C7-C8
87	A2	849	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
87	C6	517	CLA	C10-C11-C12-C13
87	c6	614	CLA	C8-C10-C11-C12
87	cL	509	CLA	C13-C15-C16-C17
87	AN	827	CLA	O1A-CGA-O2A-C1
87	ON	202	CLA	O1A-CGA-O2A-C1
87	12	602	CLA	O1A-CGA-O2A-C1
87	A2	813	CLA	O1A-CGA-O2A-C1
87	A2	827	CLA	O1A-CGA-O2A-C1
87	O2	202	CLA	O1A-CGA-O2A-C1
87	C6	509	CLA	O1A-CGA-O2A-C1
87	d6	406	CLA	O1A-CGA-O2A-C1
87	1N	602	CLA	O1A-CGA-O2A-C1
91	A6	407	PHO	O1A-CGA-O2A-C1
87	DL	404	CLA	C16-C17-C18-C20
87	AN	839	CLA	C16-C17-C18-C19
87	BN	819	CLA	C16-C17-C18-C20
87	IN	102	CLA	C16-C17-C18-C19
87	42	602	CLA	C16-C17-C18-C20
87	82	302	CLA	C16-C17-C18-C20
87	A2	839	CLA	C16-C17-C18-C19
87	B2	818	CLA	C16-C17-C18-C20
87	I2	102	CLA	C16-C17-C18-C19
87	B6	611	CLA	C16-C17-C18-C20
87	C6	510	CLA	C16-C17-C18-C20
87	b6	605	CLA	C16-C17-C18-C19
87	4N	602	CLA	C16-C17-C18-C20
87	8N	303	CLA	C16-C17-C18-C20
92	D6	409	LMG	O6-C5-C6-O5
84	r3	1001	CYC	NB-C1B-CHB-C4A
87	22	605	CLA	C4-C3-C5-C6
87	B6	611	CLA	C4-C3-C5-C6
87	dL	401	CLA	C4-C3-C5-C6
87	2N	301	CLA	C4-C3-C5-C6
94	D6	408	PL9	C35-C34-C36-C37
94	dL	406	PL9	C35-C34-C36-C37
88	DL	407	LHG	C10-C11-C12-C13
92	ML	101	LMG	C13-C14-C15-C16
92	aL	611	LMG	C19-C20-C21-C22
92	bL	610	LMG	C32-C33-C34-C35
95	BN	844	DGD	CDA-CEA-CFA-CGA
95	B2	844	DGD	CDA-CEA-CFA-CGA
95	cL	502	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
87	b6	608	CLA	C2-C3-C5-C6
87	BL	601	CLA	C14-C13-C15-C16
87	BL	602	CLA	C11-C12-C13-C14
87	CL	510	CLA	C11-C10-C8-C9
87	DL	404	CLA	C6-C7-C8-C9
87	AN	840	CLA	C6-C7-C8-C9
87	BN	813	CLA	C6-C7-C8-C9
87	BN	823	CLA	C6-C7-C8-C9
87	A2	840	CLA	C6-C7-C8-C9
87	B2	812	CLA	C6-C7-C8-C9
87	B2	822	CLA	C6-C7-C8-C9
87	C6	512	CLA	C14-C13-C15-C16
87	bL	606	CLA	C6-C7-C8-C9
87	bL	617	CLA	C14-C13-C15-C16
87	cL	505	CLA	C6-C7-C8-C9
91	a6	613	PHO	C11-C12-C13-C14
87	AN	836	CLA	O1D-CGD-O2D-CED
87	A2	836	CLA	O1D-CGD-O2D-CED
87	dL	409	CLA	O1D-CGD-O2D-CED
95	C6	523	DGD	O6D-C5D-C6D-O5D
95	c6	620	DGD	O6D-C5D-C6D-O5D
88	B6	617	LHG	C23-C24-C25-C26
87	CL	507	CLA	C4C-C3C-CAC-CBC
87	BN	817	CLA	C10-C11-C12-C13
87	bL	619	CLA	C10-C11-C12-C13
88	D6	406	LHG	C10-C11-C12-C13
88	m6	102	LHG	C10-C11-C12-C13
88	dL	405	LHG	C10-C11-C12-C13
88	dL	408	LHG	C30-C31-C32-C33
92	CL	519	LMG	C20-C21-C22-C23
95	CL	517	DGD	C8A-C9A-CAA-CBA
95	BN	844	DGD	CBA-CCA-CDA-CEA
95	B2	844	DGD	CBA-CCA-CDA-CEA
95	C6	502	DGD	C5A-C6A-C7A-C8A
95	c6	601	DGD	C5A-C6A-C7A-C8A
95	lL	101	DGD	C5A-C6A-C7A-C8A
100	J2	104	3XQ	C6-C7-C8-C9
87	AN	851	CLA	C15-C16-C17-C18
87	A2	851	CLA	C15-C16-C17-C18
87	d6	406	CLA	C15-C16-C17-C18
87	AN	836	CLA	C2A-CAA-CBA-CGA
87	BN	809	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	BN	827	CLA	C2A-CAA-CBA-CGA
87	A2	836	CLA	C2A-CAA-CBA-CGA
87	B2	808	CLA	C2A-CAA-CBA-CGA
87	B2	827	CLA	C2A-CAA-CBA-CGA
87	bL	620	CLA	C2A-CAA-CBA-CGA
87	cL	514	CLA	C2A-CAA-CBA-CGA
82	SA	201	PEB	C2B-C1B-CHA-C4A
82	UA	201	PEB	C2B-C1B-CHA-C4A
82	JB	201	PEB	C2B-C1B-CHA-C4A
82	TB	201	PEB	C2B-C1B-CHA-C4A
82	HD	202	PEB	C2B-C1B-CHA-C4A
82	SF	202	PEB	C2B-C1B-CHA-C4A
82	QH	202	PEB	C2B-C1B-CHA-C4A
82	SK	202	PEB	C2B-C1B-CHA-C4A
82	UO	201	PEB	C2B-C1B-CHA-C4A
82	HQ	202	PEB	C2B-C1B-CHA-C4A
82	Q1	202	PEB	C2B-C1B-CHA-C4A
82	U4	201	PEB	C2B-C1B-CHA-C4A
82	S7	201	PEB	C2B-C1B-CHA-C4A
82	U7	201	PEB	C2B-C1B-CHA-C4A
84	BE	1002	CYC	C3A-C4A-CHB-C1B
84	LE	1001	CYC	C3A-C4A-CHB-C1B
84	BG	1002	CYC	C3A-C4A-CHB-C1B
84	LG	1001	CYC	C3A-C4A-CHB-C1B
84	JO	1001	CYC	C3A-C4A-CHB-C1B
84	LO	1001	CYC	C3A-C4A-CHB-C1B
84	A3	1001	CYC	C3A-C4A-CHB-C1B
84	B3	1001	CYC	C3A-C4A-CHB-C1B
84	C3	1001	CYC	C3A-C4A-CHB-C1B
84	D3	1001	CYC	C3A-C4A-CHB-C1B
84	E3	1001	CYC	C3A-C4A-CHB-C1B
84	F3	1001	CYC	C3A-C4A-CHB-C1B
84	G3	1001	CYC	C3A-C4A-CHB-C1B
84	H3	1001	CYC	C3A-C4A-CHB-C1B
84	I3	1001	CYC	C3A-C4A-CHB-C1B
84	J3	1001	CYC	C3A-C4A-CHB-C1B
84	K3	1001	CYC	C3A-C4A-CHB-C1B
84	L3	1001	CYC	C3A-C4A-CHB-C1B
84	M3	1001	CYC	C3A-C4A-CHB-C1B
84	N3	1001	CYC	C3A-C4A-CHB-C1B
84	O3	1001	CYC	C3A-C4A-CHB-C1B
84	P3	1001	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
84	Q3	1001	CYC	C3A-C4A-CHB-C1B
84	R3	1001	CYC	C3A-C4A-CHB-C1B
84	S3	1001	CYC	C3A-C4A-CHB-C1B
84	T3	1001	CYC	C3A-C4A-CHB-C1B
84	U3	1001	CYC	C3A-C4A-CHB-C1B
84	V3	1001	CYC	C3A-C4A-CHB-C1B
84	W3	1001	CYC	C3A-C4A-CHB-C1B
84	c3	1001	CYC	C3A-C4A-CHB-C1B
84	d3	1001	CYC	C3A-C4A-CHB-C1B
84	e3	1001	CYC	C3A-C4A-CHB-C1B
84	f3	1001	CYC	C3A-C4A-CHB-C1B
84	g3	1001	CYC	C3A-C4A-CHB-C1B
84	h3	1001	CYC	C3A-C4A-CHB-C1B
84	i3	1001	CYC	C3A-C4A-CHB-C1B
84	j3	1001	CYC	C3A-C4A-CHB-C1B
84	k3	1001	CYC	C3A-C4A-CHB-C1B
84	l3	1001	CYC	C3A-C4A-CHB-C1B
84	m3	1001	CYC	C3A-C4A-CHB-C1B
84	n3	1001	CYC	C3A-C4A-CHB-C1B
84	o3	1001	CYC	C3A-C4A-CHB-C1B
84	p3	1001	CYC	C3A-C4A-CHB-C1B
84	q3	1001	CYC	C3A-C4A-CHB-C1B
84	t3	1001	CYC	C3A-C4A-CHB-C1B
84	u3	1001	CYC	C3A-C4A-CHB-C1B
84	v3	1001	CYC	C3A-C4A-CHB-C1B
84	w3	1001	CYC	C3A-C4A-CHB-C1B
84	x3	1001	CYC	C3A-C4A-CHB-C1B
84	y3	1001	CYC	C3A-C4A-CHB-C1B
84	73	1001	CYC	C3A-C4A-CHB-C1B
84	J4	1001	CYC	C3A-C4A-CHB-C1B
84	L4	1001	CYC	C3A-C4A-CHB-C1B
95	CL	523	DGD	C4E-C5E-C6E-O5E
95	cL	520	DGD	C4E-C5E-C6E-O5E
87	CL	518	CLA	O1A-CGA-O2A-C1
87	AN	813	CLA	O1A-CGA-O2A-C1
87	AN	832	CLA	O1A-CGA-O2A-C1
87	BN	832	CLA	O1A-CGA-O2A-C1
87	A2	832	CLA	O1A-CGA-O2A-C1
87	B2	832	CLA	O1A-CGA-O2A-C1
87	B6	603	CLA	O1A-CGA-O2A-C1
87	bL	622	CLA	O1A-CGA-O2A-C1
87	cL	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
85	BL	617	BCR	C7-C8-C9-C34
85	AN	846	BCR	C36-C18-C19-C20
85	FN	204	BCR	C37-C22-C23-C24
85	JN	102	BCR	C37-C22-C23-C24
85	A2	846	BCR	C36-C18-C19-C20
85	J2	102	BCR	C37-C22-C23-C24
85	B6	602	BCR	C7-C8-C9-C34
103	82	309	ZEX	C27-C28-C29-C39
103	8N	309	ZEX	C27-C28-C29-C39
87	B2	816	CLA	C10-C11-C12-C13
92	yL	101	LMG	C41-C42-C43-C44
95	C6	504	DGD	C2A-C3A-C4A-C5A
100	JN	104	3XQ	C5-C6-C7-C8
82	IF	202	PEB	NA-C4A-CHA-C1B
82	IK	202	PEB	NA-C4A-CHA-C1B
88	AN	844	LHG	O1-C1-C2-C3
88	A2	844	LHG	O1-C1-C2-C3
88	B6	617	LHG	O1-C1-C2-C3
88	aL	607	LHG	O1-C1-C2-C3
85	CL	516	BCR	C7-C8-C9-C10
85	AN	846	BCR	C17-C18-C19-C20
85	BN	842	BCR	C21-C22-C23-C24
85	JN	103	BCR	C11-C12-C13-C14
85	JN	103	BCR	C21-C22-C23-C24
85	A2	846	BCR	C17-C18-C19-C20
85	B2	842	BCR	C21-C22-C23-C24
85	J2	103	BCR	C11-C12-C13-C14
85	J2	103	BCR	C21-C22-C23-C24
85	B6	602	BCR	C7-C8-C9-C10
103	82	309	ZEX	C27-C28-C29-C30
103	8N	309	ZEX	C27-C28-C29-C30
87	CL	508	CLA	C3-C5-C6-C7
87	22	602	CLA	C3-C5-C6-C7
87	2N	303	CLA	C3-C5-C6-C7
88	A2	843	LHG	O9-C7-O7-C5
92	yL	101	LMG	O9-C10-O7-C8
87	AN	835	CLA	C10-C11-C12-C13
87	A2	835	CLA	C10-C11-C12-C13
87	C6	515	CLA	C10-C11-C12-C13
87	c6	616	CLA	C10-C11-C12-C13
92	ML	101	LMG	C11-C10-O7-C8
92	D6	409	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
92	mL	101	LMG	C11-C10-O7-C8
84	KO	1001	CYC	C2B-C3B-CAB-CBB
84	K4	1001	CYC	C2B-C3B-CAB-CBB
88	I6	101	LHG	C33-C34-C35-C36
92	A6	408	LMG	C19-C20-C21-C22
92	J6	102	LMG	C13-C14-C15-C16
92	j6	101	LMG	C13-C14-C15-C16
95	J6	101	DGD	C5A-C6A-C7A-C8A
92	b6	619	LMG	C28-C29-C30-C31
87	CL	506	CLA	O1D-CGD-O2D-CED
87	d6	406	CLA	O1D-CGD-O2D-CED
87	cL	505	CLA	O1D-CGD-O2D-CED
87	BL	604	CLA	C10-C11-C12-C13
88	AL	406	LHG	C13-C14-C15-C16
88	M6	101	LHG	C11-C10-C9-C8
88	d6	407	LHG	C11-C10-C9-C8
92	D6	409	LMG	C21-C22-C23-C24
92	b6	623	LMG	C14-C15-C16-C17
92	b6	623	LMG	C15-C16-C17-C18
92	m6	103	LMG	C11-C12-C13-C14
95	AL	414	DGD	CAB-CBB-CCB-CDB
95	hL	101	DGD	CAA-CBA-CCA-CDA
95	JL	101	DGD	O6E-C5E-C6E-O5E
87	AL	404	CLA	C4B-C3B-CAB-CBB
87	BL	609	CLA	C4B-C3B-CAB-CBB
87	CL	505	CLA	C4B-C3B-CAB-CBB
87	CL	508	CLA	C4B-C3B-CAB-CBB
87	CL	509	CLA	C4B-C3B-CAB-CBB
87	CL	515	CLA	C4B-C3B-CAB-CBB
87	AN	802	CLA	C4B-C3B-CAB-CBB
87	AN	807	CLA	C4B-C3B-CAB-CBB
87	AN	814	CLA	C4B-C3B-CAB-CBB
87	AN	824	CLA	C4B-C3B-CAB-CBB
87	AN	831	CLA	C4B-C3B-CAB-CBB
87	AN	841	CLA	C4B-C3B-CAB-CBB
87	BN	811	CLA	C4B-C3B-CAB-CBB
87	BN	813	CLA	C4B-C3B-CAB-CBB
87	BN	821	CLA	C4B-C3B-CAB-CBB
87	BN	822	CLA	C4B-C3B-CAB-CBB
87	FN	201	CLA	C4B-C3B-CAB-CBB
87	IN	102	CLA	C4B-C3B-CAB-CBB
87	KN	102	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	LN	203	CLA	C4B-C3B-CAB-CBB
87	RN	202	CLA	C4B-C3B-CAB-CBB
87	RN	204	CLA	C4B-C3B-CAB-CBB
87	12	604	CLA	C4B-C3B-CAB-CBB
87	12	608	CLA	C4B-C3B-CAB-CBB
87	12	609	CLA	C4B-C3B-CAB-CBB
87	12	610	CLA	C4B-C3B-CAB-CBB
87	12	611	CLA	C4B-C3B-CAB-CBB
87	22	606	CLA	C4B-C3B-CAB-CBB
87	32	304	CLA	C4B-C3B-CAB-CBB
87	32	306	CLA	C4B-C3B-CAB-CBB
87	32	310	CLA	C4B-C3B-CAB-CBB
87	32	312	CLA	C4B-C3B-CAB-CBB
87	42	607	CLA	C4B-C3B-CAB-CBB
87	42	609	CLA	C4B-C3B-CAB-CBB
87	42	611	CLA	C4B-C3B-CAB-CBB
87	52	604	CLA	C4B-C3B-CAB-CBB
87	62	305	CLA	C4B-C3B-CAB-CBB
87	62	306	CLA	C4B-C3B-CAB-CBB
87	62	307	CLA	C4B-C3B-CAB-CBB
87	62	310	CLA	C4B-C3B-CAB-CBB
87	72	603	CLA	C4B-C3B-CAB-CBB
87	72	608	CLA	C4B-C3B-CAB-CBB
87	82	303	CLA	C4B-C3B-CAB-CBB
87	82	307	CLA	C4B-C3B-CAB-CBB
87	A2	801	CLA	C4B-C3B-CAB-CBB
87	A2	807	CLA	C4B-C3B-CAB-CBB
87	A2	814	CLA	C4B-C3B-CAB-CBB
87	A2	824	CLA	C4B-C3B-CAB-CBB
87	A2	831	CLA	C4B-C3B-CAB-CBB
87	A2	841	CLA	C4B-C3B-CAB-CBB
87	B2	810	CLA	C4B-C3B-CAB-CBB
87	B2	812	CLA	C4B-C3B-CAB-CBB
87	B2	820	CLA	C4B-C3B-CAB-CBB
87	B2	821	CLA	C4B-C3B-CAB-CBB
87	F2	202	CLA	C4B-C3B-CAB-CBB
87	I2	102	CLA	C4B-C3B-CAB-CBB
87	K2	101	CLA	C4B-C3B-CAB-CBB
87	K2	103	CLA	C4B-C3B-CAB-CBB
87	L2	203	CLA	C4B-C3B-CAB-CBB
87	R2	202	CLA	C4B-C3B-CAB-CBB
87	R2	204	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	B6	613	CLA	C4B-C3B-CAB-CBB
87	c6	612	CLA	C4B-C3B-CAB-CBB
87	bL	606	CLA	C4B-C3B-CAB-CBB
87	bL	608	CLA	C4B-C3B-CAB-CBB
87	cL	506	CLA	C4B-C3B-CAB-CBB
87	cL	507	CLA	C4B-C3B-CAB-CBB
87	cL	516	CLA	C4B-C3B-CAB-CBB
87	cL	517	CLA	C4B-C3B-CAB-CBB
87	dL	401	CLA	C4B-C3B-CAB-CBB
87	dL	404	CLA	C4B-C3B-CAB-CBB
87	1N	604	CLA	C4B-C3B-CAB-CBB
87	1N	608	CLA	C4B-C3B-CAB-CBB
87	1N	609	CLA	C4B-C3B-CAB-CBB
87	1N	610	CLA	C4B-C3B-CAB-CBB
87	1N	611	CLA	C4B-C3B-CAB-CBB
87	3N	305	CLA	C4B-C3B-CAB-CBB
87	3N	307	CLA	C4B-C3B-CAB-CBB
87	3N	310	CLA	C4B-C3B-CAB-CBB
87	3N	312	CLA	C4B-C3B-CAB-CBB
87	4N	607	CLA	C4B-C3B-CAB-CBB
87	4N	609	CLA	C4B-C3B-CAB-CBB
87	4N	611	CLA	C4B-C3B-CAB-CBB
87	5N	604	CLA	C4B-C3B-CAB-CBB
87	6N	604	CLA	C4B-C3B-CAB-CBB
87	6N	605	CLA	C4B-C3B-CAB-CBB
87	6N	606	CLA	C4B-C3B-CAB-CBB
87	6N	609	CLA	C4B-C3B-CAB-CBB
87	7N	603	CLA	C4B-C3B-CAB-CBB
87	7N	608	CLA	C4B-C3B-CAB-CBB
87	8N	304	CLA	C4B-C3B-CAB-CBB
87	8N	307	CLA	C4B-C3B-CAB-CBB
87	BL	608	CLA	C16-C17-C18-C19
87	AN	812	CLA	C6-C7-C8-C9
87	AN	812	CLA	C6-C7-C8-C10
87	BN	823	CLA	C16-C17-C18-C20
87	BN	835	CLA	C16-C17-C18-C19
87	22	605	CLA	C6-C7-C8-C9
87	A2	812	CLA	C6-C7-C8-C9
87	A2	812	CLA	C6-C7-C8-C10
87	B2	822	CLA	C16-C17-C18-C20
87	B2	835	CLA	C16-C17-C18-C19
87	C6	519	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
87	b6	604	CLA	C16-C17-C18-C20
87	b6	617	CLA	C16-C17-C18-C19
87	c6	604	CLA	C16-C17-C18-C20
87	c6	615	CLA	C6-C7-C8-C10
87	2N	301	CLA	C6-C7-C8-C9
95	L6	102	DGD	O6E-C1E-O5D-C6D
87	HL	102	CLA	C13-C15-C16-C17
87	AN	810	CLA	C10-C11-C12-C13
87	AN	820	CLA	C5-C6-C7-C8
87	AN	823	CLA	C15-C16-C17-C18
87	A2	810	CLA	C10-C11-C12-C13
87	A2	820	CLA	C5-C6-C7-C8
87	A2	823	CLA	C15-C16-C17-C18
87	b6	618	CLA	C10-C11-C12-C13
88	I6	101	LHG	C10-C11-C12-C13
100	JN	104	3XQ	C13-C14-C15-C16
95	BL	614	DGD	C4D-C5D-C6D-O5D
83	AH	304	PUB	C3C-C2C-CAC-CBC
83	A1	304	PUB	C3C-C2C-CAC-CBC
87	dL	401	CLA	O1D-CGD-O2D-CED
87	1N	603	CLA	O1D-CGD-O2D-CED
88	CL	521	LHG	C27-C28-C29-C30
88	AN	844	LHG	C25-C26-C27-C28
88	A2	844	LHG	C25-C26-C27-C28
88	iL	101	LHG	C27-C28-C29-C30
92	B6	622	LMG	C15-C16-C17-C18
95	AL	414	DGD	CBA-CCA-CDA-CEA
95	BL	614	DGD	C3B-C4B-C5B-C6B
95	b6	622	DGD	C3A-C4A-C5A-C6A
95	cL	502	DGD	C5A-C6A-C7A-C8A
88	mL	102	LHG	C23-C24-C25-C26
87	B6	604	CLA	C5-C6-C7-C8
87	c6	604	CLA	C10-C11-C12-C13
87	nL	101	CLA	C8-C10-C11-C12
91	AL	410	PHO	C8-C10-C11-C12
91	aL	610	PHO	C8-C10-C11-C12
87	22	605	CLA	O1A-CGA-O2A-C1
87	2N	301	CLA	O1A-CGA-O2A-C1
91	a6	613	PHO	O1A-CGA-O2A-C1
88	C6	505	LHG	C27-C28-C29-C30
88	I6	101	LHG	C27-C28-C29-C30
92	J6	102	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
92	j6	101	LMG	C11-C12-C13-C14
92	bL	609	LMG	C32-C33-C34-C35
95	hL	101	DGD	C6A-C7A-C8A-C9A
100	J2	104	3XQ	C13-C14-C15-C16
87	B6	614	CLA	C3-C5-C6-C7
87	c6	615	CLA	C3-C5-C6-C7
87	BL	609	CLA	CBA-CGA-O2A-C1
87	BN	831	CLA	CBA-CGA-O2A-C1
87	B2	831	CLA	CBA-CGA-O2A-C1
87	c6	605	CLA	CBA-CGA-O2A-C1
92	D6	407	LMG	C29-C28-O8-C9
92	qL	301	LMG	C29-C28-O8-C9
88	bL	612	LHG	C29-C30-C31-C32
88	iL	101	LHG	C34-C35-C36-C37
92	BL	611	LMG	C17-C18-C19-C20
92	C6	501	LMG	C41-C42-C43-C44
92	m6	101	LMG	C11-C12-C13-C14
95	D6	410	DGD	C6B-C7B-C8B-C9B
87	AN	820	CLA	O1D-CGD-O2D-CED
87	AN	823	CLA	O1D-CGD-O2D-CED
87	BN	831	CLA	O1D-CGD-O2D-CED
87	BN	833	CLA	O1D-CGD-O2D-CED
87	LN	206	CLA	O1D-CGD-O2D-CED
87	12	603	CLA	O1D-CGD-O2D-CED
87	A2	820	CLA	O1D-CGD-O2D-CED
87	A2	823	CLA	O1D-CGD-O2D-CED
87	B2	831	CLA	O1D-CGD-O2D-CED
87	B2	833	CLA	O1D-CGD-O2D-CED
87	CL	514	CLA	C3A-C2A-CAA-CBA
87	DL	404	CLA	C3A-C2A-CAA-CBA
87	AN	805	CLA	C3A-C2A-CAA-CBA
87	AN	807	CLA	C3A-C2A-CAA-CBA
87	AN	808	CLA	C3A-C2A-CAA-CBA
87	AN	809	CLA	C3A-C2A-CAA-CBA
87	AN	826	CLA	C3A-C2A-CAA-CBA
87	AN	833	CLA	C3A-C2A-CAA-CBA
87	AN	837	CLA	C3A-C2A-CAA-CBA
87	AN	852	CLA	C3A-C2A-CAA-CBA
87	BN	806	CLA	C3A-C2A-CAA-CBA
87	BN	811	CLA	C3A-C2A-CAA-CBA
87	BN	812	CLA	C3A-C2A-CAA-CBA
87	BN	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	BN	822	CLA	C3A-C2A-CAA-CBA
87	12	602	CLA	C3A-C2A-CAA-CBA
87	12	605	CLA	C3A-C2A-CAA-CBA
87	12	611	CLA	C3A-C2A-CAA-CBA
87	22	608	CLA	C3A-C2A-CAA-CBA
87	32	305	CLA	C3A-C2A-CAA-CBA
87	32	313	CLA	C3A-C2A-CAA-CBA
87	42	606	CLA	C3A-C2A-CAA-CBA
87	62	313	CLA	C3A-C2A-CAA-CBA
87	72	605	CLA	C3A-C2A-CAA-CBA
87	72	606	CLA	C3A-C2A-CAA-CBA
87	A2	805	CLA	C3A-C2A-CAA-CBA
87	A2	807	CLA	C3A-C2A-CAA-CBA
87	A2	808	CLA	C3A-C2A-CAA-CBA
87	A2	809	CLA	C3A-C2A-CAA-CBA
87	A2	826	CLA	C3A-C2A-CAA-CBA
87	A2	833	CLA	C3A-C2A-CAA-CBA
87	A2	837	CLA	C3A-C2A-CAA-CBA
87	A2	852	CLA	C3A-C2A-CAA-CBA
87	B2	805	CLA	C3A-C2A-CAA-CBA
87	B2	810	CLA	C3A-C2A-CAA-CBA
87	B2	811	CLA	C3A-C2A-CAA-CBA
87	B2	812	CLA	C3A-C2A-CAA-CBA
87	B2	821	CLA	C3A-C2A-CAA-CBA
87	C6	518	CLA	C3A-C2A-CAA-CBA
87	C6	519	CLA	C3A-C2A-CAA-CBA
87	b6	608	CLA	C3A-C2A-CAA-CBA
87	c6	615	CLA	C3A-C2A-CAA-CBA
87	cL	516	CLA	C3A-C2A-CAA-CBA
87	dL	402	CLA	C3A-C2A-CAA-CBA
87	1N	602	CLA	C3A-C2A-CAA-CBA
87	1N	605	CLA	C3A-C2A-CAA-CBA
87	1N	611	CLA	C3A-C2A-CAA-CBA
87	2N	308	CLA	C3A-C2A-CAA-CBA
87	3N	306	CLA	C3A-C2A-CAA-CBA
87	3N	313	CLA	C3A-C2A-CAA-CBA
87	4N	606	CLA	C3A-C2A-CAA-CBA
87	6N	612	CLA	C3A-C2A-CAA-CBA
87	7N	605	CLA	C3A-C2A-CAA-CBA
87	7N	606	CLA	C3A-C2A-CAA-CBA
87	b6	618	CLA	C5-C6-C7-C8
95	AL	415	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
88	BL	610	LHG	C9-C10-C11-C12
87	12	602	CLA	O1D-CGD-O2D-CED
87	L2	206	CLA	O1D-CGD-O2D-CED
87	bL	616	CLA	O1D-CGD-O2D-CED
87	1N	602	CLA	O1D-CGD-O2D-CED
87	cL	506	CLA	O1A-CGA-O2A-C1
87	BN	822	CLA	C6-C7-C8-C9
87	B2	821	CLA	C6-C7-C8-C9
87	C6	510	CLA	C16-C17-C18-C19
87	C6	519	CLA	C6-C7-C8-C9
87	D6	402	CLA	C16-C17-C18-C19
87	K6	101	CLA	C16-C17-C18-C20
87	b6	607	CLA	C16-C17-C18-C19
87	b6	607	CLA	C16-C17-C18-C20
87	c6	604	CLA	C16-C17-C18-C19
87	c6	615	CLA	C6-C7-C8-C9
87	nL	101	CLA	C16-C17-C18-C19
92	CL	519	LMG	C35-C36-C37-C38
92	B6	619	LMG	C13-C14-C15-C16
92	b6	620	LMG	O1-C7-C8-C9
87	AN	831	CLA	CBD-CGD-O2D-CED
87	BN	836	CLA	CBD-CGD-O2D-CED
87	A2	831	CLA	CBD-CGD-O2D-CED
87	B2	836	CLA	CBD-CGD-O2D-CED
87	bL	608	CLA	CBD-CGD-O2D-CED
87	cL	512	CLA	CBD-CGD-O2D-CED
84	BE	1001	CYC	C4B-C3B-CAB-CBB
84	BG	1001	CYC	C4B-C3B-CAB-CBB
84	FO	1001	CYC	C4B-C3B-CAB-CBB
84	W3	1001	CYC	C4B-C3B-CAB-CBB
84	y3	1001	CYC	C4B-C3B-CAB-CBB
84	F4	1001	CYC	C4B-C3B-CAB-CBB
82	IA	201	PEB	NC-C1C-CHB-C4B
82	YE	202	PEB	NC-C1C-CHB-C4B
82	SF	203	PEB	NC-C1C-CHB-C4B
82	YG	202	PEB	NC-C1C-CHB-C4B
82	SK	203	PEB	NC-C1C-CHB-C4B
82	WK	203	PEB	NC-C1C-CHB-C4B
82	OQ	202	PEB	NC-C1C-CHB-C4B
82	I7	201	PEB	NC-C1C-CHB-C4B
82	s8	203	PEB	NC-C1C-CHB-C4B
82	w8	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	sC	203	PEB	NC-C1C-CHB-C4B
82	wC	203	PEB	NC-C1C-CHB-C4B
82	kE	202	PEB	NC-C1C-CHB-C4B
82	kG	202	PEB	NC-C1C-CHB-C4B
82	cH	202	PEB	NC-C1C-CHB-C4B
83	AM	303	PUB	NB-C4B-CHB-C1C
92	k6	101	LMG	O6-C5-C6-O5
92	CL	519	LMG	C12-C13-C14-C15
87	bL	614	CLA	O1A-CGA-O2A-C1
87	AN	851	CLA	C4-C3-C5-C6
87	A2	851	CLA	C4-C3-C5-C6
87	b6	610	CLA	C4-C3-C5-C6
94	a6	601	PL9	C35-C34-C36-C37
87	c6	606	CLA	CBA-CGA-O2A-C1
95	cL	519	DGD	C4E-C5E-C6E-O5E
87	DL	403	CLA	C2-C3-C5-C6
87	AN	851	CLA	C2-C3-C5-C6
87	BN	813	CLA	C2-C3-C5-C6
87	A2	851	CLA	C2-C3-C5-C6
87	B2	812	CLA	C2-C3-C5-C6
87	B6	610	CLA	C2-C3-C5-C6
87	B6	611	CLA	C2-C3-C5-C6
87	c6	608	CLA	C2-C3-C5-C6
87	dL	401	CLA	C2-C3-C5-C6
94	DL	401	PL9	C12-C11-C9-C8
94	a6	601	PL9	C12-C11-C9-C8
94	dL	406	PL9	C33-C34-C36-C37
88	iL	101	LHG	C8-C7-O7-C5
95	AL	416	DGD	C2B-C1B-O2G-C2G
82	XA	203	PEB	C3C-C2C-CAC-CBC
82	KB	301	PEB	C3C-C2C-CAC-CBC
82	ED	201	PEB	C3C-C2C-CAC-CBC
82	SP	203	PEB	C3C-C2C-CAC-CBC
82	EQ	201	PEB	C3C-C2C-CAC-CBC
82	X7	203	PEB	C3C-C2C-CAC-CBC
82	qF	202	PEB	C3C-C2C-CAC-CBC
82	qK	202	PEB	C3C-C2C-CAC-CBC
83	AH	303	PUB	C2B-C3B-CAB-CBB
83	A1	303	PUB	C2B-C3B-CAB-CBB
95	DL	408	DGD	CAB-CBB-CCB-CDB
82	YE	202	PEB	C2C-C1C-CHB-C4B
82	YG	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	JJ	202	PEB	C2C-C1C-CHB-C4B
82	LJ	202	PEB	C2C-C1C-CHB-C4B
82	RJ	202	PEB	C2C-C1C-CHB-C4B
82	f1	203	PEB	C2C-C1C-CHB-C4B
82	g4	203	PEB	C2C-C1C-CHB-C4B
82	H5	202	PEB	C2C-C1C-CHB-C4B
82	J5	203	PEB	C2C-C1C-CHB-C4B
82	gF	202	PEB	C2C-C1C-CHB-C4B
82	uF	201	PEB	C2C-C1C-CHB-C4B
82	fH	203	PEB	C2C-C1C-CHB-C4B
82	gK	202	PEB	C2C-C1C-CHB-C4B
82	tK	203	PEB	C2C-C1C-CHB-C4B
82	gO	203	PEB	C2C-C1C-CHB-C4B
87	BL	604	CLA	C2A-CAA-CBA-CGA
88	B6	617	LHG	O1-C1-C2-O2
88	C6	522	LHG	O1-C1-C2-O2
88	I6	101	LHG	O1-C1-C2-O2
88	bL	612	LHG	O1-C1-C2-O2
88	cL	501	LHG	O1-C1-C2-O2
87	b6	617	CLA	C15-C16-C17-C18
95	AL	416	DGD	C1B-C2B-C3B-C4B
95	b6	621	DGD	C1B-C2B-C3B-C4B
87	cL	508	CLA	O1A-CGA-O2A-C1
87	4N	608	CLA	O1A-CGA-O2A-C1
95	C6	504	DGD	C1A-C2A-C3A-C4A
92	A6	408	LMG	O6-C5-C6-O5
87	AN	839	CLA	C16-C17-C18-C20
87	A2	839	CLA	C16-C17-C18-C20
87	AL	404	CLA	C2B-C3B-CAB-CBB
87	BL	609	CLA	C2B-C3B-CAB-CBB
87	CL	504	CLA	C2B-C3B-CAB-CBB
87	CL	505	CLA	C2B-C3B-CAB-CBB
87	CL	506	CLA	C2B-C3B-CAB-CBB
87	CL	508	CLA	C2B-C3B-CAB-CBB
87	CL	509	CLA	C2B-C3B-CAB-CBB
87	CL	515	CLA	C2B-C3B-CAB-CBB
87	HL	102	CLA	C2B-C3B-CAB-CBB
87	AN	802	CLA	C2B-C3B-CAB-CBB
87	AN	805	CLA	C2B-C3B-CAB-CBB
87	AN	807	CLA	C2B-C3B-CAB-CBB
87	AN	812	CLA	C2B-C3B-CAB-CBB
87	AN	814	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	AN	815	CLA	C2B-C3B-CAB-CBB
87	AN	816	CLA	C2B-C3B-CAB-CBB
87	AN	828	CLA	C2B-C3B-CAB-CBB
87	AN	831	CLA	C2B-C3B-CAB-CBB
87	AN	838	CLA	C2B-C3B-CAB-CBB
87	AN	841	CLA	C2B-C3B-CAB-CBB
87	BN	808	CLA	C2B-C3B-CAB-CBB
87	BN	811	CLA	C2B-C3B-CAB-CBB
87	BN	813	CLA	C2B-C3B-CAB-CBB
87	BN	816	CLA	C2B-C3B-CAB-CBB
87	BN	820	CLA	C2B-C3B-CAB-CBB
87	BN	821	CLA	C2B-C3B-CAB-CBB
87	BN	822	CLA	C2B-C3B-CAB-CBB
87	BN	825	CLA	C2B-C3B-CAB-CBB
87	BN	828	CLA	C2B-C3B-CAB-CBB
87	BN	829	CLA	C2B-C3B-CAB-CBB
87	FN	201	CLA	C2B-C3B-CAB-CBB
87	IN	102	CLA	C2B-C3B-CAB-CBB
87	KN	102	CLA	C2B-C3B-CAB-CBB
87	LN	203	CLA	C2B-C3B-CAB-CBB
87	LN	204	CLA	C2B-C3B-CAB-CBB
87	RN	201	CLA	C2B-C3B-CAB-CBB
87	RN	202	CLA	C2B-C3B-CAB-CBB
87	RN	204	CLA	C2B-C3B-CAB-CBB
87	12	602	CLA	C2B-C3B-CAB-CBB
87	12	604	CLA	C2B-C3B-CAB-CBB
87	12	605	CLA	C2B-C3B-CAB-CBB
87	12	608	CLA	C2B-C3B-CAB-CBB
87	12	609	CLA	C2B-C3B-CAB-CBB
87	12	610	CLA	C2B-C3B-CAB-CBB
87	12	611	CLA	C2B-C3B-CAB-CBB
87	22	606	CLA	C2B-C3B-CAB-CBB
87	22	608	CLA	C2B-C3B-CAB-CBB
87	32	306	CLA	C2B-C3B-CAB-CBB
87	32	309	CLA	C2B-C3B-CAB-CBB
87	32	310	CLA	C2B-C3B-CAB-CBB
87	32	311	CLA	C2B-C3B-CAB-CBB
87	32	312	CLA	C2B-C3B-CAB-CBB
87	32	313	CLA	C2B-C3B-CAB-CBB
87	42	607	CLA	C2B-C3B-CAB-CBB
87	42	609	CLA	C2B-C3B-CAB-CBB
87	42	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	52	601	CLA	C2B-C3B-CAB-CBB
87	52	604	CLA	C2B-C3B-CAB-CBB
87	52	610	CLA	C2B-C3B-CAB-CBB
87	62	304	CLA	C2B-C3B-CAB-CBB
87	62	305	CLA	C2B-C3B-CAB-CBB
87	62	306	CLA	C2B-C3B-CAB-CBB
87	62	307	CLA	C2B-C3B-CAB-CBB
87	62	310	CLA	C2B-C3B-CAB-CBB
87	72	603	CLA	C2B-C3B-CAB-CBB
87	72	606	CLA	C2B-C3B-CAB-CBB
87	72	608	CLA	C2B-C3B-CAB-CBB
87	72	609	CLA	C2B-C3B-CAB-CBB
87	82	305	CLA	C2B-C3B-CAB-CBB
87	82	307	CLA	C2B-C3B-CAB-CBB
87	A2	801	CLA	C2B-C3B-CAB-CBB
87	A2	805	CLA	C2B-C3B-CAB-CBB
87	A2	807	CLA	C2B-C3B-CAB-CBB
87	A2	812	CLA	C2B-C3B-CAB-CBB
87	A2	814	CLA	C2B-C3B-CAB-CBB
87	A2	815	CLA	C2B-C3B-CAB-CBB
87	A2	816	CLA	C2B-C3B-CAB-CBB
87	A2	828	CLA	C2B-C3B-CAB-CBB
87	A2	831	CLA	C2B-C3B-CAB-CBB
87	A2	838	CLA	C2B-C3B-CAB-CBB
87	A2	841	CLA	C2B-C3B-CAB-CBB
87	B2	807	CLA	C2B-C3B-CAB-CBB
87	B2	810	CLA	C2B-C3B-CAB-CBB
87	B2	812	CLA	C2B-C3B-CAB-CBB
87	B2	815	CLA	C2B-C3B-CAB-CBB
87	B2	819	CLA	C2B-C3B-CAB-CBB
87	B2	820	CLA	C2B-C3B-CAB-CBB
87	B2	821	CLA	C2B-C3B-CAB-CBB
87	B2	824	CLA	C2B-C3B-CAB-CBB
87	B2	828	CLA	C2B-C3B-CAB-CBB
87	B2	829	CLA	C2B-C3B-CAB-CBB
87	F2	202	CLA	C2B-C3B-CAB-CBB
87	I2	102	CLA	C2B-C3B-CAB-CBB
87	K2	101	CLA	C2B-C3B-CAB-CBB
87	K2	103	CLA	C2B-C3B-CAB-CBB
87	L2	203	CLA	C2B-C3B-CAB-CBB
87	L2	204	CLA	C2B-C3B-CAB-CBB
87	R2	201	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	R2	202	CLA	C2B-C3B-CAB-CBB
87	R2	204	CLA	C2B-C3B-CAB-CBB
87	B6	613	CLA	C2B-C3B-CAB-CBB
87	B6	616	CLA	C2B-C3B-CAB-CBB
87	c6	612	CLA	C2B-C3B-CAB-CBB
87	d6	406	CLA	C2B-C3B-CAB-CBB
87	bL	604	CLA	C2B-C3B-CAB-CBB
87	bL	606	CLA	C2B-C3B-CAB-CBB
87	bL	608	CLA	C2B-C3B-CAB-CBB
87	bL	622	CLA	C2B-C3B-CAB-CBB
87	cL	507	CLA	C2B-C3B-CAB-CBB
87	cL	516	CLA	C2B-C3B-CAB-CBB
87	cL	517	CLA	C2B-C3B-CAB-CBB
87	dL	401	CLA	C2B-C3B-CAB-CBB
87	dL	404	CLA	C2B-C3B-CAB-CBB
87	1N	602	CLA	C2B-C3B-CAB-CBB
87	1N	604	CLA	C2B-C3B-CAB-CBB
87	1N	605	CLA	C2B-C3B-CAB-CBB
87	1N	608	CLA	C2B-C3B-CAB-CBB
87	1N	609	CLA	C2B-C3B-CAB-CBB
87	1N	610	CLA	C2B-C3B-CAB-CBB
87	1N	611	CLA	C2B-C3B-CAB-CBB
87	2N	306	CLA	C2B-C3B-CAB-CBB
87	2N	308	CLA	C2B-C3B-CAB-CBB
87	3N	307	CLA	C2B-C3B-CAB-CBB
87	3N	309	CLA	C2B-C3B-CAB-CBB
87	3N	310	CLA	C2B-C3B-CAB-CBB
87	3N	311	CLA	C2B-C3B-CAB-CBB
87	3N	312	CLA	C2B-C3B-CAB-CBB
87	3N	313	CLA	C2B-C3B-CAB-CBB
87	4N	607	CLA	C2B-C3B-CAB-CBB
87	4N	609	CLA	C2B-C3B-CAB-CBB
87	4N	611	CLA	C2B-C3B-CAB-CBB
87	5N	601	CLA	C2B-C3B-CAB-CBB
87	5N	604	CLA	C2B-C3B-CAB-CBB
87	5N	610	CLA	C2B-C3B-CAB-CBB
87	6N	603	CLA	C2B-C3B-CAB-CBB
87	6N	604	CLA	C2B-C3B-CAB-CBB
87	6N	605	CLA	C2B-C3B-CAB-CBB
87	6N	606	CLA	C2B-C3B-CAB-CBB
87	6N	609	CLA	C2B-C3B-CAB-CBB
87	7N	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	7N	606	CLA	C2B-C3B-CAB-CBB
87	7N	608	CLA	C2B-C3B-CAB-CBB
87	7N	609	CLA	C2B-C3B-CAB-CBB
87	8N	306	CLA	C2B-C3B-CAB-CBB
87	8N	307	CLA	C2B-C3B-CAB-CBB
87	BL	605	CLA	C13-C15-C16-C17
87	CL	505	CLA	C10-C11-C12-C13
92	m6	101	LMG	C16-C17-C18-C19
95	BN	844	DGD	C9B-CAB-CBB-CCB
95	B2	844	DGD	C9B-CAB-CBB-CCB
87	c6	609	CLA	C3-C5-C6-C7
95	cL	519	DGD	C2A-C1A-O1G-C1G
88	L6	101	LHG	C18-C19-C20-C21
88	l6	101	LHG	C18-C19-C20-C21
95	JL	101	DGD	C4A-C5A-C6A-C7A
87	CL	508	CLA	O1A-CGA-O2A-C1
87	42	608	CLA	O1A-CGA-O2A-C1
87	62	309	CLA	O1A-CGA-O2A-C1
87	C6	511	CLA	O1A-CGA-O2A-C1
87	D6	403	CLA	O1A-CGA-O2A-C1
87	6N	608	CLA	O1A-CGA-O2A-C1
92	bL	609	LMG	C10-C11-C12-C13
87	CL	515	CLA	C8-C10-C11-C12
88	AL	406	LHG	C28-C29-C30-C31
88	m6	102	LHG	C12-C13-C14-C15
92	BL	612	LMG	C13-C14-C15-C16
92	bL	624	LMG	C29-C30-C31-C32
95	C6	521	DGD	C8A-C9A-CAA-CBA
95	hL	101	DGD	C2A-C3A-C4A-C5A
88	iL	101	LHG	O9-C7-O7-C5
92	ML	101	LMG	O9-C10-O7-C8
92	mL	101	LMG	O9-C10-O7-C8
87	bL	619	CLA	C2-C1-O2A-CGA
87	dL	401	CLA	C2-C1-O2A-CGA
88	AN	843	LHG	C25-C26-C27-C28
88	A2	843	LHG	C25-C26-C27-C28
88	a6	610	LHG	C25-C26-C27-C28
92	b6	620	LMG	C29-C30-C31-C32
92	dL	407	LMG	C29-C30-C31-C32
87	CL	507	CLA	C13-C15-C16-C17
87	AN	830	CLA	C8-C10-C11-C12
87	A2	830	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
87	A6	402	CLA	C13-C15-C16-C17
87	C6	510	CLA	C13-C15-C16-C17
87	C6	520	CLA	C10-C11-C12-C13
87	a6	608	CLA	C8-C10-C11-C12
87	bL	618	CLA	C10-C11-C12-C13
87	bL	621	CLA	C15-C16-C17-C18
87	cL	517	CLA	C8-C10-C11-C12
82	GA	202	PEB	C4D-C3D-CAD-CBD
82	IA	201	PEB	C4D-C3D-CAD-CBD
82	YA	301	PEB	C4D-C3D-CAD-CBD
82	IB	202	PEB	C4D-C3D-CAD-CBD
82	OB	201	PEB	C4D-C3D-CAD-CBD
82	AD	301	PEB	C4D-C3D-CAD-CBD
82	HD	202	PEB	C4D-C3D-CAD-CBD
82	QD	202	PEB	C4D-C3D-CAD-CBD
82	IF	202	PEB	C4D-C3D-CAD-CBD
82	OF	202	PEB	C4D-C3D-CAD-CBD
82	RF	202	PEB	C4D-C3D-CAD-CBD
82	TH	201	PEB	C4D-C3D-CAD-CBD
82	WH	201	PEB	C4D-C3D-CAD-CBD
82	AI	203	PEB	C4D-C3D-CAD-CBD
82	BI	202	PEB	C4D-C3D-CAD-CBD
82	HI	202	PEB	C4D-C3D-CAD-CBD
82	II	203	PEB	C4D-C3D-CAD-CBD
82	NI	203	PEB	C4D-C3D-CAD-CBD
82	OI	202	PEB	C4D-C3D-CAD-CBD
82	RI	203	PEB	C4D-C3D-CAD-CBD
82	TI	201	PEB	C4D-C3D-CAD-CBD
82	IK	202	PEB	C4D-C3D-CAD-CBD
82	OK	202	PEB	C4D-C3D-CAD-CBD
82	RK	202	PEB	C4D-C3D-CAD-CBD
82	EM	203	PEB	C4D-C3D-CAD-CBD
82	KM	202	PEB	C4D-C3D-CAD-CBD
82	QM	204	PEB	C4D-C3D-CAD-CBD
82	YM	203	PEB	C4D-C3D-CAD-CBD
82	LO	1002	PEB	C4D-C3D-CAD-CBD
82	CP	201	PEB	C4D-C3D-CAD-CBD
82	AQ	301	PEB	C4D-C3D-CAD-CBD
82	HQ	202	PEB	C4D-C3D-CAD-CBD
82	QQ	202	PEB	C4D-C3D-CAD-CBD
82	T1	201	PEB	C4D-C3D-CAD-CBD
82	W1	201	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
82	b1	201	PEB	C4D-C3D-CAD-CBD
82	L4	1002	PEB	C4D-C3D-CAD-CBD
82	c4	202	PEB	C4D-C3D-CAD-CBD
82	H5	201	PEB	C4D-C3D-CAD-CBD
82	U5	201	PEB	C4D-C3D-CAD-CBD
82	G7	202	PEB	C4D-C3D-CAD-CBD
82	I7	201	PEB	C4D-C3D-CAD-CBD
82	Y7	301	PEB	C4D-C3D-CAD-CBD
82	y8	203	PEB	C4D-C3D-CAD-CBD
82	W9	201	PEB	C4D-C3D-CAD-CBD
82	yC	203	PEB	C4D-C3D-CAD-CBD
82	oF	202	PEB	C4D-C3D-CAD-CBD
82	xF	303	PEB	C4D-C3D-CAD-CBD
82	lG	202	PEB	C4D-C3D-CAD-CBD
82	bH	201	PEB	C4D-C3D-CAD-CBD
82	oK	202	PEB	C4D-C3D-CAD-CBD
82	xK	303	PEB	C4D-C3D-CAD-CBD
82	cO	202	PEB	C4D-C3D-CAD-CBD
82	Z9	301	PEB	C4D-C3D-CAD-CBD
82	M9	302	PEB	C4D-C3D-CAD-CBD
92	bL	611	LMG	O10-C28-O8-C9
92	bL	610	LMG	C4-C5-C6-O5
87	CL	507	CLA	C2C-C3C-CAC-CBC
88	I6	101	LHG	C24-C25-C26-C27
92	BL	611	LMG	C16-C17-C18-C19
92	mL	101	LMG	C13-C14-C15-C16
100	JN	104	3XQ	C14-C15-C16-C17
87	DL	404	CLA	C16-C17-C18-C19
87	IN	102	CLA	C16-C17-C18-C20
87	I2	102	CLA	C16-C17-C18-C20
87	c6	609	CLA	C16-C17-C18-C19
87	bL	604	CLA	O1A-CGA-O2A-C1
85	AL	401	BCR	C23-C24-C25-C26
85	BL	616	BCR	C1-C6-C7-C8
85	BL	616	BCR	C5-C6-C7-C8
85	BL	618	BCR	C23-C24-C25-C26
85	BL	618	BCR	C23-C24-C25-C30
85	CL	502	BCR	C1-C6-C7-C8
85	CL	502	BCR	C5-C6-C7-C8
85	KL	100	BCR	C5-C6-C7-C8
85	AN	845	BCR	C1-C6-C7-C8
85	AN	847	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
85	AN	848	BCR	C1-C6-C7-C8
85	AN	848	BCR	C5-C6-C7-C8
85	AN	848	BCR	C23-C24-C25-C30
85	BN	803	BCR	C1-C6-C7-C8
85	BN	803	BCR	C23-C24-C25-C26
85	BN	839	BCR	C23-C24-C25-C26
85	BN	842	BCR	C1-C6-C7-C8
85	BN	842	BCR	C23-C24-C25-C30
85	BN	843	BCR	C1-C6-C7-C8
85	BN	843	BCR	C5-C6-C7-C8
85	IN	101	BCR	C5-C6-C7-C8
85	JN	103	BCR	C23-C24-C25-C30
85	KN	101	BCR	C23-C24-C25-C26
85	KN	101	BCR	C23-C24-C25-C30
85	LN	201	BCR	C23-C24-C25-C26
85	LN	201	BCR	C23-C24-C25-C30
85	A2	845	BCR	C1-C6-C7-C8
85	A2	847	BCR	C5-C6-C7-C8
85	A2	848	BCR	C1-C6-C7-C8
85	A2	848	BCR	C5-C6-C7-C8
85	A2	848	BCR	C23-C24-C25-C30
85	B2	802	BCR	C1-C6-C7-C8
85	B2	802	BCR	C23-C24-C25-C26
85	B2	839	BCR	C23-C24-C25-C26
85	B2	842	BCR	C1-C6-C7-C8
85	B2	842	BCR	C23-C24-C25-C30
85	B2	843	BCR	C1-C6-C7-C8
85	B2	843	BCR	C5-C6-C7-C8
85	I2	101	BCR	C5-C6-C7-C8
85	J2	103	BCR	C23-C24-C25-C30
85	K2	102	BCR	C23-C24-C25-C26
85	K2	102	BCR	C23-C24-C25-C30
85	L2	201	BCR	C23-C24-C25-C26
85	L2	201	BCR	C23-C24-C25-C30
85	K6	102	BCR	C1-C6-C7-C8
85	K6	102	BCR	C5-C6-C7-C8
85	b6	601	BCR	C23-C24-C25-C26
85	c6	603	BCR	C23-C24-C25-C26
85	c6	603	BCR	C23-C24-C25-C30
85	c6	617	BCR	C5-C6-C7-C8
85	k6	102	BCR	C1-C6-C7-C8
85	k6	102	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
85	aL	604	BCR	C23-C24-C25-C26
85	bL	601	BCR	C1-C6-C7-C8
85	bL	601	BCR	C5-C6-C7-C8
85	bL	601	BCR	C23-C24-C25-C26
85	bL	601	BCR	C23-C24-C25-C30
85	bL	603	BCR	C23-C24-C25-C26
85	cL	504	BCR	C1-C6-C7-C8
85	cL	504	BCR	C5-C6-C7-C8
85	kL	100	BCR	C5-C6-C7-C8
87	DL	406	CLA	C3-C5-C6-C7
87	AN	823	CLA	C3-C5-C6-C7
87	A2	823	CLA	C3-C5-C6-C7
87	F2	205	CLA	C3-C5-C6-C7
103	82	309	ZEX	C1-C6-C7-C8
103	82	309	ZEX	C5-C6-C7-C8
103	82	310	ZEX	C1-C6-C7-C8
103	82	310	ZEX	C5-C6-C7-C8
103	8N	309	ZEX	C1-C6-C7-C8
103	8N	309	ZEX	C5-C6-C7-C8
103	8N	310	ZEX	C1-C6-C7-C8
103	8N	310	ZEX	C5-C6-C7-C8
95	a6	602	DGD	O6E-C5E-C6E-O5E
87	d6	401	CLA	C2C-C3C-CAC-CBC
88	d6	402	LHG	C9-C10-C11-C12
88	bL	612	LHG	C28-C29-C30-C31
87	CL	505	CLA	CBA-CGA-O2A-C1
87	AN	833	CLA	CBA-CGA-O2A-C1
87	BN	801	CLA	CBA-CGA-O2A-C1
87	BN	813	CLA	CBA-CGA-O2A-C1
87	A2	833	CLA	CBA-CGA-O2A-C1
87	B2	812	CLA	CBA-CGA-O2A-C1
87	B2	825	CLA	CBA-CGA-O2A-C1
87	cL	507	CLA	CBA-CGA-O2A-C1
87	AN	813	CLA	C8-C10-C11-C12
87	AN	813	CLA	C13-C15-C16-C17
87	AN	830	CLA	C15-C16-C17-C18
87	BN	826	CLA	C13-C15-C16-C17
87	32	304	CLA	C13-C15-C16-C17
87	A2	813	CLA	C8-C10-C11-C12
87	A2	813	CLA	C13-C15-C16-C17
87	A2	830	CLA	C15-C16-C17-C18
87	B2	826	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
87	A6	403	CLA	C8-C10-C11-C12
87	a6	607	CLA	C8-C10-C11-C12
87	a6	607	CLA	C15-C16-C17-C18
87	c6	605	CLA	C5-C6-C7-C8
87	c6	606	CLA	C5-C6-C7-C8
87	bL	605	CLA	C5-C6-C7-C8
87	cL	517	CLA	C10-C11-C12-C13
87	3N	305	CLA	C13-C15-C16-C17
82	CA	202	PEB	C2C-CAC-CBC-CGC
82	IA	201	PEB	C2C-CAC-CBC-CGC
82	KA	201	PEB	C2C-CAC-CBC-CGC
82	LA	201	PEB	C2C-CAC-CBC-CGC
82	TA	201	PEB	C2C-CAC-CBC-CGC
82	VA	201	PEB	C2C-CAC-CBC-CGC
82	DB	202	PEB	C3B-CAB-CBB-CGB
82	GD	201	PEB	C2C-CAC-CBC-CGC
82	HD	201	PEB	C2C-CAC-CBC-CGC
82	MD	201	PEB	C2C-CAC-CBC-CGC
82	UD	201	PEB	C3B-CAB-CBB-CGB
82	DE	1002	PEB	C3B-CAB-CBB-CGB
82	KE	201	PEB	C2C-CAC-CBC-CGC
82	QE	201	PEB	C2C-CAC-CBC-CGC
82	AF	201	PEB	C3B-CAB-CBB-CGB
82	HF	201	PEB	C3B-CAB-CBB-CGB
82	KF	201	PEB	C3B-CAB-CBB-CGB
82	PF	202	PEB	C3B-CAB-CBB-CGB
82	RF	202	PEB	C2C-CAC-CBC-CGC
82	XF	201	PEB	C3B-CAB-CBB-CGB
82	YF	202	PEB	C3B-CAB-CBB-CGB
82	DG	1002	PEB	C3B-CAB-CBB-CGB
82	KG	201	PEB	C2C-CAC-CBC-CGC
82	QG	201	PEB	C2C-CAC-CBC-CGC
82	WG	201	PEB	C2C-CAC-CBC-CGC
82	RH	201	PEB	C2C-CAC-CBC-CGC
82	ZH	202	PEB	C3B-CAB-CBB-CGB
82	ZH	203	PEB	C2C-CAC-CBC-CGC
82	IJ	202	PEB	C2C-CAC-CBC-CGC
82	IJ	202	PEB	C3B-CAB-CBB-CGB
82	NJ	201	PEB	C2C-CAC-CBC-CGC
82	AK	201	PEB	C3B-CAB-CBB-CGB
82	HK	201	PEB	C3B-CAB-CBB-CGB
82	KK	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	PK	202	PEB	C3B-CAB-CBB-CGB
82	RK	202	PEB	C2C-CAC-CBC-CGC
82	XK	201	PEB	C3B-CAB-CBB-CGB
82	YK	202	PEB	C3B-CAB-CBB-CGB
82	AM	301	PEB	C2C-CAC-CBC-CGC
82	BM	301	PEB	C2C-CAC-CBC-CGC
82	GM	202	PEB	C2C-CAC-CBC-CGC
82	OM	202	PEB	C3B-CAB-CBB-CGB
82	TM	202	PEB	C2C-CAC-CBC-CGC
82	AO	301	PEB	C2C-CAC-CBC-CGC
82	GQ	201	PEB	C2C-CAC-CBC-CGC
82	HQ	201	PEB	C2C-CAC-CBC-CGC
82	MQ	201	PEB	C2C-CAC-CBC-CGC
82	UQ	201	PEB	C3B-CAB-CBB-CGB
82	R1	201	PEB	C2C-CAC-CBC-CGC
82	Z1	202	PEB	C3B-CAB-CBB-CGB
82	Z1	203	PEB	C2C-CAC-CBC-CGC
82	h1	203	PEB	C3B-CAB-CBB-CGB
82	j1	203	PEB	C3B-CAB-CBB-CGB
82	k1	201	PEB	C2C-CAC-CBC-CGC
82	A4	301	PEB	C2C-CAC-CBC-CGC
82	c4	202	PEB	C3B-CAB-CBB-CGB
82	h4	202	PEB	C2C-CAC-CBC-CGC
82	A5	201	PEB	C2C-CAC-CBC-CGC
82	C5	201	PEB	C2C-CAC-CBC-CGC
82	D5	203	PEB	C2C-CAC-CBC-CGC
82	E5	201	PEB	C2C-CAC-CBC-CGC
82	G5	201	PEB	C2C-CAC-CBC-CGC
82	I5	201	PEB	C2C-CAC-CBC-CGC
82	K5	201	PEB	C2C-CAC-CBC-CGC
82	N5	201	PEB	C2C-CAC-CBC-CGC
82	P5	201	PEB	C2C-CAC-CBC-CGC
82	R5	201	PEB	C2C-CAC-CBC-CGC
82	S5	203	PEB	C2C-CAC-CBC-CGC
82	T5	201	PEB	C2C-CAC-CBC-CGC
82	V5	201	PEB	C2C-CAC-CBC-CGC
82	W5	203	PEB	C2C-CAC-CBC-CGC
82	X5	201	PEB	C2C-CAC-CBC-CGC
82	Y5	202	PEB	C3B-CAB-CBB-CGB
82	Y5	203	PEB	C2C-CAC-CBC-CGC
82	C7	202	PEB	C2C-CAC-CBC-CGC
82	I7	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	K7	201	PEB	C2C-CAC-CBC-CGC
82	L7	201	PEB	C2C-CAC-CBC-CGC
82	T7	201	PEB	C2C-CAC-CBC-CGC
82	V7	201	PEB	C2C-CAC-CBC-CGC
82	s8	201	PEB	C3B-CAB-CBB-CGB
82	t8	201	PEB	C2C-CAC-CBC-CGC
82	B9	203	PEB	C3B-CAB-CBB-CGB
82	Q9	203	PEB	C3B-CAB-CBB-CGB
82	S9	203	PEB	C3B-CAB-CBB-CGB
82	U9	201	PEB	C3B-CAB-CBB-CGB
82	yC	201	PEB	C3B-CAB-CBB-CGB
82	yC	202	PEB	C2C-CAC-CBC-CGC
82	sC	201	PEB	C3B-CAB-CBB-CGB
82	tC	201	PEB	C2C-CAC-CBC-CGC
82	dE	203	PEB	C3B-CAB-CBB-CGB
82	fE	202	PEB	C2C-CAC-CBC-CGC
82	jF	202	PEB	C2C-CAC-CBC-CGC
82	lF	202	PEB	C3B-CAB-CBB-CGB
82	qF	203	PEB	C3B-CAB-CBB-CGB
82	xF	303	PEB	C2C-CAC-CBC-CGC
82	dG	203	PEB	C3B-CAB-CBB-CGB
82	fG	202	PEB	C2C-CAC-CBC-CGC
82	hH	202	PEB	C3B-CAB-CBB-CGB
82	jH	203	PEB	C3B-CAB-CBB-CGB
82	kH	201	PEB	C2C-CAC-CBC-CGC
82	kJ	202	PEB	C2C-CAC-CBC-CGC
82	jK	202	PEB	C2C-CAC-CBC-CGC
82	lK	202	PEB	C3B-CAB-CBB-CGB
82	qK	203	PEB	C3B-CAB-CBB-CGB
82	xK	303	PEB	C2C-CAC-CBC-CGC
82	cO	202	PEB	C3B-CAB-CBB-CGB
82	hO	202	PEB	C2C-CAC-CBC-CGC
83	xF	305	PUB	C2C-CAC-CBC-CGC
83	xK	305	PUB	C2C-CAC-CBC-CGC
84	JH	1003	CYC	C2A-CAA-CBA-CGA
84	M1	201	CYC	C2A-CAA-CBA-CGA
92	AL	411	LMG	C11-C10-O7-C8
92	aL	611	LMG	C11-C10-O7-C8
92	bL	610	LMG	C11-C10-O7-C8
95	CL	523	DGD	C2B-C1B-O2G-C2G
95	cL	520	DGD	C2B-C1B-O2G-C2G
95	lL	101	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
84	DG	1001	CYC	C2B-C3B-CAB-CBB
87	a6	607	CLA	C2C-C3C-CAC-CBC
88	bL	612	LHG	C31-C32-C33-C34
92	a6	614	LMG	C19-C20-C21-C22
95	BN	844	DGD	C1A-C2A-C3A-C4A
95	B2	844	DGD	C1A-C2A-C3A-C4A
95	a6	604	DGD	C1B-C2B-C3B-C4B
92	k6	101	LMG	C39-C40-C41-C42
92	yL	101	LMG	C33-C34-C35-C36
87	A2	801	CLA	C10-C11-C12-C13
87	d6	406	CLA	C10-C11-C12-C13
92	bL	623	LMG	O6-C5-C6-O5
95	DL	408	DGD	O6E-C5E-C6E-O5E
84	DE	1001	CYC	C2B-C3B-CAB-CBB
100	J2	104	3XQ	C11-C12-C13-C14
87	DL	404	CLA	C4-C3-C5-C6
87	BN	813	CLA	C4-C3-C5-C6
87	B6	610	CLA	C4-C3-C5-C6
87	D6	403	CLA	C4-C3-C5-C6
87	b6	616	CLA	C4-C3-C5-C6
87	c6	608	CLA	C4-C3-C5-C6
87	bL	615	CLA	C4-C3-C5-C6
94	a6	601	PL9	C12-C11-C9-C10
94	a6	601	PL9	C30-C29-C31-C32
94	dL	406	PL9	C12-C11-C9-C10
87	BL	601	CLA	O1D-CGD-O2D-CED
87	d6	403	CLA	O1D-CGD-O2D-CED
87	BL	601	CLA	C12-C13-C15-C16
87	BL	621	CLA	C11-C12-C13-C15
87	CL	503	CLA	C11-C12-C13-C15
87	CL	510	CLA	C11-C10-C8-C7
87	AN	802	CLA	C12-C13-C15-C16
87	AN	805	CLA	C6-C7-C8-C10
87	AN	830	CLA	C6-C7-C8-C10
87	AN	830	CLA	C11-C12-C13-C15
87	AN	830	CLA	C12-C13-C15-C16
87	AN	841	CLA	C12-C13-C15-C16
87	BN	823	CLA	C6-C7-C8-C10
87	BN	825	CLA	C6-C7-C8-C10
87	BN	825	CLA	C11-C10-C8-C7
87	BN	825	CLA	C11-C12-C13-C15
87	BN	830	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
87	BN	835	CLA	C11-C10-C8-C7
87	LN	202	CLA	C2-C3-C5-C6
87	22	605	CLA	C2-C3-C5-C6
87	32	304	CLA	C12-C13-C15-C16
87	A2	805	CLA	C6-C7-C8-C10
87	A2	830	CLA	C6-C7-C8-C10
87	A2	830	CLA	C11-C12-C13-C15
87	A2	830	CLA	C12-C13-C15-C16
87	A2	841	CLA	C12-C13-C15-C16
87	B2	822	CLA	C6-C7-C8-C10
87	B2	824	CLA	C6-C7-C8-C10
87	B2	824	CLA	C11-C10-C8-C7
87	B2	824	CLA	C11-C12-C13-C15
87	B2	830	CLA	C11-C10-C8-C7
87	B2	835	CLA	C11-C10-C8-C7
87	L2	202	CLA	C2-C3-C5-C6
87	B6	611	CLA	C6-C7-C8-C10
87	B6	616	CLA	C6-C7-C8-C10
87	C6	511	CLA	C11-C10-C8-C7
87	C6	512	CLA	C12-C13-C15-C16
87	D6	405	CLA	C11-C12-C13-C15
87	D6	405	CLA	C12-C13-C15-C16
87	H6	103	CLA	C2-C3-C5-C6
87	b6	610	CLA	C2-C3-C5-C6
87	b6	611	CLA	C12-C13-C15-C16
87	b6	612	CLA	C12-C13-C15-C16
87	b6	613	CLA	C12-C13-C15-C16
87	b6	616	CLA	C2-C3-C5-C6
87	c6	608	CLA	C6-C7-C8-C10
87	c6	608	CLA	C11-C10-C8-C7
87	c6	608	CLA	C12-C13-C15-C16
87	c6	613	CLA	C6-C7-C8-C10
87	c6	616	CLA	C2-C3-C5-C6
87	d6	406	CLA	C11-C12-C13-C15
87	bL	606	CLA	C6-C7-C8-C10
87	bL	615	CLA	C2-C3-C5-C6
87	bL	617	CLA	C12-C13-C15-C16
87	2N	301	CLA	C2-C3-C5-C6
87	3N	305	CLA	C12-C13-C15-C16
91	D6	404	PHO	C2-C3-C5-C6
94	D6	408	PL9	C33-C34-C36-C37
94	a6	601	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
94	d6	408	PL9	C28-C29-C31-C32
98	BN	837	PQN	C16-C17-C18-C20
98	B2	837	PQN	C16-C17-C18-C20
82	IB	203	PEB	NC-C1C-CHB-C4B
82	SB	203	PEB	NC-C1C-CHB-C4B
82	EF	202	PEB	NC-C1C-CHB-C4B
82	BI	203	PEB	NC-C1C-CHB-C4B
82	EK	202	PEB	NC-C1C-CHB-C4B
82	J5	202	PEB	NC-C1C-CHB-C4B
82	O5	202	PEB	NC-C1C-CHB-C4B
82	dD	401	PEB	NC-C1C-CHB-C4B
82	dQ	401	PEB	NC-C1C-CHB-C4B
83	AH	304	PUB	NB-C4B-CHB-C1C
83	A1	304	PUB	NB-C4B-CHB-C1C
87	FN	205	CLA	C3-C5-C6-C7
87	BN	831	CLA	O1A-CGA-O2A-C1
87	B2	831	CLA	O1A-CGA-O2A-C1
87	c6	605	CLA	O1A-CGA-O2A-C1
92	XL	601	LMG	O10-C28-O8-C9
92	D6	407	LMG	O10-C28-O8-C9
92	qL	301	LMG	O10-C28-O8-C9
95	cL	519	DGD	O1A-C1A-O1G-C1G
87	c6	604	CLA	C2C-C3C-CAC-CBC
95	C6	504	DGD	C4A-C5A-C6A-C7A
87	AN	802	CLA	C10-C11-C12-C13
87	bL	615	CLA	C15-C16-C17-C18
82	AA	201	PEB	C4B-C3B-CAB-CBB
82	A7	201	PEB	C4B-C3B-CAB-CBB
82	J9	201	PEB	C4B-C3B-CAB-CBB
82	wF	303	PEB	C4B-C3B-CAB-CBB
82	wK	303	PEB	C4B-C3B-CAB-CBB
83	AH	304	PUB	C1C-C2C-CAC-CBC
83	A1	304	PUB	C1C-C2C-CAC-CBC
85	C6	508	BCR	C19-C20-C21-C22
85	fL	101	BCR	C19-C20-C21-C22
87	42	602	CLA	C16-C17-C18-C19
87	82	302	CLA	C16-C17-C18-C19
87	B6	604	CLA	C16-C17-C18-C19
87	4N	602	CLA	C16-C17-C18-C19
87	8N	303	CLA	C16-C17-C18-C19
87	CL	504	CLA	O1D-CGD-O2D-CED
87	AN	803	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
87	BN	822	CLA	O1D-CGD-O2D-CED
87	A2	803	CLA	O1D-CGD-O2D-CED
87	B2	821	CLA	O1D-CGD-O2D-CED
92	aL	611	LMG	O9-C10-O7-C8
95	lL	101	DGD	O1B-C1B-O2G-C2G
88	D6	401	LHG	C7-C8-C9-C10
87	DL	404	CLA	CBA-CGA-O2A-C1
87	BN	833	CLA	CBA-CGA-O2A-C1
87	BN	835	CLA	CBA-CGA-O2A-C1
87	B2	833	CLA	CBA-CGA-O2A-C1
87	B2	835	CLA	CBA-CGA-O2A-C1
87	D6	405	CLA	CBA-CGA-O2A-C1
87	b6	613	CLA	CBA-CGA-O2A-C1
87	bL	619	CLA	CBA-CGA-O2A-C1
92	J6	102	LMG	C29-C28-O8-C9
92	b6	623	LMG	C29-C28-O8-C9
92	j6	101	LMG	C29-C28-O8-C9
88	DL	407	LHG	C13-C14-C15-C16
92	b6	623	LMG	C12-C13-C14-C15
87	CL	503	CLA	C2A-CAA-CBA-CGA
87	CL	507	CLA	C2A-CAA-CBA-CGA
87	AN	833	CLA	C2A-CAA-CBA-CGA
87	AN	841	CLA	C2A-CAA-CBA-CGA
87	22	605	CLA	C2A-CAA-CBA-CGA
87	A2	833	CLA	C2A-CAA-CBA-CGA
87	A2	841	CLA	C2A-CAA-CBA-CGA
87	B6	605	CLA	C2A-CAA-CBA-CGA
87	c6	604	CLA	C2A-CAA-CBA-CGA
87	cL	509	CLA	C2A-CAA-CBA-CGA
87	AN	835	CLA	C15-C16-C17-C18
87	A2	835	CLA	C15-C16-C17-C18
87	B2	808	CLA	C13-C15-C16-C17
87	b6	604	CLA	C13-C15-C16-C17
87	c6	606	CLA	C13-C15-C16-C17
87	c6	611	CLA	C13-C15-C16-C17
88	BL	615	LHG	C26-C27-C28-C29
92	b6	619	LMG	C12-C13-C14-C15
87	cL	517	CLA	O1D-CGD-O2D-CED
88	D6	401	LHG	C30-C31-C32-C33
92	A6	408	LMG	C34-C35-C36-C37
92	D6	409	LMG	C16-C17-C18-C19
92	d6	409	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
82	XF	203	PEB	C2C-C1C-CHB-C4B
82	XK	203	PEB	C2C-C1C-CHB-C4B
82	iJ	202	PEB	C2C-C1C-CHB-C4B
82	cK	202	PEB	C2C-C1C-CHB-C4B
92	d6	409	LMG	C10-C11-C12-C13
95	DL	408	DGD	C1B-C2B-C3B-C4B
92	bL	610	LMG	O6-C5-C6-O5
87	22	610	CLA	O1D-CGD-O2D-CED
87	2N	310	CLA	O1D-CGD-O2D-CED
87	AN	831	CLA	C5-C6-C7-C8
87	BN	809	CLA	C13-C15-C16-C17
87	c6	612	CLA	C5-C6-C7-C8
87	cL	509	CLA	C10-C11-C12-C13
87	nL	101	CLA	C13-C15-C16-C17
84	GG	1001	CYC	C2B-C3B-CAB-CBB
87	A6	402	CLA	C4C-C3C-CAC-CBC
87	b6	606	CLA	C2C-C3C-CAC-CBC
95	D6	410	DGD	CBB-CCB-CDB-CEB
82	FA	202	PEB	C2D-C3D-CAD-CBD
82	GA	202	PEB	C2D-C3D-CAD-CBD
82	IA	201	PEB	C2D-C3D-CAD-CBD
82	YA	301	PEB	C2D-C3D-CAD-CBD
82	GB	203	PEB	C2D-C3D-CAD-CBD
82	IB	202	PEB	C2D-C3D-CAD-CBD
82	QB	201	PEB	C2D-C3D-CAD-CBD
82	AD	301	PEB	C2D-C3D-CAD-CBD
82	HD	201	PEB	C2D-C3D-CAD-CBD
82	HD	202	PEB	C2D-C3D-CAD-CBD
82	QD	202	PEB	C2D-C3D-CAD-CBD
82	VD	203	PEB	C2D-C3D-CAD-CBD
82	YD	201	PEB	C2D-C3D-CAD-CBD
82	IF	202	PEB	C2D-C3D-CAD-CBD
82	OF	202	PEB	C2D-C3D-CAD-CBD
82	RF	202	PEB	C2D-C3D-CAD-CBD
82	TH	201	PEB	C2D-C3D-CAD-CBD
82	TH	202	PEB	C2D-C3D-CAD-CBD
82	WH	201	PEB	C2D-C3D-CAD-CBD
82	AI	203	PEB	C2D-C3D-CAD-CBD
82	BI	202	PEB	C2D-C3D-CAD-CBD
82	HI	202	PEB	C2D-C3D-CAD-CBD
82	II	203	PEB	C2D-C3D-CAD-CBD
82	KI	201	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
82	NI	203	PEB	C2D-C3D-CAD-CBD
82	OI	202	PEB	C2D-C3D-CAD-CBD
82	RI	203	PEB	C2D-C3D-CAD-CBD
82	TI	201	PEB	C2D-C3D-CAD-CBD
82	WI	202	PEB	C2D-C3D-CAD-CBD
82	IK	202	PEB	C2D-C3D-CAD-CBD
82	OK	202	PEB	C2D-C3D-CAD-CBD
82	RK	202	PEB	C2D-C3D-CAD-CBD
82	EM	203	PEB	C2D-C3D-CAD-CBD
82	QM	204	PEB	C2D-C3D-CAD-CBD
82	LO	1002	PEB	C2D-C3D-CAD-CBD
82	CP	201	PEB	C2D-C3D-CAD-CBD
82	AQ	301	PEB	C2D-C3D-CAD-CBD
82	HQ	201	PEB	C2D-C3D-CAD-CBD
82	HQ	202	PEB	C2D-C3D-CAD-CBD
82	JQ	201	PEB	C2D-C3D-CAD-CBD
82	QQ	202	PEB	C2D-C3D-CAD-CBD
82	VQ	203	PEB	C2D-C3D-CAD-CBD
82	YQ	201	PEB	C2D-C3D-CAD-CBD
82	T1	201	PEB	C2D-C3D-CAD-CBD
82	T1	202	PEB	C2D-C3D-CAD-CBD
82	W1	201	PEB	C2D-C3D-CAD-CBD
82	b1	201	PEB	C2D-C3D-CAD-CBD
82	e1	202	PEB	C2D-C3D-CAD-CBD
82	L4	1002	PEB	C2D-C3D-CAD-CBD
82	c4	202	PEB	C2D-C3D-CAD-CBD
82	H5	201	PEB	C2D-C3D-CAD-CBD
82	U5	201	PEB	C2D-C3D-CAD-CBD
82	F7	202	PEB	C2D-C3D-CAD-CBD
82	G7	202	PEB	C2D-C3D-CAD-CBD
82	I7	201	PEB	C2D-C3D-CAD-CBD
82	Y7	301	PEB	C2D-C3D-CAD-CBD
82	y8	203	PEB	C2D-C3D-CAD-CBD
82	W9	201	PEB	C2D-C3D-CAD-CBD
82	yC	203	PEB	C2D-C3D-CAD-CBD
82	oF	202	PEB	C2D-C3D-CAD-CBD
82	xF	303	PEB	C2D-C3D-CAD-CBD
82	lG	202	PEB	C2D-C3D-CAD-CBD
82	bH	201	PEB	C2D-C3D-CAD-CBD
82	eH	202	PEB	C2D-C3D-CAD-CBD
82	cK	202	PEB	C2D-C3D-CAD-CBD
82	oK	202	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
82	xK	303	PEB	C2D-C3D-CAD-CBD
82	cO	202	PEB	C2D-C3D-CAD-CBD
96	FL	102	HEM	C2C-C3C-CAC-CBC
87	AN	838	CLA	C3-C5-C6-C7
87	A2	838	CLA	C3-C5-C6-C7
87	A2	849	CLA	O1D-CGD-O2D-CED
84	GE	1001	CYC	C2B-C3B-CAB-CBB
92	yL	101	LMG	C20-C21-C22-C23
95	B6	620	DGD	C6A-C7A-C8A-C9A
100	J2	104	3XQ	C12-C13-C14-C15
87	BL	609	CLA	O1A-CGA-O2A-C1
87	c6	606	CLA	O1A-CGA-O2A-C1
87	B6	605	CLA	CBD-CGD-O2D-CED
87	32	304	CLA	C16-C17-C18-C19
87	3N	305	CLA	C16-C17-C18-C19
92	DL	402	LMG	O6-C1-O1-C7
95	B6	620	DGD	O6D-C1D-O3G-C3G
87	AN	840	CLA	C13-C15-C16-C17
87	BN	826	CLA	C15-C16-C17-C18
87	A2	831	CLA	C5-C6-C7-C8
87	A2	840	CLA	C13-C15-C16-C17
87	aL	606	CLA	C10-C11-C12-C13
82	z8	202	PEB	NB-C4B-CHB-C1C
82	p8	202	PEB	NB-C4B-CHB-C1C
82	r8	202	PEB	NB-C4B-CHB-C1C
82	t8	202	PEB	NB-C4B-CHB-C1C
82	v8	202	PEB	NB-C4B-CHB-C1C
82	x8	202	PEB	NB-C4B-CHB-C1C
82	A9	202	PEB	NB-C4B-CHB-C1C
82	C9	202	PEB	NB-C4B-CHB-C1C
82	E9	202	PEB	NB-C4B-CHB-C1C
82	G9	202	PEB	NB-C4B-CHB-C1C
82	I9	202	PEB	NB-C4B-CHB-C1C
82	K9	202	PEB	NB-C4B-CHB-C1C
82	N9	202	PEB	NB-C4B-CHB-C1C
82	P9	202	PEB	NB-C4B-CHB-C1C
82	R9	202	PEB	NB-C4B-CHB-C1C
82	T9	202	PEB	NB-C4B-CHB-C1C
82	V9	202	PEB	NB-C4B-CHB-C1C
82	X9	202	PEB	NB-C4B-CHB-C1C
82	zC	202	PEB	NB-C4B-CHB-C1C
82	pC	202	PEB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
82	rC	202	PEB	NB-C4B-CHB-C1C
82	tC	202	PEB	NB-C4B-CHB-C1C
82	vC	202	PEB	NB-C4B-CHB-C1C
82	xC	202	PEB	NB-C4B-CHB-C1C
82	qF	202	PEB	NB-C4B-CHB-C1C
82	qK	202	PEB	NB-C4B-CHB-C1C
87	AN	849	CLA	O1D-CGD-O2D-CED
87	b6	610	CLA	O1D-CGD-O2D-CED
87	bL	614	CLA	O1D-CGD-O2D-CED
88	AN	844	LHG	C9-C10-C11-C12
88	A2	844	LHG	C9-C10-C11-C12
88	I6	101	LHG	C15-C16-C17-C18
95	h6	101	DGD	C6A-C7A-C8A-C9A
88	a6	610	LHG	C7-C8-C9-C10
92	b6	624	LMG	C28-C29-C30-C31
88	AN	843	LHG	C8-C7-O7-C5
88	A2	843	LHG	C8-C7-O7-C5
88	C6	522	LHG	C8-C7-O7-C5
92	B6	618	LMG	C11-C10-O7-C8
92	d6	409	LMG	C11-C10-O7-C8
92	m6	101	LMG	C11-C10-O7-C8
95	AL	414	DGD	C2B-C1B-O2G-C2G
95	BL	613	DGD	C2B-C1B-O2G-C2G
95	C6	523	DGD	C2B-C1B-O2G-C2G
95	D6	410	DGD	C2B-C1B-O2G-C2G
95	a6	602	DGD	C2B-C1B-O2G-C2G
95	a6	603	DGD	C2B-C1B-O2G-C2G
95	b6	621	DGD	C2B-C1B-O2G-C2G
95	c6	620	DGD	C2B-C1B-O2G-C2G
87	b6	609	CLA	C4C-C3C-CAC-CBC
88	i6	101	LHG	C12-C13-C14-C15
92	A6	408	LMG	C35-C36-C37-C38
95	J6	101	DGD	C9B-CAB-CBB-CCB
87	AN	833	CLA	C8-C10-C11-C12
87	BN	805	CLA	C8-C10-C11-C12
87	A2	833	CLA	C8-C10-C11-C12
87	B2	804	CLA	C8-C10-C11-C12
87	B2	826	CLA	C15-C16-C17-C18
87	bL	614	CLA	C13-C15-C16-C17
87	CL	503	CLA	CBD-CGD-O2D-CED
87	D6	402	CLA	CBD-CGD-O2D-CED
88	C6	522	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
92	AL	411	LMG	O9-C10-O7-C8
92	m6	101	LMG	O9-C10-O7-C8
95	AL	416	DGD	O1B-C1B-O2G-C2G
95	BL	613	DGD	O1B-C1B-O2G-C2G
92	yL	101	LMG	C15-C16-C17-C18
92	ML	101	LMG	C2-C1-O1-C7
95	C6	502	DGD	C2E-C1E-O5D-C6D
95	c6	601	DGD	C2E-C1E-O5D-C6D
87	c6	607	CLA	C8-C10-C11-C12
91	a6	613	PHO	C8-C10-C11-C12
92	bL	609	LMG	O7-C8-C9-O8
95	BL	607	DGD	O6E-C5E-C6E-O5E
87	cL	515	CLA	CBA-CGA-O2A-C1
88	mL	102	LHG	C11-C10-C9-C8
87	BN	835	CLA	C16-C17-C18-C20
87	B2	822	CLA	C16-C17-C18-C19
87	B2	835	CLA	C16-C17-C18-C20
87	c6	605	CLA	C16-C17-C18-C20
88	BL	615	LHG	C16-C17-C18-C19
88	B6	617	LHG	C11-C10-C9-C8
88	bL	612	LHG	C14-C15-C16-C17
92	bL	610	LMG	C15-C16-C17-C18
95	BN	844	DGD	C4A-C5A-C6A-C7A
100	JN	104	3XQ	C6-C7-C8-C9
87	CL	506	CLA	C15-C16-C17-C18
87	BN	811	CLA	C10-C11-C12-C13
87	B2	810	CLA	C10-C11-C12-C13
87	dL	402	CLA	C15-C16-C17-C18
91	dL	403	PHO	C15-C16-C17-C18
87	DL	403	CLA	C4-C3-C5-C6
87	B2	812	CLA	C4-C3-C5-C6
87	H6	103	CLA	C4-C3-C5-C6
87	b6	614	CLA	C4-C3-C5-C6
94	d6	408	PL9	C40-C39-C41-C42
87	BL	620	CLA	C2-C3-C5-C6
87	CL	505	CLA	C2-C3-C5-C6
87	AN	827	CLA	C2-C3-C5-C6
87	A2	827	CLA	C2-C3-C5-C6
87	B6	608	CLA	C2-C3-C5-C6
87	K6	101	CLA	C2-C3-C5-C6
94	dL	406	PL9	C12-C11-C9-C8
94	DL	401	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
94	D6	408	PL9	C4-C3-C7-C8
94	d6	408	PL9	C4-C3-C7-C8
94	dL	406	PL9	C4-C3-C7-C8
95	B2	844	DGD	C4A-C5A-C6A-C7A
82	KB	303	PEB	C3C-C2C-CAC-CBC
82	GD	202	PEB	C3C-C2C-CAC-CBC
82	LF	202	PEB	C3C-C2C-CAC-CBC
82	LK	202	PEB	C3C-C2C-CAC-CBC
82	GQ	202	PEB	C3C-C2C-CAC-CBC
87	BL	621	CLA	C11-C12-C13-C14
87	CL	506	CLA	C11-C10-C8-C9
87	CL	507	CLA	C11-C10-C8-C9
87	CL	511	CLA	C14-C13-C15-C16
87	AN	810	CLA	C14-C13-C15-C16
87	AN	830	CLA	C11-C12-C13-C14
87	AN	830	CLA	C14-C13-C15-C16
87	BN	807	CLA	C6-C7-C8-C9
87	BN	807	CLA	C11-C10-C8-C9
87	BN	808	CLA	C6-C7-C8-C9
87	BN	811	CLA	C11-C10-C8-C9
87	BN	813	CLA	C11-C10-C8-C9
87	BN	823	CLA	C11-C12-C13-C14
87	BN	825	CLA	C11-C12-C13-C14
87	BN	830	CLA	C6-C7-C8-C9
87	BN	830	CLA	C11-C10-C8-C9
87	BN	834	CLA	C6-C7-C8-C9
87	BN	835	CLA	C11-C10-C8-C9
87	22	602	CLA	C6-C7-C8-C9
87	52	602	CLA	C6-C7-C8-C9
87	A2	810	CLA	C14-C13-C15-C16
87	A2	830	CLA	C11-C12-C13-C14
87	A2	830	CLA	C14-C13-C15-C16
87	B2	806	CLA	C6-C7-C8-C9
87	B2	806	CLA	C11-C10-C8-C9
87	B2	807	CLA	C6-C7-C8-C9
87	B2	810	CLA	C11-C10-C8-C9
87	B2	812	CLA	C11-C10-C8-C9
87	B2	822	CLA	C11-C12-C13-C14
87	B2	824	CLA	C11-C12-C13-C14
87	B2	830	CLA	C6-C7-C8-C9
87	B2	830	CLA	C11-C10-C8-C9
87	B2	834	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
87	B2	835	CLA	C11-C10-C8-C9
87	A6	402	CLA	C11-C10-C8-C9
87	B6	604	CLA	C11-C12-C13-C14
87	B6	606	CLA	C11-C10-C8-C9
87	B6	608	CLA	C11-C10-C8-C9
87	B6	612	CLA	C11-C10-C8-C9
87	B6	616	CLA	C6-C7-C8-C9
87	B6	616	CLA	C14-C13-C15-C16
87	C6	511	CLA	C14-C13-C15-C16
87	C6	512	CLA	C6-C7-C8-C9
87	C6	514	CLA	C11-C10-C8-C9
87	D6	405	CLA	C6-C7-C8-C9
87	a6	607	CLA	C11-C10-C8-C9
87	b6	608	CLA	C14-C13-C15-C16
87	b6	611	CLA	C14-C13-C15-C16
87	b6	612	CLA	C14-C13-C15-C16
87	b6	613	CLA	C6-C7-C8-C9
87	b6	617	CLA	C11-C12-C13-C14
87	c6	608	CLA	C6-C7-C8-C9
87	c6	609	CLA	C11-C12-C13-C14
87	c6	610	CLA	C6-C7-C8-C9
87	c6	611	CLA	C11-C10-C8-C9
87	c6	613	CLA	C6-C7-C8-C9
87	cL	509	CLA	C11-C10-C8-C9
87	5N	602	CLA	C6-C7-C8-C9
91	AL	410	PHO	C11-C12-C13-C14
98	BN	837	PQN	C16-C17-C18-C19
98	B2	837	PQN	C16-C17-C18-C19
92	b6	623	LMG	C8-C9-O8-C28
92	b6	623	LMG	C18-C19-C20-C21
95	BN	844	DGD	C7B-C8B-C9B-CAB
95	B2	844	DGD	C7B-C8B-C9B-CAB
87	BL	601	CLA	C2A-CAA-CBA-CGA
87	AN	810	CLA	C2A-CAA-CBA-CGA
87	AN	814	CLA	C2A-CAA-CBA-CGA
87	LN	204	CLA	C2A-CAA-CBA-CGA
87	RN	204	CLA	C2A-CAA-CBA-CGA
87	A2	810	CLA	C2A-CAA-CBA-CGA
87	A2	814	CLA	C2A-CAA-CBA-CGA
87	L2	204	CLA	C2A-CAA-CBA-CGA
87	R2	204	CLA	C2A-CAA-CBA-CGA
87	C6	509	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	H6	102	CLA	C2A-CAA-CBA-CGA
87	c6	608	CLA	C2A-CAA-CBA-CGA
87	bL	616	CLA	C2A-CAA-CBA-CGA
87	2N	301	CLA	C2A-CAA-CBA-CGA
82	cB	402	PEB	NC-C1C-CHB-C4B
87	B6	606	CLA	C2C-C3C-CAC-CBC
87	a6	608	CLA	C4C-C3C-CAC-CBC
88	AL	406	LHG	C17-C18-C19-C20
88	C6	505	LHG	C30-C31-C32-C33
92	m6	103	LMG	O6-C5-C6-O5
95	BN	844	DGD	O6E-C5E-C6E-O5E
95	B2	844	DGD	O6E-C5E-C6E-O5E
95	O6	301	DGD	O6E-C5E-C6E-O5E
82	TA	203	PEB	C4B-C3B-CAB-CBB
82	GF	203	PEB	C4B-C3B-CAB-CBB
82	GK	203	PEB	C4B-C3B-CAB-CBB
82	T7	203	PEB	C4B-C3B-CAB-CBB
82	W9	202	PEB	C4B-C3B-CAB-CBB
85	CL	516	BCR	C37-C22-C23-C24
87	DL	404	CLA	O1D-CGD-O2D-CED
87	AN	851	CLA	O1D-CGD-O2D-CED
87	C6	512	CLA	O1D-CGD-O2D-CED
87	7N	602	CLA	O1D-CGD-O2D-CED
87	cL	508	CLA	C13-C15-C16-C17
84	FO	1001	CYC	C2B-C3B-CAB-CBB
88	BL	610	LHG	C30-C31-C32-C33
88	L6	101	LHG	C15-C16-C17-C18
88	l6	101	LHG	C15-C16-C17-C18
95	CL	523	DGD	C7B-C8B-C9B-CAB
95	JL	101	DGD	C3A-C4A-C5A-C6A
95	cL	520	DGD	C7B-C8B-C9B-CAB
85	CL	516	BCR	C21-C22-C23-C24
85	K6	102	BCR	C11-C12-C13-C14
85	k6	102	BCR	C11-C12-C13-C14
87	CL	505	CLA	O1A-CGA-O2A-C1
87	AN	833	CLA	O1A-CGA-O2A-C1
87	BN	801	CLA	O1A-CGA-O2A-C1
87	BN	813	CLA	O1A-CGA-O2A-C1
87	A2	833	CLA	O1A-CGA-O2A-C1
87	B2	812	CLA	O1A-CGA-O2A-C1
87	B2	825	CLA	O1A-CGA-O2A-C1
87	bL	619	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
87	cL	507	CLA	O1A-CGA-O2A-C1
87	72	602	CLA	O1D-CGD-O2D-CED
87	A2	851	CLA	O1D-CGD-O2D-CED
87	AL	404	CLA	C1A-C2A-CAA-CBA
87	AL	405	CLA	C1A-C2A-CAA-CBA
87	BL	620	CLA	C1A-C2A-CAA-CBA
87	CL	503	CLA	C1A-C2A-CAA-CBA
87	CL	504	CLA	C1A-C2A-CAA-CBA
87	CL	506	CLA	C1A-C2A-CAA-CBA
87	CL	510	CLA	C1A-C2A-CAA-CBA
87	CL	514	CLA	C1A-C2A-CAA-CBA
87	DL	404	CLA	C1A-C2A-CAA-CBA
87	AN	805	CLA	C1A-C2A-CAA-CBA
87	AN	807	CLA	C1A-C2A-CAA-CBA
87	AN	810	CLA	C1A-C2A-CAA-CBA
87	AN	813	CLA	C1A-C2A-CAA-CBA
87	AN	825	CLA	C1A-C2A-CAA-CBA
87	AN	826	CLA	C1A-C2A-CAA-CBA
87	AN	831	CLA	C1A-C2A-CAA-CBA
87	AN	833	CLA	C1A-C2A-CAA-CBA
87	AN	834	CLA	C1A-C2A-CAA-CBA
87	AN	835	CLA	C1A-C2A-CAA-CBA
87	AN	837	CLA	C1A-C2A-CAA-CBA
87	AN	852	CLA	C1A-C2A-CAA-CBA
87	BN	801	CLA	C1A-C2A-CAA-CBA
87	BN	808	CLA	C1A-C2A-CAA-CBA
87	BN	811	CLA	C1A-C2A-CAA-CBA
87	BN	819	CLA	C1A-C2A-CAA-CBA
87	BN	826	CLA	C1A-C2A-CAA-CBA
87	BN	830	CLA	C1A-C2A-CAA-CBA
87	BN	836	CLA	C1A-C2A-CAA-CBA
87	KN	102	CLA	C1A-C2A-CAA-CBA
87	LN	202	CLA	C1A-C2A-CAA-CBA
87	LN	204	CLA	C1A-C2A-CAA-CBA
87	MN	101	CLA	C1A-C2A-CAA-CBA
87	RN	202	CLA	C1A-C2A-CAA-CBA
87	RN	203	CLA	C1A-C2A-CAA-CBA
87	12	605	CLA	C1A-C2A-CAA-CBA
87	12	607	CLA	C1A-C2A-CAA-CBA
87	12	610	CLA	C1A-C2A-CAA-CBA
87	12	611	CLA	C1A-C2A-CAA-CBA
87	22	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	22	612	CLA	C1A-C2A-CAA-CBA
87	32	305	CLA	C1A-C2A-CAA-CBA
87	32	308	CLA	C1A-C2A-CAA-CBA
87	32	309	CLA	C1A-C2A-CAA-CBA
87	32	313	CLA	C1A-C2A-CAA-CBA
87	42	605	CLA	C1A-C2A-CAA-CBA
87	42	611	CLA	C1A-C2A-CAA-CBA
87	52	602	CLA	C1A-C2A-CAA-CBA
87	52	606	CLA	C1A-C2A-CAA-CBA
87	52	610	CLA	C1A-C2A-CAA-CBA
87	62	303	CLA	C1A-C2A-CAA-CBA
87	72	605	CLA	C1A-C2A-CAA-CBA
87	72	607	CLA	C1A-C2A-CAA-CBA
87	82	308	CLA	C1A-C2A-CAA-CBA
87	A2	805	CLA	C1A-C2A-CAA-CBA
87	A2	807	CLA	C1A-C2A-CAA-CBA
87	A2	810	CLA	C1A-C2A-CAA-CBA
87	A2	813	CLA	C1A-C2A-CAA-CBA
87	A2	825	CLA	C1A-C2A-CAA-CBA
87	A2	826	CLA	C1A-C2A-CAA-CBA
87	A2	831	CLA	C1A-C2A-CAA-CBA
87	A2	833	CLA	C1A-C2A-CAA-CBA
87	A2	834	CLA	C1A-C2A-CAA-CBA
87	A2	835	CLA	C1A-C2A-CAA-CBA
87	A2	837	CLA	C1A-C2A-CAA-CBA
87	A2	852	CLA	C1A-C2A-CAA-CBA
87	B2	807	CLA	C1A-C2A-CAA-CBA
87	B2	810	CLA	C1A-C2A-CAA-CBA
87	B2	818	CLA	C1A-C2A-CAA-CBA
87	B2	825	CLA	C1A-C2A-CAA-CBA
87	B2	826	CLA	C1A-C2A-CAA-CBA
87	B2	830	CLA	C1A-C2A-CAA-CBA
87	B2	836	CLA	C1A-C2A-CAA-CBA
87	K2	103	CLA	C1A-C2A-CAA-CBA
87	L2	202	CLA	C1A-C2A-CAA-CBA
87	L2	204	CLA	C1A-C2A-CAA-CBA
87	M2	101	CLA	C1A-C2A-CAA-CBA
87	R2	202	CLA	C1A-C2A-CAA-CBA
87	R2	203	CLA	C1A-C2A-CAA-CBA
87	A6	403	CLA	C1A-C2A-CAA-CBA
87	B6	611	CLA	C1A-C2A-CAA-CBA
87	C6	509	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	C6	514	CLA	C1A-C2A-CAA-CBA
87	C6	519	CLA	C1A-C2A-CAA-CBA
87	D6	403	CLA	C1A-C2A-CAA-CBA
87	b6	605	CLA	C1A-C2A-CAA-CBA
87	c6	615	CLA	C1A-C2A-CAA-CBA
87	d6	403	CLA	C1A-C2A-CAA-CBA
87	bL	606	CLA	C1A-C2A-CAA-CBA
87	bL	620	CLA	C1A-C2A-CAA-CBA
87	cL	506	CLA	C1A-C2A-CAA-CBA
87	dL	409	CLA	C1A-C2A-CAA-CBA
87	1N	605	CLA	C1A-C2A-CAA-CBA
87	1N	607	CLA	C1A-C2A-CAA-CBA
87	1N	610	CLA	C1A-C2A-CAA-CBA
87	1N	611	CLA	C1A-C2A-CAA-CBA
87	2N	303	CLA	C1A-C2A-CAA-CBA
87	2N	312	CLA	C1A-C2A-CAA-CBA
87	3N	301	CLA	C1A-C2A-CAA-CBA
87	3N	306	CLA	C1A-C2A-CAA-CBA
87	3N	309	CLA	C1A-C2A-CAA-CBA
87	3N	313	CLA	C1A-C2A-CAA-CBA
87	4N	605	CLA	C1A-C2A-CAA-CBA
87	4N	611	CLA	C1A-C2A-CAA-CBA
87	5N	602	CLA	C1A-C2A-CAA-CBA
87	5N	606	CLA	C1A-C2A-CAA-CBA
87	5N	610	CLA	C1A-C2A-CAA-CBA
87	6N	602	CLA	C1A-C2A-CAA-CBA
87	7N	605	CLA	C1A-C2A-CAA-CBA
87	7N	607	CLA	C1A-C2A-CAA-CBA
87	8N	308	CLA	C1A-C2A-CAA-CBA
87	BL	608	CLA	C16-C17-C18-C20
87	BN	823	CLA	C16-C17-C18-C19
87	B6	604	CLA	C16-C17-C18-C20
87	K6	101	CLA	C16-C17-C18-C19
87	b6	608	CLA	C16-C17-C18-C20
92	B6	618	LMG	O9-C10-O7-C8
92	d6	409	LMG	O9-C10-O7-C8
92	bL	610	LMG	O9-C10-O7-C8
95	AL	414	DGD	O1B-C1B-O2G-C2G
95	CL	523	DGD	O1B-C1B-O2G-C2G
95	D6	410	DGD	O1B-C1B-O2G-C2G
95	cL	520	DGD	O1B-C1B-O2G-C2G
88	mL	102	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
92	x6	601	LMG	C11-C10-O7-C8
88	C6	505	LHG	C26-C27-C28-C29
95	cL	502	DGD	CAA-CBA-CCA-CDA
85	HL	103	BCR	C9-C10-C11-C12
87	DL	404	CLA	C13-C15-C16-C17
87	BN	809	CLA	C8-C10-C11-C12
87	BN	826	CLA	C10-C11-C12-C13
87	62	303	CLA	C8-C10-C11-C12
87	B2	808	CLA	C8-C10-C11-C12
87	B2	826	CLA	C10-C11-C12-C13
87	D6	405	CLA	C13-C15-C16-C17
87	6N	602	CLA	C8-C10-C11-C12
88	L6	101	LHG	C3-O3-P-O6
88	l6	101	LHG	C3-O3-P-O6
84	IO	1001	CYC	C2B-C3B-CAB-CBB
95	c6	618	DGD	CCA-CDA-CEA-CFA
88	d6	402	LHG	C23-C24-C25-C26
92	bL	611	LMG	C28-C29-C30-C31
87	AN	807	CLA	CBD-CGD-O2D-CED
87	A2	807	CLA	CBD-CGD-O2D-CED
82	GD	202	PEB	C2C-C1C-CHB-C4B
82	LF	202	PEB	C2C-C1C-CHB-C4B
82	ZJ	202	PEB	C2C-C1C-CHB-C4B
82	JK	202	PEB	C2C-C1C-CHB-C4B
82	LK	202	PEB	C2C-C1C-CHB-C4B
82	GQ	202	PEB	C2C-C1C-CHB-C4B
82	L5	202	PEB	C2C-C1C-CHB-C4B
82	O5	203	PEB	C2C-C1C-CHB-C4B
82	U5	202	PEB	C2C-C1C-CHB-C4B
82	cF	202	PEB	C2C-C1C-CHB-C4B
87	CL	513	CLA	C3-C5-C6-C7
84	r3	1001	CYC	C3C-C4C-CHD-C1D
84	I4	1001	CYC	C2B-C3B-CAB-CBB
92	J6	102	LMG	C33-C34-C35-C36
92	j6	101	LMG	C33-C34-C35-C36
87	B6	608	CLA	C8-C10-C11-C12
87	cL	510	CLA	C13-C15-C16-C17
88	AL	406	LHG	O6-C4-C5-C6
88	m6	102	LHG	O6-C4-C5-C6
88	a6	610	LHG	C24-C25-C26-C27
92	b6	623	LMG	C33-C34-C35-C36
95	C6	502	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
95	c6	601	DGD	C2B-C3B-C4B-C5B
88	BL	610	LHG	C7-C8-C9-C10
92	JL	102	LMG	C12-C13-C14-C15
92	B6	619	LMG	C29-C30-C31-C32
95	BL	614	DGD	CCA-CDA-CEA-CFA
95	C6	504	DGD	O6E-C5E-C6E-O5E
82	JA	203	PEB	C3B-CAB-CBB-CGB
82	WA	202	PEB	C3B-CAB-CBB-CGB
82	XA	202	PEB	C3B-CAB-CBB-CGB
82	IB	202	PEB	C2C-CAC-CBC-CGC
82	GD	202	PEB	C2C-CAC-CBC-CGC
82	DE	1002	PEB	C2C-CAC-CBC-CGC
82	HE	1002	PEB	C3B-CAB-CBB-CGB
82	WE	201	PEB	C2C-CAC-CBC-CGC
82	JF	202	PEB	C2C-CAC-CBC-CGC
82	NF	202	PEB	C2C-CAC-CBC-CGC
82	VF	201	PEB	C3B-CAB-CBB-CGB
82	XF	201	PEB	C2C-CAC-CBC-CGC
82	YF	203	PEB	C3B-CAB-CBB-CGB
82	DG	1002	PEB	C2C-CAC-CBC-CGC
82	HG	1002	PEB	C3B-CAB-CBB-CGB
82	PH	202	PEB	C2C-CAC-CBC-CGC
82	VH	202	PEB	C3B-CAB-CBB-CGB
82	WI	203	PEB	C2C-CAC-CBC-CGC
82	EJ	202	PEB	C3B-CAB-CBB-CGB
82	JK	202	PEB	C2C-CAC-CBC-CGC
82	NK	202	PEB	C2C-CAC-CBC-CGC
82	VK	201	PEB	C3B-CAB-CBB-CGB
82	XK	201	PEB	C2C-CAC-CBC-CGC
82	YK	203	PEB	C3B-CAB-CBB-CGB
82	GQ	202	PEB	C2C-CAC-CBC-CGC
82	P1	202	PEB	C2C-CAC-CBC-CGC
82	V1	203	PEB	C3B-CAB-CBB-CGB
82	l1	201	PEB	C2C-CAC-CBC-CGC
82	b1	203	PEB	C3B-CAB-CBB-CGB
82	J5	203	PEB	C2C-CAC-CBC-CGC
82	Q5	203	PEB	C2C-CAC-CBC-CGC
82	U5	202	PEB	C3B-CAB-CBB-CGB
82	J7	203	PEB	C3B-CAB-CBB-CGB
82	W7	202	PEB	C3B-CAB-CBB-CGB
82	X7	202	PEB	C3B-CAB-CBB-CGB
82	y8	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	y8	202	PEB	C2C-CAC-CBC-CGC
82	q8	203	PEB	C2C-CAC-CBC-CGC
82	B9	202	PEB	C3B-CAB-CBB-CGB
82	H9	201	PEB	C3B-CAB-CBB-CGB
82	S9	201	PEB	C3B-CAB-CBB-CGB
82	eB	202	PEB	C2C-CAC-CBC-CGC
82	qC	203	PEB	C2C-CAC-CBC-CGC
82	dE	202	PEB	C2C-CAC-CBC-CGC
82	hE	201	PEB	C3B-CAB-CBB-CGB
82	bF	202	PEB	C2C-CAC-CBC-CGC
82	gF	201	PEB	C3B-CAB-CBB-CGB
82	hF	201	PEB	C3B-CAB-CBB-CGB
82	hF	202	PEB	C2C-CAC-CBC-CGC
82	oF	203	PEB	C2C-CAC-CBC-CGC
82	dG	202	PEB	C2C-CAC-CBC-CGC
82	hG	201	PEB	C3B-CAB-CBB-CGB
82	kH	203	PEB	C2C-CAC-CBC-CGC
82	eH	203	PEB	C3B-CAB-CBB-CGB
82	bK	202	PEB	C2C-CAC-CBC-CGC
82	gK	201	PEB	C3B-CAB-CBB-CGB
82	hK	201	PEB	C3B-CAB-CBB-CGB
82	hK	202	PEB	C2C-CAC-CBC-CGC
82	oK	203	PEB	C2C-CAC-CBC-CGC
82	fM	203	PEB	C3B-CAB-CBB-CGB
84	NO	1001	CYC	C2A-CAA-CBA-CGA
84	N4	1001	CYC	C2A-CAA-CBA-CGA
87	BN	832	CLA	C8-C10-C11-C12
87	B2	832	CLA	C8-C10-C11-C12
87	C6	518	CLA	C5-C6-C7-C8
87	b6	605	CLA	C16-C17-C18-C20
92	bL	611	LMG	C14-C15-C16-C17
92	ML	101	LMG	C11-C12-C13-C14
87	bL	617	CLA	C13-C15-C16-C17
87	B6	614	CLA	CBD-CGD-O2D-CED
88	mL	102	LHG	C25-C26-C27-C28
87	BN	810	CLA	CBA-CGA-O2A-C1
87	B2	809	CLA	CBA-CGA-O2A-C1
87	c6	607	CLA	CBA-CGA-O2A-C1
92	C6	501	LMG	O6-C5-C6-O5
87	CL	505	CLA	C4-C3-C5-C6
87	LN	202	CLA	C4-C3-C5-C6
87	L2	202	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	c6	616	CLA	C4-C3-C5-C6
91	D6	404	PHO	C4-C3-C5-C6
91	a6	613	PHO	C4-C3-C5-C6
82	DA	202	PEB	C2A-C3A-CAA-CBA
82	EA	202	PEB	C2A-C3A-CAA-CBA
82	FA	202	PEB	C2A-C3A-CAA-CBA
82	HA	202	PEB	C2A-C3A-CAA-CBA
82	JA	202	PEB	C2A-C3A-CAA-CBA
82	LA	202	PEB	C2A-C3A-CAA-CBA
82	MA	202	PEB	C2A-C3A-CAA-CBA
82	NA	202	PEB	C2A-C3A-CAA-CBA
82	PA	202	PEB	C2A-C3A-CAA-CBA
82	QA	202	PEB	C2A-C3A-CAA-CBA
82	RA	202	PEB	C2A-C3A-CAA-CBA
82	SA	202	PEB	C2A-C3A-CAA-CBA
82	TA	202	PEB	C2A-C3A-CAA-CBA
82	UA	202	PEB	C2A-C3A-CAA-CBA
82	XA	202	PEB	C2A-C3A-CAA-CBA
82	DB	202	PEB	C2A-C3A-CAA-CBA
82	DB	203	PEB	C2A-C3A-CAA-CBA
82	HB	202	PEB	C2A-C3A-CAA-CBA
82	IB	201	PEB	C2A-C3A-CAA-CBA
82	KB	303	PEB	C2A-C3A-CAA-CBA
82	OB	201	PEB	C2A-C3A-CAA-CBA
82	QB	203	PEB	C2A-C3A-CAA-CBA
82	UB	303	PEB	C2A-C3A-CAA-CBA
82	XB	201	PEB	C2A-C3A-CAA-CBA
82	ZB	201	PEB	C2A-C3A-CAA-CBA
82	BD	203	PEB	C2A-C3A-CAA-CBA
82	DD	201	PEB	C2A-C3A-CAA-CBA
82	DD	203	PEB	C2A-C3A-CAA-CBA
82	FD	203	PEB	C2A-C3A-CAA-CBA
82	HD	201	PEB	C2A-C3A-CAA-CBA
82	HD	203	PEB	C2A-C3A-CAA-CBA
82	JD	202	PEB	C2A-C3A-CAA-CBA
82	JD	203	PEB	C2A-C3A-CAA-CBA
82	LD	201	PEB	C2A-C3A-CAA-CBA
82	ND	203	PEB	C2A-C3A-CAA-CBA
82	ND	204	PEB	C2A-C3A-CAA-CBA
82	RD	201	PEB	C2A-C3A-CAA-CBA
82	RD	202	PEB	C2A-C3A-CAA-CBA
82	TD	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	VD	202	PEB	C2A-C3A-CAA-CBA
82	VD	203	PEB	C2A-C3A-CAA-CBA
82	XD	201	PEB	C2A-C3A-CAA-CBA
82	XD	203	PEB	C2A-C3A-CAA-CBA
82	LE	1002	PEB	C2A-C3A-CAA-CBA
82	OE	201	PEB	C2A-C3A-CAA-CBA
82	OE	202	PEB	C2A-C3A-CAA-CBA
82	OE	203	PEB	C2A-C3A-CAA-CBA
82	QE	201	PEB	C2A-C3A-CAA-CBA
82	SE	201	PEB	C2A-C3A-CAA-CBA
82	SE	202	PEB	C2A-C3A-CAA-CBA
82	UE	202	PEB	C2A-C3A-CAA-CBA
82	UE	203	PEB	C2A-C3A-CAA-CBA
82	CF	202	PEB	C2A-C3A-CAA-CBA
82	CF	203	PEB	C2A-C3A-CAA-CBA
82	DF	202	PEB	C2A-C3A-CAA-CBA
82	IF	201	PEB	C2A-C3A-CAA-CBA
82	IF	203	PEB	C2A-C3A-CAA-CBA
82	JF	202	PEB	C2A-C3A-CAA-CBA
82	KF	201	PEB	C2A-C3A-CAA-CBA
82	MF	203	PEB	C2A-C3A-CAA-CBA
82	TF	202	PEB	C2A-C3A-CAA-CBA
82	UF	201	PEB	C2A-C3A-CAA-CBA
82	LG	1002	PEB	C2A-C3A-CAA-CBA
82	OG	201	PEB	C2A-C3A-CAA-CBA
82	OG	202	PEB	C2A-C3A-CAA-CBA
82	OG	203	PEB	C2A-C3A-CAA-CBA
82	QG	201	PEB	C2A-C3A-CAA-CBA
82	SG	201	PEB	C2A-C3A-CAA-CBA
82	SG	203	PEB	C2A-C3A-CAA-CBA
82	UG	202	PEB	C2A-C3A-CAA-CBA
82	UG	203	PEB	C2A-C3A-CAA-CBA
82	AH	302	PEB	C2A-C3A-CAA-CBA
82	FH	1002	PEB	C2A-C3A-CAA-CBA
82	HH	1002	PEB	C2A-C3A-CAA-CBA
82	QH	203	PEB	C2A-C3A-CAA-CBA
82	TH	201	PEB	C2A-C3A-CAA-CBA
82	UH	202	PEB	C2A-C3A-CAA-CBA
82	WH	201	PEB	C2A-C3A-CAA-CBA
82	WH	202	PEB	C2A-C3A-CAA-CBA
82	II	203	PEB	C2A-C3A-CAA-CBA
82	KI	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	SI	201	PEB	C2A-C3A-CAA-CBA
82	WI	202	PEB	C2A-C3A-CAA-CBA
82	EJ	201	PEB	C2A-C3A-CAA-CBA
82	EJ	203	PEB	C2A-C3A-CAA-CBA
82	GJ	203	PEB	C2A-C3A-CAA-CBA
82	IJ	201	PEB	C2A-C3A-CAA-CBA
82	KJ	203	PEB	C2A-C3A-CAA-CBA
82	MJ	201	PEB	C2A-C3A-CAA-CBA
82	MJ	203	PEB	C2A-C3A-CAA-CBA
82	OJ	202	PEB	C2A-C3A-CAA-CBA
82	QJ	202	PEB	C2A-C3A-CAA-CBA
82	QJ	204	PEB	C2A-C3A-CAA-CBA
82	SJ	202	PEB	C2A-C3A-CAA-CBA
82	SJ	203	PEB	C2A-C3A-CAA-CBA
82	UJ	201	PEB	C2A-C3A-CAA-CBA
82	WJ	203	PEB	C2A-C3A-CAA-CBA
82	YJ	201	PEB	C2A-C3A-CAA-CBA
82	YJ	203	PEB	C2A-C3A-CAA-CBA
82	CK	202	PEB	C2A-C3A-CAA-CBA
82	CK	203	PEB	C2A-C3A-CAA-CBA
82	DK	202	PEB	C2A-C3A-CAA-CBA
82	IK	201	PEB	C2A-C3A-CAA-CBA
82	IK	203	PEB	C2A-C3A-CAA-CBA
82	JK	202	PEB	C2A-C3A-CAA-CBA
82	KK	201	PEB	C2A-C3A-CAA-CBA
82	MK	203	PEB	C2A-C3A-CAA-CBA
82	TK	202	PEB	C2A-C3A-CAA-CBA
82	UK	201	PEB	C2A-C3A-CAA-CBA
82	BM	301	PEB	C2A-C3A-CAA-CBA
82	CM	202	PEB	C2A-C3A-CAA-CBA
82	EM	203	PEB	C2A-C3A-CAA-CBA
82	GM	202	PEB	C2A-C3A-CAA-CBA
82	GM	203	PEB	C2A-C3A-CAA-CBA
82	IM	201	PEB	C2A-C3A-CAA-CBA
82	KM	203	PEB	C2A-C3A-CAA-CBA
82	MM	201	PEB	C2A-C3A-CAA-CBA
82	MM	203	PEB	C2A-C3A-CAA-CBA
82	QM	202	PEB	C2A-C3A-CAA-CBA
82	QM	204	PEB	C2A-C3A-CAA-CBA
82	SM	201	PEB	C2A-C3A-CAA-CBA
82	SM	202	PEB	C2A-C3A-CAA-CBA
82	UM	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	WM	203	PEB	C2A-C3A-CAA-CBA
82	XM	201	PEB	C2A-C3A-CAA-CBA
82	YM	203	PEB	C2A-C3A-CAA-CBA
82	AO	305	PEB	C2A-C3A-CAA-CBA
82	DO	1002	PEB	C2A-C3A-CAA-CBA
82	JO	1002	PEB	C2A-C3A-CAA-CBA
82	NO	1002	PEB	C2A-C3A-CAA-CBA
82	QO	201	PEB	C2A-C3A-CAA-CBA
82	SO	202	PEB	C2A-C3A-CAA-CBA
82	TO	202	PEB	C2A-C3A-CAA-CBA
82	WO	201	PEB	C2A-C3A-CAA-CBA
82	ZO	201	PEB	C2A-C3A-CAA-CBA
82	AP	202	PEB	C2A-C3A-CAA-CBA
82	EP	201	PEB	C2A-C3A-CAA-CBA
82	QP	201	PEB	C2A-C3A-CAA-CBA
82	SP	203	PEB	C2A-C3A-CAA-CBA
82	BQ	203	PEB	C2A-C3A-CAA-CBA
82	DQ	201	PEB	C2A-C3A-CAA-CBA
82	DQ	203	PEB	C2A-C3A-CAA-CBA
82	FQ	203	PEB	C2A-C3A-CAA-CBA
82	HQ	201	PEB	C2A-C3A-CAA-CBA
82	HQ	203	PEB	C2A-C3A-CAA-CBA
82	JQ	202	PEB	C2A-C3A-CAA-CBA
82	JQ	203	PEB	C2A-C3A-CAA-CBA
82	LQ	201	PEB	C2A-C3A-CAA-CBA
82	NQ	203	PEB	C2A-C3A-CAA-CBA
82	NQ	204	PEB	C2A-C3A-CAA-CBA
82	RQ	201	PEB	C2A-C3A-CAA-CBA
82	RQ	202	PEB	C2A-C3A-CAA-CBA
82	TQ	201	PEB	C2A-C3A-CAA-CBA
82	VQ	202	PEB	C2A-C3A-CAA-CBA
82	VQ	203	PEB	C2A-C3A-CAA-CBA
82	XQ	201	PEB	C2A-C3A-CAA-CBA
82	XQ	203	PEB	C2A-C3A-CAA-CBA
82	T1	201	PEB	C2A-C3A-CAA-CBA
82	U1	202	PEB	C2A-C3A-CAA-CBA
82	A1	302	PEB	C2A-C3A-CAA-CBA
82	F1	1002	PEB	C2A-C3A-CAA-CBA
82	H1	1002	PEB	C2A-C3A-CAA-CBA
82	W1	201	PEB	C2A-C3A-CAA-CBA
82	W1	202	PEB	C2A-C3A-CAA-CBA
82	g1	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	b1	203	PEB	C2A-C3A-CAA-CBA
82	d1	202	PEB	C2A-C3A-CAA-CBA
82	e1	201	PEB	C2A-C3A-CAA-CBA
82	J4	1002	PEB	C2A-C3A-CAA-CBA
82	N4	1002	PEB	C2A-C3A-CAA-CBA
82	A4	305	PEB	C2A-C3A-CAA-CBA
82	D4	1002	PEB	C2A-C3A-CAA-CBA
82	Q4	201	PEB	C2A-C3A-CAA-CBA
82	S4	202	PEB	C2A-C3A-CAA-CBA
82	T4	202	PEB	C2A-C3A-CAA-CBA
82	W4	201	PEB	C2A-C3A-CAA-CBA
82	Z4	201	PEB	C2A-C3A-CAA-CBA
82	j4	201	PEB	C2A-C3A-CAA-CBA
82	k4	201	PEB	C2A-C3A-CAA-CBA
82	l4	201	PEB	C2A-C3A-CAA-CBA
82	l4	202	PEB	C2A-C3A-CAA-CBA
82	b4	201	PEB	C2A-C3A-CAA-CBA
82	f4	201	PEB	C2A-C3A-CAA-CBA
82	f4	202	PEB	C2A-C3A-CAA-CBA
82	h4	201	PEB	C2A-C3A-CAA-CBA
82	B5	202	PEB	C2A-C3A-CAA-CBA
82	F5	201	PEB	C2A-C3A-CAA-CBA
82	H5	202	PEB	C2A-C3A-CAA-CBA
82	J5	202	PEB	C2A-C3A-CAA-CBA
82	L5	202	PEB	C2A-C3A-CAA-CBA
82	O5	202	PEB	C2A-C3A-CAA-CBA
82	S5	202	PEB	C2A-C3A-CAA-CBA
82	U5	202	PEB	C2A-C3A-CAA-CBA
82	Y5	202	PEB	C2A-C3A-CAA-CBA
82	D7	202	PEB	C2A-C3A-CAA-CBA
82	E7	202	PEB	C2A-C3A-CAA-CBA
82	F7	202	PEB	C2A-C3A-CAA-CBA
82	H7	202	PEB	C2A-C3A-CAA-CBA
82	J7	202	PEB	C2A-C3A-CAA-CBA
82	L7	202	PEB	C2A-C3A-CAA-CBA
82	M7	202	PEB	C2A-C3A-CAA-CBA
82	N7	202	PEB	C2A-C3A-CAA-CBA
82	P7	202	PEB	C2A-C3A-CAA-CBA
82	Q7	202	PEB	C2A-C3A-CAA-CBA
82	R7	202	PEB	C2A-C3A-CAA-CBA
82	S7	202	PEB	C2A-C3A-CAA-CBA
82	T7	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	U7	202	PEB	C2A-C3A-CAA-CBA
82	X7	202	PEB	C2A-C3A-CAA-CBA
82	p8	201	PEB	C2A-C3A-CAA-CBA
82	q8	202	PEB	C2A-C3A-CAA-CBA
82	r8	202	PEB	C2A-C3A-CAA-CBA
82	u8	202	PEB	C2A-C3A-CAA-CBA
82	v8	202	PEB	C2A-C3A-CAA-CBA
82	w8	202	PEB	C2A-C3A-CAA-CBA
82	x8	201	PEB	C2A-C3A-CAA-CBA
82	x8	202	PEB	C2A-C3A-CAA-CBA
82	A9	202	PEB	C2A-C3A-CAA-CBA
82	C9	202	PEB	C2A-C3A-CAA-CBA
82	E9	202	PEB	C2A-C3A-CAA-CBA
82	F9	202	PEB	C2A-C3A-CAA-CBA
82	F9	203	PEB	C2A-C3A-CAA-CBA
82	G9	202	PEB	C2A-C3A-CAA-CBA
82	I9	202	PEB	C2A-C3A-CAA-CBA
82	K9	202	PEB	C2A-C3A-CAA-CBA
82	N9	202	PEB	C2A-C3A-CAA-CBA
82	P9	202	PEB	C2A-C3A-CAA-CBA
82	R9	202	PEB	C2A-C3A-CAA-CBA
82	S9	202	PEB	C2A-C3A-CAA-CBA
82	T9	202	PEB	C2A-C3A-CAA-CBA
82	U9	204	PEB	C2A-C3A-CAA-CBA
82	V9	202	PEB	C2A-C3A-CAA-CBA
82	W9	202	PEB	C2A-C3A-CAA-CBA
82	X9	202	PEB	C2A-C3A-CAA-CBA
82	dB	201	PEB	C2A-C3A-CAA-CBA
82	gB	201	PEB	C2A-C3A-CAA-CBA
82	pC	201	PEB	C2A-C3A-CAA-CBA
82	qC	202	PEB	C2A-C3A-CAA-CBA
82	rC	202	PEB	C2A-C3A-CAA-CBA
82	uC	202	PEB	C2A-C3A-CAA-CBA
82	vC	202	PEB	C2A-C3A-CAA-CBA
82	wC	202	PEB	C2A-C3A-CAA-CBA
82	xC	201	PEB	C2A-C3A-CAA-CBA
82	xC	202	PEB	C2A-C3A-CAA-CBA
82	dE	202	PEB	C2A-C3A-CAA-CBA
82	fE	201	PEB	C2A-C3A-CAA-CBA
82	hE	202	PEB	C2A-C3A-CAA-CBA
82	jE	201	PEB	C2A-C3A-CAA-CBA
82	eF	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	fF	201	PEB	C2A-C3A-CAA-CBA
82	iF	201	PEB	C2A-C3A-CAA-CBA
82	iF	202	PEB	C2A-C3A-CAA-CBA
82	iF	203	PEB	C2A-C3A-CAA-CBA
82	kF	201	PEB	C2A-C3A-CAA-CBA
82	qF	202	PEB	C2A-C3A-CAA-CBA
82	qF	203	PEB	C2A-C3A-CAA-CBA
82	sF	201	PEB	C2A-C3A-CAA-CBA
82	uF	201	PEB	C2A-C3A-CAA-CBA
82	xF	303	PEB	C2A-C3A-CAA-CBA
82	yF	301	PEB	C2A-C3A-CAA-CBA
82	zF	501	PEB	C2A-C3A-CAA-CBA
82	dG	202	PEB	C2A-C3A-CAA-CBA
82	fG	201	PEB	C2A-C3A-CAA-CBA
82	hG	202	PEB	C2A-C3A-CAA-CBA
82	jG	201	PEB	C2A-C3A-CAA-CBA
82	lG	202	PEB	C2A-C3A-CAA-CBA
82	gH	201	PEB	C2A-C3A-CAA-CBA
82	dH	202	PEB	C2A-C3A-CAA-CBA
82	eH	201	PEB	C2A-C3A-CAA-CBA
82	eH	203	PEB	C2A-C3A-CAA-CBA
82	aJ	204	PEB	C2A-C3A-CAA-CBA
82	dJ	201	PEB	C2A-C3A-CAA-CBA
82	fJ	203	PEB	C2A-C3A-CAA-CBA
82	hJ	203	PEB	C2A-C3A-CAA-CBA
82	jJ	202	PEB	C2A-C3A-CAA-CBA
82	jJ	203	PEB	C2A-C3A-CAA-CBA
82	lJ	201	PEB	C2A-C3A-CAA-CBA
82	lJ	203	PEB	C2A-C3A-CAA-CBA
82	eK	202	PEB	C2A-C3A-CAA-CBA
82	fK	201	PEB	C2A-C3A-CAA-CBA
82	iK	201	PEB	C2A-C3A-CAA-CBA
82	iK	202	PEB	C2A-C3A-CAA-CBA
82	iK	203	PEB	C2A-C3A-CAA-CBA
82	kK	201	PEB	C2A-C3A-CAA-CBA
82	qK	202	PEB	C2A-C3A-CAA-CBA
82	qK	203	PEB	C2A-C3A-CAA-CBA
82	sK	201	PEB	C2A-C3A-CAA-CBA
82	tK	203	PEB	C2A-C3A-CAA-CBA
82	xK	303	PEB	C2A-C3A-CAA-CBA
82	yK	301	PEB	C2A-C3A-CAA-CBA
82	zK	501	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	aM	204	PEB	C2A-C3A-CAA-CBA
82	cM	201	PEB	C2A-C3A-CAA-CBA
82	dM	201	PEB	C2A-C3A-CAA-CBA
82	dM	202	PEB	C2A-C3A-CAA-CBA
82	dM	203	PEB	C2A-C3A-CAA-CBA
82	fM	203	PEB	C2A-C3A-CAA-CBA
82	hM	201	PEB	C2A-C3A-CAA-CBA
82	hM	203	PEB	C2A-C3A-CAA-CBA
82	jM	203	PEB	C2A-C3A-CAA-CBA
82	lM	201	PEB	C2A-C3A-CAA-CBA
82	lM	203	PEB	C2A-C3A-CAA-CBA
82	jO	201	PEB	C2A-C3A-CAA-CBA
82	kO	201	PEB	C2A-C3A-CAA-CBA
82	lO	201	PEB	C2A-C3A-CAA-CBA
82	lO	202	PEB	C2A-C3A-CAA-CBA
82	bO	201	PEB	C2A-C3A-CAA-CBA
82	fO	201	PEB	C2A-C3A-CAA-CBA
82	fO	202	PEB	C2A-C3A-CAA-CBA
82	hO	201	PEB	C2A-C3A-CAA-CBA
82	bP	501	PEB	C2A-C3A-CAA-CBA
82	bP	502	PEB	C2A-C3A-CAA-CBA
82	Z9	301	PEB	C2A-C3A-CAA-CBA
82	M9	302	PEB	C2A-C3A-CAA-CBA
84	NE	201	CYC	C2C-C3C-CAC-CBC
84	KG	202	CYC	C2C-C3C-CAC-CBC
84	JH	1003	CYC	C2C-C3C-CAC-CBC
84	M1	201	CYC	C2C-C3C-CAC-CBC
84	A3	1001	CYC	C2C-C3C-CAC-CBC
84	C3	1001	CYC	C2C-C3C-CAC-CBC
84	E3	1001	CYC	C2C-C3C-CAC-CBC
84	G3	1001	CYC	C2C-C3C-CAC-CBC
84	J3	1001	CYC	C2C-C3C-CAC-CBC
84	K3	1001	CYC	C2C-C3C-CAC-CBC
84	N3	1001	CYC	C2C-C3C-CAC-CBC
84	P3	1001	CYC	C2C-C3C-CAC-CBC
84	R3	1001	CYC	C2C-C3C-CAC-CBC
84	T3	1001	CYC	C2C-C3C-CAC-CBC
84	c3	1001	CYC	C2C-C3C-CAC-CBC
84	e3	1001	CYC	C2C-C3C-CAC-CBC
84	g3	1001	CYC	C2C-C3C-CAC-CBC
84	i3	1001	CYC	C2C-C3C-CAC-CBC
84	l3	1001	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
84	m3	1001	CYC	C2C-C3C-CAC-CBC
84	p3	1001	CYC	C2C-C3C-CAC-CBC
84	t3	1001	CYC	C2C-C3C-CAC-CBC
84	v3	1001	CYC	C2C-C3C-CAC-CBC
87	DL	404	CLA	C2-C3-C5-C6
95	h6	101	DGD	C2B-C3B-C4B-C5B
95	cL	502	DGD	CBA-CCA-CDA-CEA
100	JN	104	3XQ	C10-C11-C12-C13
100	JN	104	3XQ	C2-C3-C4-C5
87	CL	504	CLA	C10-C11-C12-C13
87	A2	850	CLA	C15-C16-C17-C18
92	DL	402	LMG	C16-C17-C18-C19
92	k6	101	LMG	C11-C12-C13-C14
87	BN	833	CLA	O1A-CGA-O2A-C1
87	B2	833	CLA	O1A-CGA-O2A-C1
87	b6	613	CLA	O1A-CGA-O2A-C1
92	J6	102	LMG	O10-C28-O8-C9
84	F4	1001	CYC	C2B-C3B-CAB-CBB
88	DL	407	LHG	C24-C25-C26-C27
95	C6	502	DGD	C9B-CAB-CBB-CCB
95	c6	601	DGD	C9B-CAB-CBB-CCB
87	C6	514	CLA	C2A-CAA-CBA-CGA
87	D6	402	CLA	C3-C5-C6-C7
87	b6	616	CLA	C3-C5-C6-C7
88	AL	407	LHG	C30-C31-C32-C33
92	BL	612	LMG	O1-C7-C8-C9
92	JL	102	LMG	C7-C8-C9-O8
92	XL	601	LMG	C14-C15-C16-C17
92	B6	618	LMG	C7-C8-C9-O8
92	D6	409	LMG	C7-C8-C9-O8
92	j6	102	LMG	C7-C8-C9-O8
92	bL	624	LMG	O1-C7-C8-C9
92	mL	101	LMG	C7-C8-C9-O8
92	qL	301	LMG	C7-C8-C9-O8
92	yL	101	LMG	O1-C7-C8-C9
92	yL	101	LMG	C7-C8-C9-O8
95	B2	844	DGD	CFA-CGA-CHA-CIA
95	C6	523	DGD	C1G-C2G-C3G-O3G
95	O6	301	DGD	O1G-C1G-C2G-C3G
95	a6	602	DGD	C1G-C2G-C3G-O3G
95	c6	620	DGD	C1G-C2G-C3G-O3G
82	HA	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	MA	202	PEB	NC-C1C-CHB-C4B
82	RA	203	PEB	NC-C1C-CHB-C4B
82	WA	202	PEB	NC-C1C-CHB-C4B
82	JM	202	PEB	NC-C1C-CHB-C4B
82	B5	202	PEB	NC-C1C-CHB-C4B
82	H7	203	PEB	NC-C1C-CHB-C4B
82	M7	202	PEB	NC-C1C-CHB-C4B
82	R7	203	PEB	NC-C1C-CHB-C4B
82	W7	202	PEB	NC-C1C-CHB-C4B
83	AJ	303	PUB	NB-C4B-CHB-C1C
83	Z9	305	PUB	NB-C4B-CHB-C1C
87	AN	810	CLA	C15-C16-C17-C18
87	AN	850	CLA	C15-C16-C17-C18
87	AN	851	CLA	C5-C6-C7-C8
87	A2	810	CLA	C15-C16-C17-C18
87	A2	851	CLA	C5-C6-C7-C8
87	c6	604	CLA	C13-C15-C16-C17
87	cL	512	CLA	C15-C16-C17-C18
88	DL	407	LHG	C31-C32-C33-C34
88	C6	505	LHG	C11-C12-C13-C14
88	dL	405	LHG	C19-C20-C21-C22
95	BN	844	DGD	CFA-CGA-CHA-CIA
82	a4	203	PEB	C4B-C3B-CAB-CBB
82	aO	203	PEB	C4B-C3B-CAB-CBB
87	DL	404	CLA	O1A-CGA-O2A-C1
87	B2	835	CLA	O1A-CGA-O2A-C1
92	j6	101	LMG	O10-C28-O8-C9
95	BL	614	DGD	C5D-C6D-O5D-C1E
95	CL	523	DGD	C5D-C6D-O5D-C1E
95	C6	523	DGD	C5D-C6D-O5D-C1E
95	b6	622	DGD	C5D-C6D-O5D-C1E
95	c6	620	DGD	C5D-C6D-O5D-C1E
95	cL	520	DGD	C5D-C6D-O5D-C1E
95	lL	101	DGD	C5D-C6D-O5D-C1E
87	5N	607	CLA	O1D-CGD-O2D-CED
87	b6	611	CLA	C2C-C3C-CAC-CBC
87	52	607	CLA	O1D-CGD-O2D-CED
87	c6	612	CLA	O1D-CGD-O2D-CED
87	bL	621	CLA	CBD-CGD-O2D-CED
87	F2	205	CLA	C8-C10-C11-C12
87	B6	615	CLA	C5-C6-C7-C8
87	bL	619	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
88	AN	843	LHG	C11-C10-C9-C8
88	A2	843	LHG	C11-C10-C9-C8
92	AL	411	LMG	C22-C23-C24-C25
92	bL	623	LMG	C16-C17-C18-C19
92	qL	301	LMG	C12-C13-C14-C15
95	b6	622	DGD	C2A-C3A-C4A-C5A
100	J2	104	3XQ	C14-C15-C16-C17
100	J2	104	3XQ	C2-C3-C4-C5
92	yL	101	LMG	O8-C28-C29-C30
87	b6	609	CLA	O1D-CGD-O2D-CED
88	dL	408	LHG	C7-C8-C9-C10
87	BN	835	CLA	O1A-CGA-O2A-C1
87	D6	405	CLA	O1A-CGA-O2A-C1
87	cL	509	CLA	C4C-C3C-CAC-CBC
87	D6	402	CLA	C16-C17-C18-C20
87	FN	205	CLA	C8-C10-C11-C12
87	cL	508	CLA	C15-C16-C17-C18
82	NA	203	PEB	C2C-C1C-CHB-C4B
82	WA	202	PEB	C2C-C1C-CHB-C4B
82	SB	203	PEB	C2C-C1C-CHB-C4B
82	OD	202	PEB	C2C-C1C-CHB-C4B
82	VE	202	PEB	C2C-C1C-CHB-C4B
82	JF	202	PEB	C2C-C1C-CHB-C4B
82	WF	203	PEB	C2C-C1C-CHB-C4B
82	VG	202	PEB	C2C-C1C-CHB-C4B
82	WK	203	PEB	C2C-C1C-CHB-C4B
82	JM	202	PEB	C2C-C1C-CHB-C4B
82	OQ	202	PEB	C2C-C1C-CHB-C4B
82	c1	202	PEB	C2C-C1C-CHB-C4B
82	B5	202	PEB	C2C-C1C-CHB-C4B
82	O5	202	PEB	C2C-C1C-CHB-C4B
82	N7	203	PEB	C2C-C1C-CHB-C4B
82	W7	202	PEB	C2C-C1C-CHB-C4B
82	w8	203	PEB	C2C-C1C-CHB-C4B
82	kE	202	PEB	C2C-C1C-CHB-C4B
82	uF	203	PEB	C2C-C1C-CHB-C4B
82	kG	202	PEB	C2C-C1C-CHB-C4B
82	cH	202	PEB	C2C-C1C-CHB-C4B
82	uK	202	PEB	C2C-C1C-CHB-C4B
82	cM	201	PEB	C2C-C1C-CHB-C4B
82	cM	202	PEB	C2C-C1C-CHB-C4B
83	AH	304	PUB	C3B-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
83	A1	304	PUB	C3B-C4B-CHB-C1C
88	aL	607	LHG	C31-C32-C33-C34
92	bL	624	LMG	O6-C5-C6-O5
92	yL	101	LMG	O6-C5-C6-O5
88	CL	521	LHG	O1-C1-C2-O2
97	WL	101	GOL	O1-C1-C2-O2
97	wL	101	GOL	O1-C1-C2-O2
87	b6	614	CLA	C11-C12-C13-C14
95	L6	102	DGD	C7B-C8B-C9B-CAB
92	JL	102	LMG	C29-C30-C31-C32
92	D6	409	LMG	C39-C40-C41-C42
88	m6	102	LHG	C8-C7-O7-C5
88	L6	101	LHG	C29-C30-C31-C32
88	l6	101	LHG	C29-C30-C31-C32
88	bL	612	LHG	C19-C20-C21-C22
95	lL	101	DGD	C9B-CAB-CBB-CCB
87	AN	821	CLA	O1D-CGD-O2D-CED
87	A2	821	CLA	O1D-CGD-O2D-CED
87	C6	510	CLA	O1D-CGD-O2D-CED
87	BN	801	CLA	C13-C15-C16-C17
87	bL	605	CLA	C10-C11-C12-C13
92	AL	411	LMG	O6-C5-C6-O5
95	C6	523	DGD	O6E-C5E-C6E-O5E
95	a6	603	DGD	O6E-C5E-C6E-O5E
95	c6	620	DGD	O6E-C5E-C6E-O5E
87	AN	828	CLA	C4-C3-C5-C6
87	22	602	CLA	C4-C3-C5-C6
87	A2	828	CLA	C4-C3-C5-C6
87	cL	507	CLA	C4-C3-C5-C6
87	2N	303	CLA	C4-C3-C5-C6
91	AL	410	PHO	C4-C3-C5-C6
91	DL	405	PHO	C4-C3-C5-C6
91	dL	403	PHO	C4-C3-C5-C6
94	d6	408	PL9	C35-C34-C36-C37
82	QB	201	PEB	NC-C4C-CHC-C1D
82	PF	202	PEB	NC-C4C-CHC-C1D
82	PK	202	PEB	NC-C4C-CHC-C1D
82	bF	202	PEB	NC-C4C-CHC-C1D
82	bK	202	PEB	NC-C4C-CHC-C1D
87	LN	202	CLA	C8-C10-C11-C12
87	L2	202	CLA	C8-C10-C11-C12
92	m6	103	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
87	cL	507	CLA	C2-C3-C5-C6
92	DL	402	LMG	C10-C11-C12-C13
87	B6	615	CLA	C16-C17-C18-C20
87	B6	610	CLA	CBA-CGA-O2A-C1
87	b6	609	CLA	CBA-CGA-O2A-C1
82	CA	202	PEB	C3C-C2C-CAC-CBC
87	A6	404	CLA	C4C-C3C-CAC-CBC
87	BN	834	CLA	C8-C10-C11-C12
87	BN	835	CLA	C10-C11-C12-C13
87	B2	824	CLA	C10-C11-C12-C13
87	B2	825	CLA	C13-C15-C16-C17
87	B2	834	CLA	C8-C10-C11-C12
87	B2	835	CLA	C10-C11-C12-C13
87	b6	611	CLA	C5-C6-C7-C8
87	cL	506	CLA	C13-C15-C16-C17
82	TA	203	PEB	C2B-C3B-CAB-CBB
82	a4	203	PEB	C2B-C3B-CAB-CBB
82	T7	203	PEB	C2B-C3B-CAB-CBB
82	W9	202	PEB	C2B-C3B-CAB-CBB
82	aO	203	PEB	C2B-C3B-CAB-CBB
87	b6	605	CLA	C2C-C3C-CAC-CBC
95	B6	620	DGD	C5A-C6A-C7A-C8A
95	J6	101	DGD	C4A-C5A-C6A-C7A
82	GD	202	PEB	C1C-C2C-CAC-CBC
82	WM	202	PEB	C1C-C2C-CAC-CBC
82	jM	202	PEB	C1C-C2C-CAC-CBC
92	d6	409	LMG	C9-C8-O7-C10
87	AN	826	CLA	C2A-CAA-CBA-CGA
87	AN	832	CLA	C2A-CAA-CBA-CGA
87	AN	852	CLA	C2A-CAA-CBA-CGA
87	RN	202	CLA	C2A-CAA-CBA-CGA
87	A2	826	CLA	C2A-CAA-CBA-CGA
87	A2	832	CLA	C2A-CAA-CBA-CGA
87	A2	852	CLA	C2A-CAA-CBA-CGA
87	R2	202	CLA	C2A-CAA-CBA-CGA
87	CL	503	CLA	C8-C10-C11-C12
87	BN	806	CLA	C10-C11-C12-C13
87	BN	825	CLA	C10-C11-C12-C13
87	B2	805	CLA	C10-C11-C12-C13
87	CL	507	CLA	C2-C1-O2A-CGA
87	b6	613	CLA	C2-C1-O2A-CGA
87	B6	612	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
92	BL	612	LMG	O6-C5-C6-O5
95	J6	101	DGD	O6E-C5E-C6E-O5E
87	bL	617	CLA	C3-C5-C6-C7
88	B6	617	LHG	C19-C20-C21-C22
87	CL	509	CLA	C15-C16-C17-C18
87	AN	827	CLA	C5-C6-C7-C8
87	A2	827	CLA	C5-C6-C7-C8
87	bL	607	CLA	C15-C16-C17-C18
87	dL	401	CLA	C15-C16-C17-C18
87	BL	603	CLA	CBA-CGA-O2A-C1
87	CL	515	CLA	CBA-CGA-O2A-C1
87	AN	834	CLA	CBA-CGA-O2A-C1
87	A2	834	CLA	CBA-CGA-O2A-C1
87	H6	103	CLA	CBA-CGA-O2A-C1
87	bL	615	CLA	CBA-CGA-O2A-C1
88	C6	505	LHG	O6-C4-C5-O7
88	M6	101	LHG	O6-C4-C5-O7
87	AN	815	CLA	C16-C17-C18-C19
87	A2	815	CLA	C16-C17-C18-C19
82	XJ	202	PEB	NC-C1C-CHB-C4B
82	S5	203	PEB	NC-C1C-CHB-C4B
82	W5	202	PEB	NC-C1C-CHB-C4B
82	hF	201	PEB	NC-C1C-CHB-C4B
82	hK	201	PEB	NC-C1C-CHB-C4B
82	c4	203	PEB	C4B-C3B-CAB-CBB
82	cO	203	PEB	C4B-C3B-CAB-CBB
95	cL	502	DGD	O6D-C5D-C6D-O5D
87	AN	835	CLA	C5-C6-C7-C8
87	A2	835	CLA	C5-C6-C7-C8
87	c6	604	CLA	O1D-CGD-O2D-CED
87	cL	515	CLA	O1A-CGA-O2A-C1
92	b6	623	LMG	O10-C28-O8-C9
82	PA	202	PEB	C2C-CAC-CBC-CGC
82	RA	202	PEB	C2C-CAC-CBC-CGC
82	RA	203	PEB	C3B-CAB-CBB-CGB
82	GB	203	PEB	C3B-CAB-CBB-CGB
82	ED	201	PEB	C2C-CAC-CBC-CGC
82	KD	201	PEB	C2C-CAC-CBC-CGC
82	GE	1002	PEB	C3B-CAB-CBB-CGB
82	QF	203	PEB	C3B-CAB-CBB-CGB
82	GG	1002	PEB	C3B-CAB-CBB-CGB
82	PH	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	UH	203	PEB	C2C-CAC-CBC-CGC
82	WH	202	PEB	C3B-CAB-CBB-CGB
82	FJ	202	PEB	C2C-CAC-CBC-CGC
82	MJ	203	PEB	C3B-CAB-CBB-CGB
82	QK	203	PEB	C3B-CAB-CBB-CGB
82	QM	204	PEB	C3B-CAB-CBB-CGB
82	RM	202	PEB	C2C-CAC-CBC-CGC
82	PO	201	PEB	C2C-CAC-CBC-CGC
82	TO	201	PEB	C2C-CAC-CBC-CGC
82	JP	201	PEB	C2C-CAC-CBC-CGC
82	EQ	201	PEB	C2C-CAC-CBC-CGC
82	KQ	201	PEB	C2C-CAC-CBC-CGC
82	P1	201	PEB	C2C-CAC-CBC-CGC
82	U1	203	PEB	C2C-CAC-CBC-CGC
82	W1	202	PEB	C3B-CAB-CBB-CGB
82	a1	202	PEB	C3B-CAB-CBB-CGB
82	P4	201	PEB	C2C-CAC-CBC-CGC
82	T4	201	PEB	C2C-CAC-CBC-CGC
82	B5	202	PEB	C3B-CAB-CBB-CGB
82	D5	202	PEB	C3B-CAB-CBB-CGB
82	N7	201	PEB	C2C-CAC-CBC-CGC
82	P7	202	PEB	C2C-CAC-CBC-CGC
82	R7	202	PEB	C2C-CAC-CBC-CGC
82	R7	203	PEB	C3B-CAB-CBB-CGB
82	y8	202	PEB	C3B-CAB-CBB-CGB
82	H9	202	PEB	C2C-CAC-CBC-CGC
82	O9	203	PEB	C3B-CAB-CBB-CGB
82	eA	301	PEB	C2C-CAC-CBC-CGC
82	yC	202	PEB	C3B-CAB-CBB-CGB
82	kE	201	PEB	C2C-CAC-CBC-CGC
82	gF	203	PEB	C2C-CAC-CBC-CGC
82	kG	201	PEB	C2C-CAC-CBC-CGC
82	aH	202	PEB	C3B-CAB-CBB-CGB
82	dJ	201	PEB	C3B-CAB-CBB-CGB
82	gK	203	PEB	C2C-CAC-CBC-CGC
82	aM	204	PEB	C3B-CAB-CBB-CGB
82	Z9	301	PEB	C3B-CAB-CBB-CGB
82	M9	302	PEB	C3B-CAB-CBB-CGB
83	xF	301	PUB	C3B-CAB-CBB-CGB
83	xK	301	PUB	C3B-CAB-CBB-CGB
87	AN	828	CLA	C15-C16-C17-C18
87	BN	819	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
87	A2	828	CLA	C15-C16-C17-C18
87	B2	818	CLA	C5-C6-C7-C8
87	C6	510	CLA	C5-C6-C7-C8
87	b6	607	CLA	C5-C6-C7-C8
87	bL	614	CLA	C15-C16-C17-C18
87	CL	518	CLA	CAA-CBA-CGA-O2A
92	j6	102	LMG	O7-C8-C9-O8
88	aL	607	LHG	C30-C31-C32-C33
100	JN	104	3XQ	C3-C4-C5-C6
88	mL	102	LHG	O9-C7-O7-C5
95	b6	621	DGD	O1B-C1B-O2G-C2G
82	wC	203	PEB	C2C-C1C-CHB-C4B
82	aJ	203	PEB	C2C-C1C-CHB-C4B
87	BN	807	CLA	C10-C11-C12-C13
87	B2	806	CLA	C10-C11-C12-C13
91	DL	405	PHO	CHA-CBD-CGD-O2D
91	d6	404	PHO	CHA-CBD-CGD-O1D
91	d6	404	PHO	CHA-CBD-CGD-O2D
91	aL	610	PHO	CHA-CBD-CGD-O2D
91	dL	403	PHO	CHA-CBD-CGD-O1D
91	dL	403	PHO	CHA-CBD-CGD-O2D
87	BL	621	CLA	O1D-CGD-O2D-CED
88	BL	615	LHG	C14-C15-C16-C17
88	iL	101	LHG	C11-C10-C9-C8
92	m6	101	LMG	C18-C19-C20-C21
87	AN	803	CLA	C4-C3-C5-C6
87	AN	823	CLA	C4-C3-C5-C6
87	AN	826	CLA	C4-C3-C5-C6
87	BN	826	CLA	C4-C3-C5-C6
87	A2	803	CLA	C4-C3-C5-C6
87	A2	823	CLA	C4-C3-C5-C6
87	A2	826	CLA	C4-C3-C5-C6
87	B2	826	CLA	C4-C3-C5-C6
87	cL	515	CLA	C4-C3-C5-C6
94	DL	401	PL9	C35-C34-C36-C37
87	BL	603	CLA	C11-C10-C8-C7
87	CL	507	CLA	C11-C10-C8-C7
87	CL	508	CLA	C11-C12-C13-C15
87	CL	508	CLA	C12-C13-C15-C16
87	CL	513	CLA	C11-C10-C8-C7
87	HL	101	CLA	C11-C12-C13-C15
87	AN	803	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	AN	805	CLA	C12-C13-C15-C16
87	AN	809	CLA	C11-C12-C13-C15
87	AN	811	CLA	C11-C10-C8-C7
87	AN	815	CLA	C11-C12-C13-C15
87	AN	823	CLA	C6-C7-C8-C10
87	AN	826	CLA	C2-C3-C5-C6
87	AN	828	CLA	C2-C3-C5-C6
87	AN	834	CLA	C6-C7-C8-C10
87	AN	835	CLA	C11-C12-C13-C15
87	AN	851	CLA	C11-C12-C13-C15
87	BN	802	CLA	C6-C7-C8-C10
87	BN	806	CLA	C11-C10-C8-C7
87	BN	807	CLA	C6-C7-C8-C10
87	BN	807	CLA	C11-C10-C8-C7
87	BN	808	CLA	C6-C7-C8-C10
87	BN	810	CLA	C12-C13-C15-C16
87	BN	811	CLA	C6-C7-C8-C10
87	BN	811	CLA	C11-C10-C8-C7
87	BN	813	CLA	C11-C10-C8-C7
87	BN	813	CLA	C12-C13-C15-C16
87	BN	823	CLA	C11-C12-C13-C15
87	BN	826	CLA	C2-C3-C5-C6
87	BN	827	CLA	C11-C10-C8-C7
87	BN	830	CLA	C6-C7-C8-C10
87	BN	830	CLA	C11-C12-C13-C15
87	BN	831	CLA	C6-C7-C8-C10
87	BN	834	CLA	C11-C12-C13-C15
87	IN	102	CLA	C6-C7-C8-C10
87	IN	103	CLA	C6-C7-C8-C10
87	IN	103	CLA	C11-C12-C13-C15
87	LN	203	CLA	C11-C10-C8-C7
87	22	602	CLA	C2-C3-C5-C6
87	22	602	CLA	C6-C7-C8-C10
87	52	602	CLA	C6-C7-C8-C10
87	62	303	CLA	C12-C13-C15-C16
87	82	302	CLA	C6-C7-C8-C10
87	A2	803	CLA	C2-C3-C5-C6
87	A2	805	CLA	C12-C13-C15-C16
87	A2	809	CLA	C11-C12-C13-C15
87	A2	811	CLA	C11-C10-C8-C7
87	A2	815	CLA	C11-C12-C13-C15
87	A2	823	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
87	A2	826	CLA	C2-C3-C5-C6
87	A2	828	CLA	C2-C3-C5-C6
87	A2	834	CLA	C6-C7-C8-C10
87	A2	835	CLA	C11-C12-C13-C15
87	A2	851	CLA	C11-C12-C13-C15
87	B2	801	CLA	C6-C7-C8-C10
87	B2	805	CLA	C11-C10-C8-C7
87	B2	806	CLA	C6-C7-C8-C10
87	B2	806	CLA	C11-C10-C8-C7
87	B2	807	CLA	C6-C7-C8-C10
87	B2	809	CLA	C12-C13-C15-C16
87	B2	810	CLA	C6-C7-C8-C10
87	B2	810	CLA	C11-C10-C8-C7
87	B2	812	CLA	C11-C10-C8-C7
87	B2	812	CLA	C12-C13-C15-C16
87	B2	822	CLA	C11-C12-C13-C15
87	B2	826	CLA	C2-C3-C5-C6
87	B2	827	CLA	C11-C10-C8-C7
87	B2	830	CLA	C6-C7-C8-C10
87	B2	830	CLA	C11-C12-C13-C15
87	B2	831	CLA	C6-C7-C8-C10
87	B2	834	CLA	C11-C12-C13-C15
87	I2	102	CLA	C6-C7-C8-C10
87	I2	103	CLA	C6-C7-C8-C10
87	I2	103	CLA	C11-C12-C13-C15
87	K2	101	CLA	C11-C12-C13-C15
87	L2	203	CLA	C11-C10-C8-C7
87	B6	604	CLA	C11-C12-C13-C15
87	B6	608	CLA	C11-C10-C8-C7
87	B6	608	CLA	C12-C13-C15-C16
87	B6	609	CLA	C11-C10-C8-C7
87	B6	613	CLA	C11-C12-C13-C15
87	C6	512	CLA	C11-C10-C8-C7
87	C6	515	CLA	C6-C7-C8-C10
87	C6	515	CLA	C12-C13-C15-C16
87	C6	516	CLA	C12-C13-C15-C16
87	D6	405	CLA	C6-C7-C8-C10
87	H6	103	CLA	C12-C13-C15-C16
87	K6	101	CLA	C11-C10-C8-C7
87	a6	607	CLA	C12-C13-C15-C16
87	b6	608	CLA	C12-C13-C15-C16
87	b6	609	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
87	b6	613	CLA	C11-C10-C8-C7
87	b6	613	CLA	C11-C12-C13-C15
87	b6	617	CLA	C11-C12-C13-C15
87	b6	618	CLA	C6-C7-C8-C10
87	c6	606	CLA	C11-C10-C8-C7
87	c6	607	CLA	C11-C12-C13-C15
87	c6	609	CLA	C11-C12-C13-C15
87	c6	610	CLA	C6-C7-C8-C10
87	c6	612	CLA	C6-C7-C8-C10
87	c6	614	CLA	C6-C7-C8-C10
87	d6	403	CLA	C6-C7-C8-C10
87	bL	607	CLA	C12-C13-C15-C16
87	bL	618	CLA	C11-C10-C8-C7
87	cL	509	CLA	C11-C10-C8-C7
87	cL	510	CLA	C11-C12-C13-C15
87	cL	510	CLA	C12-C13-C15-C16
87	cL	515	CLA	C2-C3-C5-C6
87	nL	101	CLA	C11-C12-C13-C15
87	2N	303	CLA	C2-C3-C5-C6
87	2N	303	CLA	C6-C7-C8-C10
87	5N	602	CLA	C6-C7-C8-C10
87	6N	602	CLA	C12-C13-C15-C16
87	8N	303	CLA	C6-C7-C8-C10
91	DL	405	PHO	C2-C3-C5-C6
94	DL	401	PL9	C33-C34-C36-C37
94	d6	408	PL9	C33-C34-C36-C37
82	GF	203	PEB	C2B-C3B-CAB-CBB
82	GK	203	PEB	C2B-C3B-CAB-CBB
82	wF	303	PEB	C2B-C3B-CAB-CBB
82	wK	303	PEB	C2B-C3B-CAB-CBB
87	BL	602	CLA	C3-C5-C6-C7
87	cL	508	CLA	C3-C5-C6-C7
100	JN	104	3XQ	C7-C8-C9-C10
100	J2	104	3XQ	C11-C10-C9-C8
82	C7	202	PEB	C3C-C2C-CAC-CBC
87	BL	608	CLA	C11-C12-C13-C14
87	BL	620	CLA	C6-C7-C8-C9
87	CL	508	CLA	C6-C7-C8-C9
87	CL	508	CLA	C11-C12-C13-C14
87	CL	510	CLA	C11-C12-C13-C14
87	AN	805	CLA	C14-C13-C15-C16
87	AN	808	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
87	AN	809	CLA	C11-C12-C13-C14
87	AN	811	CLA	C11-C10-C8-C9
87	AN	813	CLA	C11-C12-C13-C14
87	AN	815	CLA	C11-C12-C13-C14
87	AN	819	CLA	C11-C12-C13-C14
87	AN	821	CLA	C11-C12-C13-C14
87	AN	834	CLA	C6-C7-C8-C9
87	AN	838	CLA	C6-C7-C8-C9
87	AN	841	CLA	C14-C13-C15-C16
87	AN	851	CLA	C11-C12-C13-C14
87	BN	802	CLA	C6-C7-C8-C9
87	BN	806	CLA	C11-C12-C13-C14
87	BN	813	CLA	C14-C13-C15-C16
87	BN	818	CLA	C11-C10-C8-C9
87	BN	827	CLA	C11-C10-C8-C9
87	BN	831	CLA	C6-C7-C8-C9
87	FN	205	CLA	C6-C7-C8-C9
87	FN	205	CLA	C14-C13-C15-C16
87	IN	102	CLA	C6-C7-C8-C9
87	IN	103	CLA	C11-C10-C8-C9
87	LN	203	CLA	C14-C13-C15-C16
87	42	602	CLA	C6-C7-C8-C9
87	82	302	CLA	C6-C7-C8-C9
87	A2	805	CLA	C14-C13-C15-C16
87	A2	808	CLA	C11-C10-C8-C9
87	A2	809	CLA	C11-C12-C13-C14
87	A2	811	CLA	C11-C10-C8-C9
87	A2	813	CLA	C11-C12-C13-C14
87	A2	815	CLA	C11-C12-C13-C14
87	A2	819	CLA	C11-C12-C13-C14
87	A2	821	CLA	C11-C12-C13-C14
87	A2	834	CLA	C6-C7-C8-C9
87	A2	838	CLA	C6-C7-C8-C9
87	A2	841	CLA	C14-C13-C15-C16
87	A2	851	CLA	C11-C12-C13-C14
87	B2	801	CLA	C6-C7-C8-C9
87	B2	805	CLA	C11-C12-C13-C14
87	B2	812	CLA	C14-C13-C15-C16
87	B2	817	CLA	C11-C10-C8-C9
87	B2	827	CLA	C11-C10-C8-C9
87	B2	831	CLA	C6-C7-C8-C9
87	F2	205	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
87	F2	205	CLA	C14-C13-C15-C16
87	I2	102	CLA	C6-C7-C8-C9
87	I2	103	CLA	C11-C10-C8-C9
87	K2	101	CLA	C11-C12-C13-C14
87	L2	203	CLA	C14-C13-C15-C16
87	B6	608	CLA	C14-C13-C15-C16
87	B6	611	CLA	C11-C10-C8-C9
87	C6	515	CLA	C6-C7-C8-C9
87	K6	101	CLA	C11-C10-C8-C9
87	b6	606	CLA	C11-C10-C8-C9
87	b6	606	CLA	C11-C12-C13-C14
87	b6	613	CLA	C11-C10-C8-C9
87	b6	618	CLA	C6-C7-C8-C9
87	c6	605	CLA	C11-C12-C13-C14
87	c6	606	CLA	C11-C12-C13-C14
87	c6	607	CLA	C6-C7-C8-C9
87	d6	401	CLA	C14-C13-C15-C16
87	bL	607	CLA	C14-C13-C15-C16
87	bL	613	CLA	C14-C13-C15-C16
87	bL	622	CLA	C6-C7-C8-C9
87	cL	510	CLA	C11-C12-C13-C14
87	cL	511	CLA	C6-C7-C8-C9
87	cL	514	CLA	C11-C12-C13-C14
87	2N	303	CLA	C6-C7-C8-C9
87	4N	602	CLA	C6-C7-C8-C9
87	8N	303	CLA	C6-C7-C8-C9
98	AN	842	PQN	C16-C17-C18-C19
98	A2	842	PQN	C16-C17-C18-C19
103	82	310	ZEX	C33-C34-C35-C15
91	DL	405	PHO	CBD-CGD-O2D-CED
95	hL	101	DGD	C4A-C5A-C6A-C7A
87	AL	403	CLA	CBA-CGA-O2A-C1
87	BL	608	CLA	CBA-CGA-O2A-C1
87	CL	506	CLA	CBA-CGA-O2A-C1
87	CL	507	CLA	C10-C11-C12-C13
91	DL	405	PHO	C15-C16-C17-C18
87	52	611	CLA	C2A-CAA-CBA-CGA
87	c6	616	CLA	C2A-CAA-CBA-CGA
87	aL	606	CLA	C2A-CAA-CBA-CGA
87	5N	611	CLA	C2A-CAA-CBA-CGA
95	h6	101	DGD	C6B-C7B-C8B-C9B
85	Z6	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
87	B6	611	CLA	C16-C17-C18-C19
82	GF	203	PEB	NA-C4A-CHA-C1B
82	GK	203	PEB	NA-C4A-CHA-C1B
82	A5	202	PEB	NA-C4A-CHA-C1B
82	C5	202	PEB	NA-C4A-CHA-C1B
82	E5	202	PEB	NA-C4A-CHA-C1B
82	G5	202	PEB	NA-C4A-CHA-C1B
82	I5	202	PEB	NA-C4A-CHA-C1B
82	K5	202	PEB	NA-C4A-CHA-C1B
82	N5	202	PEB	NA-C4A-CHA-C1B
82	P5	202	PEB	NA-C4A-CHA-C1B
82	R5	202	PEB	NA-C4A-CHA-C1B
82	T5	202	PEB	NA-C4A-CHA-C1B
82	V5	202	PEB	NA-C4A-CHA-C1B
82	X5	202	PEB	NA-C4A-CHA-C1B
82	z8	202	PEB	NA-C4A-CHA-C1B
82	p8	202	PEB	NA-C4A-CHA-C1B
82	r8	202	PEB	NA-C4A-CHA-C1B
82	t8	202	PEB	NA-C4A-CHA-C1B
82	v8	202	PEB	NA-C4A-CHA-C1B
82	x8	202	PEB	NA-C4A-CHA-C1B
82	A9	202	PEB	NA-C4A-CHA-C1B
82	C9	202	PEB	NA-C4A-CHA-C1B
82	E9	202	PEB	NA-C4A-CHA-C1B
82	G9	202	PEB	NA-C4A-CHA-C1B
82	I9	202	PEB	NA-C4A-CHA-C1B
82	K9	202	PEB	NA-C4A-CHA-C1B
82	N9	202	PEB	NA-C4A-CHA-C1B
82	P9	202	PEB	NA-C4A-CHA-C1B
82	R9	202	PEB	NA-C4A-CHA-C1B
82	T9	202	PEB	NA-C4A-CHA-C1B
82	V9	202	PEB	NA-C4A-CHA-C1B
82	X9	202	PEB	NA-C4A-CHA-C1B
82	zC	202	PEB	NA-C4A-CHA-C1B
82	pC	202	PEB	NA-C4A-CHA-C1B
82	rC	202	PEB	NA-C4A-CHA-C1B
82	tC	202	PEB	NA-C4A-CHA-C1B
82	vC	202	PEB	NA-C4A-CHA-C1B
82	xC	202	PEB	NA-C4A-CHA-C1B
82	mF	202	PEB	NA-C4A-CHA-C1B
82	mK	202	PEB	NA-C4A-CHA-C1B
87	D6	403	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
85	AN	804	BCR	C7-C8-C9-C10
85	A2	804	BCR	C7-C8-C9-C10
85	Z6	101	BCR	C21-C22-C23-C24
92	J6	102	LMG	C32-C33-C34-C35
95	a6	602	DGD	O1B-C1B-O2G-C2G
87	AN	849	CLA	C10-C11-C12-C13
87	A2	849	CLA	C10-C11-C12-C13
87	C6	509	CLA	C5-C6-C7-C8
87	D6	403	CLA	C10-C11-C12-C13
87	b6	617	CLA	C10-C11-C12-C13
92	j6	101	LMG	C32-C33-C34-C35
95	JL	101	DGD	C9A-CAA-CBA-CCA
87	b6	614	CLA	CBA-CGA-O2A-C1
95	JL	101	DGD	C2A-C1A-O1G-C1G
95	DL	408	DGD	C6B-C7B-C8B-C9B
95	DL	408	DGD	C7B-C8B-C9B-CAB
88	BL	610	LHG	C23-C24-C25-C26
87	BN	830	CLA	C8-C10-C11-C12
87	B2	830	CLA	C8-C10-C11-C12
87	B6	615	CLA	C8-C10-C11-C12
87	C6	509	CLA	C15-C16-C17-C18
87	cL	507	CLA	C8-C10-C11-C12
87	cL	511	CLA	C5-C6-C7-C8
82	IA	202	PEB	NC-C1C-CHB-C4B
82	OB	201	PEB	NC-C1C-CHB-C4B
82	ND	204	PEB	NC-C1C-CHB-C4B
82	OI	203	PEB	NC-C1C-CHB-C4B
82	VJ	202	PEB	NC-C1C-CHB-C4B
82	KM	202	PEB	NC-C1C-CHB-C4B
82	NQ	204	PEB	NC-C1C-CHB-C4B
82	RQ	202	PEB	NC-C1C-CHB-C4B
82	U5	203	PEB	NC-C1C-CHB-C4B
82	w8	201	PEB	NC-C1C-CHB-C4B
82	F9	201	PEB	NC-C1C-CHB-C4B
82	wC	201	PEB	NC-C1C-CHB-C4B
82	cM	201	PEB	NC-C1C-CHB-C4B
82	cM	202	PEB	NC-C1C-CHB-C4B
82	Z9	303	PEB	NC-C1C-CHB-C4B
82	M9	304	PEB	NC-C1C-CHB-C4B
84	LG	1001	CYC	C2B-C3B-CAB-CBB
87	B6	612	CLA	C10-C11-C12-C13
88	AL	407	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
88	AN	843	LHG	C9-C10-C11-C12
88	A2	843	LHG	C9-C10-C11-C12
95	c6	618	DGD	C2B-C3B-C4B-C5B
100	J2	104	3XQ	C3-C4-C5-C6
82	LE	1002	PEB	C4B-C3B-CAB-CBB
82	LG	1002	PEB	C4B-C3B-CAB-CBB
82	ZK	201	PEB	C4B-C3B-CAB-CBB
82	S5	201	PEB	C4B-C3B-CAB-CBB
82	dE	204	PEB	C4B-C3B-CAB-CBB
82	lF	201	PEB	C4B-C3B-CAB-CBB
82	dG	204	PEB	C4B-C3B-CAB-CBB
82	lK	201	PEB	C4B-C3B-CAB-CBB
84	BE	1001	CYC	C1A-C2A-CAA-CBA
84	BG	1001	CYC	C1A-C2A-CAA-CBA
95	aL	603	DGD	CBB-CCB-CDB-CEB
87	BL	608	CLA	C4B-C3B-CAB-CBB
87	BL	623	CLA	C4B-C3B-CAB-CBB
87	CL	504	CLA	C4B-C3B-CAB-CBB
87	CL	506	CLA	C4B-C3B-CAB-CBB
87	CL	513	CLA	C4B-C3B-CAB-CBB
87	CL	514	CLA	C4B-C3B-CAB-CBB
87	HL	102	CLA	C4B-C3B-CAB-CBB
87	AN	810	CLA	C4B-C3B-CAB-CBB
87	AN	815	CLA	C4B-C3B-CAB-CBB
87	AN	816	CLA	C4B-C3B-CAB-CBB
87	AN	819	CLA	C4B-C3B-CAB-CBB
87	AN	827	CLA	C4B-C3B-CAB-CBB
87	AN	828	CLA	C4B-C3B-CAB-CBB
87	AN	836	CLA	C4B-C3B-CAB-CBB
87	AN	851	CLA	C4B-C3B-CAB-CBB
87	BN	815	CLA	C4B-C3B-CAB-CBB
87	BN	816	CLA	C4B-C3B-CAB-CBB
87	BN	823	CLA	C4B-C3B-CAB-CBB
87	BN	826	CLA	C4B-C3B-CAB-CBB
87	BN	827	CLA	C4B-C3B-CAB-CBB
87	BN	829	CLA	C4B-C3B-CAB-CBB
87	BN	833	CLA	C4B-C3B-CAB-CBB
87	LN	204	CLA	C4B-C3B-CAB-CBB
87	ON	201	CLA	C4B-C3B-CAB-CBB
87	22	611	CLA	C4B-C3B-CAB-CBB
87	42	602	CLA	C4B-C3B-CAB-CBB
87	42	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	52	610	CLA	C4B-C3B-CAB-CBB
87	62	303	CLA	C4B-C3B-CAB-CBB
87	62	304	CLA	C4B-C3B-CAB-CBB
87	62	312	CLA	C4B-C3B-CAB-CBB
87	72	601	CLA	C4B-C3B-CAB-CBB
87	72	609	CLA	C4B-C3B-CAB-CBB
87	82	302	CLA	C4B-C3B-CAB-CBB
87	82	305	CLA	C4B-C3B-CAB-CBB
87	82	306	CLA	C4B-C3B-CAB-CBB
87	A2	810	CLA	C4B-C3B-CAB-CBB
87	A2	815	CLA	C4B-C3B-CAB-CBB
87	A2	816	CLA	C4B-C3B-CAB-CBB
87	A2	819	CLA	C4B-C3B-CAB-CBB
87	A2	827	CLA	C4B-C3B-CAB-CBB
87	A2	828	CLA	C4B-C3B-CAB-CBB
87	A2	836	CLA	C4B-C3B-CAB-CBB
87	A2	851	CLA	C4B-C3B-CAB-CBB
87	B2	814	CLA	C4B-C3B-CAB-CBB
87	B2	815	CLA	C4B-C3B-CAB-CBB
87	B2	822	CLA	C4B-C3B-CAB-CBB
87	B2	826	CLA	C4B-C3B-CAB-CBB
87	B2	827	CLA	C4B-C3B-CAB-CBB
87	B2	829	CLA	C4B-C3B-CAB-CBB
87	B2	833	CLA	C4B-C3B-CAB-CBB
87	L2	204	CLA	C4B-C3B-CAB-CBB
87	O2	201	CLA	C4B-C3B-CAB-CBB
87	B6	603	CLA	C4B-C3B-CAB-CBB
87	b6	615	CLA	C4B-C3B-CAB-CBB
87	d6	406	CLA	C4B-C3B-CAB-CBB
87	bL	607	CLA	C4B-C3B-CAB-CBB
87	bL	613	CLA	C4B-C3B-CAB-CBB
87	bL	620	CLA	C4B-C3B-CAB-CBB
87	cL	508	CLA	C4B-C3B-CAB-CBB
87	2N	311	CLA	C4B-C3B-CAB-CBB
87	4N	602	CLA	C4B-C3B-CAB-CBB
87	4N	610	CLA	C4B-C3B-CAB-CBB
87	5N	610	CLA	C4B-C3B-CAB-CBB
87	6N	602	CLA	C4B-C3B-CAB-CBB
87	6N	603	CLA	C4B-C3B-CAB-CBB
87	6N	611	CLA	C4B-C3B-CAB-CBB
87	7N	601	CLA	C4B-C3B-CAB-CBB
87	7N	609	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	8N	301	CLA	C4B-C3B-CAB-CBB
87	8N	303	CLA	C4B-C3B-CAB-CBB
87	8N	306	CLA	C4B-C3B-CAB-CBB
87	32	304	CLA	C16-C17-C18-C20
87	3N	305	CLA	C16-C17-C18-C20
87	B6	607	CLA	C13-C15-C16-C17
88	AL	407	LHG	O6-C4-C5-C6
88	a6	610	LHG	O6-C4-C5-C6
88	c6	619	LHG	O6-C4-C5-C6
88	aL	607	LHG	O6-C4-C5-C6
88	dL	408	LHG	O6-C4-C5-C6
88	iL	101	LHG	O6-C4-C5-C6
88	bL	612	LHG	C15-C16-C17-C18
87	A6	402	CLA	CBA-CGA-O2A-C1
87	B6	609	CLA	CBD-CGD-O2D-CED
87	BN	807	CLA	C15-C16-C17-C18
87	B2	806	CLA	C15-C16-C17-C18
87	bL	608	CLA	C13-C15-C16-C17
82	c4	203	PEB	C2B-C3B-CAB-CBB
82	cO	203	PEB	C2B-C3B-CAB-CBB
87	C6	511	CLA	O1D-CGD-O2D-CED
87	CL	503	CLA	C4-C3-C5-C6
87	CL	508	CLA	C4-C3-C5-C6
87	AN	821	CLA	C4-C3-C5-C6
87	A2	821	CLA	C4-C3-C5-C6
87	C6	514	CLA	C4-C3-C5-C6
87	b6	615	CLA	C4-C3-C5-C6
94	A6	410	PL9	C40-C39-C41-C42
94	dL	406	PL9	C20-C19-C21-C22
87	AN	821	CLA	C2-C3-C5-C6
87	AN	823	CLA	C2-C3-C5-C6
87	A2	823	CLA	C2-C3-C5-C6
87	C6	514	CLA	C2-C3-C5-C6
91	a6	613	PHO	C2-C3-C5-C6
91	dL	403	PHO	C2-C3-C5-C6
94	d6	408	PL9	C38-C39-C41-C42
82	IB	203	PEB	C2C-C1C-CHB-C4B
82	GQ	202	PEB	C1C-C2C-CAC-CBC
82	S5	203	PEB	C2C-C1C-CHB-C4B
82	y8	201	PEB	C1C-C2C-CAC-CBC
82	dE	201	PEB	C1C-C2C-CAC-CBC
82	dG	201	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
82	aM	203	PEB	C1C-C2C-CAC-CBC
95	D6	410	DGD	C1B-C2B-C3B-C4B
98	BN	837	PQN	C25-C26-C27-C28
98	B2	837	PQN	C25-C26-C27-C28
88	cL	501	LHG	O2-C2-C3-O3
92	x6	601	LMG	O9-C10-O7-C8
95	C6	523	DGD	O1B-C1B-O2G-C2G
95	a6	603	DGD	O1B-C1B-O2G-C2G
95	c6	620	DGD	O1B-C1B-O2G-C2G
87	B6	610	CLA	O1A-CGA-O2A-C1
87	c6	607	CLA	O1A-CGA-O2A-C1
92	B6	619	LMG	C11-C12-C13-C14
87	cL	512	CLA	O1D-CGD-O2D-CED
87	cL	510	CLA	C3-C5-C6-C7
95	cL	502	DGD	C4D-C5D-C6D-O5D
87	CL	504	CLA	C16-C17-C18-C20
83	QM	201	PUB	C4A-C3A-CAA-CBA
88	C6	505	LHG	C11-C10-C9-C8
95	AL	414	DGD	C5A-C6A-C7A-C8A
95	C6	521	DGD	C3A-C4A-C5A-C6A
87	A2	831	CLA	O1D-CGD-O2D-CED
87	BN	819	CLA	CBA-CGA-O2A-C1
87	B2	818	CLA	CBA-CGA-O2A-C1
92	JL	102	LMG	C29-C28-O8-C9
95	J6	101	DGD	C2A-C1A-O1G-C1G
84	LE	1001	CYC	C2B-C3B-CAB-CBB
88	ML	102	LHG	C11-C10-C9-C8
92	J6	102	LMG	C12-C13-C14-C15
92	j6	101	LMG	C12-C13-C14-C15
95	BL	614	DGD	C4A-C5A-C6A-C7A
88	M6	101	LHG	C5-C4-O6-P
87	AN	831	CLA	O1D-CGD-O2D-CED
87	b6	609	CLA	O1A-CGA-O2A-C1
87	AN	824	CLA	C3A-C2A-CAA-CBA
87	BN	826	CLA	C3A-C2A-CAA-CBA
87	ON	202	CLA	C3A-C2A-CAA-CBA
87	52	601	CLA	C3A-C2A-CAA-CBA
87	62	312	CLA	C3A-C2A-CAA-CBA
87	82	305	CLA	C3A-C2A-CAA-CBA
87	A2	824	CLA	C3A-C2A-CAA-CBA
87	B2	826	CLA	C3A-C2A-CAA-CBA
87	O2	202	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	B6	611	CLA	C3A-C2A-CAA-CBA
87	C6	514	CLA	C3A-C2A-CAA-CBA
87	H6	102	CLA	C3A-C2A-CAA-CBA
87	b6	618	CLA	C3A-C2A-CAA-CBA
87	5N	601	CLA	C3A-C2A-CAA-CBA
87	6N	611	CLA	C3A-C2A-CAA-CBA
87	8N	306	CLA	C3A-C2A-CAA-CBA
85	AN	845	BCR	C15-C16-C17-C18
85	A2	845	BCR	C15-C16-C17-C18
103	8N	310	ZEX	C33-C34-C35-C15
88	AN	843	LHG	C17-C18-C19-C20
88	AN	844	LHG	C13-C14-C15-C16
88	A2	843	LHG	C17-C18-C19-C20
88	A2	844	LHG	C13-C14-C15-C16
95	BN	844	DGD	C2A-C3A-C4A-C5A
95	B2	844	DGD	C2A-C3A-C4A-C5A
95	C6	521	DGD	C5B-C6B-C7B-C8B
95	lL	101	DGD	C8B-C9B-CAB-CBB
87	B6	606	CLA	C13-C15-C16-C17
88	m6	102	LHG	C11-C10-C9-C8
92	DL	402	LMG	C35-C36-C37-C38
92	k6	101	LMG	C33-C34-C35-C36
95	lL	101	DGD	CCA-CDA-CEA-CFA
82	IA	202	PEB	C3B-CAB-CBB-CGB
82	JA	202	PEB	C3B-CAB-CBB-CGB
82	LA	203	PEB	C3B-CAB-CBB-CGB
82	NA	201	PEB	C2C-CAC-CBC-CGC
82	OA	202	PEB	C3B-CAB-CBB-CGB
82	RA	202	PEB	C3B-CAB-CBB-CGB
82	TA	202	PEB	C3B-CAB-CBB-CGB
82	BB	202	PEB	C3B-CAB-CBB-CGB
82	HB	203	PEB	C2C-CAC-CBC-CGC
82	HB	203	PEB	C3B-CAB-CBB-CGB
82	VB	202	PEB	C3B-CAB-CBB-CGB
82	WB	402	PEB	C2C-CAC-CBC-CGC
82	BD	201	PEB	C3B-CAB-CBB-CGB
82	DD	201	PEB	C3B-CAB-CBB-CGB
82	HD	202	PEB	C2C-CAC-CBC-CGC
82	ID	201	PEB	C2C-CAC-CBC-CGC
82	JD	201	PEB	C2C-CAC-CBC-CGC
82	JD	203	PEB	C3B-CAB-CBB-CGB
82	ND	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	ND	204	PEB	C3B-CAB-CBB-CGB
82	OD	202	PEB	C3B-CAB-CBB-CGB
82	RD	201	PEB	C3B-CAB-CBB-CGB
82	WD	202	PEB	C3B-CAB-CBB-CGB
82	UE	201	PEB	C3B-CAB-CBB-CGB
82	DF	202	PEB	C3B-CAB-CBB-CGB
82	JF	201	PEB	C2C-CAC-CBC-CGC
82	LF	202	PEB	C3B-CAB-CBB-CGB
82	TF	202	PEB	C2C-CAC-CBC-CGC
82	VF	201	PEB	C2C-CAC-CBC-CGC
82	UG	201	PEB	C3B-CAB-CBB-CGB
82	NH	1002	PEB	C3B-CAB-CBB-CGB
82	QH	202	PEB	C2C-CAC-CBC-CGC
82	TH	202	PEB	C3B-CAB-CBB-CGB
82	FI	201	PEB	C2C-CAC-CBC-CGC
82	SI	201	PEB	C2C-CAC-CBC-CGC
82	BJ	301	PEB	C2C-CAC-CBC-CGC
82	IJ	203	PEB	C3B-CAB-CBB-CGB
82	RJ	201	PEB	C2C-CAC-CBC-CGC
82	SJ	203	PEB	C2C-CAC-CBC-CGC
82	TJ	202	PEB	C2C-CAC-CBC-CGC
82	DK	202	PEB	C3B-CAB-CBB-CGB
82	JK	201	PEB	C2C-CAC-CBC-CGC
82	LK	202	PEB	C3B-CAB-CBB-CGB
82	VK	201	PEB	C2C-CAC-CBC-CGC
82	FM	202	PEB	C2C-CAC-CBC-CGC
82	GM	202	PEB	C3B-CAB-CBB-CGB
82	HM	201	PEB	C2C-CAC-CBC-CGC
82	MM	201	PEB	C3B-CAB-CBB-CGB
82	OM	201	PEB	C2C-CAC-CBC-CGC
82	QM	202	PEB	C2C-CAC-CBC-CGC
82	XM	201	PEB	C2C-CAC-CBC-CGC
82	NO	1002	PEB	C2C-CAC-CBC-CGC
82	RO	202	PEB	C2C-CAC-CBC-CGC
82	ZO	202	PEB	C2C-CAC-CBC-CGC
82	DP	201	PEB	C2C-CAC-CBC-CGC
82	LP	201	PEB	C2C-CAC-CBC-CGC
82	PP	201	PEB	C2C-CAC-CBC-CGC
82	VP	201	PEB	C2C-CAC-CBC-CGC
82	YP	501	PEB	C2C-CAC-CBC-CGC
82	YP	502	PEB	C3B-CAB-CBB-CGB
82	BQ	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	DQ	201	PEB	C3B-CAB-CBB-CGB
82	HQ	202	PEB	C2C-CAC-CBC-CGC
82	IQ	201	PEB	C2C-CAC-CBC-CGC
82	JQ	201	PEB	C2C-CAC-CBC-CGC
82	JQ	203	PEB	C3B-CAB-CBB-CGB
82	NQ	202	PEB	C2C-CAC-CBC-CGC
82	NQ	204	PEB	C3B-CAB-CBB-CGB
82	OQ	202	PEB	C3B-CAB-CBB-CGB
82	RQ	201	PEB	C3B-CAB-CBB-CGB
82	WQ	202	PEB	C3B-CAB-CBB-CGB
82	N1	1002	PEB	C3B-CAB-CBB-CGB
82	Q1	202	PEB	C2C-CAC-CBC-CGC
82	T1	202	PEB	C3B-CAB-CBB-CGB
82	i1	201	PEB	C2C-CAC-CBC-CGC
82	j1	201	PEB	C2C-CAC-CBC-CGC
82	m1	201	PEB	C2C-CAC-CBC-CGC
82	e1	201	PEB	C2C-CAC-CBC-CGC
82	N4	1002	PEB	C2C-CAC-CBC-CGC
82	R4	202	PEB	C2C-CAC-CBC-CGC
82	Z4	202	PEB	C2C-CAC-CBC-CGC
82	F5	202	PEB	C2C-CAC-CBC-CGC
82	F5	202	PEB	C3B-CAB-CBB-CGB
82	H5	203	PEB	C2C-CAC-CBC-CGC
82	J5	202	PEB	C3B-CAB-CBB-CGB
82	O5	202	PEB	C3B-CAB-CBB-CGB
82	O5	203	PEB	C2C-CAC-CBC-CGC
82	Q5	202	PEB	C3B-CAB-CBB-CGB
82	U5	203	PEB	C2C-CAC-CBC-CGC
82	I7	202	PEB	C3B-CAB-CBB-CGB
82	J7	202	PEB	C3B-CAB-CBB-CGB
82	L7	203	PEB	C3B-CAB-CBB-CGB
82	O7	202	PEB	C3B-CAB-CBB-CGB
82	R7	202	PEB	C3B-CAB-CBB-CGB
82	T7	202	PEB	C3B-CAB-CBB-CGB
82	e7	301	PEB	C2C-CAC-CBC-CGC
82	y8	201	PEB	C2C-CAC-CBC-CGC
82	18	202	PEB	C2C-CAC-CBC-CGC
82	p8	201	PEB	C2C-CAC-CBC-CGC
82	p8	202	PEB	C2C-CAC-CBC-CGC
82	s8	202	PEB	C2C-CAC-CBC-CGC
82	D9	202	PEB	C2C-CAC-CBC-CGC
82	F9	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	F9	202	PEB	C2C-CAC-CBC-CGC
82	L9	202	PEB	C2C-CAC-CBC-CGC
82	Q9	202	PEB	C2C-CAC-CBC-CGC
82	U9	202	PEB	C2C-CAC-CBC-CGC
82	W9	202	PEB	C2C-CAC-CBC-CGC
82	Y9	201	PEB	C2C-CAC-CBC-CGC
82	cB	403	PEB	C2C-CAC-CBC-CGC
82	1C	202	PEB	C2C-CAC-CBC-CGC
82	pC	201	PEB	C2C-CAC-CBC-CGC
82	pC	202	PEB	C2C-CAC-CBC-CGC
82	sC	202	PEB	C2C-CAC-CBC-CGC
82	fE	201	PEB	C2C-CAC-CBC-CGC
82	cF	203	PEB	C3B-CAB-CBB-CGB
82	fF	202	PEB	C3B-CAB-CBB-CGB
82	kF	201	PEB	C2C-CAC-CBC-CGC
82	kF	203	PEB	C2C-CAC-CBC-CGC
82	qF	203	PEB	C2C-CAC-CBC-CGC
82	wF	302	PEB	C2C-CAC-CBC-CGC
82	fG	201	PEB	C2C-CAC-CBC-CGC
82	iH	201	PEB	C2C-CAC-CBC-CGC
82	jH	201	PEB	C2C-CAC-CBC-CGC
82	mH	201	PEB	C2C-CAC-CBC-CGC
82	eH	201	PEB	C2C-CAC-CBC-CGC
82	dJ	202	PEB	C3B-CAB-CBB-CGB
82	hJ	202	PEB	C2C-CAC-CBC-CGC
82	hJ	203	PEB	C2C-CAC-CBC-CGC
82	cK	203	PEB	C3B-CAB-CBB-CGB
82	fK	202	PEB	C3B-CAB-CBB-CGB
82	gK	202	PEB	C3B-CAB-CBB-CGB
82	kK	201	PEB	C2C-CAC-CBC-CGC
82	kK	203	PEB	C2C-CAC-CBC-CGC
82	qK	203	PEB	C2C-CAC-CBC-CGC
82	wK	302	PEB	C2C-CAC-CBC-CGC
82	dM	202	PEB	C2C-CAC-CBC-CGC
82	fM	201	PEB	C2C-CAC-CBC-CGC
82	iM	201	PEB	C2C-CAC-CBC-CGC
82	lM	203	PEB	C3B-CAB-CBB-CGB
83	AE	303	PUB	C3B-CAB-CBB-CGB
83	AG	303	PUB	C3B-CAB-CBB-CGB
83	AH	303	PUB	C2C-CAC-CBC-CGC
83	AO	303	PUB	C3B-CAB-CBB-CGB
83	A1	303	PUB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
83	A4	303	PUB	C3B-CAB-CBB-CGB
83	xF	306	PUB	C2C-CAC-CBC-CGC
83	xK	306	PUB	C2C-CAC-CBC-CGC
84	BE	1001	CYC	C2A-CAA-CBA-CGA
84	BG	1001	CYC	C2A-CAA-CBA-CGA
82	CA	202	PEB	NB-C4B-CHB-C1C
82	C7	202	PEB	NB-C4B-CHB-C1C
87	C6	518	CLA	CBA-CGA-O2A-C1
87	c6	609	CLA	CBA-CGA-O2A-C1
95	C6	503	DGD	C2A-C1A-O1G-C1G
84	J3	1001	CYC	C2B-C3B-CAB-CBB
84	N3	1001	CYC	C2B-C3B-CAB-CBB
95	BL	614	DGD	CAA-CBA-CCA-CDA
87	AN	841	CLA	C13-C15-C16-C17
87	A2	841	CLA	C13-C15-C16-C17
87	c6	607	CLA	C15-C16-C17-C18
88	AL	406	LHG	C4-C5-C6-O8
88	AL	407	LHG	C4-C5-C6-O8
88	AN	843	LHG	C4-C5-C6-O8
88	A2	843	LHG	C4-C5-C6-O8
88	i6	101	LHG	C4-C5-C6-O8
88	aL	607	LHG	C4-C5-C6-O8
92	ML	101	LMG	C7-C8-C9-O8
92	B6	622	LMG	O1-C7-C8-C9
92	J6	102	LMG	C7-C8-C9-O8
92	d6	409	LMG	C7-C8-C9-O8
92	j6	101	LMG	C7-C8-C9-O8
92	j6	102	LMG	O1-C7-C8-C9
92	bL	609	LMG	C7-C8-C9-O8
95	CL	520	DGD	O1G-C1G-C2G-C3G
95	BN	844	DGD	C1G-C2G-C3G-O3G
95	B2	844	DGD	C1G-C2G-C3G-O3G
95	C6	503	DGD	O6E-C5E-C6E-O5E
95	L6	102	DGD	O1G-C1G-C2G-C3G
95	hL	101	DGD	O1G-C1G-C2G-C3G
84	A3	1001	CYC	C2B-C3B-CAB-CBB
84	FE	1001	CYC	C4B-C3B-CAB-CBB
84	CG	1001	CYC	C4B-C3B-CAB-CBB
84	EO	1001	CYC	C4B-C3B-CAB-CBB
84	E4	1001	CYC	C4B-C3B-CAB-CBB
87	bL	615	CLA	O1A-CGA-O2A-C1
82	RD	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
84	r3	1001	CYC	C2B-C1B-CHB-C4A
84	C3	1001	CYC	C2B-C3B-CAB-CBB
84	K3	1001	CYC	C2B-C3B-CAB-CBB
84	c3	1001	CYC	C2B-C3B-CAB-CBB
84	g3	1001	CYC	C2B-C3B-CAB-CBB
84	m3	1001	CYC	C2B-C3B-CAB-CBB
88	AN	844	LHG	C26-C27-C28-C29
88	A2	844	LHG	C26-C27-C28-C29
92	ML	101	LMG	C19-C20-C21-C22
92	B6	622	LMG	C16-C17-C18-C19
95	CL	517	DGD	C5B-C6B-C7B-C8B
82	ZF	201	PEB	C4B-C3B-CAB-CBB
87	AN	823	CLA	C8-C10-C11-C12
87	A2	823	CLA	C8-C10-C11-C12
87	d6	403	CLA	CAA-CBA-CGA-O2A
84	l3	1001	CYC	C2B-C3B-CAB-CBB
92	JL	102	LMG	C33-C34-C35-C36
92	bL	611	LMG	C41-C42-C43-C44
82	DA	201	PEB	C2B-C3B-CAB-CBB
82	QE	201	PEB	C2B-C3B-CAB-CBB
82	QG	201	PEB	C2B-C3B-CAB-CBB
82	PM	201	PEB	C2B-C3B-CAB-CBB
82	D7	201	PEB	C2B-C3B-CAB-CBB
87	CL	505	CLA	O1D-CGD-O2D-CED
84	E3	1001	CYC	C2B-C3B-CAB-CBB
84	G3	1001	CYC	C2B-C3B-CAB-CBB
84	P3	1001	CYC	C2B-C3B-CAB-CBB
84	R3	1001	CYC	C2B-C3B-CAB-CBB
84	e3	1001	CYC	C2B-C3B-CAB-CBB
84	i3	1001	CYC	C2B-C3B-CAB-CBB
84	p3	1001	CYC	C2B-C3B-CAB-CBB
84	v3	1001	CYC	C2B-C3B-CAB-CBB
92	d6	409	LMG	C16-C17-C18-C19
95	C6	502	DGD	C6A-C7A-C8A-C9A
95	b6	621	DGD	C3A-C4A-C5A-C6A
95	c6	601	DGD	C6A-C7A-C8A-C9A
87	BL	603	CLA	O1A-CGA-O2A-C1
98	AN	842	PQN	C25-C26-C27-C28
98	A2	842	PQN	C25-C26-C27-C28
87	B6	605	CLA	C4-C3-C5-C6
87	C6	519	CLA	C4-C3-C5-C6
87	c6	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
87	cL	505	CLA	C4-C3-C5-C6
87	b6	608	CLA	C16-C17-C18-C19
87	CL	508	CLA	C2-C3-C5-C6
87	A2	821	CLA	C2-C3-C5-C6
84	T3	1001	CYC	C2B-C3B-CAB-CBB
84	t3	1001	CYC	C2B-C3B-CAB-CBB
87	d6	401	CLA	C4C-C3C-CAC-CBC
88	BL	615	LHG	C9-C10-C11-C12
87	bL	607	CLA	O1D-CGD-O2D-CED
82	DD	202	PEB	C2C-C1C-CHB-C4B
82	OI	203	PEB	C2C-C1C-CHB-C4B
82	VJ	202	PEB	C2C-C1C-CHB-C4B
82	XJ	202	PEB	C2C-C1C-CHB-C4B
82	F9	201	PEB	C2C-C1C-CHB-C4B
82	fM	202	PEB	C2C-C1C-CHB-C4B
87	AN	806	CLA	C3-C5-C6-C7
87	42	602	CLA	C3-C5-C6-C7
87	A2	806	CLA	C3-C5-C6-C7
87	4N	602	CLA	C3-C5-C6-C7
87	b6	611	CLA	C2A-CAA-CBA-CGA
91	D6	404	PHO	C2A-CAA-CBA-CGA
88	CL	522	LHG	O1-C1-C2-O2
88	aL	607	LHG	O1-C1-C2-O2
87	32	304	CLA	C8-C10-C11-C12
87	3N	305	CLA	C8-C10-C11-C12
88	L6	101	LHG	O6-C4-C5-O7
88	l6	101	LHG	O6-C4-C5-O7
88	iL	101	LHG	O6-C4-C5-O7
87	b6	612	CLA	CBA-CGA-O2A-C1
87	bL	608	CLA	CBA-CGA-O2A-C1
88	C6	522	LHG	C10-C11-C12-C13
87	B6	615	CLA	C16-C17-C18-C19
87	BN	823	CLA	C8-C10-C11-C12
91	aL	610	PHO	C10-C11-C12-C13
88	D6	406	LHG	C26-C27-C28-C29
92	JL	102	LMG	C36-C37-C38-C39
87	AN	808	CLA	CBD-CGD-O2D-CED
87	BL	623	CLA	C2B-C3B-CAB-CBB
87	CL	514	CLA	C2B-C3B-CAB-CBB
87	AN	819	CLA	C2B-C3B-CAB-CBB
87	AN	851	CLA	C2B-C3B-CAB-CBB
87	BN	815	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	BN	823	CLA	C2B-C3B-CAB-CBB
87	BN	826	CLA	C2B-C3B-CAB-CBB
87	BN	827	CLA	C2B-C3B-CAB-CBB
87	BN	833	CLA	C2B-C3B-CAB-CBB
87	ON	201	CLA	C2B-C3B-CAB-CBB
87	42	602	CLA	C2B-C3B-CAB-CBB
87	42	610	CLA	C2B-C3B-CAB-CBB
87	62	303	CLA	C2B-C3B-CAB-CBB
87	62	312	CLA	C2B-C3B-CAB-CBB
87	82	303	CLA	C2B-C3B-CAB-CBB
87	A2	819	CLA	C2B-C3B-CAB-CBB
87	A2	851	CLA	C2B-C3B-CAB-CBB
87	B2	814	CLA	C2B-C3B-CAB-CBB
87	B2	822	CLA	C2B-C3B-CAB-CBB
87	B2	826	CLA	C2B-C3B-CAB-CBB
87	B2	827	CLA	C2B-C3B-CAB-CBB
87	B2	833	CLA	C2B-C3B-CAB-CBB
87	O2	201	CLA	C2B-C3B-CAB-CBB
87	B6	603	CLA	C2B-C3B-CAB-CBB
87	bL	607	CLA	C2B-C3B-CAB-CBB
87	bL	620	CLA	C2B-C3B-CAB-CBB
87	cL	508	CLA	C2B-C3B-CAB-CBB
87	4N	602	CLA	C2B-C3B-CAB-CBB
87	4N	610	CLA	C2B-C3B-CAB-CBB
87	6N	602	CLA	C2B-C3B-CAB-CBB
87	6N	611	CLA	C2B-C3B-CAB-CBB
87	8N	304	CLA	C2B-C3B-CAB-CBB
92	AL	411	LMG	C19-C20-C21-C22
92	XL	601	LMG	C40-C41-C42-C43
95	a6	604	DGD	C3A-C4A-C5A-C6A
87	C6	518	CLA	C8-C10-C11-C12
87	c6	616	CLA	C8-C10-C11-C12
87	AL	403	CLA	O1A-CGA-O2A-C1
87	CL	506	CLA	O1A-CGA-O2A-C1
87	CL	515	CLA	O1A-CGA-O2A-C1
87	AN	834	CLA	O1A-CGA-O2A-C1
87	A2	834	CLA	O1A-CGA-O2A-C1
88	AL	407	LHG	O7-C5-C6-O8
88	i6	101	LHG	O7-C5-C6-O8
92	BL	612	LMG	O1-C7-C8-O7
92	DL	402	LMG	O7-C8-C9-O8
92	b6	620	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
92	b6	620	LMG	O7-C8-C9-O8
92	bL	624	LMG	O1-C7-C8-O7
95	BL	614	DGD	O2G-C2G-C3G-O3G
95	BN	844	DGD	O2G-C2G-C3G-O3G
95	B2	844	DGD	O2G-C2G-C3G-O3G
95	O6	301	DGD	O1G-C1G-C2G-O2G
87	A2	808	CLA	CBD-CGD-O2D-CED
87	K2	101	CLA	CBA-CGA-O2A-C1
87	BL	601	CLA	C15-C16-C17-C18
87	B2	822	CLA	C8-C10-C11-C12
87	cL	509	CLA	C15-C16-C17-C18
88	D6	406	LHG	C13-C14-C15-C16
95	J6	101	DGD	C3A-C4A-C5A-C6A
82	J9	201	PEB	C2B-C3B-CAB-CBB
92	C6	501	LMG	C37-C38-C39-C40
92	dL	407	LMG	O6-C1-O1-C7
87	BN	809	CLA	C5-C6-C7-C8
87	22	605	CLA	C5-C6-C7-C8
87	B2	808	CLA	C5-C6-C7-C8
87	B6	609	CLA	C5-C6-C7-C8
87	2N	301	CLA	C5-C6-C7-C8
82	I7	202	PEB	NC-C1C-CHB-C4B
88	i6	101	LHG	C1-C2-C3-O3
94	A6	410	PL9	C19-C21-C22-C23
88	i6	101	LHG	C18-C19-C20-C21
92	AL	411	LMG	C20-C21-C22-C23
95	BN	844	DGD	C2B-C3B-C4B-C5B
95	B2	844	DGD	C2B-C3B-C4B-C5B
95	C6	502	DGD	CDB-CEB-CFB-CGB
95	c6	601	DGD	CDB-CEB-CFB-CGB
88	m6	102	LHG	O9-C7-O7-C5
87	AN	806	CLA	C2-C1-O2A-CGA
87	AN	819	CLA	C2-C1-O2A-CGA
87	A2	806	CLA	C2-C1-O2A-CGA
87	A2	819	CLA	C2-C1-O2A-CGA
87	B6	614	CLA	C2-C1-O2A-CGA
87	b6	616	CLA	C2-C1-O2A-CGA
87	c6	609	CLA	C2-C1-O2A-CGA
87	CL	511	CLA	O1D-CGD-O2D-CED
87	CL	509	CLA	C5-C6-C7-C8
82	YE	201	PEB	C3C-C2C-CAC-CBC
82	YG	201	PEB	C3C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
87	BL	601	CLA	C11-C12-C13-C14
87	BL	623	CLA	C14-C13-C15-C16
87	CL	507	CLA	C14-C13-C15-C16
87	HL	101	CLA	C11-C12-C13-C14
87	AN	810	CLA	C11-C10-C8-C9
87	AN	813	CLA	C11-C10-C8-C9
87	AN	826	CLA	C6-C7-C8-C9
87	AN	830	CLA	C6-C7-C8-C9
87	AN	835	CLA	C6-C7-C8-C9
87	BN	801	CLA	C14-C13-C15-C16
87	BN	806	CLA	C6-C7-C8-C9
87	BN	830	CLA	C11-C12-C13-C14
87	IN	103	CLA	C6-C7-C8-C9
87	LN	202	CLA	C11-C10-C8-C9
87	A2	810	CLA	C11-C10-C8-C9
87	A2	813	CLA	C11-C10-C8-C9
87	A2	826	CLA	C6-C7-C8-C9
87	A2	830	CLA	C6-C7-C8-C9
87	A2	835	CLA	C6-C7-C8-C9
87	B2	805	CLA	C6-C7-C8-C9
87	B2	825	CLA	C14-C13-C15-C16
87	B2	830	CLA	C11-C12-C13-C14
87	I2	103	CLA	C6-C7-C8-C9
87	L2	202	CLA	C11-C10-C8-C9
87	C6	517	CLA	C14-C13-C15-C16
87	b6	605	CLA	C6-C7-C8-C9
87	b6	614	CLA	C6-C7-C8-C9
87	b6	615	CLA	C14-C13-C15-C16
87	c6	612	CLA	C11-C10-C8-C9
87	cL	509	CLA	C14-C13-C15-C16
87	cL	510	CLA	C6-C7-C8-C9
87	nL	101	CLA	C11-C12-C13-C14
92	b6	624	LMG	C30-C31-C32-C33
95	c6	620	DGD	C6B-C7B-C8B-C9B
87	AN	850	CLA	C10-C11-C12-C13
87	BN	807	CLA	C5-C6-C7-C8
87	A2	850	CLA	C10-C11-C12-C13
87	B2	806	CLA	C5-C6-C7-C8
87	A6	403	CLA	C5-C6-C7-C8
87	c6	613	CLA	C8-C10-C11-C12
82	FA	202	PEB	C4D-C3D-CAD-CBD
82	SD	202	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
82	KI	201	PEB	C4D-C3D-CAD-CBD
82	SQ	202	PEB	C4D-C3D-CAD-CBD
82	e1	202	PEB	C4D-C3D-CAD-CBD
82	F7	202	PEB	C4D-C3D-CAD-CBD
82	eH	202	PEB	C4D-C3D-CAD-CBD
82	cK	202	PEB	C4D-C3D-CAD-CBD
88	m6	102	LHG	C5-C4-O6-P
88	iL	101	LHG	C2-C3-O3-P
88	mL	102	LHG	C5-C4-O6-P
87	BL	608	CLA	O1A-CGA-O2A-C1
87	H6	103	CLA	O1A-CGA-O2A-C1
87	b6	614	CLA	O1A-CGA-O2A-C1
92	BL	611	LMG	C13-C14-C15-C16
92	bL	623	LMG	C13-C14-C15-C16
95	C6	503	DGD	C3A-C4A-C5A-C6A
87	AN	815	CLA	C16-C17-C18-C20
87	AN	834	CLA	C16-C17-C18-C20
87	A2	815	CLA	C16-C17-C18-C20
87	A2	834	CLA	C16-C17-C18-C19
87	A2	834	CLA	C16-C17-C18-C20
87	A6	403	CLA	C11-C12-C13-C14
87	b6	606	CLA	C16-C17-C18-C20
87	b6	610	CLA	C16-C17-C18-C19
87	b6	616	CLA	C16-C17-C18-C20
85	KL	100	BCR	C1-C6-C7-C8
85	AN	846	BCR	C23-C24-C25-C26
85	BN	803	BCR	C23-C24-C25-C30
85	BN	839	BCR	C23-C24-C25-C30
85	FN	202	BCR	C23-C24-C25-C26
85	FN	204	BCR	C1-C6-C7-C8
85	FN	204	BCR	C5-C6-C7-C8
85	IN	101	BCR	C1-C6-C7-C8
85	JN	102	BCR	C1-C6-C7-C8
85	JN	102	BCR	C5-C6-C7-C8
85	A2	846	BCR	C23-C24-C25-C26
85	B2	802	BCR	C23-C24-C25-C30
85	B2	839	BCR	C23-C24-C25-C30
85	F2	203	BCR	C23-C24-C25-C26
85	F2	204	BCR	C1-C6-C7-C8
85	F2	204	BCR	C5-C6-C7-C8
85	I2	101	BCR	C1-C6-C7-C8
85	J2	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
85	J2	102	BCR	C5-C6-C7-C8
85	C6	508	BCR	C1-C6-C7-C8
85	C6	508	BCR	C5-C6-C7-C8
85	F6	101	BCR	C5-C6-C7-C8
85	c6	603	BCR	C1-C6-C7-C8
85	c6	603	BCR	C5-C6-C7-C8
85	d6	405	BCR	C23-C24-C25-C26
85	aL	604	BCR	C23-C24-C25-C30
85	kL	100	BCR	C1-C6-C7-C8
87	I2	102	CLA	C13-C15-C16-C17
87	cL	509	CLA	C2C-C3C-CAC-CBC
88	D6	401	LHG	C32-C33-C34-C35
88	i6	101	LHG	C29-C30-C31-C32
92	bL	609	LMG	C33-C34-C35-C36
95	C6	523	DGD	C6B-C7B-C8B-C9B
95	L6	102	DGD	CAA-CBA-CCA-CDA
95	c6	618	DGD	C8A-C9A-CAA-CBA
85	AN	804	BCR	C7-C8-C9-C34
85	A2	804	BCR	C7-C8-C9-C34
85	c6	603	BCR	C11-C12-C13-C35
85	bL	601	BCR	C36-C18-C19-C20
82	HD	202	PEB	C2C-C1C-CHB-C4B
82	DQ	202	PEB	C2C-C1C-CHB-C4B
82	HQ	202	PEB	C2C-C1C-CHB-C4B
82	T1	202	PEB	C2C-C1C-CHB-C4B
82	S5	202	PEB	C2C-C1C-CHB-C4B
82	U5	203	PEB	C2C-C1C-CHB-C4B
82	cB	402	PEB	C2C-C1C-CHB-C4B
82	aF	203	PEB	C2C-C1C-CHB-C4B
82	aK	203	PEB	C2C-C1C-CHB-C4B
83	AM	303	PUB	C3B-C4B-CHB-C1C
87	bL	608	CLA	O1D-CGD-O2D-CED
82	EA	201	PEB	C4A-C3A-CAA-CBA
82	YA	303	PEB	C4A-C3A-CAA-CBA
82	IB	201	PEB	C4A-C3A-CAA-CBA
82	RD	201	PEB	C4A-C3A-CAA-CBA
82	PE	202	PEB	C4A-C3A-CAA-CBA
82	QE	203	PEB	C4A-C3A-CAA-CBA
82	CF	203	PEB	C4A-C3A-CAA-CBA
82	PG	202	PEB	C4A-C3A-CAA-CBA
82	QG	203	PEB	C4A-C3A-CAA-CBA
82	TH	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	TH	202	PEB	C4A-C3A-CAA-CBA
82	WH	203	PEB	C4A-C3A-CAA-CBA
82	CK	203	PEB	C4A-C3A-CAA-CBA
82	OM	203	PEB	C4A-C3A-CAA-CBA
82	ZM	201	PEB	C4A-C3A-CAA-CBA
82	QP	201	PEB	C4A-C3A-CAA-CBA
82	RP	201	PEB	C4A-C3A-CAA-CBA
82	RQ	201	PEB	C4A-C3A-CAA-CBA
82	T1	201	PEB	C4A-C3A-CAA-CBA
82	T1	202	PEB	C4A-C3A-CAA-CBA
82	W1	203	PEB	C4A-C3A-CAA-CBA
82	m1	202	PEB	C4A-C3A-CAA-CBA
82	d1	203	PEB	C4A-C3A-CAA-CBA
82	e4	202	PEB	C4A-C3A-CAA-CBA
82	E7	201	PEB	C4A-C3A-CAA-CBA
82	Y7	303	PEB	C4A-C3A-CAA-CBA
82	fB	301	PEB	C4A-C3A-CAA-CBA
82	hB	301	PEB	C4A-C3A-CAA-CBA
82	cF	203	PEB	C4A-C3A-CAA-CBA
82	gF	203	PEB	C4A-C3A-CAA-CBA
82	lF	202	PEB	C4A-C3A-CAA-CBA
82	wF	301	PEB	C4A-C3A-CAA-CBA
82	mH	202	PEB	C4A-C3A-CAA-CBA
82	dH	203	PEB	C4A-C3A-CAA-CBA
82	cK	203	PEB	C4A-C3A-CAA-CBA
82	gK	203	PEB	C4A-C3A-CAA-CBA
82	lK	202	PEB	C4A-C3A-CAA-CBA
82	wK	301	PEB	C4A-C3A-CAA-CBA
82	eO	202	PEB	C4A-C3A-CAA-CBA
84	NE	201	CYC	C4C-C3C-CAC-CBC
84	KG	202	CYC	C4C-C3C-CAC-CBC
85	BN	803	BCR	C7-C8-C9-C10
85	BN	840	BCR	C21-C22-C23-C24
85	JN	102	BCR	C17-C18-C19-C20
85	B2	802	BCR	C7-C8-C9-C10
85	B2	840	BCR	C21-C22-C23-C24
85	J2	102	BCR	C17-C18-C19-C20
85	C6	508	BCR	C7-C8-C9-C10
85	d6	405	BCR	C21-C22-C23-C24
85	bL	601	BCR	C21-C22-C23-C24
87	AN	817	CLA	C1A-C2A-CAA-CBA
87	12	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	22	611	CLA	C1A-C2A-CAA-CBA
87	32	306	CLA	C1A-C2A-CAA-CBA
87	32	311	CLA	C1A-C2A-CAA-CBA
87	72	604	CLA	C1A-C2A-CAA-CBA
87	72	609	CLA	C1A-C2A-CAA-CBA
87	A2	817	CLA	C1A-C2A-CAA-CBA
87	1N	609	CLA	C1A-C2A-CAA-CBA
87	2N	311	CLA	C1A-C2A-CAA-CBA
87	3N	307	CLA	C1A-C2A-CAA-CBA
87	3N	311	CLA	C1A-C2A-CAA-CBA
87	7N	604	CLA	C1A-C2A-CAA-CBA
87	7N	609	CLA	C1A-C2A-CAA-CBA
103	82	310	ZEX	C11-C12-C13-C14
103	8N	310	ZEX	C11-C12-C13-C14
87	CL	506	CLA	C13-C15-C16-C17
87	IN	102	CLA	C13-C15-C16-C17
82	MA	201	PEB	C3B-CAB-CBB-CGB
82	DB	201	PEB	C2C-CAC-CBC-CGC
82	KB	301	PEB	C2C-CAC-CBC-CGC
82	QB	202	PEB	C2C-CAC-CBC-CGC
82	QD	202	PEB	C3B-CAB-CBB-CGB
82	HE	1002	PEB	C2C-CAC-CBC-CGC
82	FF	201	PEB	C3B-CAB-CBB-CGB
82	GF	203	PEB	C3B-CAB-CBB-CGB
82	TF	201	PEB	C3B-CAB-CBB-CGB
82	HG	1002	PEB	C2C-CAC-CBC-CGC
82	SI	202	PEB	C2C-CAC-CBC-CGC
82	OJ	203	PEB	C3B-CAB-CBB-CGB
82	YJ	203	PEB	C3B-CAB-CBB-CGB
82	FK	201	PEB	C3B-CAB-CBB-CGB
82	GK	203	PEB	C3B-CAB-CBB-CGB
82	TK	201	PEB	C3B-CAB-CBB-CGB
82	TK	202	PEB	C2C-CAC-CBC-CGC
82	KM	201	PEB	C2C-CAC-CBC-CGC
82	LM	202	PEB	C3B-CAB-CBB-CGB
82	SO	201	PEB	C3B-CAB-CBB-CGB
82	HP	201	PEB	C2C-CAC-CBC-CGC
82	RP	201	PEB	C2C-CAC-CBC-CGC
82	TP	201	PEB	C2C-CAC-CBC-CGC
82	QQ	202	PEB	C3B-CAB-CBB-CGB
82	d1	201	PEB	C3B-CAB-CBB-CGB
82	S4	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	S5	202	PEB	C3B-CAB-CBB-CGB
82	W5	202	PEB	C3B-CAB-CBB-CGB
82	M7	201	PEB	C3B-CAB-CBB-CGB
82	B9	202	PEB	C2C-CAC-CBC-CGC
82	U9	202	PEB	C3B-CAB-CBB-CGB
82	Y9	202	PEB	C2C-CAC-CBC-CGC
82	lE	201	PEB	C3B-CAB-CBB-CGB
82	gF	202	PEB	C3B-CAB-CBB-CGB
82	lF	202	PEB	C2C-CAC-CBC-CGC
82	pF	202	PEB	C3B-CAB-CBB-CGB
82	lG	201	PEB	C3B-CAB-CBB-CGB
82	dH	201	PEB	C3B-CAB-CBB-CGB
82	iJ	201	PEB	C2C-CAC-CBC-CGC
82	lK	202	PEB	C2C-CAC-CBC-CGC
82	pK	202	PEB	C3B-CAB-CBB-CGB
82	kM	202	PEB	C2C-CAC-CBC-CGC
84	DE	1001	CYC	C2A-CAA-CBA-CGA
84	DG	1001	CYC	C2A-CAA-CBA-CGA
84	r3	1001	CYC	C2A-CAA-CBA-CGA
92	dL	407	LMG	C35-C36-C37-C38
95	CL	517	DGD	C3A-C4A-C5A-C6A
95	J6	101	DGD	CDA-CEA-CFA-CGA
95	a6	604	DGD	C4A-C5A-C6A-C7A
87	d6	403	CLA	C13-C15-C16-C17
95	DL	408	DGD	CCB-CDB-CEB-CFB
95	hL	101	DGD	C2B-C3B-C4B-C5B
87	AN	834	CLA	C16-C17-C18-C19
87	B6	607	CLA	C16-C17-C18-C19
87	aL	606	CLA	C11-C12-C13-C15
91	A6	407	PHO	C16-C17-C18-C19
87	BN	830	CLA	C3-C5-C6-C7
87	B2	830	CLA	C3-C5-C6-C7
82	ID	202	PEB	C2B-C3B-CAB-CBB
82	LE	1002	PEB	C2B-C3B-CAB-CBB
82	IQ	202	PEB	C2B-C3B-CAB-CBB
92	C6	501	LMG	C28-C29-C30-C31
92	bL	610	LMG	C18-C19-C20-C21
83	AE	302	PUB	C2D-C1D-CHC-C4C
83	AE	303	PUB	C3A-C4A-CHA-C1B
83	AG	302	PUB	C2D-C1D-CHC-C4C
83	AG	303	PUB	C3A-C4A-CHA-C1B
83	AH	303	PUB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
83	AJ	303	PUB	C2D-C1D-CHC-C4C
83	AJ	304	PUB	C3A-C4A-CHA-C1B
83	BJ	302	PUB	C3A-C4A-CHA-C1B
83	AM	303	PUB	C2D-C1D-CHC-C4C
83	AM	304	PUB	C3A-C4A-CHA-C1B
83	BM	302	PUB	C3A-C4A-CHA-C1B
83	AO	302	PUB	C3A-C4A-CHA-C1B
83	A1	303	PUB	C3A-C4A-CHA-C1B
83	A4	302	PUB	C3A-C4A-CHA-C1B
83	wF	304	PUB	C3A-C4A-CHA-C1B
83	wK	304	PUB	C3A-C4A-CHA-C1B
83	Z9	302	PUB	C3A-C4A-CHA-C1B
83	Z9	305	PUB	C3A-C4A-CHA-C1B
83	M9	303	PUB	C3A-C4A-CHA-C1B
87	b6	606	CLA	C4C-C3C-CAC-CBC
92	A6	408	LMG	C12-C13-C14-C15
87	D6	403	CLA	C8-C10-C11-C12
88	BL	615	LHG	O6-C4-C5-C6
88	C6	522	LHG	O6-C4-C5-C6
87	6N	608	CLA	CAA-CBA-CGA-O2A
87	a6	607	CLA	C4C-C3C-CAC-CBC
88	dL	405	LHG	C31-C32-C33-C34
87	BL	608	CLA	C11-C12-C13-C15
87	BL	609	CLA	C6-C7-C8-C10
87	BL	620	CLA	C6-C7-C8-C10
87	BL	621	CLA	C12-C13-C15-C16
87	BL	623	CLA	C12-C13-C15-C16
87	CL	506	CLA	C11-C10-C8-C7
87	CL	507	CLA	C12-C13-C15-C16
87	CL	508	CLA	C6-C7-C8-C10
87	CL	509	CLA	C12-C13-C15-C16
87	CL	510	CLA	C11-C12-C13-C15
87	DL	404	CLA	C11-C10-C8-C7
87	HL	101	CLA	C12-C13-C15-C16
87	AN	808	CLA	C11-C10-C8-C7
87	AN	808	CLA	C11-C12-C13-C15
87	AN	810	CLA	C11-C10-C8-C7
87	AN	810	CLA	C11-C12-C13-C15
87	AN	813	CLA	C11-C12-C13-C15
87	AN	815	CLA	C6-C7-C8-C10
87	AN	821	CLA	C11-C12-C13-C15
87	AN	834	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
87	AN	835	CLA	C6-C7-C8-C10
87	AN	838	CLA	C6-C7-C8-C10
87	AN	849	CLA	C12-C13-C15-C16
87	BN	801	CLA	C12-C13-C15-C16
87	BN	811	CLA	C11-C12-C13-C15
87	BN	818	CLA	C11-C10-C8-C7
87	BN	824	CLA	C12-C13-C15-C16
87	BN	832	CLA	C12-C13-C15-C16
87	BN	834	CLA	C11-C10-C8-C7
87	FN	205	CLA	C6-C7-C8-C10
87	FN	205	CLA	C12-C13-C15-C16
87	LN	202	CLA	C11-C10-C8-C7
87	LN	203	CLA	C12-C13-C15-C16
87	42	602	CLA	C6-C7-C8-C10
87	72	602	CLA	C12-C13-C15-C16
87	A2	808	CLA	C11-C10-C8-C7
87	A2	808	CLA	C11-C12-C13-C15
87	A2	810	CLA	C11-C10-C8-C7
87	A2	810	CLA	C11-C12-C13-C15
87	A2	813	CLA	C11-C12-C13-C15
87	A2	815	CLA	C6-C7-C8-C10
87	A2	821	CLA	C11-C12-C13-C15
87	A2	834	CLA	C11-C10-C8-C7
87	A2	835	CLA	C6-C7-C8-C10
87	A2	838	CLA	C6-C7-C8-C10
87	A2	849	CLA	C12-C13-C15-C16
87	B2	810	CLA	C11-C12-C13-C15
87	B2	817	CLA	C11-C10-C8-C7
87	B2	823	CLA	C12-C13-C15-C16
87	B2	825	CLA	C12-C13-C15-C16
87	B2	832	CLA	C12-C13-C15-C16
87	B2	834	CLA	C11-C10-C8-C7
87	F2	205	CLA	C6-C7-C8-C10
87	F2	205	CLA	C12-C13-C15-C16
87	L2	202	CLA	C11-C10-C8-C7
87	L2	203	CLA	C12-C13-C15-C16
87	A6	403	CLA	C11-C10-C8-C7
87	B6	603	CLA	C11-C10-C8-C7
87	B6	607	CLA	C11-C10-C8-C7
87	B6	607	CLA	C12-C13-C15-C16
87	B6	610	CLA	C12-C13-C15-C16
87	B6	611	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
87	B6	615	CLA	C6-C7-C8-C10
87	C6	509	CLA	C12-C13-C15-C16
87	C6	513	CLA	C11-C10-C8-C7
87	C6	513	CLA	C12-C13-C15-C16
87	C6	517	CLA	C6-C7-C8-C10
87	D6	402	CLA	C12-C13-C15-C16
87	a6	608	CLA	C11-C10-C8-C7
87	b6	605	CLA	C6-C7-C8-C10
87	b6	606	CLA	C11-C12-C13-C15
87	b6	607	CLA	C11-C12-C13-C15
87	b6	609	CLA	C12-C13-C15-C16
87	b6	611	CLA	C11-C12-C13-C15
87	b6	617	CLA	C11-C10-C8-C7
87	c6	604	CLA	C11-C12-C13-C15
87	c6	604	CLA	C12-C13-C15-C16
87	c6	607	CLA	C11-C10-C8-C7
87	c6	608	CLA	C11-C12-C13-C15
87	c6	612	CLA	C11-C10-C8-C7
87	bL	613	CLA	C12-C13-C15-C16
87	bL	622	CLA	C6-C7-C8-C10
87	cL	505	CLA	C12-C13-C15-C16
87	cL	509	CLA	C11-C12-C13-C15
87	cL	510	CLA	C6-C7-C8-C10
87	cL	510	CLA	C11-C10-C8-C7
87	cL	511	CLA	C6-C7-C8-C10
87	cL	512	CLA	C11-C12-C13-C15
87	nL	101	CLA	C11-C10-C8-C7
87	4N	602	CLA	C6-C7-C8-C10
87	7N	602	CLA	C12-C13-C15-C16
91	aL	610	PHO	C11-C10-C8-C7
98	AN	842	PQN	C16-C17-C18-C20
98	A2	842	PQN	C16-C17-C18-C20
92	CL	519	LMG	C36-C37-C38-C39
95	AL	414	DGD	C3B-C4B-C5B-C6B
85	BN	841	BCR	C19-C20-C21-C22
85	KN	104	BCR	C13-C14-C15-C16
85	B2	841	BCR	C19-C20-C21-C22
85	K2	105	BCR	C13-C14-C15-C16
85	C6	507	BCR	C9-C10-C11-C12
87	CL	504	CLA	C16-C17-C18-C19
87	A6	402	CLA	C16-C17-C18-C19
100	JN	104	3XQ	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
92	XL	601	LMG	C28-C29-C30-C31
100	JN	104	3XQ	C1-C2-C3-C4
87	AN	851	CLA	CBA-CGA-O2A-C1
87	A2	851	CLA	CBA-CGA-O2A-C1
87	AN	838	CLA	C8-C10-C11-C12
87	A2	807	CLA	C5-C6-C7-C8
87	A2	834	CLA	C15-C16-C17-C18
87	A2	838	CLA	C8-C10-C11-C12
87	B6	613	CLA	C15-C16-C17-C18
87	D6	403	CLA	C5-C6-C7-C8
87	bL	616	CLA	C15-C16-C17-C18
87	62	309	CLA	CAA-CBA-CGA-O2A
87	22	612	CLA	C2A-CAA-CBA-CGA
87	2N	312	CLA	C2A-CAA-CBA-CGA
87	AN	807	CLA	C5-C6-C7-C8
87	AN	834	CLA	C15-C16-C17-C18
87	nL	101	CLA	C5-C6-C7-C8
88	B6	617	LHG	C28-C29-C30-C31
87	BL	619	CLA	C3-C5-C6-C7
87	B6	615	CLA	C3-C5-C6-C7
87	C6	520	CLA	C3-C5-C6-C7
87	BN	810	CLA	O1A-CGA-O2A-C1
87	b6	612	CLA	C16-C17-C18-C19
87	bL	622	CLA	C16-C17-C18-C19
98	AN	842	PQN	C26-C27-C28-C30
98	A2	842	PQN	C26-C27-C28-C30
87	BN	808	CLA	C15-C16-C17-C18
87	B2	807	CLA	C15-C16-C17-C18
87	B6	611	CLA	C13-C15-C16-C17
87	b6	608	CLA	C5-C6-C7-C8
87	BL	622	CLA	CBA-CGA-O2A-C1
87	BN	823	CLA	CBA-CGA-O2A-C1
87	B2	822	CLA	CBA-CGA-O2A-C1
87	b6	608	CLA	CBA-CGA-O2A-C1
87	aL	605	CLA	CBA-CGA-O2A-C1
92	B6	622	LMG	C29-C28-O8-C9
95	BL	614	DGD	C2A-C1A-O1G-C1G
88	m6	102	LHG	C9-C10-C11-C12
92	dL	407	LMG	C11-C12-C13-C14
82	TH	202	PEB	C2C-C1C-CHB-C4B
82	LG	1002	PEB	C2B-C3B-CAB-CBB
82	dE	204	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
82	dG	204	PEB	C2B-C3B-CAB-CBB
87	b6	606	CLA	C8-C10-C11-C12
87	B2	809	CLA	O1A-CGA-O2A-C1
84	CO	1001	CYC	C2B-C3B-CAB-CBB
84	C4	1001	CYC	C2B-C3B-CAB-CBB
88	I6	101	LHG	C29-C30-C31-C32
88	i6	101	LHG	C26-C27-C28-C29
95	L6	102	DGD	C2A-C3A-C4A-C5A
82	JD	201	PEB	C2D-C3D-CAD-CBD
82	SD	202	PEB	C2D-C3D-CAD-CBD
82	XD	202	PEB	C2D-C3D-CAD-CBD
82	KM	202	PEB	C2D-C3D-CAD-CBD
82	YM	203	PEB	C2D-C3D-CAD-CBD
82	SQ	202	PEB	C2D-C3D-CAD-CBD
82	XQ	202	PEB	C2D-C3D-CAD-CBD
82	f1	201	PEB	C2D-C3D-CAD-CBD
82	b1	202	PEB	C2D-C3D-CAD-CBD
82	c1	202	PEB	C2D-C3D-CAD-CBD
82	fH	201	PEB	C2D-C3D-CAD-CBD
82	bH	202	PEB	C2D-C3D-CAD-CBD
82	cH	202	PEB	C2D-C3D-CAD-CBD
87	BL	604	CLA	CAD-CBD-CGD-O2D
87	BL	621	CLA	CAD-CBD-CGD-O2D
87	CL	509	CLA	CAD-CBD-CGD-O2D
87	CL	514	CLA	CAD-CBD-CGD-O2D
87	HL	102	CLA	CAD-CBD-CGD-O2D
87	AN	805	CLA	CAD-CBD-CGD-O2D
87	AN	821	CLA	CAD-CBD-CGD-O2D
87	AN	833	CLA	CAD-CBD-CGD-O2D
87	AN	837	CLA	CAD-CBD-CGD-O2D
87	BN	809	CLA	CAD-CBD-CGD-O2D
87	BN	816	CLA	CAD-CBD-CGD-O2D
87	BN	823	CLA	CAD-CBD-CGD-O2D
87	BN	832	CLA	CAD-CBD-CGD-O2D
87	BN	835	CLA	CAD-CBD-CGD-O2D
87	FN	205	CLA	CAD-CBD-CGD-O2D
87	IN	102	CLA	CAD-CBD-CGD-O2D
87	12	605	CLA	CAD-CBD-CGD-O2D
87	12	609	CLA	CAD-CBD-CGD-O2D
87	22	608	CLA	CAD-CBD-CGD-O2D
87	22	612	CLA	CAD-CBD-CGD-O2D
87	42	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	42	607	CLA	CAD-CBD-CGD-O2D
87	42	609	CLA	CAD-CBD-CGD-O2D
87	52	606	CLA	CAD-CBD-CGD-O2D
87	52	611	CLA	CAD-CBD-CGD-O2D
87	62	301	CLA	CAD-CBD-CGD-O2D
87	62	313	CLA	CAD-CBD-CGD-O2D
87	A2	805	CLA	CAD-CBD-CGD-O2D
87	A2	821	CLA	CAD-CBD-CGD-O2D
87	A2	833	CLA	CAD-CBD-CGD-O2D
87	A2	837	CLA	CAD-CBD-CGD-O2D
87	B2	808	CLA	CAD-CBD-CGD-O2D
87	B2	815	CLA	CAD-CBD-CGD-O2D
87	B2	822	CLA	CAD-CBD-CGD-O2D
87	B2	832	CLA	CAD-CBD-CGD-O2D
87	B2	835	CLA	CAD-CBD-CGD-O2D
87	F2	205	CLA	CAD-CBD-CGD-O2D
87	I2	102	CLA	CAD-CBD-CGD-O2D
87	K2	101	CLA	CAD-CBD-CGD-O2D
87	B6	605	CLA	CAD-CBD-CGD-O2D
87	B6	606	CLA	CAD-CBD-CGD-O2D
87	B6	614	CLA	CAD-CBD-CGD-O2D
87	C6	512	CLA	CAD-CBD-CGD-O2D
87	bL	607	CLA	CAD-CBD-CGD-O2D
87	bL	619	CLA	CAD-CBD-CGD-O2D
87	cL	509	CLA	CAD-CBD-CGD-O2D
87	cL	517	CLA	CAD-CBD-CGD-O2D
87	dL	404	CLA	CAD-CBD-CGD-O2D
87	1N	605	CLA	CAD-CBD-CGD-O2D
87	1N	609	CLA	CAD-CBD-CGD-O2D
87	2N	308	CLA	CAD-CBD-CGD-O2D
87	2N	312	CLA	CAD-CBD-CGD-O2D
87	4N	604	CLA	CAD-CBD-CGD-O2D
87	4N	607	CLA	CAD-CBD-CGD-O2D
87	4N	609	CLA	CAD-CBD-CGD-O2D
87	5N	606	CLA	CAD-CBD-CGD-O2D
87	5N	611	CLA	CAD-CBD-CGD-O2D
87	6N	612	CLA	CAD-CBD-CGD-O2D
87	6N	613	CLA	CAD-CBD-CGD-O2D
88	iL	101	LHG	C6-C5-O7-C7
91	D6	404	PHO	CAD-CBD-CGD-O2D
92	C6	501	LMG	C9-C8-O7-C10
92	D6	409	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
92	yL	101	LMG	C9-C8-O7-C10
87	C6	512	CLA	C3-C5-C6-C7
92	bL	610	LMG	C30-C31-C32-C33
92	bL	624	LMG	C14-C15-C16-C17
92	yL	101	LMG	C39-C40-C41-C42
87	B6	614	CLA	C5-C6-C7-C8
87	C6	514	CLA	C15-C16-C17-C18
98	BN	837	PQN	C23-C25-C26-C27
98	B2	837	PQN	C23-C25-C26-C27
95	BN	844	DGD	C1B-C2B-C3B-C4B
95	B2	844	DGD	C1B-C2B-C3B-C4B
84	FG	1001	CYC	C2B-C3B-CAB-CBB
88	AN	844	LHG	C14-C15-C16-C17
95	c6	618	DGD	C7B-C8B-C9B-CAB
83	QJ	201	PUB	C4A-C3A-CAA-CBA
87	AN	809	CLA	CBA-CGA-O2A-C1
87	A2	809	CLA	CBA-CGA-O2A-C1
87	c6	612	CLA	CBA-CGA-O2A-C1
88	a6	610	LHG	C24-C23-O8-C6
87	AN	829	CLA	C4-C3-C5-C6
87	AN	840	CLA	C4-C3-C5-C6
87	A2	829	CLA	C4-C3-C5-C6
87	A2	840	CLA	C4-C3-C5-C6
94	a6	601	PL9	C40-C39-C41-C42
87	AN	831	CLA	C16-C17-C18-C19
87	BN	813	CLA	C16-C17-C18-C19
87	A2	831	CLA	C16-C17-C18-C19
87	B2	812	CLA	C16-C17-C18-C19
87	C6	511	CLA	C16-C17-C18-C19
84	FE	1002	CYC	C2B-C3B-CAB-CBB
88	A2	844	LHG	C14-C15-C16-C17
92	C6	501	LMG	C19-C20-C21-C22
95	hL	101	DGD	O6D-C1D-O3G-C3G
87	D6	403	CLA	C2-C3-C5-C6
91	AL	410	PHO	C2-C3-C5-C6
94	a6	601	PL9	C38-C39-C41-C42
95	h6	101	DGD	C1B-C2B-C3B-C4B
92	DL	402	LMG	C7-C8-C9-O8
92	b6	620	LMG	C7-C8-C9-O8
92	b6	624	LMG	O1-C7-C8-C9
92	m6	101	LMG	O1-C7-C8-C9
92	dL	407	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
95	AL	414	DGD	C1G-C2G-C3G-O3G
95	CL	523	DGD	C1G-C2G-C3G-O3G
95	C6	502	DGD	C1G-C2G-C3G-O3G
95	c6	601	DGD	C1G-C2G-C3G-O3G
95	cL	520	DGD	C1G-C2G-C3G-O3G
87	b6	612	CLA	O1A-CGA-O2A-C1
88	BL	615	LHG	O6-C4-C5-O7
88	C6	522	LHG	O6-C4-C5-O7
88	dL	408	LHG	O6-C4-C5-O7
87	BN	827	CLA	C8-C10-C11-C12
87	B2	827	CLA	C8-C10-C11-C12
87	B6	603	CLA	C15-C16-C17-C18
87	B6	612	CLA	C5-C6-C7-C8
84	IE	1001	CYC	C4B-C3B-CAB-CBB
84	NE	201	CYC	C4B-C3B-CAB-CBB
84	IG	1001	CYC	C4B-C3B-CAB-CBB
84	KG	202	CYC	C4B-C3B-CAB-CBB
84	GO	1001	CYC	C4B-C3B-CAB-CBB
84	G4	1001	CYC	C4B-C3B-CAB-CBB
82	JA	203	PEB	NC-C1C-CHB-C4B
82	BB	203	PEB	NC-C1C-CHB-C4B
82	OK	203	PEB	NC-C1C-CHB-C4B
82	D5	202	PEB	NC-C1C-CHB-C4B
82	J7	203	PEB	NC-C1C-CHB-C4B
82	fJ	202	PEB	NC-C1C-CHB-C4B
87	B6	611	CLA	C2C-C3C-CAC-CBC
82	QE	201	PEB	C4B-C3B-CAB-CBB
82	QG	201	PEB	C4B-C3B-CAB-CBB
96	GN	201	HEM	C4C-C3C-CAC-CBC
96	G2	201	HEM	C4C-C3C-CAC-CBC
87	AN	820	CLA	C2A-CAA-CBA-CGA
87	AN	820	CLA	C13-C15-C16-C17
92	d6	409	LMG	C29-C30-C31-C32
95	hL	101	DGD	CBB-CCB-CDB-CEB
83	Z5	303	PUB	C4A-C3A-CAA-CBA
92	JL	102	LMG	O10-C28-O8-C9
87	b6	616	CLA	C16-C17-C18-C19
87	CL	503	CLA	O1D-CGD-O2D-CED
83	M5	303	PUB	C4A-C3A-CAA-CBA
82	NJ	202	PEB	C3B-CAB-CBB-CGB
82	A1	301	PEB	C2C-CAC-CBC-CGC
82	dJ	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	lJ	202	PEB	C2C-CAC-CBC-CGC
87	AL	405	CLA	CHA-CBD-CGD-O1D
87	AL	405	CLA	CHA-CBD-CGD-O2D
87	CL	503	CLA	CHA-CBD-CGD-O1D
87	CL	503	CLA	CHA-CBD-CGD-O2D
87	CL	507	CLA	CHA-CBD-CGD-O1D
87	CL	507	CLA	CHA-CBD-CGD-O2D
87	CL	508	CLA	CHA-CBD-CGD-O1D
87	CL	511	CLA	CHA-CBD-CGD-O1D
87	AN	815	CLA	CHA-CBD-CGD-O1D
87	AN	815	CLA	CHA-CBD-CGD-O2D
87	AN	817	CLA	CHA-CBD-CGD-O1D
87	AN	817	CLA	CHA-CBD-CGD-O2D
87	AN	830	CLA	CHA-CBD-CGD-O1D
87	AN	830	CLA	CHA-CBD-CGD-O2D
87	AN	834	CLA	CHA-CBD-CGD-O1D
87	AN	834	CLA	CHA-CBD-CGD-O2D
87	AN	836	CLA	CHA-CBD-CGD-O1D
87	AN	836	CLA	CHA-CBD-CGD-O2D
87	BN	801	CLA	CHA-CBD-CGD-O2D
87	BN	813	CLA	CHA-CBD-CGD-O1D
87	BN	825	CLA	CHA-CBD-CGD-O2D
87	BN	831	CLA	CHA-CBD-CGD-O1D
87	BN	831	CLA	CHA-CBD-CGD-O2D
87	BN	836	CLA	CHA-CBD-CGD-O1D
87	KN	103	CLA	CHA-CBD-CGD-O1D
87	LN	204	CLA	CHA-CBD-CGD-O2D
87	ON	201	CLA	CHA-CBD-CGD-O1D
87	ON	203	CLA	CHA-CBD-CGD-O1D
87	ON	203	CLA	CHA-CBD-CGD-O2D
87	12	607	CLA	CHA-CBD-CGD-O1D
87	12	607	CLA	CHA-CBD-CGD-O2D
87	22	603	CLA	CHA-CBD-CGD-O1D
87	22	603	CLA	CHA-CBD-CGD-O2D
87	22	611	CLA	CHA-CBD-CGD-O2D
87	32	303	CLA	CHA-CBD-CGD-O1D
87	32	303	CLA	CHA-CBD-CGD-O2D
87	72	604	CLA	CHA-CBD-CGD-O1D
87	A2	815	CLA	CHA-CBD-CGD-O1D
87	A2	815	CLA	CHA-CBD-CGD-O2D
87	A2	817	CLA	CHA-CBD-CGD-O1D
87	A2	817	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	A2	830	CLA	CHA-CBD-CGD-O1D
87	A2	830	CLA	CHA-CBD-CGD-O2D
87	A2	834	CLA	CHA-CBD-CGD-O1D
87	A2	834	CLA	CHA-CBD-CGD-O2D
87	A2	836	CLA	CHA-CBD-CGD-O1D
87	A2	836	CLA	CHA-CBD-CGD-O2D
87	B2	812	CLA	CHA-CBD-CGD-O1D
87	B2	824	CLA	CHA-CBD-CGD-O2D
87	B2	825	CLA	CHA-CBD-CGD-O2D
87	B2	831	CLA	CHA-CBD-CGD-O1D
87	B2	831	CLA	CHA-CBD-CGD-O2D
87	B2	836	CLA	CHA-CBD-CGD-O1D
87	K2	104	CLA	CHA-CBD-CGD-O1D
87	L2	204	CLA	CHA-CBD-CGD-O2D
87	O2	201	CLA	CHA-CBD-CGD-O1D
87	O2	203	CLA	CHA-CBD-CGD-O1D
87	O2	203	CLA	CHA-CBD-CGD-O2D
87	A6	404	CLA	CHA-CBD-CGD-O1D
87	A6	404	CLA	CHA-CBD-CGD-O2D
87	B6	604	CLA	CHA-CBD-CGD-O1D
87	B6	604	CLA	CHA-CBD-CGD-O2D
87	B6	609	CLA	CHA-CBD-CGD-O2D
87	B6	612	CLA	CHA-CBD-CGD-O2D
87	B6	615	CLA	CHA-CBD-CGD-O1D
87	B6	615	CLA	CHA-CBD-CGD-O2D
87	C6	513	CLA	CHA-CBD-CGD-O1D
87	C6	513	CLA	CHA-CBD-CGD-O2D
87	C6	514	CLA	CHA-CBD-CGD-O2D
87	C6	517	CLA	CHA-CBD-CGD-O1D
87	C6	517	CLA	CHA-CBD-CGD-O2D
87	K6	101	CLA	CHA-CBD-CGD-O1D
87	K6	101	CLA	CHA-CBD-CGD-O2D
87	b6	607	CLA	CHA-CBD-CGD-O1D
87	b6	611	CLA	CHA-CBD-CGD-O1D
87	b6	611	CLA	CHA-CBD-CGD-O2D
87	b6	616	CLA	CHA-CBD-CGD-O1D
87	b6	616	CLA	CHA-CBD-CGD-O2D
87	c6	609	CLA	CHA-CBD-CGD-O1D
87	c6	610	CLA	CHA-CBD-CGD-O1D
87	c6	611	CLA	CHA-CBD-CGD-O1D
87	c6	611	CLA	CHA-CBD-CGD-O2D
87	c6	615	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	c6	615	CLA	CHA-CBD-CGD-O2D
87	bL	617	CLA	CHA-CBD-CGD-O1D
87	bL	617	CLA	CHA-CBD-CGD-O2D
87	bL	618	CLA	CHA-CBD-CGD-O1D
87	cL	509	CLA	CHA-CBD-CGD-O2D
87	cL	512	CLA	CHA-CBD-CGD-O1D
87	cL	512	CLA	CHA-CBD-CGD-O2D
87	1N	607	CLA	CHA-CBD-CGD-O1D
87	1N	607	CLA	CHA-CBD-CGD-O2D
87	2N	304	CLA	CHA-CBD-CGD-O1D
87	2N	304	CLA	CHA-CBD-CGD-O2D
87	2N	311	CLA	CHA-CBD-CGD-O1D
87	2N	311	CLA	CHA-CBD-CGD-O2D
87	3N	304	CLA	CHA-CBD-CGD-O1D
87	3N	304	CLA	CHA-CBD-CGD-O2D
87	7N	604	CLA	CHA-CBD-CGD-O1D
87	BN	823	CLA	C5-C6-C7-C8
87	A2	820	CLA	C13-C15-C16-C17
87	B2	822	CLA	C5-C6-C7-C8
87	c6	609	CLA	C13-C15-C16-C17
87	BL	604	CLA	C3-C5-C6-C7
87	AN	815	CLA	C3-C5-C6-C7
87	A2	815	CLA	C3-C5-C6-C7
87	AN	851	CLA	O1A-CGA-O2A-C1
87	BN	819	CLA	O1A-CGA-O2A-C1
87	A2	851	CLA	O1A-CGA-O2A-C1
87	B2	818	CLA	O1A-CGA-O2A-C1
87	B2	822	CLA	O1A-CGA-O2A-C1
87	A6	402	CLA	O1A-CGA-O2A-C1
95	JL	101	DGD	O1A-C1A-O1G-C1G
95	J6	101	DGD	O1A-C1A-O1G-C1G
92	bL	623	LMG	C32-C33-C34-C35
92	d6	409	LMG	C2-C1-O1-C7
95	C6	502	DGD	CAB-CBB-CCB-CDB
95	c6	601	DGD	CAB-CBB-CCB-CDB
95	cL	502	DGD	CAB-CBB-CCB-CDB
88	AL	406	LHG	O7-C5-C6-O8
92	ML	101	LMG	O7-C8-C9-O8
92	B6	618	LMG	O7-C8-C9-O8
92	D6	409	LMG	O7-C8-C9-O8
92	J6	102	LMG	O7-C8-C9-O8
92	d6	409	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
92	j6	101	LMG	O7-C8-C9-O8
92	dL	407	LMG	O7-C8-C9-O8
95	AL	414	DGD	O2G-C2G-C3G-O3G
95	CL	523	DGD	O2G-C2G-C3G-O3G
95	C6	523	DGD	O2G-C2G-C3G-O3G
95	L6	102	DGD	O1G-C1G-C2G-O2G
95	a6	602	DGD	O2G-C2G-C3G-O3G
95	c6	620	DGD	O2G-C2G-C3G-O3G
95	cL	502	DGD	O2G-C2G-C3G-O3G
95	cL	520	DGD	O2G-C2G-C3G-O3G
95	hL	101	DGD	O1G-C1G-C2G-O2G
92	CL	519	LMG	C29-C28-O8-C9
82	CA	202	PEB	C3B-C4B-CHB-C1C
82	J5	202	PEB	C2C-C1C-CHB-C4B
82	C7	202	PEB	C3B-C4B-CHB-C1C
87	b6	605	CLA	C15-C16-C17-C18
87	BN	823	CLA	O1A-CGA-O2A-C1
87	C6	518	CLA	O1A-CGA-O2A-C1
87	c6	609	CLA	O1A-CGA-O2A-C1
87	bL	608	CLA	O1A-CGA-O2A-C1
95	C6	503	DGD	O1A-C1A-O1G-C1G
87	c6	608	CLA	C16-C17-C18-C20
88	AN	844	LHG	O1-C1-C2-O2
88	A2	844	LHG	O1-C1-C2-O2
87	AN	808	CLA	O1D-CGD-O2D-CED
87	A2	808	CLA	O1D-CGD-O2D-CED
87	B6	605	CLA	O1D-CGD-O2D-CED
87	D6	402	CLA	O1D-CGD-O2D-CED
95	C6	523	DGD	C8B-C9B-CAB-CBB
95	D6	410	DGD	C8B-C9B-CAB-CBB
87	c6	613	CLA	C10-C11-C12-C13
87	HL	102	CLA	C4-C3-C5-C6
87	AN	807	CLA	C4-C3-C5-C6
87	82	302	CLA	C4-C3-C5-C6
87	A2	807	CLA	C4-C3-C5-C6
87	B6	615	CLA	C4-C3-C5-C6
87	C6	520	CLA	C4-C3-C5-C6
87	8N	303	CLA	C4-C3-C5-C6
88	BL	610	LHG	C16-C17-C18-C19
88	BL	615	LHG	C24-C25-C26-C27
92	BL	611	LMG	C29-C30-C31-C32
92	ML	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
87	HL	102	CLA	C2-C3-C5-C6
87	AN	807	CLA	C2-C3-C5-C6
87	A2	807	CLA	C2-C3-C5-C6
87	b6	614	CLA	C2-C3-C5-C6
87	B6	606	CLA	C4C-C3C-CAC-CBC
87	DL	406	CLA	C15-C16-C17-C18
87	BL	621	CLA	C14-C13-C15-C16
87	AN	823	CLA	C11-C12-C13-C14
87	BN	825	CLA	C14-C13-C15-C16
87	A2	823	CLA	C11-C12-C13-C14
87	B2	824	CLA	C14-C13-C15-C16
87	B6	610	CLA	C14-C13-C15-C16
87	C6	513	CLA	C11-C10-C8-C9
87	C6	514	CLA	C14-C13-C15-C16
87	b6	607	CLA	C11-C12-C13-C14
87	c6	604	CLA	C14-C13-C15-C16
87	cL	508	CLA	C14-C13-C15-C16
87	cL	510	CLA	C11-C10-C8-C9
87	cL	512	CLA	C11-C12-C13-C14
87	AN	807	CLA	O1D-CGD-O2D-CED
87	A2	807	CLA	O1D-CGD-O2D-CED
87	B6	614	CLA	O1D-CGD-O2D-CED
87	BL	622	CLA	O1A-CGA-O2A-C1
87	AN	809	CLA	O1A-CGA-O2A-C1
87	b6	608	CLA	O1A-CGA-O2A-C1
87	bL	607	CLA	C13-C15-C16-C17
87	D6	402	CLA	C2C-C3C-CAC-CBC
92	bL	624	LMG	C13-C14-C15-C16
95	c6	620	DGD	C8B-C9B-CAB-CBB
82	UP	203	PEB	NC-C4C-CHC-C1D
82	dF	202	PEB	NC-C4C-CHC-C1D
82	fJ	202	PEB	NC-C4C-CHC-C1D
82	dK	202	PEB	NC-C4C-CHC-C1D
87	AN	840	CLA	C2A-CAA-CBA-CGA
87	A2	820	CLA	C2A-CAA-CBA-CGA
87	A2	840	CLA	C2A-CAA-CBA-CGA
87	cL	506	CLA	C2A-CAA-CBA-CGA
87	7N	603	CLA	C2A-CAA-CBA-CGA
82	FB	201	PEB	NC-C1C-CHB-C4B
82	OF	203	PEB	NC-C1C-CHB-C4B
82	DJ	201	PEB	NC-C1C-CHB-C4B
82	DM	201	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	z8	201	PEB	NC-C1C-CHB-C4B
82	zC	201	PEB	NC-C1C-CHB-C4B
82	uC	201	PEB	NC-C1C-CHB-C4B
82	lH	202	PEB	NC-C1C-CHB-C4B
87	bL	621	CLA	O1D-CGD-O2D-CED
88	CL	521	LHG	C31-C32-C33-C34
87	A2	809	CLA	O1A-CGA-O2A-C1
82	ID	202	PEB	C4B-C3B-CAB-CBB
82	PM	201	PEB	C4B-C3B-CAB-CBB
82	IQ	202	PEB	C4B-C3B-CAB-CBB
85	BN	803	BCR	C36-C18-C19-C20
85	LN	201	BCR	C37-C22-C23-C24
85	B2	802	BCR	C36-C18-C19-C20
85	L2	201	BCR	C37-C22-C23-C24
85	H6	101	BCR	C7-C8-C9-C34
85	c6	603	BCR	C37-C22-C23-C24
88	i6	101	LHG	C10-C11-C12-C13
92	bL	610	LMG	C19-C20-C21-C22
82	JA	203	PEB	C2B-C3B-CAB-CBB
82	J7	203	PEB	C2B-C3B-CAB-CBB
85	BL	618	BCR	C21-C22-C23-C24
85	LN	201	BCR	C21-C22-C23-C24
85	L2	201	BCR	C21-C22-C23-C24
85	c6	602	BCR	C17-C18-C19-C20
85	c6	603	BCR	C21-C22-C23-C24
82	VE	201	PEB	C1C-C2C-CAC-CBC
82	VG	201	PEB	C1C-C2C-CAC-CBC
82	BA	203	PEB	C2D-C1D-CHC-C4C
82	HA	201	PEB	C2D-C1D-CHC-C4C
82	JA	203	PEB	C2D-C1D-CHC-C4C
82	PA	203	PEB	C2D-C1D-CHC-C4C
82	QA	201	PEB	C2D-C1D-CHC-C4C
82	QA	202	PEB	C2D-C1D-CHC-C4C
82	IB	202	PEB	C2D-C1D-CHC-C4C
82	JB	202	PEB	C2D-C1D-CHC-C4C
82	TB	202	PEB	C2D-C1D-CHC-C4C
82	WB	402	PEB	C2D-C1D-CHC-C4C
82	XB	201	PEB	C2D-C1D-CHC-C4C
82	YB	202	PEB	C2D-C1D-CHC-C4C
82	DD	201	PEB	C2D-C1D-CHC-C4C
82	PD	201	PEB	C2D-C1D-CHC-C4C
82	VD	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	AE	304	PEB	C2D-C1D-CHC-C4C
82	PE	201	PEB	C2D-C1D-CHC-C4C
82	RE	202	PEB	C2D-C1D-CHC-C4C
82	ZE	202	PEB	C2D-C1D-CHC-C4C
82	CF	202	PEB	C2D-C1D-CHC-C4C
82	IF	202	PEB	C2D-C1D-CHC-C4C
82	OF	201	PEB	C2D-C1D-CHC-C4C
82	WF	203	PEB	C2D-C1D-CHC-C4C
82	AG	304	PEB	C2D-C1D-CHC-C4C
82	PG	201	PEB	C2D-C1D-CHC-C4C
82	RG	202	PEB	C2D-C1D-CHC-C4C
82	UG	202	PEB	C2D-C1D-CHC-C4C
82	FH	1002	PEB	C2D-C1D-CHC-C4C
82	JH	1002	PEB	C2D-C1D-CHC-C4C
82	NH	1002	PEB	C2D-C1D-CHC-C4C
82	PH	201	PEB	C2D-C1D-CHC-C4C
82	SH	201	PEB	C2D-C1D-CHC-C4C
82	UH	202	PEB	C2D-C1D-CHC-C4C
82	HI	201	PEB	C2D-C1D-CHC-C4C
82	OI	203	PEB	C2D-C1D-CHC-C4C
82	SI	202	PEB	C2D-C1D-CHC-C4C
82	YI	202	PEB	C2D-C1D-CHC-C4C
82	BJ	301	PEB	C2D-C1D-CHC-C4C
82	KJ	201	PEB	C2D-C1D-CHC-C4C
82	QJ	204	PEB	C2D-C1D-CHC-C4C
82	CK	202	PEB	C2D-C1D-CHC-C4C
82	IK	202	PEB	C2D-C1D-CHC-C4C
82	OK	201	PEB	C2D-C1D-CHC-C4C
82	WK	203	PEB	C2D-C1D-CHC-C4C
82	CM	201	PEB	C2D-C1D-CHC-C4C
82	HM	202	PEB	C2D-C1D-CHC-C4C
82	JM	202	PEB	C2D-C1D-CHC-C4C
82	OM	201	PEB	C2D-C1D-CHC-C4C
82	OM	202	PEB	C2D-C1D-CHC-C4C
82	RM	202	PEB	C2D-C1D-CHC-C4C
82	SO	201	PEB	C2D-C1D-CHC-C4C
82	VO	202	PEB	C2D-C1D-CHC-C4C
82	BP	201	PEB	C2D-C1D-CHC-C4C
82	DP	201	PEB	C2D-C1D-CHC-C4C
82	EP	202	PEB	C2D-C1D-CHC-C4C
82	IP	201	PEB	C2D-C1D-CHC-C4C
82	NP	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	PP	201	PEB	C2D-C1D-CHC-C4C
82	XP	201	PEB	C2D-C1D-CHC-C4C
82	YP	501	PEB	C2D-C1D-CHC-C4C
82	YP	503	PEB	C2D-C1D-CHC-C4C
82	DQ	201	PEB	C2D-C1D-CHC-C4C
82	PQ	201	PEB	C2D-C1D-CHC-C4C
82	VQ	203	PEB	C2D-C1D-CHC-C4C
82	N1	1002	PEB	C2D-C1D-CHC-C4C
82	P1	201	PEB	C2D-C1D-CHC-C4C
82	S1	201	PEB	C2D-C1D-CHC-C4C
82	U1	202	PEB	C2D-C1D-CHC-C4C
82	F1	1002	PEB	C2D-C1D-CHC-C4C
82	J1	1002	PEB	C2D-C1D-CHC-C4C
82	f1	202	PEB	C2D-C1D-CHC-C4C
82	g1	202	PEB	C2D-C1D-CHC-C4C
82	h1	202	PEB	C2D-C1D-CHC-C4C
82	c1	201	PEB	C2D-C1D-CHC-C4C
82	S4	201	PEB	C2D-C1D-CHC-C4C
82	V4	202	PEB	C2D-C1D-CHC-C4C
82	i4	201	PEB	C2D-C1D-CHC-C4C
82	k4	201	PEB	C2D-C1D-CHC-C4C
82	b4	201	PEB	C2D-C1D-CHC-C4C
82	b4	202	PEB	C2D-C1D-CHC-C4C
82	D5	202	PEB	C2D-C1D-CHC-C4C
82	F5	201	PEB	C2D-C1D-CHC-C4C
82	L5	201	PEB	C2D-C1D-CHC-C4C
82	O5	202	PEB	C2D-C1D-CHC-C4C
82	S5	201	PEB	C2D-C1D-CHC-C4C
82	S5	202	PEB	C2D-C1D-CHC-C4C
82	W5	202	PEB	C2D-C1D-CHC-C4C
82	Y5	201	PEB	C2D-C1D-CHC-C4C
82	B7	203	PEB	C2D-C1D-CHC-C4C
82	H7	201	PEB	C2D-C1D-CHC-C4C
82	J7	203	PEB	C2D-C1D-CHC-C4C
82	P7	203	PEB	C2D-C1D-CHC-C4C
82	Q7	201	PEB	C2D-C1D-CHC-C4C
82	Q7	202	PEB	C2D-C1D-CHC-C4C
82	q8	201	PEB	C2D-C1D-CHC-C4C
82	v8	202	PEB	C2D-C1D-CHC-C4C
82	aB	202	PEB	C2D-C1D-CHC-C4C
82	dB	201	PEB	C2D-C1D-CHC-C4C
82	eB	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	qC	201	PEB	C2D-C1D-CHC-C4C
82	vC	202	PEB	C2D-C1D-CHC-C4C
82	dD	401	PEB	C2D-C1D-CHC-C4C
82	jE	201	PEB	C2D-C1D-CHC-C4C
82	jE	202	PEB	C2D-C1D-CHC-C4C
82	kE	201	PEB	C2D-C1D-CHC-C4C
82	aF	201	PEB	C2D-C1D-CHC-C4C
82	eF	201	PEB	C2D-C1D-CHC-C4C
82	fF	201	PEB	C2D-C1D-CHC-C4C
82	gF	202	PEB	C2D-C1D-CHC-C4C
82	oF	202	PEB	C2D-C1D-CHC-C4C
82	pF	201	PEB	C2D-C1D-CHC-C4C
82	qF	202	PEB	C2D-C1D-CHC-C4C
82	zF	501	PEB	C2D-C1D-CHC-C4C
82	jG	201	PEB	C2D-C1D-CHC-C4C
82	jG	202	PEB	C2D-C1D-CHC-C4C
82	kG	201	PEB	C2D-C1D-CHC-C4C
82	fH	202	PEB	C2D-C1D-CHC-C4C
82	gH	202	PEB	C2D-C1D-CHC-C4C
82	hH	201	PEB	C2D-C1D-CHC-C4C
82	cH	201	PEB	C2D-C1D-CHC-C4C
82	aJ	202	PEB	C2D-C1D-CHC-C4C
82	kJ	201	PEB	C2D-C1D-CHC-C4C
82	aK	201	PEB	C2D-C1D-CHC-C4C
82	eK	201	PEB	C2D-C1D-CHC-C4C
82	fK	201	PEB	C2D-C1D-CHC-C4C
82	gK	202	PEB	C2D-C1D-CHC-C4C
82	oK	202	PEB	C2D-C1D-CHC-C4C
82	pK	201	PEB	C2D-C1D-CHC-C4C
82	qK	202	PEB	C2D-C1D-CHC-C4C
82	zK	501	PEB	C2D-C1D-CHC-C4C
82	aM	203	PEB	C2D-C1D-CHC-C4C
82	dM	203	PEB	C2D-C1D-CHC-C4C
82	fM	201	PEB	C2D-C1D-CHC-C4C
82	iM	201	PEB	C2D-C1D-CHC-C4C
82	iO	201	PEB	C2D-C1D-CHC-C4C
82	kO	201	PEB	C2D-C1D-CHC-C4C
82	bO	201	PEB	C2D-C1D-CHC-C4C
82	bO	202	PEB	C2D-C1D-CHC-C4C
82	bP	501	PEB	C2D-C1D-CHC-C4C
82	bP	502	PEB	C2D-C1D-CHC-C4C
82	dQ	401	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
87	DL	406	CLA	C1A-C2A-CAA-CBA
87	AN	832	CLA	C1A-C2A-CAA-CBA
87	BN	825	CLA	C1A-C2A-CAA-CBA
87	12	602	CLA	C1A-C2A-CAA-CBA
87	22	601	CLA	C1A-C2A-CAA-CBA
87	42	601	CLA	C1A-C2A-CAA-CBA
87	42	602	CLA	C1A-C2A-CAA-CBA
87	42	606	CLA	C1A-C2A-CAA-CBA
87	42	607	CLA	C1A-C2A-CAA-CBA
87	62	302	CLA	C1A-C2A-CAA-CBA
87	62	313	CLA	C1A-C2A-CAA-CBA
87	A2	832	CLA	C1A-C2A-CAA-CBA
87	B2	824	CLA	C1A-C2A-CAA-CBA
87	B6	605	CLA	C1A-C2A-CAA-CBA
87	dL	404	CLA	C1A-C2A-CAA-CBA
87	1N	602	CLA	C1A-C2A-CAA-CBA
87	2N	302	CLA	C1A-C2A-CAA-CBA
87	4N	601	CLA	C1A-C2A-CAA-CBA
87	4N	602	CLA	C1A-C2A-CAA-CBA
87	4N	606	CLA	C1A-C2A-CAA-CBA
87	4N	607	CLA	C1A-C2A-CAA-CBA
87	6N	601	CLA	C1A-C2A-CAA-CBA
87	6N	612	CLA	C1A-C2A-CAA-CBA
100	JN	104	3XQ	O20-C21-C22-O23
87	d6	401	CLA	C16-C17-C18-C20
87	C6	517	CLA	C2-C1-O2A-CGA
95	AL	414	DGD	O6D-C5D-C6D-O5D
87	CL	510	CLA	CBA-CGA-O2A-C1
87	LN	203	CLA	CBA-CGA-O2A-C1
87	L2	203	CLA	CBA-CGA-O2A-C1
88	D6	406	LHG	C9-C10-C11-C12
92	b6	624	LMG	C12-C13-C14-C15
85	BN	842	BCR	C9-C10-C11-C12
85	B2	842	BCR	C9-C10-C11-C12
87	BN	836	CLA	O1D-CGD-O2D-CED
87	B2	836	CLA	O1D-CGD-O2D-CED
87	C6	511	CLA	C10-C11-C12-C13
87	C6	514	CLA	C13-C15-C16-C17
88	m6	102	LHG	C4-O6-P-O3
88	cL	501	LHG	C3-O3-P-O6
92	x6	601	LMG	C15-C16-C17-C18
95	BL	614	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
95	C6	521	DGD	C3B-C4B-C5B-C6B
91	DL	405	PHO	O1D-CGD-O2D-CED
83	Z9	305	PUB	C3B-C4B-CHB-C1C
87	cL	511	CLA	C4-C3-C5-C6
88	ML	102	LHG	O8-C23-C24-C25
87	LN	203	CLA	C8-C10-C11-C12
87	AN	840	CLA	C3-C5-C6-C7
87	A2	840	CLA	C3-C5-C6-C7
87	cL	511	CLA	C3-C5-C6-C7
88	I6	101	LHG	C2-C3-O3-P
87	82	302	CLA	C2-C3-C5-C6
87	8N	303	CLA	C2-C3-C5-C6
94	a6	601	PL9	C33-C34-C36-C37
94	dL	406	PL9	C18-C19-C21-C22
87	c6	604	CLA	C4C-C3C-CAC-CBC
88	aL	607	LHG	C34-C35-C36-C37
87	K2	101	CLA	O1A-CGA-O2A-C1
87	aL	605	CLA	O1A-CGA-O2A-C1
82	TD	201	PEB	ND-C1D-CHC-C4C
82	VD	203	PEB	ND-C1D-CHC-C4C
82	OF	201	PEB	ND-C1D-CHC-C4C
82	SF	202	PEB	ND-C1D-CHC-C4C
82	AH	302	PEB	ND-C1D-CHC-C4C
82	JH	1002	PEB	ND-C1D-CHC-C4C
82	SH	203	PEB	ND-C1D-CHC-C4C
82	AI	201	PEB	ND-C1D-CHC-C4C
82	CI	201	PEB	ND-C1D-CHC-C4C
82	EI	201	PEB	ND-C1D-CHC-C4C
82	FI	202	PEB	ND-C1D-CHC-C4C
82	GI	202	PEB	ND-C1D-CHC-C4C
82	II	201	PEB	ND-C1D-CHC-C4C
82	KI	202	PEB	ND-C1D-CHC-C4C
82	NI	201	PEB	ND-C1D-CHC-C4C
82	PI	201	PEB	ND-C1D-CHC-C4C
82	RI	201	PEB	ND-C1D-CHC-C4C
82	TI	202	PEB	ND-C1D-CHC-C4C
82	VI	201	PEB	ND-C1D-CHC-C4C
82	XI	201	PEB	ND-C1D-CHC-C4C
82	OK	201	PEB	ND-C1D-CHC-C4C
82	SK	202	PEB	ND-C1D-CHC-C4C
82	BM	301	PEB	ND-C1D-CHC-C4C
82	IM	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	EP	202	PEB	ND-C1D-CHC-C4C
82	KP	201	PEB	ND-C1D-CHC-C4C
82	NQ	204	PEB	ND-C1D-CHC-C4C
82	TQ	201	PEB	ND-C1D-CHC-C4C
82	A1	302	PEB	ND-C1D-CHC-C4C
82	J1	1002	PEB	ND-C1D-CHC-C4C
82	V1	202	PEB	ND-C1D-CHC-C4C
82	k1	202	PEB	ND-C1D-CHC-C4C
82	l1	201	PEB	ND-C1D-CHC-C4C
82	j4	203	PEB	ND-C1D-CHC-C4C
82	D5	202	PEB	ND-C1D-CHC-C4C
82	S5	202	PEB	ND-C1D-CHC-C4C
82	W5	202	PEB	ND-C1D-CHC-C4C
82	S9	202	PEB	ND-C1D-CHC-C4C
82	kH	202	PEB	ND-C1D-CHC-C4C
82	kH	203	PEB	ND-C1D-CHC-C4C
82	kO	202	PEB	ND-C1D-CHC-C4C
87	CL	518	CLA	C4B-C3B-CAB-CBB
87	BN	817	CLA	C4B-C3B-CAB-CBB
87	FN	203	CLA	C4B-C3B-CAB-CBB
87	B2	816	CLA	C4B-C3B-CAB-CBB
87	F2	201	CLA	C4B-C3B-CAB-CBB
87	B6	607	CLA	C4B-C3B-CAB-CBB
87	b6	607	CLA	C4B-C3B-CAB-CBB
87	b6	610	CLA	C4B-C3B-CAB-CBB
87	b6	611	CLA	C4B-C3B-CAB-CBB
88	BL	610	LHG	C3-O3-P-O5
88	BL	610	LHG	C4-O6-P-O4
88	CL	521	LHG	C3-O3-P-O5
88	DL	407	LHG	C3-O3-P-O5
88	ML	102	LHG	C3-O3-P-O5
88	ML	102	LHG	C4-O6-P-O5
88	AN	843	LHG	C4-O6-P-O4
88	AN	844	LHG	C4-O6-P-O5
88	A2	843	LHG	C4-O6-P-O4
88	A2	844	LHG	C4-O6-P-O5
88	D6	406	LHG	C3-O3-P-O5
88	I6	101	LHG	C3-O3-P-O5
88	L6	101	LHG	C3-O3-P-O4
88	M6	101	LHG	C3-O3-P-O5
88	a6	610	LHG	C4-O6-P-O4
88	d6	407	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
88	i6	101	LHG	C4-O6-P-O5
88	l6	101	LHG	C3-O3-P-O4
88	m6	102	LHG	C4-O6-P-O5
88	bL	612	LHG	C3-O3-P-O4
88	bL	612	LHG	C4-O6-P-O4
88	dL	405	LHG	C3-O3-P-O5
88	dL	408	LHG	C4-O6-P-O4
88	iL	101	LHG	C3-O3-P-O5
88	mL	102	LHG	C3-O3-P-O5
87	DL	406	CLA	C16-C17-C18-C20
87	AN	810	CLA	C16-C17-C18-C19
87	BN	825	CLA	C16-C17-C18-C19
87	A2	810	CLA	C16-C17-C18-C19
87	B2	824	CLA	C16-C17-C18-C19
87	A6	403	CLA	C11-C12-C13-C15
87	B6	613	CLA	C16-C17-C18-C20
87	b6	610	CLA	C16-C17-C18-C20
87	aL	606	CLA	C11-C12-C13-C14
91	A6	407	PHO	C16-C17-C18-C20
92	A6	408	LMG	C28-C29-C30-C31
95	L6	102	DGD	C5A-C6A-C7A-C8A
95	C6	521	DGD	O6D-C1D-O3G-C3G
87	L2	203	CLA	C8-C10-C11-C12
88	dL	405	LHG	C24-C23-O8-C6
92	k6	101	LMG	C29-C28-O8-C9
95	B6	620	DGD	C2A-C1A-O1G-C1G
95	D6	410	DGD	C2A-C1A-O1G-C1G
88	C6	505	LHG	O6-C4-C5-C6
88	L6	101	LHG	O6-C4-C5-C6
88	M6	101	LHG	O6-C4-C5-C6
88	l6	101	LHG	O6-C4-C5-C6
95	AL	414	DGD	C4D-C5D-C6D-O5D
87	CL	507	CLA	C15-C16-C17-C18
95	lL	101	DGD	C1B-C2B-C3B-C4B
87	CL	504	CLA	C2A-CAA-CBA-CGA
87	AN	850	CLA	C2A-CAA-CBA-CGA
87	BN	805	CLA	C2A-CAA-CBA-CGA
87	BN	828	CLA	C2A-CAA-CBA-CGA
87	BN	836	CLA	C2A-CAA-CBA-CGA
87	72	603	CLA	C2A-CAA-CBA-CGA
87	A2	850	CLA	C2A-CAA-CBA-CGA
87	B2	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	B2	836	CLA	C2A-CAA-CBA-CGA
87	b6	609	CLA	C2A-CAA-CBA-CGA
87	C6	515	CLA	C3-C5-C6-C7
87	bL	615	CLA	C3-C5-C6-C7
82	RF	201	PEB	C3B-CAB-CBB-CGB
82	YF	201	PEB	C3B-CAB-CBB-CGB
82	AH	301	PEB	C2C-CAC-CBC-CGC
82	RK	201	PEB	C3B-CAB-CBB-CGB
82	YK	201	PEB	C3B-CAB-CBB-CGB
82	IM	202	PEB	C2C-CAC-CBC-CGC
82	YM	202	PEB	C3B-CAB-CBB-CGB
82	DO	1002	PEB	C3B-CAB-CBB-CGB
82	BP	201	PEB	C2C-CAC-CBC-CGC
82	D4	1002	PEB	C3B-CAB-CBB-CGB
82	u8	201	PEB	C3B-CAB-CBB-CGB
82	L9	202	PEB	C3B-CAB-CBB-CGB
82	dF	202	PEB	C2C-CAC-CBC-CGC
82	dK	202	PEB	C2C-CAC-CBC-CGC
82	Z9	303	PEB	C2C-CAC-CBC-CGC
82	M9	304	PEB	C2C-CAC-CBC-CGC
83	KA	203	PUB	C3B-CAB-CBB-CGB
83	K7	203	PUB	C3B-CAB-CBB-CGB
82	lF	201	PEB	C2B-C3B-CAB-CBB
92	dL	407	LMG	C12-C13-C14-C15
95	J6	101	DGD	C8B-C9B-CAB-CBB
95	BL	614	DGD	O1A-C1A-O1G-C1G
95	cL	502	DGD	C2B-C1B-O2G-C2G
82	NE	202	PEB	NC-C1C-CHB-C4B
82	JI	202	PEB	NC-C1C-CHB-C4B
82	PJ	202	PEB	NC-C1C-CHB-C4B
82	TJ	202	PEB	NC-C1C-CHB-C4B
82	l1	203	PEB	NC-C1C-CHB-C4B
82	Y5	202	PEB	NC-C1C-CHB-C4B
82	u8	201	PEB	NC-C1C-CHB-C4B
82	J9	203	PEB	NC-C1C-CHB-C4B
82	dE	204	PEB	NC-C1C-CHB-C4B
82	eF	203	PEB	NC-C1C-CHB-C4B
82	tF	201	PEB	NC-C1C-CHB-C4B
82	xF	304	PEB	NC-C1C-CHB-C4B
82	dG	204	PEB	NC-C1C-CHB-C4B
82	eK	203	PEB	NC-C1C-CHB-C4B
82	tK	201	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
87	BL	609	CLA	C16-C17-C18-C19
87	B6	606	CLA	C16-C17-C18-C19
87	b6	606	CLA	C16-C17-C18-C19
98	AN	842	PQN	C26-C27-C28-C29
98	A2	842	PQN	C26-C27-C28-C29
95	C6	502	DGD	CDA-CEA-CFA-CGA
95	c6	601	DGD	CDA-CEA-CFA-CGA
87	BL	605	CLA	CAD-CBD-CGD-O1D
87	BL	609	CLA	CAD-CBD-CGD-O1D
87	BL	620	CLA	CAD-CBD-CGD-O1D
87	CL	503	CLA	CAD-CBD-CGD-O1D
87	CL	507	CLA	CAD-CBD-CGD-O1D
87	CL	508	CLA	CAD-CBD-CGD-O1D
87	CL	518	CLA	CAD-CBD-CGD-O1D
87	AN	803	CLA	CAD-CBD-CGD-O1D
87	AN	809	CLA	CAD-CBD-CGD-O1D
87	AN	811	CLA	CAD-CBD-CGD-O1D
87	AN	815	CLA	CAD-CBD-CGD-O1D
87	AN	838	CLA	CAD-CBD-CGD-O1D
87	BN	806	CLA	CAD-CBD-CGD-O1D
87	BN	825	CLA	CAD-CBD-CGD-O1D
87	BN	831	CLA	CAD-CBD-CGD-O1D
87	BN	836	CLA	CAD-CBD-CGD-O1D
87	FN	205	CLA	CAD-CBD-CGD-O1D
87	ON	201	CLA	CAD-CBD-CGD-O1D
87	ON	203	CLA	CAD-CBD-CGD-O1D
87	22	603	CLA	CAD-CBD-CGD-O1D
87	32	303	CLA	CAD-CBD-CGD-O1D
87	32	309	CLA	CAD-CBD-CGD-O1D
87	52	601	CLA	CAD-CBD-CGD-O1D
87	A2	803	CLA	CAD-CBD-CGD-O1D
87	A2	809	CLA	CAD-CBD-CGD-O1D
87	A2	811	CLA	CAD-CBD-CGD-O1D
87	A2	815	CLA	CAD-CBD-CGD-O1D
87	A2	838	CLA	CAD-CBD-CGD-O1D
87	B2	805	CLA	CAD-CBD-CGD-O1D
87	B2	824	CLA	CAD-CBD-CGD-O1D
87	B2	831	CLA	CAD-CBD-CGD-O1D
87	B2	836	CLA	CAD-CBD-CGD-O1D
87	F2	205	CLA	CAD-CBD-CGD-O1D
87	O2	201	CLA	CAD-CBD-CGD-O1D
87	O2	203	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	B6	609	CLA	CAD-CBD-CGD-O1D
87	C6	513	CLA	CAD-CBD-CGD-O1D
87	C6	514	CLA	CAD-CBD-CGD-O1D
87	C6	517	CLA	CAD-CBD-CGD-O1D
87	b6	605	CLA	CAD-CBD-CGD-O1D
87	b6	607	CLA	CAD-CBD-CGD-O1D
87	b6	611	CLA	CAD-CBD-CGD-O1D
87	c6	609	CLA	CAD-CBD-CGD-O1D
87	bL	615	CLA	CAD-CBD-CGD-O1D
87	bL	618	CLA	CAD-CBD-CGD-O1D
87	bL	622	CLA	CAD-CBD-CGD-O1D
87	cL	505	CLA	CAD-CBD-CGD-O1D
87	cL	508	CLA	CAD-CBD-CGD-O1D
87	cL	510	CLA	CAD-CBD-CGD-O1D
87	cL	511	CLA	CAD-CBD-CGD-O1D
87	2N	304	CLA	CAD-CBD-CGD-O1D
87	3N	304	CLA	CAD-CBD-CGD-O1D
87	3N	309	CLA	CAD-CBD-CGD-O1D
87	5N	601	CLA	CAD-CBD-CGD-O1D
92	qL	301	LMG	C28-C29-C30-C31
82	JA	203	PEB	C4B-C3B-CAB-CBB
82	J7	203	PEB	C4B-C3B-CAB-CBB
87	CL	505	CLA	C13-C15-C16-C17
87	B6	616	CLA	C10-C11-C12-C13
87	C6	514	CLA	C8-C10-C11-C12
88	d6	407	LHG	C15-C16-C17-C18
87	BN	810	CLA	C3-C5-C6-C7
87	B2	809	CLA	C3-C5-C6-C7
87	BL	608	CLA	C13-C15-C16-C17
95	AL	414	DGD	C1B-C2B-C3B-C4B
88	ML	102	LHG	C12-C13-C14-C15
87	22	609	CLA	CBA-CGA-O2A-C1
87	B6	613	CLA	CBA-CGA-O2A-C1
87	bL	617	CLA	CBA-CGA-O2A-C1
87	2N	309	CLA	CBA-CGA-O2A-C1
87	BN	811	CLA	C8-C10-C11-C12
84	LH	1001	CYC	C2B-C3B-CAB-CBB
95	C6	502	DGD	C3B-C4B-C5B-C6B
95	c6	601	DGD	C3B-C4B-C5B-C6B
87	BL	619	CLA	C16-C17-C18-C20
87	C6	516	CLA	C16-C17-C18-C19
87	a6	608	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
87	cL	515	CLA	C11-C12-C13-C15
87	LN	203	CLA	C4-C3-C5-C6
87	L2	203	CLA	C4-C3-C5-C6
82	ED	201	PEB	C2A-C3A-CAA-CBA
82	WD	202	PEB	C2A-C3A-CAA-CBA
82	PE	202	PEB	C2A-C3A-CAA-CBA
82	QE	203	PEB	C2A-C3A-CAA-CBA
82	PG	202	PEB	C2A-C3A-CAA-CBA
82	QG	203	PEB	C2A-C3A-CAA-CBA
82	QH	201	PEB	C2A-C3A-CAA-CBA
82	HI	201	PEB	C2A-C3A-CAA-CBA
82	HO	1002	PEB	C2A-C3A-CAA-CBA
82	GP	201	PEB	C2A-C3A-CAA-CBA
82	PP	201	PEB	C2A-C3A-CAA-CBA
82	QP	203	PEB	C2A-C3A-CAA-CBA
82	RP	201	PEB	C2A-C3A-CAA-CBA
82	EQ	201	PEB	C2A-C3A-CAA-CBA
82	WQ	202	PEB	C2A-C3A-CAA-CBA
82	Q1	201	PEB	C2A-C3A-CAA-CBA
82	Q1	203	PEB	C2A-C3A-CAA-CBA
82	H4	1002	PEB	C2A-C3A-CAA-CBA
82	a4	202	PEB	C2A-C3A-CAA-CBA
82	M5	301	PEB	C2A-C3A-CAA-CBA
82	Z5	301	PEB	C2A-C3A-CAA-CBA
82	S9	201	PEB	C2A-C3A-CAA-CBA
82	cK	202	PEB	C2A-C3A-CAA-CBA
82	aO	202	PEB	C2A-C3A-CAA-CBA
82	Z9	304	PEB	C2A-C3A-CAA-CBA
82	M9	305	PEB	C2A-C3A-CAA-CBA
83	ND	201	PUB	C3C-C4C-CHC-C1D
83	NQ	201	PUB	C3C-C4C-CHC-C1D
83	xF	306	PUB	C3C-C4C-CHC-C1D
83	xK	306	PUB	C3C-C4C-CHC-C1D
84	EH	1001	CYC	C2C-C3C-CAC-CBC
84	E1	1001	CYC	C2C-C3C-CAC-CBC
87	BL	602	CLA	C12-C13-C15-C16
87	CL	503	CLA	C2-C3-C5-C6
87	CL	503	CLA	C12-C13-C15-C16
87	AN	801	CLA	C3A-C2A-CAA-CBA
87	AN	813	CLA	C11-C10-C8-C7
87	AN	821	CLA	C6-C7-C8-C10
87	AN	851	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
87	BN	835	CLA	C11-C12-C13-C15
87	42	604	CLA	C3A-C2A-CAA-CBA
87	62	309	CLA	C3A-C2A-CAA-CBA
87	82	302	CLA	C12-C13-C15-C16
87	A2	802	CLA	C3A-C2A-CAA-CBA
87	A2	813	CLA	C11-C10-C8-C7
87	A2	821	CLA	C6-C7-C8-C10
87	A2	851	CLA	C11-C10-C8-C7
87	B2	835	CLA	C11-C12-C13-C15
87	B6	603	CLA	C11-C12-C13-C15
87	B6	604	CLA	C6-C7-C8-C10
87	B6	610	CLA	C6-C7-C8-C10
87	C6	509	CLA	C11-C12-C13-C15
87	C6	510	CLA	C6-C7-C8-C10
87	C6	515	CLA	C11-C10-C8-C7
87	C6	518	CLA	C11-C10-C8-C7
87	C6	520	CLA	C11-C10-C8-C7
87	D6	403	CLA	C11-C10-C8-C7
87	H6	103	CLA	C6-C7-C8-C10
87	a6	608	CLA	C6-C7-C8-C10
87	b6	604	CLA	C6-C7-C8-C10
87	b6	612	CLA	C6-C7-C8-C10
87	b6	618	CLA	C12-C13-C15-C16
87	c6	610	CLA	C11-C10-C8-C7
87	c6	612	CLA	C11-C12-C13-C15
87	d6	403	CLA	C11-C12-C13-C15
87	bL	608	CLA	C12-C13-C15-C16
87	cL	513	CLA	C12-C13-C15-C16
87	dL	402	CLA	C11-C10-C8-C7
87	4N	604	CLA	C3A-C2A-CAA-CBA
87	6N	608	CLA	C3A-C2A-CAA-CBA
87	8N	303	CLA	C12-C13-C15-C16
88	c6	619	LHG	O6-C4-C5-O7
88	m6	102	LHG	O6-C4-C5-O7
88	mL	102	LHG	O6-C4-C5-O7
91	AL	410	PHO	C11-C10-C8-C7
91	A6	407	PHO	C11-C10-C8-C7
87	B2	810	CLA	C8-C10-C11-C12
87	BL	603	CLA	C3-C5-C6-C7
87	c6	612	CLA	O1A-CGA-O2A-C1
88	d6	407	LHG	C24-C25-C26-C27
82	EF	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	SF	203	PEB	C2C-C1C-CHB-C4B
82	dD	401	PEB	C2C-C1C-CHB-C4B
103	82	309	ZEX	C9-C10-C11-C12
103	8N	309	ZEX	C9-C10-C11-C12
84	I1	1001	CYC	C2B-C3B-CAB-CBB
87	BN	834	CLA	C13-C15-C16-C17
87	B2	834	CLA	C13-C15-C16-C17
87	c6	609	CLA	C8-C10-C11-C12
87	bL	605	CLA	C13-C15-C16-C17
92	bL	609	LMG	C28-C29-C30-C31
88	i6	101	LHG	C11-C12-C13-C14
95	L6	102	DGD	C3A-C4A-C5A-C6A
88	a6	610	LHG	O10-C23-O8-C6
88	i6	101	LHG	O2-C2-C3-O3
87	BL	602	CLA	C8-C10-C11-C12
82	lK	201	PEB	C2B-C3B-CAB-CBB
82	pK	202	PEB	C2B-C3B-CAB-CBB
82	hM	202	PEB	C2B-C3B-CAB-CBB
84	BE	1001	CYC	C3A-C2A-CAA-CBA
84	BG	1001	CYC	C3A-C2A-CAA-CBA
87	B2	804	CLA	C2A-CAA-CBA-CGA
87	CL	513	CLA	C11-C12-C13-C15
87	bL	622	CLA	C16-C17-C18-C20
82	k4	202	PEB	NB-C4B-CHB-C1C
82	kO	203	PEB	NB-C4B-CHB-C1C
88	DL	407	LHG	C12-C13-C14-C15
82	KB	303	PEB	C1C-C2C-CAC-CBC
87	BN	817	CLA	CAA-CBA-CGA-O2A
82	RJ	201	PEB	C3C-C4C-CHC-C1D
82	TJ	201	PEB	C3C-C4C-CHC-C1D
82	TM	201	PEB	C3C-C4C-CHC-C1D
82	CP	201	PEB	C3C-C4C-CHC-C1D
82	GP	201	PEB	C3C-C4C-CHC-C1D
82	OP	201	PEB	C3C-C4C-CHC-C1D
82	SP	201	PEB	C3C-C4C-CHC-C1D
82	gB	203	PEB	C3C-C4C-CHC-C1D
82	rF	202	PEB	C3C-C4C-CHC-C1D
82	rK	202	PEB	C3C-C4C-CHC-C1D
82	iM	201	PEB	C3C-C4C-CHC-C1D
92	CL	519	LMG	C21-C22-C23-C24
92	A6	408	LMG	C40-C41-C42-C43
95	D6	410	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
88	aL	607	LHG	O7-C5-C6-O8
92	JL	102	LMG	O7-C8-C9-O8
92	j6	102	LMG	O1-C7-C8-O7
92	yL	101	LMG	O7-C8-C9-O8
95	BL	607	DGD	O1G-C1G-C2G-O2G
95	C6	502	DGD	O2G-C2G-C3G-O3G
95	c6	601	DGD	O2G-C2G-C3G-O3G
92	DL	402	LMG	C15-C16-C17-C18
92	dL	407	LMG	C18-C19-C20-C21
87	bL	617	CLA	C8-C10-C11-C12
92	dL	407	LMG	C15-C16-C17-C18
95	L6	102	DGD	C5D-C6D-O5D-C1E
87	B2	816	CLA	CAA-CBA-CGA-O2A
87	c6	611	CLA	C16-C17-C18-C19
87	CL	508	CLA	C15-C16-C17-C18
87	42	602	CLA	C13-C15-C16-C17
87	b6	612	CLA	C8-C10-C11-C12
87	4N	602	CLA	C13-C15-C16-C17
87	cL	505	CLA	C3-C5-C6-C7
87	BN	811	CLA	O1A-CGA-O2A-C1
87	LN	203	CLA	O1A-CGA-O2A-C1
87	B2	810	CLA	O1A-CGA-O2A-C1
87	L2	203	CLA	O1A-CGA-O2A-C1
87	B6	613	CLA	O1A-CGA-O2A-C1
92	B6	622	LMG	O10-C28-O8-C9
87	c6	612	CLA	C8-C10-C11-C12
87	HL	101	CLA	CBA-CGA-O2A-C1
87	BN	811	CLA	CBA-CGA-O2A-C1
87	BN	827	CLA	CBA-CGA-O2A-C1
87	B2	810	CLA	CBA-CGA-O2A-C1
87	B2	827	CLA	CBA-CGA-O2A-C1
87	bL	618	CLA	CBA-CGA-O2A-C1
95	B6	620	DGD	C7A-C8A-C9A-CAA
87	B6	615	CLA	C2-C3-C5-C6
87	BN	811	CLA	CAA-CBA-CGA-O2A
87	B2	810	CLA	CAA-CBA-CGA-O2A
87	BN	825	CLA	C13-C15-C16-C17
87	B2	824	CLA	C13-C15-C16-C17
87	BL	602	CLA	C14-C13-C15-C16
87	BL	603	CLA	C11-C10-C8-C9
87	BL	609	CLA	C6-C7-C8-C9
87	DL	404	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
87	HL	101	CLA	C14-C13-C15-C16
87	AN	808	CLA	C11-C12-C13-C14
87	AN	810	CLA	C11-C12-C13-C14
87	AN	815	CLA	C6-C7-C8-C9
87	AN	823	CLA	C6-C7-C8-C9
87	AN	851	CLA	C11-C10-C8-C9
87	BN	809	CLA	C11-C10-C8-C9
87	BN	811	CLA	C11-C12-C13-C14
87	BN	824	CLA	C14-C13-C15-C16
87	BN	834	CLA	C11-C10-C8-C9
87	LN	203	CLA	C11-C10-C8-C9
87	62	303	CLA	C6-C7-C8-C9
87	62	303	CLA	C11-C12-C13-C14
87	72	602	CLA	C14-C13-C15-C16
87	A2	808	CLA	C11-C12-C13-C14
87	A2	810	CLA	C11-C12-C13-C14
87	A2	815	CLA	C6-C7-C8-C9
87	A2	823	CLA	C6-C7-C8-C9
87	A2	851	CLA	C11-C10-C8-C9
87	B2	808	CLA	C11-C10-C8-C9
87	B2	810	CLA	C6-C7-C8-C9
87	B2	810	CLA	C11-C12-C13-C14
87	B2	823	CLA	C14-C13-C15-C16
87	B2	834	CLA	C11-C10-C8-C9
87	L2	203	CLA	C11-C10-C8-C9
87	B6	615	CLA	C14-C13-C15-C16
87	C6	509	CLA	C14-C13-C15-C16
87	C6	513	CLA	C14-C13-C15-C16
87	C6	516	CLA	C11-C10-C8-C9
87	C6	517	CLA	C6-C7-C8-C9
87	H6	103	CLA	C11-C12-C13-C14
87	K6	101	CLA	C14-C13-C15-C16
87	a6	607	CLA	C6-C7-C8-C9
87	b6	609	CLA	C6-C7-C8-C9
87	b6	615	CLA	C6-C7-C8-C9
87	b6	615	CLA	C11-C12-C13-C14
87	c6	616	CLA	C14-C13-C15-C16
87	bL	607	CLA	C11-C12-C13-C14
87	bL	616	CLA	C14-C13-C15-C16
87	cL	505	CLA	C14-C13-C15-C16
87	6N	602	CLA	C6-C7-C8-C9
87	6N	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
87	7N	602	CLA	C14-C13-C15-C16
91	aL	610	PHO	C11-C10-C8-C9
87	bL	617	CLA	O1A-CGA-O2A-C1
92	CL	519	LMG	O10-C28-O8-C9
95	B2	844	DGD	CEA-CFA-CGA-CHA
87	b6	609	CLA	C16-C17-C18-C19
92	d6	409	LMG	C39-C40-C41-C42
95	BN	844	DGD	CEA-CFA-CGA-CHA
95	AL	416	DGD	O6E-C1E-O5D-C6D
82	pF	202	PEB	C2B-C3B-CAB-CBB
82	EK	202	PEB	C2C-C1C-CHB-C4B
82	SK	203	PEB	C2C-C1C-CHB-C4B
82	l1	203	PEB	C2C-C1C-CHB-C4B
82	s8	203	PEB	C2C-C1C-CHB-C4B
82	w8	201	PEB	C2C-C1C-CHB-C4B
82	w8	204	PEB	C2C-C1C-CHB-C4B
82	sC	203	PEB	C2C-C1C-CHB-C4B
82	wC	201	PEB	C2C-C1C-CHB-C4B
82	wC	204	PEB	C2C-C1C-CHB-C4B
82	lH	202	PEB	C2C-C1C-CHB-C4B
82	dQ	401	PEB	C2C-C1C-CHB-C4B
82	VA	202	PEB	C3B-CAB-CBB-CGB
82	CB	201	PEB	C2C-CAC-CBC-CGC
82	DB	203	PEB	C2C-CAC-CBC-CGC
82	QB	204	PEB	C2C-CAC-CBC-CGC
82	YH	202	PEB	C2C-CAC-CBC-CGC
82	EJ	201	PEB	C3B-CAB-CBB-CGB
82	YO	201	PEB	C2C-CAC-CBC-CGC
82	YP	502	PEB	C2C-CAC-CBC-CGC
82	Y4	201	PEB	C2C-CAC-CBC-CGC
82	B5	201	PEB	C3B-CAB-CBB-CGB
82	V7	202	PEB	C3B-CAB-CBB-CGB
82	S9	202	PEB	C2C-CAC-CBC-CGC
82	W9	202	PEB	C3B-CAB-CBB-CGB
82	bB	201	PEB	C2C-CAC-CBC-CGC
82	uC	201	PEB	C3B-CAB-CBB-CGB
82	iF	202	PEB	C3B-CAB-CBB-CGB
82	vF	201	PEB	C3B-CAB-CBB-CGB
82	iK	202	PEB	C3B-CAB-CBB-CGB
82	vK	201	PEB	C3B-CAB-CBB-CGB
82	dM	201	PEB	C3B-CAB-CBB-CGB
82	kM	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
83	AJ	303	PUB	C3B-CAB-CBB-CGB
87	22	609	CLA	O1A-CGA-O2A-C1
87	2N	309	CLA	O1A-CGA-O2A-C1
95	B6	620	DGD	O1A-C1A-O1G-C1G
84	D1	1001	CYC	C2B-C3B-CAB-CBB
85	BL	617	BCR	C18-C19-C20-C21
85	FL	101	BCR	C18-C19-C20-C21
85	KL	100	BCR	C10-C11-C12-C13
85	KL	100	BCR	C18-C19-C20-C21
85	AN	848	BCR	C18-C19-C20-C21
85	BN	803	BCR	C18-C19-C20-C21
85	BN	838	BCR	C10-C11-C12-C13
85	BN	842	BCR	C10-C11-C12-C13
85	KN	101	BCR	C10-C11-C12-C13
85	LN	205	BCR	C10-C11-C12-C13
85	A2	848	BCR	C18-C19-C20-C21
85	B2	802	BCR	C18-C19-C20-C21
85	B2	838	BCR	C10-C11-C12-C13
85	B2	842	BCR	C10-C11-C12-C13
85	K2	102	BCR	C10-C11-C12-C13
85	L2	205	BCR	C10-C11-C12-C13
85	C6	508	BCR	C18-C19-C20-C21
85	K6	102	BCR	C10-C11-C12-C13
85	K6	102	BCR	C18-C19-C20-C21
85	b6	602	BCR	C18-C19-C20-C21
85	c6	617	BCR	C10-C11-C12-C13
85	c6	617	BCR	C18-C19-C20-C21
85	k6	102	BCR	C10-C11-C12-C13
85	k6	102	BCR	C18-C19-C20-C21
85	bL	602	BCR	C18-C19-C20-C21
85	fL	101	BCR	C18-C19-C20-C21
85	kL	100	BCR	C10-C11-C12-C13
85	kL	100	BCR	C18-C19-C20-C21
88	AL	406	LHG	C11-C12-C13-C14
88	a6	610	LHG	C31-C32-C33-C34
92	b6	623	LMG	C13-C14-C15-C16
92	dL	407	LMG	C16-C17-C18-C19
95	C6	503	DGD	C2B-C3B-C4B-C5B
85	AN	846	BCR	C7-C8-C9-C34
85	A2	846	BCR	C7-C8-C9-C34
85	bL	603	BCR	C37-C22-C23-C24
87	A2	834	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
87	K2	101	CLA	C10-C11-C12-C13
98	AN	842	PQN	C15-C16-C17-C18
98	A2	842	PQN	C15-C16-C17-C18
88	D6	401	LHG	C12-C13-C14-C15
88	d6	402	LHG	C32-C33-C34-C35
95	b6	621	DGD	C4D-C5D-C6D-O5D
84	ME	1001	CYC	C2B-C3B-CAB-CBB
92	aL	611	LMG	C18-C19-C20-C21
92	dL	407	LMG	C19-C20-C21-C22
95	a6	603	DGD	C2A-C3A-C4A-C5A
85	B2	839	BCR	C7-C8-C9-C10
85	a6	605	BCR	C7-C8-C9-C10
87	AN	834	CLA	C13-C15-C16-C17
84	MG	1001	CYC	C2B-C3B-CAB-CBB
87	L2	204	CLA	C4C-C3C-CAC-CBC
88	AL	407	LHG	C34-C35-C36-C37
82	NG	201	PEB	NC-C1C-CHB-C4B
87	BL	602	CLA	C2B-C3B-CAB-CBB
87	BL	608	CLA	C2B-C3B-CAB-CBB
87	CL	512	CLA	C2B-C3B-CAB-CBB
87	CL	513	CLA	C2B-C3B-CAB-CBB
87	AN	810	CLA	C2B-C3B-CAB-CBB
87	AN	820	CLA	C2B-C3B-CAB-CBB
87	AN	827	CLA	C2B-C3B-CAB-CBB
87	AN	835	CLA	C2B-C3B-CAB-CBB
87	AN	836	CLA	C2B-C3B-CAB-CBB
87	BN	809	CLA	C2B-C3B-CAB-CBB
87	BN	817	CLA	C2B-C3B-CAB-CBB
87	FN	203	CLA	C2B-C3B-CAB-CBB
87	12	607	CLA	C2B-C3B-CAB-CBB
87	22	609	CLA	C2B-C3B-CAB-CBB
87	22	611	CLA	C2B-C3B-CAB-CBB
87	32	304	CLA	C2B-C3B-CAB-CBB
87	52	602	CLA	C2B-C3B-CAB-CBB
87	72	601	CLA	C2B-C3B-CAB-CBB
87	82	302	CLA	C2B-C3B-CAB-CBB
87	82	306	CLA	C2B-C3B-CAB-CBB
87	A2	810	CLA	C2B-C3B-CAB-CBB
87	A2	820	CLA	C2B-C3B-CAB-CBB
87	A2	827	CLA	C2B-C3B-CAB-CBB
87	A2	835	CLA	C2B-C3B-CAB-CBB
87	A2	836	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	B2	808	CLA	C2B-C3B-CAB-CBB
87	B2	816	CLA	C2B-C3B-CAB-CBB
87	F2	201	CLA	C2B-C3B-CAB-CBB
87	b6	610	CLA	C2B-C3B-CAB-CBB
87	b6	615	CLA	C2B-C3B-CAB-CBB
87	c6	605	CLA	C2B-C3B-CAB-CBB
87	bL	613	CLA	C2B-C3B-CAB-CBB
87	bL	615	CLA	C2B-C3B-CAB-CBB
87	cL	515	CLA	C2B-C3B-CAB-CBB
87	1N	607	CLA	C2B-C3B-CAB-CBB
87	2N	309	CLA	C2B-C3B-CAB-CBB
87	2N	311	CLA	C2B-C3B-CAB-CBB
87	3N	305	CLA	C2B-C3B-CAB-CBB
87	5N	602	CLA	C2B-C3B-CAB-CBB
87	7N	601	CLA	C2B-C3B-CAB-CBB
87	8N	301	CLA	C2B-C3B-CAB-CBB
87	8N	303	CLA	C2B-C3B-CAB-CBB
91	D6	404	PHO	C2C-C3C-CAC-CBC
84	DH	1001	CYC	C2B-C3B-CAB-CBB
87	LN	204	CLA	C4C-C3C-CAC-CBC
87	cL	505	CLA	C8-C10-C11-C12
92	D6	407	LMG	C4-C5-C6-O5
88	m6	102	LHG	C11-C12-C13-C14
87	BN	801	CLA	C4-C3-C5-C6
87	A2	835	CLA	C4-C3-C5-C6
87	B2	825	CLA	C4-C3-C5-C6
82	YA	301	PEB	NC-C4C-CHC-C1D
82	NF	202	PEB	NC-C4C-CHC-C1D
82	NK	202	PEB	NC-C4C-CHC-C1D
82	AO	305	PEB	NC-C4C-CHC-C1D
82	A4	305	PEB	NC-C4C-CHC-C1D
82	Y7	301	PEB	NC-C4C-CHC-C1D
82	fF	202	PEB	NC-C4C-CHC-C1D
82	fK	202	PEB	NC-C4C-CHC-C1D
88	mL	102	LHG	O8-C23-C24-C25
92	yL	101	LMG	C38-C39-C40-C41
92	k6	101	LMG	O10-C28-O8-C9
87	CL	515	CLA	C15-C16-C17-C18
88	AL	406	LHG	C7-C8-C9-C10
88	m6	102	LHG	C7-C8-C9-C10
87	BL	619	CLA	C16-C17-C18-C19
87	C6	509	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
87	c6	608	CLA	C16-C17-C18-C19
88	d6	407	LHG	C31-C32-C33-C34
92	AL	411	LMG	C12-C13-C14-C15
92	bL	623	LMG	C31-C32-C33-C34
82	WM	202	PEB	C3C-C2C-CAC-CBC
87	DL	406	CLA	C8-C10-C11-C12
87	KN	105	CLA	C1-C2-C3-C4
87	K2	106	CLA	C1-C2-C3-C4
88	i6	101	LHG	C28-C29-C30-C31
87	22	605	CLA	C3-C5-C6-C7
87	2N	301	CLA	C3-C5-C6-C7
84	J4	1001	CYC	C2B-C3B-CAB-CBB
92	CL	519	LMG	C9-C8-O7-C10
92	DL	402	LMG	C9-C8-O7-C10
92	b6	623	LMG	C7-C8-O7-C10
92	k6	101	LMG	C9-C8-O7-C10
92	dL	407	LMG	C9-C8-O7-C10
87	CL	512	CLA	C2A-CAA-CBA-CGA
87	BN	834	CLA	C2A-CAA-CBA-CGA
87	12	607	CLA	C2A-CAA-CBA-CGA
87	12	610	CLA	C2A-CAA-CBA-CGA
87	B2	834	CLA	C2A-CAA-CBA-CGA
87	c6	613	CLA	C2A-CAA-CBA-CGA
87	1N	607	CLA	C2A-CAA-CBA-CGA
87	1N	610	CLA	C2A-CAA-CBA-CGA
87	AL	404	CLA	C2-C1-O2A-CGA
87	CL	508	CLA	C2-C1-O2A-CGA
87	HL	102	CLA	C2-C1-O2A-CGA
87	BN	806	CLA	C2-C1-O2A-CGA
87	LN	202	CLA	C2-C1-O2A-CGA
87	L2	202	CLA	C2-C1-O2A-CGA
87	B6	609	CLA	C2-C1-O2A-CGA
87	c6	607	CLA	C2-C1-O2A-CGA
87	cL	510	CLA	C2-C1-O2A-CGA
91	AL	410	PHO	C2-C1-O2A-CGA
87	b6	605	CLA	C4C-C3C-CAC-CBC
95	h6	101	DGD	CBB-CCB-CDB-CEB
87	AN	849	CLA	O1A-CGA-O2A-C1
87	b6	618	CLA	O1A-CGA-O2A-C1
87	bL	618	CLA	O1A-CGA-O2A-C1
87	c6	612	CLA	C3-C5-C6-C7
94	D6	408	PL9	C2-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
92	bL	610	LMG	C13-C14-C15-C16
82	GB	203	PEB	C4D-C3D-CAD-CBD
82	HD	201	PEB	C4D-C3D-CAD-CBD
82	JD	201	PEB	C4D-C3D-CAD-CBD
82	XD	202	PEB	C4D-C3D-CAD-CBD
82	YD	201	PEB	C4D-C3D-CAD-CBD
82	KJ	202	PEB	C4D-C3D-CAD-CBD
82	HQ	201	PEB	C4D-C3D-CAD-CBD
82	JQ	201	PEB	C4D-C3D-CAD-CBD
82	XQ	202	PEB	C4D-C3D-CAD-CBD
82	YQ	201	PEB	C4D-C3D-CAD-CBD
82	O5	203	PEB	C4D-C3D-CAD-CBD
82	aJ	201	PEB	C4D-C3D-CAD-CBD
88	ML	102	LHG	C2-C3-O3-P
87	C6	513	CLA	C2C-C3C-CAC-CBC
87	AN	849	CLA	CBA-CGA-O2A-C1
87	A2	849	CLA	CBA-CGA-O2A-C1
87	HL	101	CLA	O1A-CGA-O2A-C1
87	A2	849	CLA	O1A-CGA-O2A-C1
88	dL	405	LHG	O10-C23-O8-C6
95	AL	414	DGD	C2B-C3B-C4B-C5B
87	AN	808	CLA	C16-C17-C18-C19
87	A2	808	CLA	C16-C17-C18-C19
82	DD	202	PEB	NC-C1C-CHB-C4B
82	VD	203	PEB	NC-C1C-CHB-C4B
82	WM	202	PEB	NC-C1C-CHB-C4B
82	j4	202	PEB	NC-C1C-CHB-C4B
82	mH	201	PEB	NC-C1C-CHB-C4B
82	hJ	203	PEB	NC-C1C-CHB-C4B
82	mJ	201	PEB	NC-C1C-CHB-C4B
82	xK	304	PEB	NC-C1C-CHB-C4B
82	jO	202	PEB	NC-C1C-CHB-C4B
87	CL	504	CLA	C13-C15-C16-C17
87	AN	835	CLA	C4-C3-C5-C6
95	B2	844	DGD	C6B-C7B-C8B-C9B
87	B6	609	CLA	O1D-CGD-O2D-CED
85	FN	202	BCR	C23-C24-C25-C30
85	KN	101	BCR	C5-C6-C7-C8
85	F2	203	BCR	C23-C24-C25-C30
85	K2	102	BCR	C5-C6-C7-C8
85	F6	101	BCR	C1-C6-C7-C8
85	a6	605	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
85	a6	605	BCR	C23-C24-C25-C30
85	d6	405	BCR	C1-C6-C7-C8
85	d6	405	BCR	C23-C24-C25-C30
85	aL	604	BCR	C1-C6-C7-C8
85	aL	604	BCR	C5-C6-C7-C8
87	C6	514	CLA	C3-C5-C6-C7
87	AN	829	CLA	C2-C3-C5-C6
87	A2	829	CLA	C2-C3-C5-C6
88	B6	617	LHG	C9-C10-C11-C12
95	BN	844	DGD	C6B-C7B-C8B-C9B
84	JO	1001	CYC	C2B-C3B-CAB-CBB
92	bL	624	LMG	C28-C29-C30-C31
87	b6	618	CLA	CBA-CGA-O2A-C1
87	BN	807	CLA	CAA-CBA-CGA-O2A
87	B2	806	CLA	CAA-CBA-CGA-O2A
95	hL	101	DGD	C4B-C5B-C6B-C7B
87	AN	839	CLA	C13-C15-C16-C17
87	BN	827	CLA	O1A-CGA-O2A-C1
82	YB	202	PEB	C2C-CAC-CBC-CGC
82	QD	201	PEB	C2C-CAC-CBC-CGC
82	PM	201	PEB	C3B-CAB-CBB-CGB
82	RO	201	PEB	C2C-CAC-CBC-CGC
82	MP	203	PEB	C2C-CAC-CBC-CGC
82	QQ	201	PEB	C2C-CAC-CBC-CGC
82	Y1	202	PEB	C2C-CAC-CBC-CGC
82	R4	201	PEB	C2C-CAC-CBC-CGC
82	H5	201	PEB	C3B-CAB-CBB-CGB
82	r8	201	PEB	C3B-CAB-CBB-CGB
82	rC	201	PEB	C3B-CAB-CBB-CGB
82	rF	201	PEB	C3B-CAB-CBB-CGB
100	J2	104	3XQ	O20-C21-C22-O23
87	A6	402	CLA	C16-C17-C18-C20
87	c6	612	CLA	C16-C17-C18-C20
87	d6	406	CLA	C16-C17-C18-C20
95	L6	102	DGD	C2B-C1B-O2G-C2G
95	C6	521	DGD	C4A-C5A-C6A-C7A
87	DL	406	CLA	C10-C11-C12-C13
87	BN	806	CLA	C15-C16-C17-C18
87	A2	839	CLA	C13-C15-C16-C17
87	B2	805	CLA	C15-C16-C17-C18
87	82	302	CLA	C2A-CAA-CBA-CGA
87	D6	403	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
87	8N	303	CLA	C2A-CAA-CBA-CGA
92	x6	601	LMG	C2-C1-O1-C7
95	C6	521	DGD	C2D-C1D-O3G-C3G
87	B2	827	CLA	O1A-CGA-O2A-C1
92	qL	301	LMG	O7-C8-C9-O8
92	yL	101	LMG	O1-C7-C8-O7
95	h6	101	DGD	CDB-CEB-CFB-CGB
95	lL	101	DGD	C3A-C4A-C5A-C6A
88	AL	406	LHG	C4-O6-P-O3
88	B6	617	LHG	C3-O3-P-O6
88	I6	101	LHG	C4-O6-P-O3
88	m6	102	LHG	C3-O3-P-O6
88	iL	101	LHG	C4-O6-P-O3
88	D6	401	LHG	C23-C24-C25-C26
95	L6	102	DGD	C7A-C8A-C9A-CAA
82	VF	202	PEB	C2C-C1C-CHB-C4B
82	TJ	202	PEB	C2C-C1C-CHB-C4B
82	VK	202	PEB	C2C-C1C-CHB-C4B
82	DM	201	PEB	C2C-C1C-CHB-C4B
87	DL	403	CLA	C15-C16-C17-C18
87	A2	808	CLA	C15-C16-C17-C18
88	D6	401	LHG	C24-C25-C26-C27
87	DL	406	CLA	C16-C17-C18-C19
91	AL	410	PHO	CHA-CBD-CGD-O1D
91	AL	410	PHO	CHA-CBD-CGD-O2D
91	DL	405	PHO	CHA-CBD-CGD-O1D
91	a6	613	PHO	CHA-CBD-CGD-O2D
91	aL	610	PHO	CHA-CBD-CGD-O1D
87	c6	605	CLA	C2C-C3C-CAC-CBC
87	AN	808	CLA	C15-C16-C17-C18
87	bL	607	CLA	CBA-CGA-O2A-C1
95	C6	504	DGD	C1G-C2G-C3G-O3G
87	IN	103	CLA	C5-C6-C7-C8
87	I2	103	CLA	C5-C6-C7-C8
87	cL	513	CLA	C15-C16-C17-C18
87	BL	601	CLA	C11-C10-C8-C7
87	CL	507	CLA	C11-C12-C13-C15
87	CL	511	CLA	C12-C13-C15-C16
87	AN	840	CLA	C2-C3-C5-C6
87	BN	831	CLA	C11-C10-C8-C7
87	A2	840	CLA	C2-C3-C5-C6
87	B2	831	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
87	B6	615	CLA	C12-C13-C15-C16
87	C6	510	CLA	C11-C12-C13-C15
87	b6	615	CLA	C2-C3-C5-C6
87	c6	609	CLA	C11-C10-C8-C7
87	d6	401	CLA	C11-C12-C13-C15
87	bL	607	CLA	C11-C12-C13-C15
83	BJ	302	PUB	C4D-C3D-CAD-CBD
83	BM	302	PUB	C4D-C3D-CAD-CBD
84	NO	1001	CYC	C4B-C3B-CAB-CBB
92	m6	103	LMG	C17-C18-C19-C20
82	ZF	201	PEB	C2B-C3B-CAB-CBB
82	ZK	201	PEB	C2B-C3B-CAB-CBB
82	S5	201	PEB	C2B-C3B-CAB-CBB
82	RH	202	PEB	NC-C1C-CHB-C4B
82	DQ	202	PEB	NC-C1C-CHB-C4B
82	VQ	203	PEB	NC-C1C-CHB-C4B
82	R1	202	PEB	NC-C1C-CHB-C4B
82	m1	201	PEB	NC-C1C-CHB-C4B
82	mM	201	PEB	NC-C1C-CHB-C4B
82	dD	401	PEB	C3C-C2C-CAC-CBC
82	aM	203	PEB	C3C-C2C-CAC-CBC
82	jM	202	PEB	C3C-C2C-CAC-CBC
87	AL	403	CLA	C11-C12-C13-C14
87	AN	835	CLA	C11-C12-C13-C14
87	BN	811	CLA	C6-C7-C8-C9
87	BN	832	CLA	C14-C13-C15-C16
87	62	303	CLA	C14-C13-C15-C16
87	A2	835	CLA	C11-C12-C13-C14
87	B2	832	CLA	C14-C13-C15-C16
87	B6	603	CLA	C11-C12-C13-C14
87	B6	610	CLA	C6-C7-C8-C9
87	b6	612	CLA	C6-C7-C8-C9
87	b6	612	CLA	C11-C12-C13-C14
87	c6	611	CLA	C14-C13-C15-C16
87	bL	618	CLA	C11-C10-C8-C9
87	cL	509	CLA	C11-C12-C13-C14
87	6N	602	CLA	C14-C13-C15-C16
91	AL	410	PHO	C11-C10-C8-C9
91	A6	407	PHO	C11-C10-C8-C9
91	aL	610	PHO	C11-C12-C13-C14
85	AN	845	BCR	C13-C14-C15-C16
85	AN	846	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
85	JN	102	BCR	C9-C10-C11-C12
85	A2	845	BCR	C13-C14-C15-C16
85	A2	846	BCR	C15-C16-C17-C18
85	J2	102	BCR	C9-C10-C11-C12
85	H6	101	BCR	C9-C10-C11-C12
87	A2	810	CLA	C16-C17-C18-C20
87	H6	103	CLA	C16-C17-C18-C19
82	dD	401	PEB	C1C-C2C-CAC-CBC
82	dQ	401	PEB	C1C-C2C-CAC-CBC
87	aL	606	CLA	C2C-C3C-CAC-CBC
95	cL	502	DGD	O1B-C1B-O2G-C2G
88	bL	612	LHG	C7-C8-C9-C10
95	JL	101	DGD	C6A-C7A-C8A-C9A
87	a6	609	CLA	CBA-CGA-O2A-C1
87	BN	835	CLA	C8-C10-C11-C12
87	LN	203	CLA	C10-C11-C12-C13
87	B2	835	CLA	C8-C10-C11-C12
87	L2	203	CLA	C10-C11-C12-C13
87	CL	510	CLA	O1A-CGA-O2A-C1
87	b6	611	CLA	C4C-C3C-CAC-CBC
92	B6	622	LMG	C29-C30-C31-C32
95	J6	101	DGD	CAA-CBA-CCA-CDA
92	D6	409	LMG	C4-C5-C6-O5
92	yL	101	LMG	O10-C28-C29-C30
87	b6	618	CLA	C2A-CAA-CBA-CGA
87	4N	603	CLA	C2A-CAA-CBA-CGA
87	CL	511	CLA	C8-C10-C11-C12
91	AL	410	PHO	C3-C5-C6-C7
82	IB	202	PEB	CAC-CBC-CGC-O1C
82	YF	203	PEB	CAC-CBC-CGC-O1C
82	f1	201	PEB	CAC-CBC-CGC-O1C
82	fH	201	PEB	CAC-CBC-CGC-O1C
88	ML	102	LHG	C13-C14-C15-C16
87	BN	832	CLA	C15-C16-C17-C18
87	CL	513	CLA	C11-C12-C13-C14
87	AN	810	CLA	C16-C17-C18-C20
82	y8	201	PEB	NA-C4A-CHA-C1B
82	yC	201	PEB	NA-C4A-CHA-C1B
88	M6	101	LHG	O1-C1-C2-C3
88	ML	102	LHG	C5-C4-O6-P
88	AN	844	LHG	C2-C3-O3-P
88	A2	844	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
88	dL	408	LHG	C2-C3-O3-P
88	mL	102	LHG	C2-C3-O3-P
82	AK	202	PEB	CAB-CBB-CGB-O1B
82	YK	203	PEB	CAC-CBC-CGC-O1C
82	BQ	201	PEB	CAB-CBB-CGB-O1B
82	v8	201	PEB	CAC-CBC-CGC-O1C
82	fB	301	PEB	CAB-CBB-CGB-O1B
82	hB	301	PEB	CAB-CBB-CGB-O1B
82	vC	201	PEB	CAC-CBC-CGC-O1C
87	82	304	CLA	CAA-CBA-CGA-O1A
87	8N	305	CLA	CAA-CBA-CGA-O1A
87	B2	832	CLA	C15-C16-C17-C18
85	BN	839	BCR	C7-C8-C9-C10
83	wK	304	PUB	C2D-C3D-CAD-CBD
82	OB	201	PEB	C2C-C1C-CHB-C4B
82	J7	203	PEB	C2C-C1C-CHB-C4B
87	b6	610	CLA	C13-C15-C16-C17
92	CL	519	LMG	C23-C24-C25-C26
87	AN	811	CLA	C4-C3-C5-C6
87	A2	811	CLA	C4-C3-C5-C6
82	RO	202	PEB	C2B-C3B-CAB-CBB
82	R4	202	PEB	C2B-C3B-CAB-CBB
82	oF	203	PEB	C2B-C3B-CAB-CBB
82	oK	203	PEB	C2B-C3B-CAB-CBB
82	XQ	203	PEB	CAB-CBB-CGB-O1B
84	DE	1001	CYC	CAA-CBA-CGA-O1A
95	BL	614	DGD	O1G-C1A-C2A-C3A
87	B6	605	CLA	C2-C3-C5-C6
87	cL	505	CLA	C2-C3-C5-C6
87	C6	513	CLA	C4C-C3C-CAC-CBC
87	BL	609	CLA	C16-C17-C18-C20
87	b6	617	CLA	CBA-CGA-O2A-C1
88	C6	522	LHG	C24-C23-O8-C6
82	HA	203	PEB	C2D-C3D-CAD-CBD
82	XA	202	PEB	C2D-C3D-CAD-CBD
82	O5	203	PEB	C2D-C3D-CAD-CBD
82	H7	203	PEB	C2D-C3D-CAD-CBD
82	X7	202	PEB	C2D-C3D-CAD-CBD
82	aJ	201	PEB	C2D-C3D-CAD-CBD
87	b6	613	CLA	C3-C5-C6-C7
82	TA	203	PEB	C2C-CAC-CBC-CGC
82	XA	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	YA	304	PEB	C2C-CAC-CBC-CGC
82	UB	301	PEB	C2C-CAC-CBC-CGC
82	BD	203	PEB	C3B-CAB-CBB-CGB
82	SD	201	PEB	C3B-CAB-CBB-CGB
82	GE	1002	PEB	C2C-CAC-CBC-CGC
82	NF	201	PEB	C3B-CAB-CBB-CGB
82	GG	1002	PEB	C2C-CAC-CBC-CGC
82	JI	202	PEB	C2C-CAC-CBC-CGC
82	QJ	203	PEB	C2C-CAC-CBC-CGC
82	NK	201	PEB	C3B-CAB-CBB-CGB
82	HM	202	PEB	C2C-CAC-CBC-CGC
82	OM	201	PEB	C3B-CAB-CBB-CGB
82	QP	203	PEB	C2C-CAC-CBC-CGC
82	BQ	203	PEB	C3B-CAB-CBB-CGB
82	SQ	201	PEB	C3B-CAB-CBB-CGB
82	e1	202	PEB	C2C-CAC-CBC-CGC
82	i4	203	PEB	C2C-CAC-CBC-CGC
82	m4	202	PEB	C2C-CAC-CBC-CGC
82	T7	203	PEB	C2C-CAC-CBC-CGC
82	X7	201	PEB	C2C-CAC-CBC-CGC
82	Y7	304	PEB	C2C-CAC-CBC-CGC
82	z8	201	PEB	C3B-CAB-CBB-CGB
82	eB	201	PEB	C2C-CAC-CBC-CGC
82	zC	201	PEB	C3B-CAB-CBB-CGB
82	dD	401	PEB	C2C-CAC-CBC-CGC
82	aE	202	PEB	C2C-CAC-CBC-CGC
82	dE	204	PEB	C3B-CAB-CBB-CGB
82	aF	203	PEB	C3B-CAB-CBB-CGB
82	aG	202	PEB	C2C-CAC-CBC-CGC
82	dG	204	PEB	C3B-CAB-CBB-CGB
82	eG	202	PEB	C3B-CAB-CBB-CGB
82	eH	202	PEB	C2C-CAC-CBC-CGC
82	kJ	201	PEB	C3B-CAB-CBB-CGB
82	aK	203	PEB	C3B-CAB-CBB-CGB
82	rK	201	PEB	C3B-CAB-CBB-CGB
82	iO	203	PEB	C2C-CAC-CBC-CGC
82	mO	202	PEB	C2C-CAC-CBC-CGC
82	dQ	401	PEB	C2C-CAC-CBC-CGC
83	YA	302	PUB	C2C-CAC-CBC-CGC
83	Y7	302	PUB	C2C-CAC-CBC-CGC
82	AA	201	PEB	CAC-CBC-CGC-O2C
82	EA	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	MA	201	PEB	CAC-CBC-CGC-O2C
82	GB	203	PEB	CAC-CBC-CGC-O2C
82	NB	202	PEB	CAB-CBB-CGB-O1B
82	ZB	201	PEB	CAB-CBB-CGB-O2B
82	JD	202	PEB	CAB-CBB-CGB-O2B
82	KD	201	PEB	CAC-CBC-CGC-O2C
82	XD	203	PEB	CAB-CBB-CGB-O1B
82	QE	201	PEB	CAC-CBC-CGC-O2C
82	KF	203	PEB	CAC-CBC-CGC-O2C
82	QG	201	PEB	CAC-CBC-CGC-O2C
82	QG	203	PEB	CAB-CBB-CGB-O2B
82	FH	1002	PEB	CAC-CBC-CGC-O2C
82	VH	202	PEB	CAB-CBB-CGB-O2B
82	AI	203	PEB	CAC-CBC-CGC-O2C
82	WI	201	PEB	CAC-CBC-CGC-O2C
82	AJ	301	PEB	CAB-CBB-CGB-O2B
82	AJ	302	PEB	CAC-CBC-CGC-O2C
82	IJ	203	PEB	CAC-CBC-CGC-O2C
82	WJ	202	PEB	CAC-CBC-CGC-O2C
82	KK	203	PEB	CAC-CBC-CGC-O2C
82	JM	202	PEB	CAC-CBC-CGC-O2C
82	RM	202	PEB	CAC-CBC-CGC-O2C
82	SM	201	PEB	CAC-CBC-CGC-O2C
82	WM	201	PEB	CAC-CBC-CGC-O2C
82	PO	202	PEB	CAB-CBB-CGB-O1B
82	GP	201	PEB	CAB-CBB-CGB-O2B
82	QP	202	PEB	CAB-CBB-CGB-O2B
82	EQ	202	PEB	CAB-CBB-CGB-O2B
82	KQ	201	PEB	CAC-CBC-CGC-O2C
82	F1	1002	PEB	CAC-CBC-CGC-O2C
82	V1	202	PEB	CAC-CBC-CGC-O2C
82	h1	202	PEB	CAC-CBC-CGC-O2C
82	P4	202	PEB	CAB-CBB-CGB-O1B
82	m4	201	PEB	CAC-CBC-CGC-O1C
82	a4	202	PEB	CAB-CBB-CGB-O1B
82	b4	201	PEB	CAB-CBB-CGB-O1B
82	b4	202	PEB	CAC-CBC-CGC-O2C
82	A7	201	PEB	CAC-CBC-CGC-O2C
82	M7	201	PEB	CAC-CBC-CGC-O2C
82	H9	201	PEB	CAC-CBC-CGC-O2C
82	U9	201	PEB	CAC-CBC-CGC-O2C
82	U9	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	eB	202	PEB	CAB-CBB-CGB-O1B
82	gE	201	PEB	CAC-CBC-CGC-O2C
82	kE	202	PEB	CAB-CBB-CGB-O1B
82	jF	202	PEB	CAB-CBB-CGB-O2B
82	kF	203	PEB	CAC-CBC-CGC-O1C
82	qF	201	PEB	CAC-CBC-CGC-O2C
82	rF	201	PEB	CAB-CBB-CGB-O2B
82	gG	201	PEB	CAC-CBC-CGC-O2C
82	kG	202	PEB	CAB-CBB-CGB-O1B
82	hH	201	PEB	CAC-CBC-CGC-O2C
82	aJ	202	PEB	CAC-CBC-CGC-O2C
82	cJ	202	PEB	CAC-CBC-CGC-O2C
82	eJ	202	PEB	CAC-CBC-CGC-O2C
82	jJ	203	PEB	CAC-CBC-CGC-O2C
82	lJ	203	PEB	CAB-CBB-CGB-O2B
82	jK	202	PEB	CAB-CBB-CGB-O2B
82	kK	203	PEB	CAC-CBC-CGC-O1C
82	qK	201	PEB	CAC-CBC-CGC-O2C
82	rK	201	PEB	CAB-CBB-CGB-O2B
82	vK	202	PEB	CAB-CBB-CGB-O2B
82	fM	201	PEB	CAC-CBC-CGC-O2C
82	mO	201	PEB	CAC-CBC-CGC-O1C
82	aO	202	PEB	CAB-CBB-CGB-O1B
82	aO	203	PEB	CAC-CBC-CGC-O1C
82	bO	202	PEB	CAC-CBC-CGC-O2C
83	AH	304	PUB	CAB-CBB-CGB-O2B
83	BJ	302	PUB	CAB-CBB-CGB-O2B
83	A1	304	PUB	CAB-CBB-CGB-O2B
84	DE	1001	CYC	CAD-CBD-CGD-O1D
84	DG	1001	CYC	CAA-CBA-CGA-O1A
84	DG	1001	CYC	CAD-CBD-CGD-O1D
84	L1	1001	CYC	CAD-CBD-CGD-O1D
84	63	901	CYC	CAD-CBD-CGD-O1D
84	73	1002	CYC	CAD-CBD-CGD-O1D
84	K4	1001	CYC	CAA-CBA-CGA-O2A
82	DA	201	PEB	C4B-C3B-CAB-CBB
82	D7	201	PEB	C4B-C3B-CAB-CBB
82	hM	202	PEB	C4B-C3B-CAB-CBB
83	wF	304	PUB	C2D-C3D-CAD-CBD
88	AL	406	LHG	C12-C13-C14-C15
92	C6	501	LMG	C32-C33-C34-C35
87	LN	203	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
87	L2	203	CLA	C13-C15-C16-C17
87	b6	617	CLA	C13-C15-C16-C17
95	CL	523	DGD	O6D-C5D-C6D-O5D
95	cL	520	DGD	O6D-C5D-C6D-O5D
87	a6	609	CLA	O1A-CGA-O2A-C1
87	bL	607	CLA	O1A-CGA-O2A-C1
87	BL	621	CLA	CBA-CGA-O2A-C1
92	m6	101	LMG	C10-C11-C12-C13
95	BN	844	DGD	C5B-C6B-C7B-C8B
95	B2	844	DGD	C5B-C6B-C7B-C8B
87	BL	602	CLA	C4B-C3B-CAB-CBB
87	CL	512	CLA	C4B-C3B-CAB-CBB
87	AN	820	CLA	C4B-C3B-CAB-CBB
87	AN	835	CLA	C4B-C3B-CAB-CBB
87	BN	809	CLA	C4B-C3B-CAB-CBB
87	22	609	CLA	C4B-C3B-CAB-CBB
87	52	602	CLA	C4B-C3B-CAB-CBB
87	A2	820	CLA	C4B-C3B-CAB-CBB
87	A2	835	CLA	C4B-C3B-CAB-CBB
87	B2	808	CLA	C4B-C3B-CAB-CBB
87	c6	605	CLA	C4B-C3B-CAB-CBB
87	bL	614	CLA	C4B-C3B-CAB-CBB
87	bL	615	CLA	C4B-C3B-CAB-CBB
87	cL	515	CLA	C4B-C3B-CAB-CBB
87	2N	309	CLA	C4B-C3B-CAB-CBB
87	5N	602	CLA	C4B-C3B-CAB-CBB
87	BL	605	CLA	C2A-CAA-CBA-CGA
87	42	603	CLA	C2A-CAA-CBA-CGA
87	52	602	CLA	C2A-CAA-CBA-CGA
87	5N	602	CLA	C2A-CAA-CBA-CGA
82	BA	202	PEB	CAB-CBB-CGB-O2B
82	HA	203	PEB	CAB-CBB-CGB-O2B
82	OA	202	PEB	CAC-CBC-CGC-O1C
82	KB	304	PEB	CAC-CBC-CGC-O1C
82	KB	304	PEB	CAB-CBB-CGB-O1B
82	QB	204	PEB	CAB-CBB-CGB-O2B
82	YB	202	PEB	CAB-CBB-CGB-O1B
82	ZB	203	PEB	CAC-CBC-CGC-O2C
82	BD	201	PEB	CAB-CBB-CGB-O1B
82	ED	202	PEB	CAB-CBB-CGB-O2B
82	PD	202	PEB	CAB-CBB-CGB-O2B
82	RD	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	TD	203	PEB	CAB-CBB-CGB-O2B
82	WD	202	PEB	CAC-CBC-CGC-O1C
82	QE	203	PEB	CAB-CBB-CGB-O2B
82	AF	202	PEB	CAB-CBB-CGB-O1B
82	CF	203	PEB	CAB-CBB-CGB-O2B
82	JF	202	PEB	CAB-CBB-CGB-O2B
82	SF	202	PEB	CAC-CBC-CGC-O2C
82	AH	302	PEB	CAB-CBB-CGB-O2B
82	SH	203	PEB	CAC-CBC-CGC-O2C
82	ZH	203	PEB	CAC-CBC-CGC-O2C
82	YJ	203	PEB	CAB-CBB-CGB-O2B
82	JK	202	PEB	CAB-CBB-CGB-O2B
82	EM	201	PEB	CAC-CBC-CGC-O2C
82	MM	202	PEB	CAC-CBC-CGC-O2C
82	MM	203	PEB	CAB-CBB-CGB-O2B
82	VM	202	PEB	CAC-CBC-CGC-O2C
82	AO	305	PEB	CAB-CBB-CGB-O2B
82	PO	202	PEB	CAC-CBC-CGC-O1C
82	AP	203	PEB	CAC-CBC-CGC-O1C
82	JQ	202	PEB	CAB-CBB-CGB-O2B
82	PQ	202	PEB	CAB-CBB-CGB-O2B
82	TQ	203	PEB	CAB-CBB-CGB-O2B
82	WQ	202	PEB	CAC-CBC-CGC-O1C
82	A1	302	PEB	CAB-CBB-CGB-O2B
82	V1	203	PEB	CAB-CBB-CGB-O2B
82	Z1	203	PEB	CAC-CBC-CGC-O2C
82	c1	201	PEB	CAC-CBC-CGC-O2C
82	O4	201	PEB	CAB-CBB-CGB-O1B
82	P4	202	PEB	CAC-CBC-CGC-O1C
82	l4	202	PEB	CAC-CBC-CGC-O2C
82	a4	203	PEB	CAC-CBC-CGC-O1C
82	S5	203	PEB	CAB-CBB-CGB-O2B
82	B7	202	PEB	CAB-CBB-CGB-O2B
82	E7	202	PEB	CAB-CBB-CGB-O2B
82	H7	203	PEB	CAB-CBB-CGB-O2B
82	O7	202	PEB	CAC-CBC-CGC-O1C
82	vC	201	PEB	CAB-CBB-CGB-O2B
82	vF	202	PEB	CAB-CBB-CGB-O2B
82	gH	201	PEB	CAB-CBB-CGB-O1B
82	kJ	202	PEB	CAC-CBC-CGC-O1C
82	lO	202	PEB	CAC-CBC-CGC-O2C
82	bO	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
84	LH	1002	CYC	CAD-CBD-CGD-O1D
84	KO	1001	CYC	CAA-CBA-CGA-O2A
84	NO	1001	CYC	CAD-CBD-CGD-O1D
84	N4	1001	CYC	CAD-CBD-CGD-O1D
85	CL	501	BCR	C9-C10-C11-C12
85	AN	848	BCR	C19-C20-C21-C22
85	A2	848	BCR	C19-C20-C21-C22
85	cL	503	BCR	C19-C20-C21-C22
95	L6	102	DGD	O1B-C1B-O2G-C2G
87	b6	617	CLA	C3-C5-C6-C7
94	AL	413	PL9	C44-C46-C47-C48
94	a6	601	PL9	C24-C26-C27-C28
88	BL	615	LHG	C18-C19-C20-C21
88	D6	401	LHG	C11-C12-C13-C14
82	HB	201	PEB	NC-C4C-CHC-C1D
82	JB	202	PEB	NC-C4C-CHC-C1D
82	TB	202	PEB	NC-C4C-CHC-C1D
82	TF	202	PEB	NC-C4C-CHC-C1D
82	YF	203	PEB	NC-C4C-CHC-C1D
82	TK	202	PEB	NC-C4C-CHC-C1D
82	YK	203	PEB	NC-C4C-CHC-C1D
82	EM	203	PEB	NC-C4C-CHC-C1D
82	AP	203	PEB	NC-C4C-CHC-C1D
83	AD	302	PUB	NB-C1B-CHA-C4A
83	AE	303	PUB	NB-C1B-CHA-C4A
83	AG	303	PUB	NB-C1B-CHA-C4A
83	AQ	302	PUB	NB-C1B-CHA-C4A
87	AN	851	CLA	C13-C15-C16-C17
87	dL	401	CLA	C13-C15-C16-C17
88	BL	610	LHG	C25-C26-C27-C28
92	dL	407	LMG	C13-C14-C15-C16
92	dL	407	LMG	C17-C18-C19-C20
82	OA	201	PEB	CAC-CBC-CGC-O2C
82	TA	201	PEB	CAC-CBC-CGC-O1C
82	UA	201	PEB	CAC-CBC-CGC-O2C
82	DB	203	PEB	CAC-CBC-CGC-O2C
82	XB	202	PEB	CAB-CBB-CGB-O2B
82	BD	202	PEB	CAB-CBB-CGB-O2B
82	DD	203	PEB	CAB-CBB-CGB-O1B
82	PD	202	PEB	CAC-CBC-CGC-O2C
82	YD	201	PEB	CAC-CBC-CGC-O2C
82	DE	1002	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	CF	202	PEB	CAC-CBC-CGC-O2C
82	SG	201	PEB	CAB-CBB-CGB-O2B
82	OH	201	PEB	CAC-CBC-CGC-O2C
82	IJ	202	PEB	CAC-CBC-CGC-O2C
82	CK	203	PEB	CAB-CBB-CGB-O2B
82	CM	201	PEB	CAC-CBC-CGC-O2C
82	MM	201	PEB	CAC-CBC-CGC-O2C
82	UM	202	PEB	CAC-CBC-CGC-O2C
82	OO	201	PEB	CAB-CBB-CGB-O1B
82	DP	202	PEB	CAB-CBB-CGB-O2B
82	EP	203	PEB	CAC-CBC-CGC-O1C
82	KP	202	PEB	CAC-CBC-CGC-O2C
82	YP	502	PEB	CAB-CBB-CGB-O1B
82	BQ	202	PEB	CAB-CBB-CGB-O2B
82	DQ	203	PEB	CAB-CBB-CGB-O1B
82	RQ	203	PEB	CAC-CBC-CGC-O2C
82	UQ	201	PEB	CAC-CBC-CGC-O2C
82	YQ	201	PEB	CAC-CBC-CGC-O2C
82	g1	201	PEB	CAB-CBB-CGB-O1B
82	c1	202	PEB	CAC-CBC-CGC-O2C
82	e4	201	PEB	CAC-CBC-CGC-O2C
82	Q5	203	PEB	CAB-CBB-CGB-O2B
82	Y5	203	PEB	CAB-CBB-CGB-O2B
82	T7	201	PEB	CAC-CBC-CGC-O1C
82	v8	201	PEB	CAB-CBB-CGB-O2B
82	cF	202	PEB	CAC-CBC-CGC-O2C
82	oF	203	PEB	CAB-CBB-CGB-O2B
82	zF	501	PEB	CAC-CBC-CGC-O2C
82	eG	201	PEB	CAB-CBB-CGB-O1B
82	lH	201	PEB	CAC-CBC-CGC-O2C
82	cH	202	PEB	CAC-CBC-CGC-O2C
82	iJ	202	PEB	CAC-CBC-CGC-O2C
82	oK	203	PEB	CAB-CBB-CGB-O2B
82	lM	203	PEB	CAC-CBC-CGC-O2C
82	eO	201	PEB	CAC-CBC-CGC-O2C
82	hO	201	PEB	CAC-CBC-CGC-O2C
83	AE	303	PUB	CAC-CBC-CGC-O1C
83	AE	303	PUB	CAB-CBB-CGB-O2B
83	AG	303	PUB	CAC-CBC-CGC-O1C
83	AG	303	PUB	CAB-CBB-CGB-O2B
88	AN	843	LHG	O6-C4-C5-O7
88	A2	843	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
88	BL	615	LHG	C10-C11-C12-C13
87	A2	851	CLA	C13-C15-C16-C17
87	BN	813	CLA	C16-C17-C18-C20
87	B2	812	CLA	C16-C17-C18-C20
87	b6	612	CLA	C16-C17-C18-C20
96	FL	102	HEM	C4C-C3C-CAC-CBC
87	BN	817	CLA	C3-C5-C6-C7
87	B2	816	CLA	C3-C5-C6-C7
91	aL	610	PHO	C3-C5-C6-C7
92	CL	519	LMG	C34-C35-C36-C37
87	BN	802	CLA	C4-C3-C5-C6
87	BN	819	CLA	C4-C3-C5-C6
87	B2	801	CLA	C4-C3-C5-C6
87	B2	818	CLA	C4-C3-C5-C6
87	C6	518	CLA	C4-C3-C5-C6
82	JA	202	PEB	CAC-CBC-CGC-O2C
82	QB	203	PEB	CAC-CBC-CGC-O1C
82	RB	202	PEB	CAB-CBB-CGB-O1B
82	BD	202	PEB	CAC-CBC-CGC-O2C
82	OD	201	PEB	CAC-CBC-CGC-O1C
82	UD	201	PEB	CAC-CBC-CGC-O2C
82	YD	202	PEB	CAC-CBC-CGC-O1C
82	YD	202	PEB	CAB-CBB-CGB-O1B
82	QE	202	PEB	CAC-CBC-CGC-O2C
82	RE	202	PEB	CAC-CBC-CGC-O2C
82	SE	201	PEB	CAB-CBB-CGB-O2B
82	EF	202	PEB	CAB-CBB-CGB-O1B
82	MF	202	PEB	CAC-CBC-CGC-O1C
82	DG	1002	PEB	CAC-CBC-CGC-O1C
82	QG	202	PEB	CAC-CBC-CGC-O2C
82	RG	202	PEB	CAC-CBC-CGC-O2C
82	VH	202	PEB	CAB-CBB-CGB-O1B
82	YH	202	PEB	CAB-CBB-CGB-O1B
82	GI	201	PEB	CAC-CBC-CGC-O1C
82	OI	201	PEB	CAC-CBC-CGC-O1C
82	CJ	202	PEB	CAC-CBC-CGC-O2C
82	CK	202	PEB	CAC-CBC-CGC-O2C
82	EK	202	PEB	CAB-CBB-CGB-O1B
82	SK	202	PEB	CAC-CBC-CGC-O2C
82	DM	202	PEB	CAC-CBC-CGC-O2C
82	GM	201	PEB	CAC-CBC-CGC-O1C
82	IM	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	OM	201	PEB	CAC-CBC-CGC-O1C
82	QM	203	PEB	CAC-CBC-CGC-O2C
82	TM	202	PEB	CAC-CBC-CGC-O2C
82	WO	201	PEB	CAC-CBC-CGC-O2C
82	BP	202	PEB	CAB-CBB-CGB-O2B
82	UP	201	PEB	CAC-CBC-CGC-O2C
82	UP	202	PEB	CAB-CBB-CGB-O1B
82	BQ	202	PEB	CAC-CBC-CGC-O2C
82	DQ	202	PEB	CAC-CBC-CGC-O2C
82	OQ	201	PEB	CAC-CBC-CGC-O1C
82	PQ	202	PEB	CAC-CBC-CGC-O2C
82	YQ	202	PEB	CAC-CBC-CGC-O1C
82	YQ	202	PEB	CAB-CBB-CGB-O1B
82	O1	201	PEB	CAC-CBC-CGC-O2C
82	V1	203	PEB	CAB-CBB-CGB-O1B
82	Y1	202	PEB	CAB-CBB-CGB-O1B
82	l1	201	PEB	CAB-CBB-CGB-O2B
82	A4	304	PEB	CAB-CBB-CGB-O1B
82	j4	201	PEB	CAC-CBC-CGC-O2C
82	m4	201	PEB	CAB-CBB-CGB-O2B
82	c4	201	PEB	CAC-CBC-CGC-O1C
82	h4	201	PEB	CAC-CBC-CGC-O2C
82	H5	203	PEB	CAB-CBB-CGB-O2B
82	L5	203	PEB	CAB-CBB-CGB-O2B
82	U5	203	PEB	CAB-CBB-CGB-O2B
82	K7	202	PEB	CAC-CBC-CGC-O2C
82	O7	201	PEB	CAC-CBC-CGC-O2C
82	U7	201	PEB	CAC-CBC-CGC-O2C
82	Y7	301	PEB	CAC-CBC-CGC-O2C
82	r8	202	PEB	CAB-CBB-CGB-O2B
82	x8	202	PEB	CAB-CBB-CGB-O2B
82	D9	201	PEB	CAB-CBB-CGB-O1B
82	J9	202	PEB	CAC-CBC-CGC-O2C
82	L9	201	PEB	CAC-CBC-CGC-O1C
82	rC	202	PEB	CAB-CBB-CGB-O2B
82	xC	202	PEB	CAB-CBB-CGB-O2B
82	eE	201	PEB	CAB-CBB-CGB-O1B
82	fE	203	PEB	CAC-CBC-CGC-O1C
82	iE	202	PEB	CAB-CBB-CGB-O1B
82	lF	202	PEB	CAC-CBC-CGC-O2C
82	oF	201	PEB	CAB-CBB-CGB-O1B
82	wF	301	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	iG	202	PEB	CAB-CBB-CGB-O1B
82	kH	203	PEB	CAB-CBB-CGB-O2B
82	cH	201	PEB	CAC-CBC-CGC-O2C
82	fJ	201	PEB	CAC-CBC-CGC-O1C
82	fJ	203	PEB	CAC-CBC-CGC-O2C
82	fJ	203	PEB	CAB-CBB-CGB-O1B
82	lJ	202	PEB	CAC-CBC-CGC-O2C
82	mJ	202	PEB	CAC-CBC-CGC-O1C
82	dK	201	PEB	CAC-CBC-CGC-O2C
82	jK	201	PEB	CAC-CBC-CGC-O2C
82	lK	202	PEB	CAC-CBC-CGC-O2C
82	zK	501	PEB	CAC-CBC-CGC-O2C
82	aM	201	PEB	CAC-CBC-CGC-O2C
82	jO	201	PEB	CAC-CBC-CGC-O2C
82	cO	201	PEB	CAC-CBC-CGC-O1C
83	AM	304	PUB	CAC-CBC-CGC-O1C
84	DH	1001	CYC	CAA-CBA-CGA-O1A
84	D1	1001	CYC	CAA-CBA-CGA-O1A
96	FL	102	HEM	CAA-CBA-CGA-O2A
87	C6	518	CLA	C2-C3-C5-C6
94	aL	601	PL9	C12-C11-C9-C8
87	b6	617	CLA	O1A-CGA-O2A-C1
87	c6	608	CLA	O1A-CGA-O2A-C1
82	CA	202	PEB	C1C-C2C-CAC-CBC
82	JA	203	PEB	C2C-C1C-CHB-C4B
82	C7	202	PEB	C1C-C2C-CAC-CBC
83	AD	302	PUB	C4B-C3B-CAB-CBB
83	AQ	302	PUB	C4B-C3B-CAB-CBB
95	cL	502	DGD	CDB-CEB-CFB-CGB
87	AN	835	CLA	C8-C10-C11-C12
87	BN	836	CLA	C15-C16-C17-C18
87	A2	835	CLA	C8-C10-C11-C12
87	B2	836	CLA	C15-C16-C17-C18
87	b6	607	CLA	C8-C10-C11-C12
82	dQ	401	PEB	C3C-C2C-CAC-CBC
82	GA	202	PEB	CAB-CBB-CGB-O2B
82	NA	203	PEB	CAB-CBB-CGB-O1B
82	SA	202	PEB	CAC-CBC-CGC-O1C
82	UA	202	PEB	CAC-CBC-CGC-O1C
82	YA	301	PEB	CAC-CBC-CGC-O2C
82	QB	201	PEB	CAB-CBB-CGB-O1B
82	QB	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	UB	303	PEB	CAC-CBC-CGC-O1C
82	ZB	202	PEB	CAB-CBB-CGB-O1B
82	DD	202	PEB	CAC-CBC-CGC-O2C
82	GD	202	PEB	CAC-CBC-CGC-O1C
82	QD	202	PEB	CAB-CBB-CGB-O1B
82	VD	201	PEB	CAB-CBB-CGB-O1B
82	AE	301	PEB	CAB-CBB-CGB-O1B
82	UE	203	PEB	CAC-CBC-CGC-O1C
82	WE	203	PEB	CAC-CBC-CGC-O1C
82	OF	203	PEB	CAC-CBC-CGC-O2C
82	SF	203	PEB	CAB-CBB-CGB-O1B
82	VF	202	PEB	CAB-CBB-CGB-O1B
82	WF	203	PEB	CAB-CBB-CGB-O1B
82	YF	202	PEB	CAB-CBB-CGB-O1B
82	AG	301	PEB	CAB-CBB-CGB-O1B
82	UG	203	PEB	CAC-CBC-CGC-O1C
82	WG	203	PEB	CAC-CBC-CGC-O1C
82	UH	201	PEB	CAC-CBC-CGC-O1C
82	JI	201	PEB	CAC-CBC-CGC-O1C
82	UI	201	PEB	CAC-CBC-CGC-O1C
82	VI	203	PEB	CAC-CBC-CGC-O2C
82	WI	202	PEB	CAC-CBC-CGC-O1C
82	EJ	201	PEB	CAC-CBC-CGC-O2C
82	FJ	202	PEB	CAC-CBC-CGC-O2C
82	GJ	201	PEB	CAC-CBC-CGC-O1C
82	HJ	202	PEB	CAC-CBC-CGC-O1C
82	KJ	202	PEB	CAC-CBC-CGC-O1C
82	QJ	203	PEB	CAC-CBC-CGC-O1C
82	YJ	202	PEB	CAC-CBC-CGC-O2C
82	MK	202	PEB	CAC-CBC-CGC-O1C
82	SK	203	PEB	CAB-CBB-CGB-O1B
82	VK	202	PEB	CAB-CBB-CGB-O1B
82	WK	203	PEB	CAB-CBB-CGB-O1B
82	YK	202	PEB	CAB-CBB-CGB-O1B
82	AM	301	PEB	CAC-CBC-CGC-O1C
82	CM	202	PEB	CAC-CBC-CGC-O1C
82	CM	202	PEB	CAB-CBB-CGB-O2B
82	QM	204	PEB	CAC-CBC-CGC-O1C
82	RM	202	PEB	CAC-CBC-CGC-O1C
82	SM	201	PEB	CAC-CBC-CGC-O1C
82	YM	201	PEB	CAC-CBC-CGC-O2C
82	ZM	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	AO	301	PEB	CAC-CBC-CGC-O1C
82	AO	304	PEB	CAB-CBB-CGB-O1B
82	AP	202	PEB	CAB-CBB-CGB-O2B
82	EP	201	PEB	CAC-CBC-CGC-O1C
82	IP	202	PEB	CAC-CBC-CGC-O1C
82	NP	202	PEB	CAB-CBB-CGB-O1B
82	OP	203	PEB	CAC-CBC-CGC-O2C
82	SP	203	PEB	CAB-CBB-CGB-O2B
82	WP	201	PEB	CAC-CBC-CGC-O1C
82	WP	202	PEB	CAC-CBC-CGC-O1C
82	DQ	203	PEB	CAC-CBC-CGC-O1C
82	GQ	202	PEB	CAC-CBC-CGC-O1C
82	JQ	203	PEB	CAC-CBC-CGC-O1C
82	OQ	202	PEB	CAC-CBC-CGC-O1C
82	QQ	202	PEB	CAB-CBB-CGB-O1B
82	XQ	203	PEB	CAC-CBC-CGC-O1C
82	YQ	202	PEB	CAB-CBB-CGB-O2B
82	Q1	202	PEB	CAC-CBC-CGC-O1C
82	U1	201	PEB	CAC-CBC-CGC-O1C
82	k1	202	PEB	CAB-CBB-CGB-O1B
82	l1	201	PEB	CAC-CBC-CGC-O1C
82	l1	202	PEB	CAC-CBC-CGC-O2C
82	A4	301	PEB	CAC-CBC-CGC-O1C
82	A4	305	PEB	CAB-CBB-CGB-O2B
82	W4	201	PEB	CAC-CBC-CGC-O2C
82	k4	202	PEB	CAC-CBC-CGC-O1C
82	a4	202	PEB	CAC-CBC-CGC-O1C
82	e4	203	PEB	CAC-CBC-CGC-O1C
82	f4	202	PEB	CAC-CBC-CGC-O1C
82	h4	202	PEB	CAC-CBC-CGC-O1C
82	H5	203	PEB	CAC-CBC-CGC-O1C
82	L5	201	PEB	CAC-CBC-CGC-O1C
82	M5	301	PEB	CAC-CBC-CGC-O1C
82	Z5	301	PEB	CAC-CBC-CGC-O1C
82	J7	202	PEB	CAC-CBC-CGC-O2C
82	N7	203	PEB	CAB-CBB-CGB-O1B
82	P7	201	PEB	CAC-CBC-CGC-O2C
82	Q7	201	PEB	CAC-CBC-CGC-O1C
82	S7	201	PEB	CAC-CBC-CGC-O2C
82	S7	202	PEB	CAC-CBC-CGC-O1C
82	W7	202	PEB	CAC-CBC-CGC-O1C
82	Y7	301	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	z8	201	PEB	CAC-CBC-CGC-O2C
82	p8	201	PEB	CAC-CBC-CGC-O1C
82	q8	202	PEB	CAB-CBB-CGB-O1B
82	r8	202	PEB	CAC-CBC-CGC-O1C
82	s8	203	PEB	CAB-CBB-CGB-O1B
82	x8	201	PEB	CAC-CBC-CGC-O1C
82	H9	201	PEB	CAB-CBB-CGB-O1B
82	zC	201	PEB	CAC-CBC-CGC-O2C
82	qC	202	PEB	CAB-CBB-CGB-O1B
82	rC	202	PEB	CAC-CBC-CGC-O1C
82	sC	203	PEB	CAB-CBB-CGB-O1B
82	xC	201	PEB	CAC-CBC-CGC-O1C
82	aE	202	PEB	CAB-CBB-CGB-O1B
82	cE	201	PEB	CAC-CBC-CGC-O1C
82	dE	201	PEB	CAC-CBC-CGC-O2C
82	eE	203	PEB	CAC-CBC-CGC-O1C
82	fE	202	PEB	CAC-CBC-CGC-O1C
82	hE	202	PEB	CAC-CBC-CGC-O1C
82	hE	202	PEB	CAB-CBB-CGB-O1B
82	jF	201	PEB	CAC-CBC-CGC-O2C
82	lF	201	PEB	CAC-CBC-CGC-O1C
82	yF	301	PEB	CAB-CBB-CGB-O1B
82	aG	202	PEB	CAB-CBB-CGB-O1B
82	cG	201	PEB	CAC-CBC-CGC-O1C
82	dG	201	PEB	CAC-CBC-CGC-O2C
82	eG	203	PEB	CAC-CBC-CGC-O1C
82	fG	201	PEB	CAC-CBC-CGC-O1C
82	fG	202	PEB	CAC-CBC-CGC-O1C
82	fG	203	PEB	CAC-CBC-CGC-O1C
82	hG	202	PEB	CAC-CBC-CGC-O1C
82	hG	202	PEB	CAB-CBB-CGB-O1B
82	lG	202	PEB	CAC-CBC-CGC-O1C
82	hH	202	PEB	CAC-CBC-CGC-O1C
82	kH	202	PEB	CAB-CBB-CGB-O1B
82	aJ	204	PEB	CAC-CBC-CGC-O1C
82	lK	201	PEB	CAC-CBC-CGC-O1C
82	oK	201	PEB	CAB-CBB-CGB-O1B
82	wK	301	PEB	CAC-CBC-CGC-O2C
82	yK	301	PEB	CAB-CBB-CGB-O1B
82	dM	201	PEB	CAC-CBC-CGC-O1C
82	dM	202	PEB	CAC-CBC-CGC-O1C
82	hM	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	mO	201	PEB	CAB-CBB-CGB-O2B
82	mO	203	PEB	CAC-CBC-CGC-O1C
82	eO	203	PEB	CAC-CBC-CGC-O1C
82	fO	202	PEB	CAC-CBC-CGC-O1C
82	hO	202	PEB	CAC-CBC-CGC-O1C
82	bP	501	PEB	CAC-CBC-CGC-O1C
82	Z9	301	PEB	CAB-CBB-CGB-O1B
82	M9	302	PEB	CAB-CBB-CGB-O1B
82	M9	304	PEB	CAC-CBC-CGC-O2C
83	AE	302	PUB	CAC-CBC-CGC-O1C
83	AG	302	PUB	CAC-CBC-CGC-O1C
83	yF	303	PUB	CAB-CBB-CGB-O1B
83	yK	303	PUB	CAB-CBB-CGB-O1B
83	Z9	305	PUB	CAC-CBC-CGC-O1C
84	CO	1001	CYC	CAA-CBA-CGA-O1A
84	C4	1001	CYC	CAA-CBA-CGA-O1A
87	32	312	CLA	CAA-CBA-CGA-O1A
87	3N	312	CLA	CAA-CBA-CGA-O1A
87	BN	826	CLA	C2-C1-O2A-CGA
87	72	607	CLA	C2-C1-O2A-CGA
87	B2	805	CLA	C2-C1-O2A-CGA
87	B2	826	CLA	C2-C1-O2A-CGA
87	B6	616	CLA	C2-C1-O2A-CGA
87	D6	403	CLA	C2-C1-O2A-CGA
87	b6	604	CLA	C2-C1-O2A-CGA
87	aL	606	CLA	C2-C1-O2A-CGA
87	cL	515	CLA	C2-C1-O2A-CGA
87	7N	607	CLA	C2-C1-O2A-CGA
87	c6	611	CLA	C16-C17-C18-C20
87	c6	612	CLA	C16-C17-C18-C19
87	cL	515	CLA	C11-C12-C13-C14
88	CL	521	LHG	C30-C31-C32-C33
95	c6	620	DGD	C7B-C8B-C9B-CAB
82	GA	202	PEB	NC-C1C-CHB-C4B
82	AF	202	PEB	NC-C1C-CHB-C4B
82	TH	202	PEB	NC-C1C-CHB-C4B
82	AK	202	PEB	NC-C1C-CHB-C4B
82	T1	202	PEB	NC-C1C-CHB-C4B
82	Y4	203	PEB	NC-C1C-CHB-C4B
82	G7	202	PEB	NC-C1C-CHB-C4B
82	S9	201	PEB	NC-C1C-CHB-C4B
82	mH	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	BA	201	PEB	CAC-CBC-CGC-O1C
82	KA	202	PEB	CAC-CBC-CGC-O2C
82	MA	202	PEB	CAC-CBC-CGC-O1C
82	OA	202	PEB	CAB-CBB-CGB-O1B
82	PA	201	PEB	CAC-CBC-CGC-O2C
82	PA	203	PEB	CAB-CBB-CGB-O1B
82	YA	301	PEB	CAB-CBB-CGB-O1B
82	BB	203	PEB	CAC-CBC-CGC-O2C
82	DB	202	PEB	CAB-CBB-CGB-O2B
82	DB	203	PEB	CAB-CBB-CGB-O1B
82	JB	202	PEB	CAB-CBB-CGB-O1B
82	NB	203	PEB	CAB-CBB-CGB-O1B
82	SB	202	PEB	CAC-CBC-CGC-O1C
82	TB	202	PEB	CAB-CBB-CGB-O1B
82	UB	303	PEB	CAB-CBB-CGB-O1B
82	VB	201	PEB	CAB-CBB-CGB-O2B
82	VB	202	PEB	CAB-CBB-CGB-O1B
82	WB	401	PEB	CAC-CBC-CGC-O1C
82	DD	201	PEB	CAC-CBC-CGC-O1C
82	DD	203	PEB	CAC-CBC-CGC-O1C
82	JD	202	PEB	CAC-CBC-CGC-O1C
82	JD	203	PEB	CAC-CBC-CGC-O1C
82	LD	202	PEB	CAB-CBB-CGB-O2B
82	OD	202	PEB	CAC-CBC-CGC-O1C
82	TD	203	PEB	CAC-CBC-CGC-O1C
82	XD	202	PEB	CAC-CBC-CGC-O1C
82	XD	202	PEB	CAB-CBB-CGB-O1B
82	XD	203	PEB	CAC-CBC-CGC-O1C
82	HE	1002	PEB	CAC-CBC-CGC-O1C
82	KE	201	PEB	CAC-CBC-CGC-O1C
82	QE	203	PEB	CAB-CBB-CGB-O1B
82	UE	203	PEB	CAB-CBB-CGB-O2B
82	ZE	203	PEB	CAC-CBC-CGC-O1C
82	CF	203	PEB	CAC-CBC-CGC-O1C
82	MF	201	PEB	CAC-CBC-CGC-O1C
82	QF	202	PEB	CAB-CBB-CGB-O1B
82	SF	202	PEB	CAC-CBC-CGC-O1C
82	HG	1002	PEB	CAC-CBC-CGC-O1C
82	KG	201	PEB	CAC-CBC-CGC-O1C
82	QG	203	PEB	CAB-CBB-CGB-O1B
82	UG	203	PEB	CAB-CBB-CGB-O2B
82	ZG	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	AH	302	PEB	CAB-CBB-CGB-O1B
82	HH	1002	PEB	CAC-CBC-CGC-O1C
82	OH	202	PEB	CAB-CBB-CGB-O1B
82	QH	202	PEB	CAC-CBC-CGC-O1C
82	QH	203	PEB	CAC-CBC-CGC-O2C
82	UH	203	PEB	CAC-CBC-CGC-O2C
82	ZH	203	PEB	CAC-CBC-CGC-O1C
82	HI	201	PEB	CAC-CBC-CGC-O1C
82	OI	201	PEB	CAC-CBC-CGC-O2C
82	GJ	202	PEB	CAC-CBC-CGC-O2C
82	JJ	202	PEB	CAC-CBC-CGC-O2C
82	SJ	203	PEB	CAC-CBC-CGC-O1C
82	WJ	202	PEB	CAB-CBB-CGB-O2B
82	WJ	203	PEB	CAC-CBC-CGC-O1C
82	MK	201	PEB	CAC-CBC-CGC-O1C
82	QK	202	PEB	CAB-CBB-CGB-O1B
82	SK	202	PEB	CAC-CBC-CGC-O1C
82	CM	202	PEB	CAB-CBB-CGB-O1B
82	EM	203	PEB	CAC-CBC-CGC-O1C
82	FM	202	PEB	CAC-CBC-CGC-O1C
82	KM	201	PEB	CAC-CBC-CGC-O2C
82	OM	202	PEB	CAB-CBB-CGB-O1B
82	AO	304	PEB	CAC-CBC-CGC-O1C
82	FO	1002	PEB	CAC-CBC-CGC-O1C
82	FO	1002	PEB	CAB-CBB-CGB-O1B
82	VO	202	PEB	CAC-CBC-CGC-O1C
82	YO	203	PEB	CAC-CBC-CGC-O1C
82	HP	202	PEB	CAB-CBB-CGB-O1B
82	JP	202	PEB	CAB-CBB-CGB-O2B
82	KP	202	PEB	CAC-CBC-CGC-O1C
82	DQ	201	PEB	CAC-CBC-CGC-O1C
82	JQ	202	PEB	CAC-CBC-CGC-O1C
82	LQ	202	PEB	CAB-CBB-CGB-O2B
82	NQ	203	PEB	CAC-CBC-CGC-O2C
82	PQ	201	PEB	CAC-CBC-CGC-O1C
82	SQ	202	PEB	CAC-CBC-CGC-O2C
82	TQ	203	PEB	CAC-CBC-CGC-O1C
82	XQ	202	PEB	CAC-CBC-CGC-O1C
82	XQ	202	PEB	CAB-CBB-CGB-O1B
82	A1	302	PEB	CAC-CBC-CGC-O2C
82	A1	302	PEB	CAB-CBB-CGB-O1B
82	h1	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	m1	201	PEB	CAB-CBB-CGB-O1B
82	F4	1002	PEB	CAC-CBC-CGC-O1C
82	V4	202	PEB	CAC-CBC-CGC-O1C
82	Y4	203	PEB	CAC-CBC-CGC-O1C
82	m4	202	PEB	CAC-CBC-CGC-O1C
82	m4	203	PEB	CAC-CBC-CGC-O1C
82	c4	202	PEB	CAC-CBC-CGC-O1C
82	S5	201	PEB	CAB-CBB-CGB-O1B
82	W5	203	PEB	CAB-CBB-CGB-O2B
82	A7	202	PEB	CAB-CBB-CGB-O1B
82	B7	201	PEB	CAC-CBC-CGC-O1C
82	G7	202	PEB	CAB-CBB-CGB-O2B
82	U7	202	PEB	CAC-CBC-CGC-O1C
82	v8	202	PEB	CAC-CBC-CGC-O2C
82	F9	201	PEB	CAC-CBC-CGC-O1C
82	J9	201	PEB	CAC-CBC-CGC-O1C
82	Q9	201	PEB	CAC-CBC-CGC-O1C
82	Q9	201	PEB	CAC-CBC-CGC-O2C
82	S9	201	PEB	CAC-CBC-CGC-O1C
82	fB	301	PEB	CAC-CBC-CGC-O1C
82	dB	202	PEB	CAB-CBB-CGB-O2B
82	gB	203	PEB	CAB-CBB-CGB-O1B
82	pC	201	PEB	CAC-CBC-CGC-O1C
82	vC	202	PEB	CAC-CBC-CGC-O2C
82	fE	201	PEB	CAC-CBC-CGC-O1C
82	gE	202	PEB	CAC-CBC-CGC-O1C
82	dF	201	PEB	CAC-CBC-CGC-O2C
82	oF	202	PEB	CAC-CBC-CGC-O1C
82	qF	203	PEB	CAC-CBC-CGC-O2C
82	sF	202	PEB	CAC-CBC-CGC-O2C
82	xF	302	PEB	CAC-CBC-CGC-O2C
82	xF	304	PEB	CAB-CBB-CGB-O1B
82	gG	202	PEB	CAC-CBC-CGC-O1C
82	lG	202	PEB	CAB-CBB-CGB-O2B
82	jH	201	PEB	CAC-CBC-CGC-O1C
82	kH	203	PEB	CAC-CBC-CGC-O1C
82	mH	201	PEB	CAB-CBB-CGB-O1B
82	cJ	202	PEB	CAC-CBC-CGC-O1C
82	eJ	202	PEB	CAC-CBC-CGC-O1C
82	hJ	202	PEB	CAC-CBC-CGC-O1C
82	hJ	203	PEB	CAC-CBC-CGC-O2C
82	jJ	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	lJ	203	PEB	CAC-CBC-CGC-O1C
82	lK	203	PEB	CAB-CBB-CGB-O1B
82	mK	201	PEB	CAC-CBC-CGC-O2C
82	oK	202	PEB	CAC-CBC-CGC-O1C
82	qK	203	PEB	CAC-CBC-CGC-O2C
82	sK	202	PEB	CAC-CBC-CGC-O2C
82	xK	302	PEB	CAC-CBC-CGC-O2C
82	cM	202	PEB	CAC-CBC-CGC-O1C
82	fM	201	PEB	CAC-CBC-CGC-O1C
82	jM	201	PEB	CAB-CBB-CGB-O1B
82	lM	203	PEB	CAC-CBC-CGC-O1C
82	mM	202	PEB	CAC-CBC-CGC-O2C
82	kO	203	PEB	CAC-CBC-CGC-O1C
82	mO	202	PEB	CAC-CBC-CGC-O1C
82	aO	202	PEB	CAC-CBC-CGC-O1C
82	bP	502	PEB	CAB-CBB-CGB-O2B
82	Z9	303	PEB	CAC-CBC-CGC-O2C
83	AH	304	PUB	CAC-CBC-CGC-O1C
83	AJ	304	PUB	CAB-CBB-CGB-O1B
83	AO	303	PUB	CAB-CBB-CGB-O2B
83	A1	304	PUB	CAC-CBC-CGC-O1C
83	Z9	305	PUB	CAB-CBB-CGB-O1B
84	GO	1001	CYC	CAA-CBA-CGA-O2A
84	IO	1001	CYC	CAA-CBA-CGA-O1A
84	G4	1001	CYC	CAA-CBA-CGA-O2A
84	I4	1001	CYC	CAA-CBA-CGA-O1A
96	FL	102	HEM	CAA-CBA-CGA-O1A
87	AN	819	CLA	C2A-CAA-CBA-CGA
87	AN	851	CLA	C2A-CAA-CBA-CGA
87	42	602	CLA	C2A-CAA-CBA-CGA
87	A2	819	CLA	C2A-CAA-CBA-CGA
87	A2	851	CLA	C2A-CAA-CBA-CGA
87	4N	602	CLA	C2A-CAA-CBA-CGA
92	bL	611	LMG	O7-C8-C9-O8
92	DL	402	LMG	C29-C30-C31-C32
92	b6	620	LMG	C29-C28-O8-C9
95	J6	101	DGD	O6D-C5D-C6D-O5D
92	AL	411	LMG	C14-C15-C16-C17
95	B6	620	DGD	C2A-C3A-C4A-C5A
95	C6	523	DGD	C7B-C8B-C9B-CAB
88	AL	406	LHG	C2-C3-O3-P
87	AN	816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	FN	203	CLA	C3A-C2A-CAA-CBA
87	12	601	CLA	C3A-C2A-CAA-CBA
87	22	606	CLA	C3A-C2A-CAA-CBA
87	42	608	CLA	C3A-C2A-CAA-CBA
87	52	607	CLA	C3A-C2A-CAA-CBA
87	A2	816	CLA	C3A-C2A-CAA-CBA
87	F2	201	CLA	C3A-C2A-CAA-CBA
87	1N	601	CLA	C3A-C2A-CAA-CBA
87	2N	306	CLA	C3A-C2A-CAA-CBA
87	4N	608	CLA	C3A-C2A-CAA-CBA
87	5N	607	CLA	C3A-C2A-CAA-CBA
82	AA	202	PEB	CAB-CBB-CGB-O1B
82	BA	202	PEB	CAB-CBB-CGB-O1B
82	BA	203	PEB	CAC-CBC-CGC-O1C
82	DA	202	PEB	CAC-CBC-CGC-O2C
82	EA	201	PEB	CAC-CBC-CGC-O1C
82	OA	201	PEB	CAB-CBB-CGB-O1B
82	QA	201	PEB	CAC-CBC-CGC-O1C
82	RA	202	PEB	CAC-CBC-CGC-O1C
82	WA	202	PEB	CAC-CBC-CGC-O1C
82	YA	304	PEB	CAC-CBC-CGC-O1C
82	AB	501	PEB	CAC-CBC-CGC-O1C
82	BB	202	PEB	CAC-CBC-CGC-O1C
82	GB	203	PEB	CAB-CBB-CGB-O1B
82	XB	201	PEB	CAC-CBC-CGC-O1C
82	ZB	203	PEB	CAB-CBB-CGB-O2B
82	BD	203	PEB	CAC-CBC-CGC-O1C
82	ED	202	PEB	CAB-CBB-CGB-O1B
82	FD	203	PEB	CAB-CBB-CGB-O2B
82	KD	202	PEB	CAC-CBC-CGC-O1C
82	LD	201	PEB	CAC-CBC-CGC-O2C
82	LD	203	PEB	CAC-CBC-CGC-O1C
82	ND	202	PEB	CAB-CBB-CGB-O2B
82	PD	201	PEB	CAC-CBC-CGC-O1C
82	PD	202	PEB	CAB-CBB-CGB-O1B
82	PD	203	PEB	CAC-CBC-CGC-O1C
82	PD	203	PEB	CAB-CBB-CGB-O1B
82	SD	202	PEB	CAC-CBC-CGC-O2C
82	TD	201	PEB	CAC-CBC-CGC-O1C
82	YD	202	PEB	CAB-CBB-CGB-O2B
82	AE	301	PEB	CAB-CBB-CGB-O2B
82	SE	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	EF	201	PEB	CAC-CBC-CGC-O2C
82	EF	202	PEB	CAC-CBC-CGC-O2C
82	JF	202	PEB	CAB-CBB-CGB-O1B
82	ZF	202	PEB	CAB-CBB-CGB-O1B
82	ZF	202	PEB	CAB-CBB-CGB-O2B
82	OG	202	PEB	CAB-CBB-CGB-O2B
82	QG	203	PEB	CAC-CBC-CGC-O2C
82	SG	201	PEB	CAC-CBC-CGC-O1C
82	CJ	202	PEB	CAC-CBC-CGC-O1C
82	DJ	202	PEB	CAC-CBC-CGC-O2C
82	EJ	202	PEB	CAC-CBC-CGC-O2C
82	ZJ	202	PEB	CAC-CBC-CGC-O2C
82	EK	201	PEB	CAC-CBC-CGC-O2C
82	EK	202	PEB	CAC-CBC-CGC-O2C
82	MK	202	PEB	CAB-CBB-CGB-O2B
82	ZK	202	PEB	CAB-CBB-CGB-O2B
82	GM	201	PEB	CAC-CBC-CGC-O2C
82	GM	202	PEB	CAC-CBC-CGC-O2C
82	JM	202	PEB	CAC-CBC-CGC-O1C
82	LM	202	PEB	CAC-CBC-CGC-O2C
82	NM	202	PEB	CAC-CBC-CGC-O2C
82	OM	203	PEB	CAC-CBC-CGC-O2C
82	QM	203	PEB	CAC-CBC-CGC-O1C
82	SM	203	PEB	CAC-CBC-CGC-O1C
82	UM	203	PEB	CAB-CBB-CGB-O1B
82	VM	202	PEB	CAC-CBC-CGC-O1C
82	YM	202	PEB	CAC-CBC-CGC-O2C
82	PO	203	PEB	CAC-CBC-CGC-O1C
82	TO	202	PEB	CAC-CBC-CGC-O1C
82	BP	202	PEB	CAB-CBB-CGB-O1B
82	DP	202	PEB	CAB-CBB-CGB-O1B
82	GP	202	PEB	CAC-CBC-CGC-O1C
82	IP	202	PEB	CAB-CBB-CGB-O2B
82	IP	203	PEB	CAC-CBC-CGC-O1C
82	KP	201	PEB	CAB-CBB-CGB-O1B
82	MP	201	PEB	CAC-CBC-CGC-O1C
82	MP	203	PEB	CAC-CBC-CGC-O1C
82	NP	202	PEB	CAB-CBB-CGB-O2B
82	OP	201	PEB	CAC-CBC-CGC-O1C
82	UP	203	PEB	CAC-CBC-CGC-O1C
82	UP	203	PEB	CAB-CBB-CGB-O1B
82	YP	502	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	AQ	304	PEB	CAC-CBC-CGC-O1C
82	BQ	203	PEB	CAC-CBC-CGC-O1C
82	KQ	202	PEB	CAC-CBC-CGC-O1C
82	LQ	203	PEB	CAC-CBC-CGC-O1C
82	PQ	202	PEB	CAB-CBB-CGB-O1B
82	PQ	203	PEB	CAC-CBC-CGC-O1C
82	PQ	203	PEB	CAB-CBB-CGB-O1B
82	QQ	202	PEB	CAC-CBC-CGC-O1C
82	TQ	201	PEB	CAC-CBC-CGC-O1C
82	O1	201	PEB	CAB-CBB-CGB-O2B
82	O1	202	PEB	CAB-CBB-CGB-O1B
82	Q1	203	PEB	CAC-CBC-CGC-O2C
82	H1	1002	PEB	CAC-CBC-CGC-O1C
82	J1	1002	PEB	CAC-CBC-CGC-O2C
82	J1	1002	PEB	CAB-CBB-CGB-O1B
82	Z1	203	PEB	CAC-CBC-CGC-O1C
82	h1	201	PEB	CAB-CBB-CGB-O1B
82	j1	201	PEB	CAC-CBC-CGC-O1C
82	l1	203	PEB	CAC-CBC-CGC-O1C
82	b1	202	PEB	CAC-CBC-CGC-O1C
82	c1	202	PEB	CAC-CBC-CGC-O1C
82	d1	202	PEB	CAB-CBB-CGB-O2B
82	F4	1002	PEB	CAB-CBB-CGB-O1B
82	T4	202	PEB	CAC-CBC-CGC-O1C
82	i4	202	PEB	CAC-CBC-CGC-O1C
82	j4	203	PEB	CAB-CBB-CGB-O1B
82	c4	203	PEB	CAC-CBC-CGC-O1C
82	M5	301	PEB	CAC-CBC-CGC-O2C
82	M5	301	PEB	CAB-CBB-CGB-O1B
82	M5	301	PEB	CAB-CBB-CGB-O2B
82	M5	305	PEB	CAB-CBB-CGB-O1B
82	O5	203	PEB	CAC-CBC-CGC-O1C
82	Z5	301	PEB	CAB-CBB-CGB-O2B
82	Z5	305	PEB	CAB-CBB-CGB-O1B
82	B7	202	PEB	CAB-CBB-CGB-O1B
82	B7	203	PEB	CAC-CBC-CGC-O1C
82	E7	201	PEB	CAC-CBC-CGC-O1C
82	M7	202	PEB	CAC-CBC-CGC-O1C
82	O7	201	PEB	CAB-CBB-CGB-O1B
82	P7	203	PEB	CAB-CBB-CGB-O1B
82	R7	202	PEB	CAC-CBC-CGC-O1C
82	Y7	304	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	y8	202	PEB	CAC-CBC-CGC-O1C
82	r8	201	PEB	CAC-CBC-CGC-O2C
82	x8	201	PEB	CAB-CBB-CGB-O1B
82	A9	201	PEB	CAC-CBC-CGC-O2C
82	E9	201	PEB	CAC-CBC-CGC-O2C
82	aB	202	PEB	CAB-CBB-CGB-O2B
82	bB	201	PEB	CAB-CBB-CGB-O1B
82	hB	301	PEB	CAC-CBC-CGC-O1C
82	yC	202	PEB	CAC-CBC-CGC-O1C
82	rC	201	PEB	CAC-CBC-CGC-O2C
82	xC	201	PEB	CAB-CBB-CGB-O1B
82	gE	202	PEB	CAB-CBB-CGB-O1B
82	hE	203	PEB	CAC-CBC-CGC-O2C
82	iE	202	PEB	CAB-CBB-CGB-O2B
82	mE	201	PEB	CAC-CBC-CGC-O1C
82	bF	202	PEB	CAB-CBB-CGB-O1B
82	eF	203	PEB	CAB-CBB-CGB-O2B
82	fF	202	PEB	CAB-CBB-CGB-O2B
82	iF	203	PEB	CAC-CBC-CGC-O2C
82	lF	203	PEB	CAB-CBB-CGB-O1B
82	mF	201	PEB	CAC-CBC-CGC-O2C
82	xF	302	PEB	CAB-CBB-CGB-O1B
82	fG	201	PEB	CAB-CBB-CGB-O1B
82	gG	202	PEB	CAB-CBB-CGB-O1B
82	hG	203	PEB	CAC-CBC-CGC-O2C
82	mG	201	PEB	CAC-CBC-CGC-O1C
82	gH	203	PEB	CAB-CBB-CGB-O1B
82	kH	202	PEB	CAB-CBB-CGB-O2B
82	bH	202	PEB	CAC-CBC-CGC-O1C
82	cH	202	PEB	CAC-CBC-CGC-O1C
82	dH	202	PEB	CAB-CBB-CGB-O2B
82	fJ	201	PEB	CAC-CBC-CGC-O2C
82	fJ	202	PEB	CAC-CBC-CGC-O1C
82	gJ	202	PEB	CAC-CBC-CGC-O1C
82	iJ	202	PEB	CAC-CBC-CGC-O1C
82	bK	202	PEB	CAB-CBB-CGB-O1B
82	eK	203	PEB	CAB-CBB-CGB-O2B
82	qK	202	PEB	CAC-CBC-CGC-O1C
82	wK	301	PEB	CAB-CBB-CGB-O1B
82	xK	302	PEB	CAB-CBB-CGB-O1B
82	aM	201	PEB	CAC-CBC-CGC-O1C
82	fM	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	hM	201	PEB	CAB-CBB-CGB-O2B
82	iO	202	PEB	CAC-CBC-CGC-O1C
82	cO	202	PEB	CAC-CBC-CGC-O1C
82	cO	203	PEB	CAC-CBC-CGC-O1C
82	bP	501	PEB	CAC-CBC-CGC-O2C
82	M9	301	PEB	CAC-CBC-CGC-O1C
83	AE	302	PUB	CAB-CBB-CGB-O2B
83	xF	301	PUB	CAB-CBB-CGB-O1B
83	xK	301	PUB	CAB-CBB-CGB-O1B
83	Z9	305	PUB	CAB-CBB-CGB-O2B
84	BE	1002	CYC	CAA-CBA-CGA-O1A
84	BG	1002	CYC	CAA-CBA-CGA-O1A
84	V3	1001	CYC	CAA-CBA-CGA-O1A
84	V3	1001	CYC	CAD-CBD-CGD-O1D
84	W3	1001	CYC	CAD-CBD-CGD-O1D
84	x3	1001	CYC	CAA-CBA-CGA-O1A
84	y3	1001	CYC	CAD-CBD-CGD-O1D
87	MN	101	CLA	CAA-CBA-CGA-O1A
87	M2	101	CLA	CAA-CBA-CGA-O1A
87	cL	508	CLA	C16-C17-C18-C19
95	lL	101	DGD	CBA-CCA-CDA-CEA
88	aL	607	LHG	O9-C7-O7-C5
92	B6	619	LMG	C29-C28-O8-C9
95	C6	521	DGD	C4D-C5D-C6D-O5D
92	B6	618	LMG	C16-C17-C18-C19
82	DA	202	PEB	CAB-CBB-CGB-O1B
82	EA	201	PEB	CAC-CBC-CGC-O2C
82	FA	203	PEB	CAC-CBC-CGC-O2C
82	HA	201	PEB	CAC-CBC-CGC-O1C
82	IA	201	PEB	CAC-CBC-CGC-O1C
82	QA	202	PEB	CAC-CBC-CGC-O2C
82	SA	201	PEB	CAC-CBC-CGC-O2C
82	WA	202	PEB	CAC-CBC-CGC-O2C
82	YA	301	PEB	CAB-CBB-CGB-O2B
82	CB	202	PEB	CAB-CBB-CGB-O2B
82	EB	501	PEB	CAB-CBB-CGB-O1B
82	FB	201	PEB	CAB-CBB-CGB-O1B
82	LB	201	PEB	CAB-CBB-CGB-O1B
82	MB	202	PEB	CAB-CBB-CGB-O2B
82	NB	203	PEB	CAC-CBC-CGC-O1C
82	QB	204	PEB	CAB-CBB-CGB-O1B
82	ZB	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	AD	303	PEB	CAB-CBB-CGB-O2B
82	AD	304	PEB	CAC-CBC-CGC-O1C
82	FD	202	PEB	CAC-CBC-CGC-O1C
82	ND	203	PEB	CAC-CBC-CGC-O2C
82	QD	202	PEB	CAC-CBC-CGC-O1C
82	UD	202	PEB	CAC-CBC-CGC-O1C
82	XD	201	PEB	CAC-CBC-CGC-O2C
82	OE	201	PEB	CAB-CBB-CGB-O1B
82	OE	202	PEB	CAC-CBC-CGC-O2C
82	OE	202	PEB	CAB-CBB-CGB-O1B
82	OE	202	PEB	CAB-CBB-CGB-O2B
82	QE	203	PEB	CAC-CBC-CGC-O2C
82	UE	203	PEB	CAB-CBB-CGB-O1B
82	YE	202	PEB	CAB-CBB-CGB-O2B
82	ZE	203	PEB	CAB-CBB-CGB-O2B
82	AF	201	PEB	CAC-CBC-CGC-O2C
82	AF	201	PEB	CAB-CBB-CGB-O2B
82	EF	201	PEB	CAB-CBB-CGB-O2B
82	EF	202	PEB	CAB-CBB-CGB-O2B
82	GF	201	PEB	CAC-CBC-CGC-O2C
82	MF	202	PEB	CAB-CBB-CGB-O2B
82	OF	203	PEB	CAB-CBB-CGB-O2B
82	AG	301	PEB	CAB-CBB-CGB-O2B
82	OG	201	PEB	CAB-CBB-CGB-O1B
82	OG	202	PEB	CAC-CBC-CGC-O2C
82	VG	202	PEB	CAC-CBC-CGC-O2C
82	WG	201	PEB	CAB-CBB-CGB-O2B
82	ZG	203	PEB	CAB-CBB-CGB-O2B
82	FH	1002	PEB	CAC-CBC-CGC-O1C
82	JH	1002	PEB	CAC-CBC-CGC-O2C
82	JH	1002	PEB	CAB-CBB-CGB-O1B
82	OH	201	PEB	CAB-CBB-CGB-O2B
82	YH	202	PEB	CAB-CBB-CGB-O2B
82	CI	202	PEB	CAB-CBB-CGB-O1B
82	EI	202	PEB	CAB-CBB-CGB-O1B
82	II	203	PEB	CAC-CBC-CGC-O1C
82	KI	203	PEB	CAB-CBB-CGB-O1B
82	PI	202	PEB	CAB-CBB-CGB-O1B
82	TI	201	PEB	CAC-CBC-CGC-O2C
82	TI	203	PEB	CAB-CBB-CGB-O1B
82	VI	203	PEB	CAC-CBC-CGC-O1C
82	WI	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	WI	202	PEB	CAC-CBC-CGC-O2C
82	AJ	301	PEB	CAB-CBB-CGB-O1B
82	CJ	203	PEB	CAC-CBC-CGC-O2C
82	DJ	202	PEB	CAB-CBB-CGB-O2B
82	GJ	202	PEB	CAC-CBC-CGC-O1C
82	GJ	202	PEB	CAB-CBB-CGB-O1B
82	KJ	202	PEB	CAC-CBC-CGC-O2C
82	KJ	202	PEB	CAB-CBB-CGB-O1B
82	QJ	204	PEB	CAC-CBC-CGC-O2C
82	RJ	202	PEB	CAC-CBC-CGC-O1C
82	SJ	202	PEB	CAB-CBB-CGB-O1B
82	YJ	201	PEB	CAC-CBC-CGC-O1C
82	YJ	203	PEB	CAB-CBB-CGB-O1B
82	AK	201	PEB	CAC-CBC-CGC-O2C
82	AK	201	PEB	CAB-CBB-CGB-O2B
82	CK	203	PEB	CAC-CBC-CGC-O1C
82	EK	201	PEB	CAB-CBB-CGB-O2B
82	EK	202	PEB	CAC-CBC-CGC-O1C
82	EK	202	PEB	CAB-CBB-CGB-O2B
82	GK	201	PEB	CAC-CBC-CGC-O2C
82	JK	202	PEB	CAB-CBB-CGB-O1B
82	OK	203	PEB	CAC-CBC-CGC-O1C
82	OK	203	PEB	CAC-CBC-CGC-O2C
82	OK	203	PEB	CAB-CBB-CGB-O2B
82	ZK	202	PEB	CAB-CBB-CGB-O1B
82	CM	202	PEB	CAC-CBC-CGC-O2C
82	HM	202	PEB	CAC-CBC-CGC-O1C
82	PM	202	PEB	CAC-CBC-CGC-O2C
82	SM	203	PEB	CAC-CBC-CGC-O2C
82	UM	201	PEB	CAC-CBC-CGC-O2C
82	YM	202	PEB	CAC-CBC-CGC-O1C
82	ZM	202	PEB	CAC-CBC-CGC-O1C
82	YO	203	PEB	CAB-CBB-CGB-O1B
82	AP	201	PEB	CAC-CBC-CGC-O1C
82	CP	201	PEB	CAC-CBC-CGC-O1C
82	CP	201	PEB	CAB-CBB-CGB-O2B
82	CP	203	PEB	CAB-CBB-CGB-O2B
82	JP	202	PEB	CAB-CBB-CGB-O1B
82	MP	201	PEB	CAC-CBC-CGC-O2C
82	PP	202	PEB	CAB-CBB-CGB-O2B
82	QP	201	PEB	CAC-CBC-CGC-O1C
82	VP	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	VP	202	PEB	CAB-CBB-CGB-O2B
82	AQ	303	PEB	CAB-CBB-CGB-O2B
82	EQ	202	PEB	CAB-CBB-CGB-O1B
82	FQ	202	PEB	CAC-CBC-CGC-O1C
82	FQ	203	PEB	CAB-CBB-CGB-O2B
82	LQ	201	PEB	CAC-CBC-CGC-O2C
82	LQ	202	PEB	CAC-CBC-CGC-O2C
82	NQ	202	PEB	CAB-CBB-CGB-O2B
82	UQ	202	PEB	CAC-CBC-CGC-O1C
82	VQ	201	PEB	CAB-CBB-CGB-O1B
82	F1	1002	PEB	CAC-CBC-CGC-O1C
82	Y1	202	PEB	CAB-CBB-CGB-O2B
82	f1	203	PEB	CAC-CBC-CGC-O2C
82	j1	203	PEB	CAC-CBC-CGC-O2C
82	k1	202	PEB	CAB-CBB-CGB-O2B
82	b1	203	PEB	CAC-CBC-CGC-O2C
82	A4	304	PEB	CAC-CBC-CGC-O1C
82	Y4	203	PEB	CAB-CBB-CGB-O1B
82	J5	201	PEB	CAC-CBC-CGC-O1C
82	L5	201	PEB	CAC-CBC-CGC-O2C
82	O5	203	PEB	CAB-CBB-CGB-O2B
82	S5	203	PEB	CAC-CBC-CGC-O1C
82	U5	201	PEB	CAC-CBC-CGC-O2C
82	Z5	301	PEB	CAC-CBC-CGC-O2C
82	Z5	301	PEB	CAB-CBB-CGB-O1B
82	D7	202	PEB	CAC-CBC-CGC-O2C
82	D7	202	PEB	CAB-CBB-CGB-O1B
82	E7	201	PEB	CAC-CBC-CGC-O2C
82	E7	202	PEB	CAC-CBC-CGC-O1C
82	F7	203	PEB	CAC-CBC-CGC-O2C
82	H7	201	PEB	CAC-CBC-CGC-O1C
82	I7	201	PEB	CAC-CBC-CGC-O1C
82	N7	203	PEB	CAB-CBB-CGB-O2B
82	O7	202	PEB	CAB-CBB-CGB-O1B
82	Q7	202	PEB	CAC-CBC-CGC-O1C
82	Q7	202	PEB	CAC-CBC-CGC-O2C
82	W7	202	PEB	CAC-CBC-CGC-O2C
82	Y7	301	PEB	CAB-CBB-CGB-O2B
82	z8	201	PEB	CAC-CBC-CGC-O1C
82	w8	201	PEB	CAC-CBC-CGC-O1C
82	C9	201	PEB	CAC-CBC-CGC-O2C
82	F9	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	G9	201	PEB	CAC-CBC-CGC-O2C
82	I9	201	PEB	CAC-CBC-CGC-O2C
82	K9	201	PEB	CAC-CBC-CGC-O2C
82	N9	201	PEB	CAC-CBC-CGC-O2C
82	O9	201	PEB	CAB-CBB-CGB-O2B
82	P9	201	PEB	CAC-CBC-CGC-O2C
82	R9	201	PEB	CAC-CBC-CGC-O2C
82	S9	201	PEB	CAB-CBB-CGB-O2B
82	T9	201	PEB	CAC-CBC-CGC-O2C
82	U9	201	PEB	CAC-CBC-CGC-O1C
82	V9	201	PEB	CAC-CBC-CGC-O2C
82	W9	201	PEB	CAC-CBC-CGC-O2C
82	X9	201	PEB	CAC-CBC-CGC-O2C
82	Y9	201	PEB	CAC-CBC-CGC-O2C
82	dB	201	PEB	CAB-CBB-CGB-O2B
82	zC	201	PEB	CAC-CBC-CGC-O1C
82	wC	201	PEB	CAC-CBC-CGC-O1C
82	dE	201	PEB	CAC-CBC-CGC-O1C
82	dE	201	PEB	CAB-CBB-CGB-O1B
82	eE	203	PEB	CAB-CBB-CGB-O1B
82	fE	201	PEB	CAB-CBB-CGB-O1B
82	lE	202	PEB	CAC-CBC-CGC-O2C
82	bF	202	PEB	CAB-CBB-CGB-O2B
82	fF	202	PEB	CAC-CBC-CGC-O1C
82	gF	202	PEB	CAC-CBC-CGC-O2C
82	kF	201	PEB	CAC-CBC-CGC-O1C
82	qF	202	PEB	CAC-CBC-CGC-O1C
82	sF	202	PEB	CAB-CBB-CGB-O1B
82	uF	202	PEB	CAC-CBC-CGC-O2C
82	uF	203	PEB	CAC-CBC-CGC-O2C
82	wF	301	PEB	CAB-CBB-CGB-O2B
82	wF	303	PEB	CAC-CBC-CGC-O1C
82	wF	303	PEB	CAC-CBC-CGC-O2C
82	eG	203	PEB	CAB-CBB-CGB-O1B
82	iG	202	PEB	CAB-CBB-CGB-O2B
82	fH	203	PEB	CAC-CBC-CGC-O2C
82	jH	203	PEB	CAC-CBC-CGC-O2C
82	lH	202	PEB	CAC-CBC-CGC-O1C
82	eH	203	PEB	CAC-CBC-CGC-O2C
82	aJ	201	PEB	CAC-CBC-CGC-O2C
82	jJ	202	PEB	CAC-CBC-CGC-O1C
82	jJ	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	lJ	203	PEB	CAB-CBB-CGB-O1B
82	mJ	202	PEB	CAB-CBB-CGB-O2B
82	fK	202	PEB	CAB-CBB-CGB-O2B
82	kK	201	PEB	CAC-CBC-CGC-O1C
82	sK	202	PEB	CAB-CBB-CGB-O1B
82	uK	201	PEB	CAC-CBC-CGC-O2C
82	uK	202	PEB	CAC-CBC-CGC-O2C
82	vK	201	PEB	CAB-CBB-CGB-O2B
82	wK	301	PEB	CAC-CBC-CGC-O1C
82	wK	301	PEB	CAB-CBB-CGB-O2B
82	wK	303	PEB	CAC-CBC-CGC-O2C
82	xK	304	PEB	CAB-CBB-CGB-O1B
82	dM	203	PEB	CAB-CBB-CGB-O1B
82	hM	202	PEB	CAB-CBB-CGB-O2B
82	Z9	303	PEB	CAB-CBB-CGB-O2B
82	M9	304	PEB	CAB-CBB-CGB-O2B
83	AG	302	PUB	CAB-CBB-CGB-O2B
84	EO	1001	CYC	CAA-CBA-CGA-O2A
84	x3	1001	CYC	CAD-CBD-CGD-O1D
84	E4	1001	CYC	CAA-CBA-CGA-O2A
87	32	305	CLA	CAA-CBA-CGA-O2A
87	3N	306	CLA	CAA-CBA-CGA-O2A
87	BL	609	CLA	C4-C3-C5-C6
94	aL	601	PL9	C12-C11-C9-C10
88	d6	402	LHG	C30-C31-C32-C33
87	AN	808	CLA	C2-C3-C5-C6
87	A2	808	CLA	C2-C3-C5-C6
87	C6	510	CLA	C3-C5-C6-C7
95	b6	621	DGD	O6D-C5D-C6D-O5D
87	BN	818	CLA	C6-C7-C8-C9
87	BN	827	CLA	C14-C13-C15-C16
87	62	303	CLA	C11-C10-C8-C9
87	82	302	CLA	C14-C13-C15-C16
87	B2	817	CLA	C6-C7-C8-C9
87	B2	827	CLA	C14-C13-C15-C16
87	A6	402	CLA	C14-C13-C15-C16
87	B6	615	CLA	C11-C10-C8-C9
87	C6	510	CLA	C11-C12-C13-C14
87	C6	520	CLA	C14-C13-C15-C16
87	b6	604	CLA	C14-C13-C15-C16
87	b6	605	CLA	C14-C13-C15-C16
87	c6	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
87	c6	616	CLA	C6-C7-C8-C9
87	bL	621	CLA	C11-C10-C8-C9
87	6N	602	CLA	C11-C10-C8-C9
87	8N	303	CLA	C14-C13-C15-C16
91	D6	404	PHO	C6-C7-C8-C9
82	CA	201	PEB	C3B-CAB-CBB-CGB
82	RA	201	PEB	C2C-CAC-CBC-CGC
82	WA	201	PEB	C3B-CAB-CBB-CGB
82	GB	203	PEB	C2C-CAC-CBC-CGC
82	RB	201	PEB	C2C-CAC-CBC-CGC
82	UB	302	PEB	C3B-CAB-CBB-CGB
82	GD	201	PEB	C3B-CAB-CBB-CGB
82	OD	202	PEB	C2C-CAC-CBC-CGC
82	RE	202	PEB	C2C-CAC-CBC-CGC
82	BF	201	PEB	C3B-CAB-CBB-CGB
82	DF	201	PEB	C3B-CAB-CBB-CGB
82	OG	202	PEB	C2C-CAC-CBC-CGC
82	RG	202	PEB	C2C-CAC-CBC-CGC
82	OH	201	PEB	C3B-CAB-CBB-CGB
82	SH	201	PEB	C3B-CAB-CBB-CGB
82	BK	201	PEB	C3B-CAB-CBB-CGB
82	DK	201	PEB	C3B-CAB-CBB-CGB
82	KM	201	PEB	C3B-CAB-CBB-CGB
82	QM	203	PEB	C2C-CAC-CBC-CGC
82	RM	202	PEB	C3B-CAB-CBB-CGB
82	WM	203	PEB	C3B-CAB-CBB-CGB
82	NO	1002	PEB	C3B-CAB-CBB-CGB
82	IP	203	PEB	C2C-CAC-CBC-CGC
82	UP	203	PEB	C2C-CAC-CBC-CGC
82	VP	201	PEB	C3B-CAB-CBB-CGB
82	GQ	201	PEB	C3B-CAB-CBB-CGB
82	OQ	202	PEB	C2C-CAC-CBC-CGC
82	O1	201	PEB	C3B-CAB-CBB-CGB
82	S1	201	PEB	C3B-CAB-CBB-CGB
82	N4	1002	PEB	C3B-CAB-CBB-CGB
82	m4	203	PEB	C3B-CAB-CBB-CGB
82	U5	201	PEB	C3B-CAB-CBB-CGB
82	C7	201	PEB	C3B-CAB-CBB-CGB
82	R7	201	PEB	C2C-CAC-CBC-CGC
82	W7	201	PEB	C3B-CAB-CBB-CGB
82	q8	201	PEB	C3B-CAB-CBB-CGB
82	F9	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	qC	201	PEB	C3B-CAB-CBB-CGB
82	hE	203	PEB	C3B-CAB-CBB-CGB
82	mE	202	PEB	C3B-CAB-CBB-CGB
82	dF	201	PEB	C3B-CAB-CBB-CGB
82	pF	201	PEB	C3B-CAB-CBB-CGB
82	mG	202	PEB	C3B-CAB-CBB-CGB
82	dK	201	PEB	C3B-CAB-CBB-CGB
82	pK	201	PEB	C3B-CAB-CBB-CGB
82	mO	203	PEB	C3B-CAB-CBB-CGB
87	b6	614	CLA	C10-C11-C12-C13
82	DA	202	PEB	CAC-CBC-CGC-O1C
82	DA	203	PEB	CAB-CBB-CGB-O1B
82	DA	203	PEB	CAB-CBB-CGB-O2B
82	EA	202	PEB	CAC-CBC-CGC-O1C
82	NA	203	PEB	CAB-CBB-CGB-O2B
82	QA	202	PEB	CAC-CBC-CGC-O1C
82	UA	202	PEB	CAC-CBC-CGC-O2C
82	AB	501	PEB	CAB-CBB-CGB-O1B
82	EB	501	PEB	CAC-CBC-CGC-O1C
82	NB	203	PEB	CAB-CBB-CGB-O2B
82	RB	202	PEB	CAB-CBB-CGB-O2B
82	VB	201	PEB	CAB-CBB-CGB-O1B
82	HD	202	PEB	CAC-CBC-CGC-O2C
82	LD	202	PEB	CAC-CBC-CGC-O2C
82	ND	203	PEB	CAC-CBC-CGC-O1C
82	OD	201	PEB	CAC-CBC-CGC-O2C
82	QD	202	PEB	CAB-CBB-CGB-O2B
82	VD	202	PEB	CAC-CBC-CGC-O2C
82	VD	202	PEB	CAB-CBB-CGB-O2B
82	VD	203	PEB	CAB-CBB-CGB-O1B
82	RE	202	PEB	CAB-CBB-CGB-O1B
82	WE	201	PEB	CAB-CBB-CGB-O2B
82	ZE	203	PEB	CAB-CBB-CGB-O1B
82	EF	202	PEB	CAC-CBC-CGC-O1C
82	HF	202	PEB	CAB-CBB-CGB-O2B
82	KF	202	PEB	CAC-CBC-CGC-O2C
82	OF	203	PEB	CAC-CBC-CGC-O1C
82	QF	202	PEB	CAB-CBB-CGB-O2B
82	TF	202	PEB	CAB-CBB-CGB-O1B
82	OG	202	PEB	CAB-CBB-CGB-O1B
82	RG	202	PEB	CAB-CBB-CGB-O1B
82	UG	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	YG	202	PEB	CAB-CBB-CGB-O1B
82	YG	202	PEB	CAB-CBB-CGB-O2B
82	AH	302	PEB	CAC-CBC-CGC-O2C
82	AH	305	PEB	CAB-CBB-CGB-O2B
82	OH	201	PEB	CAB-CBB-CGB-O1B
82	AI	202	PEB	CAB-CBB-CGB-O1B
82	AI	203	PEB	CAC-CBC-CGC-O1C
82	HI	202	PEB	CAC-CBC-CGC-O1C
82	II	203	PEB	CAC-CBC-CGC-O2C
82	JI	201	PEB	CAC-CBC-CGC-O2C
82	NI	202	PEB	CAB-CBB-CGB-O1B
82	RI	202	PEB	CAB-CBB-CGB-O1B
82	SI	201	PEB	CAC-CBC-CGC-O1C
82	VI	202	PEB	CAB-CBB-CGB-O1B
82	XI	202	PEB	CAB-CBB-CGB-O1B
82	AJ	302	PEB	CAB-CBB-CGB-O2B
82	EJ	202	PEB	CAC-CBC-CGC-O1C
82	EJ	203	PEB	CAB-CBB-CGB-O1B
82	FJ	202	PEB	CAC-CBC-CGC-O1C
82	GJ	201	PEB	CAC-CBC-CGC-O2C
82	RJ	202	PEB	CAC-CBC-CGC-O2C
82	SJ	202	PEB	CAC-CBC-CGC-O2C
82	UJ	203	PEB	CAC-CBC-CGC-O1C
82	WJ	203	PEB	CAC-CBC-CGC-O2C
82	EK	201	PEB	CAC-CBC-CGC-O1C
82	GK	202	PEB	CAC-CBC-CGC-O2C
82	KK	202	PEB	CAC-CBC-CGC-O2C
82	TK	202	PEB	CAB-CBB-CGB-O1B
82	VK	202	PEB	CAB-CBB-CGB-O2B
82	EM	203	PEB	CAC-CBC-CGC-O2C
82	FM	202	PEB	CAB-CBB-CGB-O1B
82	GM	202	PEB	CAC-CBC-CGC-O1C
82	NM	202	PEB	CAC-CBC-CGC-O1C
82	OM	201	PEB	CAC-CBC-CGC-O2C
82	OM	202	PEB	CAC-CBC-CGC-O2C
82	OM	203	PEB	CAC-CBC-CGC-O1C
82	QM	204	PEB	CAC-CBC-CGC-O2C
82	RM	202	PEB	CAB-CBB-CGB-O1B
82	SM	202	PEB	CAC-CBC-CGC-O2C
82	QO	201	PEB	CAC-CBC-CGC-O2C
82	RO	202	PEB	CAB-CBB-CGB-O1B
82	TO	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	TO	203	PEB	CAB-CBB-CGB-O2B
82	DP	201	PEB	CAB-CBB-CGB-O1B
82	GP	201	PEB	CAB-CBB-CGB-O1B
82	IP	201	PEB	CAC-CBC-CGC-O1C
82	IP	202	PEB	CAC-CBC-CGC-O2C
82	RP	202	PEB	CAB-CBB-CGB-O2B
82	SP	202	PEB	CAC-CBC-CGC-O1C
82	UP	201	PEB	CAC-CBC-CGC-O1C
82	HQ	202	PEB	CAC-CBC-CGC-O2C
82	NQ	203	PEB	CAC-CBC-CGC-O1C
82	OQ	201	PEB	CAC-CBC-CGC-O2C
82	QQ	202	PEB	CAB-CBB-CGB-O2B
82	VQ	202	PEB	CAC-CBC-CGC-O1C
82	VQ	202	PEB	CAC-CBC-CGC-O2C
82	VQ	202	PEB	CAB-CBB-CGB-O2B
82	VQ	203	PEB	CAB-CBB-CGB-O1B
82	XQ	201	PEB	CAC-CBC-CGC-O2C
82	U1	203	PEB	CAC-CBC-CGC-O2C
82	A1	305	PEB	CAB-CBB-CGB-O2B
82	h1	203	PEB	CAB-CBB-CGB-O1B
82	F4	1002	PEB	CAC-CBC-CGC-O2C
82	A4	305	PEB	CAB-CBB-CGB-O1B
82	R4	202	PEB	CAB-CBB-CGB-O1B
82	T4	202	PEB	CAC-CBC-CGC-O2C
82	T4	203	PEB	CAB-CBB-CGB-O2B
82	Z4	201	PEB	CAC-CBC-CGC-O2C
82	m4	202	PEB	CAC-CBC-CGC-O2C
82	m4	203	PEB	CAC-CBC-CGC-O2C
82	e4	202	PEB	CAC-CBC-CGC-O1C
82	g4	203	PEB	CAC-CBC-CGC-O1C
82	h4	201	PEB	CAB-CBB-CGB-O1B
82	B5	202	PEB	CAC-CBC-CGC-O2C
82	B5	203	PEB	CAC-CBC-CGC-O1C
82	B5	203	PEB	CAC-CBC-CGC-O2C
82	H5	201	PEB	CAC-CBC-CGC-O2C
82	S5	203	PEB	CAC-CBC-CGC-O2C
82	W5	201	PEB	CAC-CBC-CGC-O2C
82	D7	202	PEB	CAC-CBC-CGC-O1C
82	D7	203	PEB	CAB-CBB-CGB-O1B
82	D7	203	PEB	CAB-CBB-CGB-O2B
82	G7	202	PEB	CAB-CBB-CGB-O1B
82	U7	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	y8	201	PEB	CAC-CBC-CGC-O1C
82	r8	202	PEB	CAC-CBC-CGC-O2C
82	t8	201	PEB	CAB-CBB-CGB-O1B
82	x8	201	PEB	CAC-CBC-CGC-O2C
82	C9	202	PEB	CAC-CBC-CGC-O2C
82	H9	201	PEB	CAC-CBC-CGC-O1C
82	K9	202	PEB	CAC-CBC-CGC-O2C
82	L9	201	PEB	CAC-CBC-CGC-O2C
82	N9	202	PEB	CAC-CBC-CGC-O2C
82	Q9	201	PEB	CAB-CBB-CGB-O2B
82	Q9	203	PEB	CAB-CBB-CGB-O2B
82	S9	201	PEB	CAC-CBC-CGC-O2C
82	T9	202	PEB	CAB-CBB-CGB-O2B
82	dB	201	PEB	CAB-CBB-CGB-O1B
82	gB	201	PEB	CAC-CBC-CGC-O1C
82	gB	201	PEB	CAB-CBB-CGB-O1B
82	gB	202	PEB	CAC-CBC-CGC-O1C
82	gB	202	PEB	CAC-CBC-CGC-O2C
82	rC	202	PEB	CAC-CBC-CGC-O2C
82	tC	201	PEB	CAB-CBB-CGB-O1B
82	aE	202	PEB	CAB-CBB-CGB-O2B
82	fE	201	PEB	CAC-CBC-CGC-O2C
82	kE	202	PEB	CAC-CBC-CGC-O2C
82	gF	202	PEB	CAC-CBC-CGC-O1C
82	kF	202	PEB	CAB-CBB-CGB-O1B
82	oF	203	PEB	CAC-CBC-CGC-O1C
82	sF	202	PEB	CAC-CBC-CGC-O1C
82	wF	301	PEB	CAC-CBC-CGC-O1C
82	wF	301	PEB	CAB-CBB-CGB-O1B
82	aG	202	PEB	CAB-CBB-CGB-O2B
82	dG	201	PEB	CAC-CBC-CGC-O1C
82	dG	201	PEB	CAB-CBB-CGB-O1B
82	fG	201	PEB	CAC-CBC-CGC-O2C
82	hH	202	PEB	CAB-CBB-CGB-O1B
82	kH	201	PEB	CAB-CBB-CGB-O1B
82	eH	203	PEB	CAC-CBC-CGC-O1C
82	aJ	204	PEB	CAC-CBC-CGC-O2C
82	bK	202	PEB	CAB-CBB-CGB-O2B
82	gK	202	PEB	CAC-CBC-CGC-O2C
82	iK	202	PEB	CAC-CBC-CGC-O2C
82	iK	203	PEB	CAC-CBC-CGC-O2C
82	oK	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	pK	202	PEB	CAB-CBB-CGB-O1B
82	sK	202	PEB	CAC-CBC-CGC-O1C
82	aM	202	PEB	CAC-CBC-CGC-O1C
82	iM	202	PEB	CAC-CBC-CGC-O2C
82	iM	202	PEB	CAB-CBB-CGB-O2B
82	mM	202	PEB	CAC-CBC-CGC-O1C
82	iO	203	PEB	CAC-CBC-CGC-O1C
82	kO	202	PEB	CAB-CBB-CGB-O1B
82	lO	201	PEB	CAC-CBC-CGC-O1C
82	mO	203	PEB	CAC-CBC-CGC-O2C
82	eO	202	PEB	CAC-CBC-CGC-O1C
82	eO	203	PEB	CAC-CBC-CGC-O2C
82	hO	201	PEB	CAB-CBB-CGB-O1B
83	AJ	304	PUB	CAB-CBB-CGB-O2B
83	A4	303	PUB	CAB-CBB-CGB-O2B
83	M9	303	PUB	CAB-CBB-CGB-O1B
84	GO	1001	CYC	CAA-CBA-CGA-O1A
84	M1	201	CYC	CAA-CBA-CGA-O1A
84	G4	1001	CYC	CAA-CBA-CGA-O1A
84	K4	1001	CYC	CAA-CBA-CGA-O1A
84	C4	1001	CYC	CAA-CBA-CGA-O2A
87	BN	820	CLA	CAA-CBA-CGA-O1A
87	RN	201	CLA	CAA-CBA-CGA-O2A
87	32	312	CLA	CAA-CBA-CGA-O2A
87	B2	819	CLA	CAA-CBA-CGA-O1A
87	R2	201	CLA	CAA-CBA-CGA-O2A
87	3N	312	CLA	CAA-CBA-CGA-O2A
88	d6	407	LHG	C13-C14-C15-C16
84	EH	1001	CYC	C2B-C3B-CAB-CBB
84	E1	1001	CYC	C2B-C3B-CAB-CBB
85	AL	401	BCR	C16-C17-C18-C36
85	FL	101	BCR	C35-C13-C14-C15
85	KL	100	BCR	C16-C17-C18-C36
85	AN	846	BCR	C20-C21-C22-C37
85	AN	848	BCR	C11-C10-C9-C34
85	AN	848	BCR	C16-C17-C18-C36
85	AN	848	BCR	C20-C21-C22-C37
85	BN	839	BCR	C11-C10-C9-C34
85	BN	840	BCR	C20-C21-C22-C37
85	FN	202	BCR	C35-C13-C14-C15
85	KN	101	BCR	C35-C13-C14-C15
85	KN	104	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
85	LN	201	BCR	C11-C10-C9-C34
85	LN	205	BCR	C11-C10-C9-C34
85	LN	205	BCR	C35-C13-C14-C15
85	A2	846	BCR	C20-C21-C22-C37
85	A2	848	BCR	C11-C10-C9-C34
85	A2	848	BCR	C16-C17-C18-C36
85	A2	848	BCR	C20-C21-C22-C37
85	B2	839	BCR	C11-C10-C9-C34
85	B2	840	BCR	C20-C21-C22-C37
85	F2	203	BCR	C35-C13-C14-C15
85	K2	102	BCR	C35-C13-C14-C15
85	K2	105	BCR	C20-C21-C22-C37
85	L2	201	BCR	C11-C10-C9-C34
85	L2	205	BCR	C11-C10-C9-C34
85	L2	205	BCR	C35-C13-C14-C15
85	A6	401	BCR	C16-C17-C18-C36
85	C6	508	BCR	C20-C21-C22-C37
85	K6	102	BCR	C16-C17-C18-C36
85	c6	603	BCR	C35-C13-C14-C15
85	k6	102	BCR	C16-C17-C18-C36
85	aL	604	BCR	C16-C17-C18-C36
85	fL	101	BCR	C35-C13-C14-C15
85	kL	100	BCR	C16-C17-C18-C36
88	B6	617	LHG	C1-C2-C3-O3
88	cL	501	LHG	C1-C2-C3-O3
95	BL	607	DGD	O1G-C1G-C2G-C3G
82	DA	203	PEB	CAC-CBC-CGC-O1C
82	FA	203	PEB	CAC-CBC-CGC-O1C
82	GA	202	PEB	CAC-CBC-CGC-O1C
82	GA	202	PEB	CAB-CBB-CGB-O1B
82	QA	201	PEB	CAC-CBC-CGC-O2C
82	SA	201	PEB	CAC-CBC-CGC-O1C
82	UA	201	PEB	CAC-CBC-CGC-O1C
82	VA	202	PEB	CAB-CBB-CGB-O1B
82	WA	201	PEB	CAB-CBB-CGB-O1B
82	XA	203	PEB	CAC-CBC-CGC-O1C
82	XA	203	PEB	CAB-CBB-CGB-O2B
82	GB	202	PEB	CAC-CBC-CGC-O1C
82	HB	202	PEB	CAC-CBC-CGC-O1C
82	HB	203	PEB	CAB-CBB-CGB-O1B
82	LB	201	PEB	CAB-CBB-CGB-O2B
82	OB	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	ZB	201	PEB	CAC-CBC-CGC-O2C
82	ZB	201	PEB	CAB-CBB-CGB-O1B
82	ZB	203	PEB	CAB-CBB-CGB-O1B
82	AD	303	PEB	CAB-CBB-CGB-O1B
82	BD	201	PEB	CAC-CBC-CGC-O1C
82	FD	202	PEB	CAC-CBC-CGC-O2C
82	HD	201	PEB	CAB-CBB-CGB-O1B
82	HD	202	PEB	CAC-CBC-CGC-O1C
82	KD	201	PEB	CAC-CBC-CGC-O1C
82	LD	202	PEB	CAC-CBC-CGC-O1C
82	VD	202	PEB	CAC-CBC-CGC-O1C
82	XD	201	PEB	CAC-CBC-CGC-O1C
82	AE	301	PEB	CAC-CBC-CGC-O1C
82	OE	201	PEB	CAB-CBB-CGB-O2B
82	OE	202	PEB	CAC-CBC-CGC-O1C
82	QE	203	PEB	CAC-CBC-CGC-O1C
82	VE	202	PEB	CAB-CBB-CGB-O1B
82	AF	201	PEB	CAC-CBC-CGC-O1C
82	KF	202	PEB	CAC-CBC-CGC-O1C
82	MF	202	PEB	CAB-CBB-CGB-O1B
82	OF	202	PEB	CAC-CBC-CGC-O1C
82	VF	202	PEB	CAB-CBB-CGB-O2B
82	WF	203	PEB	CAC-CBC-CGC-O1C
82	WF	203	PEB	CAB-CBB-CGB-O2B
82	AG	301	PEB	CAC-CBC-CGC-O1C
82	OG	202	PEB	CAC-CBC-CGC-O1C
82	QG	203	PEB	CAC-CBC-CGC-O1C
82	UG	202	PEB	CAC-CBC-CGC-O1C
82	ZG	203	PEB	CAB-CBB-CGB-O1B
82	NH	1002	PEB	CAC-CBC-CGC-O2C
82	NH	1002	PEB	CAB-CBB-CGB-O1B
82	PH	202	PEB	CAC-CBC-CGC-O2C
82	QH	202	PEB	CAB-CBB-CGB-O1B
82	TH	202	PEB	CAC-CBC-CGC-O2C
82	ZH	201	PEB	CAC-CBC-CGC-O1C
82	EI	202	PEB	CAC-CBC-CGC-O1C
82	FI	201	PEB	CAC-CBC-CGC-O1C
82	GI	203	PEB	CAB-CBB-CGB-O1B
82	II	202	PEB	CAC-CBC-CGC-O1C
82	II	202	PEB	CAB-CBB-CGB-O1B
82	KI	203	PEB	CAC-CBC-CGC-O1C
82	RI	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	TI	201	PEB	CAC-CBC-CGC-O1C
82	VI	202	PEB	CAC-CBC-CGC-O1C
82	CJ	201	PEB	CAC-CBC-CGC-O1C
82	DJ	202	PEB	CAC-CBC-CGC-O1C
82	GJ	203	PEB	CAC-CBC-CGC-O1C
82	GJ	203	PEB	CAC-CBC-CGC-O2C
82	JJ	202	PEB	CAB-CBB-CGB-O2B
82	SJ	203	PEB	CAC-CBC-CGC-O2C
82	AK	201	PEB	CAC-CBC-CGC-O1C
82	EK	201	PEB	CAB-CBB-CGB-O1B
82	KK	202	PEB	CAC-CBC-CGC-O1C
82	MK	202	PEB	CAC-CBC-CGC-O2C
82	MK	202	PEB	CAB-CBB-CGB-O1B
82	OK	202	PEB	CAC-CBC-CGC-O1C
82	WK	203	PEB	CAB-CBB-CGB-O2B
82	XK	201	PEB	CAC-CBC-CGC-O1C
82	KM	201	PEB	CAC-CBC-CGC-O1C
82	LM	202	PEB	CAC-CBC-CGC-O1C
82	MM	203	PEB	CAC-CBC-CGC-O1C
82	OM	202	PEB	CAC-CBC-CGC-O1C
82	PM	202	PEB	CAC-CBC-CGC-O1C
82	RM	202	PEB	CAB-CBB-CGB-O2B
82	YM	203	PEB	CAC-CBC-CGC-O1C
82	AO	301	PEB	CAB-CBB-CGB-O2B
82	AO	305	PEB	CAB-CBB-CGB-O1B
82	RO	203	PEB	CAB-CBB-CGB-O1B
82	ZO	201	PEB	CAC-CBC-CGC-O2C
82	CP	202	PEB	CAC-CBC-CGC-O2C
82	CP	203	PEB	CAB-CBB-CGB-O1B
82	EP	202	PEB	CAB-CBB-CGB-O2B
82	GP	201	PEB	CAC-CBC-CGC-O1C
82	IP	202	PEB	CAB-CBB-CGB-O1B
82	IP	203	PEB	CAB-CBB-CGB-O1B
82	IP	203	PEB	CAB-CBB-CGB-O2B
82	OP	201	PEB	CAB-CBB-CGB-O2B
82	QP	203	PEB	CAC-CBC-CGC-O1C
82	QP	203	PEB	CAB-CBB-CGB-O1B
82	RP	202	PEB	CAB-CBB-CGB-O1B
82	TP	201	PEB	CAB-CBB-CGB-O1B
82	TP	202	PEB	CAB-CBB-CGB-O2B
82	UP	202	PEB	CAB-CBB-CGB-O2B
82	AQ	303	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	AQ	304	PEB	CAB-CBB-CGB-O1B
82	BQ	203	PEB	CAB-CBB-CGB-O2B
82	FQ	202	PEB	CAC-CBC-CGC-O2C
82	HQ	201	PEB	CAB-CBB-CGB-O1B
82	HQ	202	PEB	CAC-CBC-CGC-O1C
82	KQ	201	PEB	CAC-CBC-CGC-O1C
82	LQ	202	PEB	CAB-CBB-CGB-O1B
82	MQ	202	PEB	CAC-CBC-CGC-O2C
82	OQ	202	PEB	CAB-CBB-CGB-O1B
82	XQ	201	PEB	CAC-CBC-CGC-O1C
82	N1	1002	PEB	CAC-CBC-CGC-O2C
82	Q1	202	PEB	CAB-CBB-CGB-O1B
82	Z1	201	PEB	CAC-CBC-CGC-O1C
82	h1	201	PEB	CAC-CBC-CGC-O1C
82	h1	203	PEB	CAC-CBC-CGC-O2C
82	j1	202	PEB	CAC-CBC-CGC-O1C
82	k1	201	PEB	CAB-CBB-CGB-O1B
82	A4	301	PEB	CAB-CBB-CGB-O2B
82	D4	1002	PEB	CAB-CBB-CGB-O1B
82	Q4	201	PEB	CAC-CBC-CGC-O2C
82	i4	203	PEB	CAC-CBC-CGC-O1C
82	l4	201	PEB	CAC-CBC-CGC-O1C
82	b4	201	PEB	CAB-CBB-CGB-O2B
82	e4	203	PEB	CAC-CBC-CGC-O2C
82	f4	201	PEB	CAB-CBB-CGB-O1B
82	B5	201	PEB	CAC-CBC-CGC-O1C
82	C5	201	PEB	CAB-CBB-CGB-O1B
82	I5	201	PEB	CAB-CBB-CGB-O1B
82	K5	201	PEB	CAB-CBB-CGB-O1B
82	O5	201	PEB	CAB-CBB-CGB-O1B
82	R5	201	PEB	CAB-CBB-CGB-O1B
82	U5	201	PEB	CAC-CBC-CGC-O1C
82	U5	203	PEB	CAC-CBC-CGC-O1C
82	B7	202	PEB	CAC-CBC-CGC-O1C
82	D7	203	PEB	CAC-CBC-CGC-O1C
82	E7	202	PEB	CAB-CBB-CGB-O1B
82	F7	203	PEB	CAC-CBC-CGC-O1C
82	G7	202	PEB	CAC-CBC-CGC-O1C
82	H7	203	PEB	CAC-CBC-CGC-O1C
82	Q7	201	PEB	CAC-CBC-CGC-O2C
82	V7	202	PEB	CAB-CBB-CGB-O1B
82	p8	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	r8	201	PEB	CAC-CBC-CGC-O1C
82	r8	201	PEB	CAB-CBB-CGB-O1B
82	v8	202	PEB	CAC-CBC-CGC-O1C
82	w8	201	PEB	CAC-CBC-CGC-O2C
82	x8	202	PEB	CAB-CBB-CGB-O1B
82	A9	201	PEB	CAC-CBC-CGC-O1C
82	A9	202	PEB	CAC-CBC-CGC-O2C
82	C9	201	PEB	CAC-CBC-CGC-O1C
82	E9	201	PEB	CAC-CBC-CGC-O1C
82	E9	202	PEB	CAC-CBC-CGC-O2C
82	F9	203	PEB	CAB-CBB-CGB-O1B
82	G9	201	PEB	CAC-CBC-CGC-O1C
82	G9	202	PEB	CAC-CBC-CGC-O2C
82	I9	201	PEB	CAC-CBC-CGC-O1C
82	I9	202	PEB	CAC-CBC-CGC-O2C
82	J9	202	PEB	CAC-CBC-CGC-O1C
82	K9	201	PEB	CAC-CBC-CGC-O1C
82	L9	201	PEB	CAB-CBB-CGB-O1B
82	N9	201	PEB	CAC-CBC-CGC-O1C
82	O9	201	PEB	CAC-CBC-CGC-O1C
82	P9	201	PEB	CAC-CBC-CGC-O1C
82	P9	202	PEB	CAC-CBC-CGC-O2C
82	R9	201	PEB	CAC-CBC-CGC-O1C
82	R9	202	PEB	CAC-CBC-CGC-O2C
82	T9	202	PEB	CAC-CBC-CGC-O2C
82	V9	202	PEB	CAC-CBC-CGC-O2C
82	W9	201	PEB	CAC-CBC-CGC-O1C
82	X9	202	PEB	CAC-CBC-CGC-O2C
82	dB	201	PEB	CAC-CBC-CGC-O1C
82	yC	201	PEB	CAB-CBB-CGB-O2B
82	pC	201	PEB	CAB-CBB-CGB-O1B
82	rC	201	PEB	CAC-CBC-CGC-O1C
82	rC	201	PEB	CAB-CBB-CGB-O1B
82	vC	202	PEB	CAC-CBC-CGC-O1C
82	wC	201	PEB	CAC-CBC-CGC-O2C
82	xC	201	PEB	CAC-CBC-CGC-O2C
82	dE	203	PEB	CAB-CBB-CGB-O1B
82	fE	202	PEB	CAB-CBB-CGB-O2B
82	jE	201	PEB	CAB-CBB-CGB-O2B
82	kE	201	PEB	CAB-CBB-CGB-O1B
82	lE	202	PEB	CAC-CBC-CGC-O1C
82	aF	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	eF	201	PEB	CAB-CBB-CGB-O1B
82	qF	202	PEB	CAC-CBC-CGC-O2C
82	tF	201	PEB	CAC-CBC-CGC-O2C
82	xF	302	PEB	CAC-CBC-CGC-O1C
82	xF	304	PEB	CAC-CBC-CGC-O2C
82	yF	301	PEB	CAC-CBC-CGC-O1C
82	dG	203	PEB	CAB-CBB-CGB-O1B
82	eG	201	PEB	CAC-CBC-CGC-O1C
82	fG	202	PEB	CAB-CBB-CGB-O2B
82	jG	201	PEB	CAB-CBB-CGB-O2B
82	kG	201	PEB	CAB-CBB-CGB-O1B
82	kG	202	PEB	CAC-CBC-CGC-O2C
82	lG	202	PEB	CAB-CBB-CGB-O1B
82	fH	202	PEB	CAC-CBC-CGC-O1C
82	hH	202	PEB	CAC-CBC-CGC-O2C
82	aJ	201	PEB	CAC-CBC-CGC-O1C
82	dJ	201	PEB	CAC-CBC-CGC-O1C
82	hJ	203	PEB	CAC-CBC-CGC-O1C
82	aK	203	PEB	CAB-CBB-CGB-O1B
82	eK	201	PEB	CAB-CBB-CGB-O1B
82	fK	202	PEB	CAC-CBC-CGC-O1C
82	fK	202	PEB	CAB-CBB-CGB-O1B
82	gK	201	PEB	CAC-CBC-CGC-O1C
82	gK	202	PEB	CAB-CBB-CGB-O2B
82	kK	202	PEB	CAB-CBB-CGB-O1B
82	mK	201	PEB	CAC-CBC-CGC-O1C
82	mK	202	PEB	CAC-CBC-CGC-O1C
82	qK	202	PEB	CAC-CBC-CGC-O2C
82	tK	201	PEB	CAC-CBC-CGC-O2C
82	uK	201	PEB	CAC-CBC-CGC-O1C
82	wK	302	PEB	CAB-CBB-CGB-O1B
82	wK	303	PEB	CAC-CBC-CGC-O1C
82	aM	203	PEB	CAC-CBC-CGC-O2C
82	aM	204	PEB	CAC-CBC-CGC-O1C
82	dM	201	PEB	CAC-CBC-CGC-O2C
82	fM	202	PEB	CAB-CBB-CGB-O1B
82	hM	201	PEB	CAC-CBC-CGC-O1C
82	kM	202	PEB	CAC-CBC-CGC-O1C
82	lM	201	PEB	CAC-CBC-CGC-O1C
82	mO	202	PEB	CAC-CBC-CGC-O2C
82	bO	201	PEB	CAB-CBB-CGB-O2B
82	gO	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	bP	502	PEB	CAB-CBB-CGB-O1B
82	Z9	303	PEB	CAC-CBC-CGC-O1C
82	M9	304	PEB	CAC-CBC-CGC-O1C
83	AJ	303	PUB	CAB-CBB-CGB-O2B
83	AM	304	PUB	CAC-CBC-CGC-O2C
83	M5	302	PUB	CAB-CBB-CGB-O1B
83	Z5	302	PUB	CAB-CBB-CGB-O1B
83	Z9	302	PUB	CAB-CBB-CGB-O1B
84	HE	1001	CYC	CAA-CBA-CGA-O2A
84	HG	1001	CYC	CAA-CBA-CGA-O2A
84	JH	1003	CYC	CAA-CBA-CGA-O1A
84	DO	1001	CYC	CAA-CBA-CGA-O1A
84	EO	1001	CYC	CAA-CBA-CGA-O1A
84	JO	1001	CYC	CAA-CBA-CGA-O2A
84	F4	1001	CYC	CAA-CBA-CGA-O1A
84	J4	1001	CYC	CAA-CBA-CGA-O1A
84	E4	1001	CYC	CAA-CBA-CGA-O1A
87	52	605	CLA	CAA-CBA-CGA-O2A
87	1N	605	CLA	CAA-CBA-CGA-O1A
87	5N	605	CLA	CAA-CBA-CGA-O2A
84	N4	1001	CYC	C4B-C3B-CAB-CBB
95	C6	521	DGD	C6B-C7B-C8B-C9B
95	c6	601	DGD	C7A-C8A-C9A-CAA
95	hL	101	DGD	C7B-C8B-C9B-CAB
82	FI	202	PEB	NC-C1C-CHB-C4B
87	BN	825	CLA	C16-C17-C18-C20
87	B2	824	CLA	C16-C17-C18-C20
87	c6	613	CLA	C16-C17-C18-C19
87	d6	401	CLA	C16-C17-C18-C19
87	d6	406	CLA	C16-C17-C18-C19
87	B6	603	CLA	O2A-C1-C2-C3
87	B6	604	CLA	O2A-C1-C2-C3
87	B6	614	CLA	O2A-C1-C2-C3
87	H6	103	CLA	O2A-C1-C2-C3
87	b6	610	CLA	O2A-C1-C2-C3
87	b6	617	CLA	O2A-C1-C2-C3
87	c6	612	CLA	O2A-C1-C2-C3
82	oF	203	PEB	C4B-C3B-CAB-CBB
92	d6	409	LMG	O6-C1-O1-C7
87	b6	609	CLA	C15-C16-C17-C18
87	D6	402	CLA	C4C-C3C-CAC-CBC
82	BA	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	EA	202	PEB	CAB-CBB-CGB-O1B
82	HA	203	PEB	CAC-CBC-CGC-O1C
82	LA	203	PEB	CAB-CBB-CGB-O1B
82	VA	201	PEB	CAC-CBC-CGC-O1C
82	WA	201	PEB	CAC-CBC-CGC-O1C
82	BB	203	PEB	CAC-CBC-CGC-O1C
82	CB	202	PEB	CAB-CBB-CGB-O1B
82	OB	201	PEB	CAB-CBB-CGB-O2B
82	QB	203	PEB	CAB-CBB-CGB-O1B
82	DD	202	PEB	CAC-CBC-CGC-O1C
82	FD	203	PEB	CAB-CBB-CGB-O1B
82	LD	201	PEB	CAC-CBC-CGC-O1C
82	LD	202	PEB	CAB-CBB-CGB-O1B
82	LD	203	PEB	CAC-CBC-CGC-O2C
82	MD	202	PEB	CAC-CBC-CGC-O2C
82	RD	201	PEB	CAB-CBB-CGB-O1B
82	VD	203	PEB	CAB-CBB-CGB-O2B
82	AE	304	PEB	CAB-CBB-CGB-O1B
82	UE	202	PEB	CAC-CBC-CGC-O1C
82	WE	201	PEB	CAB-CBB-CGB-O1B
82	YE	202	PEB	CAB-CBB-CGB-O1B
82	ZE	202	PEB	CAC-CBC-CGC-O1C
82	AF	201	PEB	CAB-CBB-CGB-O1B
82	EF	201	PEB	CAC-CBC-CGC-O1C
82	GF	201	PEB	CAC-CBC-CGC-O1C
82	GF	202	PEB	CAC-CBC-CGC-O2C
82	MF	202	PEB	CAC-CBC-CGC-O2C
82	OF	203	PEB	CAB-CBB-CGB-O1B
82	TF	201	PEB	CAB-CBB-CGB-O1B
82	NG	201	PEB	CAC-CBC-CGC-O1C
82	OG	201	PEB	CAB-CBB-CGB-O2B
82	VG	202	PEB	CAB-CBB-CGB-O1B
82	WG	201	PEB	CAB-CBB-CGB-O1B
82	DH	1002	PEB	CAC-CBC-CGC-O1C
82	JH	1002	PEB	CAB-CBB-CGB-O2B
82	OH	202	PEB	CAB-CBB-CGB-O2B
82	WH	203	PEB	CAC-CBC-CGC-O1C
82	AI	202	PEB	CAC-CBC-CGC-O1C
82	DI	201	PEB	CAC-CBC-CGC-O1C
82	GI	201	PEB	CAC-CBC-CGC-O2C
82	JI	202	PEB	CAB-CBB-CGB-O1B
82	OI	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	TI	203	PEB	CAC-CBC-CGC-O1C
82	UI	201	PEB	CAB-CBB-CGB-O1B
82	XI	202	PEB	CAC-CBC-CGC-O1C
82	CJ	203	PEB	CAC-CBC-CGC-O1C
82	EJ	203	PEB	CAC-CBC-CGC-O2C
82	KJ	201	PEB	CAC-CBC-CGC-O1C
82	MJ	203	PEB	CAC-CBC-CGC-O1C
82	NJ	202	PEB	CAC-CBC-CGC-O1C
82	NJ	202	PEB	CAB-CBB-CGB-O1B
82	PJ	201	PEB	CAC-CBC-CGC-O1C
82	QJ	204	PEB	CAC-CBC-CGC-O1C
82	SJ	202	PEB	CAC-CBC-CGC-O1C
82	VJ	202	PEB	CAC-CBC-CGC-O1C
82	ZJ	202	PEB	CAC-CBC-CGC-O1C
82	GK	201	PEB	CAC-CBC-CGC-O1C
82	OK	203	PEB	CAB-CBB-CGB-O1B
82	QK	202	PEB	CAB-CBB-CGB-O2B
82	TK	201	PEB	CAB-CBB-CGB-O2B
82	WK	203	PEB	CAC-CBC-CGC-O1C
82	AM	302	PEB	CAC-CBC-CGC-O1C
82	DM	202	PEB	CAC-CBC-CGC-O1C
82	UM	203	PEB	CAC-CBC-CGC-O1C
82	VM	201	PEB	CAC-CBC-CGC-O1C
82	AO	301	PEB	CAC-CBC-CGC-O2C
82	DO	1002	PEB	CAB-CBB-CGB-O1B
82	FO	1002	PEB	CAC-CBC-CGC-O2C
82	JO	1002	PEB	CAC-CBC-CGC-O1C
82	PO	203	PEB	CAB-CBB-CGB-O1B
82	RO	202	PEB	CAC-CBC-CGC-O1C
82	RO	203	PEB	CAB-CBB-CGB-O2B
82	SO	202	PEB	CAB-CBB-CGB-O2B
82	EP	203	PEB	CAB-CBB-CGB-O1B
82	MP	203	PEB	CAB-CBB-CGB-O1B
82	PP	201	PEB	CAB-CBB-CGB-O1B
82	PP	202	PEB	CAB-CBB-CGB-O1B
82	SP	203	PEB	CAB-CBB-CGB-O1B
82	DQ	202	PEB	CAC-CBC-CGC-O1C
82	FQ	203	PEB	CAB-CBB-CGB-O1B
82	JQ	203	PEB	CAB-CBB-CGB-O1B
82	LQ	201	PEB	CAC-CBC-CGC-O1C
82	LQ	202	PEB	CAC-CBC-CGC-O1C
82	LQ	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	RQ	201	PEB	CAC-CBC-CGC-O1C
82	RQ	201	PEB	CAB-CBB-CGB-O1B
82	VQ	203	PEB	CAB-CBB-CGB-O2B
82	N1	1002	PEB	CAB-CBB-CGB-O1B
82	O1	201	PEB	CAB-CBB-CGB-O1B
82	O1	202	PEB	CAB-CBB-CGB-O2B
82	P1	202	PEB	CAC-CBC-CGC-O2C
82	S1	202	PEB	CAC-CBC-CGC-O1C
82	T1	202	PEB	CAC-CBC-CGC-O2C
82	D1	1002	PEB	CAC-CBC-CGC-O1C
82	J1	1002	PEB	CAB-CBB-CGB-O2B
82	W1	203	PEB	CAC-CBC-CGC-O1C
82	h1	202	PEB	CAB-CBB-CGB-O1B
82	b1	201	PEB	CAB-CBB-CGB-O1B
82	b1	203	PEB	CAC-CBC-CGC-O1C
82	J4	1002	PEB	CAC-CBC-CGC-O1C
82	J4	1002	PEB	CAB-CBB-CGB-O1B
82	A4	301	PEB	CAC-CBC-CGC-O2C
82	R4	202	PEB	CAC-CBC-CGC-O1C
82	R4	203	PEB	CAB-CBB-CGB-O1B
82	R4	203	PEB	CAB-CBB-CGB-O2B
82	S4	202	PEB	CAB-CBB-CGB-O2B
82	c4	201	PEB	CAC-CBC-CGC-O2C
82	A5	201	PEB	CAB-CBB-CGB-O1B
82	E5	201	PEB	CAB-CBB-CGB-O1B
82	F5	203	PEB	CAC-CBC-CGC-O1C
82	G5	201	PEB	CAB-CBB-CGB-O1B
82	L5	203	PEB	CAC-CBC-CGC-O2C
82	N5	201	PEB	CAB-CBB-CGB-O1B
82	O5	201	PEB	CAB-CBB-CGB-O2B
82	P5	201	PEB	CAB-CBB-CGB-O1B
82	T5	201	PEB	CAB-CBB-CGB-O1B
82	U5	202	PEB	CAC-CBC-CGC-O1C
82	V5	201	PEB	CAB-CBB-CGB-O1B
82	W5	201	PEB	CAC-CBC-CGC-O1C
82	X5	201	PEB	CAB-CBB-CGB-O1B
82	Y5	201	PEB	CAC-CBC-CGC-O1C
82	M7	202	PEB	CAC-CBC-CGC-O2C
82	S7	201	PEB	CAC-CBC-CGC-O1C
82	U7	201	PEB	CAC-CBC-CGC-O1C
82	V7	201	PEB	CAC-CBC-CGC-O1C
82	W7	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	X7	203	PEB	CAB-CBB-CGB-O2B
82	p8	201	PEB	CAC-CBC-CGC-O2C
82	q8	202	PEB	CAB-CBB-CGB-O2B
82	r8	202	PEB	CAB-CBB-CGB-O1B
82	A9	202	PEB	CAB-CBB-CGB-O2B
82	C9	202	PEB	CAB-CBB-CGB-O2B
82	D9	203	PEB	CAB-CBB-CGB-O1B
82	E9	202	PEB	CAB-CBB-CGB-O2B
82	G9	202	PEB	CAB-CBB-CGB-O2B
82	H9	201	PEB	CAB-CBB-CGB-O2B
82	I9	202	PEB	CAB-CBB-CGB-O2B
82	K9	202	PEB	CAB-CBB-CGB-O2B
82	N9	202	PEB	CAB-CBB-CGB-O2B
82	P9	202	PEB	CAB-CBB-CGB-O2B
82	R9	202	PEB	CAB-CBB-CGB-O2B
82	S9	201	PEB	CAB-CBB-CGB-O1B
82	T9	201	PEB	CAC-CBC-CGC-O1C
82	V9	201	PEB	CAC-CBC-CGC-O1C
82	V9	202	PEB	CAB-CBB-CGB-O2B
82	X9	201	PEB	CAC-CBC-CGC-O1C
82	X9	202	PEB	CAB-CBB-CGB-O2B
82	aB	202	PEB	CAB-CBB-CGB-O1B
82	pC	201	PEB	CAC-CBC-CGC-O2C
82	qC	202	PEB	CAB-CBB-CGB-O2B
82	xC	202	PEB	CAB-CBB-CGB-O1B
82	bE	202	PEB	CAB-CBB-CGB-O1B
82	eE	201	PEB	CAC-CBC-CGC-O1C
82	fE	203	PEB	CAC-CBC-CGC-O2C
82	hE	203	PEB	CAC-CBC-CGC-O1C
82	jE	202	PEB	CAB-CBB-CGB-O2B
82	fF	202	PEB	CAB-CBB-CGB-O1B
82	gF	201	PEB	CAC-CBC-CGC-O1C
82	gF	201	PEB	CAC-CBC-CGC-O2C
82	gF	202	PEB	CAB-CBB-CGB-O2B
82	iF	202	PEB	CAC-CBC-CGC-O2C
82	jF	201	PEB	CAC-CBC-CGC-O1C
82	kF	203	PEB	CAC-CBC-CGC-O2C
82	mF	201	PEB	CAC-CBC-CGC-O1C
82	oF	201	PEB	CAB-CBB-CGB-O2B
82	rF	202	PEB	CAB-CBB-CGB-O1B
82	sF	203	PEB	CAC-CBC-CGC-O1C
82	uF	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	vF	201	PEB	CAB-CBB-CGB-O2B
82	fG	203	PEB	CAC-CBC-CGC-O2C
82	hG	203	PEB	CAC-CBC-CGC-O1C
82	gH	203	PEB	CAC-CBC-CGC-O1C
82	hH	201	PEB	CAB-CBB-CGB-O1B
82	jH	202	PEB	CAC-CBC-CGC-O1C
82	lH	201	PEB	CAB-CBB-CGB-O1B
82	bH	201	PEB	CAB-CBB-CGB-O1B
82	aJ	203	PEB	CAC-CBC-CGC-O1C
82	eK	203	PEB	CAB-CBB-CGB-O1B
82	gK	201	PEB	CAC-CBC-CGC-O2C
82	jK	201	PEB	CAC-CBC-CGC-O1C
82	lK	202	PEB	CAB-CBB-CGB-O1B
82	oK	201	PEB	CAB-CBB-CGB-O2B
82	sK	203	PEB	CAC-CBC-CGC-O1C
82	xK	302	PEB	CAC-CBC-CGC-O1C
82	aM	203	PEB	CAC-CBC-CGC-O1C
82	dM	202	PEB	CAC-CBC-CGC-O2C
82	dM	203	PEB	CAB-CBB-CGB-O2B
82	hM	203	PEB	CAC-CBC-CGC-O2C
82	iM	202	PEB	CAB-CBB-CGB-O1B
82	jM	202	PEB	CAB-CBB-CGB-O1B
82	jM	203	PEB	CAC-CBC-CGC-O1C
82	mM	202	PEB	CAB-CBB-CGB-O1B
82	cO	201	PEB	CAC-CBC-CGC-O2C
82	bP	501	PEB	CAB-CBB-CGB-O1B
82	Z9	303	PEB	CAB-CBB-CGB-O1B
82	M9	304	PEB	CAB-CBB-CGB-O1B
83	AE	302	PUB	CAB-CBB-CGB-O1B
83	AG	302	PUB	CAB-CBB-CGB-O1B
83	BM	302	PUB	CAC-CBC-CGC-O1C
83	M5	303	PUB	CAB-CBB-CGB-O2B
83	Z5	303	PUB	CAB-CBB-CGB-O2B
83	yF	303	PUB	CAB-CBB-CGB-O2B
83	yK	303	PUB	CAB-CBB-CGB-O2B
84	DH	1001	CYC	CAA-CBA-CGA-O2A
84	CO	1001	CYC	CAA-CBA-CGA-O2A
84	FO	1001	CYC	CAA-CBA-CGA-O1A
84	JO	1001	CYC	CAA-CBA-CGA-O1A
84	KO	1001	CYC	CAA-CBA-CGA-O1A
84	D1	1001	CYC	CAA-CBA-CGA-O2A
84	73	1002	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
84	J4	1001	CYC	CAA-CBA-CGA-O2A
87	72	605	CLA	CAA-CBA-CGA-O1A
87	7N	605	CLA	CAA-CBA-CGA-O1A
96	f6	101	HEM	CAA-CBA-CGA-O1A
94	a6	601	PL9	C44-C46-C47-C48
88	D6	401	LHG	C29-C30-C31-C32
92	b6	623	LMG	C32-C33-C34-C35
82	RE	201	PEB	C2B-C3B-CAB-CBB
82	RG	201	PEB	C2B-C3B-CAB-CBB
87	C6	514	CLA	C10-C11-C12-C13
88	i6	101	LHG	C32-C33-C34-C35
92	yL	101	LMG	C34-C35-C36-C37
95	C6	502	DGD	C7A-C8A-C9A-CAA
82	AA	202	PEB	CAC-CBC-CGC-O1C
82	BA	202	PEB	CAC-CBC-CGC-O2C
82	BA	203	PEB	CAB-CBB-CGB-O2B
82	MA	202	PEB	CAC-CBC-CGC-O2C
82	NA	203	PEB	CAC-CBC-CGC-O1C
82	RA	203	PEB	CAB-CBB-CGB-O2B
82	XA	203	PEB	CAB-CBB-CGB-O1B
82	YA	303	PEB	CAB-CBB-CGB-O1B
82	YA	304	PEB	CAB-CBB-CGB-O1B
82	YA	304	PEB	CAB-CBB-CGB-O2B
82	DB	202	PEB	CAB-CBB-CGB-O1B
82	PB	201	PEB	CAB-CBB-CGB-O1B
82	XB	201	PEB	CAB-CBB-CGB-O2B
82	AD	304	PEB	CAB-CBB-CGB-O1B
82	BD	203	PEB	CAB-CBB-CGB-O2B
82	RD	201	PEB	CAC-CBC-CGC-O1C
82	VD	201	PEB	CAC-CBC-CGC-O1C
82	VD	203	PEB	CAC-CBC-CGC-O1C
82	NE	202	PEB	CAC-CBC-CGC-O1C
82	UE	203	PEB	CAC-CBC-CGC-O2C
82	VE	202	PEB	CAC-CBC-CGC-O2C
82	WE	202	PEB	CAC-CBC-CGC-O1C
82	DF	201	PEB	CAB-CBB-CGB-O2B
82	EF	201	PEB	CAB-CBB-CGB-O1B
82	LF	201	PEB	CAC-CBC-CGC-O2C
82	PF	202	PEB	CAB-CBB-CGB-O1B
82	SF	203	PEB	CAB-CBB-CGB-O2B
82	TF	202	PEB	CAC-CBC-CGC-O1C
82	UF	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	YF	203	PEB	CAC-CBC-CGC-O2C
82	AG	304	PEB	CAB-CBB-CGB-O1B
82	RG	202	PEB	CAB-CBB-CGB-O2B
82	UG	203	PEB	CAC-CBC-CGC-O2C
82	WG	202	PEB	CAC-CBC-CGC-O1C
82	JH	1002	PEB	CAC-CBC-CGC-O1C
82	OH	202	PEB	CAC-CBC-CGC-O2C
82	PH	202	PEB	CAB-CBB-CGB-O1B
82	QH	201	PEB	CAB-CBB-CGB-O2B
82	ZH	203	PEB	CAB-CBB-CGB-O1B
82	BI	202	PEB	CAC-CBC-CGC-O1C
82	CI	202	PEB	CAC-CBC-CGC-O1C
82	GI	203	PEB	CAC-CBC-CGC-O1C
82	LI	202	PEB	CAB-CBB-CGB-O1B
82	NI	202	PEB	CAC-CBC-CGC-O1C
82	OI	202	PEB	CAC-CBC-CGC-O1C
82	PI	202	PEB	CAC-CBC-CGC-O1C
82	RI	203	PEB	CAC-CBC-CGC-O2C
82	ZI	401	PEB	CAC-CBC-CGC-O1C
82	AJ	302	PEB	CAB-CBB-CGB-O1B
82	DJ	202	PEB	CAB-CBB-CGB-O1B
82	IJ	201	PEB	CAC-CBC-CGC-O1C
82	JJ	202	PEB	CAB-CBB-CGB-O1B
82	MJ	203	PEB	CAC-CBC-CGC-O2C
82	MJ	203	PEB	CAB-CBB-CGB-O1B
82	OJ	203	PEB	CAC-CBC-CGC-O1C
82	QJ	202	PEB	CAC-CBC-CGC-O2C
82	QJ	203	PEB	CAC-CBC-CGC-O2C
82	SJ	201	PEB	CAC-CBC-CGC-O2C
82	TJ	202	PEB	CAB-CBB-CGB-O1B
82	WJ	202	PEB	CAB-CBB-CGB-O1B
82	ZJ	202	PEB	CAB-CBB-CGB-O1B
82	AK	201	PEB	CAB-CBB-CGB-O1B
82	BK	201	PEB	CAC-CBC-CGC-O2C
82	CK	202	PEB	CAC-CBC-CGC-O1C
82	CK	203	PEB	CAC-CBC-CGC-O2C
82	DK	201	PEB	CAB-CBB-CGB-O2B
82	HK	202	PEB	CAB-CBB-CGB-O2B
82	PK	202	PEB	CAB-CBB-CGB-O1B
82	TK	201	PEB	CAB-CBB-CGB-O1B
82	TK	202	PEB	CAC-CBC-CGC-O1C
82	AM	301	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	GM	203	PEB	CAC-CBC-CGC-O1C
82	QM	202	PEB	CAC-CBC-CGC-O1C
82	WM	203	PEB	CAC-CBC-CGC-O1C
82	AP	202	PEB	CAB-CBB-CGB-O1B
82	CP	201	PEB	CAB-CBB-CGB-O1B
82	FP	201	PEB	CAB-CBB-CGB-O1B
82	GP	203	PEB	CAB-CBB-CGB-O1B
82	IP	201	PEB	CAC-CBC-CGC-O2C
82	LP	202	PEB	CAB-CBB-CGB-O1B
82	LP	202	PEB	CAB-CBB-CGB-O2B
82	MP	202	PEB	CAB-CBB-CGB-O1B
82	OP	202	PEB	CAC-CBC-CGC-O1C
82	RP	201	PEB	CAB-CBB-CGB-O1B
82	SP	201	PEB	CAC-CBC-CGC-O1C
82	XP	202	PEB	CAB-CBB-CGB-O2B
82	YP	502	PEB	CAC-CBC-CGC-O1C
82	AQ	303	PEB	CAC-CBC-CGC-O1C
82	FQ	201	PEB	CAB-CBB-CGB-O1B
82	JQ	203	PEB	CAB-CBB-CGB-O2B
82	NQ	203	PEB	CAB-CBB-CGB-O1B
82	UQ	202	PEB	CAB-CBB-CGB-O1B
82	VQ	203	PEB	CAC-CBC-CGC-O1C
82	N1	1002	PEB	CAC-CBC-CGC-O1C
82	O1	202	PEB	CAC-CBC-CGC-O2C
82	Q1	201	PEB	CAB-CBB-CGB-O2B
82	T1	202	PEB	CAC-CBC-CGC-O1C
82	U1	202	PEB	CAC-CBC-CGC-O1C
82	U1	203	PEB	CAB-CBB-CGB-O2B
82	J1	1002	PEB	CAC-CBC-CGC-O1C
82	W1	203	PEB	CAC-CBC-CGC-O2C
82	f1	202	PEB	CAC-CBC-CGC-O1C
82	j1	203	PEB	CAC-CBC-CGC-O1C
82	l1	202	PEB	CAB-CBB-CGB-O1B
82	l1	203	PEB	CAB-CBB-CGB-O1B
82	a1	201	PEB	CAB-CBB-CGB-O1B
82	a1	202	PEB	CAB-CBB-CGB-O1B
82	d1	203	PEB	CAB-CBB-CGB-O1B
82	R4	203	PEB	CAC-CBC-CGC-O1C
82	j4	201	PEB	CAB-CBB-CGB-O1B
82	m4	201	PEB	CAC-CBC-CGC-O2C
82	e4	203	PEB	CAB-CBB-CGB-O2B
82	f4	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	D5	203	PEB	CAC-CBC-CGC-O1C
82	D5	203	PEB	CAB-CBB-CGB-O2B
82	M5	304	PEB	CAB-CBB-CGB-O1B
82	U5	202	PEB	CAC-CBC-CGC-O2C
82	W5	203	PEB	CAC-CBC-CGC-O1C
82	A7	202	PEB	CAC-CBC-CGC-O1C
82	B7	202	PEB	CAC-CBC-CGC-O2C
82	B7	203	PEB	CAB-CBB-CGB-O2B
82	N7	203	PEB	CAC-CBC-CGC-O1C
82	R7	201	PEB	CAB-CBB-CGB-O1B
82	R7	203	PEB	CAB-CBB-CGB-O2B
82	W7	201	PEB	CAC-CBC-CGC-O1C
82	X7	203	PEB	CAC-CBC-CGC-O1C
82	X7	203	PEB	CAB-CBB-CGB-O1B
82	Y7	303	PEB	CAB-CBB-CGB-O1B
82	s8	203	PEB	CAB-CBB-CGB-O2B
82	t8	202	PEB	CAC-CBC-CGC-O2C
82	u8	202	PEB	CAC-CBC-CGC-O1C
82	v8	201	PEB	CAC-CBC-CGC-O2C
82	B9	201	PEB	CAB-CBB-CGB-O1B
82	D9	201	PEB	CAB-CBB-CGB-O2B
82	H9	203	PEB	CAB-CBB-CGB-O1B
82	L9	201	PEB	CAB-CBB-CGB-O2B
82	O9	202	PEB	CAC-CBC-CGC-O1C
82	O9	202	PEB	CAC-CBC-CGC-O2C
82	Q9	201	PEB	CAB-CBB-CGB-O1B
82	U9	203	PEB	CAB-CBB-CGB-O1B
82	U9	204	PEB	CAC-CBC-CGC-O2C
82	Y9	201	PEB	CAC-CBC-CGC-O1C
82	cB	402	PEB	CAB-CBB-CGB-O1B
82	hB	301	PEB	CAB-CBB-CGB-O2B
82	rC	202	PEB	CAB-CBB-CGB-O1B
82	sC	203	PEB	CAB-CBB-CGB-O2B
82	tC	202	PEB	CAC-CBC-CGC-O1C
82	uC	202	PEB	CAC-CBC-CGC-O1C
82	cE	202	PEB	CAB-CBB-CGB-O2B
82	lE	203	PEB	CAB-CBB-CGB-O1B
82	mE	203	PEB	CAB-CBB-CGB-O1B
82	aF	202	PEB	CAB-CBB-CGB-O1B
82	cF	201	PEB	CAB-CBB-CGB-O1B
82	eF	202	PEB	CAC-CBC-CGC-O1C
82	eF	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	mF	202	PEB	CAC-CBC-CGC-O1C
82	qF	201	PEB	CAB-CBB-CGB-O2B
82	tF	202	PEB	CAC-CBC-CGC-O1C
82	zF	501	PEB	CAC-CBC-CGC-O1C
82	cG	202	PEB	CAB-CBB-CGB-O2B
82	jG	202	PEB	CAB-CBB-CGB-O2B
82	mG	203	PEB	CAB-CBB-CGB-O1B
82	gH	203	PEB	CAC-CBC-CGC-O2C
82	hH	202	PEB	CAB-CBB-CGB-O2B
82	jH	203	PEB	CAC-CBC-CGC-O1C
82	lH	202	PEB	CAB-CBB-CGB-O1B
82	aH	201	PEB	CAB-CBB-CGB-O1B
82	aH	202	PEB	CAB-CBB-CGB-O1B
82	hJ	201	PEB	CAC-CBC-CGC-O2C
82	cK	201	PEB	CAB-CBB-CGB-O1B
82	eK	202	PEB	CAC-CBC-CGC-O1C
82	gK	202	PEB	CAC-CBC-CGC-O1C
82	kK	203	PEB	CAC-CBC-CGC-O2C
82	qK	201	PEB	CAB-CBB-CGB-O2B
82	rK	202	PEB	CAB-CBB-CGB-O1B
82	tK	202	PEB	CAC-CBC-CGC-O1C
82	xK	304	PEB	CAC-CBC-CGC-O2C
82	yK	301	PEB	CAC-CBC-CGC-O1C
82	zK	501	PEB	CAC-CBC-CGC-O1C
82	lM	202	PEB	CAC-CBC-CGC-O2C
82	mM	202	PEB	CAB-CBB-CGB-O2B
82	jO	201	PEB	CAB-CBB-CGB-O1B
82	mO	201	PEB	CAC-CBC-CGC-O2C
82	fO	201	PEB	CAC-CBC-CGC-O1C
82	fO	201	PEB	CAB-CBB-CGB-O1B
82	hO	202	PEB	CAC-CBC-CGC-O2C
82	Z9	301	PEB	CAC-CBC-CGC-O2C
82	M9	302	PEB	CAC-CBC-CGC-O2C
83	M5	302	PUB	CAB-CBB-CGB-O2B
84	IO	1001	CYC	CAA-CBA-CGA-O2A
84	y3	1001	CYC	CAD-CBD-CGD-O2D
84	D4	1001	CYC	CAA-CBA-CGA-O1A
87	12	605	CLA	CAA-CBA-CGA-O1A
87	12	605	CLA	CAA-CBA-CGA-O2A
87	1N	605	CLA	CAA-CBA-CGA-O2A
96	E6	101	HEM	CAA-CBA-CGA-O1A
92	XL	601	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
92	bL	611	LMG	C9-C8-O7-C10
87	AN	808	CLA	C4-C3-C5-C6
87	A2	808	CLA	C4-C3-C5-C6
87	CL	513	CLA	C1A-C2A-CAA-CBA
87	AN	816	CLA	C1A-C2A-CAA-CBA
87	BN	829	CLA	C1A-C2A-CAA-CBA
87	FN	203	CLA	C1A-C2A-CAA-CBA
87	LN	206	CLA	C1A-C2A-CAA-CBA
87	12	601	CLA	C1A-C2A-CAA-CBA
87	22	606	CLA	C1A-C2A-CAA-CBA
87	52	611	CLA	C1A-C2A-CAA-CBA
87	A2	816	CLA	C1A-C2A-CAA-CBA
87	B2	829	CLA	C1A-C2A-CAA-CBA
87	F2	201	CLA	C1A-C2A-CAA-CBA
87	K2	101	CLA	C1A-C2A-CAA-CBA
87	L2	206	CLA	C1A-C2A-CAA-CBA
87	H6	102	CLA	C1A-C2A-CAA-CBA
87	b6	618	CLA	C1A-C2A-CAA-CBA
87	c6	604	CLA	C1A-C2A-CAA-CBA
87	1N	601	CLA	C1A-C2A-CAA-CBA
87	2N	306	CLA	C1A-C2A-CAA-CBA
87	5N	611	CLA	C1A-C2A-CAA-CBA
87	BN	836	CLA	C16-C17-C18-C19
87	B2	836	CLA	C16-C17-C18-C19
87	bL	615	CLA	C16-C17-C18-C19
87	AL	403	CLA	C11-C12-C13-C15
87	BL	603	CLA	C6-C7-C8-C10
87	BL	605	CLA	C12-C13-C15-C16
87	AN	802	CLA	C6-C7-C8-C10
87	AN	823	CLA	C11-C12-C13-C15
87	BN	805	CLA	C11-C10-C8-C7
87	BN	810	CLA	C6-C7-C8-C10
87	A2	801	CLA	C6-C7-C8-C10
87	A2	823	CLA	C11-C12-C13-C15
87	B2	804	CLA	C11-C10-C8-C7
87	B2	809	CLA	C6-C7-C8-C10
87	B6	605	CLA	C11-C10-C8-C7
87	B6	606	CLA	C12-C13-C15-C16
87	B6	616	CLA	C11-C10-C8-C7
87	C6	514	CLA	C6-C7-C8-C10
87	C6	520	CLA	C6-C7-C8-C10
87	D6	403	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
87	b6	616	CLA	C11-C12-C13-C15
87	c6	605	CLA	C2-C3-C5-C6
87	cL	508	CLA	C6-C7-C8-C10
87	cL	509	CLA	C12-C13-C15-C16
87	AN	820	CLA	C15-C16-C17-C18
87	A2	820	CLA	C15-C16-C17-C18
82	IA	202	PEB	CAC-CBC-CGC-O2C
82	RA	201	PEB	CAB-CBB-CGB-O1B
82	DB	203	PEB	CAB-CBB-CGB-O2B
82	EB	501	PEB	CAB-CBB-CGB-O2B
82	GB	202	PEB	CAB-CBB-CGB-O1B
82	JB	202	PEB	CAB-CBB-CGB-O2B
82	KB	304	PEB	CAB-CBB-CGB-O2B
82	TB	202	PEB	CAB-CBB-CGB-O2B
82	WB	401	PEB	CAB-CBB-CGB-O1B
82	XB	201	PEB	CAB-CBB-CGB-O1B
82	ZB	202	PEB	CAB-CBB-CGB-O2B
82	AD	304	PEB	CAB-CBB-CGB-O2B
82	BD	201	PEB	CAC-CBC-CGC-O2C
82	FD	201	PEB	CAB-CBB-CGB-O2B
82	GD	202	PEB	CAC-CBC-CGC-O2C
82	JD	203	PEB	CAC-CBC-CGC-O2C
82	JD	203	PEB	CAB-CBB-CGB-O1B
82	JD	203	PEB	CAB-CBB-CGB-O2B
82	PD	201	PEB	CAC-CBC-CGC-O2C
82	PD	203	PEB	CAC-CBC-CGC-O2C
82	TD	201	PEB	CAB-CBB-CGB-O2B
82	UD	202	PEB	CAB-CBB-CGB-O1B
82	VD	201	PEB	CAC-CBC-CGC-O2C
82	PE	202	PEB	CAB-CBB-CGB-O2B
82	RE	202	PEB	CAB-CBB-CGB-O2B
82	VE	202	PEB	CAC-CBC-CGC-O1C
82	WE	203	PEB	CAC-CBC-CGC-O2C
82	BF	201	PEB	CAC-CBC-CGC-O2C
82	CF	203	PEB	CAC-CBC-CGC-O2C
82	MF	201	PEB	CAC-CBC-CGC-O2C
82	TF	201	PEB	CAB-CBB-CGB-O2B
82	WF	203	PEB	CAC-CBC-CGC-O2C
82	XF	201	PEB	CAC-CBC-CGC-O1C
82	PG	202	PEB	CAB-CBB-CGB-O2B
82	VG	202	PEB	CAC-CBC-CGC-O1C
82	ZG	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	AH	305	PEB	CAC-CBC-CGC-O1C
82	FH	1002	PEB	CAB-CBB-CGB-O1B
82	NH	1002	PEB	CAC-CBC-CGC-O1C
82	NH	1002	PEB	CAB-CBB-CGB-O2B
82	OH	203	PEB	CAC-CBC-CGC-O2C
82	SH	201	PEB	CAC-CBC-CGC-O2C
82	SH	202	PEB	CAC-CBC-CGC-O1C
82	TH	202	PEB	CAC-CBC-CGC-O1C
82	UH	203	PEB	CAB-CBB-CGB-O2B
82	WH	203	PEB	CAC-CBC-CGC-O2C
82	FI	202	PEB	CAB-CBB-CGB-O1B
82	HI	201	PEB	CAC-CBC-CGC-O2C
82	HI	201	PEB	CAB-CBB-CGB-O1B
82	JI	202	PEB	CAB-CBB-CGB-O2B
82	KI	201	PEB	CAC-CBC-CGC-O1C
82	KI	201	PEB	CAC-CBC-CGC-O2C
82	NI	203	PEB	CAC-CBC-CGC-O1C
82	NI	203	PEB	CAC-CBC-CGC-O2C
82	SI	202	PEB	CAB-CBB-CGB-O1B
82	HJ	202	PEB	CAC-CBC-CGC-O2C
82	HJ	202	PEB	CAB-CBB-CGB-O1B
82	NJ	202	PEB	CAB-CBB-CGB-O2B
82	OJ	201	PEB	CAC-CBC-CGC-O2C
82	PJ	201	PEB	CAC-CBC-CGC-O2C
82	FK	202	PEB	CAC-CBC-CGC-O1C
82	LK	201	PEB	CAC-CBC-CGC-O2C
82	MK	201	PEB	CAC-CBC-CGC-O2C
82	WK	203	PEB	CAC-CBC-CGC-O2C
82	YK	203	PEB	CAC-CBC-CGC-O2C
82	DM	201	PEB	CAC-CBC-CGC-O2C
82	DM	202	PEB	CAB-CBB-CGB-O1B
82	GM	202	PEB	CAB-CBB-CGB-O1B
82	GM	203	PEB	CAC-CBC-CGC-O2C
82	IM	202	PEB	CAC-CBC-CGC-O2C
82	IM	203	PEB	CAC-CBC-CGC-O2C
82	KM	202	PEB	CAB-CBB-CGB-O1B
82	MM	203	PEB	CAC-CBC-CGC-O2C
82	OM	202	PEB	CAB-CBB-CGB-O2B
82	AO	301	PEB	CAB-CBB-CGB-O1B
82	AO	304	PEB	CAC-CBC-CGC-O2C
82	JO	1002	PEB	CAB-CBB-CGB-O1B
82	PO	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	PO	203	PEB	CAB-CBB-CGB-O2B
82	QO	201	PEB	CAC-CBC-CGC-O1C
82	AP	203	PEB	CAB-CBB-CGB-O2B
82	EP	201	PEB	CAC-CBC-CGC-O2C
82	MP	202	PEB	CAB-CBB-CGB-O2B
82	MP	203	PEB	CAC-CBC-CGC-O2C
82	OP	201	PEB	CAC-CBC-CGC-O2C
82	QP	203	PEB	CAB-CBB-CGB-O2B
82	XP	202	PEB	CAB-CBB-CGB-O1B
82	YP	503	PEB	CAB-CBB-CGB-O1B
82	AQ	304	PEB	CAB-CBB-CGB-O2B
82	BQ	201	PEB	CAC-CBC-CGC-O1C
82	BQ	201	PEB	CAC-CBC-CGC-O2C
82	GQ	202	PEB	CAC-CBC-CGC-O2C
82	HQ	201	PEB	CAB-CBB-CGB-O2B
82	PQ	201	PEB	CAC-CBC-CGC-O2C
82	PQ	203	PEB	CAC-CBC-CGC-O2C
82	QQ	202	PEB	CAC-CBC-CGC-O2C
82	TQ	201	PEB	CAB-CBB-CGB-O2B
82	TQ	203	PEB	CAC-CBC-CGC-O2C
82	VQ	201	PEB	CAC-CBC-CGC-O1C
82	VQ	201	PEB	CAC-CBC-CGC-O2C
82	N1	1002	PEB	CAB-CBB-CGB-O2B
82	O1	203	PEB	CAC-CBC-CGC-O2C
82	R1	202	PEB	CAB-CBB-CGB-O1B
82	A1	305	PEB	CAC-CBC-CGC-O1C
82	Z1	203	PEB	CAB-CBB-CGB-O1B
82	h1	201	PEB	CAC-CBC-CGC-O2C
82	j1	202	PEB	CAC-CBC-CGC-O2C
82	l1	203	PEB	CAB-CBB-CGB-O2B
82	a1	202	PEB	CAB-CBB-CGB-O2B
82	b1	201	PEB	CAB-CBB-CGB-O2B
82	b1	202	PEB	CAB-CBB-CGB-O1B
82	J4	1002	PEB	CAC-CBC-CGC-O2C
82	A4	304	PEB	CAB-CBB-CGB-O2B
82	P4	202	PEB	CAC-CBC-CGC-O2C
82	l4	202	PEB	CAB-CBB-CGB-O2B
82	d4	201	PEB	CAB-CBB-CGB-O1B
82	h4	202	PEB	CAC-CBC-CGC-O2C
82	D5	201	PEB	CAC-CBC-CGC-O1C
82	F5	203	PEB	CAB-CBB-CGB-O2B
82	H5	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	J5	201	PEB	CAC-CBC-CGC-O2C
82	L5	203	PEB	CAC-CBC-CGC-O1C
82	S5	201	PEB	CAB-CBB-CGB-O2B
82	U5	203	PEB	CAC-CBC-CGC-O2C
82	Z5	304	PEB	CAB-CBB-CGB-O1B
82	D7	202	PEB	CAB-CBB-CGB-O2B
82	I7	202	PEB	CAC-CBC-CGC-O2C
82	L7	203	PEB	CAB-CBB-CGB-O1B
82	Y7	304	PEB	CAB-CBB-CGB-O1B
82	Y7	304	PEB	CAB-CBB-CGB-O2B
82	t8	202	PEB	CAC-CBC-CGC-O1C
82	x8	201	PEB	CAB-CBB-CGB-O2B
82	x8	202	PEB	CAC-CBC-CGC-O2C
82	B9	201	PEB	CAB-CBB-CGB-O2B
82	D9	201	PEB	CAC-CBC-CGC-O1C
82	J9	201	PEB	CAC-CBC-CGC-O2C
82	O9	203	PEB	CAB-CBB-CGB-O1B
82	Q9	203	PEB	CAB-CBB-CGB-O1B
82	gB	203	PEB	CAC-CBC-CGC-O1C
82	1C	201	PEB	CAB-CBB-CGB-O2B
82	tC	202	PEB	CAC-CBC-CGC-O2C
82	vC	201	PEB	CAC-CBC-CGC-O2C
82	xC	201	PEB	CAB-CBB-CGB-O2B
82	xC	202	PEB	CAC-CBC-CGC-O1C
82	xC	202	PEB	CAC-CBC-CGC-O2C
82	cE	202	PEB	CAC-CBC-CGC-O1C
82	cE	202	PEB	CAC-CBC-CGC-O2C
82	eE	203	PEB	CAC-CBC-CGC-O2C
82	fE	201	PEB	CAB-CBB-CGB-O2B
82	fE	202	PEB	CAC-CBC-CGC-O2C
82	hE	202	PEB	CAC-CBC-CGC-O2C
82	iE	201	PEB	CAC-CBC-CGC-O1C
82	dF	202	PEB	CAB-CBB-CGB-O2B
82	iF	203	PEB	CAC-CBC-CGC-O1C
82	lF	202	PEB	CAB-CBB-CGB-O1B
82	pF	202	PEB	CAB-CBB-CGB-O1B
82	sF	201	PEB	CAB-CBB-CGB-O1B
82	tF	202	PEB	CAB-CBB-CGB-O2B
82	eG	203	PEB	CAC-CBC-CGC-O2C
82	fG	201	PEB	CAB-CBB-CGB-O2B
82	fG	202	PEB	CAC-CBC-CGC-O2C
82	hG	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	iG	201	PEB	CAC-CBC-CGC-O1C
82	lG	202	PEB	CAC-CBC-CGC-O2C
82	lG	203	PEB	CAB-CBB-CGB-O1B
82	fH	201	PEB	CAC-CBC-CGC-O2C
82	jH	202	PEB	CAC-CBC-CGC-O2C
82	lH	202	PEB	CAB-CBB-CGB-O2B
82	aH	202	PEB	CAB-CBB-CGB-O2B
82	bH	201	PEB	CAB-CBB-CGB-O2B
82	bH	202	PEB	CAB-CBB-CGB-O1B
82	dH	203	PEB	CAC-CBC-CGC-O2C
82	dH	203	PEB	CAB-CBB-CGB-O1B
82	aJ	203	PEB	CAC-CBC-CGC-O2C
82	fJ	203	PEB	CAB-CBB-CGB-O2B
82	gJ	202	PEB	CAC-CBC-CGC-O2C
82	gJ	202	PEB	CAB-CBB-CGB-O1B
82	jJ	201	PEB	CAC-CBC-CGC-O2C
82	lJ	203	PEB	CAC-CBC-CGC-O2C
82	mJ	202	PEB	CAC-CBC-CGC-O2C
82	mJ	202	PEB	CAB-CBB-CGB-O1B
82	aK	202	PEB	CAB-CBB-CGB-O1B
82	iK	203	PEB	CAC-CBC-CGC-O1C
82	sK	201	PEB	CAB-CBB-CGB-O1B
82	dM	203	PEB	CAC-CBC-CGC-O1C
82	fM	203	PEB	CAC-CBC-CGC-O1C
82	jM	201	PEB	CAB-CBB-CGB-O2B
82	jM	202	PEB	CAB-CBB-CGB-O2B
82	kM	202	PEB	CAB-CBB-CGB-O1B
82	lM	201	PEB	CAC-CBC-CGC-O2C
82	kO	202	PEB	CAB-CBB-CGB-O2B
82	lO	202	PEB	CAB-CBB-CGB-O2B
82	dO	201	PEB	CAB-CBB-CGB-O1B
82	eO	203	PEB	CAB-CBB-CGB-O2B
82	M9	301	PEB	CAB-CBB-CGB-O1B
83	BM	302	PUB	CAB-CBB-CGB-O2B
83	M5	303	PUB	CAC-CBC-CGC-O1C
83	Z5	302	PUB	CAB-CBB-CGB-O2B
83	Z5	303	PUB	CAC-CBC-CGC-O1C
83	wF	304	PUB	CAB-CBB-CGB-O1B
83	wK	304	PUB	CAB-CBB-CGB-O1B
83	Z9	305	PUB	CAC-CBC-CGC-O2C
84	DE	1001	CYC	CAA-CBA-CGA-O2A
84	DG	1001	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
84	HG	1001	CYC	CAA-CBA-CGA-O1A
84	DO	1001	CYC	CAA-CBA-CGA-O2A
84	V3	1001	CYC	CAA-CBA-CGA-O2A
84	W3	1001	CYC	CAD-CBD-CGD-O2D
84	x3	1001	CYC	CAA-CBA-CGA-O2A
84	I4	1001	CYC	CAA-CBA-CGA-O2A
84	D4	1001	CYC	CAA-CBA-CGA-O2A
87	AN	818	CLA	CAA-CBA-CGA-O1A
87	42	605	CLA	CAA-CBA-CGA-O1A
87	62	306	CLA	CAA-CBA-CGA-O1A
87	A2	818	CLA	CAA-CBA-CGA-O1A
87	B2	819	CLA	CAA-CBA-CGA-O2A
87	3N	306	CLA	CAA-CBA-CGA-O1A
87	4N	605	CLA	CAA-CBA-CGA-O1A
87	6N	605	CLA	CAA-CBA-CGA-O1A
96	f6	101	HEM	CAA-CBA-CGA-O2A
88	L6	101	LHG	C31-C32-C33-C34
87	CL	518	CLA	CAA-CBA-CGA-O1A
85	LN	205	BCR	C9-C10-C11-C12
85	L2	205	BCR	C9-C10-C11-C12
85	cL	503	BCR	C9-C10-C11-C12
85	hL	102	BCR	C9-C10-C11-C12
92	XL	601	LMG	C42-C43-C44-C45
95	C6	521	DGD	O6D-C5D-C6D-O5D
87	BL	621	CLA	O1A-CGA-O2A-C1
82	BA	201	PEB	CAC-CBC-CGC-O2C
82	DA	202	PEB	CAB-CBB-CGB-O2B
82	FA	202	PEB	CAC-CBC-CGC-O1C
82	GA	202	PEB	CAC-CBC-CGC-O2C
82	IA	202	PEB	CAC-CBC-CGC-O1C
82	IA	202	PEB	CAB-CBB-CGB-O2B
82	JA	203	PEB	CAB-CBB-CGB-O1B
82	JA	203	PEB	CAB-CBB-CGB-O2B
82	MA	201	PEB	CAC-CBC-CGC-O1C
82	PA	201	PEB	CAC-CBC-CGC-O1C
82	WA	201	PEB	CAB-CBB-CGB-O2B
82	BB	202	PEB	CAB-CBB-CGB-O1B
82	DB	203	PEB	CAC-CBC-CGC-O1C
82	FB	201	PEB	CAC-CBC-CGC-O1C
82	GB	203	PEB	CAB-CBB-CGB-O2B
82	HB	201	PEB	CAB-CBB-CGB-O1B
82	HB	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	IB	202	PEB	CAC-CBC-CGC-O2C
82	QB	202	PEB	CAC-CBC-CGC-O2C
82	QB	203	PEB	CAB-CBB-CGB-O2B
82	UB	303	PEB	CAC-CBC-CGC-O2C
82	VB	201	PEB	CAC-CBC-CGC-O2C
82	XB	201	PEB	CAC-CBC-CGC-O2C
82	ZB	201	PEB	CAC-CBC-CGC-O1C
82	AD	303	PEB	CAC-CBC-CGC-O1C
82	AD	303	PEB	CAC-CBC-CGC-O2C
82	FD	201	PEB	CAB-CBB-CGB-O1B
82	HD	201	PEB	CAB-CBB-CGB-O2B
82	HD	203	PEB	CAC-CBC-CGC-O2C
82	HD	203	PEB	CAB-CBB-CGB-O2B
82	ND	203	PEB	CAB-CBB-CGB-O1B
82	RD	202	PEB	CAB-CBB-CGB-O2B
82	TD	201	PEB	CAB-CBB-CGB-O1B
82	VD	201	PEB	CAB-CBB-CGB-O2B
82	VD	203	PEB	CAC-CBC-CGC-O2C
82	WD	201	PEB	CAC-CBC-CGC-O2C
82	AE	301	PEB	CAC-CBC-CGC-O2C
82	AE	304	PEB	CAB-CBB-CGB-O2B
82	QE	202	PEB	CAC-CBC-CGC-O1C
82	YE	202	PEB	CAC-CBC-CGC-O2C
82	ZE	202	PEB	CAB-CBB-CGB-O1B
82	CF	202	PEB	CAC-CBC-CGC-O1C
82	GF	202	PEB	CAC-CBC-CGC-O1C
82	PF	202	PEB	CAB-CBB-CGB-O2B
82	TF	202	PEB	CAC-CBC-CGC-O2C
82	XF	201	PEB	CAC-CBC-CGC-O2C
82	AG	301	PEB	CAC-CBC-CGC-O2C
82	AG	304	PEB	CAB-CBB-CGB-O2B
82	WG	203	PEB	CAC-CBC-CGC-O2C
82	YG	202	PEB	CAC-CBC-CGC-O2C
82	ZG	202	PEB	CAB-CBB-CGB-O1B
82	AH	302	PEB	CAC-CBC-CGC-O1C
82	OH	203	PEB	CAC-CBC-CGC-O1C
82	QH	203	PEB	CAC-CBC-CGC-O1C
82	RH	201	PEB	CAB-CBB-CGB-O1B
82	RH	202	PEB	CAC-CBC-CGC-O1C
82	RH	202	PEB	CAB-CBB-CGB-O1B
82	UH	201	PEB	CAC-CBC-CGC-O2C
82	ZH	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	OI	202	PEB	CAC-CBC-CGC-O2C
82	SI	201	PEB	CAC-CBC-CGC-O2C
82	CJ	201	PEB	CAC-CBC-CGC-O2C
82	IJ	202	PEB	CAC-CBC-CGC-O1C
82	JJ	202	PEB	CAC-CBC-CGC-O1C
82	KJ	201	PEB	CAC-CBC-CGC-O2C
82	WJ	201	PEB	CAC-CBC-CGC-O2C
82	GK	202	PEB	CAC-CBC-CGC-O1C
82	SK	203	PEB	CAB-CBB-CGB-O2B
82	UK	202	PEB	CAB-CBB-CGB-O1B
82	XK	201	PEB	CAC-CBC-CGC-O2C
82	DM	201	PEB	CAC-CBC-CGC-O1C
82	EM	203	PEB	CAB-CBB-CGB-O1B
82	KM	202	PEB	CAC-CBC-CGC-O2C
82	SM	202	PEB	CAC-CBC-CGC-O1C
82	UM	203	PEB	CAC-CBC-CGC-O2C
82	WM	201	PEB	CAC-CBC-CGC-O1C
82	XM	202	PEB	CAC-CBC-CGC-O1C
82	YM	203	PEB	CAC-CBC-CGC-O2C
82	AO	304	PEB	CAB-CBB-CGB-O2B
82	FO	1002	PEB	CAB-CBB-CGB-O2B
82	JO	1002	PEB	CAC-CBC-CGC-O2C
82	RO	203	PEB	CAC-CBC-CGC-O1C
82	ZO	201	PEB	CAC-CBC-CGC-O1C
82	CP	201	PEB	CAC-CBC-CGC-O2C
82	FP	202	PEB	CAB-CBB-CGB-O1B
82	GP	201	PEB	CAC-CBC-CGC-O2C
82	OP	202	PEB	CAC-CBC-CGC-O2C
82	SP	201	PEB	CAB-CBB-CGB-O1B
82	SP	201	PEB	CAB-CBB-CGB-O2B
82	TP	202	PEB	CAB-CBB-CGB-O1B
82	UP	203	PEB	CAC-CBC-CGC-O2C
82	WP	201	PEB	CAB-CBB-CGB-O1B
82	WP	202	PEB	CAC-CBC-CGC-O2C
82	XP	201	PEB	CAB-CBB-CGB-O2B
82	AQ	303	PEB	CAC-CBC-CGC-O2C
82	AQ	304	PEB	CAC-CBC-CGC-O2C
82	HQ	203	PEB	CAC-CBC-CGC-O2C
82	HQ	203	PEB	CAB-CBB-CGB-O1B
82	HQ	203	PEB	CAB-CBB-CGB-O2B
82	RQ	202	PEB	CAB-CBB-CGB-O1B
82	RQ	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	SQ	202	PEB	CAB-CBB-CGB-O1B
82	TQ	201	PEB	CAB-CBB-CGB-O1B
82	VQ	201	PEB	CAB-CBB-CGB-O2B
82	VQ	203	PEB	CAC-CBC-CGC-O2C
82	WQ	201	PEB	CAC-CBC-CGC-O2C
82	YQ	201	PEB	CAC-CBC-CGC-O1C
82	O1	203	PEB	CAC-CBC-CGC-O1C
82	P1	202	PEB	CAB-CBB-CGB-O1B
82	R1	201	PEB	CAB-CBB-CGB-O1B
82	R1	202	PEB	CAC-CBC-CGC-O1C
82	S1	201	PEB	CAC-CBC-CGC-O2C
82	U1	201	PEB	CAC-CBC-CGC-O2C
82	A1	302	PEB	CAC-CBC-CGC-O1C
82	F1	1002	PEB	CAB-CBB-CGB-O1B
82	f1	201	PEB	CAC-CBC-CGC-O2C
82	f1	202	PEB	CAC-CBC-CGC-O2C
82	g1	201	PEB	CAC-CBC-CGC-O1C
82	g1	202	PEB	CAB-CBB-CGB-O1B
82	h1	202	PEB	CAB-CBB-CGB-O2B
82	d1	202	PEB	CAC-CBC-CGC-O1C
82	d1	203	PEB	CAC-CBC-CGC-O1C
82	A4	301	PEB	CAB-CBB-CGB-O1B
82	A4	304	PEB	CAC-CBC-CGC-O2C
82	Q4	201	PEB	CAC-CBC-CGC-O1C
82	Z4	201	PEB	CAC-CBC-CGC-O1C
82	l4	202	PEB	CAB-CBB-CGB-O1B
82	a4	202	PEB	CAC-CBC-CGC-O2C
82	b4	202	PEB	CAC-CBC-CGC-O1C
82	d4	201	PEB	CAB-CBB-CGB-O2B
82	B5	201	PEB	CAC-CBC-CGC-O2C
82	B5	202	PEB	CAC-CBC-CGC-O1C
82	D5	203	PEB	CAB-CBB-CGB-O1B
82	H5	203	PEB	CAC-CBC-CGC-O2C
82	J5	203	PEB	CAC-CBC-CGC-O2C
82	J5	203	PEB	CAB-CBB-CGB-O2B
82	M5	304	PEB	CAB-CBB-CGB-O2B
82	Y5	201	PEB	CAC-CBC-CGC-O2C
82	Y5	203	PEB	CAC-CBC-CGC-O1C
82	Z5	304	PEB	CAB-CBB-CGB-O2B
82	A7	201	PEB	CAC-CBC-CGC-O1C
82	B7	201	PEB	CAC-CBC-CGC-O2C
82	F7	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	H7	203	PEB	CAC-CBC-CGC-O2C
82	I7	201	PEB	CAC-CBC-CGC-O2C
82	I7	202	PEB	CAC-CBC-CGC-O1C
82	I7	202	PEB	CAB-CBB-CGB-O2B
82	J7	203	PEB	CAB-CBB-CGB-O1B
82	J7	203	PEB	CAB-CBB-CGB-O2B
82	L7	203	PEB	CAB-CBB-CGB-O2B
82	O7	202	PEB	CAB-CBB-CGB-O2B
82	P7	201	PEB	CAC-CBC-CGC-O1C
82	R7	202	PEB	CAC-CBC-CGC-O2C
82	y8	201	PEB	CAB-CBB-CGB-O1B
82	y8	202	PEB	CAC-CBC-CGC-O2C
82	18	201	PEB	CAB-CBB-CGB-O2B
82	J9	203	PEB	CAB-CBB-CGB-O1B
82	U9	201	PEB	CAB-CBB-CGB-O1B
82	Y9	203	PEB	CAB-CBB-CGB-O1B
82	gB	203	PEB	CAC-CBC-CGC-O2C
82	gB	203	PEB	CAB-CBB-CGB-O2B
82	yC	202	PEB	CAC-CBC-CGC-O2C
82	bE	201	PEB	CAC-CBC-CGC-O1C
82	eE	201	PEB	CAC-CBC-CGC-O2C
82	gE	201	PEB	CAC-CBC-CGC-O1C
82	jE	201	PEB	CAC-CBC-CGC-O2C
82	jE	202	PEB	CAC-CBC-CGC-O1C
82	lE	202	PEB	CAB-CBB-CGB-O1B
82	lE	202	PEB	CAB-CBB-CGB-O2B
82	lE	203	PEB	CAB-CBB-CGB-O2B
82	aF	202	PEB	CAB-CBB-CGB-O2B
82	eF	201	PEB	CAB-CBB-CGB-O2B
82	fF	202	PEB	CAC-CBC-CGC-O2C
82	gF	202	PEB	CAB-CBB-CGB-O1B
82	xF	302	PEB	CAB-CBB-CGB-O2B
82	xF	303	PEB	CAB-CBB-CGB-O2B
82	xF	304	PEB	CAB-CBB-CGB-O2B
82	bG	201	PEB	CAC-CBC-CGC-O1C
82	cG	202	PEB	CAC-CBC-CGC-O1C
82	cG	202	PEB	CAC-CBC-CGC-O2C
82	gG	201	PEB	CAC-CBC-CGC-O1C
82	jG	201	PEB	CAC-CBC-CGC-O2C
82	jG	202	PEB	CAC-CBC-CGC-O1C
82	lG	203	PEB	CAB-CBB-CGB-O2B
82	fH	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	gH	201	PEB	CAC-CBC-CGC-O1C
82	hH	201	PEB	CAB-CBB-CGB-O2B
82	jH	202	PEB	CAB-CBB-CGB-O1B
82	lH	201	PEB	CAC-CBC-CGC-O1C
82	bH	201	PEB	CAC-CBC-CGC-O2C
82	dH	202	PEB	CAC-CBC-CGC-O1C
82	dJ	201	PEB	CAC-CBC-CGC-O2C
82	eJ	202	PEB	CAB-CBB-CGB-O1B
82	fJ	203	PEB	CAC-CBC-CGC-O1C
82	jJ	201	PEB	CAC-CBC-CGC-O1C
82	lJ	201	PEB	CAC-CBC-CGC-O1C
82	aK	202	PEB	CAB-CBB-CGB-O2B
82	aK	203	PEB	CAB-CBB-CGB-O2B
82	cK	202	PEB	CAC-CBC-CGC-O2C
82	dK	201	PEB	CAC-CBC-CGC-O1C
82	dK	201	PEB	CAB-CBB-CGB-O1B
82	dK	202	PEB	CAB-CBB-CGB-O2B
82	fK	202	PEB	CAC-CBC-CGC-O2C
82	gK	202	PEB	CAB-CBB-CGB-O1B
82	iK	202	PEB	CAC-CBC-CGC-O1C
82	lK	202	PEB	CAB-CBB-CGB-O2B
82	tK	202	PEB	CAB-CBB-CGB-O2B
82	xK	303	PEB	CAB-CBB-CGB-O1B
82	xK	303	PEB	CAB-CBB-CGB-O2B
82	xK	304	PEB	CAB-CBB-CGB-O2B
82	aM	202	PEB	CAC-CBC-CGC-O2C
82	cM	201	PEB	CAC-CBC-CGC-O2C
82	fM	203	PEB	CAC-CBC-CGC-O2C
82	hM	201	PEB	CAC-CBC-CGC-O2C
82	hM	202	PEB	CAB-CBB-CGB-O1B
82	lM	202	PEB	CAC-CBC-CGC-O1C
82	aO	202	PEB	CAC-CBC-CGC-O2C
82	bO	202	PEB	CAC-CBC-CGC-O1C
82	cO	202	PEB	CAB-CBB-CGB-O1B
82	dO	201	PEB	CAB-CBB-CGB-O2B
82	eO	201	PEB	CAC-CBC-CGC-O1C
82	Z9	304	PEB	CAB-CBB-CGB-O1B
82	Z9	304	PEB	CAB-CBB-CGB-O2B
82	M9	301	PEB	CAB-CBB-CGB-O2B
82	M9	302	PEB	CAB-CBB-CGB-O2B
82	M9	305	PEB	CAB-CBB-CGB-O1B
82	M9	305	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
83	AH	304	PUB	CAC-CBC-CGC-O2C
83	AJ	303	PUB	CAB-CBB-CGB-O1B
83	A1	304	PUB	CAC-CBC-CGC-O2C
83	M5	303	PUB	CAB-CBB-CGB-O1B
83	Z5	303	PUB	CAB-CBB-CGB-O1B
83	xF	301	PUB	CAB-CBB-CGB-O2B
84	BE	1001	CYC	CAD-CBD-CGD-O2D
84	HE	1001	CYC	CAA-CBA-CGA-O1A
84	JH	1003	CYC	CAA-CBA-CGA-O2A
84	M1	201	CYC	CAA-CBA-CGA-O2A
87	BN	820	CLA	CAA-CBA-CGA-O2A
87	32	305	CLA	CAA-CBA-CGA-O1A
87	42	606	CLA	CAA-CBA-CGA-O1A
87	52	601	CLA	CAA-CBA-CGA-O2A
87	4N	606	CLA	CAA-CBA-CGA-O1A
87	5N	601	CLA	CAA-CBA-CGA-O2A
88	l6	101	LHG	C31-C32-C33-C34
82	BI	203	PEB	C2C-C1C-CHB-C4B
82	kO	203	PEB	C3B-C4B-CHB-C1C
82	Z9	303	PEB	C2C-C1C-CHB-C4B
83	AJ	303	PUB	C3B-C4B-CHB-C1C
87	C6	511	CLA	C16-C17-C18-C20
95	JL	101	DGD	C2B-C3B-C4B-C5B
87	CL	503	CLA	C3-C5-C6-C7
87	b6	607	CLA	C3-C5-C6-C7
88	d6	402	LHG	C2-C3-O3-P
87	BL	620	CLA	C2A-CAA-CBA-CGA
87	AN	805	CLA	C2A-CAA-CBA-CGA
87	IN	103	CLA	C2A-CAA-CBA-CGA
87	42	611	CLA	C2A-CAA-CBA-CGA
87	A2	805	CLA	C2A-CAA-CBA-CGA
87	I2	103	CLA	C2A-CAA-CBA-CGA
87	cL	505	CLA	C2A-CAA-CBA-CGA
87	cL	510	CLA	C2A-CAA-CBA-CGA
87	dL	409	CLA	C2A-CAA-CBA-CGA
87	4N	611	CLA	C2A-CAA-CBA-CGA
91	A6	407	PHO	C2A-CAA-CBA-CGA
95	c6	618	DGD	O6D-C5D-C6D-O5D
87	B2	818	CLA	C10-C11-C12-C13
87	B6	605	CLA	C15-C16-C17-C18
87	K6	101	CLA	C13-C15-C16-C17
82	AA	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	AA	202	PEB	CAB-CBB-CGB-O2B
82	BA	203	PEB	CAB-CBB-CGB-O1B
82	CA	201	PEB	CAC-CBC-CGC-O1C
82	CA	201	PEB	CAC-CBC-CGC-O2C
82	HA	203	PEB	CAC-CBC-CGC-O2C
82	IA	201	PEB	CAC-CBC-CGC-O2C
82	IA	202	PEB	CAB-CBB-CGB-O1B
82	LA	202	PEB	CAC-CBC-CGC-O1C
82	LA	203	PEB	CAB-CBB-CGB-O2B
82	OA	201	PEB	CAC-CBC-CGC-O1C
82	OA	202	PEB	CAB-CBB-CGB-O2B
82	RA	202	PEB	CAC-CBC-CGC-O2C
82	YA	301	PEB	CAC-CBC-CGC-O1C
82	YA	303	PEB	CAC-CBC-CGC-O1C
82	YA	303	PEB	CAC-CBC-CGC-O2C
82	YA	303	PEB	CAB-CBB-CGB-O2B
82	AB	501	PEB	CAC-CBC-CGC-O2C
82	HB	201	PEB	CAC-CBC-CGC-O1C
82	WB	401	PEB	CAC-CBC-CGC-O2C
82	HD	203	PEB	CAB-CBB-CGB-O1B
82	OD	202	PEB	CAC-CBC-CGC-O2C
82	OD	202	PEB	CAB-CBB-CGB-O1B
82	PD	202	PEB	CAC-CBC-CGC-O1C
82	PD	203	PEB	CAB-CBB-CGB-O2B
82	QD	202	PEB	CAC-CBC-CGC-O2C
82	RD	201	PEB	CAC-CBC-CGC-O2C
82	RD	202	PEB	CAB-CBB-CGB-O1B
82	SD	202	PEB	CAB-CBB-CGB-O1B
82	SD	202	PEB	CAB-CBB-CGB-O2B
82	TD	203	PEB	CAC-CBC-CGC-O2C
82	UD	202	PEB	CAC-CBC-CGC-O2C
82	VD	202	PEB	CAB-CBB-CGB-O1B
82	WD	202	PEB	CAC-CBC-CGC-O2C
82	XD	202	PEB	CAC-CBC-CGC-O2C
82	XD	202	PEB	CAB-CBB-CGB-O2B
82	PE	202	PEB	CAB-CBB-CGB-O1B
82	QE	201	PEB	CAC-CBC-CGC-O1C
82	ZE	203	PEB	CAC-CBC-CGC-O2C
82	AF	202	PEB	CAB-CBB-CGB-O2B
82	FF	202	PEB	CAC-CBC-CGC-O1C
82	NF	201	PEB	CAC-CBC-CGC-O2C
82	YF	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	PG	202	PEB	CAB-CBB-CGB-O1B
82	QG	202	PEB	CAC-CBC-CGC-O1C
82	WG	202	PEB	CAB-CBB-CGB-O1B
82	DH	1002	PEB	CAC-CBC-CGC-O2C
82	QH	201	PEB	CAB-CBB-CGB-O1B
82	RH	202	PEB	CAB-CBB-CGB-O2B
82	SH	201	PEB	CAC-CBC-CGC-O1C
82	UH	202	PEB	CAC-CBC-CGC-O1C
82	UH	202	PEB	CAC-CBC-CGC-O2C
82	UH	203	PEB	CAB-CBB-CGB-O1B
82	ZH	203	PEB	CAB-CBB-CGB-O2B
82	MI	401	PEB	CAB-CBB-CGB-O2B
82	IJ	201	PEB	CAC-CBC-CGC-O2C
82	OJ	203	PEB	CAC-CBC-CGC-O2C
82	PJ	202	PEB	CAB-CBB-CGB-O2B
82	SJ	202	PEB	CAB-CBB-CGB-O2B
82	WJ	201	PEB	CAC-CBC-CGC-O1C
82	XJ	202	PEB	CAB-CBB-CGB-O1B
82	HK	202	PEB	CAB-CBB-CGB-O1B
82	KK	203	PEB	CAC-CBC-CGC-O1C
82	LK	201	PEB	CAC-CBC-CGC-O1C
82	NK	201	PEB	CAC-CBC-CGC-O2C
82	PK	202	PEB	CAB-CBB-CGB-O2B
82	TK	202	PEB	CAC-CBC-CGC-O2C
82	YK	202	PEB	CAB-CBB-CGB-O2B
82	AM	301	PEB	CAB-CBB-CGB-O2B
82	AM	302	PEB	CAB-CBB-CGB-O2B
82	CM	201	PEB	CAC-CBC-CGC-O1C
82	IM	203	PEB	CAC-CBC-CGC-O1C
82	JM	202	PEB	CAB-CBB-CGB-O1B
82	MM	202	PEB	CAC-CBC-CGC-O1C
82	WM	203	PEB	CAC-CBC-CGC-O2C
82	YM	203	PEB	CAB-CBB-CGB-O2B
82	YO	203	PEB	CAB-CBB-CGB-O2B
82	AP	203	PEB	CAB-CBB-CGB-O1B
82	CP	202	PEB	CAC-CBC-CGC-O1C
82	FP	202	PEB	CAB-CBB-CGB-O2B
82	HP	202	PEB	CAB-CBB-CGB-O2B
82	OP	201	PEB	CAB-CBB-CGB-O1B
82	QP	201	PEB	CAC-CBC-CGC-O2C
82	SP	202	PEB	CAC-CBC-CGC-O2C
82	BQ	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	DQ	201	PEB	CAC-CBC-CGC-O2C
82	FQ	201	PEB	CAB-CBB-CGB-O2B
82	JQ	203	PEB	CAC-CBC-CGC-O2C
82	MQ	202	PEB	CAB-CBB-CGB-O1B
82	NQ	202	PEB	CAB-CBB-CGB-O1B
82	OQ	202	PEB	CAC-CBC-CGC-O2C
82	OQ	202	PEB	CAB-CBB-CGB-O2B
82	PQ	202	PEB	CAC-CBC-CGC-O1C
82	RQ	201	PEB	CAC-CBC-CGC-O2C
82	SQ	202	PEB	CAB-CBB-CGB-O2B
82	VQ	202	PEB	CAB-CBB-CGB-O1B
82	WQ	202	PEB	CAC-CBC-CGC-O2C
82	XQ	202	PEB	CAC-CBC-CGC-O2C
82	XQ	202	PEB	CAB-CBB-CGB-O2B
82	O1	202	PEB	CAC-CBC-CGC-O1C
82	Q1	203	PEB	CAC-CBC-CGC-O1C
82	U1	202	PEB	CAC-CBC-CGC-O2C
82	U1	203	PEB	CAC-CBC-CGC-O1C
82	U1	203	PEB	CAB-CBB-CGB-O1B
82	j1	201	PEB	CAC-CBC-CGC-O2C
82	j1	202	PEB	CAB-CBB-CGB-O1B
82	l1	202	PEB	CAC-CBC-CGC-O1C
82	m1	201	PEB	CAB-CBB-CGB-O2B
82	b1	202	PEB	CAB-CBB-CGB-O2B
82	d1	203	PEB	CAC-CBC-CGC-O2C
82	F4	1002	PEB	CAB-CBB-CGB-O2B
82	Y4	203	PEB	CAB-CBB-CGB-O2B
82	i4	203	PEB	CAC-CBC-CGC-O2C
82	j4	203	PEB	CAB-CBB-CGB-O2B
82	k4	202	PEB	CAC-CBC-CGC-O2C
82	b4	201	PEB	CAC-CBC-CGC-O1C
82	c4	202	PEB	CAB-CBB-CGB-O1B
82	c4	202	PEB	CAB-CBB-CGB-O2B
82	e4	201	PEB	CAC-CBC-CGC-O1C
82	D5	203	PEB	CAC-CBC-CGC-O2C
82	F5	203	PEB	CAB-CBB-CGB-O1B
82	O5	203	PEB	CAC-CBC-CGC-O2C
82	O5	203	PEB	CAB-CBB-CGB-O1B
82	B7	203	PEB	CAB-CBB-CGB-O1B
82	C7	201	PEB	CAC-CBC-CGC-O1C
82	C7	201	PEB	CAC-CBC-CGC-O2C
82	G7	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	I7	202	PEB	CAB-CBB-CGB-O1B
82	L7	202	PEB	CAC-CBC-CGC-O1C
82	M7	201	PEB	CAC-CBC-CGC-O1C
82	O7	201	PEB	CAC-CBC-CGC-O1C
82	W7	201	PEB	CAB-CBB-CGB-O2B
82	Y7	303	PEB	CAC-CBC-CGC-O1C
82	Y7	303	PEB	CAC-CBC-CGC-O2C
82	Y7	303	PEB	CAB-CBB-CGB-O2B
82	x8	202	PEB	CAC-CBC-CGC-O1C
82	A9	202	PEB	CAC-CBC-CGC-O1C
82	B9	201	PEB	CAC-CBC-CGC-O2C
82	C9	202	PEB	CAC-CBC-CGC-O1C
82	E9	202	PEB	CAC-CBC-CGC-O1C
82	F9	201	PEB	CAB-CBB-CGB-O1B
82	F9	201	PEB	CAB-CBB-CGB-O2B
82	K9	202	PEB	CAC-CBC-CGC-O1C
82	N9	202	PEB	CAC-CBC-CGC-O1C
82	P9	202	PEB	CAC-CBC-CGC-O1C
82	U9	204	PEB	CAC-CBC-CGC-O1C
82	X9	202	PEB	CAC-CBC-CGC-O1C
82	fB	301	PEB	CAB-CBB-CGB-O2B
82	dB	202	PEB	CAB-CBB-CGB-O1B
82	gB	201	PEB	CAC-CBC-CGC-O2C
82	wC	201	PEB	CAB-CBB-CGB-O1B
82	cE	202	PEB	CAB-CBB-CGB-O1B
82	jE	201	PEB	CAB-CBB-CGB-O1B
82	kE	202	PEB	CAC-CBC-CGC-O1C
82	aF	203	PEB	CAB-CBB-CGB-O2B
82	dF	201	PEB	CAC-CBC-CGC-O1C
82	dF	201	PEB	CAB-CBB-CGB-O1B
82	dF	202	PEB	CAC-CBC-CGC-O1C
82	iF	202	PEB	CAC-CBC-CGC-O1C
82	kF	201	PEB	CAC-CBC-CGC-O2C
82	lF	201	PEB	CAC-CBC-CGC-O2C
82	lF	202	PEB	CAB-CBB-CGB-O2B
82	pF	201	PEB	CAB-CBB-CGB-O2B
82	tF	202	PEB	CAB-CBB-CGB-O1B
82	wF	302	PEB	CAB-CBB-CGB-O1B
82	xF	303	PEB	CAB-CBB-CGB-O1B
82	cG	202	PEB	CAB-CBB-CGB-O1B
82	eG	201	PEB	CAC-CBC-CGC-O2C
82	gG	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	jG	201	PEB	CAB-CBB-CGB-O1B
82	fH	203	PEB	CAC-CBC-CGC-O1C
82	gH	202	PEB	CAB-CBB-CGB-O1B
82	jH	201	PEB	CAC-CBC-CGC-O2C
82	lH	202	PEB	CAC-CBC-CGC-O2C
82	mH	201	PEB	CAB-CBB-CGB-O2B
82	bH	202	PEB	CAB-CBB-CGB-O2B
82	dH	203	PEB	CAC-CBC-CGC-O1C
82	dJ	201	PEB	CAB-CBB-CGB-O1B
82	hJ	202	PEB	CAC-CBC-CGC-O2C
82	eK	201	PEB	CAB-CBB-CGB-O2B
82	kK	201	PEB	CAC-CBC-CGC-O2C
82	lK	201	PEB	CAC-CBC-CGC-O2C
82	nK	201	PEB	CAC-CBC-CGC-O1C
82	pK	201	PEB	CAB-CBB-CGB-O2B
82	tK	202	PEB	CAB-CBB-CGB-O1B
82	xK	302	PEB	CAB-CBB-CGB-O2B
82	xK	304	PEB	CAC-CBC-CGC-O1C
82	aM	204	PEB	CAC-CBC-CGC-O2C
82	kM	202	PEB	CAC-CBC-CGC-O2C
82	mM	201	PEB	CAC-CBC-CGC-O2C
82	iO	203	PEB	CAC-CBC-CGC-O2C
82	kO	203	PEB	CAC-CBC-CGC-O2C
82	lO	202	PEB	CAB-CBB-CGB-O1B
82	bO	201	PEB	CAC-CBC-CGC-O1C
82	cO	202	PEB	CAB-CBB-CGB-O2B
82	Z9	301	PEB	CAC-CBC-CGC-O1C
82	Z9	301	PEB	CAB-CBB-CGB-O2B
82	M9	302	PEB	CAC-CBC-CGC-O1C
83	AJ	304	PUB	CAC-CBC-CGC-O1C
83	BM	302	PUB	CAB-CBB-CGB-O1B
83	xK	301	PUB	CAB-CBB-CGB-O2B
84	CG	1001	CYC	CAA-CBA-CGA-O2A
84	MO	1001	CYC	CAA-CBA-CGA-O1A
84	63	901	CYC	CAD-CBD-CGD-O2D
87	AN	818	CLA	CAA-CBA-CGA-O2A
87	52	605	CLA	CAA-CBA-CGA-O1A
87	82	304	CLA	CAA-CBA-CGA-O2A
87	A2	818	CLA	CAA-CBA-CGA-O2A
87	5N	601	CLA	CAA-CBA-CGA-O1A
87	5N	605	CLA	CAA-CBA-CGA-O1A
88	iL	101	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
92	AL	411	LMG	C37-C38-C39-C40
95	AL	416	DGD	C2A-C3A-C4A-C5A
100	JN	104	3XQ	C15-C16-C17-C18
82	YO	203	PEB	NC-C1C-CHB-C4B
95	BL	613	DGD	C1B-C2B-C3B-C4B
87	C6	516	CLA	C5-C6-C7-C8
87	C6	520	CLA	C8-C10-C11-C12
87	bL	613	CLA	C13-C15-C16-C17
92	j6	102	LMG	C29-C28-O8-C9
82	BA	201	PEB	C4B-C3B-CAB-CBB
82	oK	203	PEB	C4B-C3B-CAB-CBB
87	CL	503	CLA	C5-C6-C7-C8
87	c6	604	CLA	C8-C10-C11-C12
82	EA	202	PEB	CAC-CBC-CGC-O2C
82	JA	202	PEB	CAC-CBC-CGC-O1C
82	LA	202	PEB	CAC-CBC-CGC-O2C
82	OA	201	PEB	CAB-CBB-CGB-O2B
82	RA	203	PEB	CAB-CBB-CGB-O1B
82	SA	202	PEB	CAC-CBC-CGC-O2C
82	VA	202	PEB	CAB-CBB-CGB-O2B
82	AB	501	PEB	CAB-CBB-CGB-O2B
82	FB	201	PEB	CAB-CBB-CGB-O2B
82	HB	203	PEB	CAB-CBB-CGB-O2B
82	LB	201	PEB	CAC-CBC-CGC-O2C
82	NB	203	PEB	CAC-CBC-CGC-O2C
82	AD	304	PEB	CAC-CBC-CGC-O2C
82	BD	203	PEB	CAB-CBB-CGB-O1B
82	DD	201	PEB	CAC-CBC-CGC-O2C
82	DD	203	PEB	CAC-CBC-CGC-O2C
82	DD	203	PEB	CAB-CBB-CGB-O2B
82	MD	202	PEB	CAC-CBC-CGC-O1C
82	MD	202	PEB	CAB-CBB-CGB-O1B
82	ND	202	PEB	CAB-CBB-CGB-O1B
82	OD	202	PEB	CAB-CBB-CGB-O2B
82	SD	202	PEB	CAC-CBC-CGC-O1C
82	YD	201	PEB	CAC-CBC-CGC-O1C
82	HE	1002	PEB	CAC-CBC-CGC-O2C
82	KE	201	PEB	CAC-CBC-CGC-O2C
82	WE	202	PEB	CAB-CBB-CGB-O1B
82	WE	202	PEB	CAB-CBB-CGB-O2B
82	BF	201	PEB	CAB-CBB-CGB-O1B
82	BF	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	CF	201	PEB	CAB-CBB-CGB-O2B
82	KF	203	PEB	CAC-CBC-CGC-O1C
82	KF	203	PEB	CAB-CBB-CGB-O2B
82	LF	201	PEB	CAC-CBC-CGC-O1C
82	HG	1002	PEB	CAC-CBC-CGC-O2C
82	KG	201	PEB	CAC-CBC-CGC-O2C
82	QG	201	PEB	CAC-CBC-CGC-O1C
82	SG	202	PEB	CAB-CBB-CGB-O2B
82	WG	202	PEB	CAB-CBB-CGB-O2B
82	ZG	203	PEB	CAC-CBC-CGC-O2C
82	AH	305	PEB	CAB-CBB-CGB-O1B
82	QH	202	PEB	CAC-CBC-CGC-O2C
82	QH	202	PEB	CAB-CBB-CGB-O2B
82	BI	201	PEB	CAC-CBC-CGC-O2C
82	BI	203	PEB	CAB-CBB-CGB-O1B
82	FI	201	PEB	CAC-CBC-CGC-O2C
82	RI	203	PEB	CAC-CBC-CGC-O1C
82	AJ	302	PEB	CAC-CBC-CGC-O1C
82	IJ	203	PEB	CAB-CBB-CGB-O1B
82	QJ	202	PEB	CAC-CBC-CGC-O1C
82	SJ	201	PEB	CAC-CBC-CGC-O1C
82	XJ	202	PEB	CAB-CBB-CGB-O2B
82	YJ	201	PEB	CAC-CBC-CGC-O2C
82	BK	201	PEB	CAB-CBB-CGB-O1B
82	CK	201	PEB	CAB-CBB-CGB-O2B
82	DM	201	PEB	CAB-CBB-CGB-O1B
82	IM	201	PEB	CAC-CBC-CGC-O1C
82	IM	203	PEB	CAB-CBB-CGB-O2B
82	VM	202	PEB	CAB-CBB-CGB-O2B
82	RO	202	PEB	CAC-CBC-CGC-O2C
82	TO	203	PEB	CAB-CBB-CGB-O1B
82	YO	203	PEB	CAC-CBC-CGC-O2C
82	EP	202	PEB	CAB-CBB-CGB-O1B
82	GP	203	PEB	CAB-CBB-CGB-O2B
82	KP	201	PEB	CAB-CBB-CGB-O2B
82	LP	201	PEB	CAB-CBB-CGB-O1B
82	DQ	203	PEB	CAC-CBC-CGC-O2C
82	JQ	202	PEB	CAC-CBC-CGC-O2C
82	MQ	202	PEB	CAC-CBC-CGC-O1C
82	SQ	202	PEB	CAC-CBC-CGC-O1C
82	UQ	202	PEB	CAC-CBC-CGC-O2C
82	P1	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	Q1	201	PEB	CAB-CBB-CGB-O1B
82	Q1	202	PEB	CAC-CBC-CGC-O2C
82	Q1	202	PEB	CAB-CBB-CGB-O2B
82	S1	201	PEB	CAC-CBC-CGC-O1C
82	A1	305	PEB	CAB-CBB-CGB-O1B
82	D1	1002	PEB	CAC-CBC-CGC-O2C
82	Z1	201	PEB	CAC-CBC-CGC-O2C
82	Z1	201	PEB	CAB-CBB-CGB-O2B
82	Z1	203	PEB	CAB-CBB-CGB-O2B
82	f1	203	PEB	CAC-CBC-CGC-O1C
82	h1	201	PEB	CAB-CBB-CGB-O2B
82	b1	202	PEB	CAC-CBC-CGC-O2C
82	c1	201	PEB	CAC-CBC-CGC-O1C
82	d1	202	PEB	CAB-CBB-CGB-O1B
82	R4	202	PEB	CAC-CBC-CGC-O2C
82	T4	203	PEB	CAB-CBB-CGB-O1B
82	V4	202	PEB	CAC-CBC-CGC-O2C
82	Y4	203	PEB	CAC-CBC-CGC-O2C
82	i4	202	PEB	CAC-CBC-CGC-O2C
82	b4	202	PEB	CAB-CBB-CGB-O2B
82	c4	203	PEB	CAC-CBC-CGC-O2C
82	e4	202	PEB	CAC-CBC-CGC-O2C
82	e4	203	PEB	CAB-CBB-CGB-O1B
82	g4	203	PEB	CAC-CBC-CGC-O2C
82	F5	202	PEB	CAC-CBC-CGC-O1C
82	F5	203	PEB	CAC-CBC-CGC-O2C
82	J5	203	PEB	CAC-CBC-CGC-O1C
82	J5	203	PEB	CAB-CBB-CGB-O1B
82	L5	202	PEB	CAC-CBC-CGC-O1C
82	Q5	201	PEB	CAC-CBC-CGC-O1C
82	A7	202	PEB	CAB-CBB-CGB-O2B
82	E7	202	PEB	CAC-CBC-CGC-O2C
82	L7	202	PEB	CAC-CBC-CGC-O2C
82	O7	201	PEB	CAB-CBB-CGB-O2B
82	R7	203	PEB	CAB-CBB-CGB-O1B
82	S7	202	PEB	CAC-CBC-CGC-O2C
82	V7	202	PEB	CAB-CBB-CGB-O2B
82	Y7	301	PEB	CAC-CBC-CGC-O1C
82	w8	201	PEB	CAB-CBB-CGB-O1B
82	D9	202	PEB	CAC-CBC-CGC-O1C
82	G9	202	PEB	CAC-CBC-CGC-O1C
82	I9	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	R9	202	PEB	CAC-CBC-CGC-O1C
82	T9	202	PEB	CAC-CBC-CGC-O1C
82	V9	202	PEB	CAC-CBC-CGC-O1C
82	W9	202	PEB	CAC-CBC-CGC-O1C
82	dB	201	PEB	CAC-CBC-CGC-O2C
82	yC	201	PEB	CAB-CBB-CGB-O1B
82	bE	202	PEB	CAB-CBB-CGB-O2B
82	eE	203	PEB	CAB-CBB-CGB-O2B
82	fE	202	PEB	CAB-CBB-CGB-O1B
82	gE	202	PEB	CAC-CBC-CGC-O2C
82	jE	202	PEB	CAB-CBB-CGB-O1B
82	nF	201	PEB	CAC-CBC-CGC-O1C
82	sF	202	PEB	CAB-CBB-CGB-O2B
82	tF	201	PEB	CAC-CBC-CGC-O1C
82	vF	201	PEB	CAB-CBB-CGB-O1B
82	xF	304	PEB	CAC-CBC-CGC-O1C
82	eG	203	PEB	CAB-CBB-CGB-O2B
82	fG	202	PEB	CAB-CBB-CGB-O1B
82	jG	202	PEB	CAB-CBB-CGB-O1B
82	kG	202	PEB	CAC-CBC-CGC-O1C
82	gH	203	PEB	CAB-CBB-CGB-O2B
82	bH	202	PEB	CAC-CBC-CGC-O2C
82	aJ	202	PEB	CAC-CBC-CGC-O1C
82	eJ	202	PEB	CAB-CBB-CGB-O2B
82	hJ	201	PEB	CAC-CBC-CGC-O1C
82	kJ	202	PEB	CAC-CBC-CGC-O2C
82	cK	201	PEB	CAC-CBC-CGC-O2C
82	dK	202	PEB	CAC-CBC-CGC-O1C
82	sK	202	PEB	CAB-CBB-CGB-O2B
82	cM	202	PEB	CAC-CBC-CGC-O2C
82	eM	202	PEB	CAB-CBB-CGB-O1B
82	fM	202	PEB	CAB-CBB-CGB-O2B
82	hM	201	PEB	CAB-CBB-CGB-O1B
82	iM	202	PEB	CAC-CBC-CGC-O1C
82	iO	202	PEB	CAC-CBC-CGC-O2C
82	bO	202	PEB	CAB-CBB-CGB-O2B
82	cO	202	PEB	CAC-CBC-CGC-O2C
82	cO	203	PEB	CAC-CBC-CGC-O2C
82	eO	203	PEB	CAB-CBB-CGB-O1B
82	fO	202	PEB	CAC-CBC-CGC-O2C
82	gO	203	PEB	CAC-CBC-CGC-O2C
83	AH	304	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
83	A1	304	PUB	CAB-CBB-CGB-O1B
83	A4	303	PUB	CAB-CBB-CGB-O1B
84	BE	1002	CYC	CAA-CBA-CGA-O2A
84	FE	1001	CYC	CAA-CBA-CGA-O2A
84	GE	1001	CYC	CAA-CBA-CGA-O1A
84	BG	1001	CYC	CAD-CBD-CGD-O2D
84	BG	1002	CYC	CAA-CBA-CGA-O2A
84	MO	1001	CYC	CAA-CBA-CGA-O2A
84	K1	1001	CYC	CAA-CBA-CGA-O2A
84	A3	1001	CYC	CAA-CBA-CGA-O1A
84	C3	1001	CYC	CAA-CBA-CGA-O1A
84	E3	1001	CYC	CAA-CBA-CGA-O1A
84	G3	1001	CYC	CAA-CBA-CGA-O1A
84	J3	1001	CYC	CAA-CBA-CGA-O1A
84	K3	1001	CYC	CAA-CBA-CGA-O1A
84	N3	1001	CYC	CAA-CBA-CGA-O1A
84	P3	1001	CYC	CAA-CBA-CGA-O1A
84	R3	1001	CYC	CAA-CBA-CGA-O1A
84	T3	1001	CYC	CAA-CBA-CGA-O1A
84	c3	1001	CYC	CAA-CBA-CGA-O1A
84	e3	1001	CYC	CAA-CBA-CGA-O1A
84	g3	1001	CYC	CAA-CBA-CGA-O1A
84	i3	1001	CYC	CAA-CBA-CGA-O1A
84	l3	1001	CYC	CAA-CBA-CGA-O1A
84	m3	1001	CYC	CAA-CBA-CGA-O1A
84	p3	1001	CYC	CAA-CBA-CGA-O1A
84	t3	1001	CYC	CAA-CBA-CGA-O1A
84	v3	1001	CYC	CAA-CBA-CGA-O1A
84	x3	1001	CYC	CAD-CBD-CGD-O2D
84	M4	1001	CYC	CAA-CBA-CGA-O1A
84	M4	1001	CYC	CAA-CBA-CGA-O2A
87	12	601	CLA	CAA-CBA-CGA-O2A
87	M2	101	CLA	CAA-CBA-CGA-O2A
87	1N	601	CLA	CAA-CBA-CGA-O2A
95	aL	603	DGD	C4D-C5D-C6D-O5D
87	IN	102	CLA	C4-C3-C5-C6
87	I2	102	CLA	C4-C3-C5-C6
87	C6	511	CLA	C4-C3-C5-C6
87	CL	518	CLA	C2B-C3B-CAB-CBB
87	BN	832	CLA	C2B-C3B-CAB-CBB
87	MN	101	CLA	C2B-C3B-CAB-CBB
87	32	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
87	B2	832	CLA	C2B-C3B-CAB-CBB
87	M2	101	CLA	C2B-C3B-CAB-CBB
87	B6	607	CLA	C2B-C3B-CAB-CBB
87	b6	607	CLA	C2B-C3B-CAB-CBB
87	b6	611	CLA	C2B-C3B-CAB-CBB
87	bL	614	CLA	C2B-C3B-CAB-CBB
87	bL	617	CLA	C2B-C3B-CAB-CBB
87	3N	306	CLA	C2B-C3B-CAB-CBB
82	ID	202	PEB	C2C-CAC-CBC-CGC
82	LI	202	PEB	C2C-CAC-CBC-CGC
82	OI	203	PEB	C2C-CAC-CBC-CGC
82	QI	201	PEB	C2C-CAC-CBC-CGC
82	UO	201	PEB	C3B-CAB-CBB-CGB
82	EP	203	PEB	C2C-CAC-CBC-CGC
82	FP	201	PEB	C2C-CAC-CBC-CGC
82	IQ	202	PEB	C2C-CAC-CBC-CGC
82	U4	201	PEB	C3B-CAB-CBB-CGB
82	k4	201	PEB	C3B-CAB-CBB-CGB
82	W9	201	PEB	C2C-CAC-CBC-CGC
82	eE	202	PEB	C3B-CAB-CBB-CGB
82	aF	202	PEB	C3B-CAB-CBB-CGB
82	hG	203	PEB	C3B-CAB-CBB-CGB
82	aK	202	PEB	C3B-CAB-CBB-CGB
82	kO	201	PEB	C3B-CAB-CBB-CGB
83	yF	302	PUB	C2C-CAC-CBC-CGC
83	yK	302	PUB	C2C-CAC-CBC-CGC
84	JH	1003	CYC	C3D-CAD-CBD-CGD
84	M1	201	CYC	C3D-CAD-CBD-CGD
82	BA	203	PEB	CAC-CBC-CGC-O2C
82	FA	202	PEB	CAC-CBC-CGC-O2C
82	HA	201	PEB	CAC-CBC-CGC-O2C
82	PA	203	PEB	CAB-CBB-CGB-O2B
82	RA	203	PEB	CAC-CBC-CGC-O2C
82	XA	203	PEB	CAC-CBC-CGC-O2C
82	NB	202	PEB	CAC-CBC-CGC-O1C
82	QB	202	PEB	CAC-CBC-CGC-O1C
82	SB	201	PEB	CAC-CBC-CGC-O2C
82	SB	202	PEB	CAC-CBC-CGC-O2C
82	UB	303	PEB	CAB-CBB-CGB-O2B
82	YB	202	PEB	CAB-CBB-CGB-O2B
82	BD	203	PEB	CAC-CBC-CGC-O2C
82	JD	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	XD	203	PEB	CAB-CBB-CGB-O2B
82	DE	1002	PEB	CAC-CBC-CGC-O2C
82	AF	202	PEB	CAC-CBC-CGC-O1C
82	DF	202	PEB	CAB-CBB-CGB-O1B
82	HF	202	PEB	CAB-CBB-CGB-O1B
82	LF	202	PEB	CAC-CBC-CGC-O1C
82	SF	202	PEB	CAB-CBB-CGB-O1B
82	SF	202	PEB	CAB-CBB-CGB-O2B
82	TF	201	PEB	CAC-CBC-CGC-O1C
82	OH	202	PEB	CAC-CBC-CGC-O1C
82	PH	202	PEB	CAC-CBC-CGC-O1C
82	UH	203	PEB	CAC-CBC-CGC-O1C
82	ZH	201	PEB	CAC-CBC-CGC-O2C
82	SI	202	PEB	CAB-CBB-CGB-O2B
82	VI	201	PEB	CAB-CBB-CGB-O2B
82	XI	201	PEB	CAB-CBB-CGB-O2B
82	YI	202	PEB	CAB-CBB-CGB-O1B
82	YI	202	PEB	CAB-CBB-CGB-O2B
82	OJ	202	PEB	CAB-CBB-CGB-O1B
82	OJ	202	PEB	CAB-CBB-CGB-O2B
82	QJ	204	PEB	CAB-CBB-CGB-O1B
82	UJ	203	PEB	CAB-CBB-CGB-O2B
82	VJ	202	PEB	CAC-CBC-CGC-O2C
82	VJ	202	PEB	CAB-CBB-CGB-O1B
82	AK	202	PEB	CAC-CBC-CGC-O1C
82	AK	202	PEB	CAB-CBB-CGB-O2B
82	BK	201	PEB	CAB-CBB-CGB-O2B
82	HK	202	PEB	CAC-CBC-CGC-O1C
82	KK	203	PEB	CAB-CBB-CGB-O1B
82	KK	203	PEB	CAB-CBB-CGB-O2B
82	SK	202	PEB	CAB-CBB-CGB-O1B
82	TK	201	PEB	CAC-CBC-CGC-O1C
82	AM	301	PEB	CAC-CBC-CGC-O2C
82	CM	203	PEB	CAC-CBC-CGC-O2C
82	FM	202	PEB	CAC-CBC-CGC-O2C
82	HM	201	PEB	CAC-CBC-CGC-O1C
82	HM	202	PEB	CAC-CBC-CGC-O2C
82	KM	202	PEB	CAC-CBC-CGC-O1C
82	NM	202	PEB	CAB-CBB-CGB-O1B
82	PM	201	PEB	CAC-CBC-CGC-O1C
82	TM	202	PEB	CAB-CBB-CGB-O1B
82	XM	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	YM	203	PEB	CAB-CBB-CGB-O1B
82	ZM	202	PEB	CAB-CBB-CGB-O1B
82	OO	201	PEB	CAB-CBB-CGB-O2B
82	UO	202	PEB	CAC-CBC-CGC-O2C
82	VO	202	PEB	CAC-CBC-CGC-O2C
82	GP	203	PEB	CAC-CBC-CGC-O2C
82	HP	201	PEB	CAB-CBB-CGB-O1B
82	HP	201	PEB	CAB-CBB-CGB-O2B
82	IP	203	PEB	CAC-CBC-CGC-O2C
82	MP	202	PEB	CAC-CBC-CGC-O1C
82	PP	201	PEB	CAB-CBB-CGB-O2B
82	SP	203	PEB	CAC-CBC-CGC-O1C
82	WP	201	PEB	CAC-CBC-CGC-O2C
82	WP	201	PEB	CAB-CBB-CGB-O2B
82	XP	201	PEB	CAB-CBB-CGB-O1B
82	BQ	203	PEB	CAC-CBC-CGC-O2C
82	DQ	203	PEB	CAB-CBB-CGB-O2B
82	OQ	201	PEB	CAB-CBB-CGB-O2B
82	RQ	203	PEB	CAC-CBC-CGC-O1C
82	O1	201	PEB	CAC-CBC-CGC-O1C
82	g1	201	PEB	CAB-CBB-CGB-O2B
82	h1	203	PEB	CAB-CBB-CGB-O2B
82	i1	201	PEB	CAC-CBC-CGC-O1C
82	l1	203	PEB	CAC-CBC-CGC-O2C
82	a1	202	PEB	CAC-CBC-CGC-O1C
82	d1	202	PEB	CAC-CBC-CGC-O2C
82	O4	201	PEB	CAB-CBB-CGB-O2B
82	b4	202	PEB	CAB-CBB-CGB-O1B
82	c4	202	PEB	CAC-CBC-CGC-O2C
82	f4	202	PEB	CAC-CBC-CGC-O2C
82	B5	203	PEB	CAB-CBB-CGB-O2B
82	D5	202	PEB	CAC-CBC-CGC-O1C
82	M5	305	PEB	CAC-CBC-CGC-O2C
82	O5	202	PEB	CAC-CBC-CGC-O1C
82	W5	203	PEB	CAB-CBB-CGB-O1B
82	B7	203	PEB	CAC-CBC-CGC-O2C
82	G7	201	PEB	CAC-CBC-CGC-O2C
82	H7	201	PEB	CAC-CBC-CGC-O2C
82	H7	203	PEB	CAB-CBB-CGB-O1B
82	J7	202	PEB	CAC-CBC-CGC-O1C
82	P7	203	PEB	CAB-CBB-CGB-O2B
82	p8	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	H9	202	PEB	CAC-CBC-CGC-O1C
82	H9	202	PEB	CAC-CBC-CGC-O2C
82	J9	201	PEB	CAB-CBB-CGB-O2B
82	S9	202	PEB	CAC-CBC-CGC-O1C
82	fB	301	PEB	CAC-CBC-CGC-O2C
82	eB	202	PEB	CAB-CBB-CGB-O2B
82	gB	201	PEB	CAB-CBB-CGB-O2B
82	hB	301	PEB	CAC-CBC-CGC-O2C
82	yC	201	PEB	CAC-CBC-CGC-O2C
82	pC	201	PEB	CAB-CBB-CGB-O2B
82	dE	201	PEB	CAB-CBB-CGB-O2B
82	dF	202	PEB	CAB-CBB-CGB-O1B
82	oF	202	PEB	CAC-CBC-CGC-O2C
82	oF	203	PEB	CAC-CBC-CGC-O2C
82	pF	201	PEB	CAB-CBB-CGB-O1B
82	qF	201	PEB	CAB-CBB-CGB-O1B
82	qF	203	PEB	CAC-CBC-CGC-O1C
82	vF	202	PEB	CAB-CBB-CGB-O1B
82	eG	201	PEB	CAB-CBB-CGB-O2B
82	hG	201	PEB	CAC-CBC-CGC-O2C
82	gH	201	PEB	CAB-CBB-CGB-O2B
82	iH	201	PEB	CAC-CBC-CGC-O1C
82	aH	202	PEB	CAC-CBC-CGC-O1C
82	aH	202	PEB	CAC-CBC-CGC-O2C
82	cJ	202	PEB	CAB-CBB-CGB-O1B
82	jJ	202	PEB	CAB-CBB-CGB-O2B
82	dK	202	PEB	CAB-CBB-CGB-O1B
82	oK	202	PEB	CAC-CBC-CGC-O2C
82	oK	203	PEB	CAC-CBC-CGC-O2C
82	pK	201	PEB	CAB-CBB-CGB-O1B
82	qK	201	PEB	CAB-CBB-CGB-O1B
82	qK	203	PEB	CAC-CBC-CGC-O1C
82	tK	201	PEB	CAC-CBC-CGC-O1C
82	vK	201	PEB	CAB-CBB-CGB-O1B
82	vK	202	PEB	CAB-CBB-CGB-O1B
82	cM	201	PEB	CAC-CBC-CGC-O1C
82	gM	202	PEB	CAB-CBB-CGB-O1B
82	jM	202	PEB	CAC-CBC-CGC-O1C
82	mM	201	PEB	CAC-CBC-CGC-O1C
82	aO	202	PEB	CAB-CBB-CGB-O2B
82	bO	202	PEB	CAB-CBB-CGB-O1B
82	eO	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
83	AE	302	PUB	CAC-CBC-CGC-O2C
83	AG	302	PUB	CAC-CBC-CGC-O2C
83	AO	303	PUB	CAB-CBB-CGB-O1B
84	EE	1001	CYC	CAA-CBA-CGA-O1A
84	ME	1001	CYC	CAA-CBA-CGA-O2A
84	EG	1001	CYC	CAA-CBA-CGA-O1A
84	GG	1001	CYC	CAA-CBA-CGA-O1A
84	MG	1001	CYC	CAA-CBA-CGA-O2A
84	JH	1003	CYC	CAD-CBD-CGD-O2D
84	LH	1002	CYC	CAD-CBD-CGD-O2D
84	NO	1001	CYC	CAD-CBD-CGD-O2D
84	M1	201	CYC	CAD-CBD-CGD-O2D
84	N4	1001	CYC	CAD-CBD-CGD-O2D
87	MN	101	CLA	CAA-CBA-CGA-O2A
87	RN	201	CLA	CAA-CBA-CGA-O1A
87	32	307	CLA	CAA-CBA-CGA-O1A
87	52	601	CLA	CAA-CBA-CGA-O1A
87	R2	201	CLA	CAA-CBA-CGA-O1A
87	3N	308	CLA	CAA-CBA-CGA-O1A
87	8N	305	CLA	CAA-CBA-CGA-O2A
87	AN	830	CLA	C10-C11-C12-C13
87	BN	819	CLA	C10-C11-C12-C13
87	A2	830	CLA	C10-C11-C12-C13
87	b6	618	CLA	C13-C15-C16-C17
87	cL	513	CLA	C8-C10-C11-C12
82	DO	1002	PEB	C3C-C2C-CAC-CBC
82	D4	1002	PEB	C3C-C2C-CAC-CBC
92	JL	102	LMG	C30-C31-C32-C33
82	JF	202	PEB	NC-C4C-CHC-C1D
82	OJ	202	PEB	NC-C4C-CHC-C1D
82	JK	202	PEB	NC-C4C-CHC-C1D
82	CP	201	PEB	NC-C4C-CHC-C1D
82	EP	203	PEB	NC-C4C-CHC-C1D
82	GP	201	PEB	NC-C4C-CHC-C1D
82	IP	203	PEB	NC-C4C-CHC-C1D
82	KP	201	PEB	NC-C4C-CHC-C1D
82	MP	203	PEB	NC-C4C-CHC-C1D
82	OP	201	PEB	NC-C4C-CHC-C1D
82	QP	203	PEB	NC-C4C-CHC-C1D
82	WP	201	PEB	NC-C4C-CHC-C1D
82	xF	302	PEB	NC-C4C-CHC-C1D
82	rK	202	PEB	NC-C4C-CHC-C1D

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Mol	Chain	Res	Type	Atoms
82	xK	302	PEB	NC-C4C-CHC-C1D
85	AL	401	BCR	C16-C17-C18-C19
85	FL	101	BCR	C12-C13-C14-C15
85	KL	100	BCR	C16-C17-C18-C19
85	AN	846	BCR	C20-C21-C22-C23
85	AN	848	BCR	C11-C10-C9-C8
85	AN	848	BCR	C16-C17-C18-C19
85	AN	848	BCR	C20-C21-C22-C23
85	BN	839	BCR	C11-C10-C9-C8
85	BN	840	BCR	C20-C21-C22-C23
85	FN	202	BCR	C12-C13-C14-C15
85	KN	101	BCR	C12-C13-C14-C15
85	KN	104	BCR	C20-C21-C22-C23
85	LN	201	BCR	C11-C10-C9-C8
85	LN	205	BCR	C11-C10-C9-C8
85	LN	205	BCR	C12-C13-C14-C15
85	A2	846	BCR	C20-C21-C22-C23
85	A2	848	BCR	C11-C10-C9-C8
85	A2	848	BCR	C16-C17-C18-C19
85	A2	848	BCR	C20-C21-C22-C23
85	B2	839	BCR	C11-C10-C9-C8
85	B2	840	BCR	C20-C21-C22-C23
85	F2	203	BCR	C12-C13-C14-C15
85	K2	102	BCR	C12-C13-C14-C15
85	K2	105	BCR	C20-C21-C22-C23
85	L2	201	BCR	C11-C10-C9-C8
85	L2	205	BCR	C11-C10-C9-C8
85	L2	205	BCR	C12-C13-C14-C15
85	A6	401	BCR	C16-C17-C18-C19
85	C6	508	BCR	C20-C21-C22-C23
85	K6	102	BCR	C16-C17-C18-C19
85	c6	603	BCR	C12-C13-C14-C15
85	k6	102	BCR	C16-C17-C18-C19
85	aL	604	BCR	C16-C17-C18-C19
85	fL	101	BCR	C12-C13-C14-C15
85	kL	100	BCR	C16-C17-C18-C19
87	A2	823	CLA	C5-C6-C7-C8
82	FA	202	PEB	CAB-CBB-CGB-O2B
82	GA	201	PEB	CAC-CBC-CGC-O2C
82	LA	202	PEB	CAB-CBB-CGB-O2B
82	LA	203	PEB	CAC-CBC-CGC-O2C
82	MA	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	UA	202	PEB	CAB-CBB-CGB-O2B
82	DB	202	PEB	CAC-CBC-CGC-O1C
82	IB	201	PEB	CAC-CBC-CGC-O2C
82	JB	201	PEB	CAC-CBC-CGC-O2C
82	QB	203	PEB	CAC-CBC-CGC-O2C
82	SB	203	PEB	CAB-CBB-CGB-O1B
82	VB	202	PEB	CAB-CBB-CGB-O2B
82	FD	202	PEB	CAB-CBB-CGB-O2B
82	MD	202	PEB	CAB-CBB-CGB-O2B
82	OD	201	PEB	CAB-CBB-CGB-O2B
82	ZE	202	PEB	CAC-CBC-CGC-O2C
82	DF	202	PEB	CAB-CBB-CGB-O2B
82	DF	203	PEB	CAC-CBC-CGC-O2C
82	HF	202	PEB	CAC-CBC-CGC-O1C
82	IF	201	PEB	CAC-CBC-CGC-O2C
82	IF	202	PEB	CAC-CBC-CGC-O1C
82	KF	203	PEB	CAB-CBB-CGB-O1B
82	TF	202	PEB	CAB-CBB-CGB-O2B
82	OH	201	PEB	CAC-CBC-CGC-O1C
82	RH	202	PEB	CAC-CBC-CGC-O2C
82	AI	201	PEB	CAB-CBB-CGB-O2B
82	CI	201	PEB	CAB-CBB-CGB-O2B
82	GI	202	PEB	CAB-CBB-CGB-O2B
82	HI	203	PEB	CAB-CBB-CGB-O1B
82	II	201	PEB	CAB-CBB-CGB-O2B
82	JI	201	PEB	CAB-CBB-CGB-O1B
82	KI	202	PEB	CAB-CBB-CGB-O2B
82	NI	201	PEB	CAB-CBB-CGB-O2B
82	PI	201	PEB	CAB-CBB-CGB-O2B
82	RI	201	PEB	CAB-CBB-CGB-O2B
82	TI	202	PEB	CAB-CBB-CGB-O2B
82	AJ	301	PEB	CAC-CBC-CGC-O2C
82	FJ	202	PEB	CAB-CBB-CGB-O1B
82	UJ	203	PEB	CAB-CBB-CGB-O1B
82	DK	202	PEB	CAB-CBB-CGB-O2B
82	SK	202	PEB	CAB-CBB-CGB-O2B
82	TK	202	PEB	CAB-CBB-CGB-O2B
82	EM	202	PEB	CAC-CBC-CGC-O2C
82	IM	203	PEB	CAB-CBB-CGB-O1B
82	KM	203	PEB	CAC-CBC-CGC-O2C
82	TM	202	PEB	CAC-CBC-CGC-O1C
82	XM	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	OO	202	PEB	CAB-CBB-CGB-O2B
82	UO	201	PEB	CAC-CBC-CGC-O2C
82	AP	201	PEB	CAC-CBC-CGC-O2C
82	BP	201	PEB	CAC-CBC-CGC-O2C
82	YP	503	PEB	CAB-CBB-CGB-O2B
82	FQ	202	PEB	CAB-CBB-CGB-O2B
82	GQ	202	PEB	CAB-CBB-CGB-O2B
82	MQ	202	PEB	CAB-CBB-CGB-O2B
82	PQ	203	PEB	CAB-CBB-CGB-O2B
82	XQ	203	PEB	CAB-CBB-CGB-O2B
82	R1	202	PEB	CAC-CBC-CGC-O2C
82	j1	202	PEB	CAB-CBB-CGB-O2B
82	a1	202	PEB	CAC-CBC-CGC-O2C
82	b1	201	PEB	CAC-CBC-CGC-O2C
82	O4	202	PEB	CAB-CBB-CGB-O2B
82	U4	201	PEB	CAC-CBC-CGC-O2C
82	U4	202	PEB	CAC-CBC-CGC-O2C
82	a4	202	PEB	CAB-CBB-CGB-O2B
82	d4	202	PEB	CAB-CBB-CGB-O2B
82	J5	202	PEB	CAC-CBC-CGC-O2C
82	Q5	202	PEB	CAC-CBC-CGC-O1C
82	Z5	305	PEB	CAC-CBC-CGC-O2C
82	L7	202	PEB	CAB-CBB-CGB-O2B
82	R7	203	PEB	CAC-CBC-CGC-O2C
82	U7	202	PEB	CAB-CBB-CGB-O2B
82	e7	301	PEB	CAB-CBB-CGB-O2B
82	B9	203	PEB	CAB-CBB-CGB-O1B
82	S9	202	PEB	CAC-CBC-CGC-O2C
82	W9	202	PEB	CAC-CBC-CGC-O2C
82	Y9	202	PEB	CAC-CBC-CGC-O1C
82	eA	301	PEB	CAB-CBB-CGB-O2B
82	eE	201	PEB	CAB-CBB-CGB-O2B
82	hE	201	PEB	CAC-CBC-CGC-O2C
82	kE	202	PEB	CAB-CBB-CGB-O2B
82	cF	201	PEB	CAC-CBC-CGC-O2C
82	lF	203	PEB	CAB-CBB-CGB-O2B
82	rF	202	PEB	CAB-CBB-CGB-O2B
82	hG	202	PEB	CAB-CBB-CGB-O2B
82	kG	202	PEB	CAB-CBB-CGB-O2B
82	cH	201	PEB	CAC-CBC-CGC-O1C
82	dH	202	PEB	CAC-CBC-CGC-O2C
82	aJ	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	iJ	202	PEB	CAB-CBB-CGB-O1B
82	jJ	202	PEB	CAB-CBB-CGB-O1B
82	kJ	202	PEB	CAB-CBB-CGB-O2B
82	kK	202	PEB	CAC-CBC-CGC-O2C
82	lK	203	PEB	CAB-CBB-CGB-O2B
82	rK	202	PEB	CAB-CBB-CGB-O2B
82	yK	301	PEB	CAC-CBC-CGC-O2C
82	aM	203	PEB	CAB-CBB-CGB-O2B
82	jM	202	PEB	CAC-CBC-CGC-O2C
82	kM	202	PEB	CAB-CBB-CGB-O2B
82	dO	202	PEB	CAB-CBB-CGB-O2B
83	M5	303	PUB	CAC-CBC-CGC-O2C
84	DG	1001	CYC	CAD-CBD-CGD-O2D
84	CH	1001	CYC	CAA-CBA-CGA-O1A
84	L1	1001	CYC	CAD-CBD-CGD-O2D
84	C1	1001	CYC	CAA-CBA-CGA-O1A
84	V3	1001	CYC	CAD-CBD-CGD-O2D
92	BL	611	LMG	O7-C8-C9-O8
92	dL	407	LMG	O1-C7-C8-O7
88	CL	522	LHG	C24-C23-O8-C6
88	bL	612	LHG	C13-C14-C15-C16
92	aL	611	LMG	C28-C29-C30-C31
92	mL	101	LMG	C10-C11-C12-C13
92	yL	101	LMG	C8-C9-O8-C28
87	AL	405	CLA	C2A-CAA-CBA-CGA
85	JN	103	BCR	C19-C20-C21-C22
85	KN	101	BCR	C15-C16-C17-C18
85	J2	103	BCR	C19-C20-C21-C22
85	K2	102	BCR	C15-C16-C17-C18
82	KA	202	PEB	CAC-CBC-CGC-O1C
82	TA	201	PEB	CAC-CBC-CGC-O2C
82	YA	304	PEB	CAC-CBC-CGC-O2C
82	DB	202	PEB	CAC-CBC-CGC-O2C
82	KB	304	PEB	CAC-CBC-CGC-O2C
82	LB	201	PEB	CAC-CBC-CGC-O1C
82	MB	202	PEB	CAB-CBB-CGB-O1B
82	NB	202	PEB	CAC-CBC-CGC-O2C
82	NB	202	PEB	CAB-CBB-CGB-O2B
82	QB	201	PEB	CAC-CBC-CGC-O1C
82	TB	201	PEB	CAC-CBC-CGC-O2C
82	VB	202	PEB	CAC-CBC-CGC-O2C
82	BD	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	GD	202	PEB	CAB-CBB-CGB-O2B
82	RD	202	PEB	CAC-CBC-CGC-O2C
82	RD	203	PEB	CAC-CBC-CGC-O1C
82	TD	202	PEB	CAC-CBC-CGC-O2C
82	TD	203	PEB	CAB-CBB-CGB-O1B
82	UD	202	PEB	CAB-CBB-CGB-O2B
82	RE	202	PEB	CAC-CBC-CGC-O1C
82	SE	201	PEB	CAB-CBB-CGB-O1B
82	UE	202	PEB	CAC-CBC-CGC-O2C
82	VE	202	PEB	CAB-CBB-CGB-O2B
82	YE	201	PEB	CAC-CBC-CGC-O1C
82	AF	202	PEB	CAC-CBC-CGC-O2C
82	DF	201	PEB	CAB-CBB-CGB-O1B
82	HF	202	PEB	CAC-CBC-CGC-O2C
82	IF	201	PEB	CAC-CBC-CGC-O1C
82	XF	203	PEB	CAC-CBC-CGC-O1C
82	DG	1002	PEB	CAC-CBC-CGC-O2C
82	PG	202	PEB	CAC-CBC-CGC-O2C
82	VG	202	PEB	CAB-CBB-CGB-O2B
82	ZG	202	PEB	CAC-CBC-CGC-O2C
82	ZG	202	PEB	CAB-CBB-CGB-O2B
82	EI	201	PEB	CAB-CBB-CGB-O2B
82	HI	203	PEB	CAB-CBB-CGB-O2B
82	ZI	401	PEB	CAC-CBC-CGC-O2C
82	EJ	203	PEB	CAC-CBC-CGC-O1C
82	IJ	203	PEB	CAB-CBB-CGB-O2B
82	JJ	201	PEB	CAC-CBC-CGC-O1C
82	RJ	202	PEB	CAB-CBB-CGB-O1B
82	DK	201	PEB	CAB-CBB-CGB-O1B
82	DK	202	PEB	CAB-CBB-CGB-O1B
82	DK	203	PEB	CAC-CBC-CGC-O2C
82	IK	202	PEB	CAC-CBC-CGC-O1C
82	LK	202	PEB	CAC-CBC-CGC-O2C
82	XK	203	PEB	CAC-CBC-CGC-O1C
82	DM	202	PEB	CAB-CBB-CGB-O2B
82	GM	202	PEB	CAB-CBB-CGB-O2B
82	QM	202	PEB	CAC-CBC-CGC-O2C
82	SM	202	PEB	CAB-CBB-CGB-O1B
82	UM	201	PEB	CAC-CBC-CGC-O1C
82	XM	202	PEB	CAB-CBB-CGB-O1B
82	MP	202	PEB	CAC-CBC-CGC-O2C
82	QP	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	UP	202	PEB	CAC-CBC-CGC-O1C
82	BQ	202	PEB	CAC-CBC-CGC-O1C
82	RQ	202	PEB	CAC-CBC-CGC-O2C
82	TQ	203	PEB	CAB-CBB-CGB-O1B
82	UQ	201	PEB	CAC-CBC-CGC-O1C
82	i1	201	PEB	CAC-CBC-CGC-O2C
82	a1	201	PEB	CAC-CBC-CGC-O1C
82	H5	201	PEB	CAC-CBC-CGC-O1C
82	Q5	203	PEB	CAB-CBB-CGB-O1B
82	U5	203	PEB	CAB-CBB-CGB-O1B
82	Z5	305	PEB	CAB-CBB-CGB-O2B
82	F7	202	PEB	CAC-CBC-CGC-O2C
82	K7	202	PEB	CAC-CBC-CGC-O1C
82	M7	201	PEB	CAB-CBB-CGB-O1B
82	R7	201	PEB	CAB-CBB-CGB-O2B
82	T7	201	PEB	CAC-CBC-CGC-O2C
82	X7	203	PEB	CAC-CBC-CGC-O2C
82	Y7	304	PEB	CAC-CBC-CGC-O2C
82	z8	202	PEB	CAC-CBC-CGC-O2C
82	p8	202	PEB	CAB-CBB-CGB-O2B
82	s8	201	PEB	CAC-CBC-CGC-O2C
82	B9	202	PEB	CAC-CBC-CGC-O1C
82	S9	203	PEB	CAB-CBB-CGB-O1B
82	Y9	202	PEB	CAC-CBC-CGC-O2C
82	zC	202	PEB	CAC-CBC-CGC-O2C
82	sC	201	PEB	CAC-CBC-CGC-O2C
82	dD	401	PEB	CAC-CBC-CGC-O1C
82	dF	202	PEB	CAC-CBC-CGC-O2C
82	kF	202	PEB	CAC-CBC-CGC-O2C
82	kF	202	PEB	CAB-CBB-CGB-O2B
82	nF	201	PEB	CAC-CBC-CGC-O2C
82	yF	301	PEB	CAC-CBC-CGC-O2C
82	cG	201	PEB	CAC-CBC-CGC-O2C
82	dG	204	PEB	CAC-CBC-CGC-O2C
82	jG	202	PEB	CAC-CBC-CGC-O2C
82	iH	201	PEB	CAC-CBC-CGC-O2C
82	aH	201	PEB	CAC-CBC-CGC-O1C
82	gJ	201	PEB	CAC-CBC-CGC-O1C
82	mJ	201	PEB	CAC-CBC-CGC-O1C
82	dK	202	PEB	CAC-CBC-CGC-O2C
82	hK	201	PEB	CAC-CBC-CGC-O1C
82	lK	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	nK	201	PEB	CAC-CBC-CGC-O2C
82	oK	203	PEB	CAB-CBB-CGB-O1B
82	rK	201	PEB	CAC-CBC-CGC-O2C
82	mO	201	PEB	CAB-CBB-CGB-O1B
83	AE	303	PUB	CAC-CBC-CGC-O2C
83	Z5	303	PUB	CAC-CBC-CGC-O2C
84	DE	1001	CYC	CAD-CBD-CGD-O2D
84	CH	1001	CYC	CAA-CBA-CGA-O2A
84	EH	1001	CYC	CAA-CBA-CGA-O1A
84	KH	1001	CYC	CAA-CBA-CGA-O2A
84	NH	1001	CYC	CAA-CBA-CGA-O1A
84	N1	1001	CYC	CAA-CBA-CGA-O1A
84	N1	1001	CYC	CAA-CBA-CGA-O2A
84	W3	1001	CYC	CAA-CBA-CGA-O2A
87	12	601	CLA	CAA-CBA-CGA-O1A
87	1N	601	CLA	CAA-CBA-CGA-O1A
96	E6	101	HEM	CAA-CBA-CGA-O2A
82	NJ	201	PEB	C2C-C1C-CHB-C4B
82	M9	304	PEB	C2C-C1C-CHB-C4B
87	AN	823	CLA	C5-C6-C7-C8
95	c6	618	DGD	CDA-CEA-CFA-CGA
82	LE	1002	PEB	C1C-C2C-CAC-CBC
82	PE	201	PEB	C1C-C2C-CAC-CBC
82	LG	1002	PEB	C1C-C2C-CAC-CBC
82	PG	201	PEB	C1C-C2C-CAC-CBC
88	AN	844	LHG	C15-C16-C17-C18
88	A2	844	LHG	C15-C16-C17-C18
82	m1	202	PEB	NC-C1C-CHB-C4B
82	p8	201	PEB	NC-C1C-CHB-C4B
82	pC	201	PEB	NC-C1C-CHB-C4B
88	c6	619	LHG	C1-C2-C3-O3
88	d6	402	LHG	C1-C2-C3-O3
82	HA	203	PEB	CAB-CBB-CGB-O1B
82	OA	202	PEB	CAC-CBC-CGC-O2C
82	RA	201	PEB	CAB-CBB-CGB-O2B
82	SA	202	PEB	CAB-CBB-CGB-O2B
82	BB	202	PEB	CAB-CBB-CGB-O2B
82	CB	202	PEB	CAC-CBC-CGC-O1C
82	IB	201	PEB	CAC-CBC-CGC-O1C
82	VB	201	PEB	CAC-CBC-CGC-O1C
82	XB	202	PEB	CAB-CBB-CGB-O1B
82	BD	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	RD	201	PEB	CAB-CBB-CGB-O2B
82	UD	201	PEB	CAC-CBC-CGC-O1C
82	WD	201	PEB	CAC-CBC-CGC-O1C
82	XD	203	PEB	CAC-CBC-CGC-O2C
82	PE	202	PEB	CAC-CBC-CGC-O2C
82	YE	202	PEB	CAC-CBC-CGC-O1C
82	ZE	202	PEB	CAB-CBB-CGB-O2B
82	LF	202	PEB	CAC-CBC-CGC-O2C
82	PG	202	PEB	CAC-CBC-CGC-O1C
82	UG	202	PEB	CAC-CBC-CGC-O2C
82	YG	201	PEB	CAC-CBC-CGC-O1C
82	QH	203	PEB	CAB-CBB-CGB-O2B
82	BI	202	PEB	CAC-CBC-CGC-O2C
82	II	202	PEB	CAC-CBC-CGC-O2C
82	LI	201	PEB	CAB-CBB-CGB-O2B
82	OI	201	PEB	CAB-CBB-CGB-O2B
82	PI	202	PEB	CAC-CBC-CGC-O2C
82	RI	202	PEB	CAC-CBC-CGC-O2C
82	SI	201	PEB	CAB-CBB-CGB-O2B
82	TI	203	PEB	CAC-CBC-CGC-O2C
82	EJ	201	PEB	CAC-CBC-CGC-O1C
82	FJ	202	PEB	CAB-CBB-CGB-O2B
82	GJ	202	PEB	CAB-CBB-CGB-O2B
82	KJ	202	PEB	CAB-CBB-CGB-O2B
82	MJ	201	PEB	CAC-CBC-CGC-O2C
82	TJ	202	PEB	CAB-CBB-CGB-O2B
82	UJ	203	PEB	CAC-CBC-CGC-O2C
82	AK	202	PEB	CAC-CBC-CGC-O2C
82	BK	201	PEB	CAC-CBC-CGC-O1C
82	HK	202	PEB	CAC-CBC-CGC-O2C
82	IK	201	PEB	CAC-CBC-CGC-O2C
82	LK	202	PEB	CAC-CBC-CGC-O1C
82	EM	203	PEB	CAB-CBB-CGB-O2B
82	LM	202	PEB	CAB-CBB-CGB-O1B
82	MM	201	PEB	CAC-CBC-CGC-O1C
82	UM	202	PEB	CAC-CBC-CGC-O1C
82	UM	203	PEB	CAB-CBB-CGB-O2B
82	PO	202	PEB	CAB-CBB-CGB-O2B
82	SO	202	PEB	CAB-CBB-CGB-O1B
82	CP	203	PEB	CAC-CBC-CGC-O1C
82	EP	203	PEB	CAC-CBC-CGC-O2C
82	RP	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	YP	502	PEB	CAB-CBB-CGB-O2B
82	BQ	201	PEB	CAB-CBB-CGB-O2B
82	RQ	201	PEB	CAB-CBB-CGB-O2B
82	UQ	202	PEB	CAB-CBB-CGB-O2B
82	WQ	201	PEB	CAC-CBC-CGC-O1C
82	XQ	203	PEB	CAC-CBC-CGC-O2C
82	YQ	202	PEB	CAC-CBC-CGC-O2C
82	Q1	203	PEB	CAB-CBB-CGB-O2B
82	R1	202	PEB	CAB-CBB-CGB-O2B
82	S1	202	PEB	CAB-CBB-CGB-O1B
82	g1	201	PEB	CAC-CBC-CGC-O2C
82	l1	201	PEB	CAC-CBC-CGC-O2C
82	l1	201	PEB	CAB-CBB-CGB-O1B
82	P4	202	PEB	CAB-CBB-CGB-O2B
82	Q4	202	PEB	CAB-CBB-CGB-O2B
82	R4	202	PEB	CAB-CBB-CGB-O2B
82	S4	202	PEB	CAB-CBB-CGB-O1B
82	f4	202	PEB	CAB-CBB-CGB-O2B
82	D5	202	PEB	CAC-CBC-CGC-O2C
82	L5	203	PEB	CAB-CBB-CGB-O1B
82	M5	305	PEB	CAB-CBB-CGB-O2B
82	Q5	201	PEB	CAC-CBC-CGC-O2C
82	S5	202	PEB	CAC-CBC-CGC-O2C
82	S5	203	PEB	CAB-CBB-CGB-O1B
82	Y5	203	PEB	CAB-CBB-CGB-O1B
82	F7	202	PEB	CAB-CBB-CGB-O2B
82	O7	202	PEB	CAC-CBC-CGC-O2C
82	S7	202	PEB	CAB-CBB-CGB-O2B
82	y8	203	PEB	CAB-CBB-CGB-O2B
82	A9	202	PEB	CAB-CBB-CGB-O1B
82	C9	202	PEB	CAB-CBB-CGB-O1B
82	D9	202	PEB	CAC-CBC-CGC-O2C
82	E9	202	PEB	CAB-CBB-CGB-O1B
82	G9	202	PEB	CAB-CBB-CGB-O1B
82	I9	202	PEB	CAB-CBB-CGB-O1B
82	K9	202	PEB	CAB-CBB-CGB-O1B
82	N9	202	PEB	CAB-CBB-CGB-O1B
82	P9	202	PEB	CAB-CBB-CGB-O1B
82	R9	202	PEB	CAB-CBB-CGB-O1B
82	T9	202	PEB	CAB-CBB-CGB-O1B
82	V9	202	PEB	CAB-CBB-CGB-O1B
82	W9	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	X9	202	PEB	CAB-CBB-CGB-O1B
82	yC	203	PEB	CAB-CBB-CGB-O2B
82	dE	204	PEB	CAC-CBC-CGC-O2C
82	dE	204	PEB	CAB-CBB-CGB-O2B
82	gE	202	PEB	CAB-CBB-CGB-O2B
82	hF	201	PEB	CAC-CBC-CGC-O1C
82	lF	202	PEB	CAC-CBC-CGC-O1C
82	mF	202	PEB	CAB-CBB-CGB-O2B
82	oF	203	PEB	CAB-CBB-CGB-O1B
82	rF	201	PEB	CAB-CBB-CGB-O1B
82	uF	202	PEB	CAB-CBB-CGB-O2B
82	wF	302	PEB	CAB-CBB-CGB-O2B
82	yF	301	PEB	CAB-CBB-CGB-O2B
82	dG	201	PEB	CAB-CBB-CGB-O2B
82	dG	204	PEB	CAB-CBB-CGB-O2B
82	gG	202	PEB	CAB-CBB-CGB-O2B
82	jH	202	PEB	CAB-CBB-CGB-O2B
82	kH	203	PEB	CAC-CBC-CGC-O2C
82	kH	203	PEB	CAB-CBB-CGB-O1B
82	dJ	201	PEB	CAB-CBB-CGB-O2B
82	hK	201	PEB	CAC-CBC-CGC-O2C
82	kK	202	PEB	CAB-CBB-CGB-O2B
82	mK	202	PEB	CAB-CBB-CGB-O2B
82	rK	201	PEB	CAB-CBB-CGB-O1B
82	rK	202	PEB	CAC-CBC-CGC-O2C
82	yK	301	PEB	CAB-CBB-CGB-O2B
82	aM	201	PEB	CAB-CBB-CGB-O2B
82	eM	202	PEB	CAB-CBB-CGB-O2B
82	bO	201	PEB	CAC-CBC-CGC-O2C
82	fO	202	PEB	CAB-CBB-CGB-O2B
82	bP	501	PEB	CAB-CBB-CGB-O2B
82	dQ	401	PEB	CAC-CBC-CGC-O1C
83	AJ	304	PUB	CAC-CBC-CGC-O2C
83	AM	303	PUB	CAB-CBB-CGB-O2B
83	wF	304	PUB	CAB-CBB-CGB-O2B
83	xF	305	PUB	CAB-CBB-CGB-O2B
84	NH	1001	CYC	CAA-CBA-CGA-O2A
84	C1	1001	CYC	CAA-CBA-CGA-O2A
84	y3	1001	CYC	CAA-CBA-CGA-O2A
87	42	605	CLA	CAA-CBA-CGA-O2A
87	62	306	CLA	CAA-CBA-CGA-O2A
87	4N	605	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
87	6N	605	CLA	CAA-CBA-CGA-O2A
92	k6	101	LMG	C23-C24-C25-C26
87	dL	404	CLA	C5-C6-C7-C8
82	B7	201	PEB	C4B-C3B-CAB-CBB
87	nL	101	CLA	C3-C5-C6-C7
87	dL	404	CLA	C4-C3-C5-C6
87	AN	810	CLA	C2-C1-O2A-CGA
87	AN	840	CLA	C2-C1-O2A-CGA
87	BN	835	CLA	C2-C1-O2A-CGA
87	BN	836	CLA	C2-C1-O2A-CGA
87	32	309	CLA	C2-C1-O2A-CGA
87	A2	810	CLA	C2-C1-O2A-CGA
87	A2	840	CLA	C2-C1-O2A-CGA
87	B2	835	CLA	C2-C1-O2A-CGA
87	B2	836	CLA	C2-C1-O2A-CGA
87	C6	513	CLA	C2-C1-O2A-CGA
87	d6	403	CLA	C2-C1-O2A-CGA
87	aL	605	CLA	C2-C1-O2A-CGA
87	cL	509	CLA	C2-C1-O2A-CGA
87	3N	309	CLA	C2-C1-O2A-CGA
83	yK	303	PUB	C4A-C3A-CAA-CBA
82	KA	202	PEB	C2A-C3A-CAA-CBA
82	XF	201	PEB	C2A-C3A-CAA-CBA
82	BI	201	PEB	C2A-C3A-CAA-CBA
82	XK	201	PEB	C2A-C3A-CAA-CBA
82	LP	201	PEB	C2A-C3A-CAA-CBA
82	SP	201	PEB	C2A-C3A-CAA-CBA
82	m1	202	PEB	C2A-C3A-CAA-CBA
82	H5	201	PEB	C2A-C3A-CAA-CBA
82	K7	202	PEB	C2A-C3A-CAA-CBA
82	gE	201	PEB	C2A-C3A-CAA-CBA
82	mH	202	PEB	C2A-C3A-CAA-CBA
82	aM	201	PEB	C2A-C3A-CAA-CBA
82	mO	202	PEB	C2A-C3A-CAA-CBA
87	BL	609	CLA	C2-C3-C5-C6
82	AA	201	PEB	CAB-CBB-CGB-O1B
82	FB	201	PEB	CAC-CBC-CGC-O2C
82	GB	203	PEB	CAC-CBC-CGC-O1C
82	OB	201	PEB	CAC-CBC-CGC-O2C
82	RB	202	PEB	CAC-CBC-CGC-O1C
82	RB	202	PEB	CAC-CBC-CGC-O2C
82	AD	301	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	GD	202	PEB	CAB-CBB-CGB-O1B
82	HD	203	PEB	CAC-CBC-CGC-O1C
82	YD	202	PEB	CAC-CBC-CGC-O2C
82	PE	202	PEB	CAC-CBC-CGC-O1C
82	BF	201	PEB	CAC-CBC-CGC-O1C
82	CF	201	PEB	CAB-CBB-CGB-O1B
82	CF	203	PEB	CAB-CBB-CGB-O1B
82	DF	203	PEB	CAC-CBC-CGC-O1C
82	NF	201	PEB	CAC-CBC-CGC-O1C
82	RG	202	PEB	CAC-CBC-CGC-O1C
82	SG	201	PEB	CAB-CBB-CGB-O1B
82	YG	202	PEB	CAC-CBC-CGC-O1C
82	AH	305	PEB	CAC-CBC-CGC-O2C
82	RH	201	PEB	CAB-CBB-CGB-O2B
82	SH	202	PEB	CAB-CBB-CGB-O1B
82	SH	202	PEB	CAB-CBB-CGB-O2B
82	SH	203	PEB	CAC-CBC-CGC-O1C
82	ZH	201	PEB	CAB-CBB-CGB-O1B
82	AI	202	PEB	CAC-CBC-CGC-O2C
82	CI	202	PEB	CAC-CBC-CGC-O2C
82	EI	202	PEB	CAC-CBC-CGC-O2C
82	FI	202	PEB	CAB-CBB-CGB-O2B
82	GI	203	PEB	CAC-CBC-CGC-O2C
82	HI	201	PEB	CAB-CBB-CGB-O2B
82	KI	203	PEB	CAC-CBC-CGC-O2C
82	LI	202	PEB	CAB-CBB-CGB-O2B
82	XI	202	PEB	CAC-CBC-CGC-O2C
82	CJ	202	PEB	CAB-CBB-CGB-O2B
82	NJ	202	PEB	CAC-CBC-CGC-O2C
82	OJ	201	PEB	CAC-CBC-CGC-O1C
82	PJ	202	PEB	CAB-CBB-CGB-O1B
82	WJ	202	PEB	CAC-CBC-CGC-O1C
82	YJ	202	PEB	CAC-CBC-CGC-O1C
82	CK	201	PEB	CAB-CBB-CGB-O1B
82	IK	201	PEB	CAC-CBC-CGC-O1C
82	NK	201	PEB	CAC-CBC-CGC-O1C
82	AM	302	PEB	CAB-CBB-CGB-O1B
82	EM	201	PEB	CAC-CBC-CGC-O1C
82	IM	202	PEB	CAC-CBC-CGC-O1C
82	JM	202	PEB	CAB-CBB-CGB-O2B
82	MM	203	PEB	CAB-CBB-CGB-O1B
82	VM	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	YM	201	PEB	CAC-CBC-CGC-O1C
82	ZM	202	PEB	CAB-CBB-CGB-O2B
82	RO	203	PEB	CAC-CBC-CGC-O2C
82	AP	202	PEB	CAC-CBC-CGC-O2C
82	AP	203	PEB	CAC-CBC-CGC-O2C
82	DP	201	PEB	CAB-CBB-CGB-O2B
82	FP	201	PEB	CAB-CBB-CGB-O2B
82	MP	203	PEB	CAB-CBB-CGB-O2B
82	OP	203	PEB	CAC-CBC-CGC-O1C
82	QP	202	PEB	CAC-CBC-CGC-O1C
82	QP	202	PEB	CAC-CBC-CGC-O2C
82	QP	202	PEB	CAB-CBB-CGB-O1B
82	AQ	301	PEB	CAB-CBB-CGB-O2B
82	GQ	202	PEB	CAB-CBB-CGB-O1B
82	HQ	203	PEB	CAC-CBC-CGC-O1C
82	JQ	202	PEB	CAB-CBB-CGB-O1B
82	TQ	202	PEB	CAC-CBC-CGC-O2C
82	S1	202	PEB	CAB-CBB-CGB-O2B
82	A1	305	PEB	CAC-CBC-CGC-O2C
82	V1	202	PEB	CAC-CBC-CGC-O1C
82	h1	202	PEB	CAC-CBC-CGC-O1C
82	b1	201	PEB	CAC-CBC-CGC-O1C
82	j4	201	PEB	CAC-CBC-CGC-O1C
82	j4	202	PEB	CAB-CBB-CGB-O2B
82	l4	201	PEB	CAC-CBC-CGC-O2C
82	l4	202	PEB	CAC-CBC-CGC-O1C
82	m4	201	PEB	CAB-CBB-CGB-O1B
82	a4	203	PEB	CAC-CBC-CGC-O2C
82	b4	201	PEB	CAC-CBC-CGC-O2C
82	d4	201	PEB	CAC-CBC-CGC-O2C
82	f4	201	PEB	CAC-CBC-CGC-O2C
82	h4	201	PEB	CAC-CBC-CGC-O1C
82	C5	201	PEB	CAB-CBB-CGB-O2B
82	H5	202	PEB	CAC-CBC-CGC-O2C
82	H5	203	PEB	CAB-CBB-CGB-O1B
82	O5	201	PEB	CAC-CBC-CGC-O1C
82	P5	201	PEB	CAB-CBB-CGB-O2B
82	W5	203	PEB	CAC-CBC-CGC-O2C
82	A7	201	PEB	CAB-CBB-CGB-O1B
82	A7	202	PEB	CAC-CBC-CGC-O2C
82	F7	202	PEB	CAB-CBB-CGB-O1B
82	L7	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	y8	201	PEB	CAB-CBB-CGB-O2B
82	z8	202	PEB	CAC-CBC-CGC-O1C
82	p8	202	PEB	CAB-CBB-CGB-O1B
82	t8	202	PEB	CAB-CBB-CGB-O2B
82	v8	201	PEB	CAB-CBB-CGB-O1B
82	F9	203	PEB	CAB-CBB-CGB-O2B
82	O9	201	PEB	CAC-CBC-CGC-O2C
82	O9	201	PEB	CAB-CBB-CGB-O1B
82	Q9	202	PEB	CAC-CBC-CGC-O2C
82	bB	201	PEB	CAC-CBC-CGC-O2C
82	zC	202	PEB	CAC-CBC-CGC-O1C
82	pC	202	PEB	CAB-CBB-CGB-O1B
82	pC	202	PEB	CAB-CBB-CGB-O2B
82	tC	202	PEB	CAB-CBB-CGB-O2B
82	vC	201	PEB	CAB-CBB-CGB-O1B
82	cE	201	PEB	CAC-CBC-CGC-O2C
82	hE	202	PEB	CAB-CBB-CGB-O2B
82	jE	202	PEB	CAC-CBC-CGC-O2C
82	cF	201	PEB	CAB-CBB-CGB-O2B
82	cF	202	PEB	CAC-CBC-CGC-O1C
82	jF	202	PEB	CAB-CBB-CGB-O1B
82	rF	201	PEB	CAC-CBC-CGC-O2C
82	vF	201	PEB	CAC-CBC-CGC-O2C
82	lG	203	PEB	CAC-CBC-CGC-O2C
82	gH	201	PEB	CAC-CBC-CGC-O2C
82	dH	202	PEB	CAB-CBB-CGB-O1B
82	lJ	202	PEB	CAC-CBC-CGC-O1C
82	cK	202	PEB	CAC-CBC-CGC-O1C
82	jK	202	PEB	CAB-CBB-CGB-O1B
82	qK	201	PEB	CAC-CBC-CGC-O1C
82	sK	201	PEB	CAB-CBB-CGB-O2B
82	sK	203	PEB	CAC-CBC-CGC-O2C
82	uK	201	PEB	CAB-CBB-CGB-O2B
82	uK	202	PEB	CAC-CBC-CGC-O1C
82	vK	201	PEB	CAC-CBC-CGC-O2C
82	wK	302	PEB	CAB-CBB-CGB-O2B
82	aM	201	PEB	CAB-CBB-CGB-O1B
82	hM	202	PEB	CAC-CBC-CGC-O1C
82	jM	203	PEB	CAC-CBC-CGC-O2C
82	kM	201	PEB	CAC-CBC-CGC-O1C
82	jO	201	PEB	CAC-CBC-CGC-O1C
82	jO	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	lO	202	PEB	CAC-CBC-CGC-O1C
82	dO	201	PEB	CAC-CBC-CGC-O2C
82	hO	201	PEB	CAC-CBC-CGC-O1C
83	AE	303	PUB	CAB-CBB-CGB-O1B
83	AG	303	PUB	CAC-CBC-CGC-O2C
83	AG	303	PUB	CAB-CBB-CGB-O1B
83	BJ	302	PUB	CAB-CBB-CGB-O1B
83	BM	302	PUB	CAC-CBC-CGC-O2C
83	wK	304	PUB	CAB-CBB-CGB-O2B
83	xK	305	PUB	CAB-CBB-CGB-O2B
84	ME	1001	CYC	CAA-CBA-CGA-O1A
84	NE	201	CYC	CAA-CBA-CGA-O2A
84	MG	1001	CYC	CAA-CBA-CGA-O1A
84	FH	1001	CYC	CAA-CBA-CGA-O2A
84	KH	1001	CYC	CAA-CBA-CGA-O1A
84	E1	1001	CYC	CAA-CBA-CGA-O1A
84	E1	1001	CYC	CAA-CBA-CGA-O2A
84	A3	1001	CYC	CAA-CBA-CGA-O2A
84	E3	1001	CYC	CAA-CBA-CGA-O2A
84	G3	1001	CYC	CAA-CBA-CGA-O2A
84	N3	1001	CYC	CAA-CBA-CGA-O2A
84	i3	1001	CYC	CAA-CBA-CGA-O2A
84	v3	1001	CYC	CAA-CBA-CGA-O2A
92	a6	614	LMG	C10-C11-C12-C13
83	yF	303	PUB	C4A-C3A-CAA-CBA
82	LE	1002	PEB	C3C-C2C-CAC-CBC
82	LG	1002	PEB	C3C-C2C-CAC-CBC
82	OJ	202	PEB	C3C-C2C-CAC-CBC
82	dE	201	PEB	C3C-C2C-CAC-CBC
82	dG	201	PEB	C3C-C2C-CAC-CBC
87	BL	608	CLA	C6-C7-C8-C9
87	AN	802	CLA	C14-C13-C15-C16
87	AN	821	CLA	C14-C13-C15-C16
87	A2	801	CLA	C14-C13-C15-C16
87	A2	821	CLA	C14-C13-C15-C16
87	c6	612	CLA	C14-C13-C15-C16
82	k4	202	PEB	C3B-C4B-CHB-C1C
88	C6	522	LHG	O10-C23-O8-C6
82	DA	201	PEB	CAB-CBB-CGB-O2B
82	FA	202	PEB	CAB-CBB-CGB-O1B
82	LA	203	PEB	CAC-CBC-CGC-O1C
82	RA	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	GB	202	PEB	CAB-CBB-CGB-O2B
82	SB	201	PEB	CAC-CBC-CGC-O1C
82	WB	401	PEB	CAB-CBB-CGB-O2B
82	JD	202	PEB	CAB-CBB-CGB-O1B
82	ND	203	PEB	CAB-CBB-CGB-O2B
82	FF	201	PEB	CAB-CBB-CGB-O2B
82	VF	202	PEB	CAC-CBC-CGC-O2C
82	BI	203	PEB	CAB-CBB-CGB-O2B
82	LI	201	PEB	CAB-CBB-CGB-O1B
82	NI	202	PEB	CAC-CBC-CGC-O2C
82	OI	203	PEB	CAB-CBB-CGB-O2B
82	UI	201	PEB	CAB-CBB-CGB-O2B
82	VI	202	PEB	CAC-CBC-CGC-O2C
82	WI	203	PEB	CAB-CBB-CGB-O2B
82	EJ	203	PEB	CAB-CBB-CGB-O2B
82	IJ	203	PEB	CAC-CBC-CGC-O1C
82	CK	203	PEB	CAB-CBB-CGB-O1B
82	DK	203	PEB	CAC-CBC-CGC-O1C
82	FK	201	PEB	CAB-CBB-CGB-O2B
82	VK	202	PEB	CAC-CBC-CGC-O2C
82	AM	302	PEB	CAC-CBC-CGC-O2C
82	FM	202	PEB	CAB-CBB-CGB-O2B
82	KM	202	PEB	CAB-CBB-CGB-O2B
82	VM	201	PEB	CAC-CBC-CGC-O2C
82	QO	202	PEB	CAB-CBB-CGB-O2B
82	WO	201	PEB	CAC-CBC-CGC-O1C
82	ZO	202	PEB	CAC-CBC-CGC-O2C
82	AP	202	PEB	CAC-CBC-CGC-O1C
82	SP	203	PEB	CAC-CBC-CGC-O2C
82	TP	201	PEB	CAB-CBB-CGB-O2B
82	NQ	203	PEB	CAB-CBB-CGB-O2B
82	TQ	201	PEB	CAC-CBC-CGC-O2C
82	R1	201	PEB	CAB-CBB-CGB-O2B
82	F1	1002	PEB	CAB-CBB-CGB-O2B
82	W4	201	PEB	CAC-CBC-CGC-O1C
82	f4	202	PEB	CAB-CBB-CGB-O1B
82	Y5	203	PEB	CAC-CBC-CGC-O2C
82	D7	201	PEB	CAB-CBB-CGB-O2B
82	R7	203	PEB	CAC-CBC-CGC-O1C
82	u8	202	PEB	CAC-CBC-CGC-O2C
82	w8	201	PEB	CAB-CBB-CGB-O2B
82	B9	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	B9	202	PEB	CAC-CBC-CGC-O2C
82	D9	201	PEB	CAC-CBC-CGC-O2C
82	D9	203	PEB	CAB-CBB-CGB-O2B
82	H9	203	PEB	CAB-CBB-CGB-O2B
82	Q9	202	PEB	CAC-CBC-CGC-O1C
82	bB	201	PEB	CAB-CBB-CGB-O2B
82	uC	202	PEB	CAC-CBC-CGC-O2C
82	iE	201	PEB	CAC-CBC-CGC-O2C
82	hF	201	PEB	CAC-CBC-CGC-O2C
82	qF	201	PEB	CAC-CBC-CGC-O1C
82	rF	201	PEB	CAC-CBC-CGC-O1C
82	rF	202	PEB	CAC-CBC-CGC-O2C
82	sF	201	PEB	CAB-CBB-CGB-O2B
82	sF	203	PEB	CAC-CBC-CGC-O2C
82	uF	203	PEB	CAC-CBC-CGC-O1C
82	iG	201	PEB	CAC-CBC-CGC-O2C
82	hH	201	PEB	CAC-CBC-CGC-O1C
82	gJ	202	PEB	CAB-CBB-CGB-O2B
82	lJ	201	PEB	CAC-CBC-CGC-O2C
82	cK	201	PEB	CAB-CBB-CGB-O2B
82	lO	201	PEB	CAC-CBC-CGC-O2C
82	fO	201	PEB	CAC-CBC-CGC-O2C
84	HG	1001	CYC	CAD-CBD-CGD-O1D
84	EH	1001	CYC	CAA-CBA-CGA-O2A
84	LH	1002	CYC	CAA-CBA-CGA-O2A
84	L1	1001	CYC	CAA-CBA-CGA-O2A
84	F1	1001	CYC	CAA-CBA-CGA-O2A
84	K1	1001	CYC	CAA-CBA-CGA-O1A
84	K3	1001	CYC	CAA-CBA-CGA-O2A
84	P3	1001	CYC	CAA-CBA-CGA-O2A
84	R3	1001	CYC	CAA-CBA-CGA-O2A
84	T3	1001	CYC	CAA-CBA-CGA-O2A
84	e3	1001	CYC	CAA-CBA-CGA-O2A
84	l3	1001	CYC	CAA-CBA-CGA-O2A
84	m3	1001	CYC	CAA-CBA-CGA-O2A
87	42	606	CLA	CAA-CBA-CGA-O2A
87	4N	606	CLA	CAA-CBA-CGA-O2A
87	a6	609	CLA	C2C-C3C-CAC-CBC
92	B6	618	LMG	C14-C15-C16-C17
92	m6	101	LMG	C31-C32-C33-C34
87	B2	827	CLA	C15-C16-C17-C18
82	kF	203	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
87	AN	808	CLA	CAA-CBA-CGA-O2A
87	72	602	CLA	CAA-CBA-CGA-O2A
87	A2	808	CLA	CAA-CBA-CGA-O2A
87	7N	602	CLA	CAA-CBA-CGA-O2A
87	BN	827	CLA	C15-C16-C17-C18
87	AN	803	CLA	C2A-CAA-CBA-CGA
87	A2	803	CLA	C2A-CAA-CBA-CGA
87	H6	103	CLA	C2A-CAA-CBA-CGA
87	AN	829	CLA	C16-C17-C18-C20
87	BN	807	CLA	C16-C17-C18-C20
87	B2	806	CLA	C16-C17-C18-C20
82	AA	202	PEB	CAC-CBC-CGC-O2C
82	DA	203	PEB	CAC-CBC-CGC-O2C
82	GA	201	PEB	CAC-CBC-CGC-O1C
82	TA	202	PEB	CAC-CBC-CGC-O1C
82	GB	202	PEB	CAC-CBC-CGC-O2C
82	QB	201	PEB	CAC-CBC-CGC-O2C
82	VB	202	PEB	CAC-CBC-CGC-O1C
82	TD	201	PEB	CAC-CBC-CGC-O2C
82	WE	201	PEB	CAC-CBC-CGC-O1C
82	IF	202	PEB	CAC-CBC-CGC-O2C
82	OF	202	PEB	CAC-CBC-CGC-O2C
82	FH	1002	PEB	CAB-CBB-CGB-O2B
82	SH	202	PEB	CAC-CBC-CGC-O2C
82	HI	202	PEB	CAC-CBC-CGC-O2C
82	JI	201	PEB	CAB-CBB-CGB-O2B
82	LI	201	PEB	CAC-CBC-CGC-O1C
82	MJ	203	PEB	CAB-CBB-CGB-O2B
82	UJ	201	PEB	CAB-CBB-CGB-O2B
82	ZJ	202	PEB	CAB-CBB-CGB-O2B
82	IK	202	PEB	CAC-CBC-CGC-O2C
82	OK	202	PEB	CAC-CBC-CGC-O2C
82	XM	202	PEB	CAC-CBC-CGC-O2C
82	BP	201	PEB	CAB-CBB-CGB-O2B
82	KP	201	PEB	CAC-CBC-CGC-O1C
82	UP	203	PEB	CAB-CBB-CGB-O2B
82	FQ	202	PEB	CAB-CBB-CGB-O1B
82	i1	201	PEB	CAB-CBB-CGB-O1B
82	l1	202	PEB	CAB-CBB-CGB-O2B
82	d1	203	PEB	CAB-CBB-CGB-O2B
82	U4	201	PEB	CAC-CBC-CGC-O1C
82	U4	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	Z4	202	PEB	CAC-CBC-CGC-O2C
82	d4	202	PEB	CAB-CBB-CGB-O1B
82	f4	201	PEB	CAB-CBB-CGB-O2B
82	O5	202	PEB	CAC-CBC-CGC-O2C
82	Q5	202	PEB	CAC-CBC-CGC-O2C
82	V5	201	PEB	CAB-CBB-CGB-O2B
82	X5	201	PEB	CAB-CBB-CGB-O2B
82	D7	203	PEB	CAC-CBC-CGC-O2C
82	G7	201	PEB	CAC-CBC-CGC-O1C
82	T7	202	PEB	CAC-CBC-CGC-O1C
82	V7	201	PEB	CAC-CBC-CGC-O2C
82	O9	203	PEB	CAB-CBB-CGB-O2B
82	S9	203	PEB	CAB-CBB-CGB-O2B
82	sC	202	PEB	CAC-CBC-CGC-O2C
82	wC	201	PEB	CAB-CBB-CGB-O2B
82	dD	401	PEB	CAC-CBC-CGC-O2C
82	dE	204	PEB	CAB-CBB-CGB-O1B
82	dF	201	PEB	CAB-CBB-CGB-O2B
82	fF	201	PEB	CAB-CBB-CGB-O2B
82	tF	202	PEB	CAC-CBC-CGC-O2C
82	dG	204	PEB	CAB-CBB-CGB-O1B
82	aH	201	PEB	CAC-CBC-CGC-O2C
82	bH	201	PEB	CAC-CBC-CGC-O1C
82	dH	203	PEB	CAB-CBB-CGB-O2B
82	eH	202	PEB	CAB-CBB-CGB-O2B
82	mJ	201	PEB	CAC-CBC-CGC-O2C
82	aK	201	PEB	CAC-CBC-CGC-O2C
82	dK	201	PEB	CAB-CBB-CGB-O2B
82	fK	201	PEB	CAB-CBB-CGB-O2B
82	tK	202	PEB	CAC-CBC-CGC-O2C
82	aM	204	PEB	CAB-CBB-CGB-O2B
82	dM	203	PEB	CAC-CBC-CGC-O2C
82	dO	202	PEB	CAB-CBB-CGB-O1B
82	fO	201	PEB	CAB-CBB-CGB-O2B
82	dQ	401	PEB	CAC-CBC-CGC-O2C
84	EE	1001	CYC	CAA-CBA-CGA-O2A
84	HE	1001	CYC	CAD-CBD-CGD-O1D
84	KG	202	CYC	CAA-CBA-CGA-O2A
84	FH	1001	CYC	CAA-CBA-CGA-O1A
84	F1	1001	CYC	CAA-CBA-CGA-O1A
84	C3	1001	CYC	CAA-CBA-CGA-O2A
84	J3	1001	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
84	W3	1001	CYC	CAA-CBA-CGA-O1A
84	c3	1001	CYC	CAA-CBA-CGA-O2A
84	g3	1001	CYC	CAA-CBA-CGA-O2A
84	p3	1001	CYC	CAA-CBA-CGA-O2A
84	t3	1001	CYC	CAA-CBA-CGA-O2A
84	y3	1001	CYC	CAA-CBA-CGA-O1A
87	62	312	CLA	CAA-CBA-CGA-O2A
87	6N	611	CLA	CAA-CBA-CGA-O2A
88	dL	408	LHG	C25-C26-C27-C28
85	AN	846	BCR	C23-C24-C25-C30
85	JN	103	BCR	C1-C6-C7-C8
85	A2	846	BCR	C23-C24-C25-C30
85	J2	103	BCR	C1-C6-C7-C8
85	A6	401	BCR	C1-C6-C7-C8
85	A6	401	BCR	C23-C24-C25-C30
85	a6	605	BCR	C1-C6-C7-C8
85	d6	405	BCR	C5-C6-C7-C8
87	D6	402	CLA	C13-C15-C16-C17
87	c6	609	CLA	C15-C16-C17-C18
88	C6	505	LHG	O8-C23-C24-C25
88	bL	612	LHG	C30-C31-C32-C33
82	MA	202	PEB	C2C-C1C-CHB-C4B
82	DJ	201	PEB	C2C-C1C-CHB-C4B
82	KJ	202	PEB	C2C-C1C-CHB-C4B
82	M7	202	PEB	C2C-C1C-CHB-C4B
82	Z9	301	PEB	C2C-C1C-CHB-C4B
82	M9	302	PEB	C2C-C1C-CHB-C4B
84	63	901	CYC	C2D-C1D-CHD-C4C
82	NA	203	PEB	CAC-CBC-CGC-O2C
82	VA	201	PEB	CAC-CBC-CGC-O2C
82	BD	202	PEB	CAB-CBB-CGB-O1B
82	FD	202	PEB	CAB-CBB-CGB-O1B
82	KD	202	PEB	CAC-CBC-CGC-O2C
82	RE	201	PEB	CAB-CBB-CGB-O1B
82	MF	203	PEB	CAB-CBB-CGB-O2B
82	RG	201	PEB	CAB-CBB-CGB-O1B
82	WG	201	PEB	CAC-CBC-CGC-O1C
82	WG	202	PEB	CAC-CBC-CGC-O2C
82	HH	1002	PEB	CAC-CBC-CGC-O2C
82	AI	202	PEB	CAB-CBB-CGB-O2B
82	CI	202	PEB	CAB-CBB-CGB-O2B
82	EI	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	GI	203	PEB	CAB-CBB-CGB-O2B
82	II	202	PEB	CAB-CBB-CGB-O2B
82	KI	203	PEB	CAB-CBB-CGB-O2B
82	MI	401	PEB	CAB-CBB-CGB-O1B
82	NI	202	PEB	CAB-CBB-CGB-O2B
82	PI	202	PEB	CAB-CBB-CGB-O2B
82	RI	202	PEB	CAB-CBB-CGB-O2B
82	TI	203	PEB	CAB-CBB-CGB-O2B
82	VI	202	PEB	CAB-CBB-CGB-O2B
82	XI	202	PEB	CAB-CBB-CGB-O2B
82	HJ	202	PEB	CAB-CBB-CGB-O2B
82	QJ	204	PEB	CAB-CBB-CGB-O2B
82	MK	203	PEB	CAB-CBB-CGB-O2B
82	OK	201	PEB	CAC-CBC-CGC-O1C
82	WK	201	PEB	CAC-CBC-CGC-O1C
82	CM	203	PEB	CAC-CBC-CGC-O1C
82	DM	201	PEB	CAB-CBB-CGB-O2B
82	KM	203	PEB	CAC-CBC-CGC-O1C
82	NM	202	PEB	CAB-CBB-CGB-O2B
82	UO	201	PEB	CAC-CBC-CGC-O1C
82	UO	202	PEB	CAC-CBC-CGC-O1C
82	CP	203	PEB	CAC-CBC-CGC-O2C
82	EP	203	PEB	CAB-CBB-CGB-O2B
82	LP	201	PEB	CAB-CBB-CGB-O2B
82	BQ	202	PEB	CAB-CBB-CGB-O1B
82	H1	1002	PEB	CAC-CBC-CGC-O2C
82	Z1	201	PEB	CAB-CBB-CGB-O1B
82	e1	202	PEB	CAB-CBB-CGB-O2B
82	R4	203	PEB	CAC-CBC-CGC-O2C
82	Z4	202	PEB	CAC-CBC-CGC-O1C
82	A5	201	PEB	CAB-CBB-CGB-O2B
82	D5	201	PEB	CAC-CBC-CGC-O2C
82	E5	201	PEB	CAB-CBB-CGB-O2B
82	F5	202	PEB	CAC-CBC-CGC-O2C
82	G5	201	PEB	CAB-CBB-CGB-O2B
82	I5	201	PEB	CAB-CBB-CGB-O2B
82	K5	201	PEB	CAB-CBB-CGB-O2B
82	N5	201	PEB	CAB-CBB-CGB-O2B
82	R5	201	PEB	CAB-CBB-CGB-O2B
82	T5	201	PEB	CAB-CBB-CGB-O2B
82	N7	203	PEB	CAC-CBC-CGC-O2C
82	p8	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	s8	201	PEB	CAC-CBC-CGC-O1C
82	s8	202	PEB	CAC-CBC-CGC-O2C
82	J9	203	PEB	CAB-CBB-CGB-O2B
82	U9	203	PEB	CAB-CBB-CGB-O2B
82	eA	301	PEB	CAB-CBB-CGB-O1B
82	eB	201	PEB	CAC-CBC-CGC-O2C
82	yC	201	PEB	CAC-CBC-CGC-O1C
82	yC	203	PEB	CAB-CBB-CGB-O1B
82	1C	201	PEB	CAB-CBB-CGB-O1B
82	pC	202	PEB	CAC-CBC-CGC-O1C
82	sC	201	PEB	CAC-CBC-CGC-O1C
82	jE	201	PEB	CAC-CBC-CGC-O1C
82	lE	203	PEB	CAC-CBC-CGC-O2C
82	mE	201	PEB	CAC-CBC-CGC-O2C
82	mE	203	PEB	CAB-CBB-CGB-O2B
82	cF	201	PEB	CAC-CBC-CGC-O1C
82	lF	203	PEB	CAC-CBC-CGC-O1C
82	jG	201	PEB	CAC-CBC-CGC-O1C
82	mG	201	PEB	CAC-CBC-CGC-O2C
82	mG	203	PEB	CAB-CBB-CGB-O2B
82	iH	201	PEB	CAB-CBB-CGB-O1B
82	eH	201	PEB	CAC-CBC-CGC-O2C
82	iJ	202	PEB	CAB-CBB-CGB-O2B
82	lK	203	PEB	CAC-CBC-CGC-O1C
82	eM	201	PEB	CAC-CBC-CGC-O2C
82	eM	202	PEB	CAC-CBC-CGC-O1C
82	aO	203	PEB	CAC-CBC-CGC-O2C
84	BE	1001	CYC	CAD-CBD-CGD-O1D
84	GE	1001	CYC	CAA-CBA-CGA-O2A
84	FO	1001	CYC	CAA-CBA-CGA-O2A
84	F4	1001	CYC	CAA-CBA-CGA-O2A
87	RN	202	CLA	CAA-CBA-CGA-O2A
87	62	312	CLA	CAA-CBA-CGA-O1A
87	72	605	CLA	CAA-CBA-CGA-O2A
87	6N	611	CLA	CAA-CBA-CGA-O1A
87	7N	605	CLA	CAA-CBA-CGA-O2A
87	AN	805	CLA	C10-C11-C12-C13
87	AN	812	CLA	C5-C6-C7-C8
87	A2	805	CLA	C10-C11-C12-C13
87	A2	812	CLA	C5-C6-C7-C8
100	J2	104	3XQ	C21-C22-C24-O25
85	CL	516	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
85	JN	103	BCR	C9-C10-C11-C12
85	JN	103	BCR	C15-C16-C17-C18
85	LN	201	BCR	C9-C10-C11-C12
85	J2	103	BCR	C9-C10-C11-C12
85	J2	103	BCR	C15-C16-C17-C18
85	L2	201	BCR	C9-C10-C11-C12
85	c6	617	BCR	C13-C14-C15-C16
95	a6	604	DGD	C2A-C3A-C4A-C5A
82	YB	202	PEB	NC-C1C-CHB-C4B
82	SI	202	PEB	NC-C1C-CHB-C4B
82	VM	202	PEB	NC-C1C-CHB-C4B
82	mJ	202	PEB	NC-C1C-CHB-C4B
87	b6	618	CLA	C4-C3-C5-C6
87	aL	606	CLA	C4-C3-C5-C6
94	AL	413	PL9	C12-C11-C9-C10
82	BA	203	PEB	C4A-C3A-CAA-CBA
82	XA	203	PEB	C4A-C3A-CAA-CBA
82	YA	304	PEB	C4A-C3A-CAA-CBA
82	AD	303	PEB	C4A-C3A-CAA-CBA
82	LE	1002	PEB	C4A-C3A-CAA-CBA
82	UE	202	PEB	C4A-C3A-CAA-CBA
82	JF	201	PEB	C4A-C3A-CAA-CBA
82	UF	202	PEB	C4A-C3A-CAA-CBA
82	WF	203	PEB	C4A-C3A-CAA-CBA
82	XF	201	PEB	C4A-C3A-CAA-CBA
82	LG	1002	PEB	C4A-C3A-CAA-CBA
82	UG	202	PEB	C4A-C3A-CAA-CBA
82	OH	203	PEB	C4A-C3A-CAA-CBA
82	UH	203	PEB	C4A-C3A-CAA-CBA
82	JK	201	PEB	C4A-C3A-CAA-CBA
82	UK	202	PEB	C4A-C3A-CAA-CBA
82	WK	203	PEB	C4A-C3A-CAA-CBA
82	BM	301	PEB	C4A-C3A-CAA-CBA
82	AQ	303	PEB	C4A-C3A-CAA-CBA
82	O1	203	PEB	C4A-C3A-CAA-CBA
82	U1	203	PEB	C4A-C3A-CAA-CBA
82	f1	203	PEB	C4A-C3A-CAA-CBA
82	g1	201	PEB	C4A-C3A-CAA-CBA
82	j1	203	PEB	C4A-C3A-CAA-CBA
82	l1	203	PEB	C4A-C3A-CAA-CBA
82	A5	201	PEB	C4A-C3A-CAA-CBA
82	C5	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	E5	201	PEB	C4A-C3A-CAA-CBA
82	G5	201	PEB	C4A-C3A-CAA-CBA
82	I5	201	PEB	C4A-C3A-CAA-CBA
82	K5	201	PEB	C4A-C3A-CAA-CBA
82	N5	201	PEB	C4A-C3A-CAA-CBA
82	P5	201	PEB	C4A-C3A-CAA-CBA
82	R5	201	PEB	C4A-C3A-CAA-CBA
82	T5	201	PEB	C4A-C3A-CAA-CBA
82	V5	201	PEB	C4A-C3A-CAA-CBA
82	X5	201	PEB	C4A-C3A-CAA-CBA
82	B7	203	PEB	C4A-C3A-CAA-CBA
82	X7	203	PEB	C4A-C3A-CAA-CBA
82	Y7	304	PEB	C4A-C3A-CAA-CBA
82	gB	201	PEB	C4A-C3A-CAA-CBA
82	sF	203	PEB	C4A-C3A-CAA-CBA
82	fH	203	PEB	C4A-C3A-CAA-CBA
82	gH	201	PEB	C4A-C3A-CAA-CBA
82	jH	203	PEB	C4A-C3A-CAA-CBA
82	lH	202	PEB	C4A-C3A-CAA-CBA
82	sK	203	PEB	C4A-C3A-CAA-CBA
85	BL	616	BCR	C17-C18-C19-C20
85	H6	101	BCR	C7-C8-C9-C10
85	bL	603	BCR	C21-C22-C23-C24
87	42	610	CLA	C1A-C2A-CAA-CBA
87	52	609	CLA	C1A-C2A-CAA-CBA
87	4N	610	CLA	C1A-C2A-CAA-CBA
87	5N	609	CLA	C1A-C2A-CAA-CBA
87	A2	829	CLA	C16-C17-C18-C20
88	D6	401	LHG	C9-C10-C11-C12
87	BN	801	CLA	C2-C3-C5-C6
87	LN	203	CLA	C2-C3-C5-C6
87	B2	825	CLA	C2-C3-C5-C6
87	L2	203	CLA	C2-C3-C5-C6
94	AL	413	PL9	C12-C11-C9-C8
94	A6	410	PL9	C38-C39-C41-C42
88	dL	408	LHG	C23-C24-C25-C26
82	DA	201	PEB	C2C-CAC-CBC-CGC
82	HA	203	PEB	C2C-CAC-CBC-CGC
82	PA	203	PEB	C2C-CAC-CBC-CGC
82	CB	202	PEB	C2C-CAC-CBC-CGC
82	IB	201	PEB	C3B-CAB-CBB-CGB
82	FD	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
82	XD	202	PEB	C2C-CAC-CBC-CGC
82	XD	202	PEB	C3B-CAB-CBB-CGB
82	OE	202	PEB	C2C-CAC-CBC-CGC
82	SE	202	PEB	C3B-CAB-CBB-CGB
82	RF	201	PEB	C2C-CAC-CBC-CGC
82	SG	203	PEB	C3B-CAB-CBB-CGB
82	WH	202	PEB	C2C-CAC-CBC-CGC
82	SI	202	PEB	C3B-CAB-CBB-CGB
82	WJ	202	PEB	C3B-CAB-CBB-CGB
82	WJ	203	PEB	C3B-CAB-CBB-CGB
82	RK	201	PEB	C2C-CAC-CBC-CGC
82	CP	201	PEB	C2C-CAC-CBC-CGC
82	FQ	203	PEB	C2C-CAC-CBC-CGC
82	XQ	202	PEB	C2C-CAC-CBC-CGC
82	W1	202	PEB	C2C-CAC-CBC-CGC
82	f4	202	PEB	C2C-CAC-CBC-CGC
82	A5	202	PEB	C3B-CAB-CBB-CGB
82	C5	202	PEB	C3B-CAB-CBB-CGB
82	E5	202	PEB	C3B-CAB-CBB-CGB
82	G5	202	PEB	C3B-CAB-CBB-CGB
82	I5	202	PEB	C3B-CAB-CBB-CGB
82	K5	202	PEB	C3B-CAB-CBB-CGB
82	N5	202	PEB	C3B-CAB-CBB-CGB
82	P5	202	PEB	C3B-CAB-CBB-CGB
82	R5	202	PEB	C3B-CAB-CBB-CGB
82	T5	202	PEB	C3B-CAB-CBB-CGB
82	V5	202	PEB	C3B-CAB-CBB-CGB
82	X5	202	PEB	C3B-CAB-CBB-CGB
82	Y5	202	PEB	C2C-CAC-CBC-CGC
82	H7	203	PEB	C2C-CAC-CBC-CGC
82	P7	203	PEB	C2C-CAC-CBC-CGC
82	iE	201	PEB	C3B-CAB-CBB-CGB
82	cF	203	PEB	C2C-CAC-CBC-CGC
82	sF	203	PEB	C3B-CAB-CBB-CGB
82	vF	202	PEB	C3B-CAB-CBB-CGB
82	dG	202	PEB	C3B-CAB-CBB-CGB
82	iG	201	PEB	C3B-CAB-CBB-CGB
82	lG	202	PEB	C2C-CAC-CBC-CGC
82	aJ	202	PEB	C2C-CAC-CBC-CGC
82	cK	203	PEB	C2C-CAC-CBC-CGC
82	sK	203	PEB	C3B-CAB-CBB-CGB
82	vK	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	aM	201	PEB	C2C-CAC-CBC-CGC
82	fO	202	PEB	C2C-CAC-CBC-CGC
83	YA	302	PUB	C3B-CAB-CBB-CGB
83	Y7	302	PUB	C3B-CAB-CBB-CGB
82	MA	201	PEB	CAB-CBB-CGB-O2B
82	XA	201	PEB	CAC-CBC-CGC-O2C
82	SB	203	PEB	CAB-CBB-CGB-O2B
82	OD	201	PEB	CAB-CBB-CGB-O1B
82	UD	201	PEB	CAB-CBB-CGB-O2B
82	SE	201	PEB	CAC-CBC-CGC-O2C
82	WE	202	PEB	CAC-CBC-CGC-O2C
82	BF	202	PEB	CAC-CBC-CGC-O2C
82	RF	201	PEB	CAB-CBB-CGB-O2B
82	TF	201	PEB	CAC-CBC-CGC-O2C
82	WF	201	PEB	CAC-CBC-CGC-O1C
82	XF	201	PEB	CAB-CBB-CGB-O2B
82	XF	203	PEB	CAC-CBC-CGC-O2C
82	SG	201	PEB	CAC-CBC-CGC-O2C
82	SG	202	PEB	CAB-CBB-CGB-O1B
82	BI	201	PEB	CAC-CBC-CGC-O1C
82	UI	201	PEB	CAC-CBC-CGC-O2C
82	AJ	301	PEB	CAC-CBC-CGC-O1C
82	RJ	202	PEB	CAB-CBB-CGB-O2B
82	VJ	202	PEB	CAB-CBB-CGB-O2B
82	FK	202	PEB	CAC-CBC-CGC-O2C
82	RK	201	PEB	CAB-CBB-CGB-O2B
82	TK	201	PEB	CAC-CBC-CGC-O2C
82	XK	203	PEB	CAC-CBC-CGC-O2C
82	PM	201	PEB	CAC-CBC-CGC-O2C
82	OO	202	PEB	CAB-CBB-CGB-O1B
82	BP	201	PEB	CAC-CBC-CGC-O1C
82	JP	201	PEB	CAB-CBB-CGB-O2B
82	KQ	202	PEB	CAC-CBC-CGC-O2C
82	NQ	204	PEB	CAC-CBC-CGC-O2C
82	NQ	204	PEB	CAB-CBB-CGB-O2B
82	OQ	201	PEB	CAB-CBB-CGB-O1B
82	RQ	202	PEB	CAC-CBC-CGC-O1C
82	UQ	201	PEB	CAB-CBB-CGB-O2B
82	S1	202	PEB	CAC-CBC-CGC-O2C
82	g1	202	PEB	CAB-CBB-CGB-O2B
82	e1	201	PEB	CAC-CBC-CGC-O2C
82	O4	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	e4	202	PEB	CAB-CBB-CGB-O1B
82	L5	202	PEB	CAC-CBC-CGC-O2C
82	L7	203	PEB	CAC-CBC-CGC-O1C
82	y8	203	PEB	CAB-CBB-CGB-O1B
82	18	201	PEB	CAB-CBB-CGB-O1B
82	aF	201	PEB	CAC-CBC-CGC-O2C
82	nF	201	PEB	CAB-CBB-CGB-O2B
82	vF	201	PEB	CAC-CBC-CGC-O1C
82	gH	202	PEB	CAB-CBB-CGB-O2B
82	lH	201	PEB	CAB-CBB-CGB-O2B
82	cK	201	PEB	CAC-CBC-CGC-O1C
82	rK	201	PEB	CAC-CBC-CGC-O1C
82	sK	201	PEB	CAC-CBC-CGC-O2C
82	aM	203	PEB	CAB-CBB-CGB-O1B
82	gM	202	PEB	CAB-CBB-CGB-O2B
82	eO	202	PEB	CAB-CBB-CGB-O1B
82	fO	202	PEB	CAB-CBB-CGB-O1B
84	BG	1001	CYC	CAD-CBD-CGD-O1D
84	EG	1001	CYC	CAA-CBA-CGA-O2A
84	GG	1001	CYC	CAA-CBA-CGA-O2A
84	JH	1003	CYC	CAD-CBD-CGD-O1D
87	FN	203	CLA	CAA-CBA-CGA-O2A
87	12	611	CLA	CAA-CBA-CGA-O2A
87	32	307	CLA	CAA-CBA-CGA-O2A
87	F2	201	CLA	CAA-CBA-CGA-O2A
87	R2	202	CLA	CAA-CBA-CGA-O2A
87	1N	611	CLA	CAA-CBA-CGA-O2A
87	3N	308	CLA	CAA-CBA-CGA-O2A
88	d6	407	LHG	C16-C17-C18-C19
92	bL	610	LMG	C14-C15-C16-C17
92	DL	402	LMG	C8-C7-O1-C1
92	m6	103	LMG	C8-C7-O1-C1
92	bL	610	LMG	C8-C7-O1-C1
82	WA	201	PEB	CAC-CBC-CGC-O2C
82	HB	203	PEB	CAC-CBC-CGC-O2C
82	NB	201	PEB	CAB-CBB-CGB-O2B
82	ND	204	PEB	CAB-CBB-CGB-O2B
82	RD	202	PEB	CAC-CBC-CGC-O1C
82	OE	203	PEB	CAC-CBC-CGC-O2C
82	FF	202	PEB	CAC-CBC-CGC-O2C
82	LF	201	PEB	CAB-CBB-CGB-O2B
82	LF	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	UF	202	PEB	CAB-CBB-CGB-O2B
82	VF	201	PEB	CAC-CBC-CGC-O2C
82	YF	202	PEB	CAC-CBC-CGC-O2C
82	OG	203	PEB	CAC-CBC-CGC-O2C
82	PH	202	PEB	CAB-CBB-CGB-O2B
82	II	203	PEB	CAB-CBB-CGB-O2B
82	JJ	201	PEB	CAC-CBC-CGC-O2C
82	BK	202	PEB	CAC-CBC-CGC-O2C
82	JK	201	PEB	CAB-CBB-CGB-O2B
82	UK	202	PEB	CAB-CBB-CGB-O2B
82	XK	201	PEB	CAB-CBB-CGB-O2B
82	EM	202	PEB	CAC-CBC-CGC-O1C
82	HM	201	PEB	CAC-CBC-CGC-O2C
82	WM	202	PEB	CAC-CBC-CGC-O2C
82	XM	202	PEB	CAB-CBB-CGB-O2B
82	NO	1002	PEB	CAB-CBB-CGB-O2B
82	OO	201	PEB	CAC-CBC-CGC-O2C
82	SP	201	PEB	CAC-CBC-CGC-O2C
82	P1	202	PEB	CAB-CBB-CGB-O2B
82	a1	201	PEB	CAC-CBC-CGC-O2C
82	d1	201	PEB	CAC-CBC-CGC-O2C
82	h4	202	PEB	CAB-CBB-CGB-O2B
82	A5	202	PEB	CAC-CBC-CGC-O2C
82	A5	202	PEB	CAB-CBB-CGB-O2B
82	B5	203	PEB	CAB-CBB-CGB-O1B
82	C5	202	PEB	CAC-CBC-CGC-O2C
82	C5	202	PEB	CAB-CBB-CGB-O2B
82	E5	202	PEB	CAC-CBC-CGC-O2C
82	E5	202	PEB	CAB-CBB-CGB-O2B
82	G5	202	PEB	CAC-CBC-CGC-O2C
82	G5	202	PEB	CAB-CBB-CGB-O2B
82	I5	202	PEB	CAC-CBC-CGC-O2C
82	I5	202	PEB	CAB-CBB-CGB-O2B
82	K5	202	PEB	CAC-CBC-CGC-O2C
82	K5	202	PEB	CAB-CBB-CGB-O2B
82	M5	305	PEB	CAC-CBC-CGC-O1C
82	N5	202	PEB	CAC-CBC-CGC-O2C
82	N5	202	PEB	CAB-CBB-CGB-O2B
82	P5	202	PEB	CAC-CBC-CGC-O2C
82	P5	202	PEB	CAB-CBB-CGB-O2B
82	R5	202	PEB	CAC-CBC-CGC-O2C
82	R5	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	T5	202	PEB	CAC-CBC-CGC-O2C
82	T5	202	PEB	CAB-CBB-CGB-O2B
82	V5	202	PEB	CAC-CBC-CGC-O2C
82	V5	202	PEB	CAB-CBB-CGB-O2B
82	W5	202	PEB	CAC-CBC-CGC-O2C
82	X5	202	PEB	CAC-CBC-CGC-O2C
82	X5	202	PEB	CAB-CBB-CGB-O2B
82	Y5	202	PEB	CAC-CBC-CGC-O2C
82	Z5	305	PEB	CAC-CBC-CGC-O1C
82	M7	201	PEB	CAB-CBB-CGB-O2B
82	U7	202	PEB	CAB-CBB-CGB-O1B
82	X7	201	PEB	CAC-CBC-CGC-O2C
82	B9	203	PEB	CAB-CBB-CGB-O2B
82	U9	202	PEB	CAC-CBC-CGC-O2C
82	W9	201	PEB	CAB-CBB-CGB-O2B
82	W9	203	PEB	CAB-CBB-CGB-O2B
82	bB	201	PEB	CAC-CBC-CGC-O1C
82	dB	202	PEB	CAC-CBC-CGC-O2C
82	kE	201	PEB	CAB-CBB-CGB-O2B
82	eF	202	PEB	CAC-CBC-CGC-O2C
82	nF	202	PEB	CAB-CBB-CGB-O2B
82	sF	201	PEB	CAC-CBC-CGC-O2C
82	gJ	201	PEB	CAC-CBC-CGC-O2C
82	eK	202	PEB	CAC-CBC-CGC-O2C
82	gK	203	PEB	CAC-CBC-CGC-O2C
82	nK	202	PEB	CAB-CBB-CGB-O2B
82	vK	201	PEB	CAC-CBC-CGC-O1C
82	kM	201	PEB	CAC-CBC-CGC-O2C
82	lM	201	PEB	CAB-CBB-CGB-O2B
84	LH	1001	CYC	CAA-CBA-CGA-O2A
84	HO	1001	CYC	CAA-CBA-CGA-O2A
84	M1	201	CYC	CAD-CBD-CGD-O1D
87	52	603	CLA	CAA-CBA-CGA-O2A
87	52	606	CLA	CAA-CBA-CGA-O2A
87	72	606	CLA	CAA-CBA-CGA-O2A
87	5N	606	CLA	CAA-CBA-CGA-O2A
87	7N	606	CLA	CAA-CBA-CGA-O2A
92	x6	601	LMG	O8-C28-C29-C30
92	m6	101	LMG	C19-C20-C21-C22
87	b6	613	CLA	C16-C17-C18-C19
87	B6	616	CLA	C8-C10-C11-C12
87	D6	403	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
91	aL	610	PHO	C15-C16-C17-C18
88	ML	102	LHG	O6-C4-C5-O7
82	cF	202	PEB	C2B-C3B-CAB-CBB
88	d6	402	LHG	C18-C19-C20-C21
82	DA	201	PEB	CAB-CBB-CGB-O1B
82	VA	201	PEB	CAB-CBB-CGB-O2B
82	BB	202	PEB	CAC-CBC-CGC-O2C
82	HB	201	PEB	CAC-CBC-CGC-O2C
82	PB	201	PEB	CAB-CBB-CGB-O2B
82	YB	201	PEB	CAC-CBC-CGC-O2C
82	CD	202	PEB	CAB-CBB-CGB-O2B
82	ND	204	PEB	CAC-CBC-CGC-O2C
82	JF	201	PEB	CAB-CBB-CGB-O2B
82	OF	201	PEB	CAC-CBC-CGC-O1C
82	VF	201	PEB	CAC-CBC-CGC-O1C
82	VF	202	PEB	CAC-CBC-CGC-O1C
82	XF	203	PEB	CAB-CBB-CGB-O2B
82	WH	202	PEB	CAC-CBC-CGC-O2C
82	AI	201	PEB	CAB-CBB-CGB-O1B
82	CI	201	PEB	CAB-CBB-CGB-O1B
82	EI	201	PEB	CAB-CBB-CGB-O1B
82	GI	202	PEB	CAB-CBB-CGB-O1B
82	II	201	PEB	CAB-CBB-CGB-O1B
82	KI	202	PEB	CAB-CBB-CGB-O1B
82	NI	201	PEB	CAB-CBB-CGB-O1B
82	PI	201	PEB	CAB-CBB-CGB-O1B
82	RI	201	PEB	CAB-CBB-CGB-O1B
82	TI	202	PEB	CAB-CBB-CGB-O1B
82	UI	202	PEB	CAB-CBB-CGB-O2B
82	VI	201	PEB	CAB-CBB-CGB-O1B
82	XI	201	PEB	CAB-CBB-CGB-O1B
82	LK	201	PEB	CAB-CBB-CGB-O2B
82	LK	202	PEB	CAB-CBB-CGB-O2B
82	RK	202	PEB	CAC-CBC-CGC-O2C
82	VK	201	PEB	CAC-CBC-CGC-O1C
82	VK	202	PEB	CAC-CBC-CGC-O1C
82	XK	203	PEB	CAB-CBB-CGB-O2B
82	YK	202	PEB	CAC-CBC-CGC-O2C
82	GM	203	PEB	CAB-CBB-CGB-O2B
82	PM	202	PEB	CAB-CBB-CGB-O2B
82	SM	202	PEB	CAB-CBB-CGB-O2B
82	SM	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	PO	203	PEB	CAC-CBC-CGC-O2C
82	ZO	202	PEB	CAC-CBC-CGC-O1C
82	EP	202	PEB	CAC-CBC-CGC-O2C
82	TP	202	PEB	CAC-CBC-CGC-O1C
82	TP	202	PEB	CAC-CBC-CGC-O2C
82	UP	202	PEB	CAC-CBC-CGC-O2C
82	CQ	202	PEB	CAB-CBB-CGB-O2B
82	W1	202	PEB	CAC-CBC-CGC-O2C
82	j1	201	PEB	CAB-CBB-CGB-O2B
82	N4	1002	PEB	CAB-CBB-CGB-O2B
82	O4	201	PEB	CAC-CBC-CGC-O2C
82	D4	1002	PEB	CAB-CBB-CGB-O2B
82	Q4	202	PEB	CAB-CBB-CGB-O1B
82	j4	202	PEB	CAB-CBB-CGB-O1B
82	d4	201	PEB	CAC-CBC-CGC-O1C
82	A5	202	PEB	CAC-CBC-CGC-O1C
82	E5	202	PEB	CAC-CBC-CGC-O1C
82	G5	202	PEB	CAC-CBC-CGC-O1C
82	K5	202	PEB	CAC-CBC-CGC-O1C
82	N5	202	PEB	CAC-CBC-CGC-O1C
82	P5	202	PEB	CAC-CBC-CGC-O1C
82	R5	202	PEB	CAC-CBC-CGC-O1C
82	T5	202	PEB	CAC-CBC-CGC-O1C
82	V5	202	PEB	CAC-CBC-CGC-O1C
82	Z5	304	PEB	CAC-CBC-CGC-O1C
82	D7	201	PEB	CAB-CBB-CGB-O1B
82	M7	202	PEB	CAB-CBB-CGB-O2B
82	V7	201	PEB	CAB-CBB-CGB-O2B
82	W7	201	PEB	CAC-CBC-CGC-O2C
82	s8	202	PEB	CAC-CBC-CGC-O1C
82	cB	402	PEB	CAB-CBB-CGB-O2B
82	sC	202	PEB	CAC-CBC-CGC-O1C
82	dD	401	PEB	CAB-CBB-CGB-O2B
82	eF	201	PEB	CAC-CBC-CGC-O2C
82	gF	203	PEB	CAC-CBC-CGC-O2C
82	kG	201	PEB	CAB-CBB-CGB-O2B
82	dH	201	PEB	CAC-CBC-CGC-O2C
82	eH	202	PEB	CAB-CBB-CGB-O1B
82	fJ	202	PEB	CAB-CBB-CGB-O2B
82	eK	201	PEB	CAC-CBC-CGC-O2C
82	nK	201	PEB	CAB-CBB-CGB-O2B
82	fM	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	jO	202	PEB	CAB-CBB-CGB-O1B
82	dO	201	PEB	CAC-CBC-CGC-O1C
82	M9	301	PEB	CAC-CBC-CGC-O2C
84	DH	1003	CYC	CAA-CBA-CGA-O2A
84	D1	1003	CYC	CAA-CBA-CGA-O2A
84	I1	1001	CYC	CAA-CBA-CGA-O2A
84	H4	1001	CYC	CAA-CBA-CGA-O2A
87	RN	202	CLA	CAA-CBA-CGA-O1A
87	RN	204	CLA	CAA-CBA-CGA-O2A
87	62	304	CLA	CAA-CBA-CGA-O2A
87	R2	202	CLA	CAA-CBA-CGA-O1A
87	5N	603	CLA	CAA-CBA-CGA-O2A
87	6N	603	CLA	CAA-CBA-CGA-O2A
83	AE	302	PUB	C3A-C4A-CHA-C1B
83	AG	302	PUB	C3A-C4A-CHA-C1B
83	AH	304	PUB	C2D-C1D-CHC-C4C
83	A1	304	PUB	C2D-C1D-CHC-C4C
83	M5	302	PUB	C3A-C4A-CHA-C1B
83	M5	303	PUB	C3A-C4A-CHA-C1B
83	Z5	302	PUB	C3A-C4A-CHA-C1B
83	Z5	303	PUB	C3A-C4A-CHA-C1B
83	yK	303	PUB	C3A-C4A-CHA-C1B
87	CL	518	CLA	C2A-CAA-CBA-CGA
87	52	603	CLA	C2A-CAA-CBA-CGA
87	5N	603	CLA	C2A-CAA-CBA-CGA
92	AL	411	LMG	C29-C28-O8-C9
92	B6	618	LMG	C30-C31-C32-C33
82	MA	202	PEB	CAB-CBB-CGB-O2B
82	UA	202	PEB	CAB-CBB-CGB-O1B
82	HB	203	PEB	CAC-CBC-CGC-O1C
82	IB	203	PEB	CAB-CBB-CGB-O1B
82	HE	1002	PEB	CAB-CBB-CGB-O2B
82	RF	202	PEB	CAC-CBC-CGC-O2C
82	UF	202	PEB	CAC-CBC-CGC-O2C
82	WF	202	PEB	CAB-CBB-CGB-O2B
82	AH	301	PEB	CAB-CBB-CGB-O2B
82	WH	202	PEB	CAC-CBC-CGC-O1C
82	WI	203	PEB	CAB-CBB-CGB-O1B
82	YI	201	PEB	CAC-CBC-CGC-O1C
82	DJ	201	PEB	CAC-CBC-CGC-O2C
82	LJ	202	PEB	CAB-CBB-CGB-O1B
82	MJ	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	CK	201	PEB	CAC-CBC-CGC-O1C
82	RK	201	PEB	CAC-CBC-CGC-O1C
82	SK	203	PEB	CAC-CBC-CGC-O2C
82	UK	202	PEB	CAC-CBC-CGC-O2C
82	VK	201	PEB	CAC-CBC-CGC-O2C
82	WK	202	PEB	CAB-CBB-CGB-O2B
82	LM	202	PEB	CAB-CBB-CGB-O2B
82	TM	202	PEB	CAB-CBB-CGB-O2B
82	WM	202	PEB	CAB-CBB-CGB-O2B
82	AO	305	PEB	CAC-CBC-CGC-O1C
82	QO	202	PEB	CAB-CBB-CGB-O1B
82	RO	202	PEB	CAB-CBB-CGB-O2B
82	GP	203	PEB	CAC-CBC-CGC-O1C
82	Q1	203	PEB	CAB-CBB-CGB-O1B
82	U1	201	PEB	CAB-CBB-CGB-O1B
82	A1	301	PEB	CAB-CBB-CGB-O2B
82	c1	202	PEB	CAB-CBB-CGB-O2B
82	e1	201	PEB	CAC-CBC-CGC-O1C
82	e1	202	PEB	CAB-CBB-CGB-O1B
82	A4	305	PEB	CAC-CBC-CGC-O1C
82	C5	202	PEB	CAC-CBC-CGC-O1C
82	I5	202	PEB	CAC-CBC-CGC-O1C
82	M5	304	PEB	CAC-CBC-CGC-O1C
82	X5	202	PEB	CAC-CBC-CGC-O1C
82	t8	202	PEB	CAB-CBB-CGB-O1B
82	u8	201	PEB	CAB-CBB-CGB-O1B
82	Y9	203	PEB	CAB-CBB-CGB-O2B
82	1C	203	PEB	CAB-CBB-CGB-O2B
82	tC	202	PEB	CAB-CBB-CGB-O1B
82	jH	201	PEB	CAB-CBB-CGB-O2B
82	cH	202	PEB	CAB-CBB-CGB-O2B
82	eH	201	PEB	CAC-CBC-CGC-O1C
82	aJ	203	PEB	CAB-CBB-CGB-O1B
82	cJ	202	PEB	CAB-CBB-CGB-O2B
82	aM	204	PEB	CAB-CBB-CGB-O1B
82	cM	202	PEB	CAB-CBB-CGB-O1B
82	hO	202	PEB	CAB-CBB-CGB-O2B
82	dQ	401	PEB	CAB-CBB-CGB-O2B
83	AM	303	PUB	CAB-CBB-CGB-O1B
84	I1	1001	CYC	CAA-CBA-CGA-O1A
87	52	606	CLA	CAA-CBA-CGA-O1A
87	5N	606	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	AN	821	CLA	C4B-C3B-CAB-CBB
87	BN	832	CLA	C4B-C3B-CAB-CBB
87	MN	101	CLA	C4B-C3B-CAB-CBB
87	12	607	CLA	C4B-C3B-CAB-CBB
87	32	305	CLA	C4B-C3B-CAB-CBB
87	A2	821	CLA	C4B-C3B-CAB-CBB
87	B2	832	CLA	C4B-C3B-CAB-CBB
87	M2	101	CLA	C4B-C3B-CAB-CBB
87	1N	607	CLA	C4B-C3B-CAB-CBB
87	3N	306	CLA	C4B-C3B-CAB-CBB
95	BL	613	DGD	O6D-C1D-O3G-C3G
87	B6	616	CLA	C13-C15-C16-C17
87	B6	611	CLA	C4C-C3C-CAC-CBC
88	mL	102	LHG	O6-C4-C5-C6
87	AN	802	CLA	C4-C3-C5-C6
87	A2	801	CLA	C4-C3-C5-C6
94	AL	413	PL9	C30-C29-C31-C32
94	A6	410	PL9	C30-C29-C31-C32
82	W5	202	PEB	C2C-C1C-CHB-C4B
94	aL	601	PL9	C9-C11-C12-C13
94	dL	406	PL9	C24-C26-C27-C28
95	aL	603	DGD	O6D-C5D-C6D-O5D
92	D6	409	LMG	C18-C19-C20-C21
87	AN	821	CLA	C12-C13-C15-C16
87	AN	826	CLA	C6-C7-C8-C10
87	BN	835	CLA	C12-C13-C15-C16
87	62	303	CLA	C11-C12-C13-C15
87	A2	821	CLA	C12-C13-C15-C16
87	A2	826	CLA	C6-C7-C8-C10
87	B2	835	CLA	C12-C13-C15-C16
87	A6	402	CLA	C11-C12-C13-C15
87	C6	511	CLA	C2-C3-C5-C6
87	C6	519	CLA	C2-C3-C5-C6
87	b6	612	CLA	C2-C3-C5-C6
87	c6	606	CLA	C12-C13-C15-C16
87	aL	606	CLA	C2-C3-C5-C6
87	6N	602	CLA	C11-C12-C13-C15
82	NA	202	PEB	CAB-CBB-CGB-O1B
82	NA	202	PEB	CAB-CBB-CGB-O2B
82	QA	202	PEB	CAB-CBB-CGB-O1B
82	DB	201	PEB	CAB-CBB-CGB-O1B
82	LD	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	ND	204	PEB	CAC-CBC-CGC-O1C
82	CF	201	PEB	CAC-CBC-CGC-O1C
82	CF	201	PEB	CAC-CBC-CGC-O2C
82	FF	201	PEB	CAB-CBB-CGB-O1B
82	GF	203	PEB	CAC-CBC-CGC-O2C
82	QF	202	PEB	CAC-CBC-CGC-O1C
82	RF	201	PEB	CAC-CBC-CGC-O1C
82	RF	201	PEB	CAC-CBC-CGC-O2C
82	SF	203	PEB	CAC-CBC-CGC-O1C
82	SF	203	PEB	CAC-CBC-CGC-O2C
82	YF	202	PEB	CAC-CBC-CGC-O1C
82	HG	1002	PEB	CAB-CBB-CGB-O2B
82	UH	201	PEB	CAB-CBB-CGB-O1B
82	BI	201	PEB	CAB-CBB-CGB-O1B
82	WI	201	PEB	CAB-CBB-CGB-O2B
82	CJ	202	PEB	CAB-CBB-CGB-O1B
82	MJ	202	PEB	CAC-CBC-CGC-O2C
82	VJ	201	PEB	CAC-CBC-CGC-O1C
82	VJ	201	PEB	CAC-CBC-CGC-O2C
82	CK	201	PEB	CAC-CBC-CGC-O2C
82	GK	203	PEB	CAC-CBC-CGC-O1C
82	GK	203	PEB	CAC-CBC-CGC-O2C
82	RK	201	PEB	CAC-CBC-CGC-O2C
82	SK	203	PEB	CAC-CBC-CGC-O1C
82	UK	201	PEB	CAC-CBC-CGC-O1C
82	YK	202	PEB	CAC-CBC-CGC-O1C
82	NM	201	PEB	CAC-CBC-CGC-O2C
82	DO	1002	PEB	CAB-CBB-CGB-O2B
82	OO	201	PEB	CAC-CBC-CGC-O1C
82	GP	202	PEB	CAC-CBC-CGC-O2C
82	LQ	203	PEB	CAB-CBB-CGB-O1B
82	NQ	204	PEB	CAC-CBC-CGC-O1C
82	L1	1002	PEB	CAB-CBB-CGB-O1B
82	W1	202	PEB	CAC-CBC-CGC-O1C
82	c1	202	PEB	CAB-CBB-CGB-O1B
82	P4	201	PEB	CAB-CBB-CGB-O2B
82	F5	201	PEB	CAC-CBC-CGC-O2C
82	W5	202	PEB	CAC-CBC-CGC-O1C
82	N7	202	PEB	CAB-CBB-CGB-O1B
82	P7	202	PEB	CAB-CBB-CGB-O1B
82	Q7	202	PEB	CAB-CBB-CGB-O1B
82	e7	301	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	18	203	PEB	CAB-CBB-CGB-O2B
82	L9	203	PEB	CAB-CBB-CGB-O1B
82	hE	201	PEB	CAC-CBC-CGC-O1C
82	mF	202	PEB	CAC-CBC-CGC-O2C
82	hG	201	PEB	CAC-CBC-CGC-O1C
82	cH	202	PEB	CAB-CBB-CGB-O1B
82	aJ	201	PEB	CAB-CBB-CGB-O1B
82	aJ	203	PEB	CAB-CBB-CGB-O2B
82	fJ	202	PEB	CAC-CBC-CGC-O2C
82	fK	201	PEB	CAB-CBB-CGB-O1B
82	mK	202	PEB	CAC-CBC-CGC-O2C
82	lM	203	PEB	CAB-CBB-CGB-O1B
83	Z9	302	PUB	CAC-CBC-CGC-O1C
83	M9	303	PUB	CAC-CBC-CGC-O1C
84	LH	1001	CYC	CAA-CBA-CGA-O1A
84	HO	1001	CYC	CAA-CBA-CGA-O1A
84	H4	1001	CYC	CAA-CBA-CGA-O1A
87	R2	204	CLA	CAA-CBA-CGA-O2A
96	GN	201	HEM	CAD-CBD-CGD-O1D
96	G2	201	HEM	CAD-CBD-CGD-O1D
87	c6	608	CLA	CBA-CGA-O2A-C1
88	a6	610	LHG	C12-C13-C14-C15
92	yL	101	LMG	C29-C30-C31-C32
82	VE	201	PEB	C3C-C2C-CAC-CBC
82	VG	201	PEB	C3C-C2C-CAC-CBC
82	kE	202	PEB	C3C-C2C-CAC-CBC
82	kG	202	PEB	C3C-C2C-CAC-CBC
83	AD	302	PUB	C2B-C3B-CAB-CBB
83	AQ	302	PUB	C2B-C3B-CAB-CBB
91	aL	610	PHO	C5-C6-C7-C8
82	RO	202	PEB	C4B-C3B-CAB-CBB
82	F5	201	PEB	C4B-C3B-CAB-CBB
85	BN	840	BCR	C15-C16-C17-C18
85	BN	841	BCR	C9-C10-C11-C12
85	B2	840	BCR	C15-C16-C17-C18
85	B2	841	BCR	C9-C10-C11-C12
85	F6	101	BCR	C19-C20-C21-C22
85	h6	102	BCR	C9-C10-C11-C12
95	D6	410	DGD	C2E-C1E-O5D-C6D
95	h6	101	DGD	CAB-CBB-CCB-CDB
82	PA	202	PEB	CAB-CBB-CGB-O1B
82	QA	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	IB	203	PEB	CAB-CBB-CGB-O2B
82	JD	201	PEB	CAB-CBB-CGB-O1B
82	LD	201	PEB	CAB-CBB-CGB-O1B
82	GF	203	PEB	CAC-CBC-CGC-O1C
82	LF	202	PEB	CAB-CBB-CGB-O1B
82	UF	201	PEB	CAC-CBC-CGC-O1C
82	UF	202	PEB	CAC-CBC-CGC-O1C
82	YF	201	PEB	CAC-CBC-CGC-O2C
82	PJ	202	PEB	CAC-CBC-CGC-O1C
82	FK	201	PEB	CAB-CBB-CGB-O1B
82	LK	202	PEB	CAB-CBB-CGB-O1B
82	QK	201	PEB	CAC-CBC-CGC-O2C
82	QK	202	PEB	CAC-CBC-CGC-O1C
82	ZM	201	PEB	CAC-CBC-CGC-O1C
82	YP	503	PEB	CAC-CBC-CGC-O1C
82	JQ	201	PEB	CAB-CBB-CGB-O1B
82	LQ	201	PEB	CAB-CBB-CGB-O1B
82	TQ	202	PEB	CAC-CBC-CGC-O1C
82	U1	201	PEB	CAB-CBB-CGB-O2B
82	O4	201	PEB	CAC-CBC-CGC-O1C
82	c4	203	PEB	CAB-CBB-CGB-O1B
82	P7	202	PEB	CAB-CBB-CGB-O2B
82	Q7	202	PEB	CAB-CBB-CGB-O2B
82	e7	301	PEB	CAB-CBB-CGB-O1B
82	uC	201	PEB	CAB-CBB-CGB-O1B
82	lE	203	PEB	CAC-CBC-CGC-O1C
82	eF	203	PEB	CAC-CBC-CGC-O2C
82	lF	201	PEB	CAB-CBB-CGB-O2B
82	dG	204	PEB	CAC-CBC-CGC-O1C
82	lK	201	PEB	CAB-CBB-CGB-O2B
82	mK	202	PEB	CAB-CBB-CGB-O1B
82	cO	203	PEB	CAB-CBB-CGB-O1B
84	IE	1001	CYC	CAA-CBA-CGA-O2A
84	IG	1001	CYC	CAA-CBA-CGA-O2A
88	M6	101	LHG	C1-C2-C3-O3
88	I6	101	LHG	O7-C5-C6-O8
92	XL	601	LMG	O7-C8-C9-O8
92	b6	624	LMG	O7-C8-C9-O8
95	C6	504	DGD	O2G-C2G-C3G-O3G
87	K6	101	CLA	O1A-CGA-O2A-C1
92	b6	620	LMG	O10-C28-O8-C9
82	SI	201	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
82	aG	202	PEB	C2B-C3B-CAB-CBB
87	AN	831	CLA	CBA-CGA-O2A-C1
87	A2	831	CLA	CBA-CGA-O2A-C1
87	b6	605	CLA	C5-C6-C7-C8
82	KA	201	PEB	CAC-CBC-CGC-O2C
82	PA	202	PEB	CAB-CBB-CGB-O2B
82	DB	201	PEB	CAB-CBB-CGB-O2B
82	JB	201	PEB	CAC-CBC-CGC-O1C
82	NB	201	PEB	CAB-CBB-CGB-O1B
82	OB	201	PEB	CAC-CBC-CGC-O1C
82	TB	201	PEB	CAC-CBC-CGC-O1C
82	ED	201	PEB	CAB-CBB-CGB-O2B
82	JD	201	PEB	CAB-CBB-CGB-O2B
82	LD	203	PEB	CAB-CBB-CGB-O2B
82	ND	204	PEB	CAB-CBB-CGB-O1B
82	TD	202	PEB	CAC-CBC-CGC-O1C
82	JF	201	PEB	CAB-CBB-CGB-O1B
82	QF	201	PEB	CAC-CBC-CGC-O2C
82	QF	202	PEB	CAC-CBC-CGC-O2C
82	PG	201	PEB	CAB-CBB-CGB-O1B
82	ZG	201	PEB	CAC-CBC-CGC-O1C
82	LH	1003	PEB	CAB-CBB-CGB-O1B
82	QH	203	PEB	CAB-CBB-CGB-O1B
82	UH	201	PEB	CAB-CBB-CGB-O2B
82	WI	201	PEB	CAB-CBB-CGB-O1B
82	HJ	201	PEB	CAC-CBC-CGC-O2C
82	PJ	202	PEB	CAC-CBC-CGC-O2C
82	YJ	203	PEB	CAC-CBC-CGC-O2C
82	JK	201	PEB	CAB-CBB-CGB-O1B
82	QK	202	PEB	CAC-CBC-CGC-O2C
82	UK	202	PEB	CAC-CBC-CGC-O1C
82	BM	301	PEB	CAB-CBB-CGB-O1B
82	EQ	201	PEB	CAB-CBB-CGB-O2B
82	JQ	201	PEB	CAB-CBB-CGB-O2B
82	LQ	203	PEB	CAB-CBB-CGB-O2B
82	NQ	204	PEB	CAB-CBB-CGB-O1B
82	d1	201	PEB	CAC-CBC-CGC-O1C
82	S4	201	PEB	CAC-CBC-CGC-O2C
82	Y4	202	PEB	CAB-CBB-CGB-O1B
82	J5	202	PEB	CAC-CBC-CGC-O1C
82	M5	304	PEB	CAC-CBC-CGC-O2C
82	Q5	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	S5	201	PEB	CAC-CBC-CGC-O2C
82	S5	202	PEB	CAC-CBC-CGC-O1C
82	X5	202	PEB	CAB-CBB-CGB-O1B
82	Z5	304	PEB	CAC-CBC-CGC-O2C
82	K7	201	PEB	CAC-CBC-CGC-O2C
82	N7	202	PEB	CAB-CBB-CGB-O2B
82	e7	301	PEB	CAC-CBC-CGC-O2C
82	18	203	PEB	CAB-CBB-CGB-O1B
82	S9	203	PEB	CAC-CBC-CGC-O2C
82	W9	201	PEB	CAB-CBB-CGB-O1B
82	1C	203	PEB	CAB-CBB-CGB-O1B
82	dE	204	PEB	CAC-CBC-CGC-O1C
82	aF	201	PEB	CAC-CBC-CGC-O1C
82	eF	201	PEB	CAC-CBC-CGC-O1C
82	gF	203	PEB	CAC-CBC-CGC-O1C
82	mF	202	PEB	CAB-CBB-CGB-O1B
82	nF	202	PEB	CAB-CBB-CGB-O1B
82	pF	202	PEB	CAB-CBB-CGB-O2B
82	rF	202	PEB	CAC-CBC-CGC-O1C
82	sF	201	PEB	CAC-CBC-CGC-O1C
82	dH	201	PEB	CAC-CBC-CGC-O1C
82	kJ	202	PEB	CAB-CBB-CGB-O1B
82	aK	201	PEB	CAC-CBC-CGC-O1C
82	eK	201	PEB	CAC-CBC-CGC-O1C
82	eK	203	PEB	CAC-CBC-CGC-O2C
82	nK	202	PEB	CAB-CBB-CGB-O1B
82	sK	201	PEB	CAC-CBC-CGC-O1C
82	cM	202	PEB	CAB-CBB-CGB-O2B
84	CG	1001	CYC	CAA-CBA-CGA-O1A
87	62	308	CLA	CAA-CBA-CGA-O2A
87	6N	607	CLA	CAA-CBA-CGA-O2A
87	CL	512	CLA	CAA-CBA-CGA-O2A
87	52	607	CLA	CAA-CBA-CGA-O2A
87	F2	205	CLA	CAA-CBA-CGA-O2A
87	5N	607	CLA	CAA-CBA-CGA-O2A
87	CL	509	CLA	C2A-CAA-CBA-CGA
87	cL	508	CLA	C16-C17-C18-C20
82	HA	202	PEB	CAC-CBC-CGC-O2C
82	LA	202	PEB	CAB-CBB-CGB-O1B
82	AD	301	PEB	CAC-CBC-CGC-O2C
82	PE	201	PEB	CAB-CBB-CGB-O1B
82	ZE	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	ZE	201	PEB	CAC-CBC-CGC-O2C
82	DF	203	PEB	CAB-CBB-CGB-O1B
82	XF	203	PEB	CAB-CBB-CGB-O1B
82	ZG	201	PEB	CAC-CBC-CGC-O2C
82	ZH	202	PEB	CAC-CBC-CGC-O2C
82	DI	202	PEB	CAB-CBB-CGB-O2B
82	KI	201	PEB	CAB-CBB-CGB-O2B
82	QI	201	PEB	CAB-CBB-CGB-O2B
82	LJ	201	PEB	CAC-CBC-CGC-O2C
82	LJ	202	PEB	CAB-CBB-CGB-O2B
82	UJ	201	PEB	CAC-CBC-CGC-O2C
82	DK	203	PEB	CAB-CBB-CGB-O1B
82	XK	203	PEB	CAB-CBB-CGB-O1B
82	YK	201	PEB	CAC-CBC-CGC-O2C
82	PM	202	PEB	CAB-CBB-CGB-O1B
82	WM	202	PEB	CAC-CBC-CGC-O1C
82	WM	202	PEB	CAB-CBB-CGB-O1B
82	ZM	201	PEB	CAC-CBC-CGC-O2C
82	PO	201	PEB	CAB-CBB-CGB-O2B
82	SO	201	PEB	CAC-CBC-CGC-O2C
82	TO	201	PEB	CAC-CBC-CGC-O2C
82	YO	202	PEB	CAB-CBB-CGB-O1B
82	BP	201	PEB	CAB-CBB-CGB-O1B
82	EP	202	PEB	CAC-CBC-CGC-O1C
82	JP	201	PEB	CAB-CBB-CGB-O1B
82	VP	201	PEB	CAB-CBB-CGB-O2B
82	EQ	202	PEB	CAC-CBC-CGC-O1C
82	Z1	202	PEB	CAC-CBC-CGC-O2C
82	H4	1002	PEB	CAB-CBB-CGB-O1B
82	T4	201	PEB	CAC-CBC-CGC-O2C
82	A5	202	PEB	CAB-CBB-CGB-O1B
82	C5	202	PEB	CAB-CBB-CGB-O1B
82	E5	202	PEB	CAB-CBB-CGB-O1B
82	G5	202	PEB	CAB-CBB-CGB-O1B
82	I5	202	PEB	CAB-CBB-CGB-O1B
82	K5	202	PEB	CAB-CBB-CGB-O1B
82	N5	202	PEB	CAB-CBB-CGB-O1B
82	P5	202	PEB	CAB-CBB-CGB-O1B
82	Q5	203	PEB	CAC-CBC-CGC-O1C
82	R5	202	PEB	CAB-CBB-CGB-O1B
82	T5	202	PEB	CAB-CBB-CGB-O1B
82	V5	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	Y5	202	PEB	CAC-CBC-CGC-O1C
82	H7	202	PEB	CAC-CBC-CGC-O2C
82	L7	202	PEB	CAB-CBB-CGB-O1B
82	V7	202	PEB	CAC-CBC-CGC-O2C
82	r8	201	PEB	CAB-CBB-CGB-O2B
82	u8	201	PEB	CAB-CBB-CGB-O2B
82	J9	201	PEB	CAB-CBB-CGB-O1B
82	L9	202	PEB	CAC-CBC-CGC-O1C
82	L9	203	PEB	CAB-CBB-CGB-O2B
82	U9	202	PEB	CAC-CBC-CGC-O1C
82	rC	201	PEB	CAB-CBB-CGB-O2B
82	uC	201	PEB	CAB-CBB-CGB-O2B
82	dD	401	PEB	CAB-CBB-CGB-O1B
82	fF	201	PEB	CAC-CBC-CGC-O2C
82	fF	201	PEB	CAB-CBB-CGB-O1B
82	hF	202	PEB	CAB-CBB-CGB-O2B
82	kF	202	PEB	CAC-CBC-CGC-O1C
82	uF	202	PEB	CAB-CBB-CGB-O1B
82	fK	201	PEB	CAC-CBC-CGC-O2C
82	gK	203	PEB	CAC-CBC-CGC-O1C
82	hK	202	PEB	CAB-CBB-CGB-O2B
82	kK	202	PEB	CAC-CBC-CGC-O1C
82	pK	202	PEB	CAB-CBB-CGB-O2B
82	rK	202	PEB	CAC-CBC-CGC-O1C
82	lM	203	PEB	CAB-CBB-CGB-O2B
84	FE	1001	CYC	CAA-CBA-CGA-O1A
84	NE	201	CYC	CAA-CBA-CGA-O1A
84	KG	202	CYC	CAA-CBA-CGA-O1A
84	HH	1001	CYC	CAA-CBA-CGA-O2A
84	JH	1001	CYC	CAA-CBA-CGA-O2A
84	H1	1001	CYC	CAA-CBA-CGA-O2A
84	J1	1001	CYC	CAA-CBA-CGA-O2A
84	73	1002	CYC	CAA-CBA-CGA-O2A
87	72	603	CLA	CAA-CBA-CGA-O2A
87	7N	603	CLA	CAA-CBA-CGA-O2A
96	GN	201	HEM	CAD-CBD-CGD-O2D
96	G2	201	HEM	CAD-CBD-CGD-O2D
88	B6	617	LHG	C24-C23-O8-C6
92	jL	101	LMG	C29-C28-O8-C9
87	AN	833	CLA	CAA-CBA-CGA-O2A
87	FN	205	CLA	CAA-CBA-CGA-O2A
87	A2	833	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
87	C6	509	CLA	CAA-CBA-CGA-O2A
87	c6	604	CLA	CAA-CBA-CGA-O2A
95	aL	603	DGD	O1G-C1A-C2A-C3A
87	cL	510	CLA	C4-C3-C5-C6
94	A6	410	PL9	C25-C24-C26-C27
87	BN	835	CLA	C15-C16-C17-C18
87	b6	613	CLA	C5-C6-C7-C8
82	IJ	203	PEB	NC-C4C-CHC-C1D
82	SP	201	PEB	NC-C4C-CHC-C1D
82	gB	203	PEB	NC-C4C-CHC-C1D
82	rF	202	PEB	NC-C4C-CHC-C1D
82	SB	202	PEB	C2C-CAC-CBC-CGC
82	JF	201	PEB	C3B-CAB-CBB-CGB
82	JK	201	PEB	C3B-CAB-CBB-CGB
82	NM	201	PEB	C3B-CAB-CBB-CGB
82	YM	202	PEB	C2C-CAC-CBC-CGC
82	XQ	202	PEB	C3B-CAB-CBB-CGB
82	D7	201	PEB	C2C-CAC-CBC-CGC
82	J9	201	PEB	C2C-CAC-CBC-CGC
82	dE	202	PEB	C3B-CAB-CBB-CGB
84	HG	1001	CYC	C2A-CAA-CBA-CGA
82	VA	202	PEB	CAC-CBC-CGC-O2C
82	XA	202	PEB	CAC-CBC-CGC-O2C
82	QB	204	PEB	CAC-CBC-CGC-O2C
82	AD	301	PEB	CAC-CBC-CGC-O1C
82	ED	202	PEB	CAC-CBC-CGC-O1C
82	LD	201	PEB	CAB-CBB-CGB-O2B
82	OE	201	PEB	CAC-CBC-CGC-O2C
82	IF	202	PEB	CAB-CBB-CGB-O1B
82	PF	201	PEB	CAB-CBB-CGB-O2B
82	WF	202	PEB	CAC-CBC-CGC-O2C
82	OG	201	PEB	CAC-CBC-CGC-O2C
82	ZH	202	PEB	CAC-CBC-CGC-O1C
82	DI	202	PEB	CAB-CBB-CGB-O1B
82	GJ	203	PEB	CAB-CBB-CGB-O2B
82	MJ	201	PEB	CAC-CBC-CGC-O1C
82	IK	202	PEB	CAB-CBB-CGB-O1B
82	LK	201	PEB	CAB-CBB-CGB-O1B
82	NK	201	PEB	CAB-CBB-CGB-O2B
82	PK	201	PEB	CAB-CBB-CGB-O2B
82	WK	202	PEB	CAC-CBC-CGC-O2C
82	TM	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	HO	1002	PEB	CAB-CBB-CGB-O1B
82	NP	201	PEB	CAB-CBB-CGB-O2B
82	OP	203	PEB	CAB-CBB-CGB-O1B
82	AQ	301	PEB	CAC-CBC-CGC-O2C
82	LQ	201	PEB	CAB-CBB-CGB-O2B
82	Q1	201	PEB	CAC-CBC-CGC-O1C
82	Z1	202	PEB	CAC-CBC-CGC-O1C
82	i4	201	PEB	CAC-CBC-CGC-O2C
82	C7	202	PEB	CAC-CBC-CGC-O2C
82	X7	202	PEB	CAC-CBC-CGC-O2C
82	t8	201	PEB	CAC-CBC-CGC-O1C
82	F9	202	PEB	CAC-CBC-CGC-O2C
82	L9	202	PEB	CAC-CBC-CGC-O2C
82	eA	301	PEB	CAC-CBC-CGC-O2C
82	cB	402	PEB	CAC-CBC-CGC-O1C
82	dB	202	PEB	CAC-CBC-CGC-O1C
82	lE	201	PEB	CAC-CBC-CGC-O2C
82	aF	203	PEB	CAC-CBC-CGC-O2C
82	hF	202	PEB	CAB-CBB-CGB-O1B
82	nF	201	PEB	CAB-CBB-CGB-O1B
82	oF	201	PEB	CAC-CBC-CGC-O2C
82	lG	201	PEB	CAC-CBC-CGC-O2C
82	lG	203	PEB	CAC-CBC-CGC-O1C
82	eJ	201	PEB	CAC-CBC-CGC-O2C
82	fJ	202	PEB	CAB-CBB-CGB-O1B
82	aK	203	PEB	CAC-CBC-CGC-O2C
82	hK	202	PEB	CAB-CBB-CGB-O1B
82	nK	201	PEB	CAB-CBB-CGB-O1B
82	oK	201	PEB	CAC-CBC-CGC-O2C
82	uK	201	PEB	CAB-CBB-CGB-O1B
82	hM	203	PEB	CAB-CBB-CGB-O1B
82	hM	203	PEB	CAB-CBB-CGB-O2B
82	jM	201	PEB	CAC-CBC-CGC-O2C
82	iO	201	PEB	CAC-CBC-CGC-O2C
82	cO	203	PEB	CAB-CBB-CGB-O2B
82	dQ	401	PEB	CAB-CBB-CGB-O1B
83	Z9	302	PUB	CAC-CBC-CGC-O2C
83	M9	303	PUB	CAC-CBC-CGC-O2C
84	NH	1001	CYC	CAD-CBD-CGD-O1D
84	N1	1001	CYC	CAD-CBD-CGD-O1D
84	73	1002	CYC	CAA-CBA-CGA-O1A
87	AN	822	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	ON	203	CLA	CAA-CBA-CGA-O1A
87	A2	822	CLA	CAA-CBA-CGA-O1A
87	C6	520	CLA	C2-C3-C5-C6
87	b6	618	CLA	C2-C3-C5-C6
87	cL	511	CLA	C2-C3-C5-C6
88	AL	406	LHG	C19-C20-C21-C22
87	B2	835	CLA	C15-C16-C17-C18
87	12	607	CLA	CAA-CBA-CGA-O2A
87	32	309	CLA	CAA-CBA-CGA-O2A
87	cL	516	CLA	CAA-CBA-CGA-O2A
87	1N	607	CLA	CAA-CBA-CGA-O2A
87	3N	309	CLA	CAA-CBA-CGA-O2A
95	CL	520	DGD	O6D-C5D-C6D-O5D
82	HA	203	PEB	C2C-C1C-CHB-C4B
82	BB	203	PEB	C2C-C1C-CHB-C4B
82	PJ	202	PEB	C2C-C1C-CHB-C4B
82	H7	203	PEB	C2C-C1C-CHB-C4B
87	CL	503	CLA	C6-C7-C8-C9
87	CL	503	CLA	C14-C13-C15-C16
87	CL	506	CLA	C11-C12-C13-C14
87	AN	821	CLA	C6-C7-C8-C9
87	BN	831	CLA	C11-C10-C8-C9
87	BN	834	CLA	C11-C12-C13-C14
87	LN	203	CLA	C6-C7-C8-C9
87	A2	821	CLA	C6-C7-C8-C9
87	B2	831	CLA	C11-C10-C8-C9
87	B2	834	CLA	C11-C12-C13-C14
87	L2	203	CLA	C6-C7-C8-C9
87	C6	510	CLA	C6-C7-C8-C9
87	C6	510	CLA	C11-C10-C8-C9
87	C6	511	CLA	C11-C10-C8-C9
87	C6	514	CLA	C6-C7-C8-C9
87	C6	520	CLA	C11-C10-C8-C9
87	D6	403	CLA	C11-C10-C8-C9
87	a6	608	CLA	C6-C7-C8-C9
87	b6	618	CLA	C14-C13-C15-C16
87	c6	608	CLA	C14-C13-C15-C16
87	c6	613	CLA	C11-C12-C13-C14
87	bL	608	CLA	C14-C13-C15-C16
87	cL	508	CLA	C11-C10-C8-C9
87	dL	402	CLA	C11-C10-C8-C9
82	CA	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	SA	202	PEB	CAB-CBB-CGB-O1B
82	VA	201	PEB	CAB-CBB-CGB-O1B
82	JB	201	PEB	CAB-CBB-CGB-O1B
82	QB	204	PEB	CAC-CBC-CGC-O1C
82	TB	201	PEB	CAB-CBB-CGB-O1B
82	FD	203	PEB	CAC-CBC-CGC-O1C
82	MD	201	PEB	CAB-CBB-CGB-O2B
82	DE	1002	PEB	CAB-CBB-CGB-O2B
82	OE	201	PEB	CAC-CBC-CGC-O1C
82	LF	201	PEB	CAB-CBB-CGB-O1B
82	WF	202	PEB	CAB-CBB-CGB-O1B
82	DG	1002	PEB	CAB-CBB-CGB-O2B
82	OG	201	PEB	CAC-CBC-CGC-O1C
82	AH	301	PEB	CAB-CBB-CGB-O1B
82	DH	1002	PEB	CAB-CBB-CGB-O1B
82	QH	201	PEB	CAC-CBC-CGC-O1C
82	TJ	201	PEB	CAC-CBC-CGC-O1C
82	BK	202	PEB	CAB-CBB-CGB-O1B
82	BM	301	PEB	CAC-CBC-CGC-O1C
82	SO	201	PEB	CAC-CBC-CGC-O1C
82	MQ	201	PEB	CAB-CBB-CGB-O2B
82	A1	301	PEB	CAB-CBB-CGB-O1B
82	D1	1002	PEB	CAB-CBB-CGB-O1B
82	a1	201	PEB	CAB-CBB-CGB-O2B
82	m4	202	PEB	CAB-CBB-CGB-O1B
82	c4	203	PEB	CAB-CBB-CGB-O2B
82	g4	201	PEB	CAC-CBC-CGC-O2C
82	S7	202	PEB	CAB-CBB-CGB-O1B
82	tC	201	PEB	CAB-CBB-CGB-O2B
82	mE	202	PEB	CAC-CBC-CGC-O2C
82	dG	203	PEB	CAB-CBB-CGB-O2B
83	Z9	302	PUB	CAB-CBB-CGB-O2B
84	DH	1003	CYC	CAA-CBA-CGA-O1A
84	JH	1001	CYC	CAA-CBA-CGA-O1A
84	D1	1003	CYC	CAA-CBA-CGA-O1A
84	J1	1001	CYC	CAA-CBA-CGA-O1A
87	22	603	CLA	CAA-CBA-CGA-O2A
87	42	603	CLA	CAA-CBA-CGA-O2A
87	62	304	CLA	CAA-CBA-CGA-O1A
87	O2	203	CLA	CAA-CBA-CGA-O1A
87	2N	306	CLA	CAA-CBA-CGA-O2A
87	3N	303	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
87	4N	603	CLA	CAA-CBA-CGA-O2A
87	6N	603	CLA	CAA-CBA-CGA-O1A
91	A6	407	PHO	C8-C10-C11-C12
87	AN	811	CLA	C3A-C2A-CAA-CBA
87	AN	828	CLA	C3A-C2A-CAA-CBA
87	BN	825	CLA	C3A-C2A-CAA-CBA
87	12	607	CLA	C3A-C2A-CAA-CBA
87	52	611	CLA	C3A-C2A-CAA-CBA
87	A2	811	CLA	C3A-C2A-CAA-CBA
87	A2	828	CLA	C3A-C2A-CAA-CBA
87	B2	824	CLA	C3A-C2A-CAA-CBA
87	C6	520	CLA	C3A-C2A-CAA-CBA
87	D6	402	CLA	C3A-C2A-CAA-CBA
87	cL	505	CLA	C3A-C2A-CAA-CBA
87	1N	607	CLA	C3A-C2A-CAA-CBA
87	5N	611	CLA	C3A-C2A-CAA-CBA
82	R4	202	PEB	C4B-C3B-CAB-CBB
95	AL	414	DGD	C4B-C5B-C6B-C7B
88	AL	407	LHG	O2-C2-C3-O3
88	CL	522	LHG	O10-C23-O8-C6
92	j6	102	LMG	O10-C28-O8-C9
92	jL	101	LMG	O10-C28-O8-C9
87	BN	802	CLA	CAA-CBA-CGA-O2A
87	LN	204	CLA	CAA-CBA-CGA-O2A
87	B2	801	CLA	CAA-CBA-CGA-O2A
87	L2	204	CLA	CAA-CBA-CGA-O2A
87	B6	604	CLA	CAA-CBA-CGA-O2A
92	m6	103	LMG	O7-C10-C11-C12
88	AL	406	LHG	C30-C31-C32-C33
82	EB	501	PEB	CAC-CBC-CGC-O2C
82	HB	202	PEB	CAC-CBC-CGC-O2C
82	CD	202	PEB	CAB-CBB-CGB-O1B
82	KD	202	PEB	CAB-CBB-CGB-O2B
82	SE	202	PEB	CAC-CBC-CGC-O2C
82	YF	201	PEB	CAC-CBC-CGC-O1C
82	SG	203	PEB	CAC-CBC-CGC-O2C
82	AH	301	PEB	CAC-CBC-CGC-O2C
82	YH	201	PEB	CAC-CBC-CGC-O2C
82	GI	201	PEB	CAB-CBB-CGB-O2B
82	LJ	202	PEB	CAC-CBC-CGC-O1C
82	UK	201	PEB	CAC-CBC-CGC-O2C
82	VK	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	WK	202	PEB	CAB-CBB-CGB-O1B
82	YK	201	PEB	CAC-CBC-CGC-O1C
82	XP	202	PEB	CAC-CBC-CGC-O2C
82	AQ	301	PEB	CAC-CBC-CGC-O1C
82	AQ	301	PEB	CAB-CBB-CGB-O1B
82	FQ	203	PEB	CAC-CBC-CGC-O1C
82	A1	301	PEB	CAC-CBC-CGC-O2C
82	Y1	201	PEB	CAC-CBC-CGC-O2C
82	S4	201	PEB	CAC-CBC-CGC-O1C
82	h4	201	PEB	CAB-CBB-CGB-O2B
82	A5	201	PEB	CAC-CBC-CGC-O2C
82	C5	201	PEB	CAC-CBC-CGC-O2C
82	E5	201	PEB	CAC-CBC-CGC-O2C
82	G5	201	PEB	CAC-CBC-CGC-O2C
82	I5	201	PEB	CAC-CBC-CGC-O2C
82	K5	201	PEB	CAC-CBC-CGC-O2C
82	N5	201	PEB	CAC-CBC-CGC-O2C
82	P5	201	PEB	CAC-CBC-CGC-O2C
82	R5	201	PEB	CAC-CBC-CGC-O2C
82	T5	201	PEB	CAC-CBC-CGC-O2C
82	V5	201	PEB	CAC-CBC-CGC-O2C
82	X5	201	PEB	CAC-CBC-CGC-O2C
82	V7	201	PEB	CAB-CBB-CGB-O1B
82	y8	201	PEB	CAC-CBC-CGC-O2C
82	t8	201	PEB	CAB-CBB-CGB-O2B
82	Y9	201	PEB	CAB-CBB-CGB-O1B
82	gB	202	PEB	CAB-CBB-CGB-O1B
82	tC	201	PEB	CAC-CBC-CGC-O1C
82	dE	203	PEB	CAB-CBB-CGB-O2B
82	hE	203	PEB	CAB-CBB-CGB-O2B
82	qF	202	PEB	CAB-CBB-CGB-O1B
82	hG	203	PEB	CAB-CBB-CGB-O2B
82	mG	202	PEB	CAC-CBC-CGC-O2C
82	kH	201	PEB	CAB-CBB-CGB-O2B
82	kJ	201	PEB	CAC-CBC-CGC-O2C
82	nK	202	PEB	CAC-CBC-CGC-O2C
82	qK	202	PEB	CAB-CBB-CGB-O1B
82	kO	201	PEB	CAC-CBC-CGC-O2C
82	mO	202	PEB	CAB-CBB-CGB-O1B
82	hO	201	PEB	CAB-CBB-CGB-O2B
82	Z9	304	PEB	CAC-CBC-CGC-O2C
83	xF	305	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
83	xK	305	PUB	CAB-CBB-CGB-O1B
84	IE	1001	CYC	CAA-CBA-CGA-O1A
84	IG	1001	CYC	CAA-CBA-CGA-O1A
87	22	606	CLA	CAA-CBA-CGA-O2A
87	32	302	CLA	CAA-CBA-CGA-O2A
87	52	611	CLA	CAA-CBA-CGA-O2A
87	82	301	CLA	CAA-CBA-CGA-O2A
87	2N	304	CLA	CAA-CBA-CGA-O2A
87	4N	607	CLA	CAA-CBA-CGA-O2A
87	8N	302	CLA	CAA-CBA-CGA-O2A
87	AL	403	CLA	CAD-CBD-CGD-O2D
87	AL	404	CLA	CAD-CBD-CGD-O2D
87	BL	601	CLA	CAD-CBD-CGD-O2D
87	BL	608	CLA	CAD-CBD-CGD-O2D
87	CL	504	CLA	CAD-CBD-CGD-O2D
87	CL	506	CLA	CAD-CBD-CGD-O2D
87	CL	515	CLA	CAD-CBD-CGD-O2D
87	AN	812	CLA	CAD-CBD-CGD-O2D
87	AN	813	CLA	CAD-CBD-CGD-O2D
87	AN	814	CLA	CAD-CBD-CGD-O2D
87	AN	818	CLA	CAD-CBD-CGD-O2D
87	AN	822	CLA	CAD-CBD-CGD-O2D
87	AN	826	CLA	CAD-CBD-CGD-O2D
87	AN	835	CLA	CAD-CBD-CGD-O2D
87	AN	840	CLA	CAD-CBD-CGD-O2D
87	BN	802	CLA	CAD-CBD-CGD-O2D
87	BN	811	CLA	CAD-CBD-CGD-O2D
87	BN	814	CLA	CAD-CBD-CGD-O2D
87	BN	824	CLA	CAD-CBD-CGD-O2D
87	BN	827	CLA	CAD-CBD-CGD-O2D
87	BN	830	CLA	CAD-CBD-CGD-O2D
87	BN	833	CLA	CAD-CBD-CGD-O2D
87	JN	101	CLA	CAD-CBD-CGD-O2D
87	KN	105	CLA	CAD-CBD-CGD-O2D
87	LN	202	CLA	CAD-CBD-CGD-O2D
87	ON	202	CLA	CAD-CBD-CGD-O2D
87	RN	202	CLA	CAD-CBD-CGD-O2D
87	12	601	CLA	CAD-CBD-CGD-O2D
87	12	610	CLA	CAD-CBD-CGD-O2D
87	22	606	CLA	CAD-CBD-CGD-O2D
87	42	602	CLA	CAD-CBD-CGD-O2D
87	42	608	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	52	603	CLA	CAD-CBD-CGD-O2D
87	62	302	CLA	CAD-CBD-CGD-O2D
87	62	303	CLA	CAD-CBD-CGD-O2D
87	62	306	CLA	CAD-CBD-CGD-O2D
87	62	309	CLA	CAD-CBD-CGD-O2D
87	62	310	CLA	CAD-CBD-CGD-O2D
87	62	311	CLA	CAD-CBD-CGD-O2D
87	72	606	CLA	CAD-CBD-CGD-O2D
87	72	610	CLA	CAD-CBD-CGD-O2D
87	82	305	CLA	CAD-CBD-CGD-O2D
87	A2	812	CLA	CAD-CBD-CGD-O2D
87	A2	813	CLA	CAD-CBD-CGD-O2D
87	A2	814	CLA	CAD-CBD-CGD-O2D
87	A2	818	CLA	CAD-CBD-CGD-O2D
87	A2	822	CLA	CAD-CBD-CGD-O2D
87	A2	826	CLA	CAD-CBD-CGD-O2D
87	A2	835	CLA	CAD-CBD-CGD-O2D
87	A2	840	CLA	CAD-CBD-CGD-O2D
87	B2	801	CLA	CAD-CBD-CGD-O2D
87	B2	810	CLA	CAD-CBD-CGD-O2D
87	B2	813	CLA	CAD-CBD-CGD-O2D
87	B2	823	CLA	CAD-CBD-CGD-O2D
87	B2	827	CLA	CAD-CBD-CGD-O2D
87	B2	830	CLA	CAD-CBD-CGD-O2D
87	B2	833	CLA	CAD-CBD-CGD-O2D
87	J2	101	CLA	CAD-CBD-CGD-O2D
87	K2	106	CLA	CAD-CBD-CGD-O2D
87	L2	202	CLA	CAD-CBD-CGD-O2D
87	O2	202	CLA	CAD-CBD-CGD-O2D
87	R2	202	CLA	CAD-CBD-CGD-O2D
87	B6	616	CLA	CAD-CBD-CGD-O2D
87	C6	509	CLA	CAD-CBD-CGD-O2D
87	C6	510	CLA	CAD-CBD-CGD-O2D
87	b6	618	CLA	CAD-CBD-CGD-O2D
87	c6	604	CLA	CAD-CBD-CGD-O2D
87	c6	608	CLA	CAD-CBD-CGD-O2D
87	c6	610	CLA	CAD-CBD-CGD-O2D
87	d6	406	CLA	CAD-CBD-CGD-O2D
87	bL	613	CLA	CAD-CBD-CGD-O2D
87	bL	616	CLA	CAD-CBD-CGD-O2D
87	cL	514	CLA	CAD-CBD-CGD-O2D
87	1N	601	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	1N	610	CLA	CAD-CBD-CGD-O2D
87	2N	306	CLA	CAD-CBD-CGD-O2D
87	4N	602	CLA	CAD-CBD-CGD-O2D
87	4N	608	CLA	CAD-CBD-CGD-O2D
87	5N	603	CLA	CAD-CBD-CGD-O2D
87	6N	601	CLA	CAD-CBD-CGD-O2D
87	6N	602	CLA	CAD-CBD-CGD-O2D
87	6N	605	CLA	CAD-CBD-CGD-O2D
87	6N	608	CLA	CAD-CBD-CGD-O2D
87	6N	609	CLA	CAD-CBD-CGD-O2D
87	6N	610	CLA	CAD-CBD-CGD-O2D
87	7N	606	CLA	CAD-CBD-CGD-O2D
87	7N	610	CLA	CAD-CBD-CGD-O2D
87	8N	306	CLA	CAD-CBD-CGD-O2D
95	L6	102	DGD	C1A-C2A-C3A-C4A
87	LN	203	CLA	C15-C16-C17-C18
87	L2	203	CLA	C15-C16-C17-C18
95	B6	620	DGD	C4D-C5D-C6D-O5D
87	AN	807	CLA	C2-C1-O2A-CGA
82	WA	202	PEB	CAB-CBB-CGB-O2B
82	AD	301	PEB	CAB-CBB-CGB-O1B
82	YE	201	PEB	CAB-CBB-CGB-O2B
82	DF	202	PEB	CAC-CBC-CGC-O2C
82	NF	201	PEB	CAB-CBB-CGB-O2B
82	PF	201	PEB	CAC-CBC-CGC-O2C
82	VF	201	PEB	CAB-CBB-CGB-O2B
82	HH	1002	PEB	CAB-CBB-CGB-O2B
82	YH	202	PEB	CAC-CBC-CGC-O2C
82	BI	201	PEB	CAB-CBB-CGB-O2B
82	MI	401	PEB	CAC-CBC-CGC-O2C
82	TI	201	PEB	CAB-CBB-CGB-O2B
82	WI	202	PEB	CAB-CBB-CGB-O2B
82	KJ	203	PEB	CAB-CBB-CGB-O2B
82	DK	202	PEB	CAC-CBC-CGC-O2C
82	JO	1002	PEB	CAB-CBB-CGB-O2B
82	CQ	202	PEB	CAB-CBB-CGB-O1B
82	KQ	202	PEB	CAB-CBB-CGB-O2B
82	H1	1002	PEB	CAB-CBB-CGB-O2B
82	Y1	202	PEB	CAC-CBC-CGC-O2C
82	f1	201	PEB	CAB-CBB-CGB-O2B
82	k1	201	PEB	CAB-CBB-CGB-O2B
82	J4	1002	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	k4	201	PEB	CAC-CBC-CGC-O2C
82	h4	202	PEB	CAB-CBB-CGB-O1B
82	K7	201	PEB	CAC-CBC-CGC-O1C
82	W7	202	PEB	CAB-CBB-CGB-O2B
82	z8	201	PEB	CAB-CBB-CGB-O2B
82	q8	202	PEB	CAC-CBC-CGC-O1C
82	u8	201	PEB	CAC-CBC-CGC-O2C
82	zC	201	PEB	CAB-CBB-CGB-O2B
82	qC	202	PEB	CAC-CBC-CGC-O1C
82	lE	201	PEB	CAC-CBC-CGC-O1C
82	eF	203	PEB	CAC-CBC-CGC-O1C
82	oF	201	PEB	CAC-CBC-CGC-O1C
82	lG	201	PEB	CAC-CBC-CGC-O1C
82	fH	201	PEB	CAB-CBB-CGB-O2B
82	aH	201	PEB	CAB-CBB-CGB-O2B
82	eK	203	PEB	CAC-CBC-CGC-O1C
82	oK	201	PEB	CAC-CBC-CGC-O1C
82	gO	201	PEB	CAC-CBC-CGC-O2C
82	hO	202	PEB	CAB-CBB-CGB-O1B
82	M9	305	PEB	CAC-CBC-CGC-O2C
83	KA	203	PUB	CAB-CBB-CGB-O2B
83	K7	203	PUB	CAB-CBB-CGB-O2B
83	M9	303	PUB	CAB-CBB-CGB-O2B
84	LO	1001	CYC	CAA-CBA-CGA-O2A
84	L4	1001	CYC	CAA-CBA-CGA-O2A
87	12	603	CLA	CAA-CBA-CGA-O2A
87	42	607	CLA	CAA-CBA-CGA-O2A
87	72	601	CLA	CAA-CBA-CGA-O2A
87	1N	603	CLA	CAA-CBA-CGA-O2A
87	5N	611	CLA	CAA-CBA-CGA-O2A
87	7N	601	CLA	CAA-CBA-CGA-O2A
87	BL	605	CLA	CAA-CBA-CGA-O2A
87	C6	517	CLA	CAA-CBA-CGA-O2A
92	BL	611	LMG	O7-C10-C11-C12
92	bL	623	LMG	O7-C10-C11-C12
95	L6	102	DGD	O1G-C1A-C2A-C3A
88	L6	101	LHG	C28-C29-C30-C31
95	C6	504	DGD	C2A-C1A-O1G-C1G
88	l6	101	LHG	C28-C29-C30-C31
87	DL	406	CLA	C4-C3-C5-C6
87	b6	613	CLA	C4-C3-C5-C6
82	JA	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	KA	201	PEB	CAC-CBC-CGC-O1C
82	LA	201	PEB	CAB-CBB-CGB-O1B
82	BB	203	PEB	CAB-CBB-CGB-O2B
82	CD	202	PEB	CAC-CBC-CGC-O1C
82	HE	1002	PEB	CAB-CBB-CGB-O1B
82	OE	203	PEB	CAC-CBC-CGC-O1C
82	BF	202	PEB	CAB-CBB-CGB-O1B
82	RF	202	PEB	CAC-CBC-CGC-O1C
82	UF	201	PEB	CAC-CBC-CGC-O2C
82	HG	1002	PEB	CAB-CBB-CGB-O1B
82	SG	202	PEB	CAC-CBC-CGC-O2C
82	OH	203	PEB	CAB-CBB-CGB-O2B
82	AI	203	PEB	CAB-CBB-CGB-O2B
82	DI	201	PEB	CAC-CBC-CGC-O2C
82	FI	201	PEB	CAB-CBB-CGB-O1B
82	UI	202	PEB	CAB-CBB-CGB-O1B
82	DJ	201	PEB	CAC-CBC-CGC-O1C
82	LJ	201	PEB	CAC-CBC-CGC-O1C
82	TJ	201	PEB	CAC-CBC-CGC-O2C
82	NK	201	PEB	CAB-CBB-CGB-O1B
82	RK	202	PEB	CAC-CBC-CGC-O1C
82	GM	203	PEB	CAB-CBB-CGB-O1B
82	JM	201	PEB	CAC-CBC-CGC-O2C
82	ZO	202	PEB	CAB-CBB-CGB-O2B
82	OP	203	PEB	CAB-CBB-CGB-O2B
82	FQ	203	PEB	CAC-CBC-CGC-O2C
82	KQ	202	PEB	CAB-CBB-CGB-O1B
82	O1	203	PEB	CAB-CBB-CGB-O2B
82	j1	201	PEB	CAB-CBB-CGB-O1B
82	Y4	202	PEB	CAC-CBC-CGC-O1C
82	i4	203	PEB	CAB-CBB-CGB-O2B
82	g4	202	PEB	CAC-CBC-CGC-O1C
82	S5	201	PEB	CAC-CBC-CGC-O1C
82	J7	203	PEB	CAC-CBC-CGC-O1C
82	X7	202	PEB	CAC-CBC-CGC-O1C
82	z8	201	PEB	CAB-CBB-CGB-O1B
82	q8	203	PEB	CAB-CBB-CGB-O2B
82	Y9	201	PEB	CAB-CBB-CGB-O2B
82	eB	201	PEB	CAC-CBC-CGC-O1C
82	zC	201	PEB	CAB-CBB-CGB-O1B
82	qC	203	PEB	CAB-CBB-CGB-O2B
82	uC	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	fF	201	PEB	CAC-CBC-CGC-O1C
82	jF	201	PEB	CAB-CBB-CGB-O2B
82	nF	202	PEB	CAC-CBC-CGC-O2C
82	jH	201	PEB	CAB-CBB-CGB-O1B
82	hJ	203	PEB	CAB-CBB-CGB-O2B
82	fK	201	PEB	CAC-CBC-CGC-O1C
82	jK	201	PEB	CAB-CBB-CGB-O2B
82	lM	201	PEB	CAB-CBB-CGB-O1B
82	iO	203	PEB	CAB-CBB-CGB-O2B
82	gO	202	PEB	CAC-CBC-CGC-O1C
83	AM	304	PUB	CAB-CBB-CGB-O2B
84	63	901	CYC	CAA-CBA-CGA-O2A
87	12	611	CLA	CAA-CBA-CGA-O1A
87	32	302	CLA	CAA-CBA-CGA-O1A
87	62	313	CLA	CAA-CBA-CGA-O2A
87	3N	303	CLA	CAA-CBA-CGA-O1A
87	6N	612	CLA	CAA-CBA-CGA-O2A
92	JL	102	LMG	C35-C36-C37-C38
87	IN	102	CLA	C2-C3-C5-C6
87	I2	102	CLA	C2-C3-C5-C6
87	cL	510	CLA	C2-C3-C5-C6
87	AN	814	CLA	CAA-CBA-CGA-O2A
87	AN	841	CLA	CAA-CBA-CGA-O2A
87	BN	813	CLA	CAA-CBA-CGA-O2A
87	A2	841	CLA	CAA-CBA-CGA-O2A
87	b6	608	CLA	CAA-CBA-CGA-O2A
87	bL	616	CLA	CAA-CBA-CGA-O2A
92	m6	101	LMG	O8-C28-C29-C30
92	bL	611	LMG	O7-C10-C11-C12
95	BL	607	DGD	O2G-C1B-C2B-C3B
92	k6	101	LMG	C35-C36-C37-C38
87	A2	831	CLA	O1A-CGA-O2A-C1
92	B6	619	LMG	O10-C28-O8-C9
85	bL	601	BCR	C17-C18-C19-C20
94	aL	601	PL9	C24-C26-C27-C28
88	BL	610	LHG	C24-C25-C26-C27
82	y8	201	PEB	C3C-C2C-CAC-CBC
95	BL	614	DGD	C1G-C2G-C3G-O3G
82	CA	202	PEB	CAC-CBC-CGC-O1C
82	HA	202	PEB	CAC-CBC-CGC-O1C
82	NA	202	PEB	CAC-CBC-CGC-O1C
82	XA	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	XA	202	PEB	CAC-CBC-CGC-O1C
82	KB	303	PEB	CAC-CBC-CGC-O2C
82	MD	201	PEB	CAB-CBB-CGB-O1B
82	XD	201	PEB	CAB-CBB-CGB-O2B
82	BF	202	PEB	CAC-CBC-CGC-O1C
82	JF	202	PEB	CAC-CBC-CGC-O2C
82	NF	201	PEB	CAB-CBB-CGB-O1B
82	PF	201	PEB	CAB-CBB-CGB-O1B
82	PF	202	PEB	CAC-CBC-CGC-O1C
82	QF	201	PEB	CAC-CBC-CGC-O1C
82	VF	201	PEB	CAB-CBB-CGB-O1B
82	OG	203	PEB	CAC-CBC-CGC-O1C
82	BI	202	PEB	CAB-CBB-CGB-O2B
82	QI	201	PEB	CAB-CBB-CGB-O1B
82	BJ	301	PEB	CAB-CBB-CGB-O1B
82	HJ	201	PEB	CAC-CBC-CGC-O1C
82	UJ	202	PEB	CAC-CBC-CGC-O2C
82	BK	202	PEB	CAC-CBC-CGC-O1C
82	IK	201	PEB	CAB-CBB-CGB-O2B
82	PK	201	PEB	CAC-CBC-CGC-O2C
82	PK	201	PEB	CAB-CBB-CGB-O1B
82	PK	202	PEB	CAC-CBC-CGC-O1C
82	QK	201	PEB	CAC-CBC-CGC-O1C
82	PO	201	PEB	CAB-CBB-CGB-O1B
82	SO	202	PEB	CAC-CBC-CGC-O2C
82	TO	203	PEB	CAC-CBC-CGC-O1C
82	YO	202	PEB	CAC-CBC-CGC-O1C
82	NP	201	PEB	CAB-CBB-CGB-O1B
82	CQ	202	PEB	CAC-CBC-CGC-O1C
82	Y1	201	PEB	CAC-CBC-CGC-O1C
82	f1	202	PEB	CAB-CBB-CGB-O2B
82	m1	202	PEB	CAB-CBB-CGB-O1B
82	Q4	201	PEB	CAB-CBB-CGB-O2B
82	S4	202	PEB	CAC-CBC-CGC-O2C
82	T4	203	PEB	CAC-CBC-CGC-O1C
82	U4	202	PEB	CAB-CBB-CGB-O1B
82	Z4	202	PEB	CAB-CBB-CGB-O2B
82	C7	202	PEB	CAC-CBC-CGC-O1C
82	H7	202	PEB	CAC-CBC-CGC-O1C
82	L7	201	PEB	CAB-CBB-CGB-O1B
82	X7	201	PEB	CAC-CBC-CGC-O1C
82	eA	301	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	aF	202	PEB	CAC-CBC-CGC-O2C
82	eJ	201	PEB	CAC-CBC-CGC-O1C
82	aK	202	PEB	CAC-CBC-CGC-O2C
82	iK	202	PEB	CAB-CBB-CGB-O1B
82	jM	201	PEB	CAC-CBC-CGC-O1C
82	jO	201	PEB	CAB-CBB-CGB-O2B
82	dO	202	PEB	CAC-CBC-CGC-O1C
82	gO	201	PEB	CAC-CBC-CGC-O1C
87	FN	203	CLA	CAA-CBA-CGA-O1A
87	72	606	CLA	CAA-CBA-CGA-O1A
87	F2	201	CLA	CAA-CBA-CGA-O1A
87	1N	611	CLA	CAA-CBA-CGA-O1A
96	fL	102	HEM	CAA-CBA-CGA-O1A
82	FI	201	PEB	C2B-C3B-CAB-CBB
82	U9	202	PEB	C2B-C3B-CAB-CBB
82	aE	202	PEB	C2B-C3B-CAB-CBB
87	AN	831	CLA	O1A-CGA-O2A-C1
95	BN	844	DGD	O6D-C5D-C6D-O5D
95	B2	844	DGD	O6D-C5D-C6D-O5D
95	b6	622	DGD	O6D-C5D-C6D-O5D
92	bL	609	LMG	C14-C15-C16-C17
84	H1	1001	CYC	C4B-C3B-CAB-CBB
82	mJ	201	PEB	C2C-C1C-CHB-C4B
87	A2	814	CLA	CAA-CBA-CGA-O2A
87	C6	519	CLA	CAA-CBA-CGA-O2A
87	cL	514	CLA	CAA-CBA-CGA-O2A
92	j6	102	LMG	O8-C28-C29-C30
95	cL	519	DGD	O1G-C1A-C2A-C3A
82	KD	202	PEB	NC-C1C-CHB-C4B
82	MD	202	PEB	NC-C1C-CHB-C4B
82	MF	202	PEB	NC-C1C-CHB-C4B
82	MK	202	PEB	NC-C1C-CHB-C4B
82	KQ	202	PEB	NC-C1C-CHB-C4B
83	xF	301	PUB	NB-C4B-CHB-C1C
83	xK	301	PUB	NB-C4B-CHB-C1C
87	d6	403	CLA	CAA-CBA-CGA-O1A
82	DA	201	PEB	CAC-CBC-CGC-O1C
82	KA	202	PEB	CAB-CBB-CGB-O1B
82	LA	201	PEB	CAB-CBB-CGB-O2B
82	VA	203	PEB	CAB-CBB-CGB-O2B
82	BB	203	PEB	CAB-CBB-CGB-O1B
82	KB	303	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	ZB	202	PEB	CAC-CBC-CGC-O1C
82	FD	203	PEB	CAC-CBC-CGC-O2C
82	HD	201	PEB	CAC-CBC-CGC-O1C
82	KD	202	PEB	CAB-CBB-CGB-O1B
82	DE	1002	PEB	CAB-CBB-CGB-O1B
82	DF	201	PEB	CAC-CBC-CGC-O1C
82	DF	201	PEB	CAC-CBC-CGC-O2C
82	GF	201	PEB	CAB-CBB-CGB-O1B
82	GF	201	PEB	CAB-CBB-CGB-O2B
82	MF	203	PEB	CAB-CBB-CGB-O1B
82	PF	202	PEB	CAC-CBC-CGC-O2C
82	ZF	201	PEB	CAC-CBC-CGC-O2C
82	DG	1002	PEB	CAB-CBB-CGB-O1B
82	AH	301	PEB	CAC-CBC-CGC-O1C
82	PH	201	PEB	CAB-CBB-CGB-O1B
82	SH	203	PEB	CAB-CBB-CGB-O1B
82	SH	203	PEB	CAB-CBB-CGB-O2B
82	YH	201	PEB	CAC-CBC-CGC-O1C
82	BI	202	PEB	CAB-CBB-CGB-O1B
82	OI	201	PEB	CAB-CBB-CGB-O1B
82	OI	202	PEB	CAB-CBB-CGB-O2B
82	SI	201	PEB	CAB-CBB-CGB-O1B
82	YI	201	PEB	CAB-CBB-CGB-O2B
82	CJ	203	PEB	CAB-CBB-CGB-O2B
82	KJ	203	PEB	CAC-CBC-CGC-O1C
82	KJ	203	PEB	CAC-CBC-CGC-O2C
82	NJ	201	PEB	CAC-CBC-CGC-O2C
82	OJ	202	PEB	CAC-CBC-CGC-O1C
82	TJ	202	PEB	CAC-CBC-CGC-O1C
82	UJ	201	PEB	CAC-CBC-CGC-O1C
82	UJ	202	PEB	CAC-CBC-CGC-O1C
82	DK	201	PEB	CAC-CBC-CGC-O1C
82	DK	201	PEB	CAC-CBC-CGC-O2C
82	GK	201	PEB	CAB-CBB-CGB-O1B
82	JK	202	PEB	CAC-CBC-CGC-O2C
82	PK	202	PEB	CAC-CBC-CGC-O2C
82	RK	201	PEB	CAB-CBB-CGB-O1B
82	ZK	201	PEB	CAC-CBC-CGC-O2C
82	SM	203	PEB	CAB-CBB-CGB-O1B
82	TM	201	PEB	CAC-CBC-CGC-O1C
82	QO	201	PEB	CAB-CBB-CGB-O2B
82	QO	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	UO	202	PEB	CAB-CBB-CGB-O1B
82	UO	202	PEB	CAB-CBB-CGB-O2B
82	ZO	202	PEB	CAB-CBB-CGB-O1B
82	FQ	201	PEB	CAC-CBC-CGC-O1C
82	XQ	201	PEB	CAB-CBB-CGB-O2B
82	A1	301	PEB	CAC-CBC-CGC-O1C
82	V1	202	PEB	CAB-CBB-CGB-O1B
82	V1	202	PEB	CAB-CBB-CGB-O2B
82	m1	202	PEB	CAB-CBB-CGB-O2B
82	Z4	202	PEB	CAB-CBB-CGB-O1B
82	i4	201	PEB	CAC-CBC-CGC-O1C
82	j4	201	PEB	CAB-CBB-CGB-O2B
82	d4	202	PEB	CAC-CBC-CGC-O1C
82	d4	202	PEB	CAC-CBC-CGC-O2C
82	g4	201	PEB	CAC-CBC-CGC-O1C
82	O5	201	PEB	CAC-CBC-CGC-O2C
82	D7	201	PEB	CAC-CBC-CGC-O1C
82	K7	202	PEB	CAB-CBB-CGB-O1B
82	T7	202	PEB	CAB-CBB-CGB-O2B
82	V7	203	PEB	CAB-CBB-CGB-O2B
82	q8	203	PEB	CAB-CBB-CGB-O1B
82	t8	201	PEB	CAC-CBC-CGC-O2C
82	qC	203	PEB	CAB-CBB-CGB-O1B
82	tC	201	PEB	CAC-CBC-CGC-O2C
82	aE	202	PEB	CAC-CBC-CGC-O1C
82	bE	201	PEB	CAC-CBC-CGC-O2C
82	bE	202	PEB	CAC-CBC-CGC-O1C
82	aF	202	PEB	CAC-CBC-CGC-O1C
82	iF	202	PEB	CAB-CBB-CGB-O1B
82	jF	202	PEB	CAC-CBC-CGC-O2C
82	aG	202	PEB	CAC-CBC-CGC-O1C
82	fH	202	PEB	CAB-CBB-CGB-O1B
82	mH	202	PEB	CAB-CBB-CGB-O1B
82	mH	202	PEB	CAB-CBB-CGB-O2B
82	cJ	201	PEB	CAC-CBC-CGC-O2C
82	kJ	201	PEB	CAC-CBC-CGC-O1C
82	aK	202	PEB	CAC-CBC-CGC-O1C
82	cK	202	PEB	CAB-CBB-CGB-O2B
82	iK	202	PEB	CAB-CBB-CGB-O2B
82	jK	202	PEB	CAC-CBC-CGC-O2C
82	eM	201	PEB	CAC-CBC-CGC-O1C
82	iO	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	iO	203	PEB	CAB-CBB-CGB-O1B
82	dO	202	PEB	CAC-CBC-CGC-O2C
82	Z9	304	PEB	CAC-CBC-CGC-O1C
82	M9	305	PEB	CAC-CBC-CGC-O1C
83	AM	304	PUB	CAB-CBB-CGB-O1B
84	HE	1001	CYC	CAD-CBD-CGD-O2D
84	HH	1001	CYC	CAA-CBA-CGA-O1A
84	LH	1002	CYC	CAA-CBA-CGA-O1A
84	L1	1001	CYC	CAA-CBA-CGA-O1A
84	D1	1003	CYC	CAD-CBD-CGD-O1D
84	H1	1001	CYC	CAA-CBA-CGA-O1A
87	42	607	CLA	CAA-CBA-CGA-O1A
87	52	603	CLA	CAA-CBA-CGA-O1A
87	82	308	CLA	CAA-CBA-CGA-O1A
87	5N	603	CLA	CAA-CBA-CGA-O1A
87	7N	606	CLA	CAA-CBA-CGA-O1A
87	8N	308	CLA	CAA-CBA-CGA-O1A
96	fL	102	HEM	CAA-CBA-CGA-O2A
87	2N	303	CLA	C15-C16-C17-C18
87	AN	811	CLA	O2A-C1-C2-C3
87	BN	806	CLA	O2A-C1-C2-C3
87	FN	205	CLA	O2A-C1-C2-C3
87	A2	811	CLA	O2A-C1-C2-C3
87	B2	805	CLA	O2A-C1-C2-C3
87	F2	205	CLA	O2A-C1-C2-C3
87	B6	612	CLA	O2A-C1-C2-C3
87	C6	516	CLA	O2A-C1-C2-C3
92	x6	601	LMG	C36-C37-C38-C39
92	bL	610	LMG	C31-C32-C33-C34
87	A2	801	CLA	C2A-CAA-CBA-CGA
87	bL	606	CLA	C2A-CAA-CBA-CGA
87	22	602	CLA	C15-C16-C17-C18
88	AL	406	LHG	C9-C10-C11-C12
87	AN	829	CLA	CAA-CBA-CGA-O2A
87	72	607	CLA	CAA-CBA-CGA-O2A
87	A2	829	CLA	CAA-CBA-CGA-O2A
87	B2	812	CLA	CAA-CBA-CGA-O2A
87	B6	612	CLA	CAA-CBA-CGA-O2A
87	b6	611	CLA	CAA-CBA-CGA-O2A
87	7N	607	CLA	CAA-CBA-CGA-O2A
92	B6	622	LMG	O7-C10-C11-C12
92	bL	609	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
82	KA	202	PEB	CAB-CBB-CGB-O2B
82	MA	202	PEB	CAB-CBB-CGB-O1B
82	TA	202	PEB	CAB-CBB-CGB-O2B
82	VA	203	PEB	CAB-CBB-CGB-O1B
82	XB	202	PEB	CAC-CBC-CGC-O1C
82	ZB	202	PEB	CAC-CBC-CGC-O2C
82	FD	201	PEB	CAC-CBC-CGC-O2C
82	HD	201	PEB	CAC-CBC-CGC-O2C
82	ID	202	PEB	CAC-CBC-CGC-O1C
82	RD	203	PEB	CAB-CBB-CGB-O2B
82	UD	201	PEB	CAB-CBB-CGB-O1B
82	XD	201	PEB	CAB-CBB-CGB-O1B
82	VE	201	PEB	CAC-CBC-CGC-O1C
82	IF	201	PEB	CAB-CBB-CGB-O1B
82	IF	201	PEB	CAB-CBB-CGB-O2B
82	RF	201	PEB	CAB-CBB-CGB-O1B
82	WF	202	PEB	CAC-CBC-CGC-O1C
82	SG	202	PEB	CAC-CBC-CGC-O1C
82	VG	201	PEB	CAC-CBC-CGC-O1C
82	YG	201	PEB	CAB-CBB-CGB-O2B
82	TH	202	PEB	CAB-CBB-CGB-O2B
82	YH	202	PEB	CAC-CBC-CGC-O1C
82	AI	203	PEB	CAB-CBB-CGB-O1B
82	FI	201	PEB	CAB-CBB-CGB-O2B
82	II	203	PEB	CAB-CBB-CGB-O1B
82	KI	201	PEB	CAB-CBB-CGB-O1B
82	MI	401	PEB	CAC-CBC-CGC-O1C
82	OI	202	PEB	CAB-CBB-CGB-O1B
82	WI	202	PEB	CAB-CBB-CGB-O1B
82	YI	201	PEB	CAB-CBB-CGB-O1B
82	OJ	202	PEB	CAC-CBC-CGC-O2C
82	UJ	201	PEB	CAB-CBB-CGB-O1B
82	YJ	203	PEB	CAC-CBC-CGC-O1C
82	FK	202	PEB	CAB-CBB-CGB-O2B
82	GK	201	PEB	CAB-CBB-CGB-O2B
82	HK	201	PEB	CAC-CBC-CGC-O1C
82	MK	203	PEB	CAB-CBB-CGB-O1B
82	VK	201	PEB	CAB-CBB-CGB-O1B
82	WK	202	PEB	CAC-CBC-CGC-O1C
82	JM	201	PEB	CAC-CBC-CGC-O1C
82	NO	1002	PEB	CAB-CBB-CGB-O1B
82	QO	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	YO	202	PEB	CAC-CBC-CGC-O2C
82	FQ	201	PEB	CAC-CBC-CGC-O2C
82	HQ	201	PEB	CAC-CBC-CGC-O1C
82	HQ	201	PEB	CAC-CBC-CGC-O2C
82	IQ	202	PEB	CAC-CBC-CGC-O1C
82	MQ	201	PEB	CAB-CBB-CGB-O1B
82	RQ	203	PEB	CAB-CBB-CGB-O2B
82	UQ	201	PEB	CAB-CBB-CGB-O1B
82	XQ	201	PEB	CAB-CBB-CGB-O1B
82	O1	203	PEB	CAB-CBB-CGB-O1B
82	P1	201	PEB	CAB-CBB-CGB-O1B
82	Q1	201	PEB	CAC-CBC-CGC-O2C
82	T1	202	PEB	CAB-CBB-CGB-O2B
82	f1	201	PEB	CAB-CBB-CGB-O1B
82	f1	202	PEB	CAB-CBB-CGB-O1B
82	i1	202	PEB	CAB-CBB-CGB-O1B
82	i1	202	PEB	CAB-CBB-CGB-O2B
82	N4	1002	PEB	CAB-CBB-CGB-O1B
82	P4	201	PEB	CAB-CBB-CGB-O1B
82	Q4	201	PEB	CAB-CBB-CGB-O1B
82	Q4	202	PEB	CAC-CBC-CGC-O2C
82	S4	202	PEB	CAC-CBC-CGC-O1C
82	U4	202	PEB	CAB-CBB-CGB-O2B
82	Y4	202	PEB	CAC-CBC-CGC-O2C
82	i4	203	PEB	CAB-CBB-CGB-O1B
82	F5	201	PEB	CAC-CBC-CGC-O1C
82	K7	202	PEB	CAB-CBB-CGB-O2B
82	N7	202	PEB	CAC-CBC-CGC-O1C
82	V7	203	PEB	CAB-CBB-CGB-O1B
82	18	201	PEB	CAC-CBC-CGC-O1C
82	18	201	PEB	CAC-CBC-CGC-O2C
82	F9	202	PEB	CAC-CBC-CGC-O1C
82	S9	203	PEB	CAC-CBC-CGC-O1C
82	1C	201	PEB	CAC-CBC-CGC-O1C
82	1C	201	PEB	CAC-CBC-CGC-O2C
82	aE	202	PEB	CAC-CBC-CGC-O2C
82	bE	202	PEB	CAC-CBC-CGC-O2C
82	iF	201	PEB	CAC-CBC-CGC-O1C
82	iF	202	PEB	CAB-CBB-CGB-O2B
82	jF	202	PEB	CAC-CBC-CGC-O1C
82	oF	202	PEB	CAB-CBB-CGB-O1B
82	aG	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	bG	201	PEB	CAC-CBC-CGC-O2C
82	fH	202	PEB	CAB-CBB-CGB-O2B
82	iH	202	PEB	CAB-CBB-CGB-O1B
82	iH	202	PEB	CAB-CBB-CGB-O2B
82	hJ	203	PEB	CAB-CBB-CGB-O1B
82	cK	202	PEB	CAB-CBB-CGB-O1B
82	iK	201	PEB	CAC-CBC-CGC-O1C
82	lK	201	PEB	CAB-CBB-CGB-O1B
82	oK	202	PEB	CAB-CBB-CGB-O1B
82	gM	201	PEB	CAC-CBC-CGC-O2C
82	hM	202	PEB	CAC-CBC-CGC-O2C
83	AO	303	PUB	CAC-CBC-CGC-O1C
83	A4	303	PUB	CAC-CBC-CGC-O1C
84	DH	1003	CYC	CAD-CBD-CGD-O1D
84	63	901	CYC	CAA-CBA-CGA-O1A
87	RN	204	CLA	CAA-CBA-CGA-O1A
87	72	603	CLA	CAA-CBA-CGA-O1A
87	82	308	CLA	CAA-CBA-CGA-O2A
87	R2	204	CLA	CAA-CBA-CGA-O1A
87	4N	607	CLA	CAA-CBA-CGA-O1A
87	6N	612	CLA	CAA-CBA-CGA-O1A
87	7N	603	CLA	CAA-CBA-CGA-O1A
87	8N	308	CLA	CAA-CBA-CGA-O2A
92	D6	409	LMG	C30-C31-C32-C33
88	B6	617	LHG	O2-C2-C3-O3
88	DL	407	LHG	C11-C12-C13-C14
82	j1	202	PEB	C3B-CAB-CBB-CGB
84	HE	1001	CYC	C2A-CAA-CBA-CGA
87	AL	404	CLA	CHA-CBD-CGD-O1D
87	BL	603	CLA	CHA-CBD-CGD-O1D
87	BL	622	CLA	CHA-CBD-CGD-O1D
87	BL	622	CLA	CHA-CBD-CGD-O2D
87	CL	505	CLA	CHA-CBD-CGD-O1D
87	CL	505	CLA	CHA-CBD-CGD-O2D
87	CL	508	CLA	CHA-CBD-CGD-O2D
87	CL	511	CLA	CHA-CBD-CGD-O2D
87	AN	801	CLA	CHA-CBD-CGD-O1D
87	AN	801	CLA	CHA-CBD-CGD-O2D
87	AN	810	CLA	CHA-CBD-CGD-O1D
87	AN	810	CLA	CHA-CBD-CGD-O2D
87	AN	816	CLA	CHA-CBD-CGD-O1D
87	AN	816	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	AN	823	CLA	CHA-CBD-CGD-O1D
87	AN	823	CLA	CHA-CBD-CGD-O2D
87	AN	831	CLA	CHA-CBD-CGD-O2D
87	AN	839	CLA	CHA-CBD-CGD-O1D
87	AN	839	CLA	CHA-CBD-CGD-O2D
87	BN	802	CLA	CHA-CBD-CGD-O2D
87	BN	808	CLA	CHA-CBD-CGD-O1D
87	BN	808	CLA	CHA-CBD-CGD-O2D
87	BN	810	CLA	CHA-CBD-CGD-O1D
87	BN	810	CLA	CHA-CBD-CGD-O2D
87	BN	813	CLA	CHA-CBD-CGD-O2D
87	BN	815	CLA	CHA-CBD-CGD-O1D
87	BN	815	CLA	CHA-CBD-CGD-O2D
87	BN	828	CLA	CHA-CBD-CGD-O1D
87	BN	828	CLA	CHA-CBD-CGD-O2D
87	BN	836	CLA	CHA-CBD-CGD-O2D
87	FN	201	CLA	CHA-CBD-CGD-O2D
87	IN	103	CLA	CHA-CBD-CGD-O1D
87	IN	103	CLA	CHA-CBD-CGD-O2D
87	KN	103	CLA	CHA-CBD-CGD-O2D
87	KN	105	CLA	CHA-CBD-CGD-O1D
87	ON	201	CLA	CHA-CBD-CGD-O2D
87	22	601	CLA	CHA-CBD-CGD-O2D
87	22	609	CLA	CHA-CBD-CGD-O1D
87	22	609	CLA	CHA-CBD-CGD-O2D
87	22	610	CLA	CHA-CBD-CGD-O2D
87	32	305	CLA	CHA-CBD-CGD-O1D
87	32	305	CLA	CHA-CBD-CGD-O2D
87	32	306	CLA	CHA-CBD-CGD-O1D
87	32	310	CLA	CHA-CBD-CGD-O2D
87	32	311	CLA	CHA-CBD-CGD-O1D
87	32	311	CLA	CHA-CBD-CGD-O2D
87	32	313	CLA	CHA-CBD-CGD-O1D
87	32	313	CLA	CHA-CBD-CGD-O2D
87	42	602	CLA	CHA-CBD-CGD-O2D
87	42	610	CLA	CHA-CBD-CGD-O1D
87	42	610	CLA	CHA-CBD-CGD-O2D
87	52	602	CLA	CHA-CBD-CGD-O1D
87	52	604	CLA	CHA-CBD-CGD-O2D
87	52	607	CLA	CHA-CBD-CGD-O2D
87	52	609	CLA	CHA-CBD-CGD-O2D
87	62	304	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	62	304	CLA	CHA-CBD-CGD-O2D
87	62	312	CLA	CHA-CBD-CGD-O2D
87	72	602	CLA	CHA-CBD-CGD-O2D
87	72	604	CLA	CHA-CBD-CGD-O2D
87	82	302	CLA	CHA-CBD-CGD-O1D
87	82	302	CLA	CHA-CBD-CGD-O2D
87	82	308	CLA	CHA-CBD-CGD-O1D
87	82	308	CLA	CHA-CBD-CGD-O2D
87	A2	802	CLA	CHA-CBD-CGD-O1D
87	A2	802	CLA	CHA-CBD-CGD-O2D
87	A2	810	CLA	CHA-CBD-CGD-O1D
87	A2	810	CLA	CHA-CBD-CGD-O2D
87	A2	816	CLA	CHA-CBD-CGD-O1D
87	A2	816	CLA	CHA-CBD-CGD-O2D
87	A2	823	CLA	CHA-CBD-CGD-O1D
87	A2	823	CLA	CHA-CBD-CGD-O2D
87	A2	839	CLA	CHA-CBD-CGD-O1D
87	A2	839	CLA	CHA-CBD-CGD-O2D
87	B2	801	CLA	CHA-CBD-CGD-O2D
87	B2	807	CLA	CHA-CBD-CGD-O1D
87	B2	807	CLA	CHA-CBD-CGD-O2D
87	B2	809	CLA	CHA-CBD-CGD-O1D
87	B2	809	CLA	CHA-CBD-CGD-O2D
87	B2	812	CLA	CHA-CBD-CGD-O2D
87	B2	814	CLA	CHA-CBD-CGD-O1D
87	B2	814	CLA	CHA-CBD-CGD-O2D
87	B2	828	CLA	CHA-CBD-CGD-O1D
87	B2	828	CLA	CHA-CBD-CGD-O2D
87	B2	836	CLA	CHA-CBD-CGD-O2D
87	F2	202	CLA	CHA-CBD-CGD-O2D
87	I2	103	CLA	CHA-CBD-CGD-O1D
87	I2	103	CLA	CHA-CBD-CGD-O2D
87	K2	104	CLA	CHA-CBD-CGD-O2D
87	K2	106	CLA	CHA-CBD-CGD-O1D
87	O2	201	CLA	CHA-CBD-CGD-O2D
87	B6	611	CLA	CHA-CBD-CGD-O1D
87	C6	518	CLA	CHA-CBD-CGD-O1D
87	C6	518	CLA	CHA-CBD-CGD-O2D
87	H6	103	CLA	CHA-CBD-CGD-O2D
87	b6	604	CLA	CHA-CBD-CGD-O1D
87	b6	604	CLA	CHA-CBD-CGD-O2D
87	b6	607	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
87	b6	617	CLA	CHA-CBD-CGD-O1D
87	b6	617	CLA	CHA-CBD-CGD-O2D
87	c6	607	CLA	CHA-CBD-CGD-O2D
87	c6	609	CLA	CHA-CBD-CGD-O2D
87	c6	610	CLA	CHA-CBD-CGD-O2D
87	bL	618	CLA	CHA-CBD-CGD-O2D
87	cL	507	CLA	CHA-CBD-CGD-O1D
87	cL	507	CLA	CHA-CBD-CGD-O2D
87	cL	513	CLA	CHA-CBD-CGD-O1D
87	nL	101	CLA	CHA-CBD-CGD-O1D
87	nL	101	CLA	CHA-CBD-CGD-O2D
87	2N	302	CLA	CHA-CBD-CGD-O2D
87	2N	309	CLA	CHA-CBD-CGD-O1D
87	2N	309	CLA	CHA-CBD-CGD-O2D
87	2N	310	CLA	CHA-CBD-CGD-O2D
87	3N	306	CLA	CHA-CBD-CGD-O1D
87	3N	306	CLA	CHA-CBD-CGD-O2D
87	3N	307	CLA	CHA-CBD-CGD-O1D
87	3N	310	CLA	CHA-CBD-CGD-O2D
87	3N	311	CLA	CHA-CBD-CGD-O1D
87	3N	311	CLA	CHA-CBD-CGD-O2D
87	3N	313	CLA	CHA-CBD-CGD-O1D
87	3N	313	CLA	CHA-CBD-CGD-O2D
87	4N	602	CLA	CHA-CBD-CGD-O2D
87	4N	610	CLA	CHA-CBD-CGD-O1D
87	4N	610	CLA	CHA-CBD-CGD-O2D
87	5N	602	CLA	CHA-CBD-CGD-O1D
87	5N	604	CLA	CHA-CBD-CGD-O2D
87	5N	607	CLA	CHA-CBD-CGD-O2D
87	5N	609	CLA	CHA-CBD-CGD-O2D
87	6N	603	CLA	CHA-CBD-CGD-O1D
87	6N	603	CLA	CHA-CBD-CGD-O2D
87	6N	611	CLA	CHA-CBD-CGD-O2D
87	7N	602	CLA	CHA-CBD-CGD-O2D
87	7N	604	CLA	CHA-CBD-CGD-O2D
87	8N	303	CLA	CHA-CBD-CGD-O1D
87	8N	303	CLA	CHA-CBD-CGD-O2D
87	8N	308	CLA	CHA-CBD-CGD-O1D
87	8N	308	CLA	CHA-CBD-CGD-O2D
87	C6	513	CLA	C10-C11-C12-C13
82	TA	202	PEB	CAB-CBB-CGB-O1B
82	VA	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	UB	302	PEB	CAC-CBC-CGC-O2C
82	XB	202	PEB	CAC-CBC-CGC-O2C
82	YB	201	PEB	CAC-CBC-CGC-O1C
82	FD	201	PEB	CAC-CBC-CGC-O1C
82	RD	203	PEB	CAB-CBB-CGB-O1B
82	FF	202	PEB	CAB-CBB-CGB-O2B
82	NF	202	PEB	CAB-CBB-CGB-O2B
82	XF	201	PEB	CAB-CBB-CGB-O1B
82	OH	203	PEB	CAB-CBB-CGB-O1B
82	QH	201	PEB	CAC-CBC-CGC-O2C
82	NI	203	PEB	CAB-CBB-CGB-O2B
82	GJ	203	PEB	CAB-CBB-CGB-O1B
82	JK	202	PEB	CAC-CBC-CGC-O1C
82	NK	202	PEB	CAB-CBB-CGB-O2B
82	PK	201	PEB	CAC-CBC-CGC-O1C
82	XK	201	PEB	CAB-CBB-CGB-O1B
82	NM	201	PEB	CAC-CBC-CGC-O1C
82	QO	202	PEB	CAC-CBC-CGC-O1C
82	SO	202	PEB	CAC-CBC-CGC-O1C
82	XP	202	PEB	CAC-CBC-CGC-O1C
82	RQ	203	PEB	CAB-CBB-CGB-O1B
82	Q4	202	PEB	CAC-CBC-CGC-O1C
82	m4	202	PEB	CAB-CBB-CGB-O2B
82	A5	201	PEB	CAC-CBC-CGC-O1C
82	C5	201	PEB	CAC-CBC-CGC-O1C
82	R5	201	PEB	CAC-CBC-CGC-O1C
82	L7	201	PEB	CAB-CBB-CGB-O2B
82	M7	202	PEB	CAB-CBB-CGB-O1B
82	T7	202	PEB	CAB-CBB-CGB-O1B
82	u8	201	PEB	CAC-CBC-CGC-O1C
82	uC	201	PEB	CAC-CBC-CGC-O1C
82	hF	201	PEB	CAB-CBB-CGB-O2B
82	lF	201	PEB	CAB-CBB-CGB-O1B
82	oF	202	PEB	CAB-CBB-CGB-O2B
82	fH	201	PEB	CAB-CBB-CGB-O1B
82	oK	202	PEB	CAB-CBB-CGB-O2B
84	LO	1001	CYC	CAA-CBA-CGA-O1A
84	L4	1001	CYC	CAA-CBA-CGA-O1A
87	12	603	CLA	CAA-CBA-CGA-O1A
87	22	603	CLA	CAA-CBA-CGA-O1A
87	22	606	CLA	CAA-CBA-CGA-O1A
87	52	611	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	62	313	CLA	CAA-CBA-CGA-O1A
87	O2	203	CLA	CAA-CBA-CGA-O2A
87	1N	603	CLA	CAA-CBA-CGA-O1A
87	2N	304	CLA	CAA-CBA-CGA-O1A
87	2N	306	CLA	CAA-CBA-CGA-O1A
87	5N	611	CLA	CAA-CBA-CGA-O1A
87	6N	607	CLA	CAA-CBA-CGA-O1A
87	BL	601	CLA	CAA-CBA-CGA-O2A
92	XL	601	LMG	O8-C28-C29-C30
92	bL	611	LMG	O8-C28-C29-C30
87	A2	835	CLA	C2-C3-C5-C6
87	c6	614	CLA	C2C-C3C-CAC-CBC
95	L6	102	DGD	C9A-CAA-CBA-CCA
84	LH	1002	CYC	C2B-C3B-CAB-CBB
84	L1	1001	CYC	C2B-C3B-CAB-CBB
92	bL	609	LMG	C17-C18-C19-C20
88	ML	102	LHG	O6-C4-C5-C6
88	d6	402	LHG	O6-C4-C5-C6
82	DA	201	PEB	CAC-CBC-CGC-O2C
82	RA	202	PEB	CAB-CBB-CGB-O2B
82	ED	201	PEB	CAB-CBB-CGB-O1B
82	UE	202	PEB	CAB-CBB-CGB-O1B
82	YE	201	PEB	CAB-CBB-CGB-O1B
82	BF	202	PEB	CAB-CBB-CGB-O2B
82	SG	203	PEB	CAC-CBC-CGC-O1C
82	UG	202	PEB	CAB-CBB-CGB-O1B
82	HH	1002	PEB	CAB-CBB-CGB-O1B
82	TH	202	PEB	CAB-CBB-CGB-O1B
82	RI	203	PEB	CAB-CBB-CGB-O2B
82	TI	201	PEB	CAB-CBB-CGB-O1B
82	CJ	203	PEB	CAB-CBB-CGB-O1B
82	KJ	203	PEB	CAB-CBB-CGB-O1B
82	LJ	202	PEB	CAC-CBC-CGC-O2C
82	NJ	201	PEB	CAC-CBC-CGC-O1C
82	TJ	202	PEB	CAC-CBC-CGC-O2C
82	BK	202	PEB	CAB-CBB-CGB-O2B
82	IK	201	PEB	CAB-CBB-CGB-O1B
82	TO	201	PEB	CAC-CBC-CGC-O1C
82	TO	203	PEB	CAC-CBC-CGC-O2C
82	W1	202	PEB	CAB-CBB-CGB-O1B
82	E5	201	PEB	CAC-CBC-CGC-O1C
82	G5	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	I5	201	PEB	CAC-CBC-CGC-O1C
82	K5	201	PEB	CAC-CBC-CGC-O1C
82	N5	201	PEB	CAC-CBC-CGC-O1C
82	P5	201	PEB	CAC-CBC-CGC-O1C
82	T5	201	PEB	CAC-CBC-CGC-O1C
82	V5	201	PEB	CAC-CBC-CGC-O1C
82	X5	201	PEB	CAC-CBC-CGC-O1C
82	D7	201	PEB	CAC-CBC-CGC-O2C
82	R7	202	PEB	CAB-CBB-CGB-O2B
82	V7	202	PEB	CAC-CBC-CGC-O1C
82	gB	202	PEB	CAB-CBB-CGB-O2B
82	hE	203	PEB	CAB-CBB-CGB-O1B
82	aF	203	PEB	CAC-CBC-CGC-O1C
82	hG	203	PEB	CAB-CBB-CGB-O1B
82	hK	201	PEB	CAB-CBB-CGB-O2B
82	jK	202	PEB	CAC-CBC-CGC-O1C
82	kO	201	PEB	CAC-CBC-CGC-O1C
82	mO	202	PEB	CAB-CBB-CGB-O2B
84	HG	1001	CYC	CAD-CBD-CGD-O2D
84	DO	1001	CYC	CAD-CBD-CGD-O1D
87	ON	203	CLA	CAA-CBA-CGA-O2A
87	62	308	CLA	CAA-CBA-CGA-O1A
87	72	601	CLA	CAA-CBA-CGA-O1A
87	BL	605	CLA	C15-C16-C17-C18
94	DL	401	PL9	C2-C3-C7-C8
87	AN	805	CLA	CAA-CBA-CGA-O2A
87	A2	805	CLA	CAA-CBA-CGA-O2A
87	B6	613	CLA	CAA-CBA-CGA-O2A
87	c6	608	CLA	CAA-CBA-CGA-O2A
88	BL	615	LHG	O7-C5-C6-O8
88	L6	101	LHG	O7-C5-C6-O8
88	l6	101	LHG	O7-C5-C6-O8
92	JL	103	LMG	O7-C8-C9-O8
92	D6	407	LMG	O7-C8-C9-O8
95	B6	620	DGD	O1G-C1G-C2G-O2G
95	C6	521	DGD	O2G-C2G-C3G-O3G
82	LJ	202	PEB	C1C-C2C-CAC-CBC
92	mL	101	LMG	C19-C20-C21-C22
95	B6	620	DGD	C6B-C7B-C8B-C9B
83	AJ	304	PUB	C4A-C3A-CAA-CBA
82	JA	203	PEB	CAC-CBC-CGC-O2C
82	JB	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
82	JB	202	PEB	CAC-CBC-CGC-O2C
82	TB	201	PEB	CAB-CBB-CGB-O2B
82	TB	202	PEB	CAC-CBC-CGC-O2C
82	CD	202	PEB	CAC-CBC-CGC-O2C
82	JD	201	PEB	CAC-CBC-CGC-O1C
82	NE	202	PEB	CAC-CBC-CGC-O2C
82	SE	202	PEB	CAC-CBC-CGC-O1C
82	VE	201	PEB	CAC-CBC-CGC-O2C
82	FF	202	PEB	CAB-CBB-CGB-O1B
82	HF	201	PEB	CAC-CBC-CGC-O1C
82	PF	201	PEB	CAC-CBC-CGC-O1C
82	ZF	201	PEB	CAC-CBC-CGC-O1C
82	NG	201	PEB	CAC-CBC-CGC-O2C
82	YG	201	PEB	CAB-CBB-CGB-O1B
82	PH	201	PEB	CAB-CBB-CGB-O2B
82	WH	202	PEB	CAB-CBB-CGB-O1B
82	FK	202	PEB	CAB-CBB-CGB-O1B
82	BM	301	PEB	CAC-CBC-CGC-O2C
82	CQ	202	PEB	CAC-CBC-CGC-O2C
82	JQ	201	PEB	CAC-CBC-CGC-O1C
82	P1	201	PEB	CAB-CBB-CGB-O2B
82	H1	1002	PEB	CAB-CBB-CGB-O1B
82	Y1	202	PEB	CAC-CBC-CGC-O1C
82	i1	201	PEB	CAB-CBB-CGB-O2B
82	k4	201	PEB	CAC-CBC-CGC-O1C
82	g4	202	PEB	CAC-CBC-CGC-O2C
82	J7	203	PEB	CAC-CBC-CGC-O2C
82	q8	202	PEB	CAC-CBC-CGC-O2C
82	mE	202	PEB	CAC-CBC-CGC-O1C
82	iH	201	PEB	CAB-CBB-CGB-O2B
82	lJ	201	PEB	CAB-CBB-CGB-O2B
84	DH	1003	CYC	CAD-CBD-CGD-O2D
84	IO	1001	CYC	CAD-CBD-CGD-O2D
84	I4	1001	CYC	CAD-CBD-CGD-O2D
84	D4	1001	CYC	CAD-CBD-CGD-O1D
87	7N	601	CLA	CAA-CBA-CGA-O1A
88	AL	407	LHG	O9-C7-O7-C5
82	IA	201	PEB	C2C-C1C-CHB-C4B
82	IA	202	PEB	C2C-C1C-CHB-C4B
82	VM	202	PEB	C2C-C1C-CHB-C4B
82	D5	202	PEB	C2C-C1C-CHB-C4B
82	Y5	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
82	I7	201	PEB	C2C-C1C-CHB-C4B
82	I7	202	PEB	C2C-C1C-CHB-C4B
82	UI	202	PEB	NC-C1C-CHB-C4B
82	CK	203	PEB	NC-C1C-CHB-C4B
88	d6	407	LHG	C10-C11-C12-C13
95	lL	101	DGD	CDA-CEA-CFA-CGA
87	B2	836	CLA	C10-C11-C12-C13
87	C6	515	CLA	O1A-CGA-O2A-C1
95	C6	504	DGD	O1A-C1A-O1G-C1G
87	22	602	CLA	CAA-CBA-CGA-O2A
87	C6	513	CLA	CAA-CBA-CGA-O2A
87	b6	615	CLA	CAA-CBA-CGA-O2A
87	c6	613	CLA	CAA-CBA-CGA-O2A
87	2N	303	CLA	CAA-CBA-CGA-O2A
92	CL	519	LMG	O8-C28-C29-C30
95	c6	618	DGD	CDB-CEB-CFB-CGB
87	AN	802	CLA	C2A-CAA-CBA-CGA
87	AN	838	CLA	C2A-CAA-CBA-CGA
87	A2	838	CLA	C2A-CAA-CBA-CGA
91	a6	613	PHO	C2A-CAA-CBA-CGA
91	dL	403	PHO	C2A-CAA-CBA-CGA
82	NA	202	PEB	CAC-CBC-CGC-O2C
82	TA	202	PEB	CAC-CBC-CGC-O2C
82	WA	202	PEB	CAB-CBB-CGB-O1B
82	GB	201	PEB	CAC-CBC-CGC-O2C
82	ED	202	PEB	CAC-CBC-CGC-O2C
82	JF	202	PEB	CAC-CBC-CGC-O1C
82	NF	202	PEB	CAB-CBB-CGB-O1B
82	VG	201	PEB	CAC-CBC-CGC-O2C
82	VI	203	PEB	CAB-CBB-CGB-O2B
82	BJ	301	PEB	CAB-CBB-CGB-O2B
82	NK	202	PEB	CAB-CBB-CGB-O1B
82	EQ	201	PEB	CAB-CBB-CGB-O1B
82	T1	202	PEB	CAB-CBB-CGB-O1B
82	T4	203	PEB	CAC-CBC-CGC-O2C
82	T7	202	PEB	CAC-CBC-CGC-O2C
82	W7	202	PEB	CAB-CBB-CGB-O1B
82	cB	402	PEB	CAC-CBC-CGC-O2C
82	qC	202	PEB	CAC-CBC-CGC-O2C
82	nF	202	PEB	CAC-CBC-CGC-O1C
82	cJ	201	PEB	CAC-CBC-CGC-O1C
82	aK	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
82	nK	202	PEB	CAC-CBC-CGC-O1C
82	gM	201	PEB	CAC-CBC-CGC-O1C
83	KA	203	PUB	CAB-CBB-CGB-O1B
83	K7	203	PUB	CAB-CBB-CGB-O1B
84	D1	1003	CYC	CAD-CBD-CGD-O2D
87	32	303	CLA	CAA-CBA-CGA-O2A
87	3N	304	CLA	CAA-CBA-CGA-O2A
88	M6	101	LHG	O1-C1-C2-O2
91	A6	407	PHO	CHA-CBD-CGD-O1D
91	A6	407	PHO	CHA-CBD-CGD-O2D
91	a6	613	PHO	CHA-CBD-CGD-O1D
87	BL	606	CLA	C10-C11-C12-C13
87	A2	810	CLA	C5-C6-C7-C8
87	c6	614	CLA	C4C-C3C-CAC-CBC
95	C6	502	DGD	C2A-C1A-O1G-C1G
95	O6	301	DGD	C2A-C1A-O1G-C1G
95	c6	601	DGD	C2A-C1A-O1G-C1G
87	b6	611	CLA	C3-C5-C6-C7
87	b6	615	CLA	C3-C5-C6-C7
87	CL	514	CLA	CAA-CBA-CGA-O2A
87	AN	811	CLA	CAA-CBA-CGA-O2A
92	b6	623	LMG	O8-C28-C29-C30
92	qL	301	LMG	O7-C10-C11-C12
92	yL	101	LMG	O7-C10-C11-C12
95	lL	101	DGD	O1G-C1A-C2A-C3A
88	l6	101	LHG	C19-C20-C21-C22
87	b6	604	CLA	CBD-CGD-O2D-CED
82	TA	203	PEB	CAB-CBB-CGB-O1B
82	HB	202	PEB	CAB-CBB-CGB-O1B
82	MB	202	PEB	CAC-CBC-CGC-O2C
82	ZK	201	PEB	CAC-CBC-CGC-O1C
82	D1	1002	PEB	CAB-CBB-CGB-O2B
82	c4	201	PEB	CAB-CBB-CGB-O1B
82	N7	202	PEB	CAC-CBC-CGC-O2C
82	T7	203	PEB	CAB-CBB-CGB-O1B
82	iF	203	PEB	CAB-CBB-CGB-O1B
82	mG	202	PEB	CAC-CBC-CGC-O1C
82	iK	203	PEB	CAB-CBB-CGB-O1B
82	cO	201	PEB	CAB-CBB-CGB-O1B
82	gO	202	PEB	CAC-CBC-CGC-O2C
82	bP	502	PEB	CAC-CBC-CGC-O1C
84	LG	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	AN	822	CLA	CAA-CBA-CGA-O2A
87	BN	836	CLA	C10-C11-C12-C13
87	CL	508	CLA	C11-C10-C8-C7
87	CL	509	CLA	C6-C7-C8-C10
87	AN	811	CLA	C2-C3-C5-C6
87	AN	835	CLA	C2-C3-C5-C6
87	BN	818	CLA	C6-C7-C8-C10
87	62	303	CLA	C6-C7-C8-C10
87	A2	811	CLA	C2-C3-C5-C6
87	B2	817	CLA	C6-C7-C8-C10
87	C6	513	CLA	C11-C12-C13-C15
87	b6	608	CLA	C6-C7-C8-C10
87	c6	604	CLA	C11-C10-C8-C7
87	d6	406	CLA	C11-C10-C8-C7
87	bL	616	CLA	C11-C12-C13-C15
87	bL	616	CLA	C12-C13-C15-C16
87	bL	621	CLA	C11-C10-C8-C7
87	6N	602	CLA	C6-C7-C8-C10
94	A6	410	PL9	C23-C24-C26-C27
87	AN	825	CLA	C6-C7-C8-C10
87	BN	836	CLA	C16-C17-C18-C20
87	A2	825	CLA	C6-C7-C8-C10
87	B2	836	CLA	C16-C17-C18-C20
82	TH	201	PEB	C2B-C3B-CAB-CBB
82	T1	201	PEB	C2B-C3B-CAB-CBB
82	j4	203	PEB	C2B-C3B-CAB-CBB
82	kO	202	PEB	C2B-C3B-CAB-CBB
88	L6	101	LHG	C19-C20-C21-C22
92	k6	101	LMG	O9-C10-O7-C8
87	82	302	CLA	C13-C15-C16-C17
87	8N	303	CLA	C13-C15-C16-C17
87	A2	811	CLA	CAA-CBA-CGA-O2A
87	B2	826	CLA	CAA-CBA-CGA-O2A
87	bL	604	CLA	CAA-CBA-CGA-O2A
88	iL	101	LHG	O7-C7-C8-C9
92	jL	101	LMG	O8-C28-C29-C30
82	DB	201	PEB	CAC-CBC-CGC-O1C
82	WE	201	PEB	CAC-CBC-CGC-O2C
82	DF	202	PEB	CAC-CBC-CGC-O1C
82	DF	203	PEB	CAB-CBB-CGB-O2B
82	PG	201	PEB	CAB-CBB-CGB-O2B
82	WG	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	YG	201	PEB	CAC-CBC-CGC-O2C
82	DH	1002	PEB	CAB-CBB-CGB-O2B
82	FJ	201	PEB	CAC-CBC-CGC-O1C
82	DK	203	PEB	CAB-CBB-CGB-O2B
82	HO	1002	PEB	CAB-CBB-CGB-O2B
82	EQ	202	PEB	CAC-CBC-CGC-O2C
84	LE	1001	CYC	CAA-CBA-CGA-O1A
87	42	603	CLA	CAA-CBA-CGA-O1A
87	82	301	CLA	CAA-CBA-CGA-O1A
87	A2	822	CLA	CAA-CBA-CGA-O2A
87	4N	603	CLA	CAA-CBA-CGA-O1A
87	8N	302	CLA	CAA-CBA-CGA-O1A
87	CL	508	CLA	C11-C10-C8-C9
87	CL	509	CLA	C6-C7-C8-C9
87	AN	849	CLA	C11-C10-C8-C9
87	BN	809	CLA	C14-C13-C15-C16
87	BN	835	CLA	C14-C13-C15-C16
87	52	602	CLA	C14-C13-C15-C16
87	A2	849	CLA	C11-C10-C8-C9
87	B2	808	CLA	C14-C13-C15-C16
87	A6	402	CLA	C11-C12-C13-C14
87	B6	611	CLA	C6-C7-C8-C9
87	B6	613	CLA	C11-C12-C13-C14
87	b6	608	CLA	C6-C7-C8-C9
87	c6	604	CLA	C11-C10-C8-C9
87	5N	602	CLA	C14-C13-C15-C16
87	cL	516	CLA	CAA-CBA-CGA-O1A
95	aL	603	DGD	O1A-C1A-C2A-C3A
85	Z6	101	BCR	C19-C20-C21-C22
87	b6	618	CLA	C2C-C3C-CAC-CBC
87	c6	605	CLA	C4C-C3C-CAC-CBC
87	AN	821	CLA	C2B-C3B-CAB-CBB
87	A2	821	CLA	C2B-C3B-CAB-CBB
87	C6	513	CLA	C2B-C3B-CAB-CBB
87	d6	403	CLA	C2B-C3B-CAB-CBB
87	cL	510	CLA	C2B-C3B-CAB-CBB
87	KN	105	CLA	O2A-C1-C2-C3
87	K2	106	CLA	O2A-C1-C2-C3
87	BL	602	CLA	O1A-CGA-O2A-C1
82	AA	201	PEB	CAB-CBB-CGB-O2B
82	CB	202	PEB	CAC-CBC-CGC-O2C
82	ID	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
82	PE	201	PEB	CAB-CBB-CGB-O2B
82	YE	201	PEB	CAC-CBC-CGC-O2C
82	SO	201	PEB	CAB-CBB-CGB-O2B
82	H4	1002	PEB	CAB-CBB-CGB-O2B
82	S4	201	PEB	CAB-CBB-CGB-O2B
82	T4	201	PEB	CAC-CBC-CGC-O1C
82	Q5	201	PEB	CAB-CBB-CGB-O2B
82	Q5	203	PEB	CAC-CBC-CGC-O2C
82	A7	201	PEB	CAB-CBB-CGB-O2B
82	iE	202	PEB	CAC-CBC-CGC-O2C
82	lF	203	PEB	CAC-CBC-CGC-O2C
82	lK	203	PEB	CAC-CBC-CGC-O2C
84	CO	1001	CYC	CAD-CBD-CGD-O2D
84	C4	1001	CYC	CAD-CBD-CGD-O2D
92	C6	501	LMG	C10-C11-C12-C13
92	jL	101	LMG	C10-C11-C12-C13
95	aL	603	DGD	C5B-C6B-C7B-C8B
87	BL	602	CLA	CBA-CGA-O2A-C1
87	K6	101	CLA	CBA-CGA-O2A-C1
92	ML	101	LMG	C29-C28-O8-C9
87	AN	851	CLA	CAA-CBA-CGA-O2A
87	A2	851	CLA	CAA-CBA-CGA-O2A
87	B6	609	CLA	CAA-CBA-CGA-O2A
95	O6	301	DGD	O2G-C1B-C2B-C3B
87	FN	205	CLA	CAA-CBA-CGA-O1A
95	O6	301	DGD	O1A-C1A-O1G-C1G
87	1N	602	CLA	C2C-C3C-CAC-CBC
88	aL	607	LHG	C8-C7-O7-C5
82	OP	203	PEB	NC-C4C-CHC-C1D
82	RE	201	PEB	CAB-CBB-CGB-O2B
82	IF	202	PEB	CAB-CBB-CGB-O2B
82	RG	201	PEB	CAB-CBB-CGB-O2B
82	GI	201	PEB	CAB-CBB-CGB-O1B
82	IK	202	PEB	CAB-CBB-CGB-O2B
82	KP	201	PEB	CAC-CBC-CGC-O2C
82	VP	201	PEB	CAB-CBB-CGB-O1B
82	IQ	202	PEB	CAC-CBC-CGC-O2C
82	p8	202	PEB	CAC-CBC-CGC-O2C
82	iG	202	PEB	CAC-CBC-CGC-O2C
84	EH	1001	CYC	CAD-CBD-CGD-O2D
84	NH	1001	CYC	CAD-CBD-CGD-O2D
84	N1	1001	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
84	E1	1001	CYC	CAD-CBD-CGD-O2D
87	AN	806	CLA	C2A-CAA-CBA-CGA
87	A2	806	CLA	C2A-CAA-CBA-CGA
87	d6	401	CLA	C2A-CAA-CBA-CGA
82	OA	202	PEB	NC-C1C-CHB-C4B
82	PD	202	PEB	NC-C1C-CHB-C4B
82	PE	202	PEB	NC-C1C-CHB-C4B
82	CF	203	PEB	NC-C1C-CHB-C4B
82	PG	202	PEB	NC-C1C-CHB-C4B
82	FP	202	PEB	NC-C1C-CHB-C4B
82	MQ	202	PEB	NC-C1C-CHB-C4B
82	O7	202	PEB	NC-C1C-CHB-C4B
82	iF	201	PEB	NC-C1C-CHB-C4B
82	iK	201	PEB	NC-C1C-CHB-C4B
82	wK	301	PEB	NC-C1C-CHB-C4B
87	AN	833	CLA	CAA-CBA-CGA-O1A
87	A2	833	CLA	CAA-CBA-CGA-O1A
87	F2	205	CLA	CAA-CBA-CGA-O1A
87	BN	826	CLA	CAA-CBA-CGA-O2A
87	C6	517	CLA	C8-C10-C11-C12
92	AL	411	LMG	O10-C28-O8-C9
87	B6	611	CLA	CBA-CGA-O2A-C1
82	U5	201	PEB	C4B-C3B-CAB-CBB
82	gB	201	PEB	C4B-C3B-CAB-CBB
82	aE	202	PEB	C4B-C3B-CAB-CBB
92	d6	409	LMG	C40-C41-C42-C43
82	DB	203	PEB	C3B-CAB-CBB-CGB
82	CD	202	PEB	C3B-CAB-CBB-CGB
82	JD	201	PEB	C3B-CAB-CBB-CGB
82	UE	203	PEB	C2C-CAC-CBC-CGC
82	OF	203	PEB	C3B-CAB-CBB-CGB
82	VF	202	PEB	C3B-CAB-CBB-CGB
82	UG	203	PEB	C2C-CAC-CBC-CGC
82	BI	203	PEB	C3B-CAB-CBB-CGB
82	OJ	202	PEB	C2C-CAC-CBC-CGC
82	ZJ	201	PEB	C2C-CAC-CBC-CGC
82	OK	203	PEB	C3B-CAB-CBB-CGB
82	VK	202	PEB	C3B-CAB-CBB-CGB
82	PM	201	PEB	C2C-CAC-CBC-CGC
82	TO	203	PEB	C3B-CAB-CBB-CGB
82	BP	201	PEB	C3B-CAB-CBB-CGB
82	VP	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
82	CQ	202	PEB	C3B-CAB-CBB-CGB
82	JQ	201	PEB	C3B-CAB-CBB-CGB
82	P1	202	PEB	C3B-CAB-CBB-CGB
82	d1	203	PEB	C3B-CAB-CBB-CGB
82	T4	203	PEB	C3B-CAB-CBB-CGB
82	g4	203	PEB	C3B-CAB-CBB-CGB
82	M5	305	PEB	C3B-CAB-CBB-CGB
82	Z5	305	PEB	C3B-CAB-CBB-CGB
82	fF	201	PEB	C3B-CAB-CBB-CGB
82	oF	202	PEB	C2C-CAC-CBC-CGC
82	jH	202	PEB	C3B-CAB-CBB-CGB
82	dH	203	PEB	C3B-CAB-CBB-CGB
82	gJ	202	PEB	C2C-CAC-CBC-CGC
82	fK	201	PEB	C3B-CAB-CBB-CGB
82	oK	202	PEB	C2C-CAC-CBC-CGC
82	aM	203	PEB	C2C-CAC-CBC-CGC
82	gO	203	PEB	C3B-CAB-CBB-CGB
84	DH	1001	CYC	C3D-CAD-CBD-CGD
84	D1	1001	CYC	C3D-CAD-CBD-CGD
82	YI	201	PEB	CAC-CBC-CGC-O2C
82	DK	202	PEB	CAC-CBC-CGC-O1C
82	YO	202	PEB	CAB-CBB-CGB-O2B
82	Y4	202	PEB	CAB-CBB-CGB-O2B
82	j4	203	PEB	CAC-CBC-CGC-O1C
82	e4	202	PEB	CAB-CBB-CGB-O2B
82	pC	202	PEB	CAC-CBC-CGC-O2C
82	qF	202	PEB	CAB-CBB-CGB-O2B
82	uF	201	PEB	CAC-CBC-CGC-O1C
82	tK	203	PEB	CAC-CBC-CGC-O1C
82	eO	202	PEB	CAB-CBB-CGB-O2B
85	HL	103	BCR	C11-C12-C13-C35
92	JL	102	LMG	C28-C29-C30-C31
87	C6	509	CLA	CAA-CBA-CGA-O1A
87	C6	519	CLA	CAA-CBA-CGA-O1A
87	AN	825	CLA	C6-C7-C8-C9
87	AN	829	CLA	C16-C17-C18-C19
87	A2	829	CLA	C16-C17-C18-C19
87	BN	831	CLA	C4-C3-C5-C6
87	B2	831	CLA	C4-C3-C5-C6
87	c6	614	CLA	C4-C3-C5-C6
92	C6	501	LMG	C21-C22-C23-C24
92	yL	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
87	AN	810	CLA	C5-C6-C7-C8
82	WF	201	PEB	CAC-CBC-CGC-O2C
82	WK	201	PEB	CAC-CBC-CGC-O2C
82	YP	503	PEB	CAC-CBC-CGC-O2C
82	a4	203	PEB	CAB-CBB-CGB-O1B
82	eM	202	PEB	CAC-CBC-CGC-O2C
82	kO	202	PEB	CAC-CBC-CGC-O1C
83	AD	302	PUB	CAC-CBC-CGC-O2C
87	52	607	CLA	CAA-CBA-CGA-O1A
87	cL	514	CLA	CAA-CBA-CGA-O1A
87	5N	607	CLA	CAA-CBA-CGA-O1A
95	cL	519	DGD	O1A-C1A-C2A-C3A
85	c6	603	BCR	C11-C12-C13-C14
87	12	602	CLA	C2C-C3C-CAC-CBC
92	bL	609	LMG	C30-C31-C32-C33
82	O9	202	PEB	C3C-C2C-CAC-CBC
82	kE	202	PEB	C1C-C2C-CAC-CBC
82	kG	202	PEB	C1C-C2C-CAC-CBC
82	FA	201	PEB	C2D-C1D-CHC-C4C
82	KA	202	PEB	C2D-C1D-CHC-C4C
82	LA	201	PEB	C2D-C1D-CHC-C4C
82	LA	203	PEB	C2D-C1D-CHC-C4C
82	XA	201	PEB	C2D-C1D-CHC-C4C
82	DB	201	PEB	C2D-C1D-CHC-C4C
82	KB	304	PEB	C2D-C1D-CHC-C4C
82	UB	303	PEB	C2D-C1D-CHC-C4C
82	AD	301	PEB	C2D-C1D-CHC-C4C
82	LD	203	PEB	C2D-C1D-CHC-C4C
82	ND	204	PEB	C2D-C1D-CHC-C4C
82	SD	202	PEB	C2D-C1D-CHC-C4C
82	ZE	203	PEB	C2D-C1D-CHC-C4C
82	MF	202	PEB	C2D-C1D-CHC-C4C
82	QF	203	PEB	C2D-C1D-CHC-C4C
82	UF	202	PEB	C2D-C1D-CHC-C4C
82	YF	202	PEB	C2D-C1D-CHC-C4C
82	ZG	203	PEB	C2D-C1D-CHC-C4C
82	LH	1003	PEB	C2D-C1D-CHC-C4C
82	SH	202	PEB	C2D-C1D-CHC-C4C
82	SH	203	PEB	C2D-C1D-CHC-C4C
82	LI	202	PEB	C2D-C1D-CHC-C4C
82	CJ	202	PEB	C2D-C1D-CHC-C4C
82	IJ	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	MJ	202	PEB	C2D-C1D-CHC-C4C
82	NJ	202	PEB	C2D-C1D-CHC-C4C
82	YJ	202	PEB	C2D-C1D-CHC-C4C
82	MK	202	PEB	C2D-C1D-CHC-C4C
82	QK	203	PEB	C2D-C1D-CHC-C4C
82	UK	202	PEB	C2D-C1D-CHC-C4C
82	YK	202	PEB	C2D-C1D-CHC-C4C
82	AM	302	PEB	C2D-C1D-CHC-C4C
82	BM	301	PEB	C2D-C1D-CHC-C4C
82	DM	202	PEB	C2D-C1D-CHC-C4C
82	KM	201	PEB	C2D-C1D-CHC-C4C
82	ZM	202	PEB	C2D-C1D-CHC-C4C
82	AO	305	PEB	C2D-C1D-CHC-C4C
82	DO	1002	PEB	C2D-C1D-CHC-C4C
82	HO	1002	PEB	C2D-C1D-CHC-C4C
82	TO	203	PEB	C2D-C1D-CHC-C4C
82	MP	201	PEB	C2D-C1D-CHC-C4C
82	AQ	301	PEB	C2D-C1D-CHC-C4C
82	LQ	203	PEB	C2D-C1D-CHC-C4C
82	NQ	204	PEB	C2D-C1D-CHC-C4C
82	SQ	202	PEB	C2D-C1D-CHC-C4C
82	L1	1002	PEB	C2D-C1D-CHC-C4C
82	S1	202	PEB	C2D-C1D-CHC-C4C
82	V1	202	PEB	C2D-C1D-CHC-C4C
82	j1	203	PEB	C2D-C1D-CHC-C4C
82	k1	202	PEB	C2D-C1D-CHC-C4C
82	l1	201	PEB	C2D-C1D-CHC-C4C
82	b1	202	PEB	C2D-C1D-CHC-C4C
82	H4	1002	PEB	C2D-C1D-CHC-C4C
82	A4	305	PEB	C2D-C1D-CHC-C4C
82	D4	1002	PEB	C2D-C1D-CHC-C4C
82	T4	203	PEB	C2D-C1D-CHC-C4C
82	Y4	201	PEB	C2D-C1D-CHC-C4C
82	d4	201	PEB	C2D-C1D-CHC-C4C
82	F5	202	PEB	C2D-C1D-CHC-C4C
82	J5	202	PEB	C2D-C1D-CHC-C4C
82	L5	202	PEB	C2D-C1D-CHC-C4C
82	U5	202	PEB	C2D-C1D-CHC-C4C
82	Y5	202	PEB	C2D-C1D-CHC-C4C
82	F7	201	PEB	C2D-C1D-CHC-C4C
82	K7	202	PEB	C2D-C1D-CHC-C4C
82	L7	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	L7	203	PEB	C2D-C1D-CHC-C4C
82	y8	201	PEB	C2D-C1D-CHC-C4C
82	y8	202	PEB	C2D-C1D-CHC-C4C
82	w8	203	PEB	C2D-C1D-CHC-C4C
82	D9	202	PEB	C2D-C1D-CHC-C4C
82	S9	202	PEB	C2D-C1D-CHC-C4C
82	U9	202	PEB	C2D-C1D-CHC-C4C
82	W9	202	PEB	C2D-C1D-CHC-C4C
82	yC	202	PEB	C2D-C1D-CHC-C4C
82	wC	203	PEB	C2D-C1D-CHC-C4C
82	cE	201	PEB	C2D-C1D-CHC-C4C
82	eE	202	PEB	C2D-C1D-CHC-C4C
82	mE	202	PEB	C2D-C1D-CHC-C4C
82	aF	203	PEB	C2D-C1D-CHC-C4C
82	gF	203	PEB	C2D-C1D-CHC-C4C
82	iF	201	PEB	C2D-C1D-CHC-C4C
82	iF	203	PEB	C2D-C1D-CHC-C4C
82	mF	202	PEB	C2D-C1D-CHC-C4C
82	sF	202	PEB	C2D-C1D-CHC-C4C
82	tF	201	PEB	C2D-C1D-CHC-C4C
82	uF	203	PEB	C2D-C1D-CHC-C4C
82	wF	301	PEB	C2D-C1D-CHC-C4C
82	cG	201	PEB	C2D-C1D-CHC-C4C
82	eG	202	PEB	C2D-C1D-CHC-C4C
82	mG	202	PEB	C2D-C1D-CHC-C4C
82	jH	203	PEB	C2D-C1D-CHC-C4C
82	kH	202	PEB	C2D-C1D-CHC-C4C
82	kH	203	PEB	C2D-C1D-CHC-C4C
82	bH	202	PEB	C2D-C1D-CHC-C4C
82	fJ	201	PEB	C2D-C1D-CHC-C4C
82	iJ	202	PEB	C2D-C1D-CHC-C4C
82	jJ	201	PEB	C2D-C1D-CHC-C4C
82	aK	203	PEB	C2D-C1D-CHC-C4C
82	gK	203	PEB	C2D-C1D-CHC-C4C
82	iK	201	PEB	C2D-C1D-CHC-C4C
82	iK	203	PEB	C2D-C1D-CHC-C4C
82	mK	202	PEB	C2D-C1D-CHC-C4C
82	sK	202	PEB	C2D-C1D-CHC-C4C
82	tK	201	PEB	C2D-C1D-CHC-C4C
82	uK	202	PEB	C2D-C1D-CHC-C4C
82	wK	301	PEB	C2D-C1D-CHC-C4C
82	dO	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
87	BL	602	CLA	C1A-C2A-CAA-CBA
87	AN	822	CLA	C1A-C2A-CAA-CBA
87	AN	828	CLA	C1A-C2A-CAA-CBA
87	BN	835	CLA	C1A-C2A-CAA-CBA
87	62	304	CLA	C1A-C2A-CAA-CBA
87	62	308	CLA	C1A-C2A-CAA-CBA
87	A2	822	CLA	C1A-C2A-CAA-CBA
87	A2	828	CLA	C1A-C2A-CAA-CBA
87	B2	835	CLA	C1A-C2A-CAA-CBA
87	C6	520	CLA	C1A-C2A-CAA-CBA
87	D6	402	CLA	C1A-C2A-CAA-CBA
87	bL	605	CLA	C1A-C2A-CAA-CBA
87	bL	614	CLA	C1A-C2A-CAA-CBA
87	cL	510	CLA	C1A-C2A-CAA-CBA
87	cL	512	CLA	C1A-C2A-CAA-CBA
87	6N	603	CLA	C1A-C2A-CAA-CBA
87	6N	607	CLA	C1A-C2A-CAA-CBA
95	hL	101	DGD	CDA-CEA-CFA-CGA
87	A2	825	CLA	C6-C7-C8-C9
87	BL	605	CLA	CAA-CBA-CGA-O1A
87	C6	517	CLA	CAA-CBA-CGA-O1A
87	bL	616	CLA	CAA-CBA-CGA-O1A
92	CL	519	LMG	O10-C28-C29-C30
92	bL	611	LMG	O10-C28-C29-C30
82	OF	201	PEB	CAC-CBC-CGC-O2C
82	HI	202	PEB	CAB-CBB-CGB-O2B
82	IQ	201	PEB	CAC-CBC-CGC-O1C
82	R7	202	PEB	CAB-CBB-CGB-O1B
82	aO	203	PEB	CAB-CBB-CGB-O1B
83	AQ	302	PUB	CAC-CBC-CGC-O2C
84	DO	1001	CYC	CAD-CBD-CGD-O2D
94	dL	406	PL9	C31-C32-C33-C34
95	C6	502	DGD	O1A-C1A-O1G-C1G
87	A2	807	CLA	C2-C1-O2A-CGA
91	aL	610	PHO	CBD-CGD-O2D-CED
92	C6	501	LMG	C36-C37-C38-C39
87	CL	512	CLA	CAA-CBA-CGA-O1A
87	LN	204	CLA	CAA-CBA-CGA-O1A
87	12	607	CLA	CAA-CBA-CGA-O1A
87	32	309	CLA	CAA-CBA-CGA-O1A
87	A2	829	CLA	CAA-CBA-CGA-O1A
87	L2	204	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	b6	608	CLA	CAA-CBA-CGA-O1A
87	3N	309	CLA	CAA-CBA-CGA-O1A
92	B6	622	LMG	O9-C10-C11-C12
92	j6	102	LMG	O10-C28-C29-C30
92	m6	103	LMG	O9-C10-C11-C12
92	jL	101	LMG	O10-C28-C29-C30
92	B6	618	LMG	C15-C16-C17-C18
82	ID	201	PEB	CAC-CBC-CGC-O1C
82	LI	201	PEB	CAC-CBC-CGC-O2C
82	NP	201	PEB	CAC-CBC-CGC-O2C
84	IO	1001	CYC	CAD-CBD-CGD-O1D
84	I4	1001	CYC	CAD-CBD-CGD-O1D
95	C6	521	DGD	C1G-C2G-C3G-O3G
95	cL	502	DGD	C1G-C2G-C3G-O3G
87	BN	805	CLA	CAA-CBA-CGA-O2A
87	B2	804	CLA	CAA-CBA-CGA-O2A
88	A2	843	LHG	C35-C36-C37-C38
88	AN	843	LHG	C35-C36-C37-C38
92	x6	601	LMG	C13-C14-C15-C16
95	AL	414	DGD	C8A-C9A-CAA-CBA
84	HH	1001	CYC	C4B-C3B-CAB-CBB
87	AN	829	CLA	CAA-CBA-CGA-O1A
87	BN	813	CLA	CAA-CBA-CGA-O1A
87	B2	812	CLA	CAA-CBA-CGA-O1A
87	1N	607	CLA	CAA-CBA-CGA-O1A
87	A6	402	CLA	C15-C16-C17-C18
87	d6	406	CLA	C8-C10-C11-C12
82	UA	202	PEB	NC-C1C-CHB-C4B
82	WB	401	PEB	NC-C1C-CHB-C4B
82	DI	202	PEB	NC-C1C-CHB-C4B
82	U7	202	PEB	NC-C1C-CHB-C4B
82	wF	301	PEB	NC-C1C-CHB-C4B
87	a6	609	CLA	C4C-C3C-CAC-CBC
95	J6	101	DGD	CBA-CCA-CDA-CEA
82	RA	202	PEB	CAB-CBB-CGB-O1B
82	NB	201	PEB	CAC-CBC-CGC-O1C
82	QJ	202	PEB	CAB-CBB-CGB-O2B
82	OK	201	PEB	CAC-CBC-CGC-O2C
82	BM	301	PEB	CAB-CBB-CGB-O2B
82	EM	202	PEB	CAB-CBB-CGB-O2B
82	V4	202	PEB	CAB-CBB-CGB-O1B
82	hF	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	qK	202	PEB	CAB-CBB-CGB-O2B
84	CG	1001	CYC	CAD-CBD-CGD-O2D
87	B2	828	CLA	CAA-CBA-CGA-O2A
82	RD	202	PEB	C2C-C1C-CHB-C4B
82	FI	202	PEB	C2C-C1C-CHB-C4B
82	RQ	202	PEB	C2C-C1C-CHB-C4B
87	BL	609	CLA	C10-C11-C12-C13
88	ML	102	LHG	O9-C7-O7-C5
82	aG	202	PEB	C4B-C3B-CAB-CBB
87	BN	802	CLA	CAA-CBA-CGA-O1A
87	72	607	CLA	CAA-CBA-CGA-O1A
87	B2	801	CLA	CAA-CBA-CGA-O1A
87	c6	604	CLA	CAA-CBA-CGA-O1A
92	BL	611	LMG	O9-C10-C11-C12
92	XL	601	LMG	O10-C28-C29-C30
92	m6	101	LMG	O10-C28-C29-C30
87	BN	802	CLA	C2-C3-C5-C6
87	B2	801	CLA	C2-C3-C5-C6
95	c6	601	DGD	O1A-C1A-O1G-C1G
82	LH	1003	PEB	CAB-CBB-CGB-O2B
82	WH	203	PEB	CAB-CBB-CGB-O2B
82	FM	201	PEB	CAC-CBC-CGC-O2C
82	AO	305	PEB	CAC-CBC-CGC-O2C
82	VO	202	PEB	CAB-CBB-CGB-O1B
82	L1	1002	PEB	CAB-CBB-CGB-O2B
82	A4	305	PEB	CAC-CBC-CGC-O2C
82	kG	201	PEB	CAC-CBC-CGC-O2C
82	lJ	201	PEB	CAB-CBB-CGB-O1B
83	AM	303	PUB	CAC-CBC-CGC-O2C
84	FE	1001	CYC	CAD-CBD-CGD-O2D
87	BN	828	CLA	CAA-CBA-CGA-O2A
87	12	606	CLA	CAA-CBA-CGA-O2A
87	1N	606	CLA	CAA-CBA-CGA-O2A
87	6N	606	CLA	CAA-CBA-CGA-O2A
92	B6	618	LMG	C2-C1-O1-C7
87	AN	823	CLA	C13-C15-C16-C17
87	A2	823	CLA	C13-C15-C16-C17
82	FA	201	PEB	ND-C1D-CHC-C4C
82	DB	202	PEB	ND-C1D-CHC-C4C
82	AD	301	PEB	ND-C1D-CHC-C4C
82	DD	201	PEB	ND-C1D-CHC-C4C
82	HD	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	LD	201	PEB	ND-C1D-CHC-C4C
82	LD	203	PEB	ND-C1D-CHC-C4C
82	ND	204	PEB	ND-C1D-CHC-C4C
82	PD	201	PEB	ND-C1D-CHC-C4C
82	YE	201	PEB	ND-C1D-CHC-C4C
82	IF	203	PEB	ND-C1D-CHC-C4C
82	MF	203	PEB	ND-C1D-CHC-C4C
82	QF	203	PEB	ND-C1D-CHC-C4C
82	XF	202	PEB	ND-C1D-CHC-C4C
82	YG	201	PEB	ND-C1D-CHC-C4C
82	OH	203	PEB	ND-C1D-CHC-C4C
82	QH	201	PEB	ND-C1D-CHC-C4C
82	QH	202	PEB	ND-C1D-CHC-C4C
82	SH	201	PEB	ND-C1D-CHC-C4C
82	UH	201	PEB	ND-C1D-CHC-C4C
82	IK	203	PEB	ND-C1D-CHC-C4C
82	MK	203	PEB	ND-C1D-CHC-C4C
82	QK	203	PEB	ND-C1D-CHC-C4C
82	XK	202	PEB	ND-C1D-CHC-C4C
82	AM	302	PEB	ND-C1D-CHC-C4C
82	EM	202	PEB	ND-C1D-CHC-C4C
82	OM	202	PEB	ND-C1D-CHC-C4C
82	RM	201	PEB	ND-C1D-CHC-C4C
82	GP	203	PEB	ND-C1D-CHC-C4C
82	HP	201	PEB	ND-C1D-CHC-C4C
82	JP	202	PEB	ND-C1D-CHC-C4C
82	RP	202	PEB	ND-C1D-CHC-C4C
82	WP	201	PEB	ND-C1D-CHC-C4C
82	YP	502	PEB	ND-C1D-CHC-C4C
82	AQ	301	PEB	ND-C1D-CHC-C4C
82	DQ	201	PEB	ND-C1D-CHC-C4C
82	HQ	201	PEB	ND-C1D-CHC-C4C
82	LQ	201	PEB	ND-C1D-CHC-C4C
82	LQ	203	PEB	ND-C1D-CHC-C4C
82	PQ	201	PEB	ND-C1D-CHC-C4C
82	O1	203	PEB	ND-C1D-CHC-C4C
82	Q1	201	PEB	ND-C1D-CHC-C4C
82	Q1	202	PEB	ND-C1D-CHC-C4C
82	S1	201	PEB	ND-C1D-CHC-C4C
82	U1	201	PEB	ND-C1D-CHC-C4C
82	f1	202	PEB	ND-C1D-CHC-C4C
82	h1	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
82	m1	202	PEB	ND-C1D-CHC-C4C
82	e4	201	PEB	ND-C1D-CHC-C4C
82	F5	202	PEB	ND-C1D-CHC-C4C
82	J5	202	PEB	ND-C1D-CHC-C4C
82	L5	202	PEB	ND-C1D-CHC-C4C
82	M5	304	PEB	ND-C1D-CHC-C4C
82	O5	202	PEB	ND-C1D-CHC-C4C
82	Q5	202	PEB	ND-C1D-CHC-C4C
82	U5	202	PEB	ND-C1D-CHC-C4C
82	Y5	202	PEB	ND-C1D-CHC-C4C
82	Z5	304	PEB	ND-C1D-CHC-C4C
82	F7	201	PEB	ND-C1D-CHC-C4C
82	u8	202	PEB	ND-C1D-CHC-C4C
82	v8	202	PEB	ND-C1D-CHC-C4C
82	D9	202	PEB	ND-C1D-CHC-C4C
82	J9	202	PEB	ND-C1D-CHC-C4C
82	U9	202	PEB	ND-C1D-CHC-C4C
82	W9	202	PEB	ND-C1D-CHC-C4C
82	uC	202	PEB	ND-C1D-CHC-C4C
82	vC	202	PEB	ND-C1D-CHC-C4C
82	aE	202	PEB	ND-C1D-CHC-C4C
82	eF	201	PEB	ND-C1D-CHC-C4C
82	gF	203	PEB	ND-C1D-CHC-C4C
82	iF	203	PEB	ND-C1D-CHC-C4C
82	qF	202	PEB	ND-C1D-CHC-C4C
82	aG	202	PEB	ND-C1D-CHC-C4C
82	fH	202	PEB	ND-C1D-CHC-C4C
82	gH	203	PEB	ND-C1D-CHC-C4C
82	mH	202	PEB	ND-C1D-CHC-C4C
82	aJ	201	PEB	ND-C1D-CHC-C4C
82	aJ	204	PEB	ND-C1D-CHC-C4C
82	jJ	203	PEB	ND-C1D-CHC-C4C
82	eK	201	PEB	ND-C1D-CHC-C4C
82	gK	203	PEB	ND-C1D-CHC-C4C
82	iK	203	PEB	ND-C1D-CHC-C4C
82	qK	202	PEB	ND-C1D-CHC-C4C
82	dM	202	PEB	ND-C1D-CHC-C4C
82	fM	202	PEB	ND-C1D-CHC-C4C
82	eO	201	PEB	ND-C1D-CHC-C4C
87	FN	205	CLA	C4B-C3B-CAB-CBB
87	F2	205	CLA	C4B-C3B-CAB-CBB
88	I6	101	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
87	B2	806	CLA	C16-C17-C18-C19
92	mL	101	LMG	O7-C8-C9-O8
87	BL	601	CLA	CAA-CBA-CGA-O1A
87	AN	814	CLA	CAA-CBA-CGA-O1A
87	A2	814	CLA	CAA-CBA-CGA-O1A
87	B6	613	CLA	CAA-CBA-CGA-O1A
87	c6	613	CLA	CAA-CBA-CGA-O1A
87	7N	607	CLA	CAA-CBA-CGA-O1A
92	bL	609	LMG	O10-C28-C29-C30
95	BL	607	DGD	O1B-C1B-C2B-C3B
95	L6	102	DGD	O1A-C1A-C2A-C3A
87	12	602	CLA	CAA-CBA-CGA-O2A
87	1N	602	CLA	CAA-CBA-CGA-O2A
92	JL	103	LMG	O8-C28-C29-C30
82	SJ	203	PEB	CAB-CBB-CGB-O2B
82	dE	203	PEB	CAC-CBC-CGC-O2C
82	kE	201	PEB	CAC-CBC-CGC-O2C
82	jK	201	PEB	CAB-CBB-CGB-O1B
83	A4	303	PUB	CAC-CBC-CGC-O2C
84	K1	1001	CYC	CAD-CBD-CGD-O2D
84	D4	1001	CYC	CAD-CBD-CGD-O2D
85	AL	401	BCR	C5-C6-C7-C8
85	JN	103	BCR	C5-C6-C7-C8
85	LN	201	BCR	C1-C6-C7-C8
85	J2	103	BCR	C5-C6-C7-C8
85	L2	201	BCR	C1-C6-C7-C8
85	a6	605	BCR	C5-C6-C7-C8
94	AL	413	PL9	C19-C21-C22-C23
87	BL	621	CLA	C15-C16-C17-C18
87	b6	616	CLA	C15-C16-C17-C18
92	ML	101	LMG	C10-C11-C12-C13
87	AN	841	CLA	CAA-CBA-CGA-O1A
87	A2	841	CLA	CAA-CBA-CGA-O1A
87	B6	612	CLA	CAA-CBA-CGA-O1A
87	C6	513	CLA	CAA-CBA-CGA-O1A
87	b6	611	CLA	CAA-CBA-CGA-O1A
92	bL	623	LMG	O9-C10-C11-C12
88	aL	607	LHG	C29-C30-C31-C32
92	DL	402	LMG	C36-C37-C38-C39
92	b6	623	LMG	C19-C20-C21-C22
87	AN	834	CLA	CAA-CBA-CGA-O2A
87	A2	834	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
92	a6	614	LMG	O7-C10-C11-C12
82	UE	202	PEB	CAB-CBB-CGB-O2B
82	RI	203	PEB	CAB-CBB-CGB-O1B
82	W1	203	PEB	CAB-CBB-CGB-O2B
82	dG	203	PEB	CAC-CBC-CGC-O2C
82	hK	201	PEB	CAB-CBB-CGB-O1B
82	iK	201	PEB	CAC-CBC-CGC-O2C
83	AJ	303	PUB	CAC-CBC-CGC-O2C
83	AO	303	PUB	CAC-CBC-CGC-O2C
84	KH	1001	CYC	CAD-CBD-CGD-O2D
84	J4	1001	CYC	CAD-CBD-CGD-O2D
87	32	303	CLA	CAA-CBA-CGA-O1A
87	62	307	CLA	CAA-CBA-CGA-O2A
87	BN	807	CLA	C16-C17-C18-C19
92	k6	101	LMG	C37-C38-C39-C40
87	BN	813	CLA	C2A-CAA-CBA-CGA
87	BN	823	CLA	C2A-CAA-CBA-CGA
87	B2	812	CLA	C2A-CAA-CBA-CGA
87	B2	822	CLA	C2A-CAA-CBA-CGA
87	B6	609	CLA	CAA-CBA-CGA-O1A
87	AN	850	CLA	O1D-CGD-O2D-CED
95	DL	408	DGD	O1A-C1A-O1G-C1G
87	12	602	CLA	C5-C6-C7-C8
92	k6	101	LMG	C36-C37-C38-C39
82	NA	202	PEB	C2C-CAC-CBC-CGC
82	AD	303	PEB	C3B-CAB-CBB-CGB
82	PH	202	PEB	C3B-CAB-CBB-CGB
82	KJ	201	PEB	C2C-CAC-CBC-CGC
82	SJ	202	PEB	C2C-CAC-CBC-CGC
82	N7	202	PEB	C2C-CAC-CBC-CGC
92	bL	609	LMG	C15-C16-C17-C18
82	HF	201	PEB	CAC-CBC-CGC-O2C
82	UG	202	PEB	CAB-CBB-CGB-O2B
82	HK	201	PEB	CAC-CBC-CGC-O2C
82	aE	201	PEB	CAB-CBB-CGB-O2B
82	iE	201	PEB	CAB-CBB-CGB-O2B
82	iF	201	PEB	CAC-CBC-CGC-O2C
82	jF	201	PEB	CAB-CBB-CGB-O1B
82	aG	201	PEB	CAB-CBB-CGB-O2B
82	iG	201	PEB	CAB-CBB-CGB-O2B
84	JO	1001	CYC	CAD-CBD-CGD-O2D
87	3N	304	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	CL	503	CLA	CAA-CBA-CGA-O2A
87	B6	606	CLA	C10-C11-C12-C13
87	1N	602	CLA	C5-C6-C7-C8
88	L6	101	LHG	C7-C8-C9-C10
88	l6	101	LHG	C7-C8-C9-C10
87	AN	851	CLA	CAA-CBA-CGA-O1A
83	Z9	302	PUB	C4A-C3A-CAA-CBA
83	M9	303	PUB	C4A-C3A-CAA-CBA
87	b6	612	CLA	C4-C3-C5-C6
87	C6	515	CLA	C2C-C3C-CAC-CBC
87	CL	510	CLA	O1D-CGD-O2D-CED
87	BN	819	CLA	C2-C3-C5-C6
87	B2	818	CLA	C2-C3-C5-C6
92	CL	519	LMG	C42-C43-C44-C45
95	CL	517	DGD	C6A-C7A-C8A-C9A
82	DB	201	PEB	CAC-CBC-CGC-O2C
82	GB	201	PEB	CAC-CBC-CGC-O1C
82	HB	202	PEB	CAB-CBB-CGB-O2B
82	TE	201	PEB	CAB-CBB-CGB-O2B
82	TG	201	PEB	CAB-CBB-CGB-O2B
82	W1	202	PEB	CAB-CBB-CGB-O2B
82	c4	201	PEB	CAB-CBB-CGB-O2B
82	iE	201	PEB	CAB-CBB-CGB-O1B
82	iG	201	PEB	CAB-CBB-CGB-O1B
82	cO	201	PEB	CAB-CBB-CGB-O2B
82	bP	502	PEB	CAC-CBC-CGC-O2C
84	LE	1001	CYC	CAA-CBA-CGA-O2A
84	LG	1001	CYC	CAA-CBA-CGA-O2A
87	62	307	CLA	CAA-CBA-CGA-O1A
87	A2	816	CLA	CAA-CBA-CGA-O2A
87	6N	606	CLA	CAA-CBA-CGA-O1A
82	YB	202	PEB	C2C-C1C-CHB-C4B
82	RH	202	PEB	C2C-C1C-CHB-C4B
82	YO	203	PEB	C2C-C1C-CHB-C4B
82	Y4	203	PEB	C2C-C1C-CHB-C4B
82	J9	203	PEB	C2C-C1C-CHB-C4B
87	BL	603	CLA	CAD-CBD-CGD-O1D
87	CL	509	CLA	CAD-CBD-CGD-O1D
87	BN	801	CLA	CAD-CBD-CGD-O1D
87	BN	813	CLA	CAD-CBD-CGD-O1D
87	BN	819	CLA	CAD-CBD-CGD-O1D
87	BN	829	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
87	32	311	CLA	CAD-CBD-CGD-O1D
87	B2	812	CLA	CAD-CBD-CGD-O1D
87	B2	818	CLA	CAD-CBD-CGD-O1D
87	B2	825	CLA	CAD-CBD-CGD-O1D
87	B2	829	CLA	CAD-CBD-CGD-O1D
87	C6	519	CLA	CAD-CBD-CGD-O1D
87	C6	520	CLA	CAD-CBD-CGD-O1D
87	D6	405	CLA	CAD-CBD-CGD-O1D
87	bL	604	CLA	CAD-CBD-CGD-O1D
87	bL	606	CLA	CAD-CBD-CGD-O1D
87	3N	311	CLA	CAD-CBD-CGD-O1D
92	XL	601	LMG	C7-C8-O7-C10
87	B6	611	CLA	O1A-CGA-O2A-C1
87	AN	805	CLA	CAA-CBA-CGA-O1A
87	82	306	CLA	CAA-CBA-CGA-O1A
87	A2	805	CLA	CAA-CBA-CGA-O1A
87	A2	851	CLA	CAA-CBA-CGA-O1A
87	b6	615	CLA	CAA-CBA-CGA-O1A
87	8N	301	CLA	CAA-CBA-CGA-O1A
92	yL	101	LMG	O9-C10-C11-C12
95	DL	408	DGD	C9A-CAA-CBA-CCA
95	c6	601	DGD	C9A-CAA-CBA-CCA
87	AN	807	CLA	CAA-CBA-CGA-O2A
87	A2	807	CLA	CAA-CBA-CGA-O2A
87	A2	839	CLA	CAA-CBA-CGA-O2A
87	aL	605	CLA	CAA-CBA-CGA-O2A
87	8N	301	CLA	CAA-CBA-CGA-O2A
92	JL	102	LMG	O7-C10-C11-C12
95	BN	844	DGD	O1G-C1A-C2A-C3A
95	B2	844	DGD	O1G-C1A-C2A-C3A
87	A2	819	CLA	C5-C6-C7-C8
95	CL	517	DGD	O6D-C5D-C6D-O5D
82	LJ	202	PEB	C3C-C2C-CAC-CBC
87	32	304	CLA	C6-C7-C8-C9
87	B2	835	CLA	C14-C13-C15-C16
87	I2	102	CLA	C11-C12-C13-C14
87	B6	610	CLA	C11-C10-C8-C9
87	b6	616	CLA	C6-C7-C8-C9
87	c6	605	CLA	C14-C13-C15-C16
87	c6	606	CLA	C11-C10-C8-C9
87	cL	508	CLA	C6-C7-C8-C9
87	3N	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
95	C6	502	DGD	C9A-CAA-CBA-CCA
82	TA	203	PEB	CAB-CBB-CGB-O2B
82	KF	201	PEB	CAC-CBC-CGC-O2C
82	WH	202	PEB	CAB-CBB-CGB-O2B
82	NI	203	PEB	CAB-CBB-CGB-O1B
82	S4	201	PEB	CAB-CBB-CGB-O1B
82	a4	203	PEB	CAB-CBB-CGB-O2B
82	T7	203	PEB	CAB-CBB-CGB-O2B
82	iK	203	PEB	CAB-CBB-CGB-O2B
82	aO	203	PEB	CAB-CBB-CGB-O2B
84	CO	1001	CYC	CAD-CBD-CGD-O1D
84	C4	1001	CYC	CAD-CBD-CGD-O1D
87	AN	816	CLA	CAA-CBA-CGA-O2A
87	BN	828	CLA	CAA-CBA-CGA-O1A
87	B2	828	CLA	CAA-CBA-CGA-O1A
87	AN	819	CLA	C5-C6-C7-C8
87	AN	831	CLA	C13-C15-C16-C17
87	BN	813	CLA	C5-C6-C7-C8
87	A2	831	CLA	C13-C15-C16-C17
87	B2	812	CLA	C5-C6-C7-C8
87	B6	611	CLA	C8-C10-C11-C12
88	B6	617	LHG	O10-C23-O8-C6
87	22	602	CLA	CAA-CBA-CGA-O1A
87	B2	826	CLA	CAA-CBA-CGA-O1A
87	2N	303	CLA	CAA-CBA-CGA-O1A
95	AL	414	DGD	C7B-C8B-C9B-CAB
87	AL	403	CLA	CAA-CBA-CGA-O2A
87	BL	604	CLA	CAA-CBA-CGA-O2A
87	AN	839	CLA	CAA-CBA-CGA-O2A
87	82	306	CLA	CAA-CBA-CGA-O2A
87	cL	505	CLA	CAA-CBA-CGA-O2A
92	j6	101	LMG	O7-C10-C11-C12
87	C6	511	CLA	C5-C6-C7-C8
87	cL	505	CLA	C10-C11-C12-C13
87	12	611	CLA	O1D-CGD-O2D-CED
82	VI	203	PEB	CAB-CBB-CGB-O1B
82	QJ	202	PEB	CAB-CBB-CGB-O1B
82	SO	201	PEB	CAB-CBB-CGB-O1B
82	iF	203	PEB	CAB-CBB-CGB-O2B
87	12	606	CLA	CAA-CBA-CGA-O1A
87	2N	307	CLA	CAA-CBA-CGA-O2A
87	BN	826	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
95	aL	603	DGD	C6B-C7B-C8B-C9B
87	BN	809	CLA	CAA-CBA-CGA-O2A
87	IN	103	CLA	CAA-CBA-CGA-O2A
87	I2	103	CLA	CAA-CBA-CGA-O2A
87	cL	511	CLA	CAA-CBA-CGA-O2A
87	5N	602	CLA	CAA-CBA-CGA-O2A
91	dL	403	PHO	CAA-CBA-CGA-O2A
82	UM	203	PEB	C2B-C3B-CAB-CBB
88	AL	407	LHG	C1-C2-C3-O3
87	72	602	CLA	C15-C16-C17-C18
87	b6	604	CLA	C15-C16-C17-C18
87	7N	602	CLA	C15-C16-C17-C18
82	MB	202	PEB	CAC-CBC-CGC-O1C
82	JD	201	PEB	CAC-CBC-CGC-O2C
82	QF	203	PEB	CAC-CBC-CGC-O2C
82	FJ	201	PEB	CAC-CBC-CGC-O2C
82	ZO	201	PEB	CAB-CBB-CGB-O2B
82	JQ	201	PEB	CAC-CBC-CGC-O2C
82	dG	203	PEB	CAC-CBC-CGC-O1C
83	AM	303	PUB	CAC-CBC-CGC-O1C
84	JO	1001	CYC	CAD-CBD-CGD-O1D
84	MO	1001	CYC	CAD-CBD-CGD-O2D
87	1N	606	CLA	CAA-CBA-CGA-O1A
96	fL	102	HEM	CAD-CBD-CGD-O2D
87	BN	813	CLA	C3-C5-C6-C7
92	qL	301	LMG	O9-C10-C11-C12
88	i6	101	LHG	O9-C7-O7-C5
87	B6	613	CLA	C16-C17-C18-C19
87	BN	807	CLA	C4-C3-C5-C6
87	B2	806	CLA	C4-C3-C5-C6
87	nL	101	CLA	C4-C3-C5-C6
94	AL	413	PL9	C20-C19-C21-C22
87	BL	603	CLA	C5-C6-C7-C8
103	8N	310	ZEX	C11-C12-C13-C20
95	C6	502	DGD	CAA-CBA-CCA-CDA
95	J6	101	DGD	C4B-C5B-C6B-C7B
82	JB	202	PEB	C2A-C3A-CAA-CBA
82	TB	202	PEB	C2A-C3A-CAA-CBA
82	JI	202	PEB	C2A-C3A-CAA-CBA
82	QK	203	PEB	C2A-C3A-CAA-CBA
82	h1	203	PEB	C2A-C3A-CAA-CBA
82	b1	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
82	m4	202	PEB	C2A-C3A-CAA-CBA
82	c4	201	PEB	C2A-C3A-CAA-CBA
82	z8	201	PEB	C2A-C3A-CAA-CBA
82	u8	201	PEB	C2A-C3A-CAA-CBA
82	zC	201	PEB	C2A-C3A-CAA-CBA
82	uC	201	PEB	C2A-C3A-CAA-CBA
82	cE	201	PEB	C2A-C3A-CAA-CBA
82	cF	201	PEB	C2A-C3A-CAA-CBA
82	xF	302	PEB	C2A-C3A-CAA-CBA
82	cG	201	PEB	C2A-C3A-CAA-CBA
82	gG	201	PEB	C2A-C3A-CAA-CBA
82	hH	202	PEB	C2A-C3A-CAA-CBA
82	bH	202	PEB	C2A-C3A-CAA-CBA
82	cK	201	PEB	C2A-C3A-CAA-CBA
82	xK	302	PEB	C2A-C3A-CAA-CBA
82	cO	201	PEB	C2A-C3A-CAA-CBA
84	EO	1001	CYC	C2C-C3C-CAC-CBC
84	E4	1001	CYC	C2C-C3C-CAC-CBC
87	BL	608	CLA	C11-C10-C8-C7
87	AN	805	CLA	C11-C10-C8-C7
87	AN	849	CLA	C11-C10-C8-C7
87	BN	806	CLA	C6-C7-C8-C10
87	BN	809	CLA	C12-C13-C15-C16
87	BN	824	CLA	C11-C12-C13-C15
87	LN	203	CLA	C6-C7-C8-C10
87	32	304	CLA	C6-C7-C8-C10
87	32	309	CLA	C3A-C2A-CAA-CBA
87	62	303	CLA	C3A-C2A-CAA-CBA
87	72	602	CLA	C3A-C2A-CAA-CBA
87	A2	805	CLA	C11-C10-C8-C7
87	A2	849	CLA	C11-C10-C8-C7
87	B2	805	CLA	C6-C7-C8-C10
87	B2	808	CLA	C12-C13-C15-C16
87	B2	823	CLA	C11-C12-C13-C15
87	L2	203	CLA	C6-C7-C8-C10
87	B6	605	CLA	C12-C13-C15-C16
87	B6	609	CLA	C11-C12-C13-C15
87	D6	402	CLA	C2-C3-C5-C6
87	c6	616	CLA	C11-C10-C8-C7
87	c6	616	CLA	C12-C13-C15-C16
87	aL	605	CLA	C11-C10-C8-C7
87	bL	605	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
87	bL	616	CLA	C11-C10-C8-C7
87	cL	508	CLA	C12-C13-C15-C16
87	dL	404	CLA	C2-C3-C5-C6
87	3N	305	CLA	C6-C7-C8-C10
87	3N	309	CLA	C3A-C2A-CAA-CBA
87	6N	602	CLA	C3A-C2A-CAA-CBA
87	7N	602	CLA	C3A-C2A-CAA-CBA
88	d6	402	LHG	O6-C4-C5-O7
87	CL	514	CLA	CAA-CBA-CGA-O1A
87	62	309	CLA	CAA-CBA-CGA-O1A
87	c6	608	CLA	CAA-CBA-CGA-O1A
87	6N	608	CLA	CAA-CBA-CGA-O1A
82	TB	202	PEB	CAC-CBC-CGC-O1C
82	RE	201	PEB	CAC-CBC-CGC-O1C
82	VE	201	PEB	CAB-CBB-CGB-O1B
82	RG	201	PEB	CAC-CBC-CGC-O1C
82	HI	202	PEB	CAB-CBB-CGB-O1B
82	SJ	203	PEB	CAB-CBB-CGB-O1B
82	XJ	202	PEB	CAC-CBC-CGC-O1C
82	KK	201	PEB	CAC-CBC-CGC-O2C
82	XK	202	PEB	CAC-CBC-CGC-O1C
82	EM	202	PEB	CAB-CBB-CGB-O1B
82	Z4	201	PEB	CAB-CBB-CGB-O2B
82	F5	201	PEB	CAB-CBB-CGB-O1B
82	dE	203	PEB	CAC-CBC-CGC-O1C
82	gM	202	PEB	CAC-CBC-CGC-O2C
84	FE	1001	CYC	CAD-CBD-CGD-O1D
84	J4	1001	CYC	CAD-CBD-CGD-O1D
84	M4	1001	CYC	CAD-CBD-CGD-O2D
87	42	601	CLA	CAA-CBA-CGA-O1A
87	2N	307	CLA	CAA-CBA-CGA-O1A
88	m6	102	LHG	C27-C28-C29-C30
87	AN	824	CLA	CAA-CBA-CGA-O2A
87	52	602	CLA	CAA-CBA-CGA-O2A
87	A2	824	CLA	CAA-CBA-CGA-O2A
87	B2	808	CLA	CAA-CBA-CGA-O2A
87	b6	614	CLA	CAA-CBA-CGA-O2A
87	bL	618	CLA	CAA-CBA-CGA-O2A
92	J6	102	LMG	O7-C10-C11-C12
95	b6	622	DGD	O1G-C1A-C2A-C3A
82	HI	203	PEB	NC-C1C-CHB-C4B
82	PQ	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
92	BL	611	LMG	C12-C13-C14-C15
87	B2	812	CLA	C3-C5-C6-C7
95	hL	101	DGD	C3B-C4B-C5B-C6B
83	QM	201	PUB	C2B-C3B-CAB-CBB
85	BL	617	BCR	C7-C8-C9-C10
85	AN	846	BCR	C7-C8-C9-C10
85	A2	846	BCR	C7-C8-C9-C10
87	A2	824	CLA	CAA-CBA-CGA-O1A
92	j6	101	LMG	O9-C10-C11-C12
82	FB	201	PEB	C2C-C1C-CHB-C4B
82	ND	204	PEB	C2C-C1C-CHB-C4B
82	AF	202	PEB	C2C-C1C-CHB-C4B
82	JI	202	PEB	C2C-C1C-CHB-C4B
82	SI	202	PEB	C2C-C1C-CHB-C4B
82	AK	202	PEB	C2C-C1C-CHB-C4B
82	NM	201	PEB	C2C-C1C-CHB-C4B
82	FP	202	PEB	C2C-C1C-CHB-C4B
82	NQ	204	PEB	C2C-C1C-CHB-C4B
82	R1	202	PEB	C2C-C1C-CHB-C4B
82	pC	201	PEB	C2C-C1C-CHB-C4B
82	JB	202	PEB	CAC-CBC-CGC-O1C
82	UB	302	PEB	CAC-CBC-CGC-O1C
82	NF	202	PEB	CAC-CBC-CGC-O2C
82	XF	202	PEB	CAC-CBC-CGC-O1C
82	GG	1002	PEB	CAC-CBC-CGC-O1C
82	VG	201	PEB	CAB-CBB-CGB-O1B
82	VG	201	PEB	CAB-CBB-CGB-O2B
82	WH	203	PEB	CAB-CBB-CGB-O1B
82	NK	202	PEB	CAC-CBC-CGC-O2C
82	QK	203	PEB	CAC-CBC-CGC-O2C
82	B5	201	PEB	CAB-CBB-CGB-O2B
82	A9	201	PEB	CAB-CBB-CGB-O1B
82	C9	201	PEB	CAB-CBB-CGB-O1B
82	E9	201	PEB	CAB-CBB-CGB-O1B
82	G9	201	PEB	CAB-CBB-CGB-O1B
82	I9	201	PEB	CAB-CBB-CGB-O1B
82	K9	201	PEB	CAB-CBB-CGB-O1B
82	N9	201	PEB	CAB-CBB-CGB-O1B
82	P9	201	PEB	CAB-CBB-CGB-O1B
82	T9	201	PEB	CAB-CBB-CGB-O1B
82	V9	201	PEB	CAB-CBB-CGB-O1B
82	X9	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
82	bE	201	PEB	CAB-CBB-CGB-O1B
82	iE	202	PEB	CAC-CBC-CGC-O1C
82	bG	201	PEB	CAB-CBB-CGB-O1B
82	iG	202	PEB	CAC-CBC-CGC-O1C
82	kO	202	PEB	CAC-CBC-CGC-O2C
83	AD	302	PUB	CAC-CBC-CGC-O1C
83	AQ	302	PUB	CAC-CBC-CGC-O1C
83	xF	306	PUB	CAB-CBB-CGB-O1B
83	xK	306	PUB	CAB-CBB-CGB-O1B
84	CG	1001	CYC	CAD-CBD-CGD-O1D
84	FO	1001	CYC	CAD-CBD-CGD-O1D
84	F4	1001	CYC	CAD-CBD-CGD-O1D
87	AN	852	CLA	CAA-CBA-CGA-O1A
87	22	607	CLA	CAA-CBA-CGA-O1A
87	22	607	CLA	CAA-CBA-CGA-O2A
87	82	305	CLA	CAA-CBA-CGA-O2A
87	A2	852	CLA	CAA-CBA-CGA-O1A
87	4N	601	CLA	CAA-CBA-CGA-O1A
87	4N	601	CLA	CAA-CBA-CGA-O2A
82	SI	201	PEB	C4B-C3B-CAB-CBB
82	j4	203	PEB	C4B-C3B-CAB-CBB
82	cF	202	PEB	C4B-C3B-CAB-CBB
82	kO	202	PEB	C4B-C3B-CAB-CBB
85	AN	846	BCR	C9-C10-C11-C12
85	A2	846	BCR	C9-C10-C11-C12
85	L2	201	BCR	C13-C14-C15-C16
95	c6	601	DGD	CAA-CBA-CCA-CDA
87	AN	823	CLA	CAA-CBA-CGA-O2A
87	LN	203	CLA	CAA-CBA-CGA-O2A
87	42	608	CLA	CAA-CBA-CGA-O2A
87	A2	823	CLA	CAA-CBA-CGA-O2A
87	L2	203	CLA	CAA-CBA-CGA-O2A
87	H6	102	CLA	CAA-CBA-CGA-O2A
87	4N	608	CLA	CAA-CBA-CGA-O2A
88	dL	405	LHG	O7-C7-C8-C9
92	B6	618	LMG	O6-C1-O1-C7
87	A2	850	CLA	O1D-CGD-O2D-CED
87	1N	611	CLA	O1D-CGD-O2D-CED
87	H6	102	CLA	C15-C16-C17-C18
87	AN	823	CLA	CAA-CBA-CGA-O1A
87	AN	824	CLA	CAA-CBA-CGA-O1A
87	BN	805	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
87	A2	823	CLA	CAA-CBA-CGA-O1A
87	H6	102	CLA	CAA-CBA-CGA-O1A
87	b6	614	CLA	CAA-CBA-CGA-O1A
87	aL	605	CLA	CAA-CBA-CGA-O1A
92	JL	102	LMG	O9-C10-C11-C12
95	lL	101	DGD	O1A-C1A-C2A-C3A
95	DL	408	DGD	C2A-C1A-O1G-C1G
82	ND	202	PEB	CAC-CBC-CGC-O1C
82	VE	201	PEB	CAB-CBB-CGB-O2B
82	VO	202	PEB	CAB-CBB-CGB-O2B
82	NQ	202	PEB	CAC-CBC-CGC-O1C
82	W1	203	PEB	CAB-CBB-CGB-O1B
82	V4	202	PEB	CAB-CBB-CGB-O2B
82	j4	203	PEB	CAC-CBC-CGC-O2C
82	R9	201	PEB	CAB-CBB-CGB-O1B
82	cB	401	PEB	CAC-CBC-CGC-O2C
82	uK	202	PEB	CAB-CBB-CGB-O1B
83	xF	306	PUB	CAB-CBB-CGB-O2B
83	xK	306	PUB	CAB-CBB-CGB-O2B
87	42	601	CLA	CAA-CBA-CGA-O2A
87	8N	306	CLA	CAA-CBA-CGA-O2A
87	CL	513	CLA	C5-C6-C7-C8
87	AN	838	CLA	C15-C16-C17-C18
87	A2	838	CLA	C15-C16-C17-C18
87	4N	602	CLA	C8-C10-C11-C12
92	CL	519	LMG	C39-C40-C41-C42
87	BL	603	CLA	CAA-CBA-CGA-O2A
87	CL	507	CLA	CAA-CBA-CGA-O2A
87	cL	509	CLA	CAA-CBA-CGA-O2A
83	BJ	302	PUB	C2D-C3D-CAD-CBD
88	BL	610	LHG	C11-C10-C9-C8
87	BL	605	CLA	C10-C11-C12-C13
87	42	602	CLA	C8-C10-C11-C12
87	H6	102	CLA	C8-C10-C11-C12
95	cL	519	DGD	C1B-C2B-C3B-C4B
87	AN	811	CLA	CAA-CBA-CGA-O1A
87	A2	811	CLA	CAA-CBA-CGA-O1A
87	B2	804	CLA	CAA-CBA-CGA-O1A
87	cL	511	CLA	CAA-CBA-CGA-O1A
88	iL	101	LHG	O9-C7-C8-C9
92	JL	103	LMG	O10-C28-C29-C30
92	J6	102	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
92	b6	623	LMG	O10-C28-C29-C30
95	O6	301	DGD	O1B-C1B-C2B-C3B
82	fB	301	PEB	C2B-C3B-CAB-CBB
82	hB	301	PEB	C2B-C3B-CAB-CBB
87	72	602	CLA	C2A-CAA-CBA-CGA
87	7N	602	CLA	C2A-CAA-CBA-CGA
82	MA	201	PEB	C2C-CAC-CBC-CGC
82	RB	202	PEB	C2C-CAC-CBC-CGC
82	ZE	201	PEB	C3B-CAB-CBB-CGB
82	YG	202	PEB	C3B-CAB-CBB-CGB
82	MJ	201	PEB	C3B-CAB-CBB-CGB
82	SM	202	PEB	C3B-CAB-CBB-CGB
82	AQ	303	PEB	C3B-CAB-CBB-CGB
82	A5	202	PEB	C2C-CAC-CBC-CGC
82	C5	202	PEB	C2C-CAC-CBC-CGC
82	E5	202	PEB	C2C-CAC-CBC-CGC
82	G5	202	PEB	C2C-CAC-CBC-CGC
82	I5	202	PEB	C2C-CAC-CBC-CGC
82	K5	202	PEB	C2C-CAC-CBC-CGC
82	N5	202	PEB	C2C-CAC-CBC-CGC
82	P5	202	PEB	C2C-CAC-CBC-CGC
82	R5	202	PEB	C2C-CAC-CBC-CGC
82	T5	202	PEB	C2C-CAC-CBC-CGC
82	V5	202	PEB	C2C-CAC-CBC-CGC
82	X5	202	PEB	C2C-CAC-CBC-CGC
82	M7	201	PEB	C2C-CAC-CBC-CGC
82	dE	201	PEB	C3B-CAB-CBB-CGB
82	aM	202	PEB	C2C-CAC-CBC-CGC
82	GE	1002	PEB	CAC-CBC-CGC-O1C
82	ZI	401	PEB	CAB-CBB-CGB-O2B
82	U4	201	PEB	CAB-CBB-CGB-O2B
82	L7	201	PEB	CAC-CBC-CGC-O2C
82	uF	203	PEB	CAB-CBB-CGB-O1B
87	B6	604	CLA	C15-C16-C17-C18
87	cL	506	CLA	C10-C11-C12-C13
87	C6	520	CLA	CBA-CGA-O2A-C1
92	jL	101	LMG	C12-C13-C14-C15
87	AL	403	CLA	CAA-CBA-CGA-O1A
87	AN	839	CLA	CAA-CBA-CGA-O1A
87	A2	839	CLA	CAA-CBA-CGA-O1A
82	DO	1002	PEB	C1C-C2C-CAC-CBC
82	UP	202	PEB	C1C-C2C-CAC-CBC

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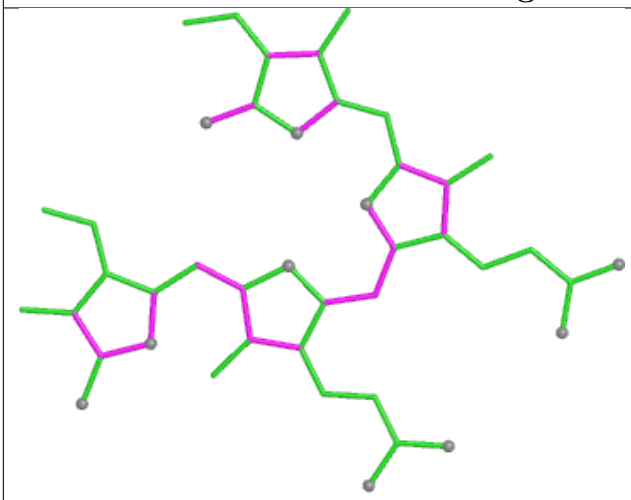
Mol	Chain	Res	Type	Atoms
82	D4	1002	PEB	C1C-C2C-CAC-CBC
83	QM	201	PUB	C4B-C3B-CAB-CBB
87	KN	105	CLA	CAA-CBA-CGA-O2A
82	NB	201	PEB	CAC-CBC-CGC-O2C
82	KK	201	PEB	CAC-CBC-CGC-O1C
82	WM	201	PEB	CAB-CBB-CGB-O2B
82	NP	201	PEB	CAC-CBC-CGC-O1C
82	bE	201	PEB	CAB-CBB-CGB-O2B
82	uF	201	PEB	CAC-CBC-CGC-O2C
82	uF	203	PEB	CAB-CBB-CGB-O2B
82	bG	201	PEB	CAB-CBB-CGB-O2B
82	tK	203	PEB	CAC-CBC-CGC-O2C
83	AJ	303	PUB	CAC-CBC-CGC-O1C
84	KG	202	CYC	CAD-CBD-CGD-O2D
84	JH	1001	CYC	CAD-CBD-CGD-O1D
84	KH	1001	CYC	CAD-CBD-CGD-O1D
84	K1	1001	CYC	CAD-CBD-CGD-O1D
87	AN	816	CLA	CAA-CBA-CGA-O1A
87	A2	816	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

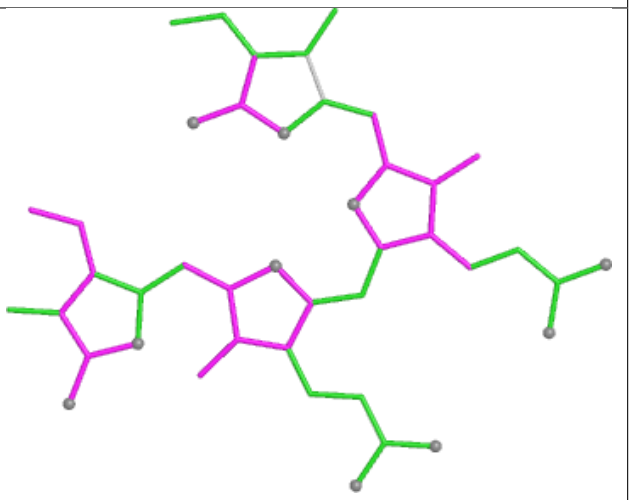
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

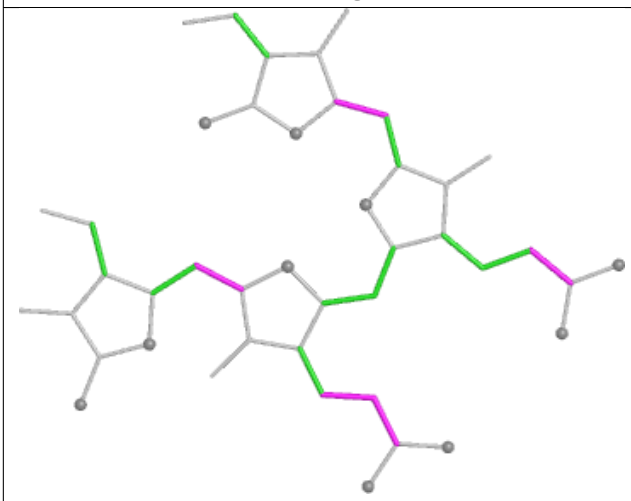
Ligand PEB rC 201



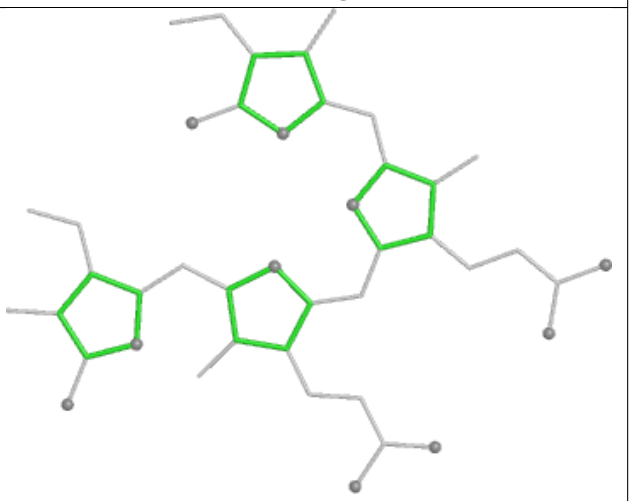
Bond lengths



Bond angles

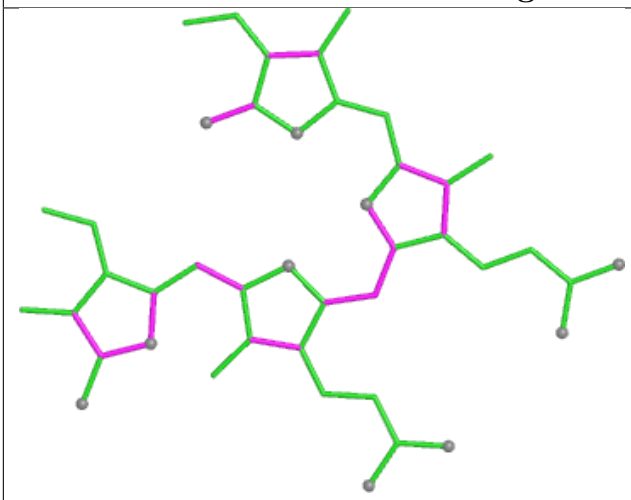


Torsions

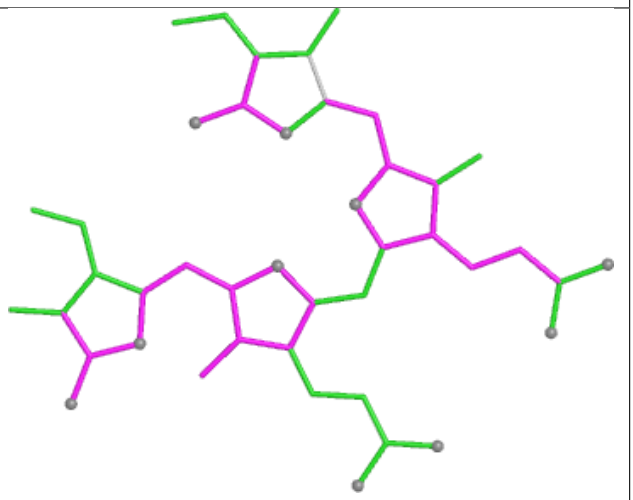


Rings

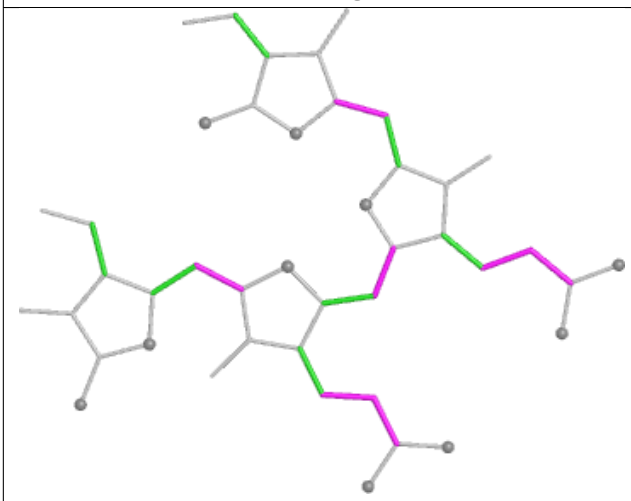
Ligand PEB F5 203



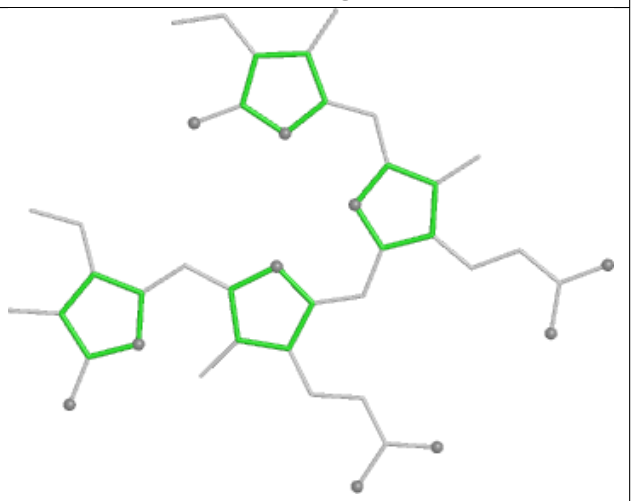
Bond lengths



Bond angles

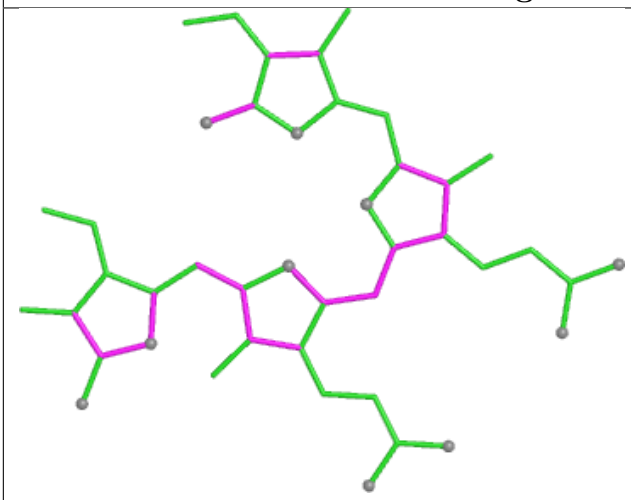


Torsions

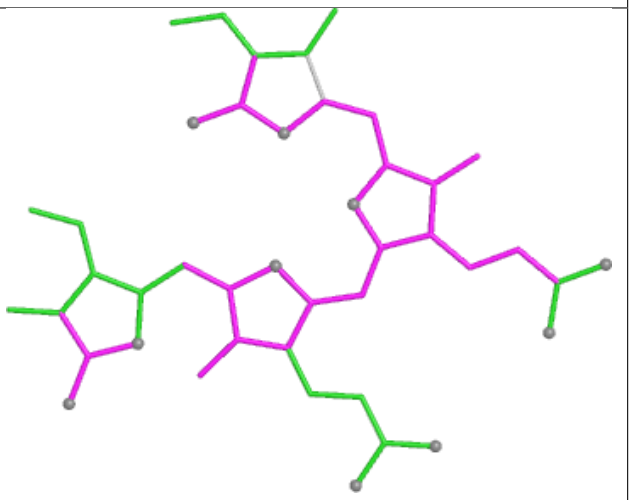


Rings

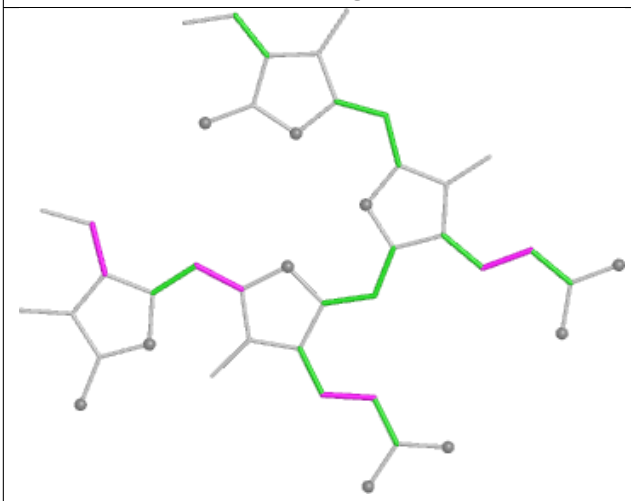
Ligand PEB cK 203



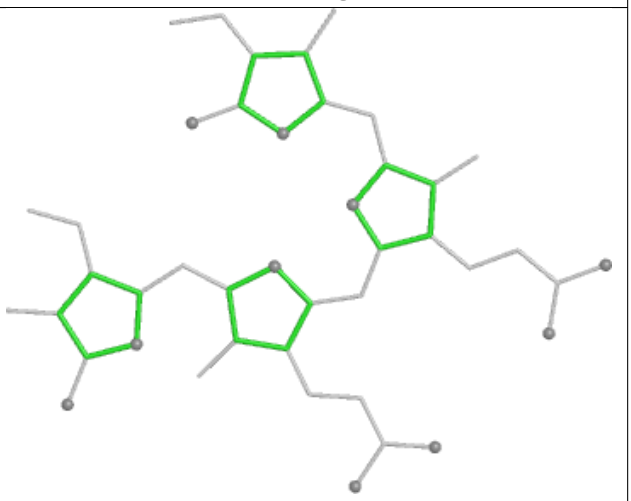
Bond lengths



Bond angles

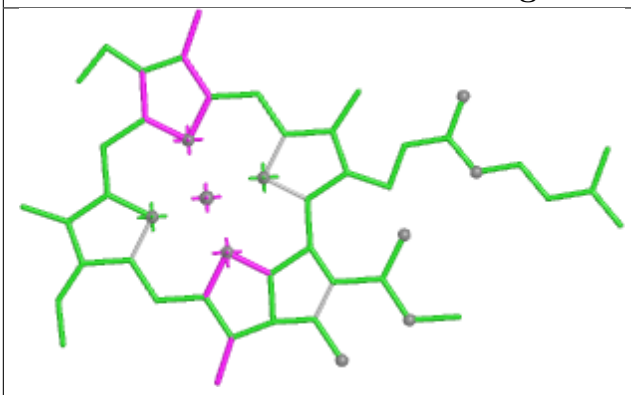


Torsions



Rings

Ligand CLA 42 608



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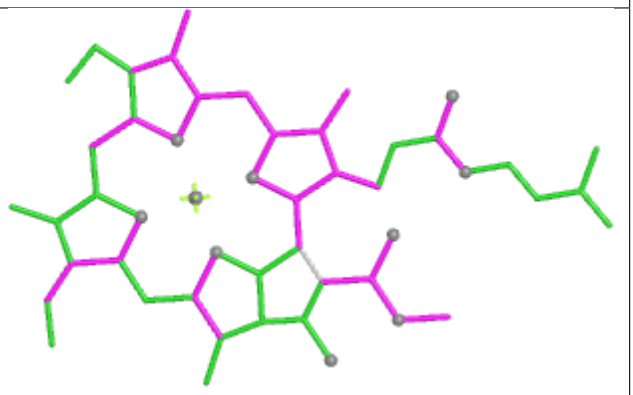
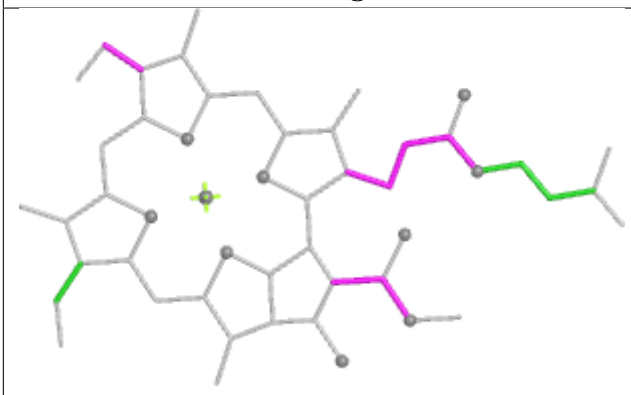
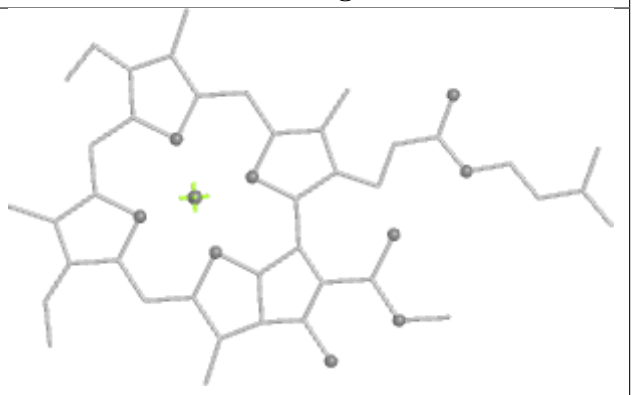


Bond angles

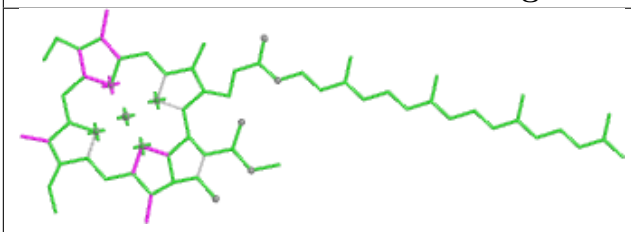


Torsions

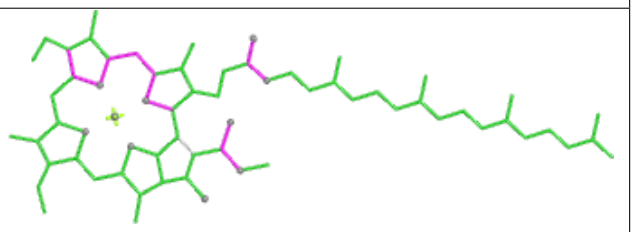


Rings

Ligand CLA I2 102



Bond lengths



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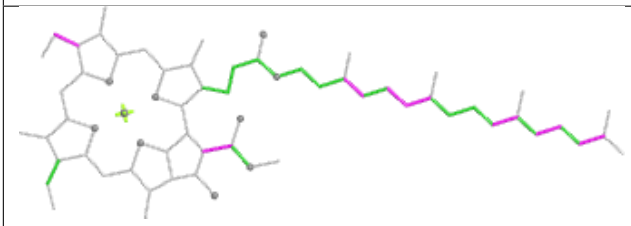

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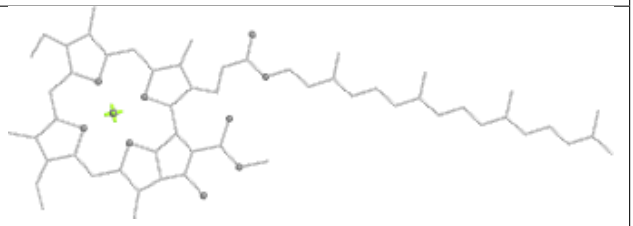
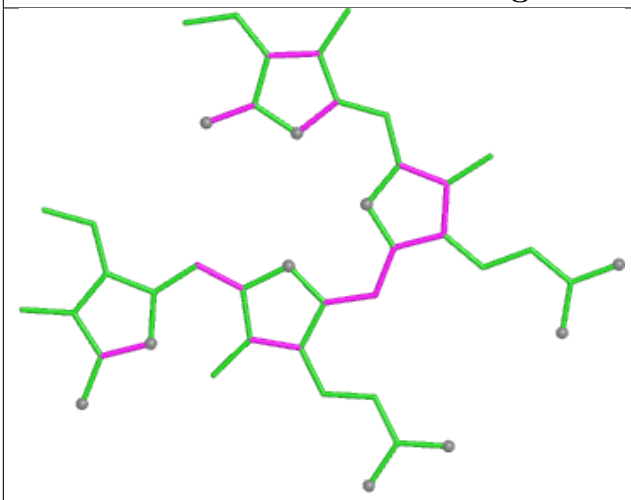


Rings

Ligand PEB TH 202



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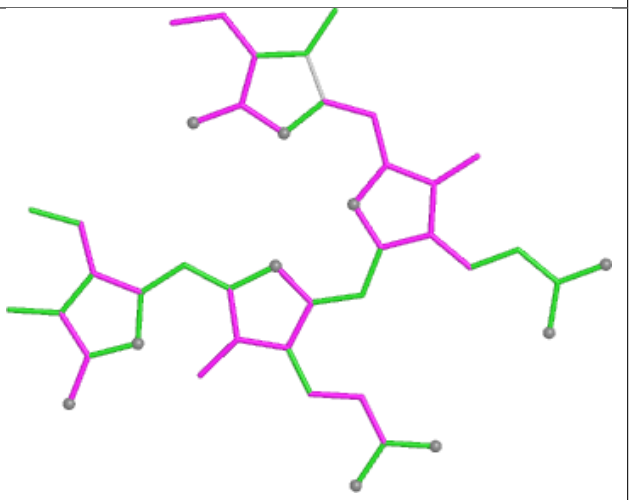

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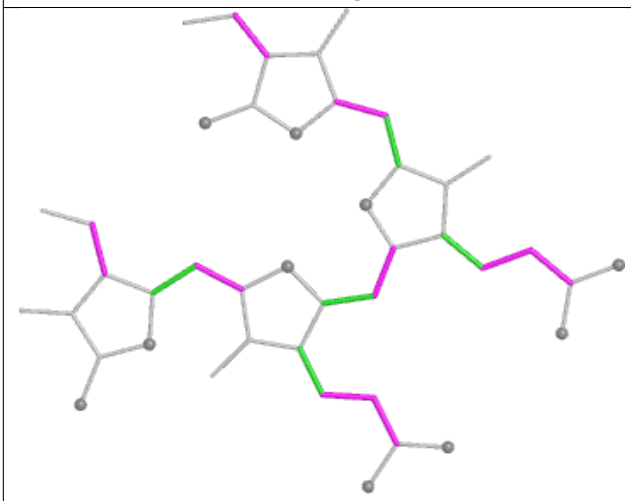
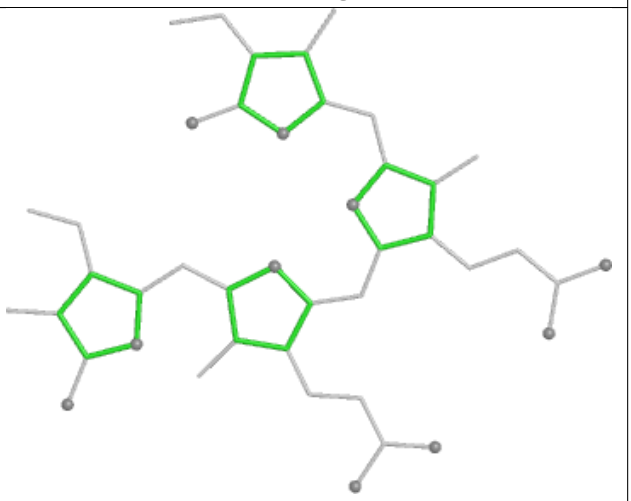
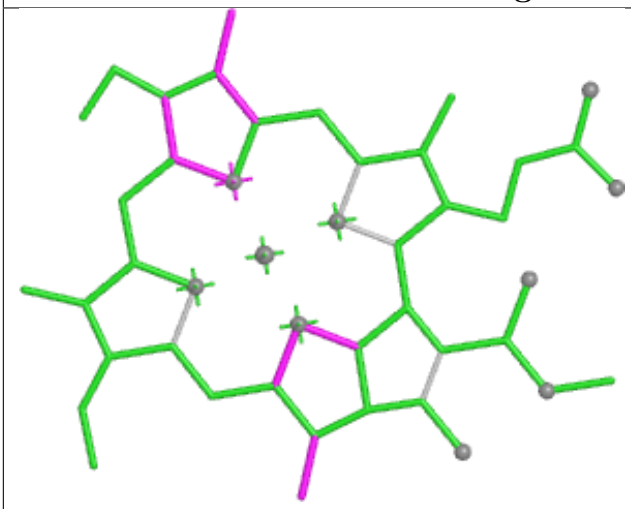


Torsions



Rings

Ligand CLA 8N 305



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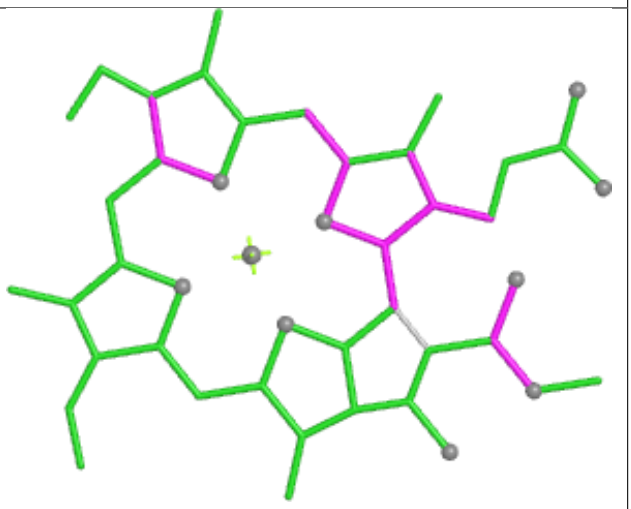
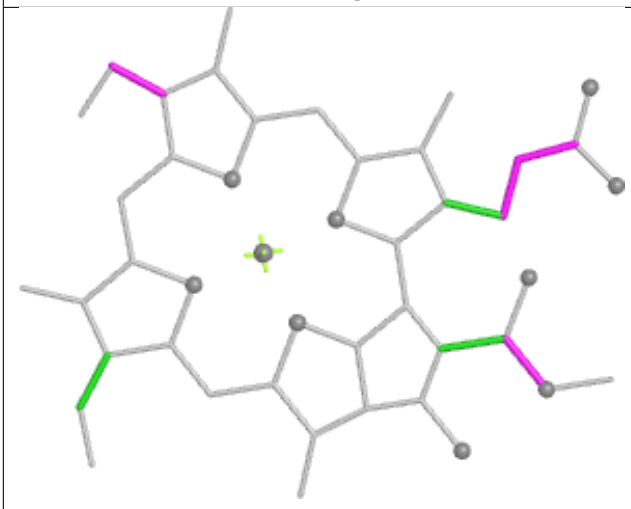


Bond angles

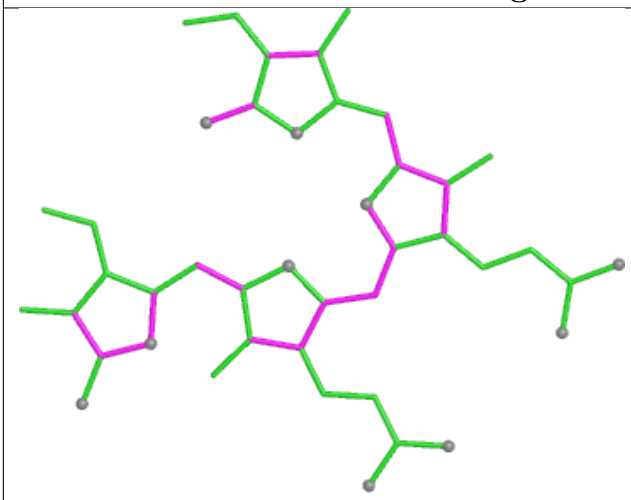


Torsions



Rings

Ligand PEB RK 202



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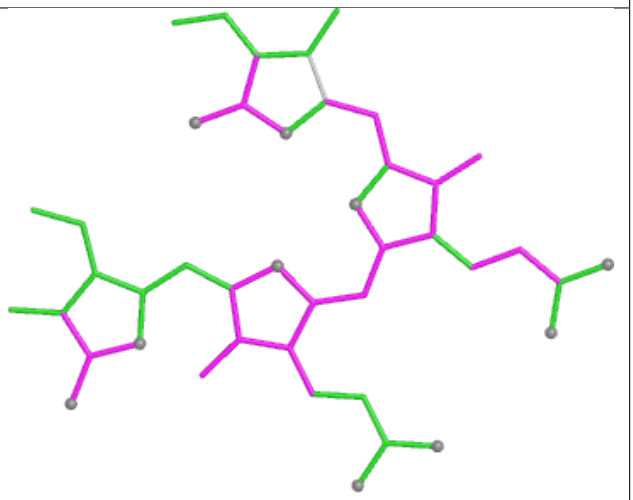
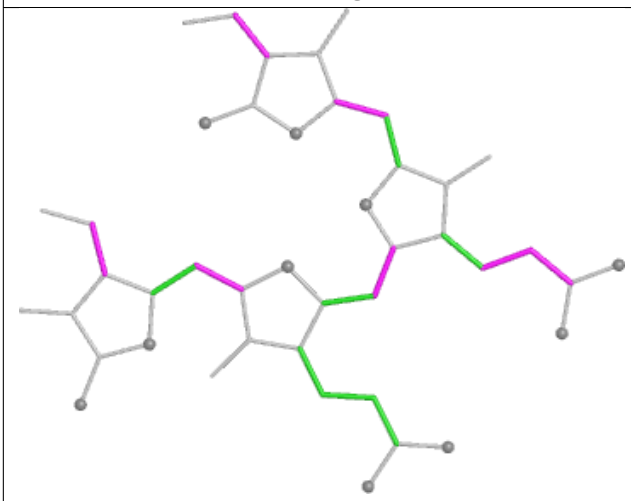
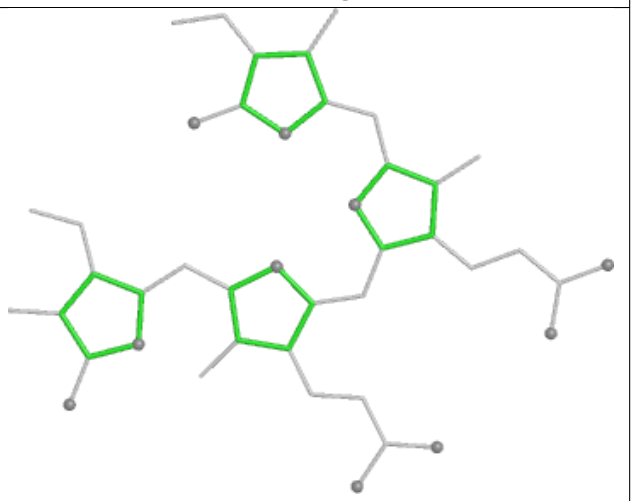


Bond angles

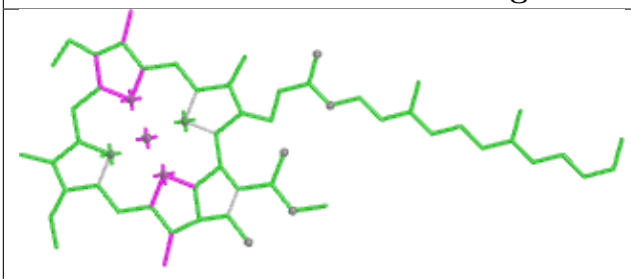


Torsions



Rings

Ligand CLA BN 817



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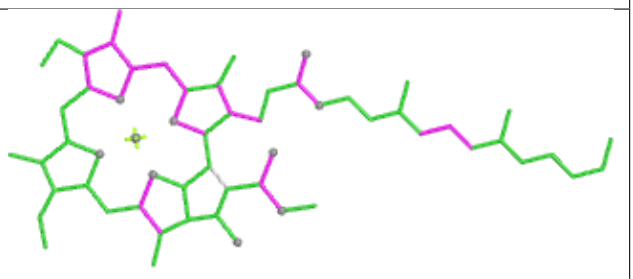

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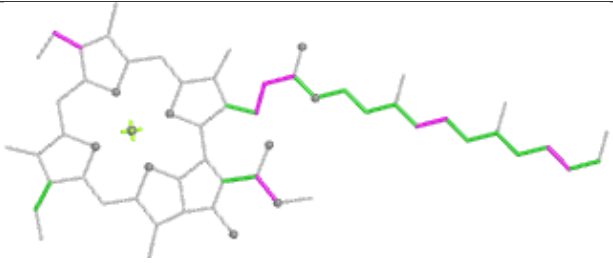

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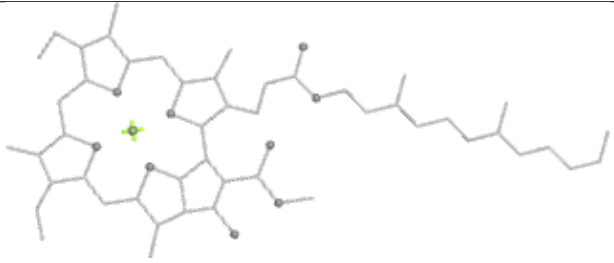
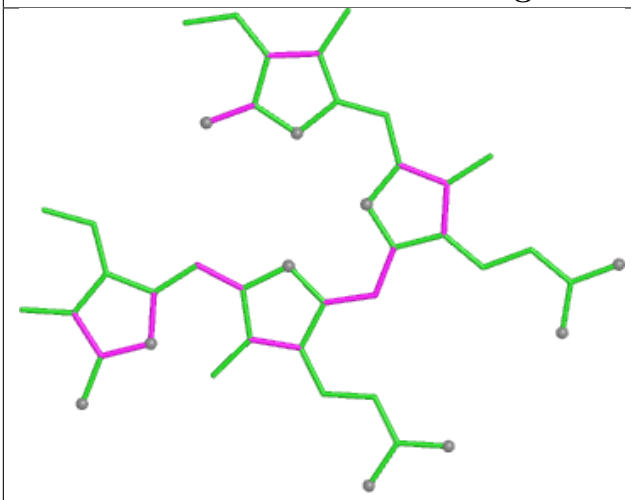


Rings

Ligand PEB dO 201



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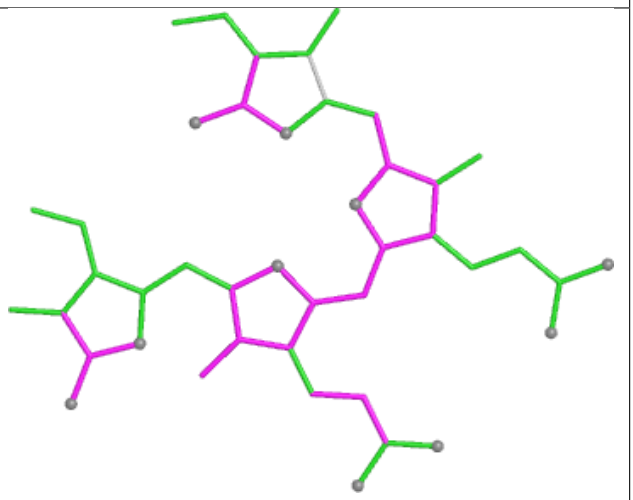

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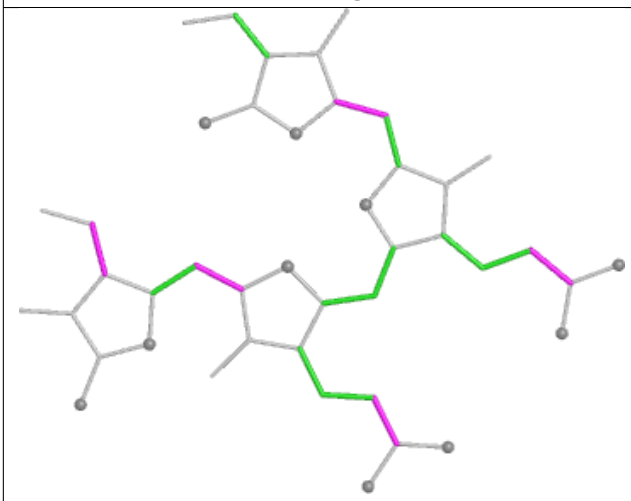

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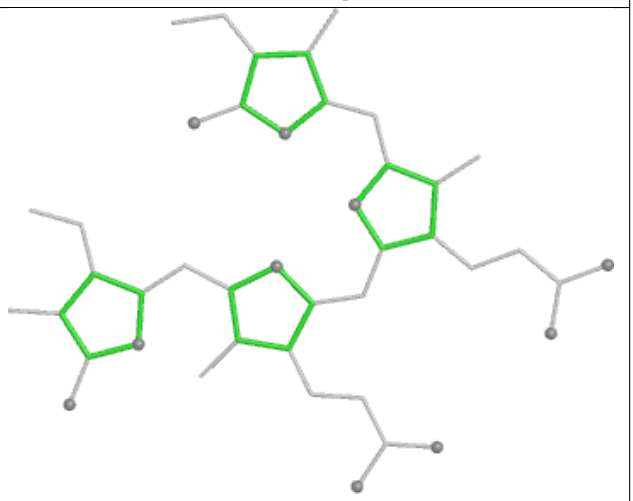
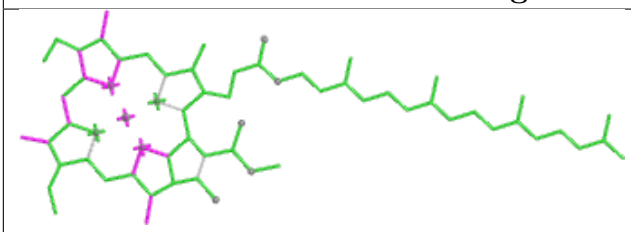


Rings

Ligand CLA BN 834



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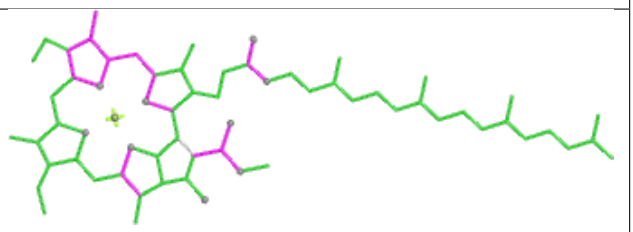

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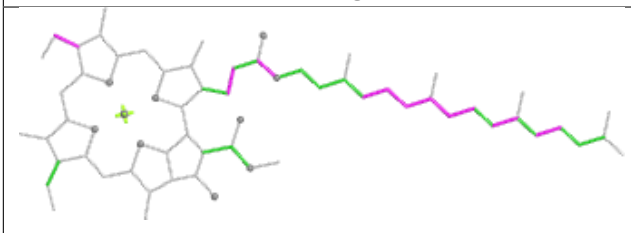

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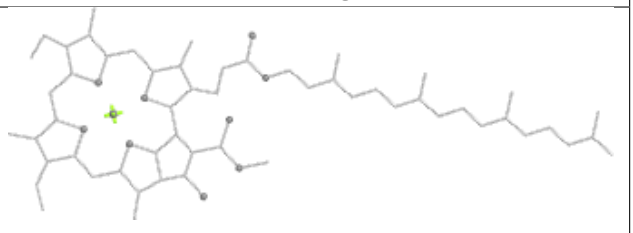

Rings

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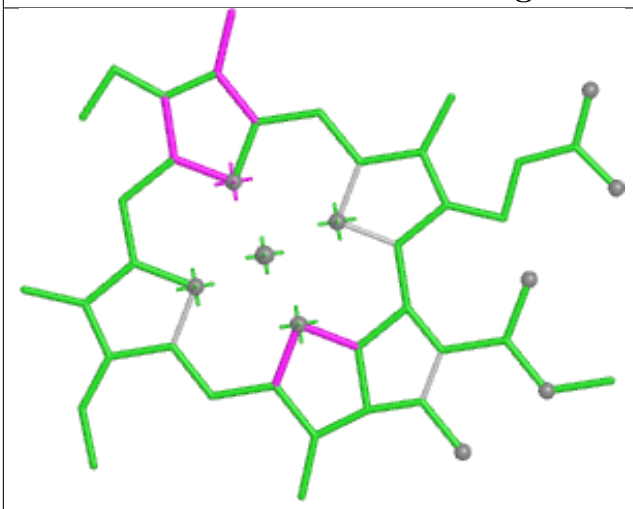

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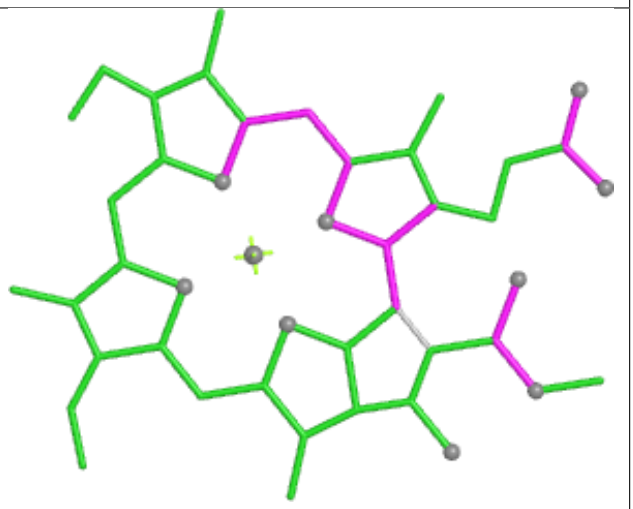

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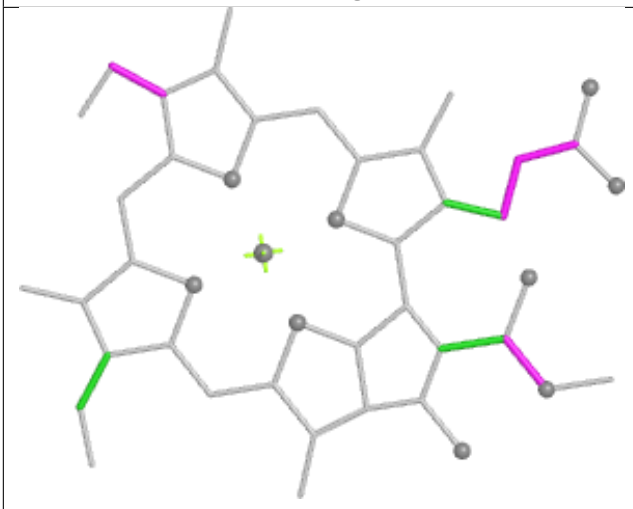
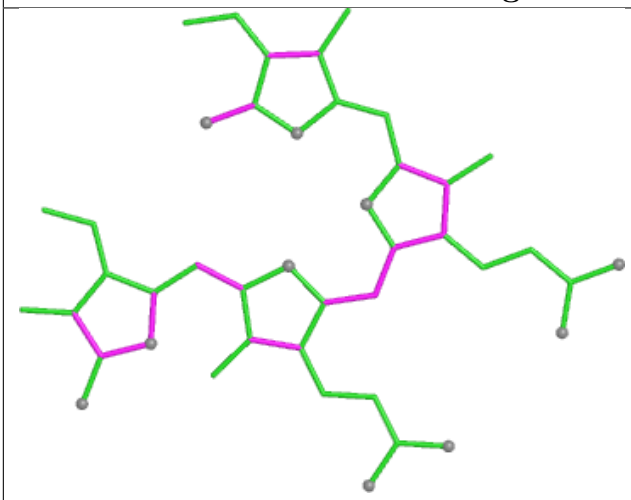


Torsions



Rings

Ligand PEB WM 201



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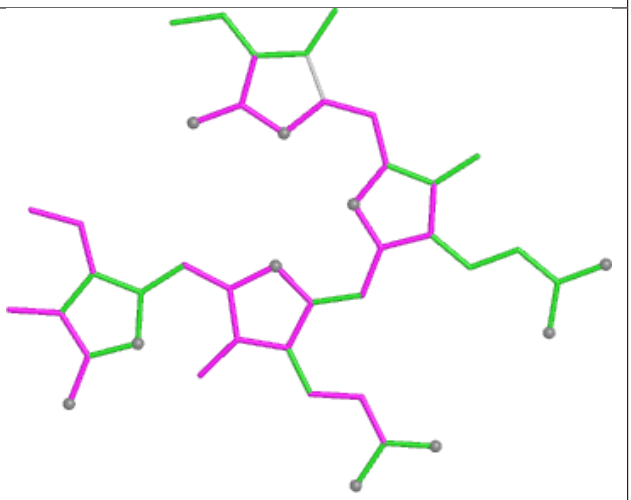

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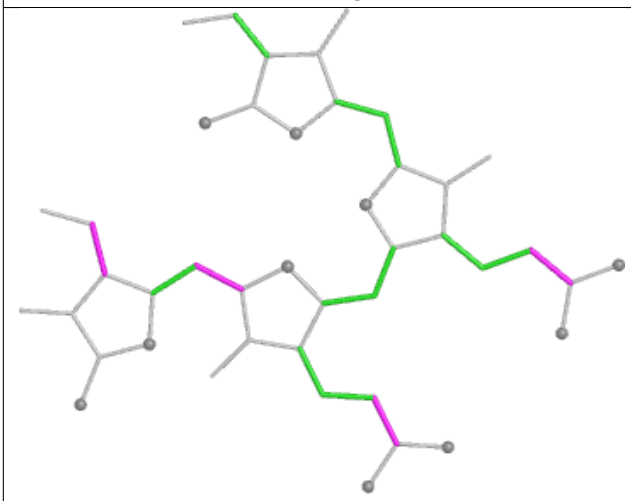

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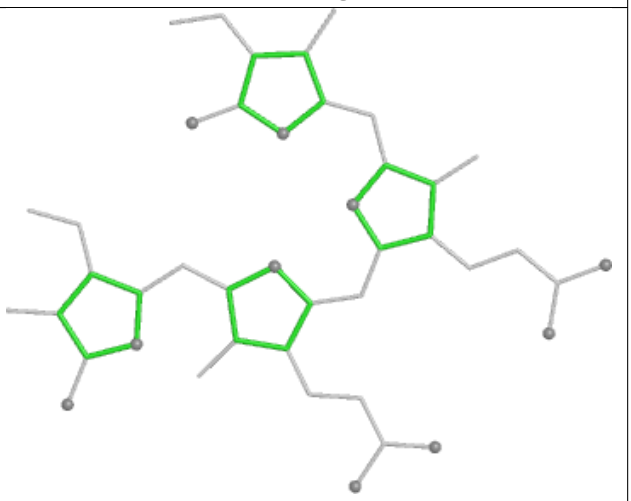
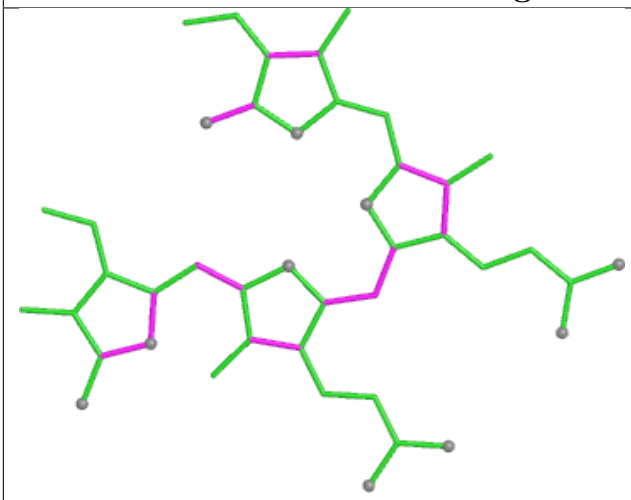


Rings

Ligand PEB dG 202



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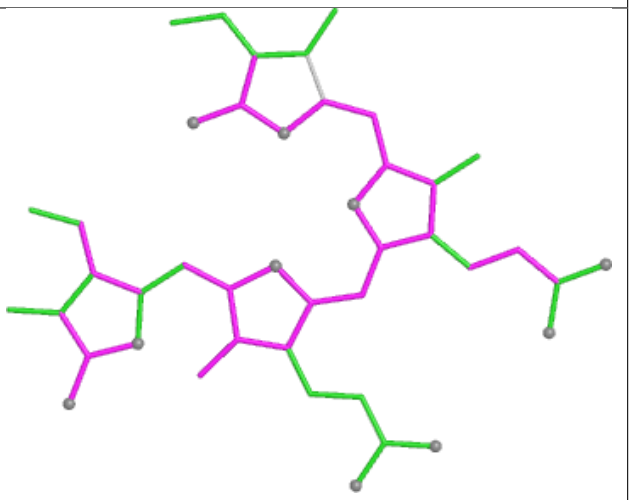

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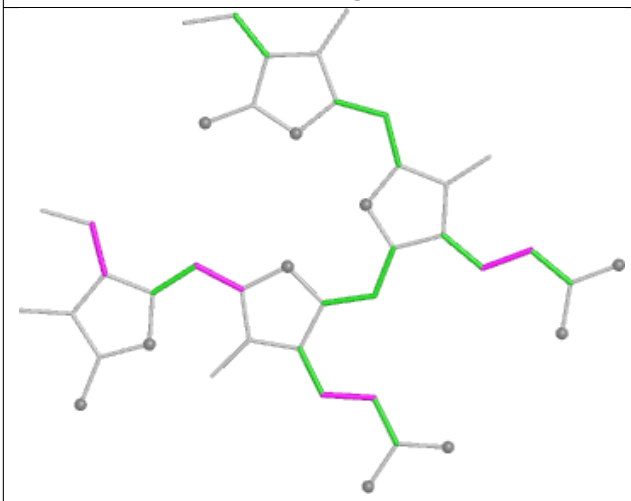

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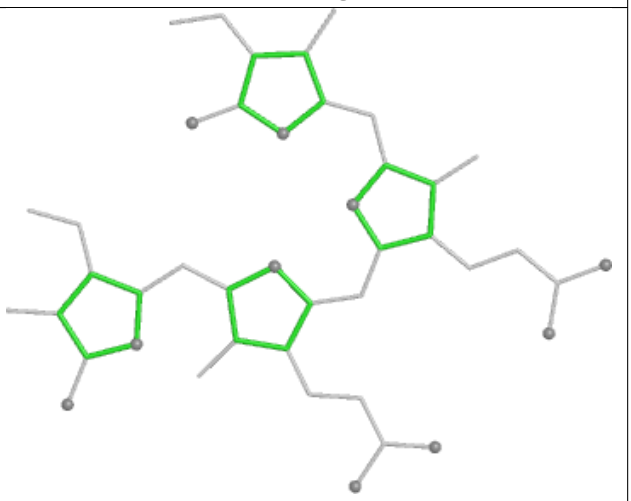
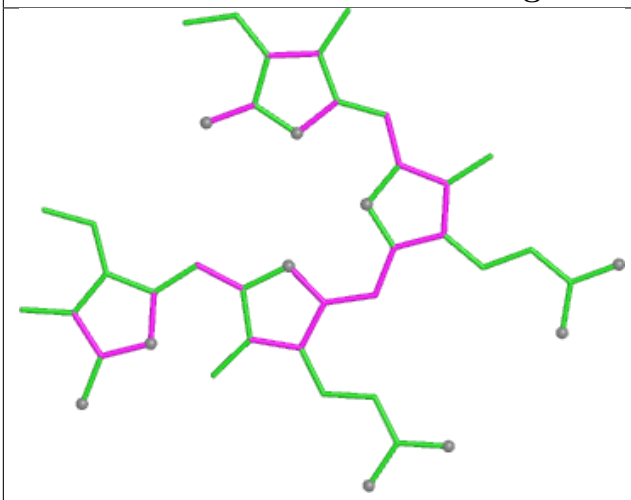


Rings

Ligand PEB j1 203



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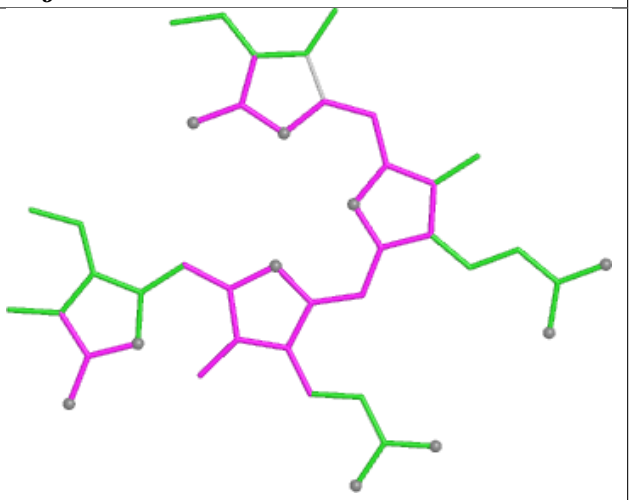

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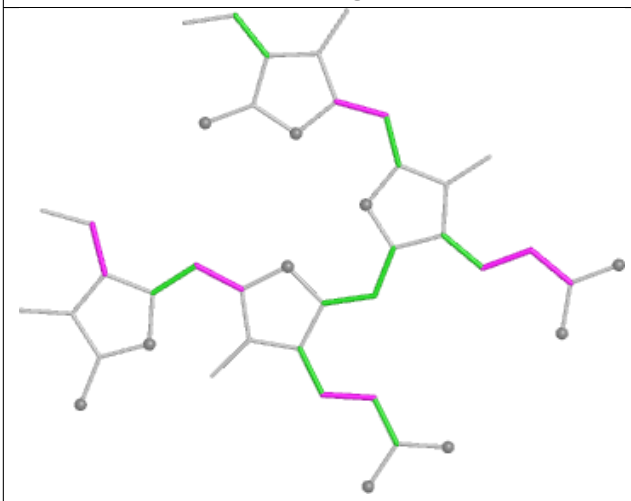

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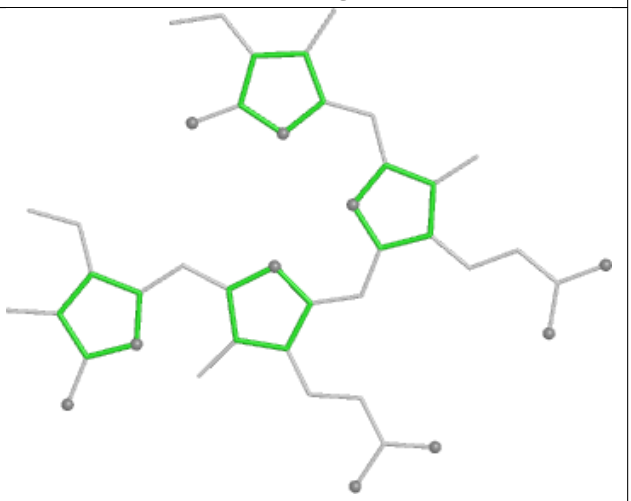
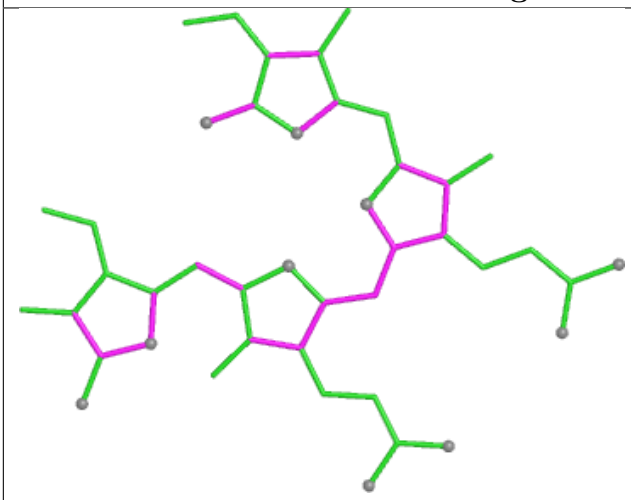


Rings

Ligand PEB QD 202



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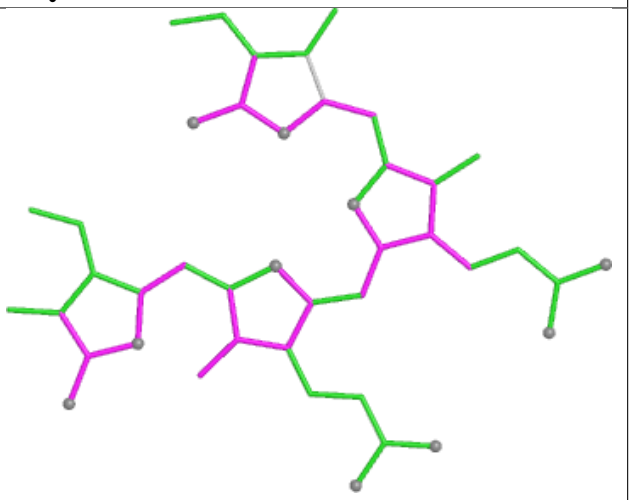

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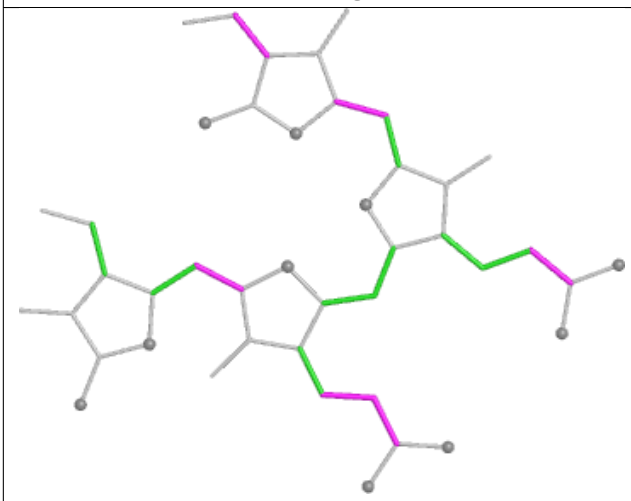

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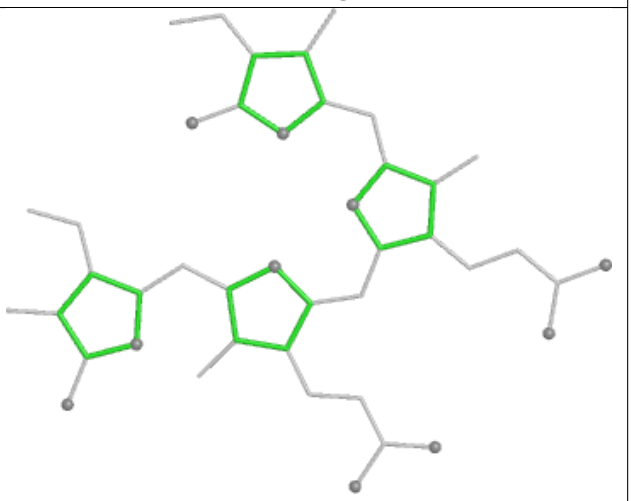
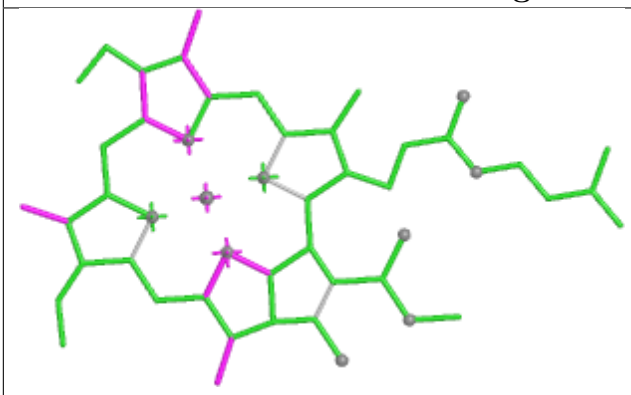


Rings

Ligand CLA AL 405



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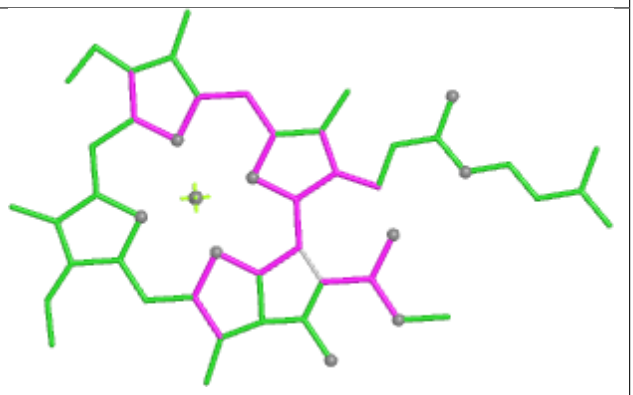

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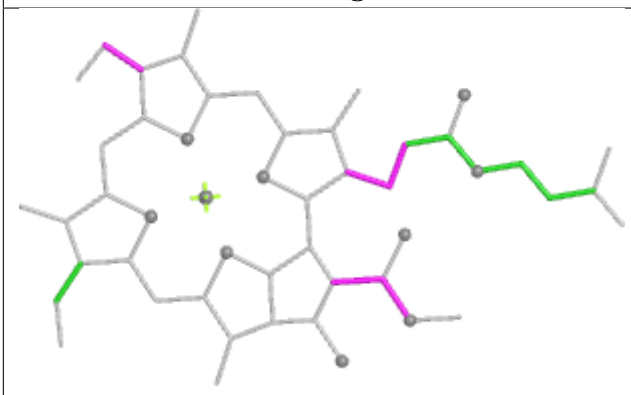

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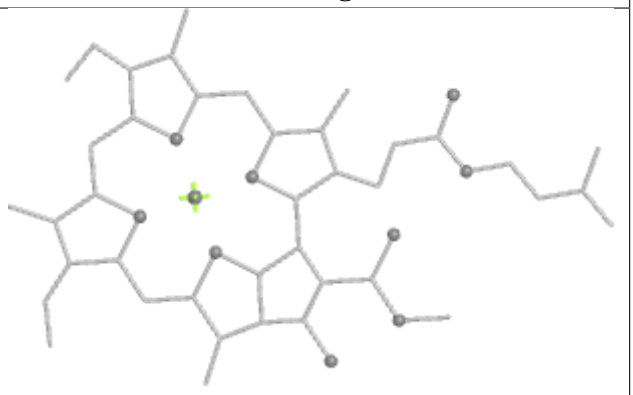
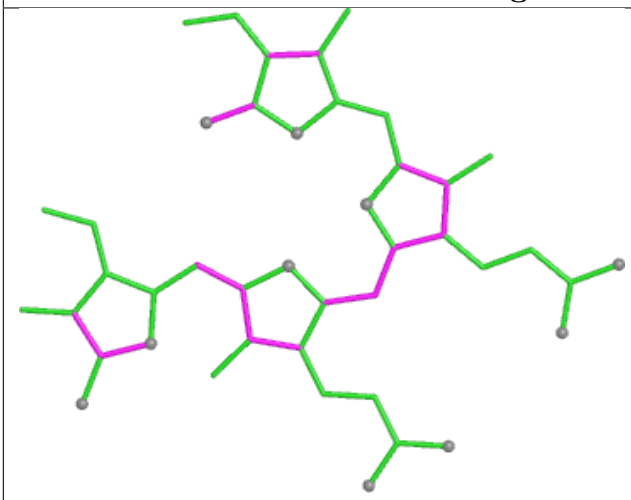


Rings

Ligand PEB YH 202



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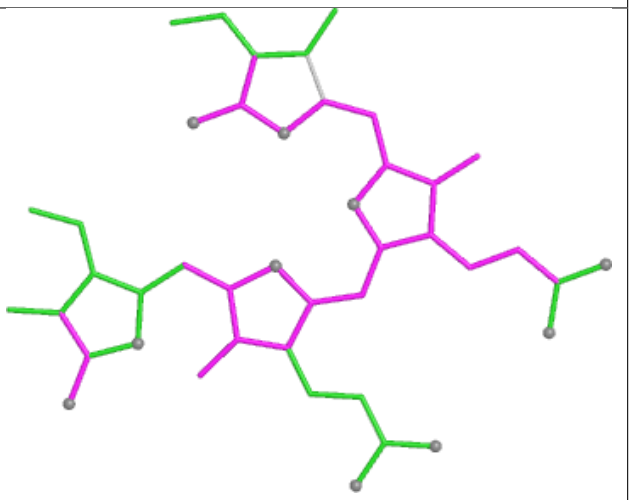

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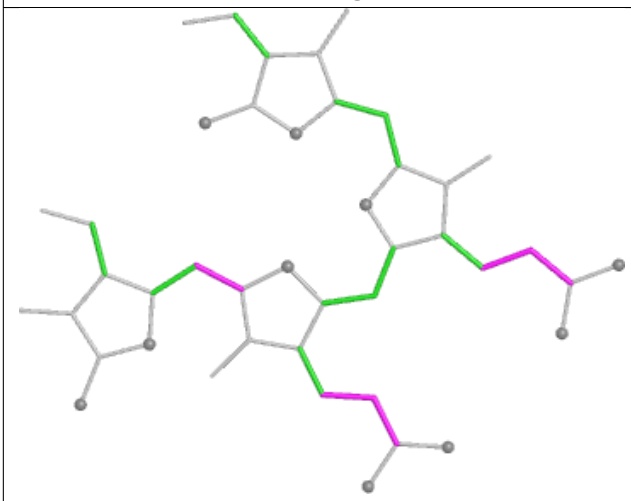

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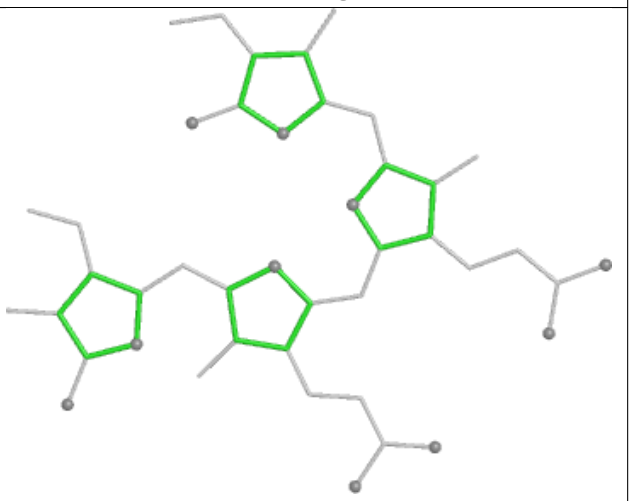
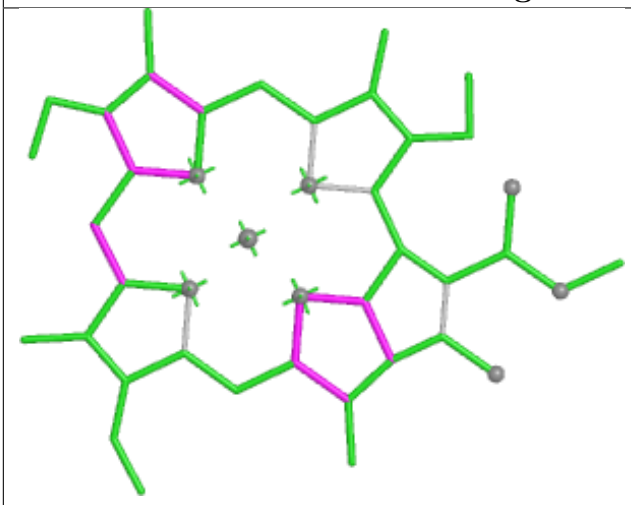


Rings

Ligand CLA 6N 604



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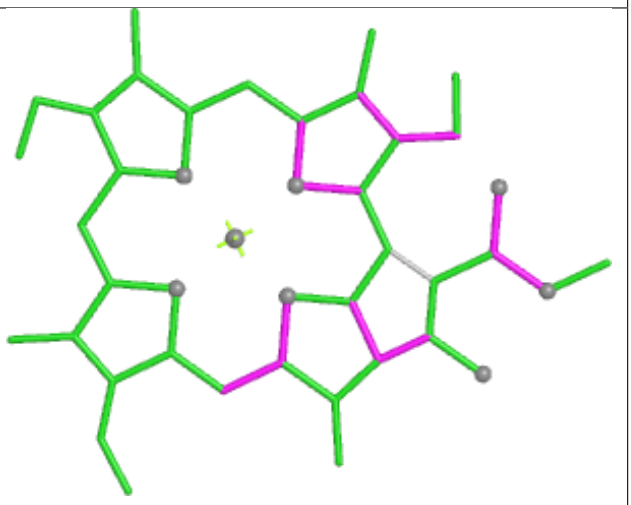

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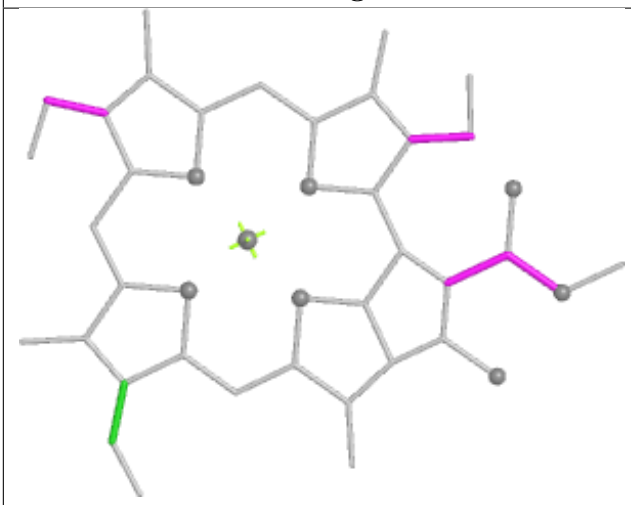
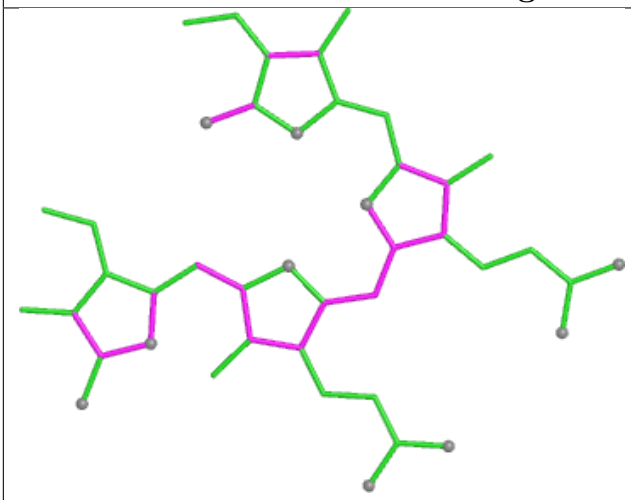


Torsions



Rings

Ligand PEB fG 202



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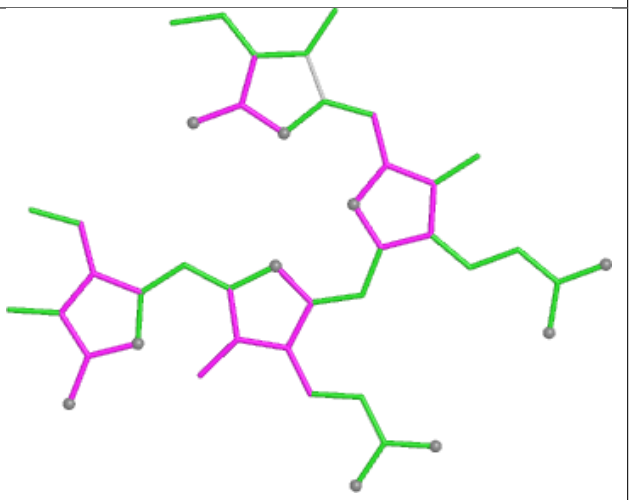

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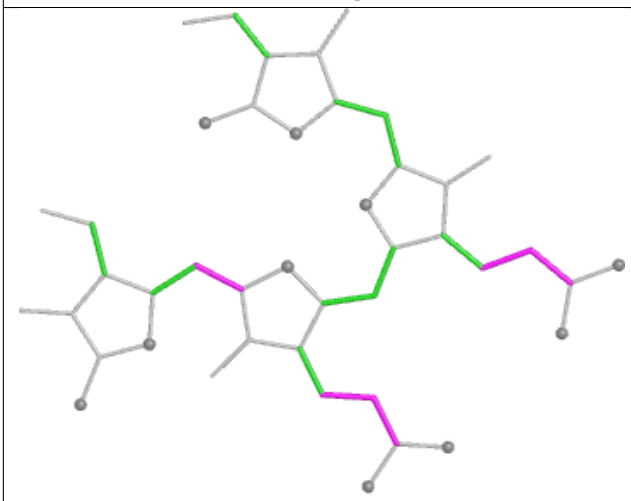

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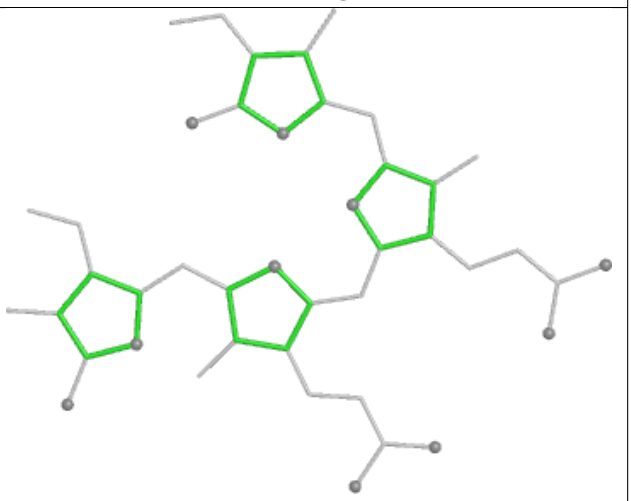
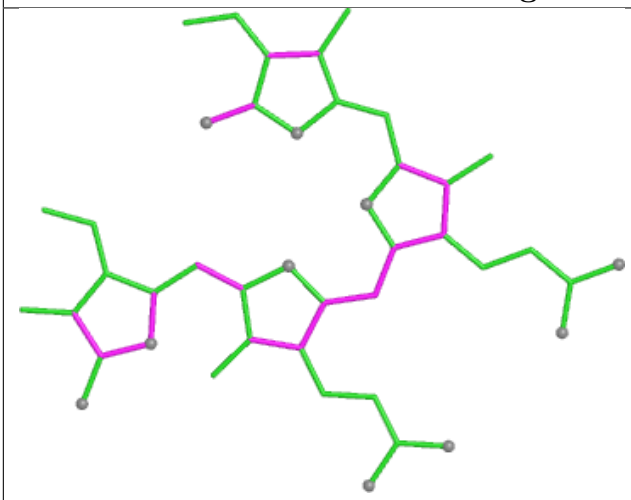


Rings

Ligand PEB g4 203



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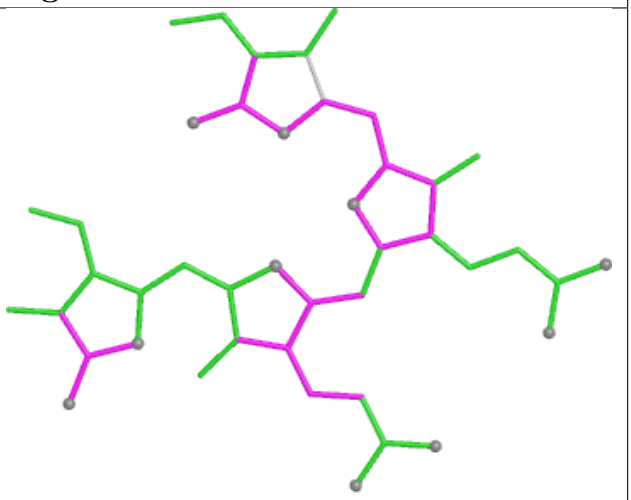
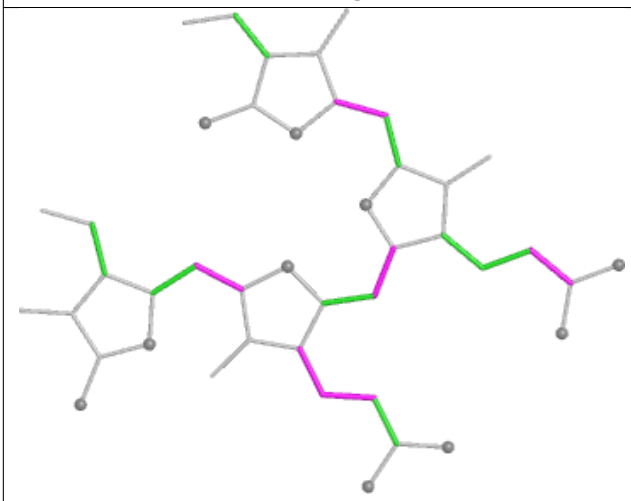


Bond angles



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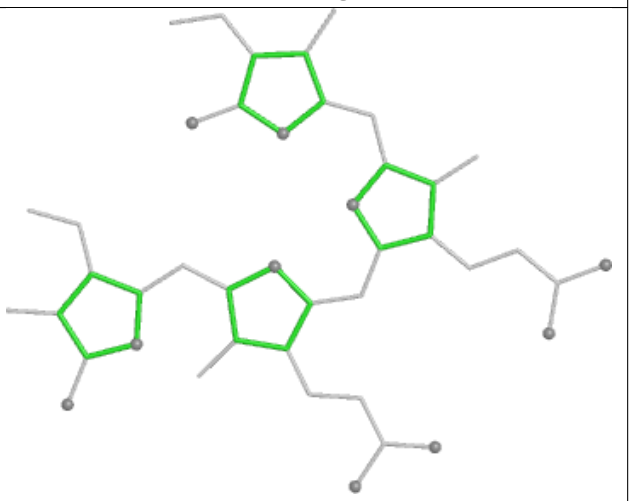
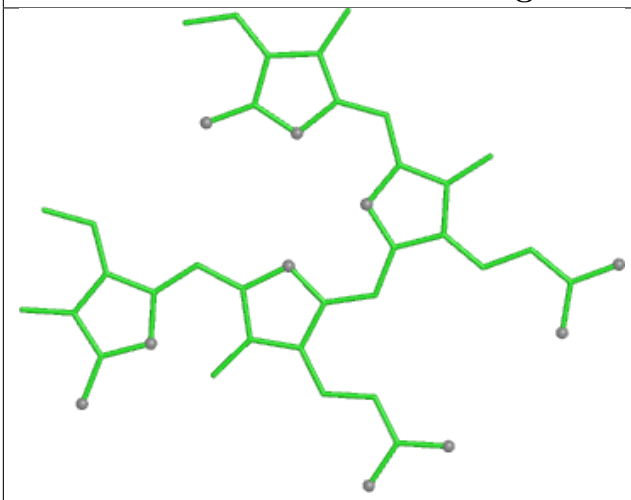


Rings

Ligand PEB C7 202



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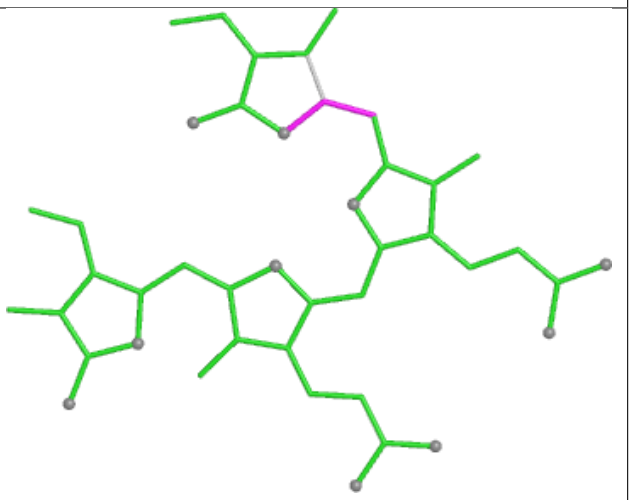
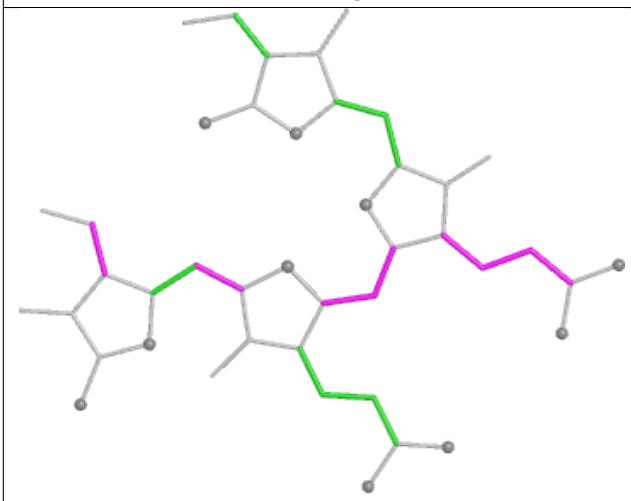


Bond angles



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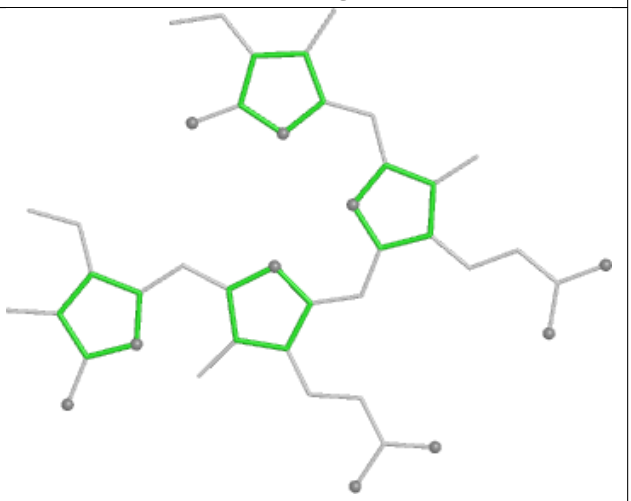
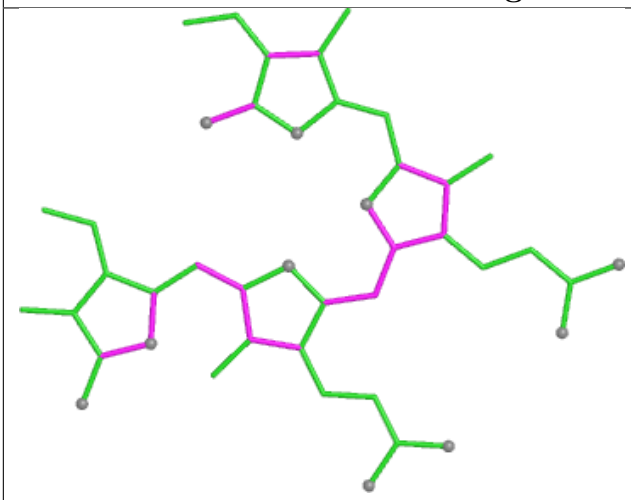
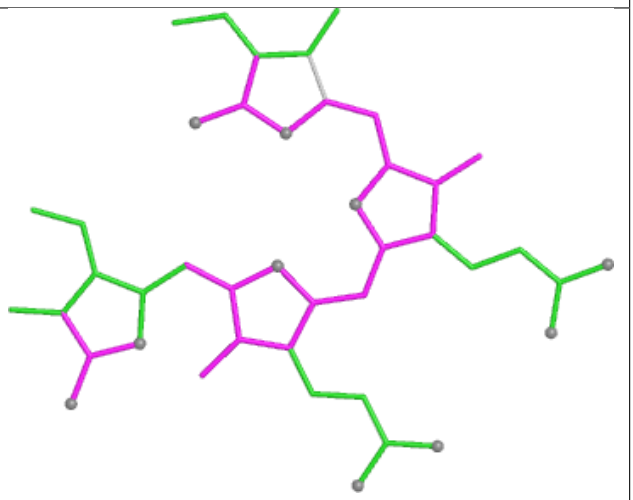


Rings

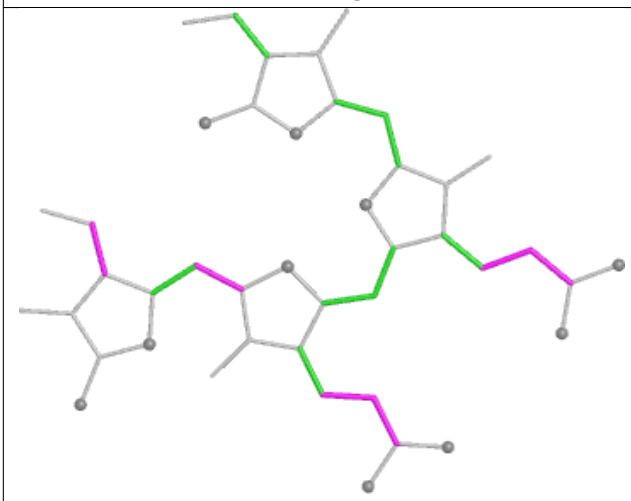
Ligand PEB WH 202



Bond lengths



Bond angles



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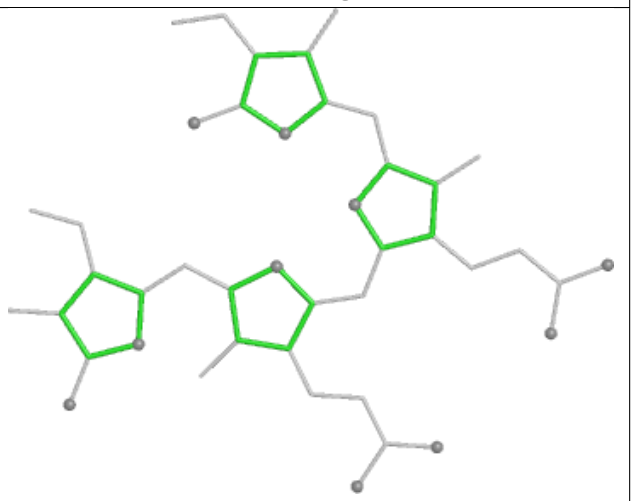
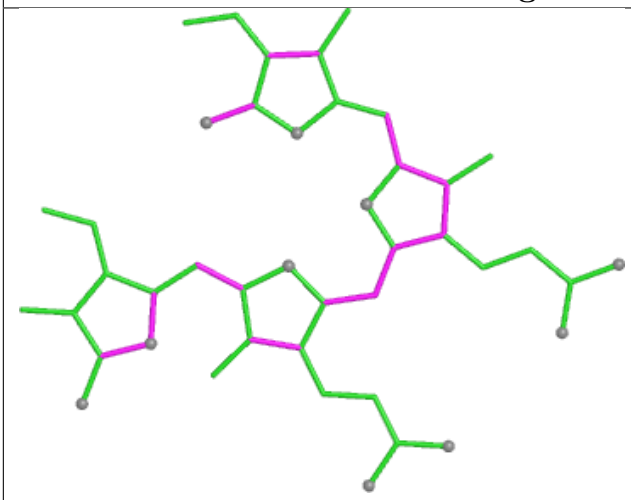


Rings

Ligand PEB iK 201



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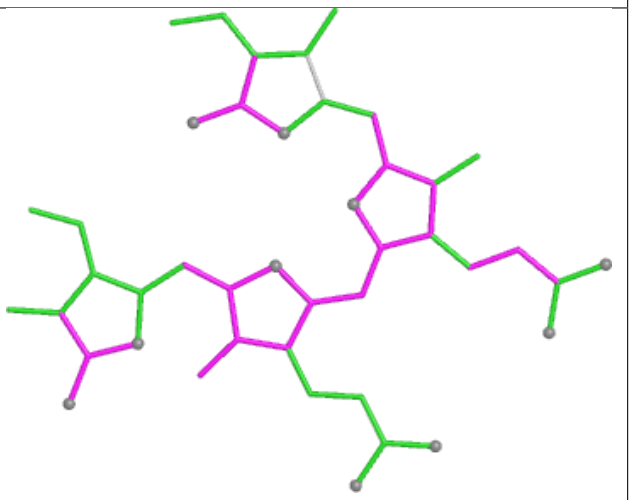

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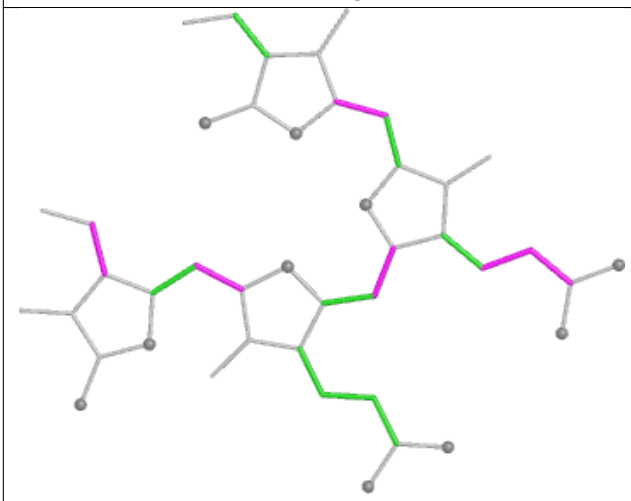

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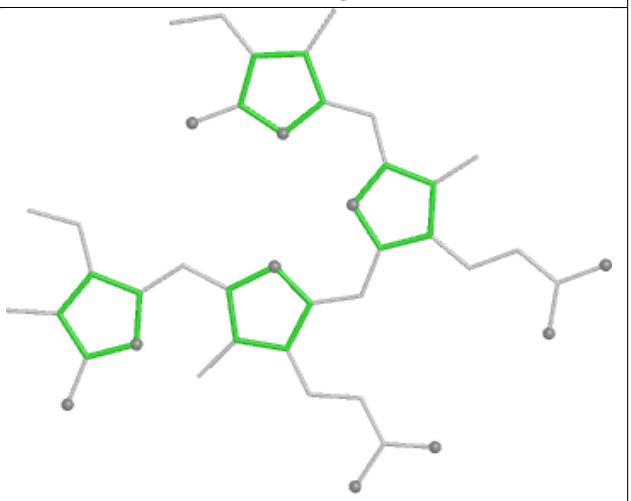
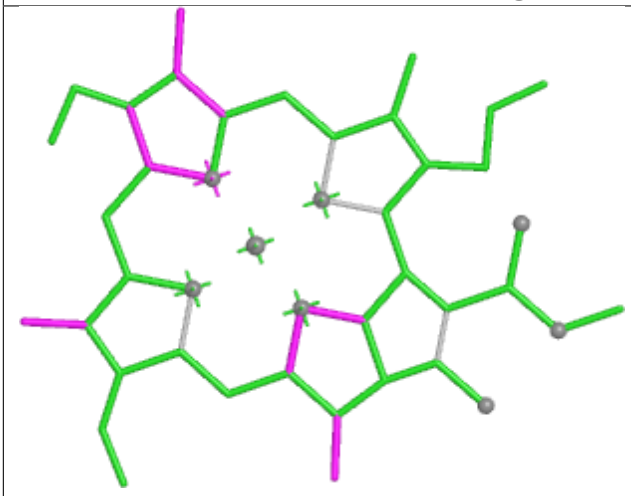
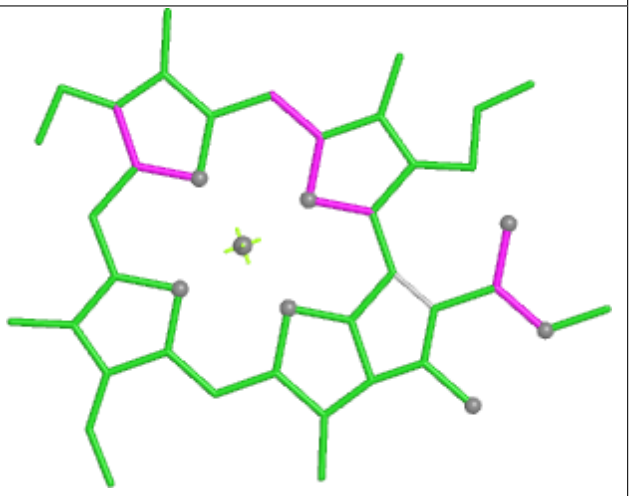


Rings

Ligand CLA BN 829	
	
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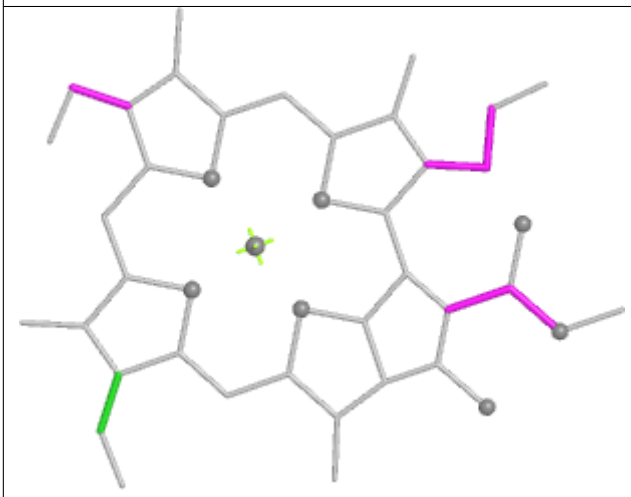
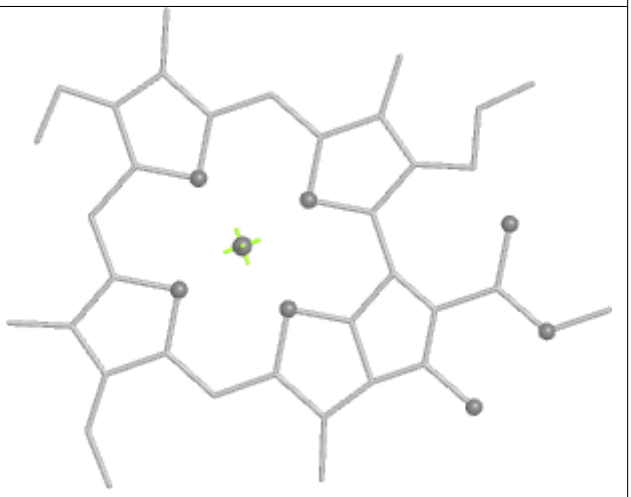
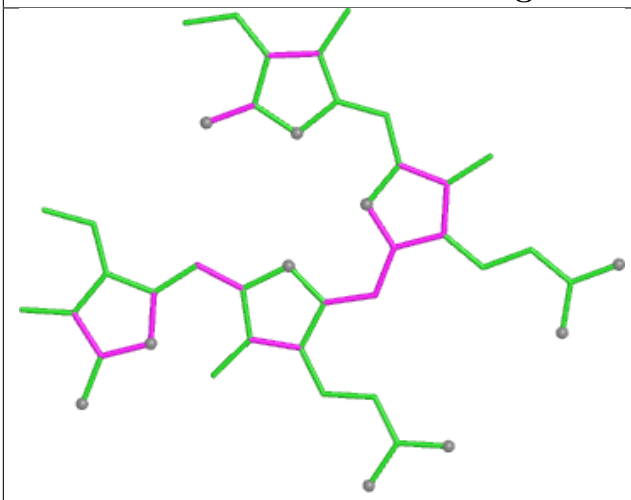
	
Torsions	**Rings**

Ligand PEB CJ 202



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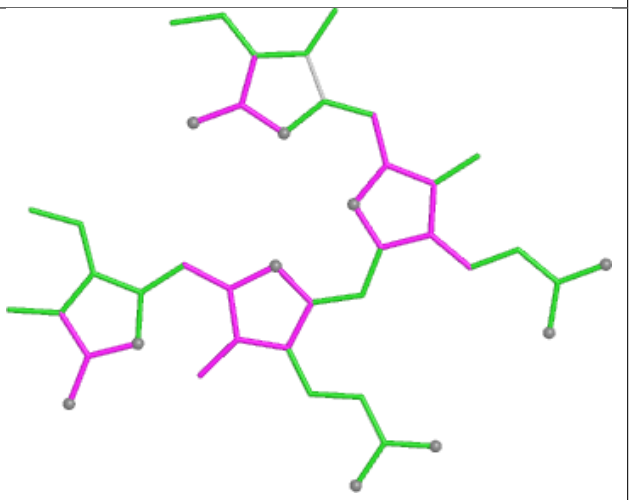

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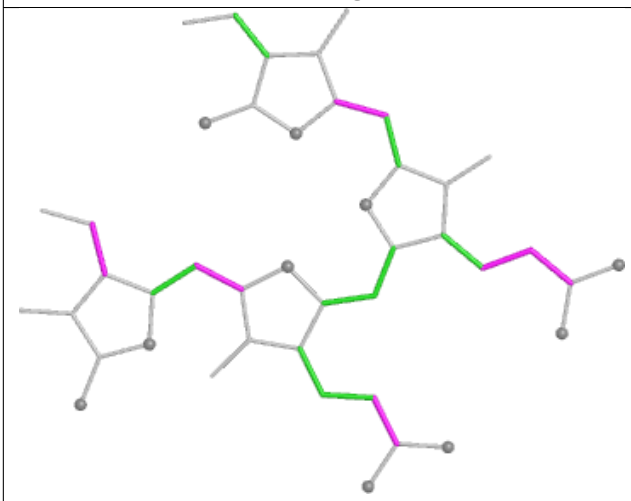

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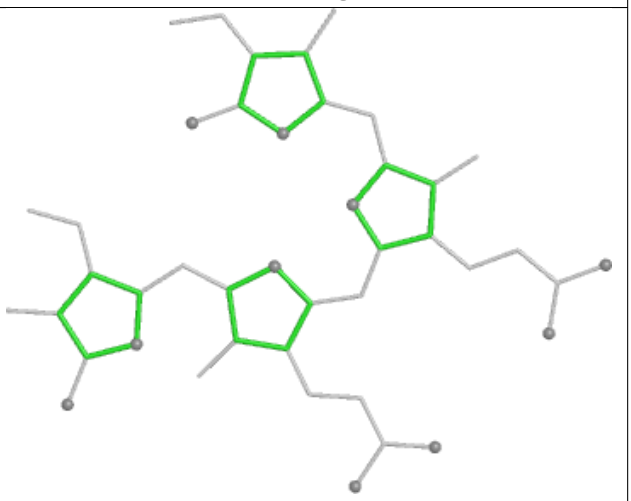
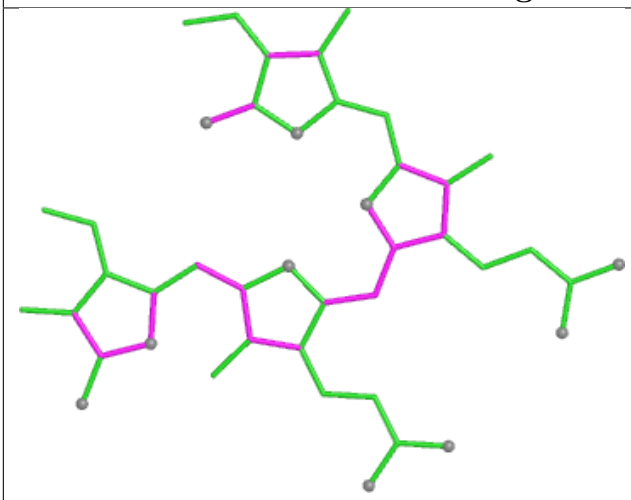


Rings

Ligand PEB SP 202



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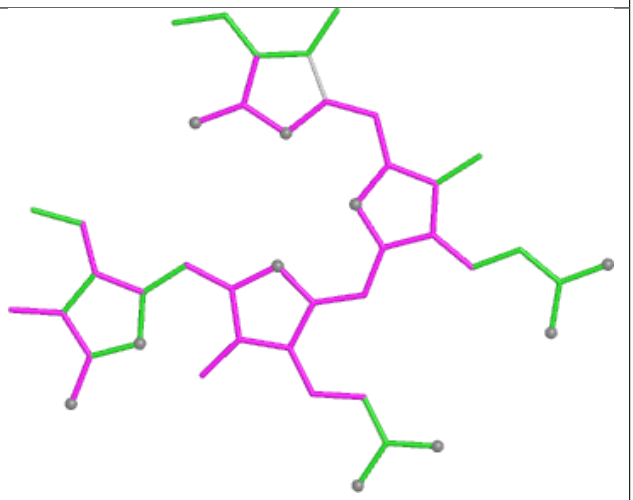

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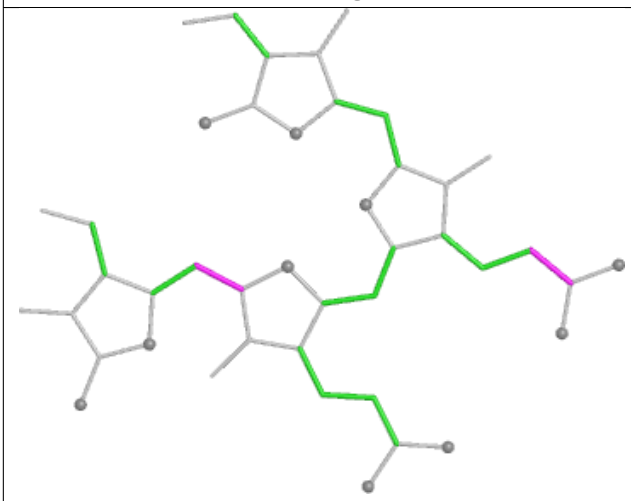

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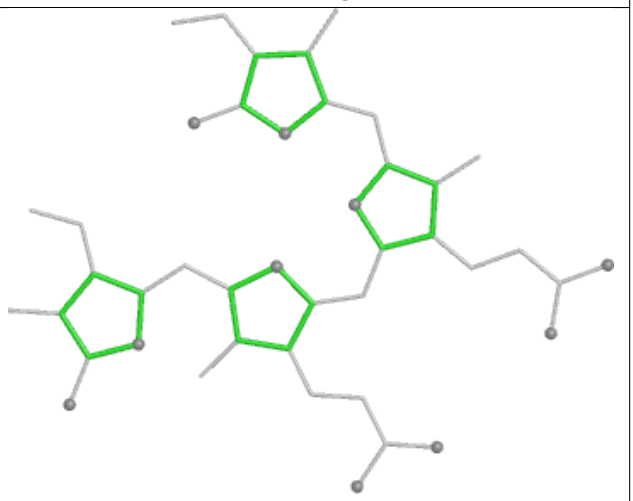
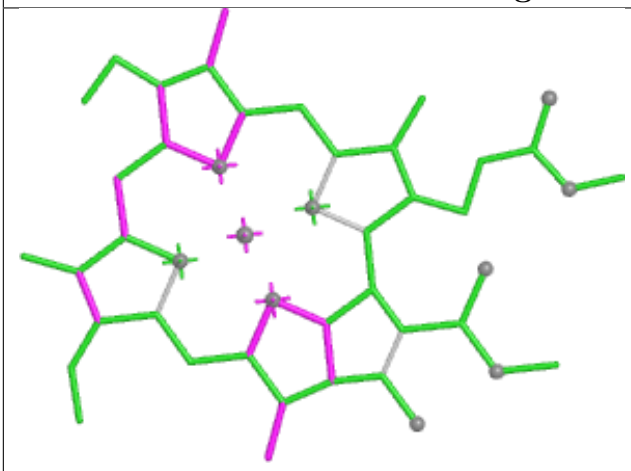


Rings

Ligand CLA 8N 301



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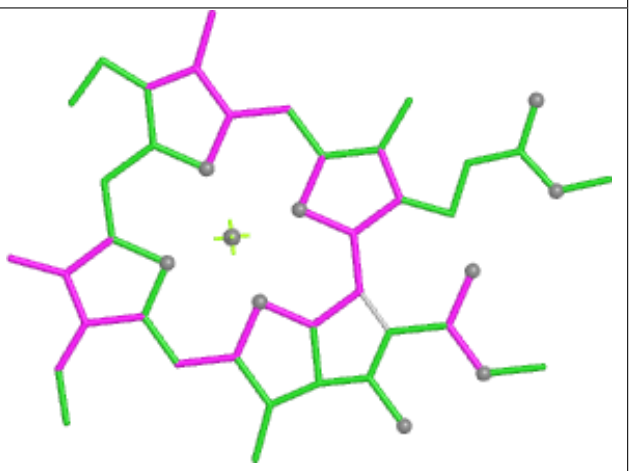

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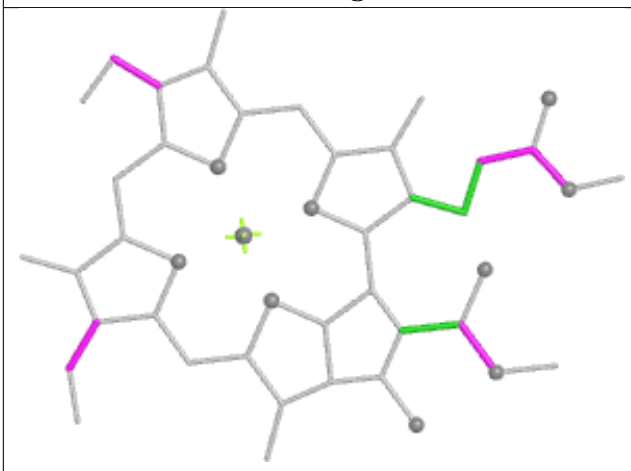

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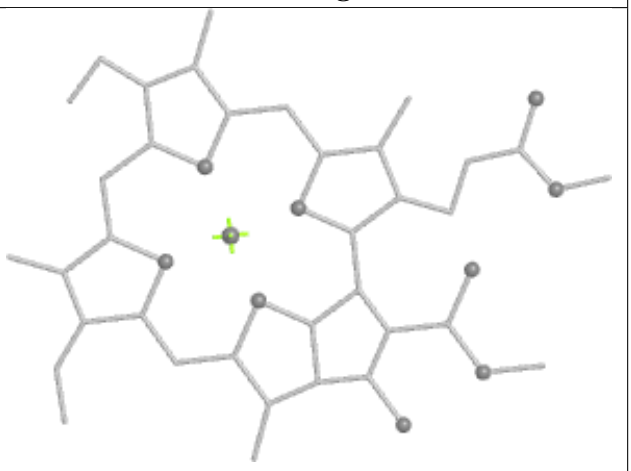
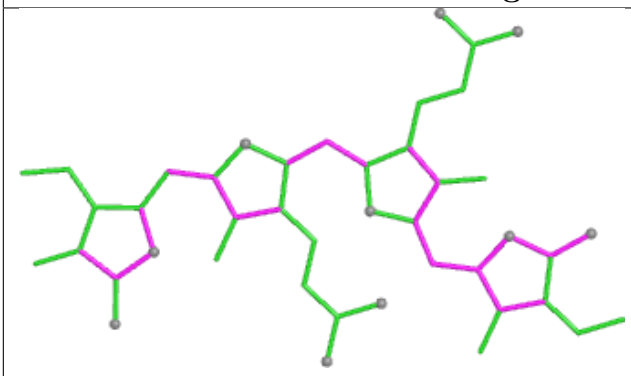


Rings

Ligand CYC H4 1001



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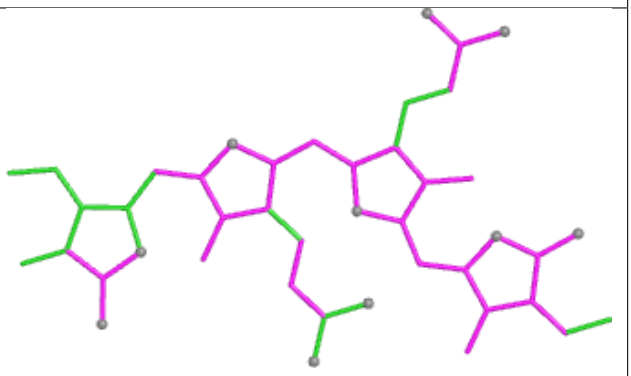

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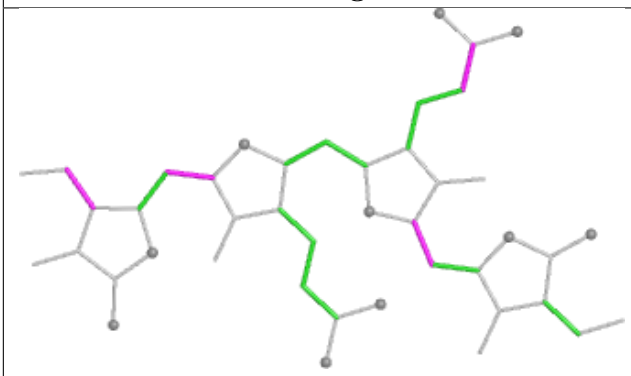

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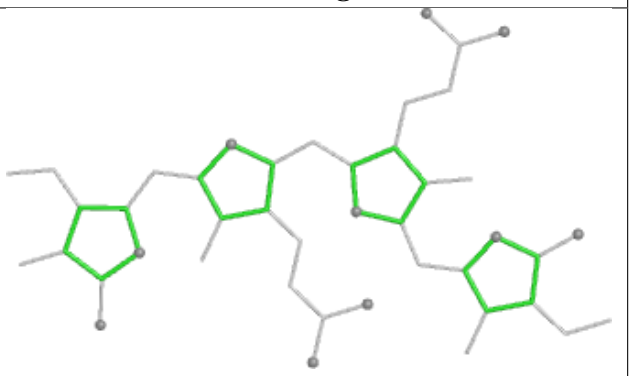
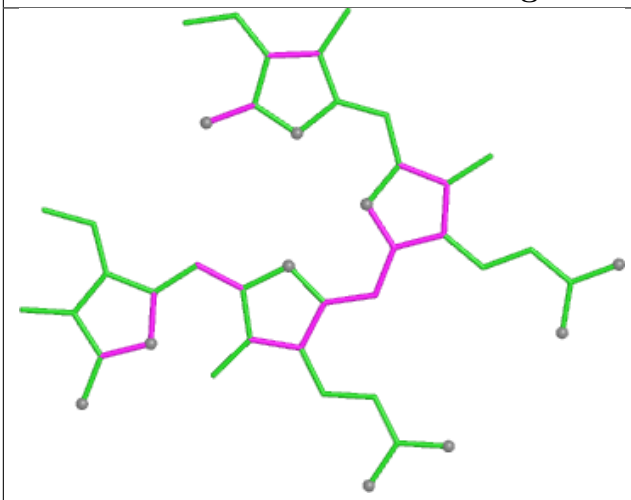


Rings

Ligand PEB z8 201



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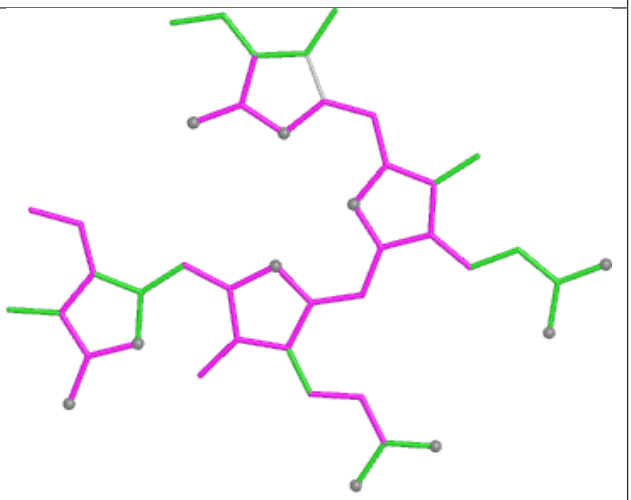

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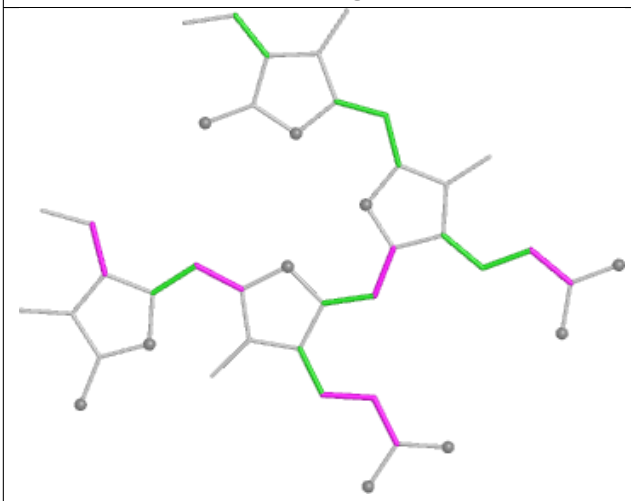

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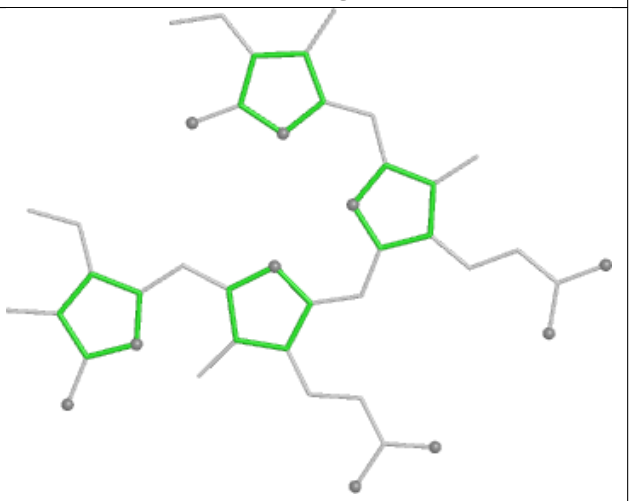
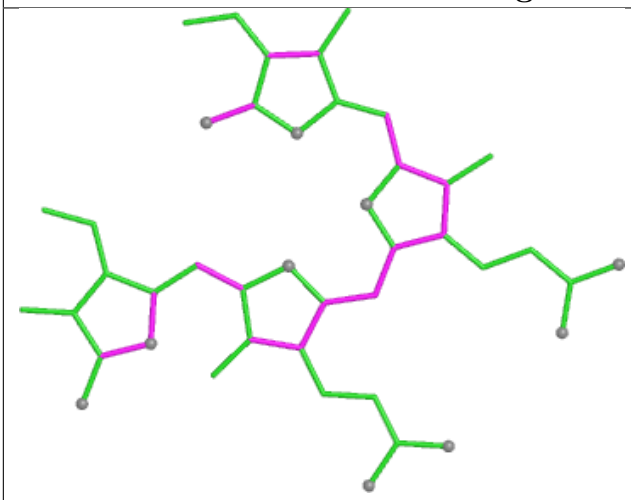


Rings

Ligand PEB lM 201



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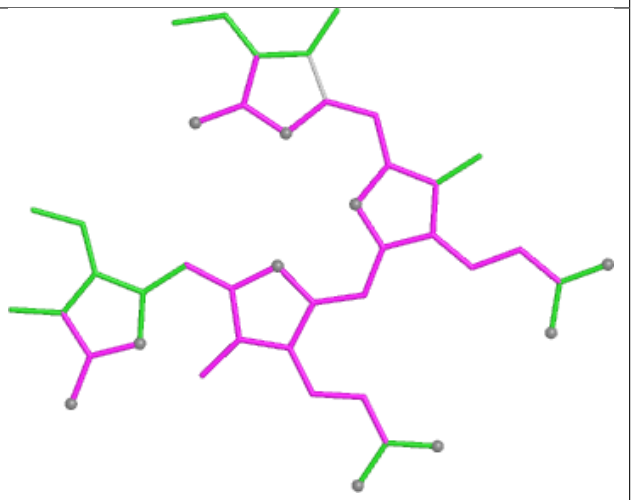

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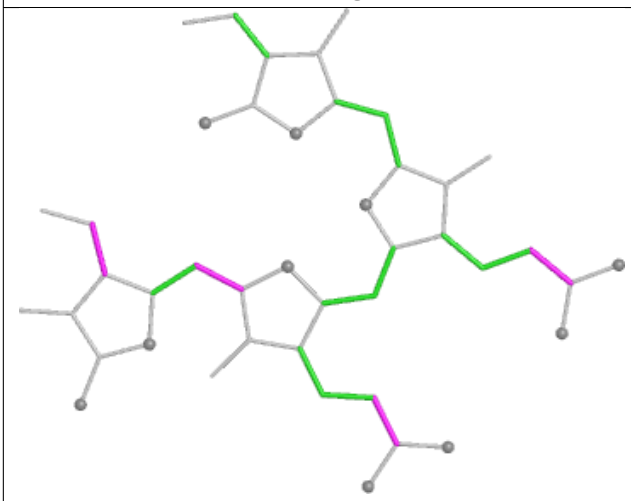

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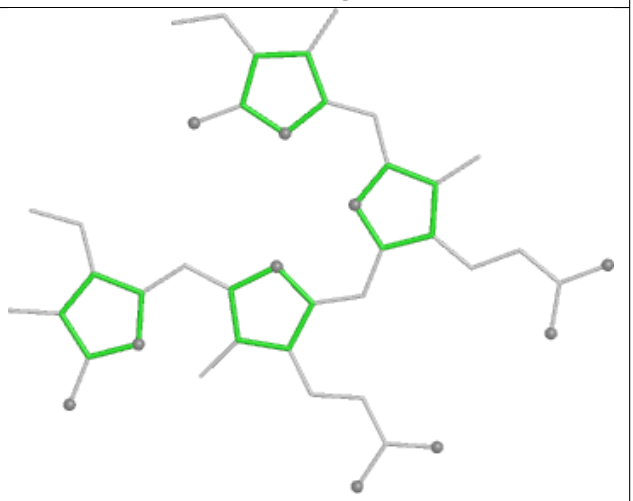
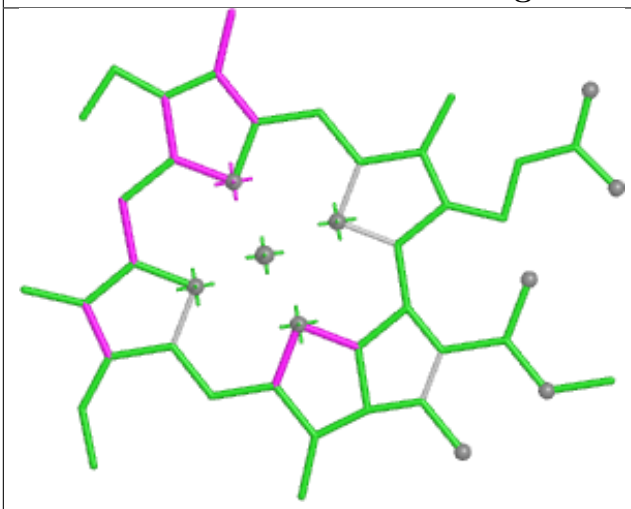


Rings

Ligand CLA 2N 312



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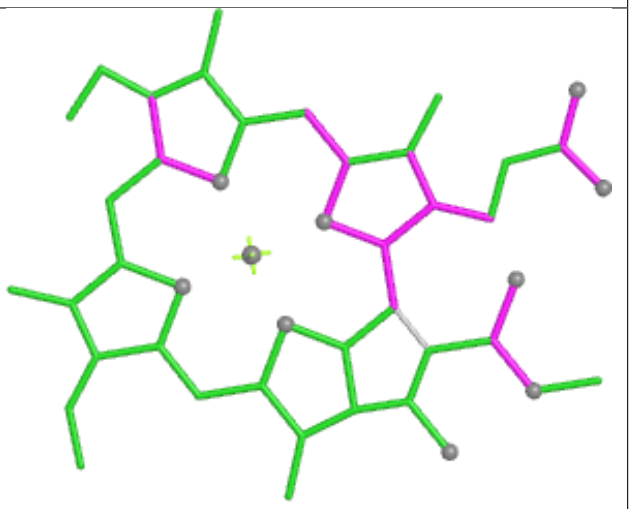

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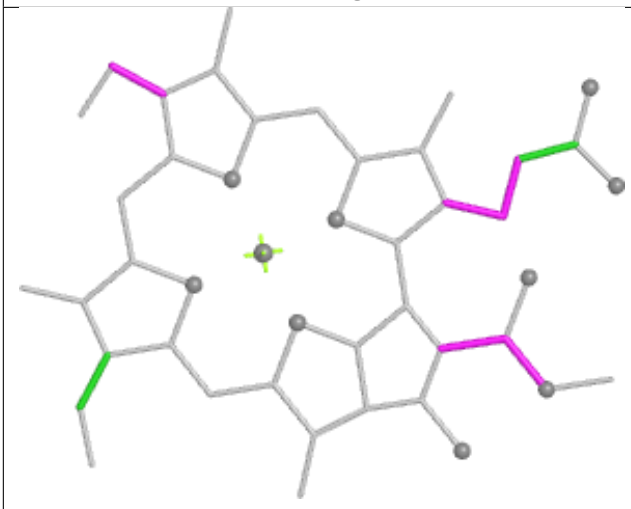
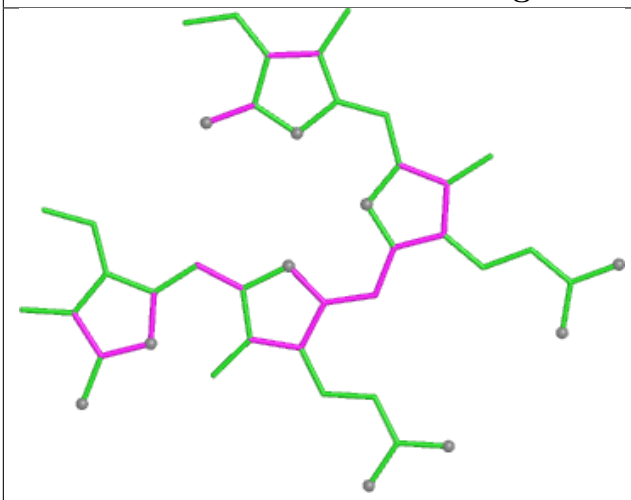


Torsions



Rings

Ligand PEB QF 203



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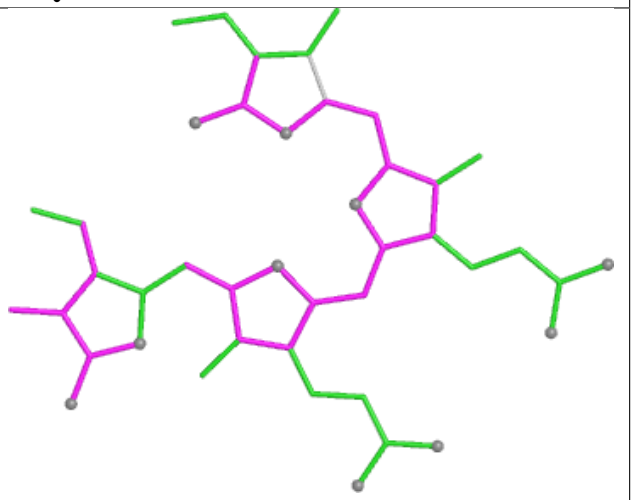
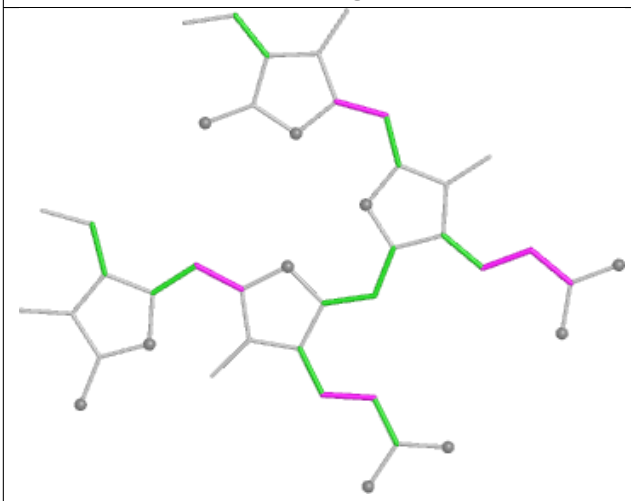


Bond angles



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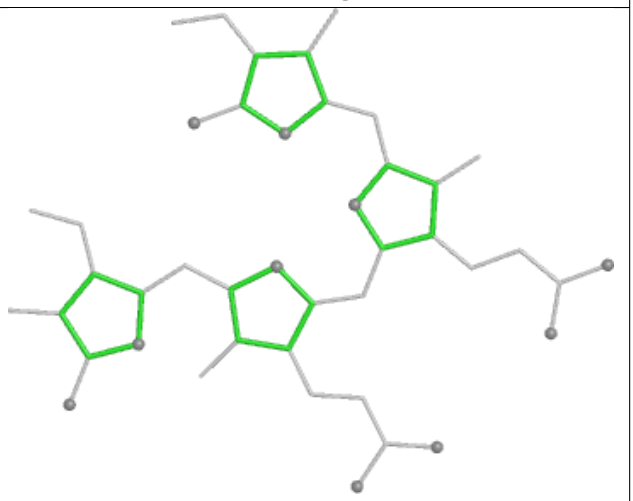
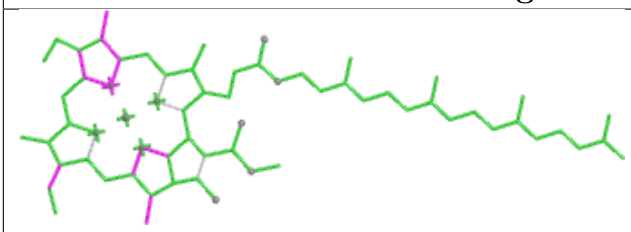


Rings

Ligand CLA dL 401



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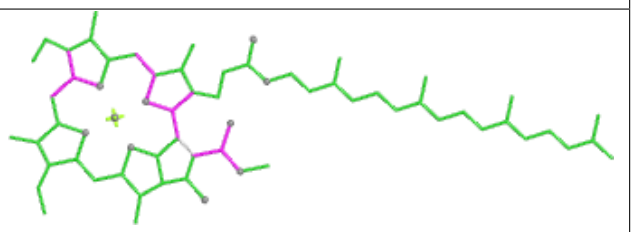
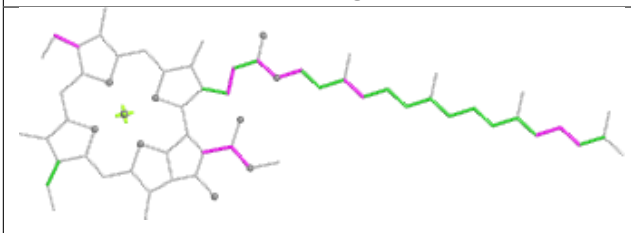


Bond angles



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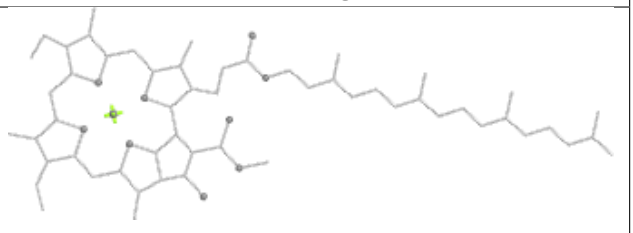
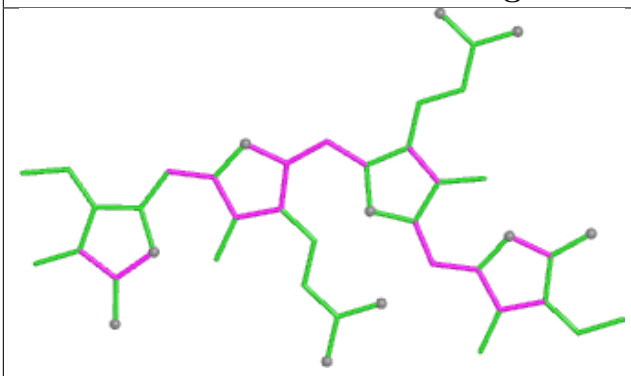


Rings

Ligand CYC V3 1001



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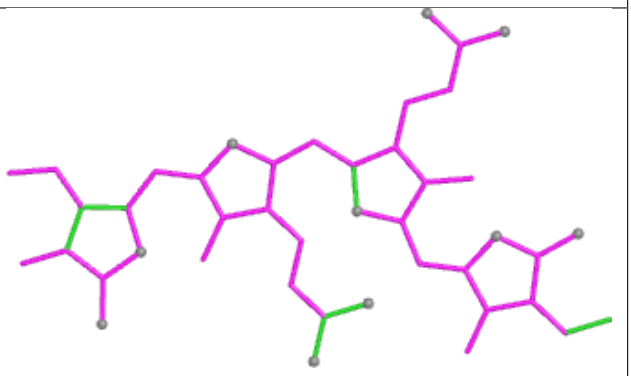
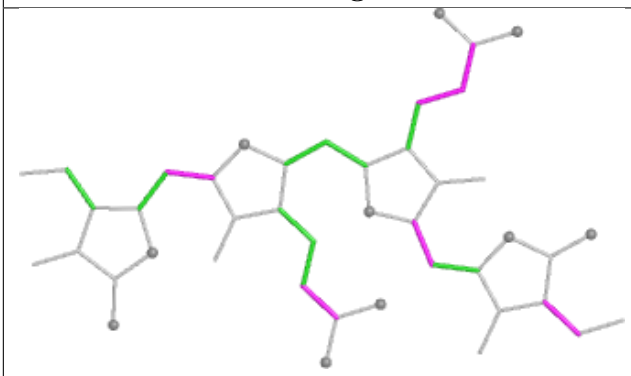


Bond angles



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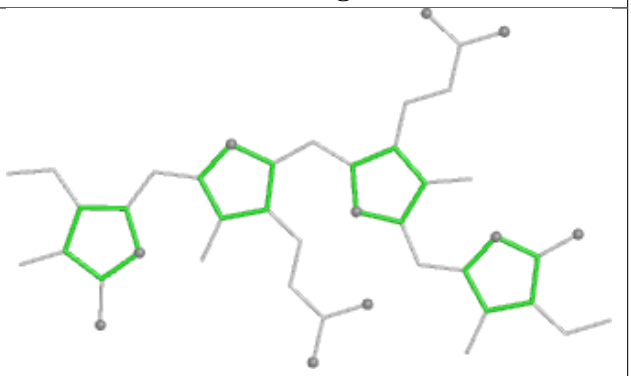
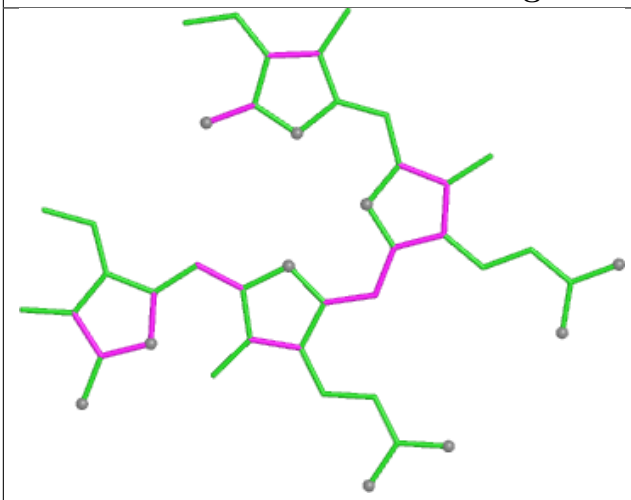


Rings

Ligand PEB lJ 201



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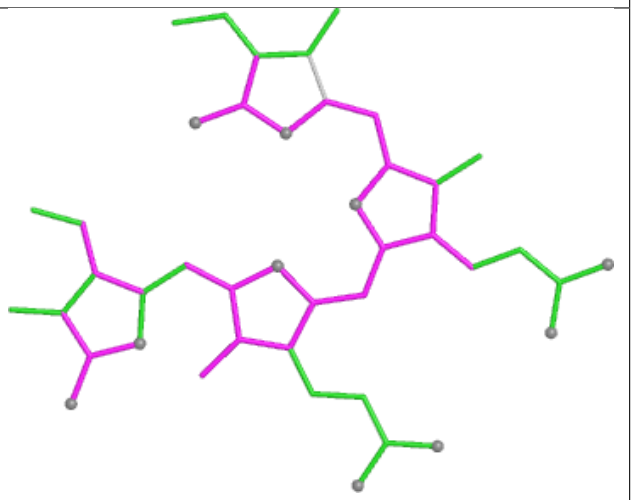
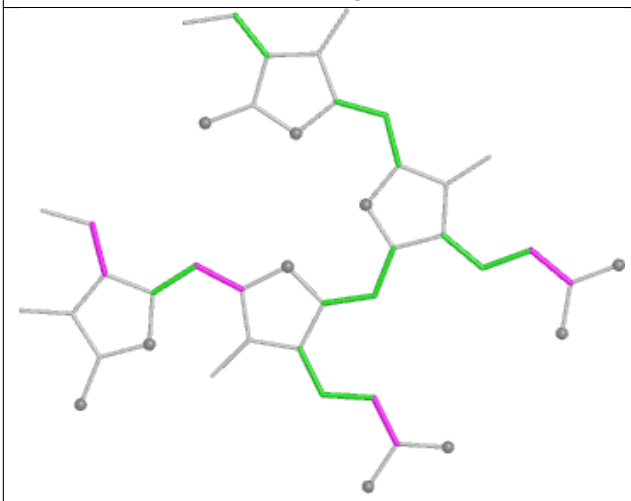


Bond angles



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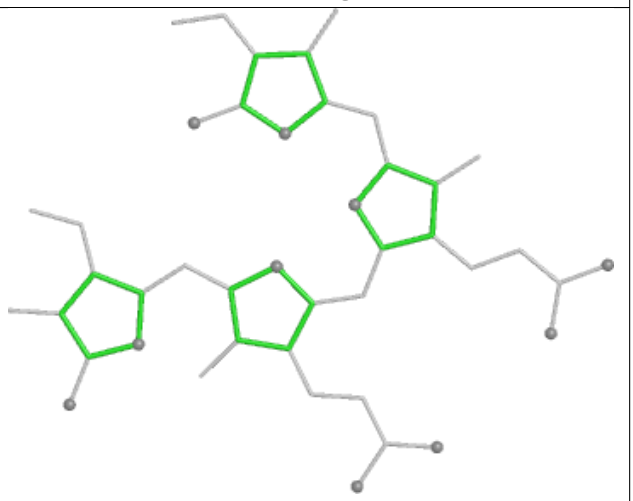
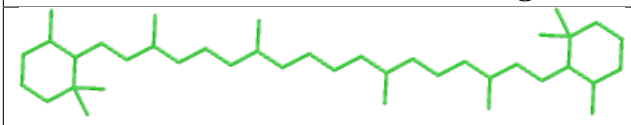


Rings

Ligand BCR d6 405



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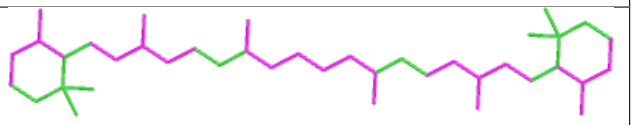
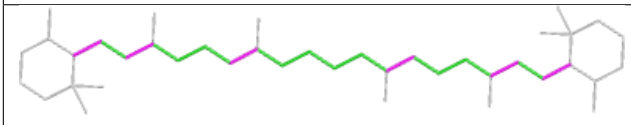


Bond angles



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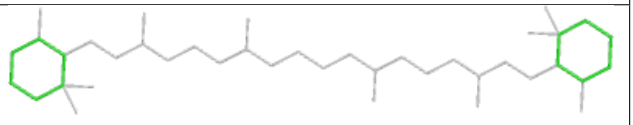
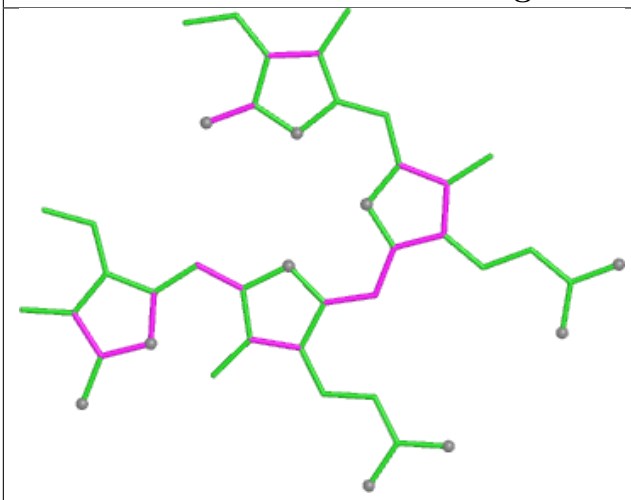


Rings

Ligand PEB IM 201



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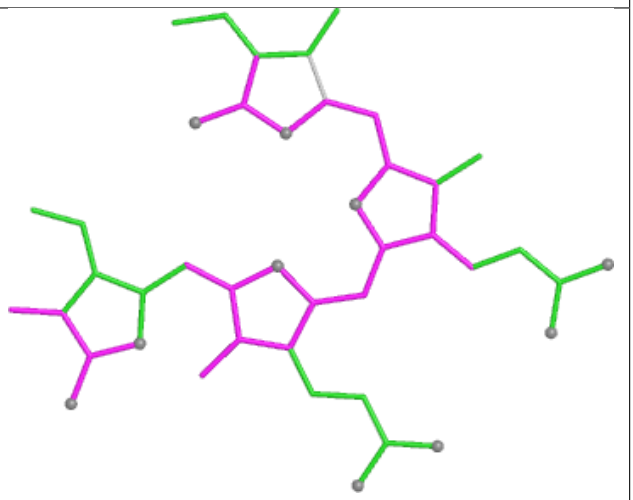

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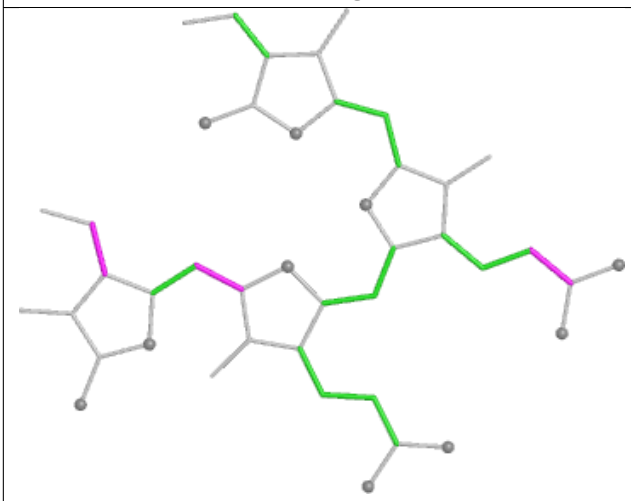

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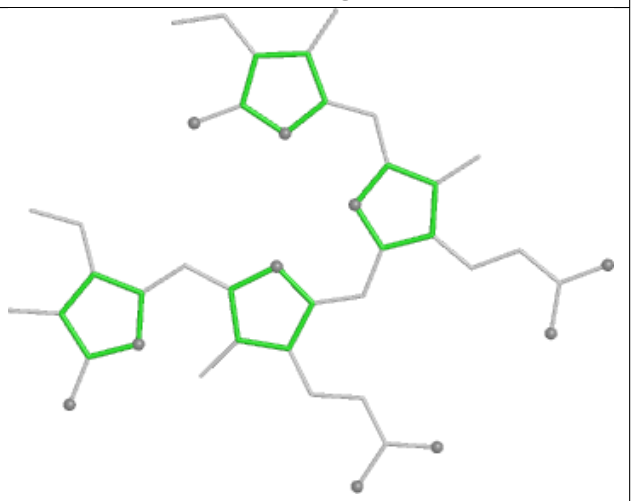
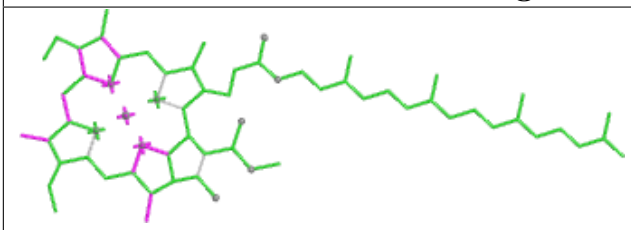


Rings

Ligand CLA B2 804



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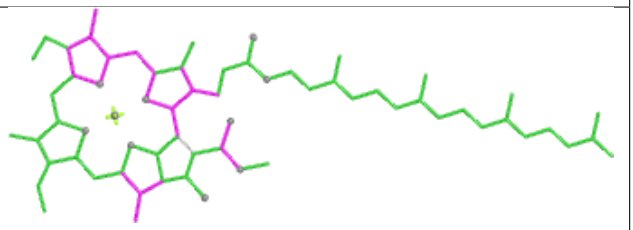

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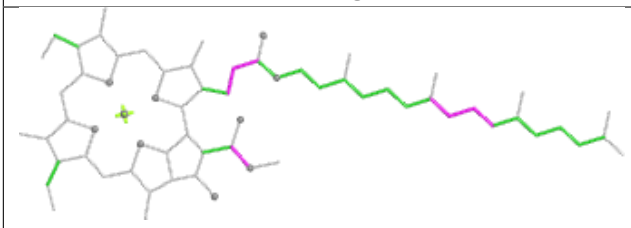

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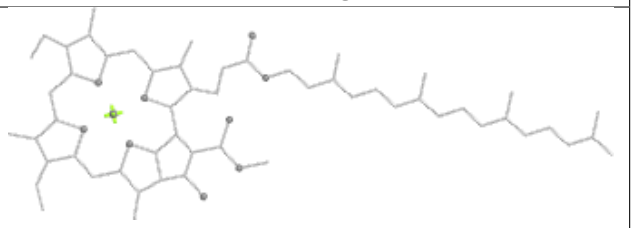
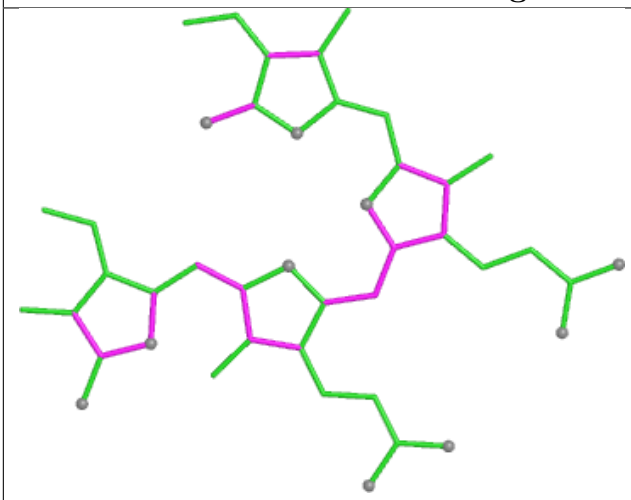


Rings

Ligand PEB FM 202



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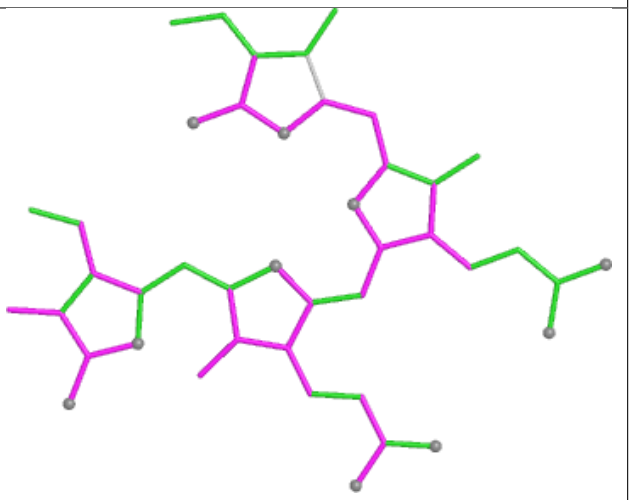

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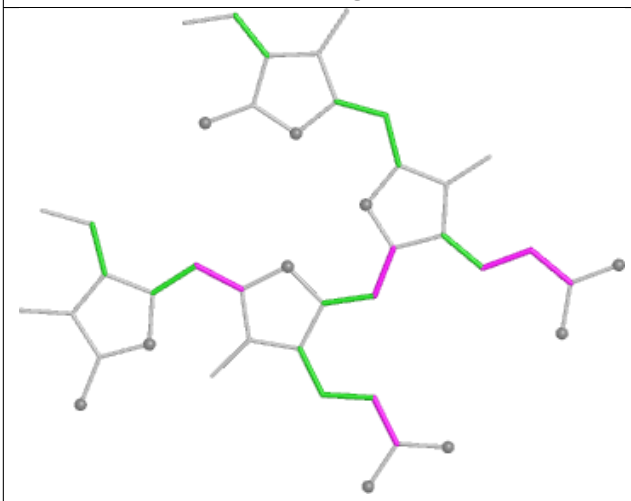

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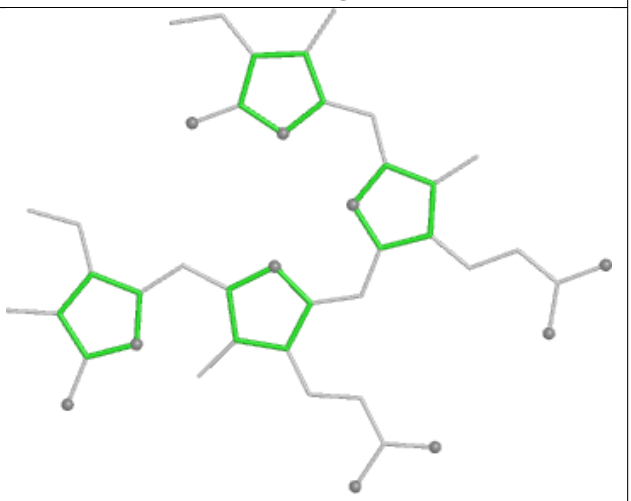
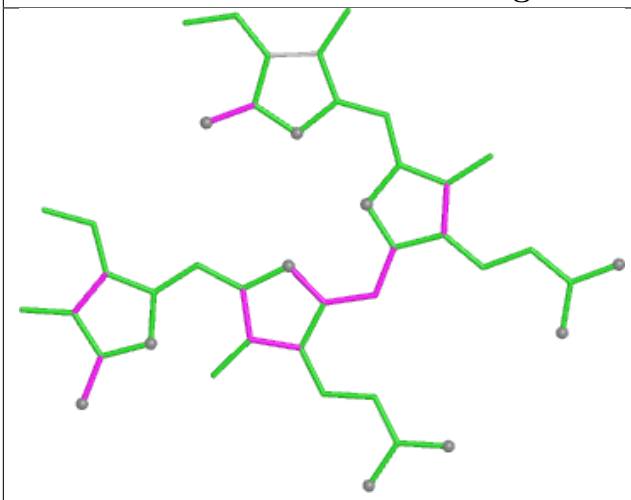


Rings

Ligand PUB AJ 304



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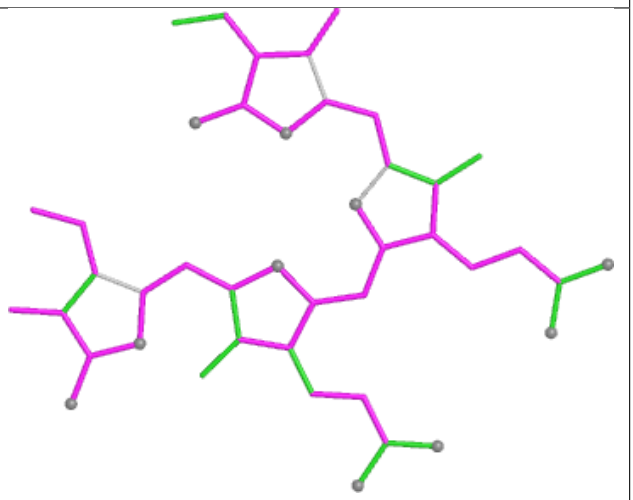

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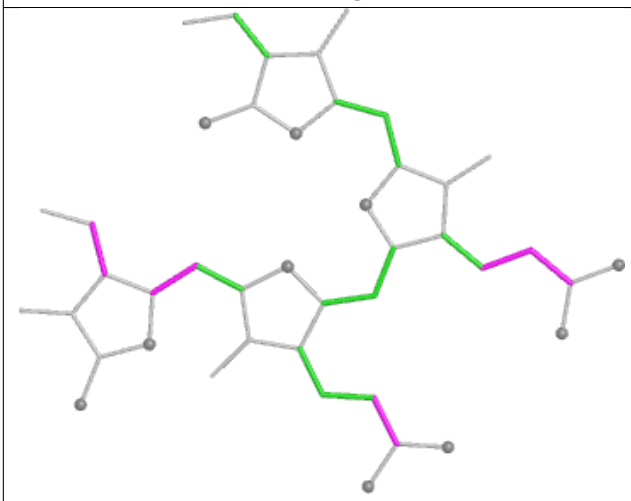

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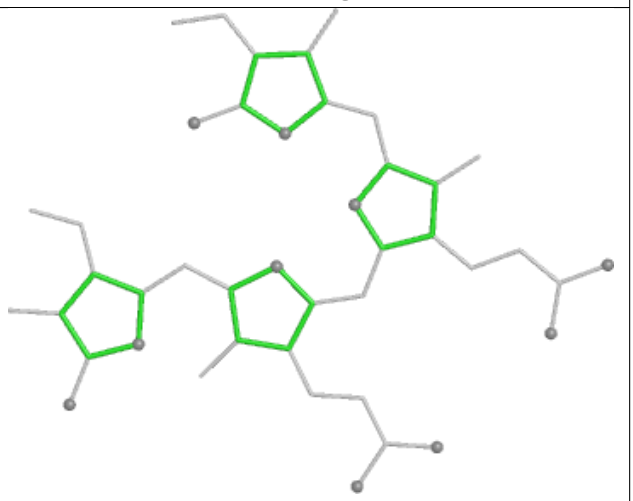
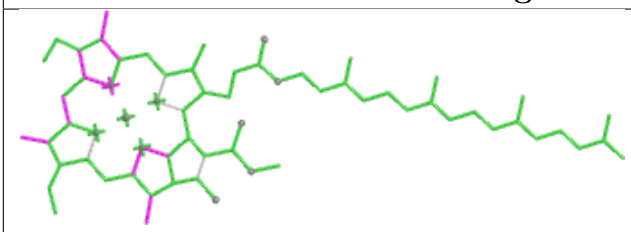


Rings

Ligand CLA H6 103



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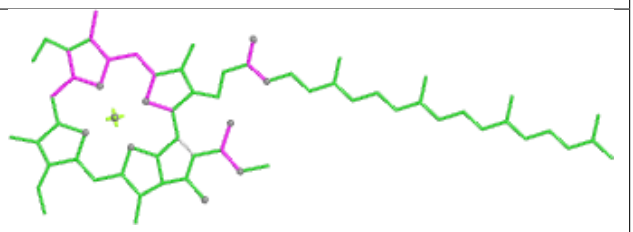

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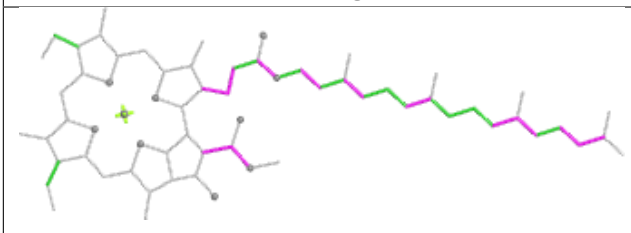

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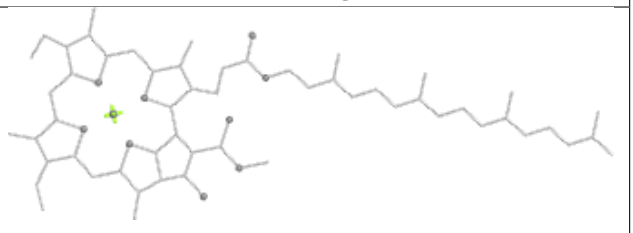
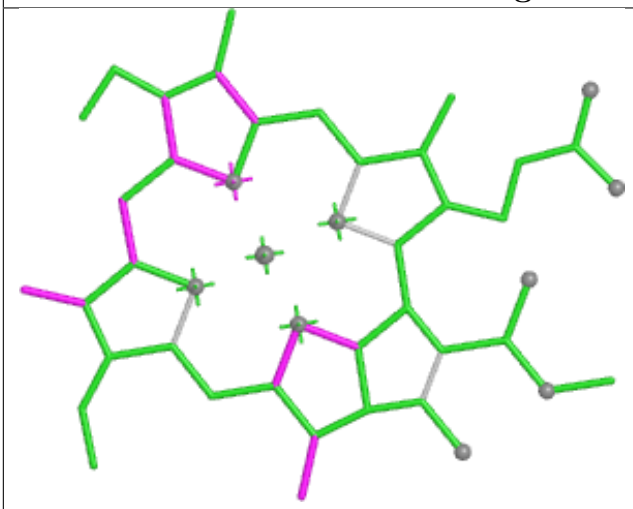


Rings

Ligand CLA 1N 601



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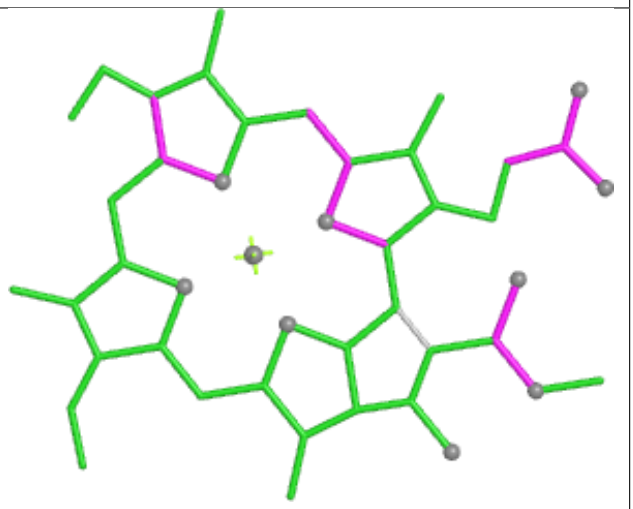

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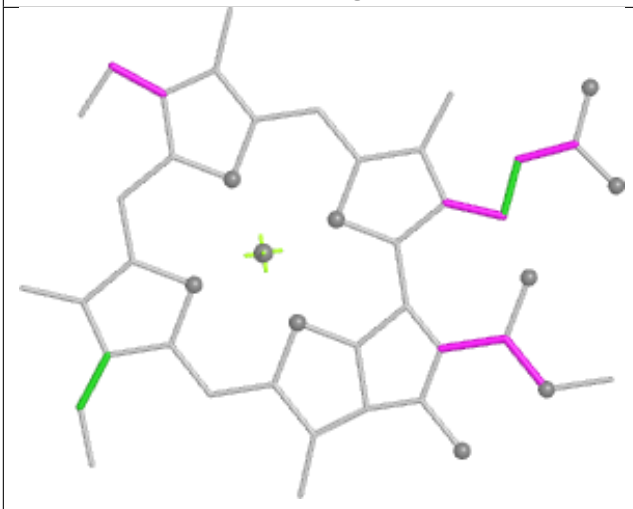
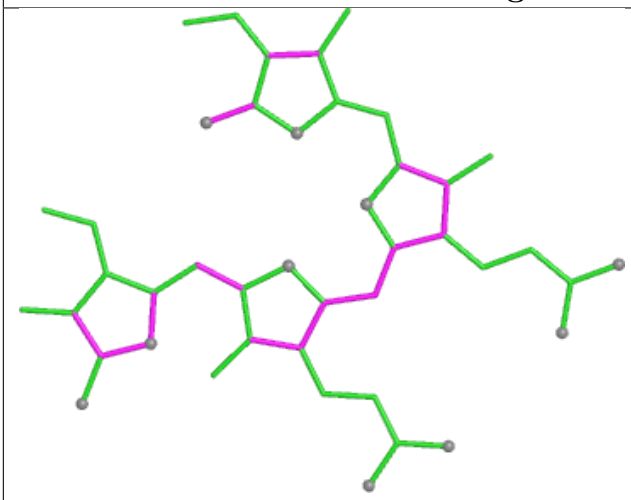


Torsions



Rings

Ligand PEB UM 203



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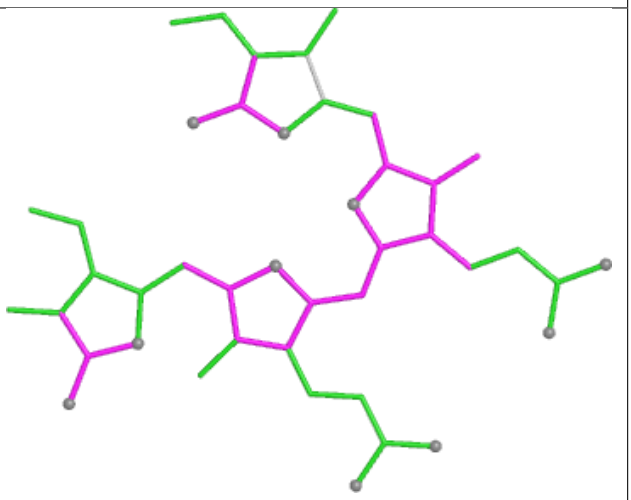

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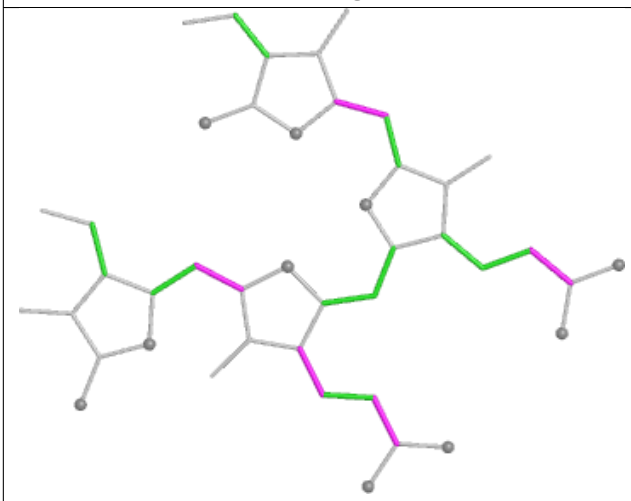

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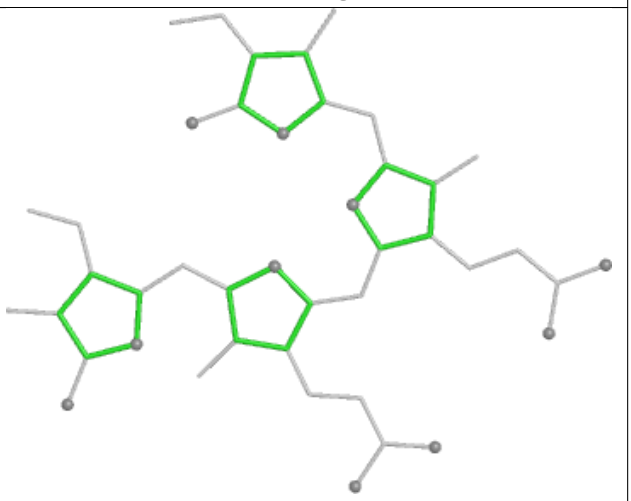
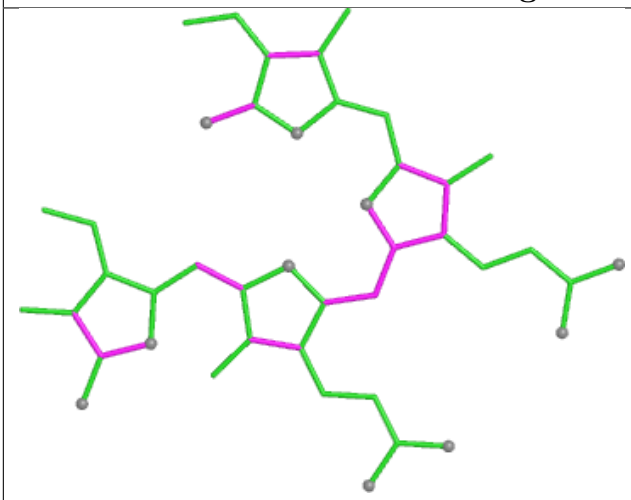


Rings

Ligand PEB J7 201



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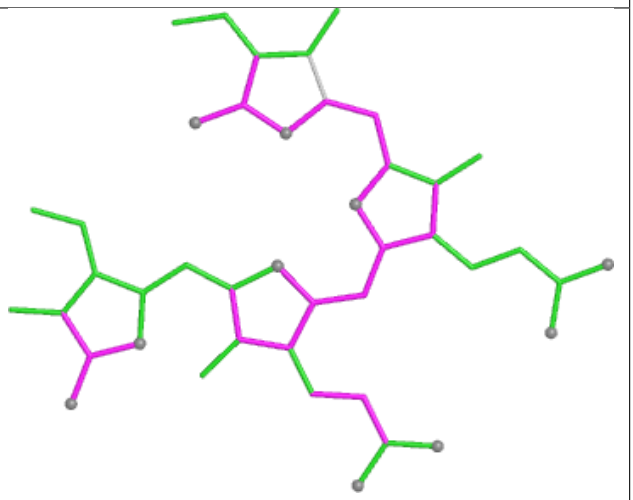

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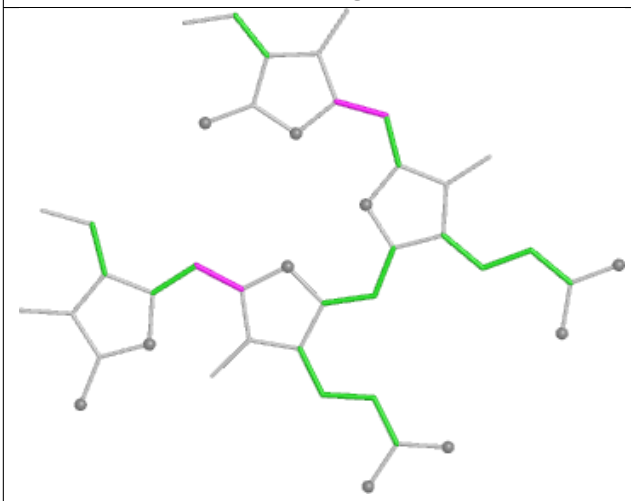

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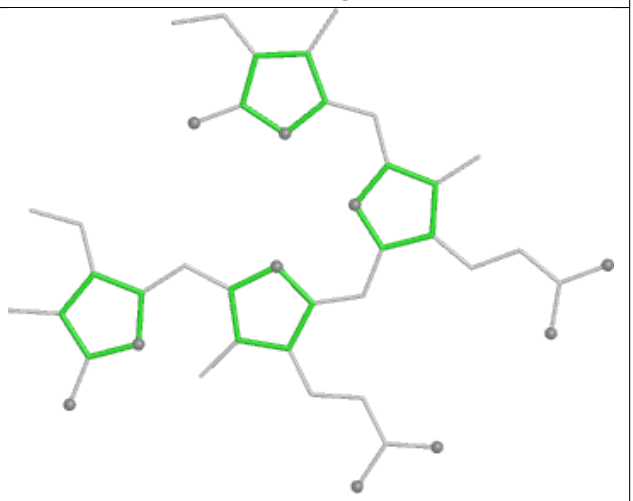
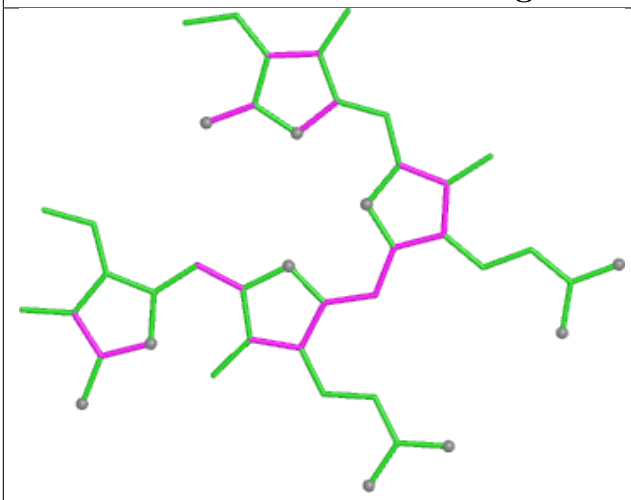


Rings

Ligand PEB Q9 202



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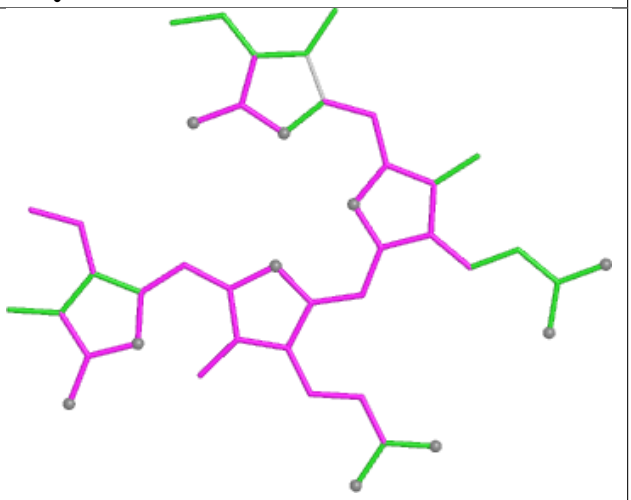

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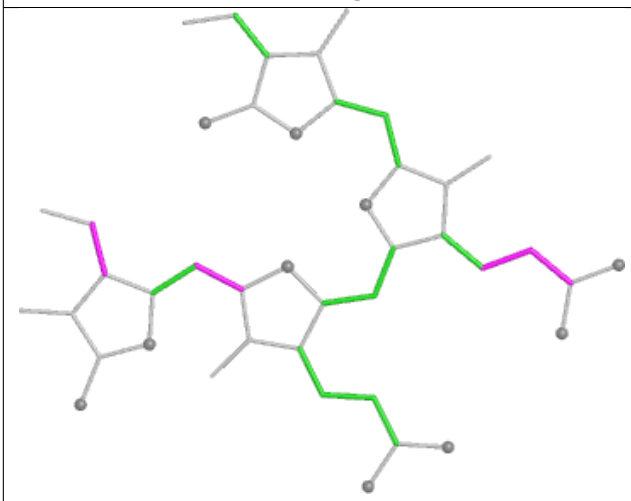

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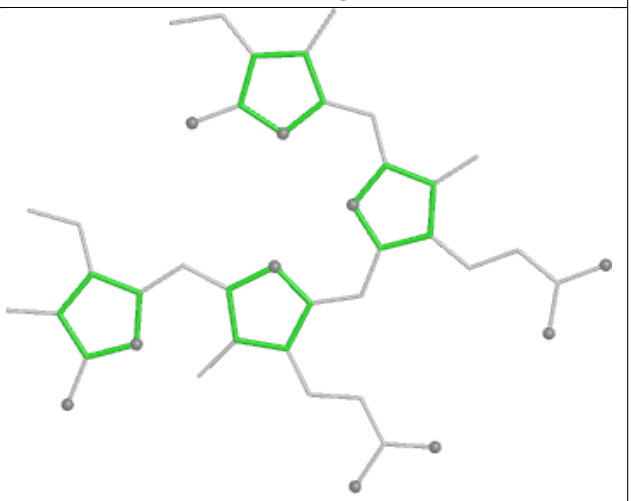
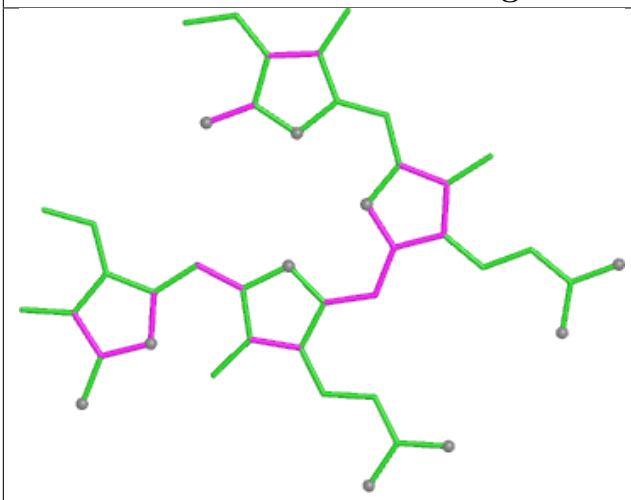


Rings

Ligand PEB NO 1002



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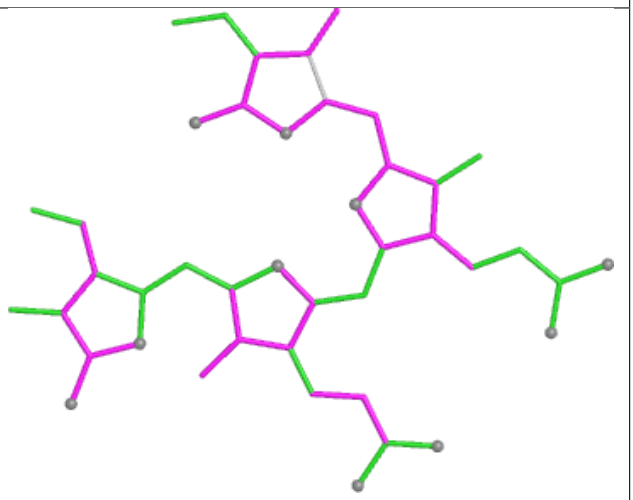

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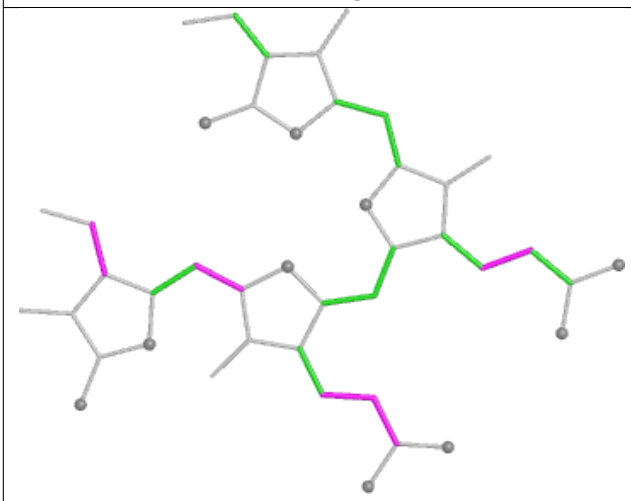

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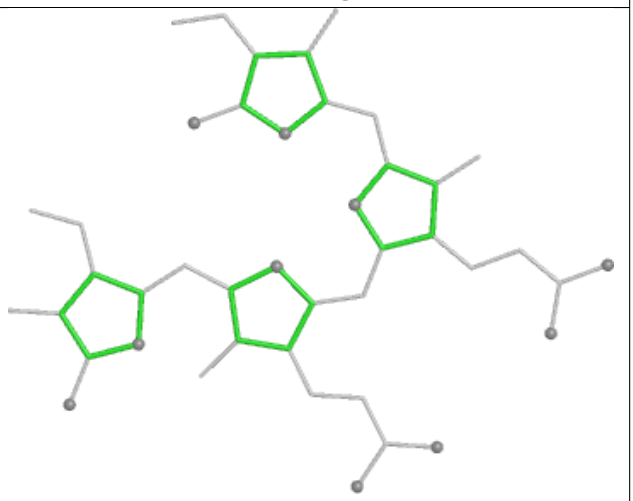

Rings

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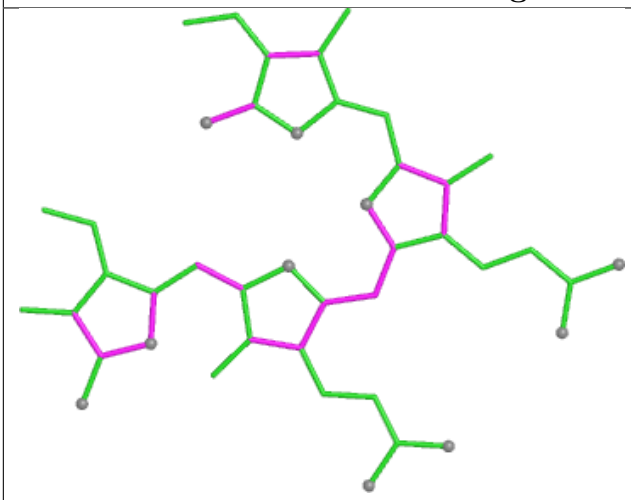

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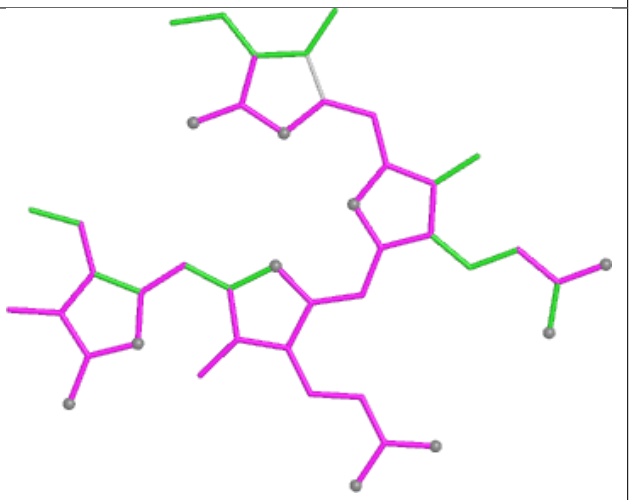

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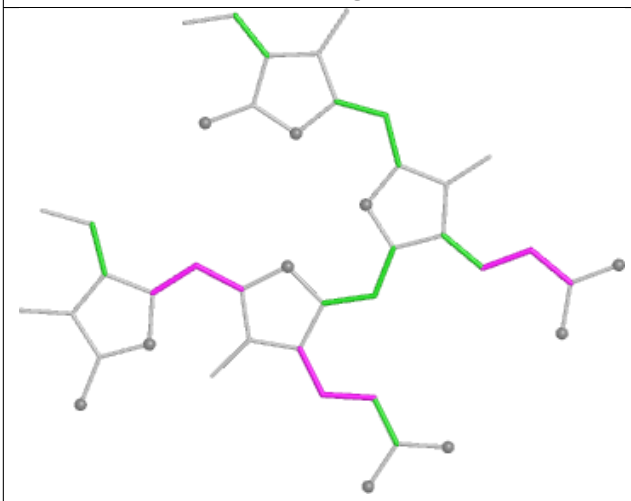

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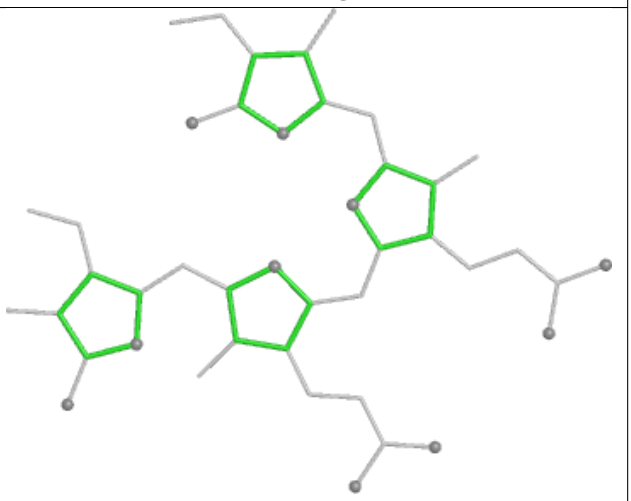
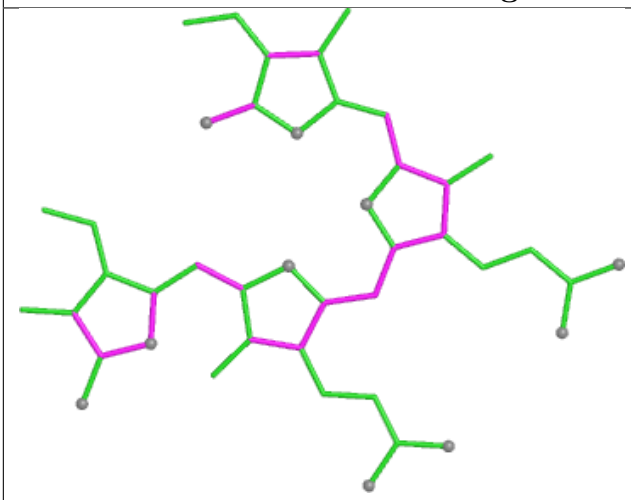


Rings

Ligand PEB HG 1002



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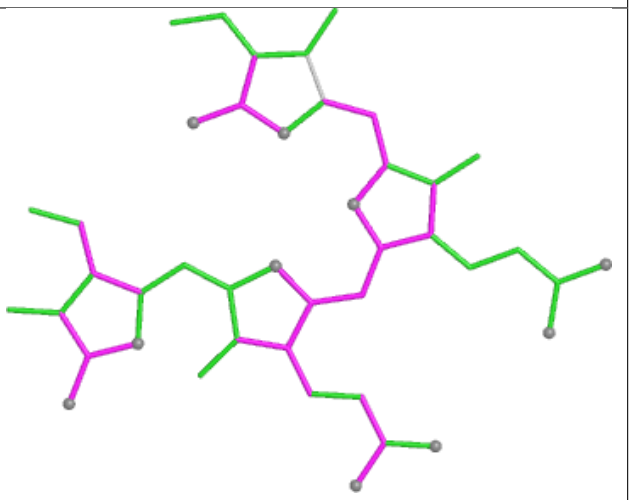

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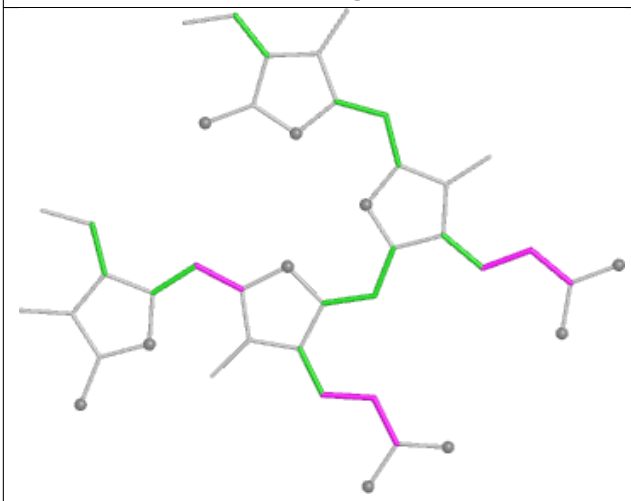

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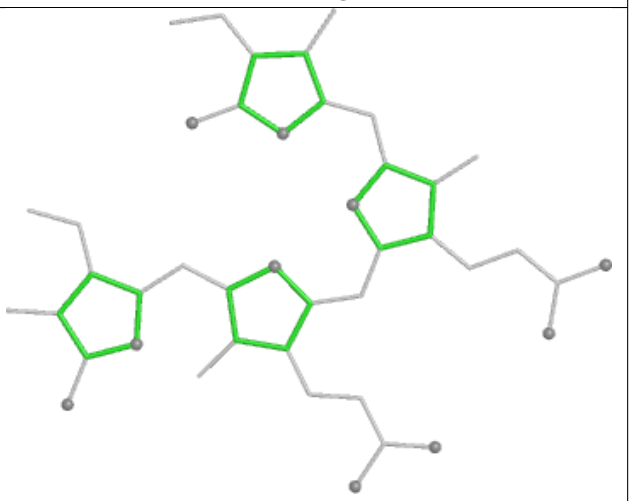
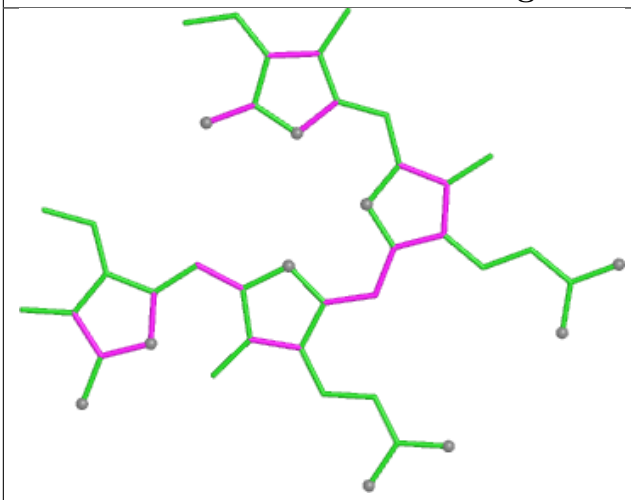


Rings

Ligand PEB IA 202



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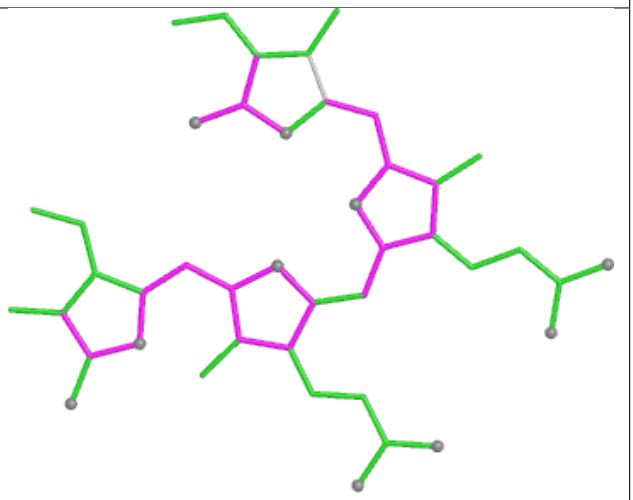
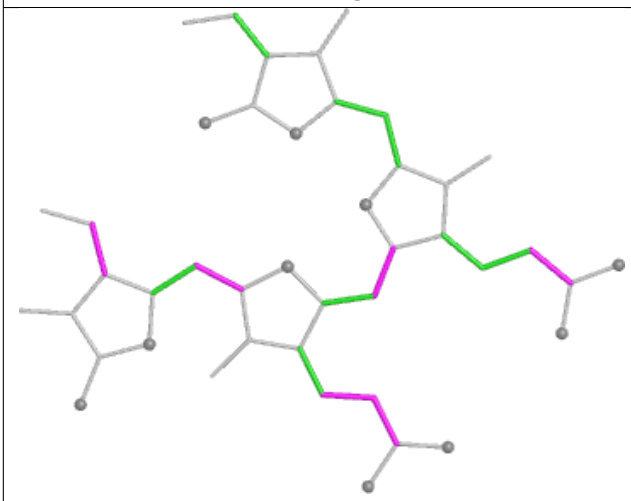


Bond angles



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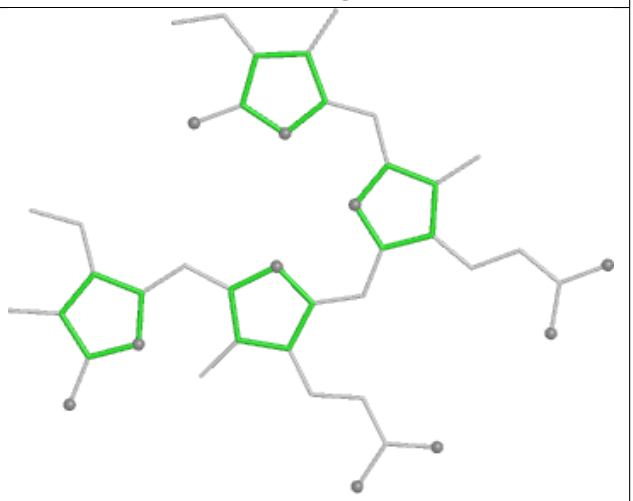
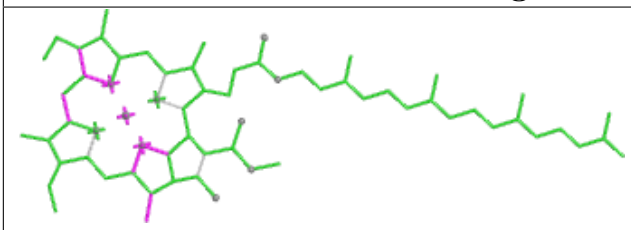


Rings

Ligand CLA BN 806



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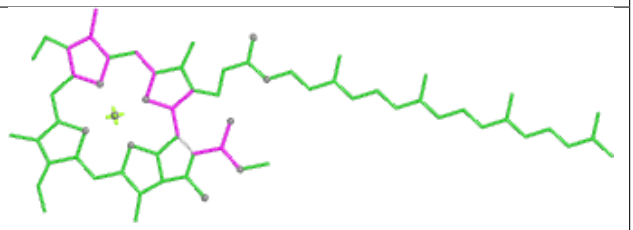
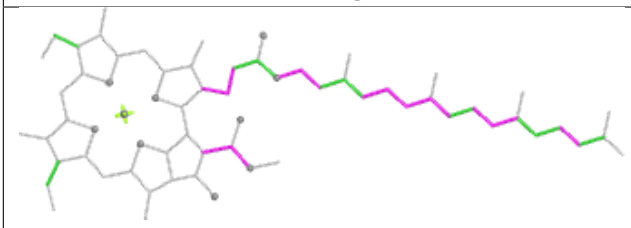


Bond angles



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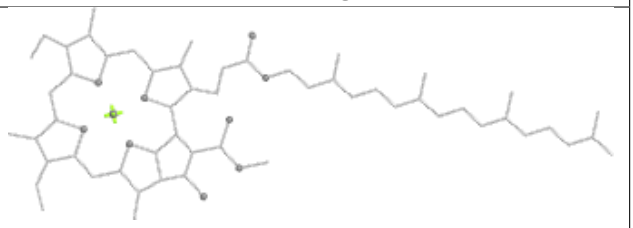
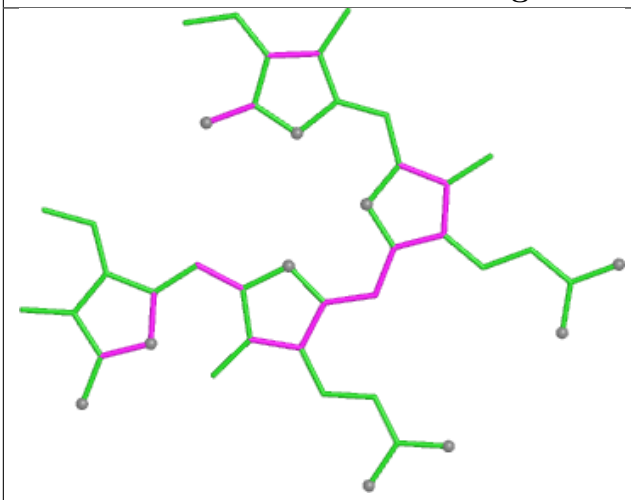


Rings

Ligand PEB XQ 201



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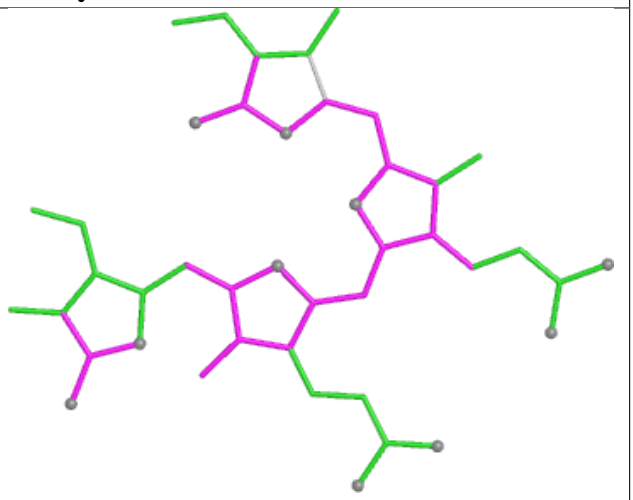
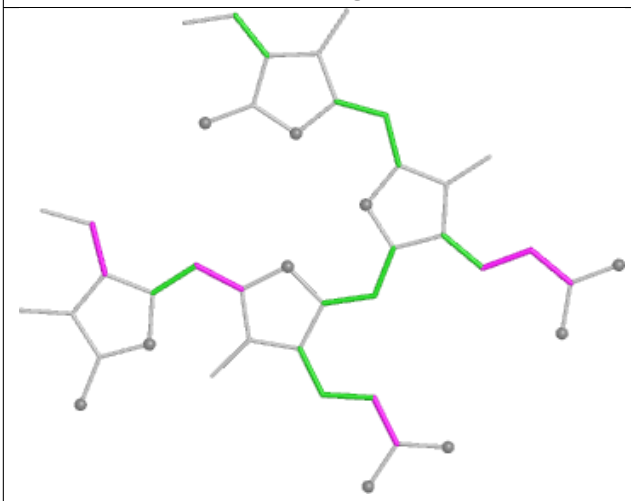


Bond angles



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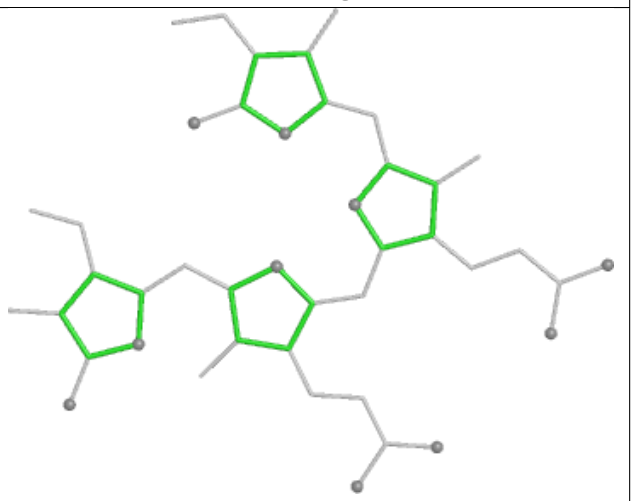
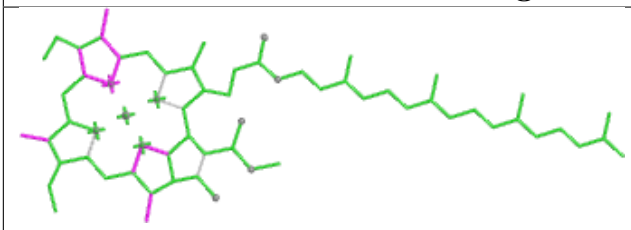


Rings

Ligand CLA B2 835



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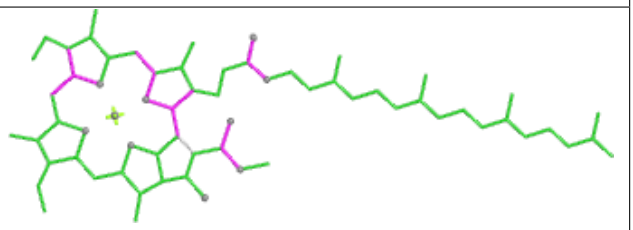
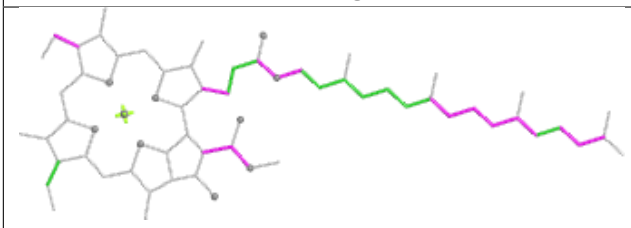
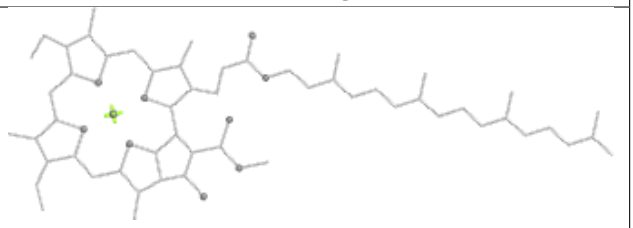


Bond angles

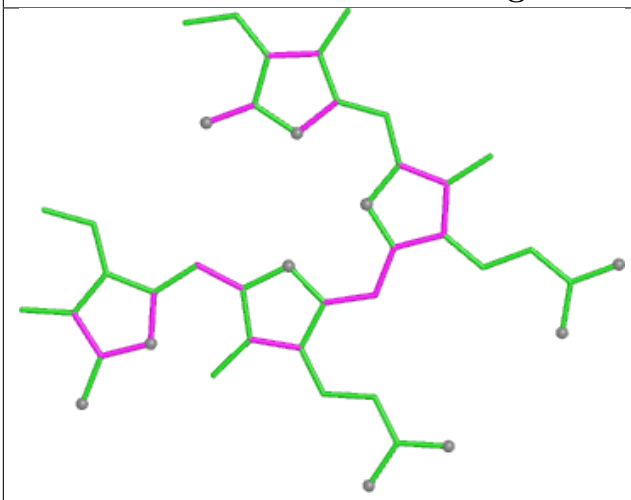


Torsions



Rings

Ligand PEB WA 202



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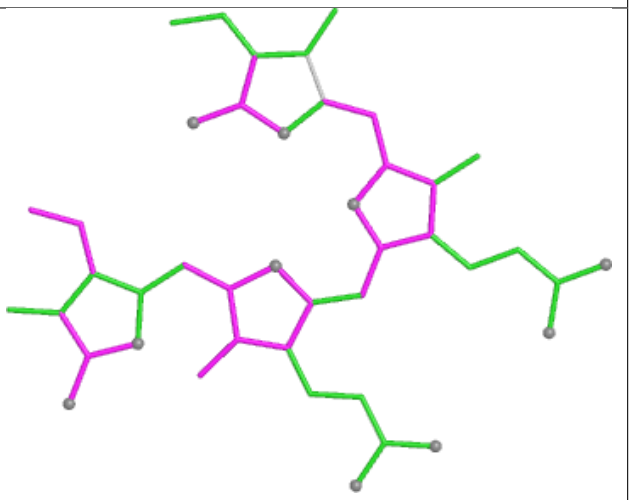

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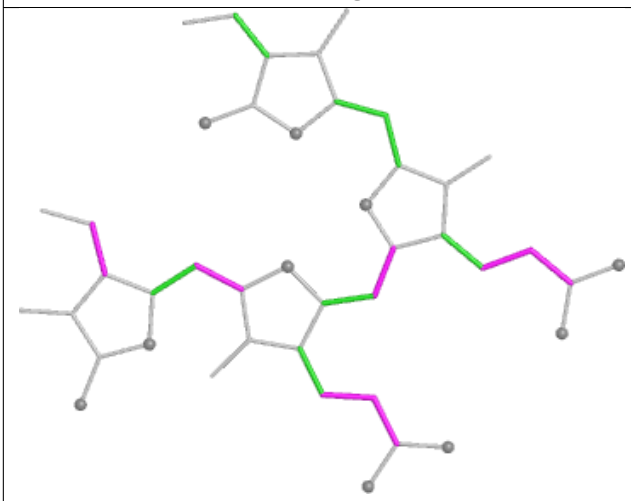

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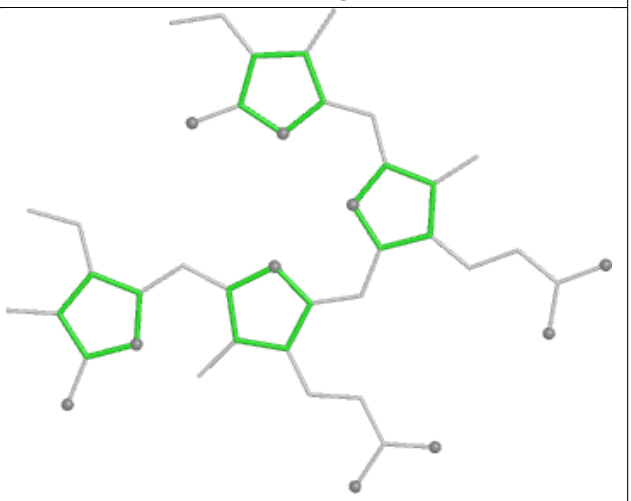
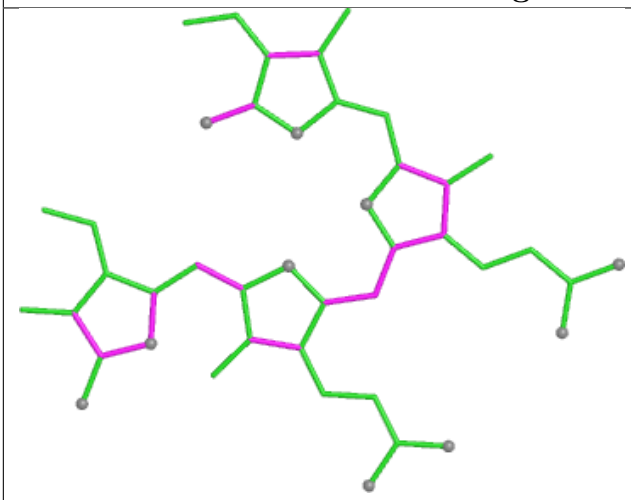


Rings

Ligand PEB YE 202



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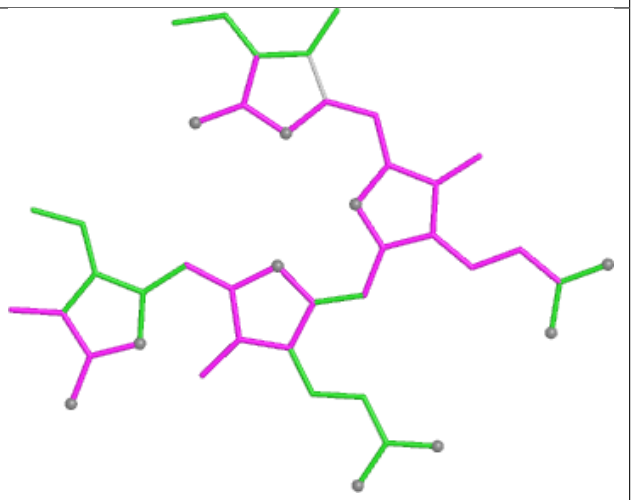

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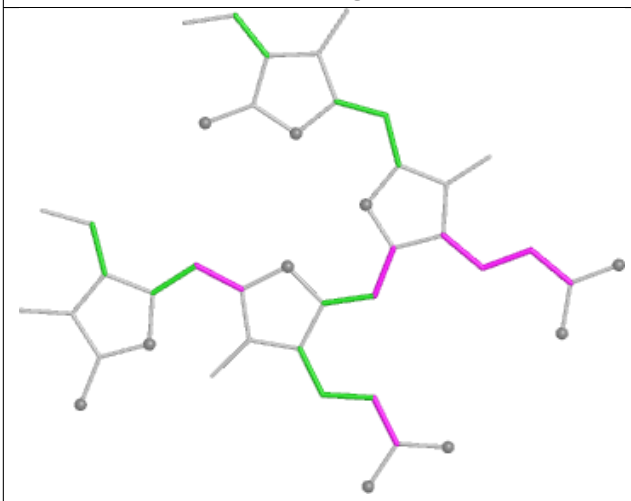

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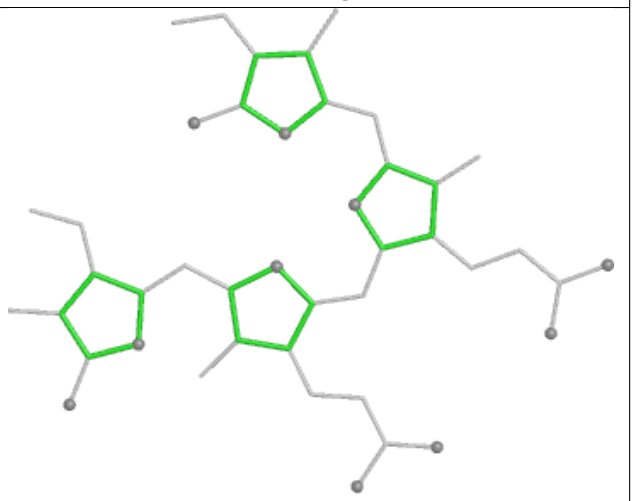
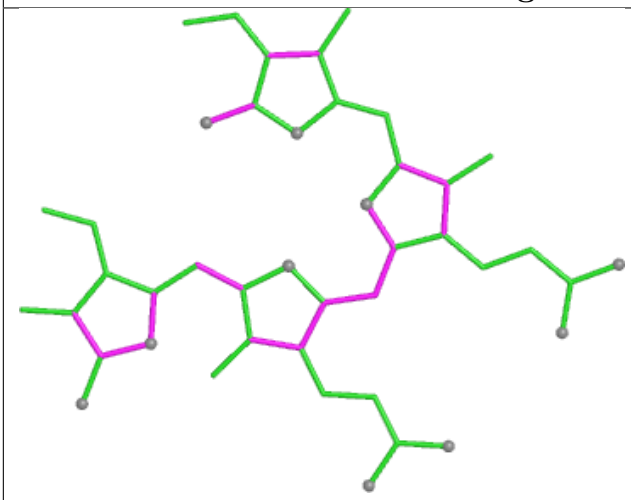


Rings

Ligand PEB ID 202



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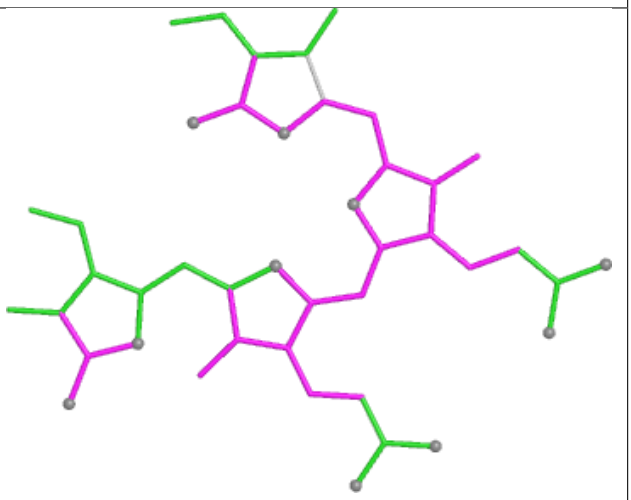

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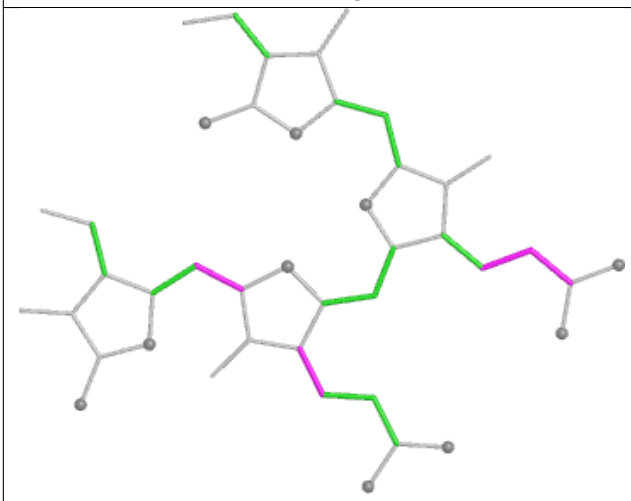

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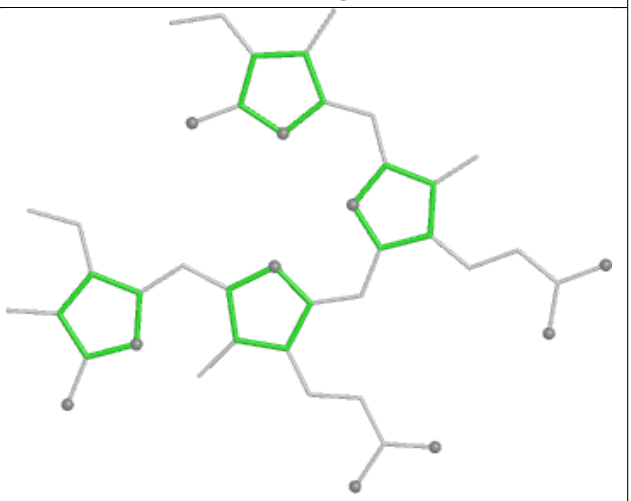
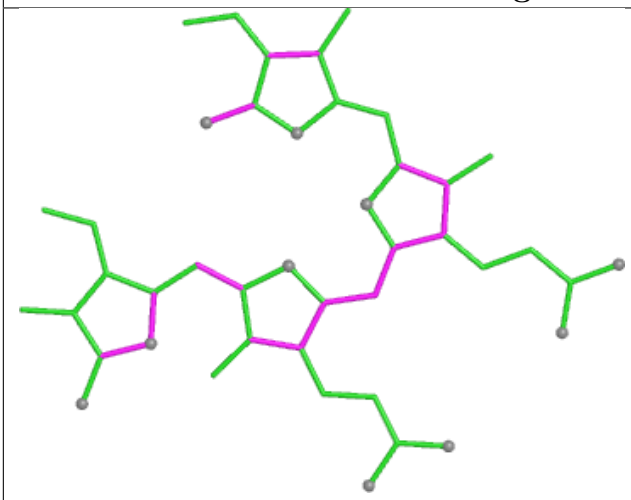


Rings

Ligand PEB LD 201



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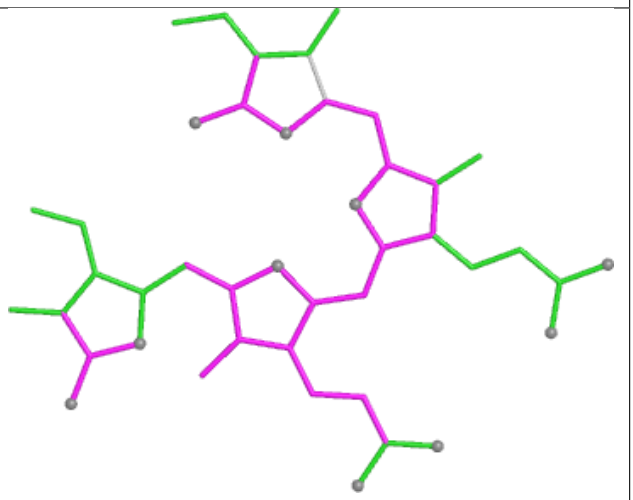

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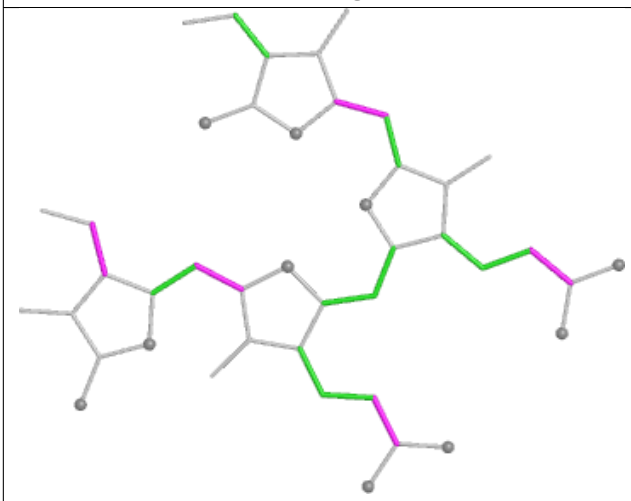

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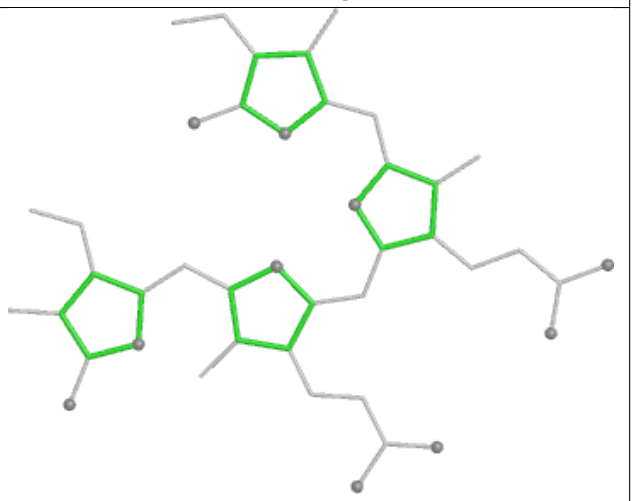
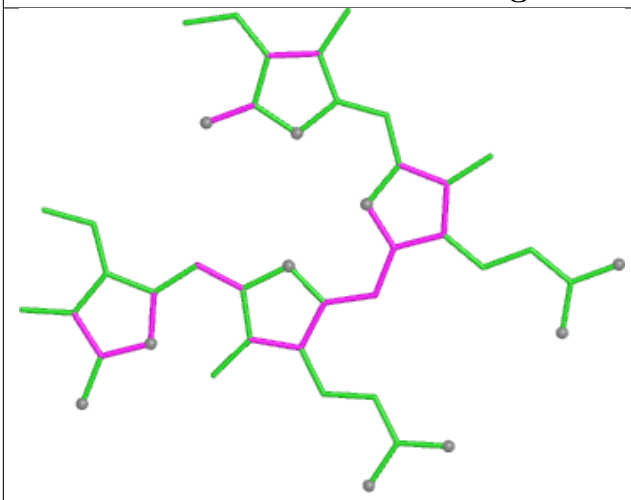


Rings

Ligand PEB VK 202



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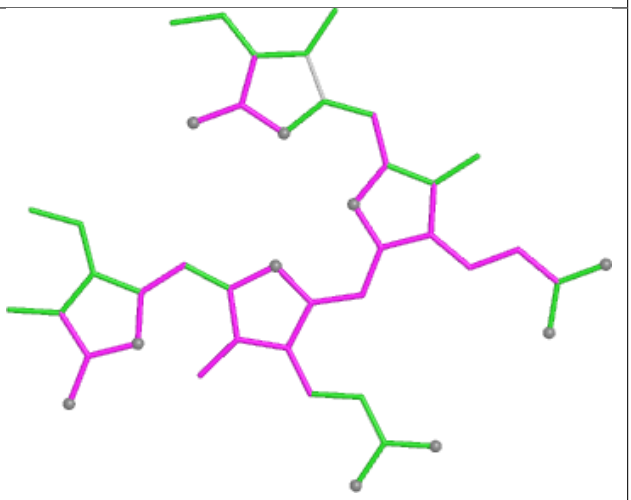

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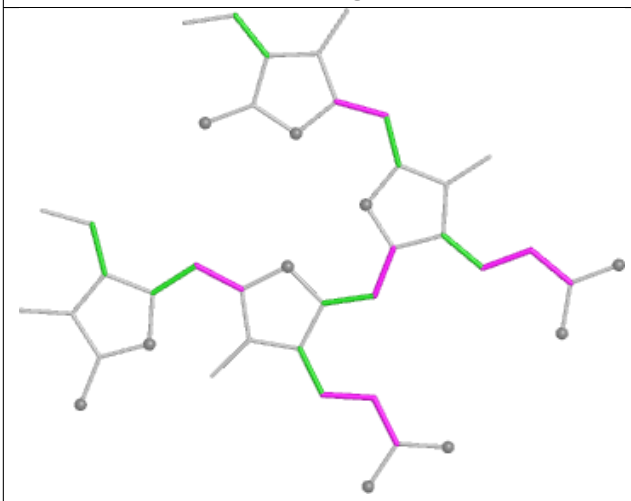

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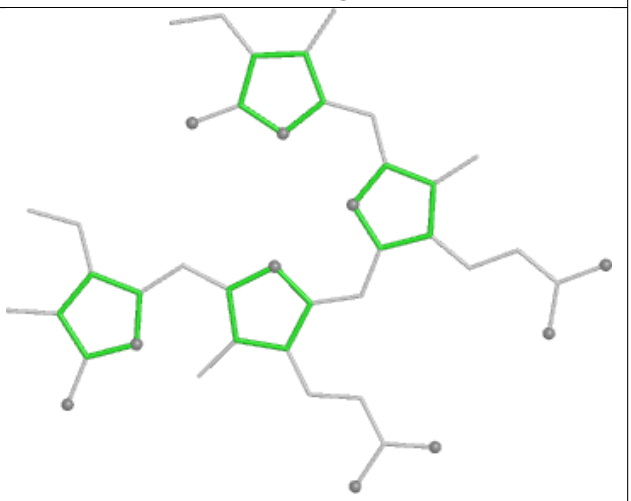
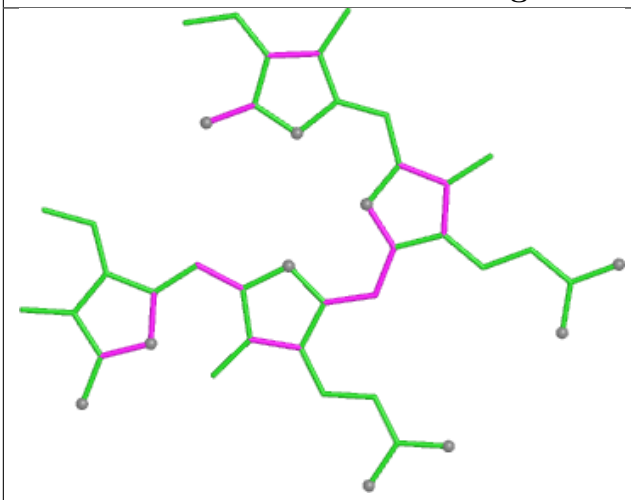


Rings

Ligand PEB OK 203



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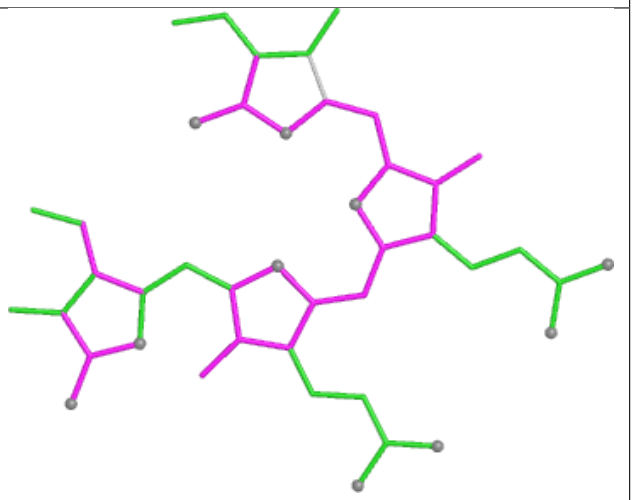

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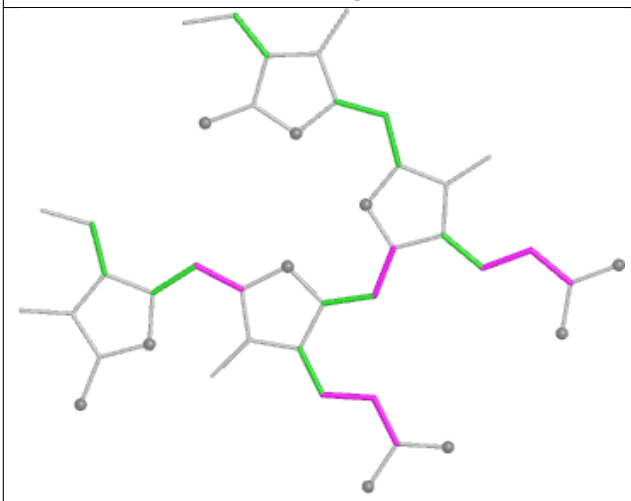

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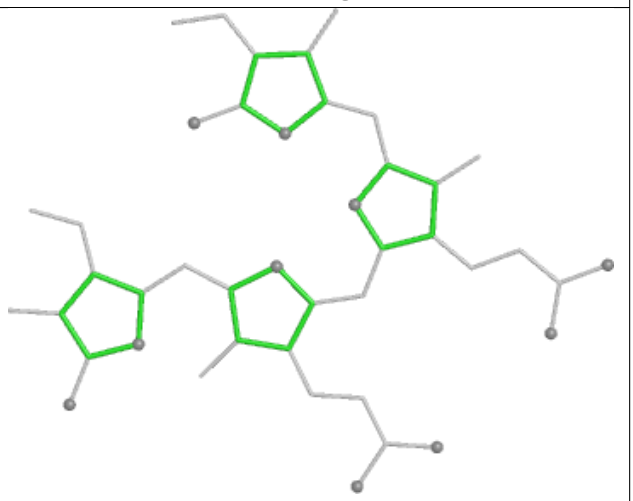
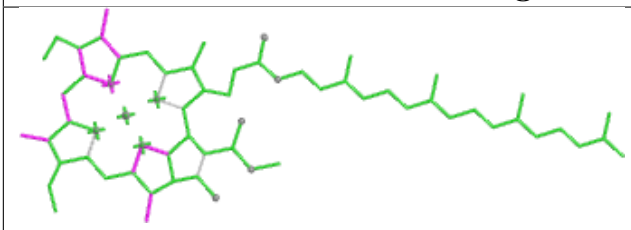


Rings

Ligand CLA D6 403



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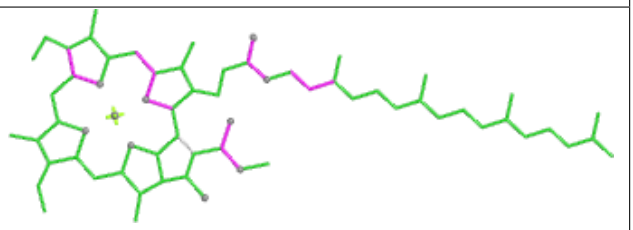

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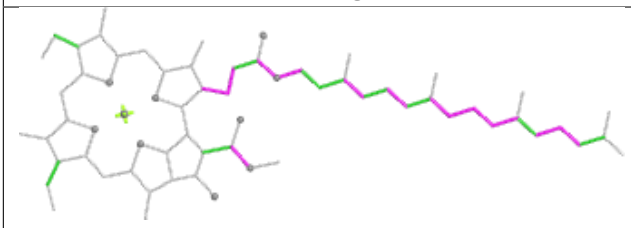

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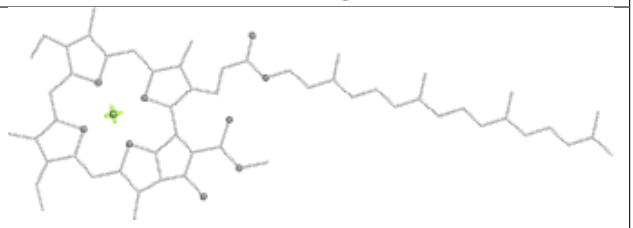
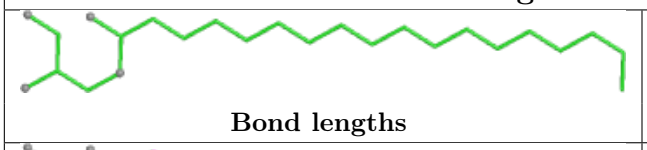


Rings

Ligand 3XQ JN 104



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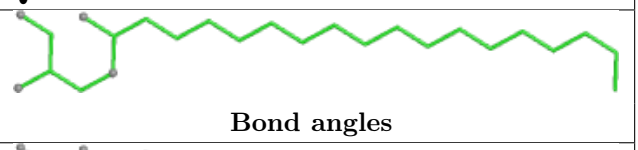

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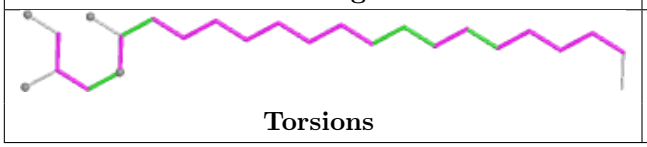

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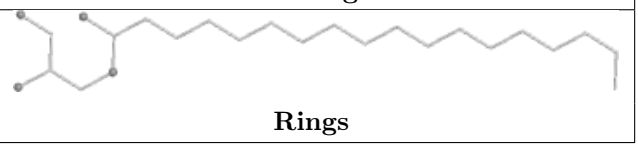
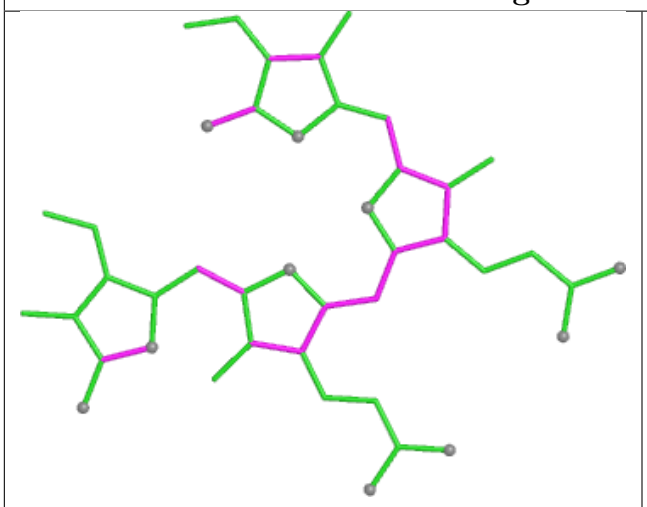


Rings

Ligand PEB wC 202



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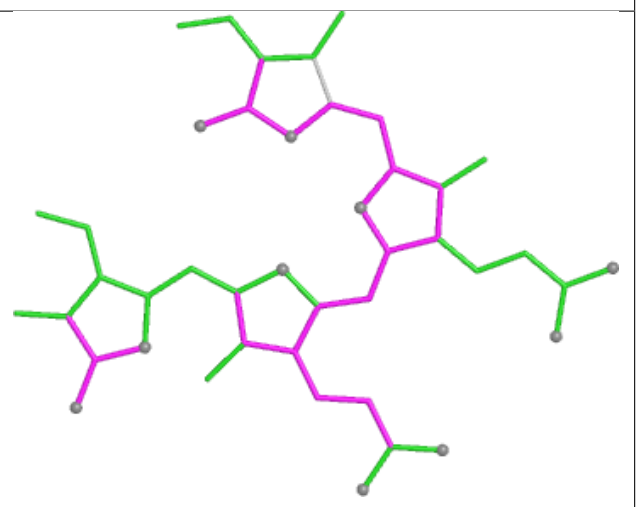

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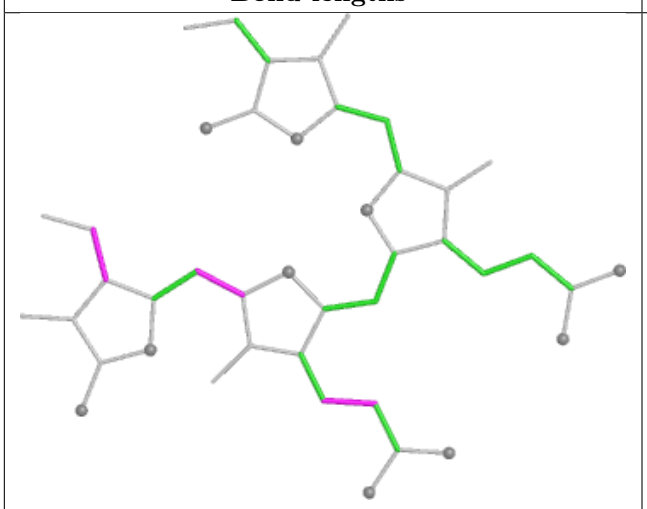

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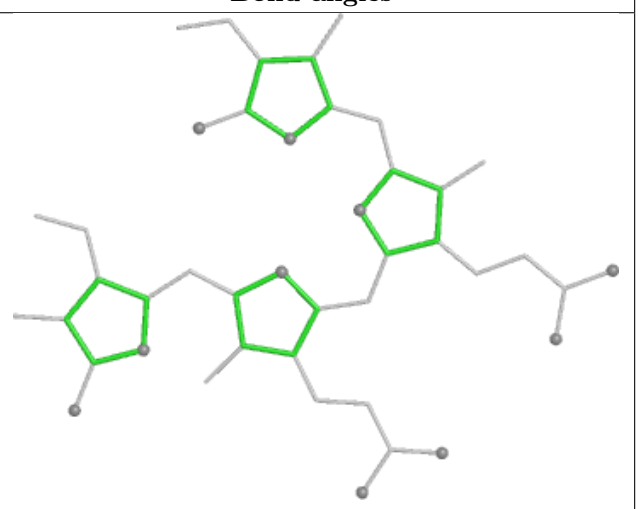
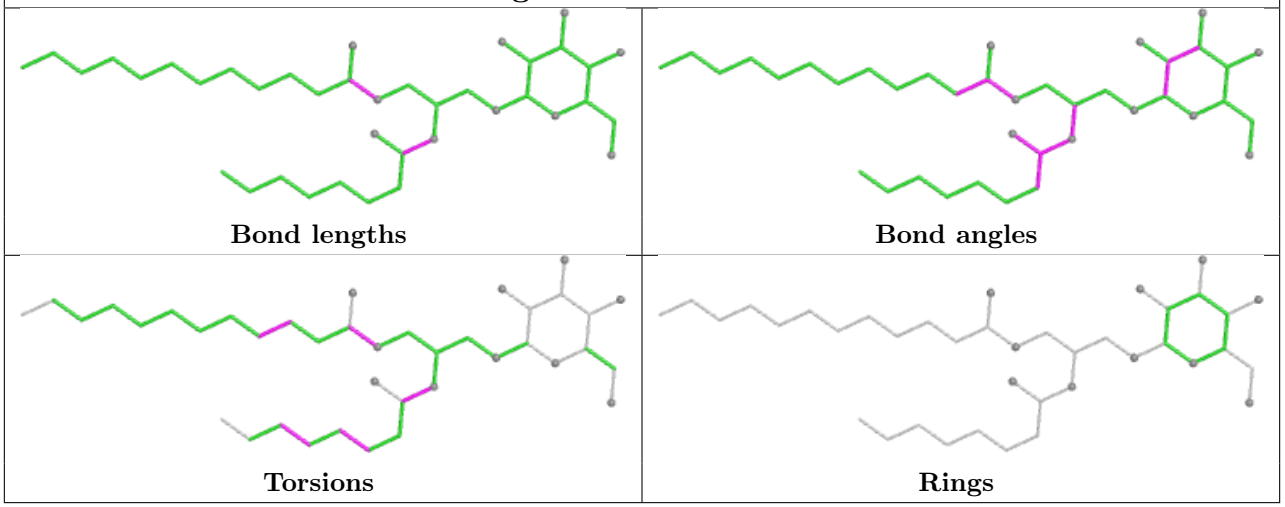
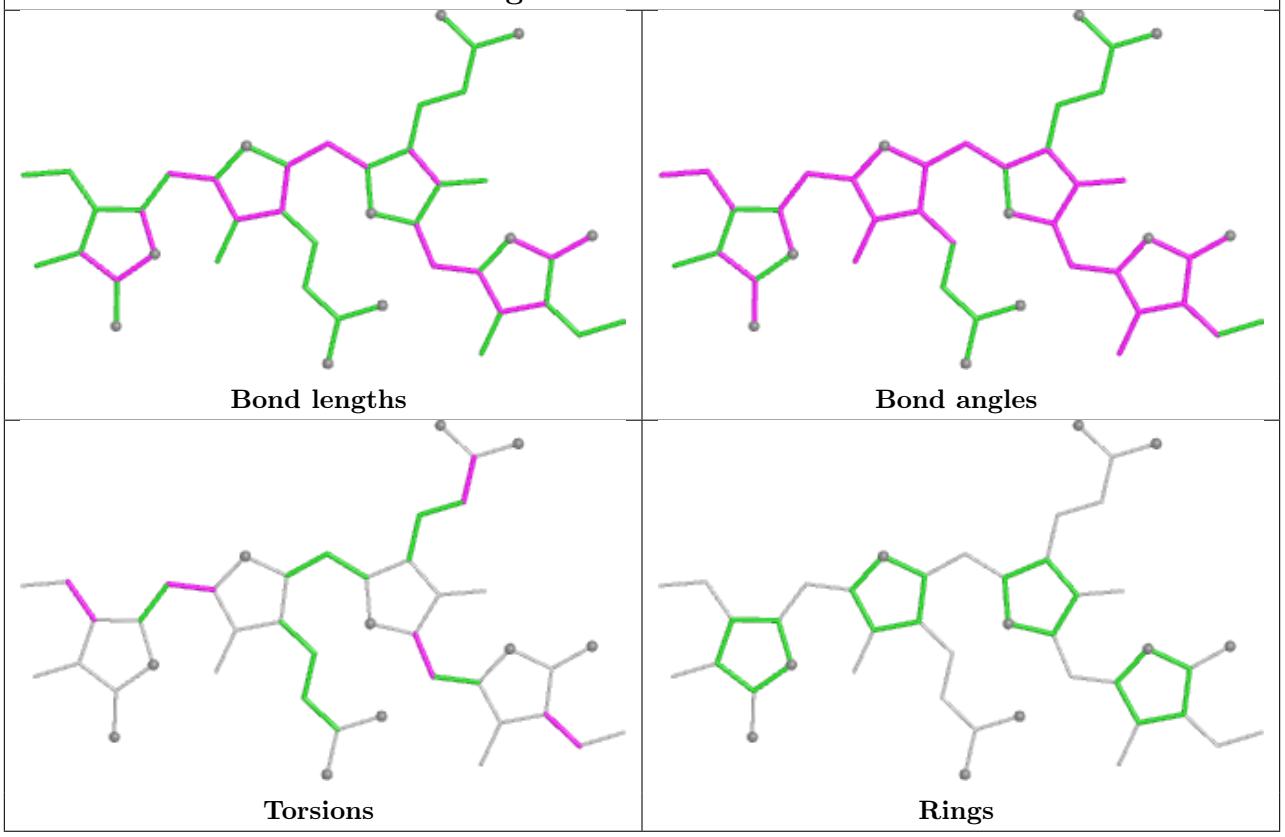


Rings

Ligand LMG B6 619



Ligand CYC T3 1001



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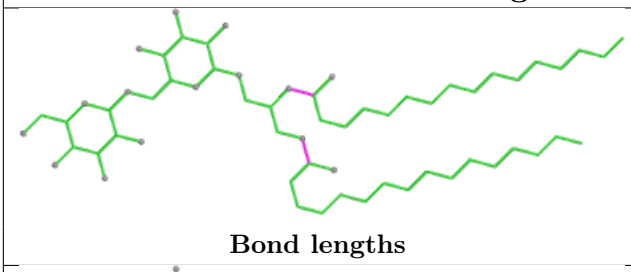

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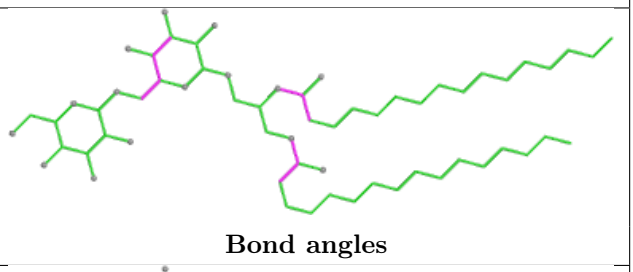
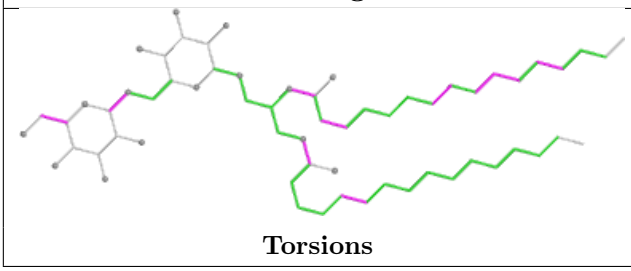


Bond angles



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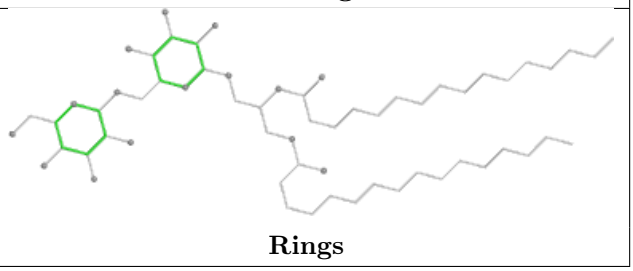
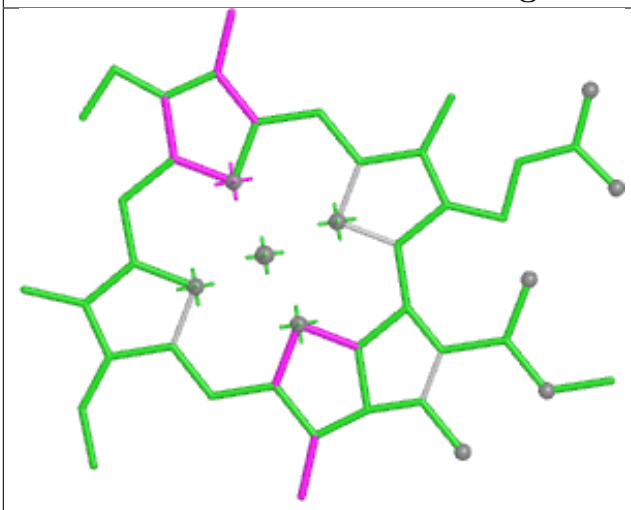


Rings

Ligand CLA 12 605



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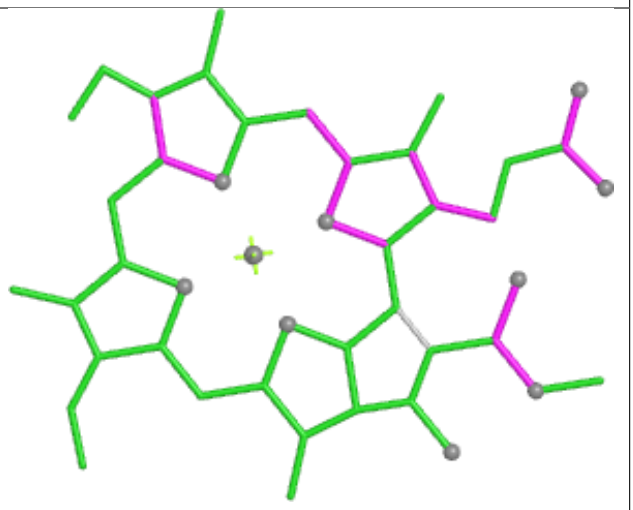

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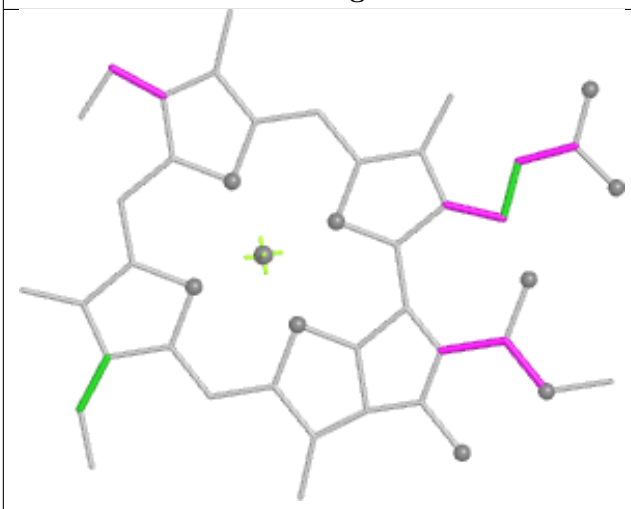
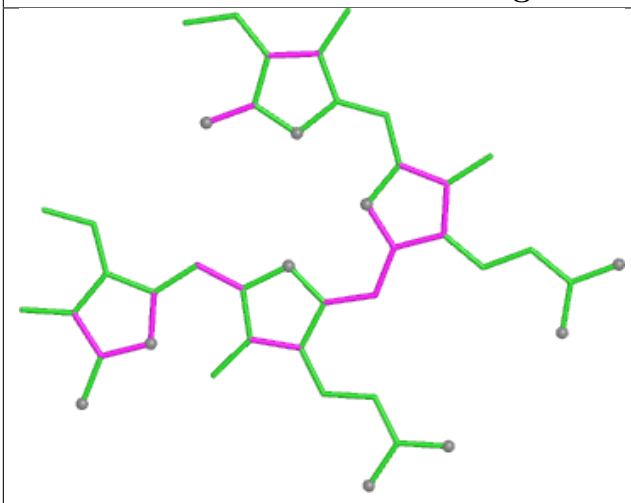


Torsions



Rings

Ligand PEB VF 202



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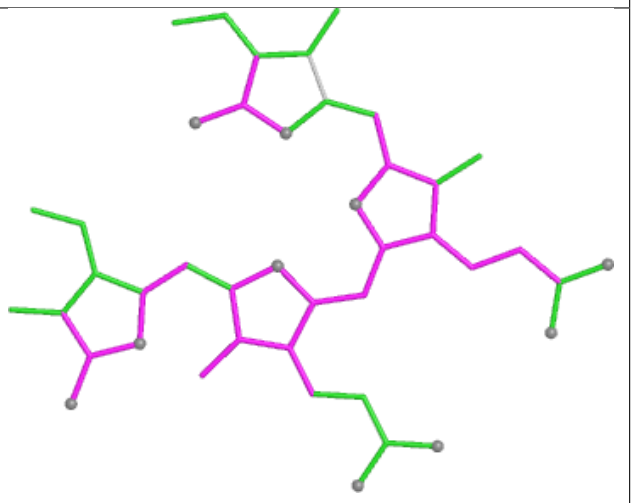
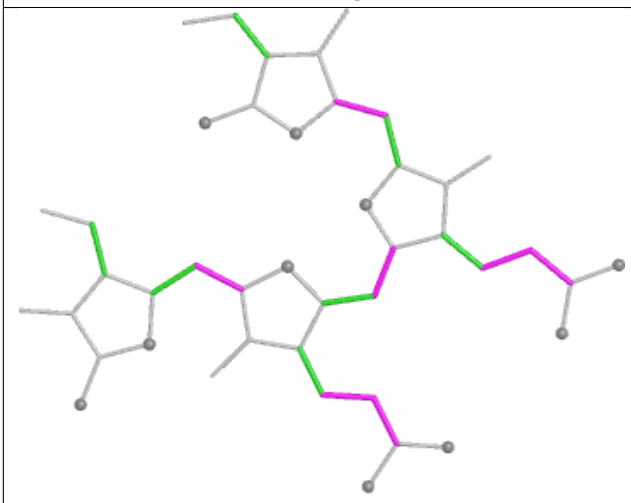


Bond angles



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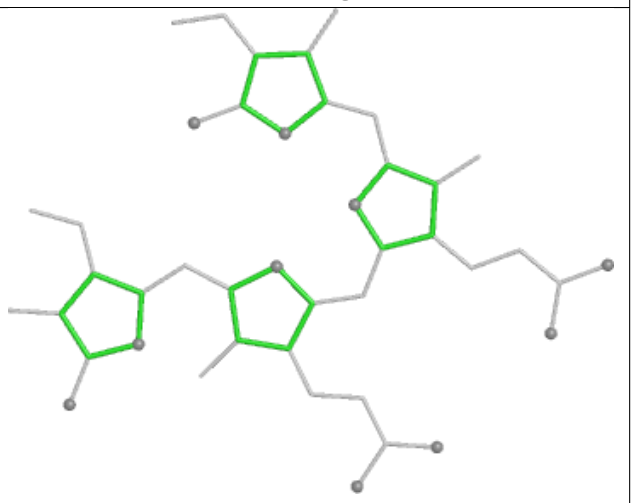
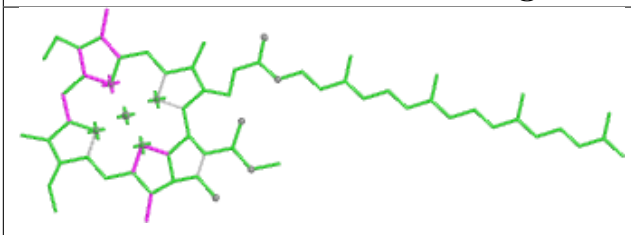


Rings

Ligand CLA d6 406



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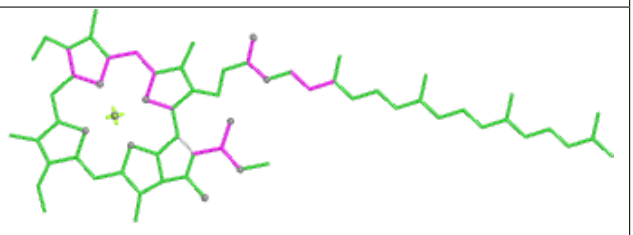

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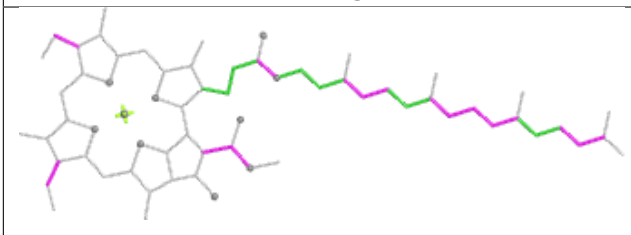

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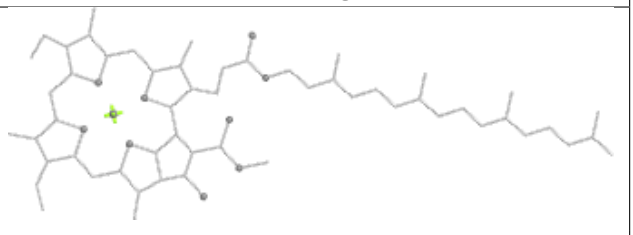
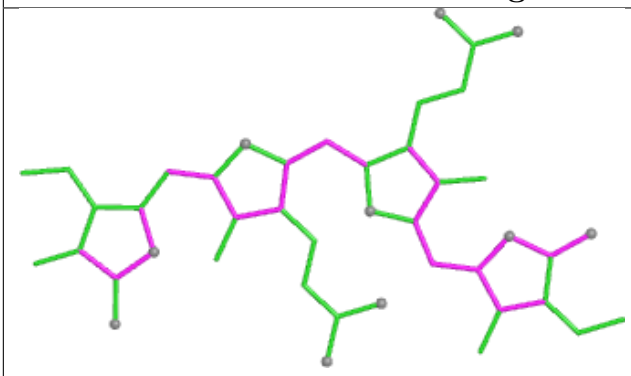
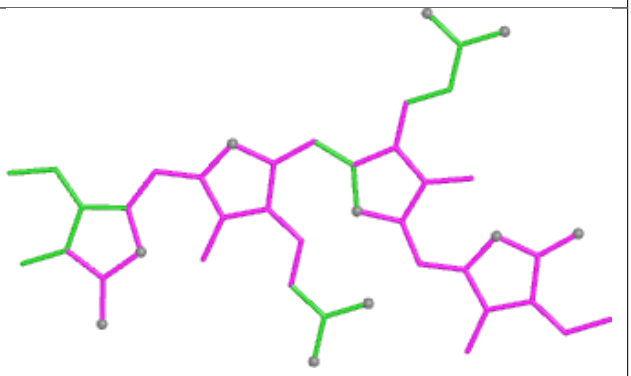


Rings

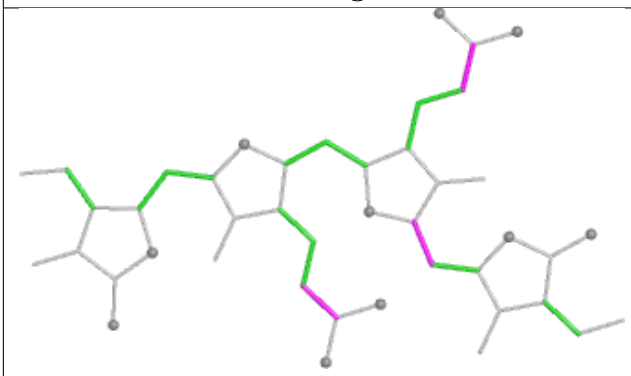
Ligand CYC 73 1002



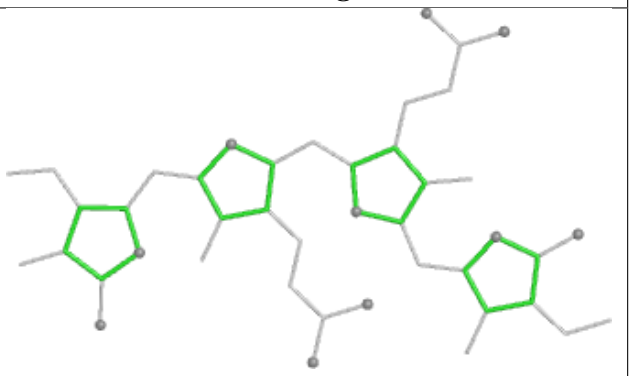
Bond lengths



Bond angles

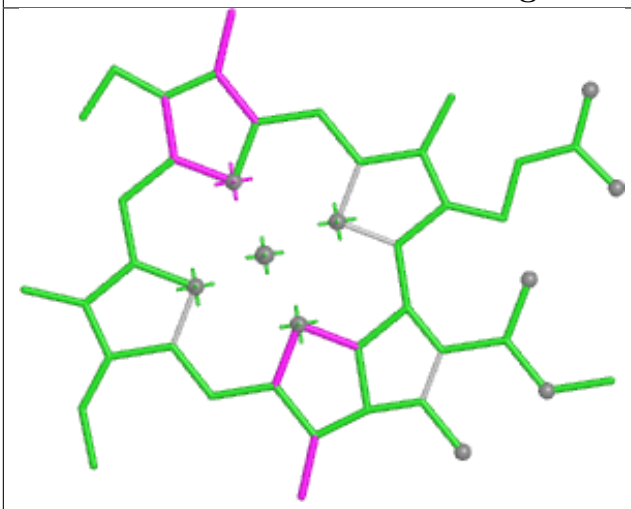


Torsions



Rings

Ligand CLA 12 606



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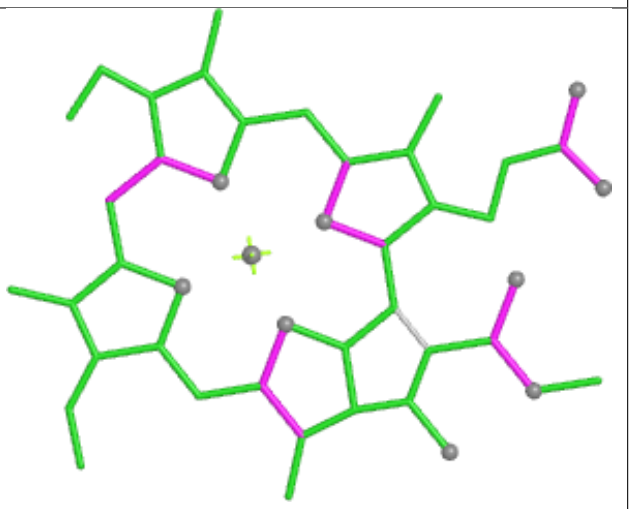

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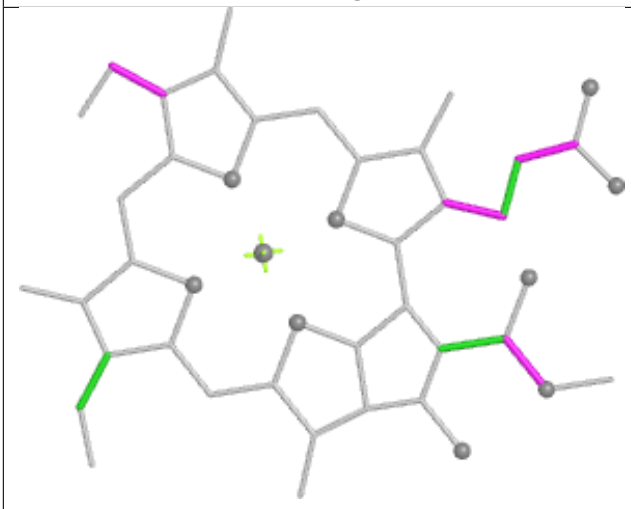
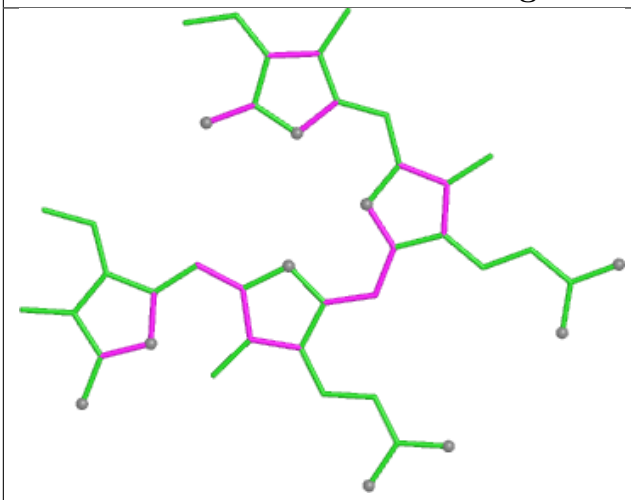


Torsions



Rings

Ligand PEB sF 201



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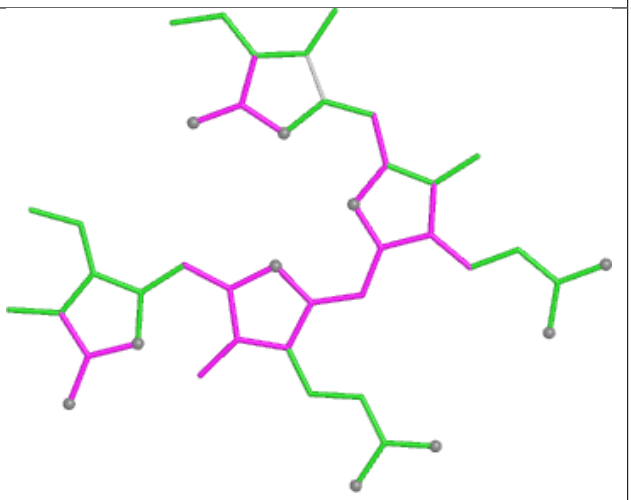

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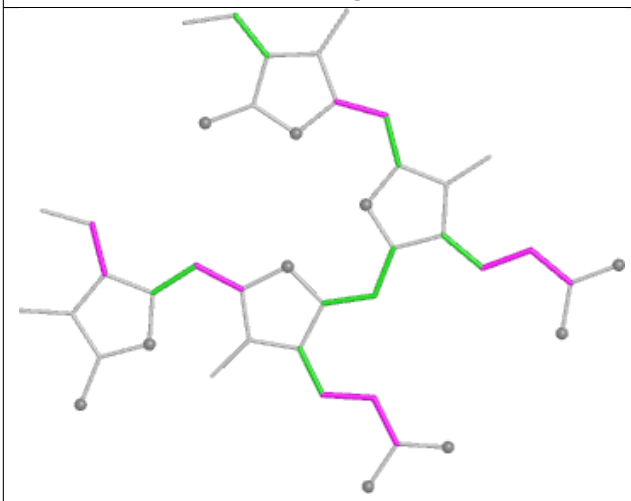

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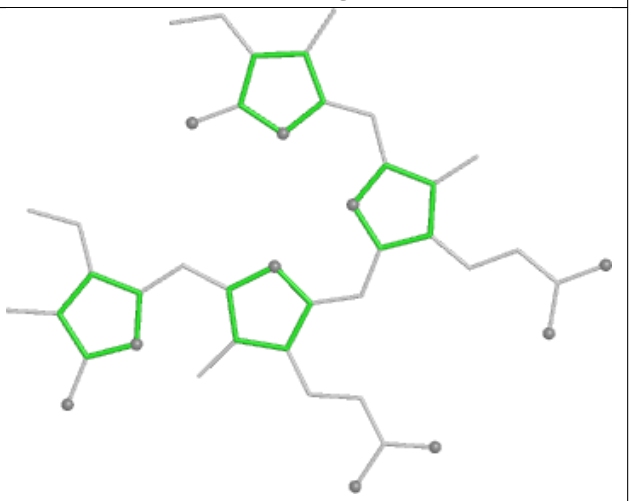

Rings

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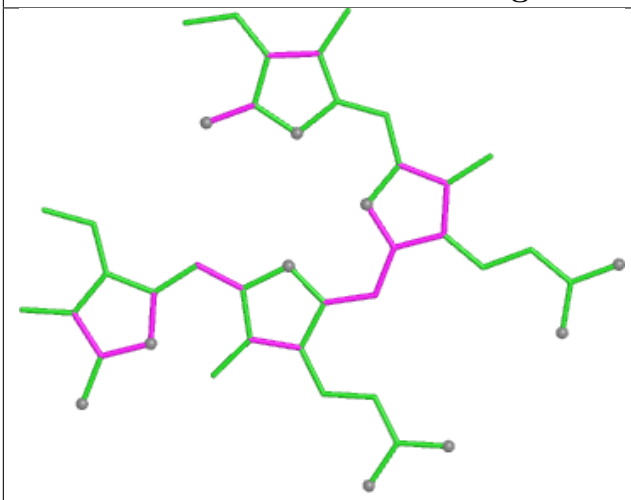

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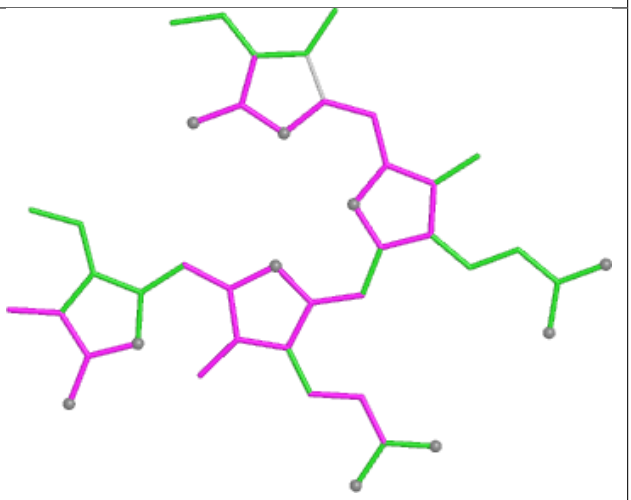

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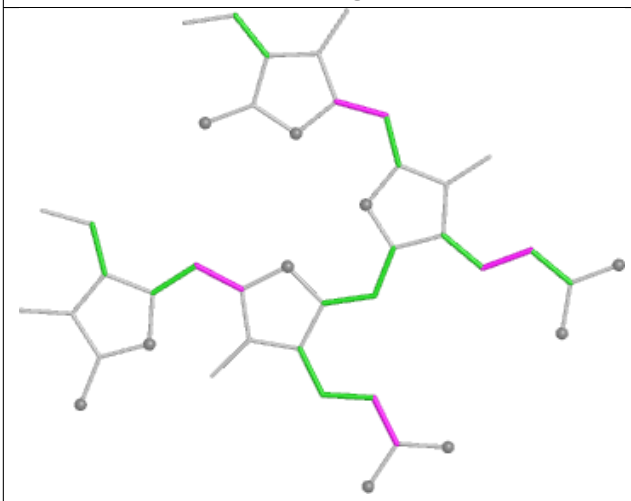

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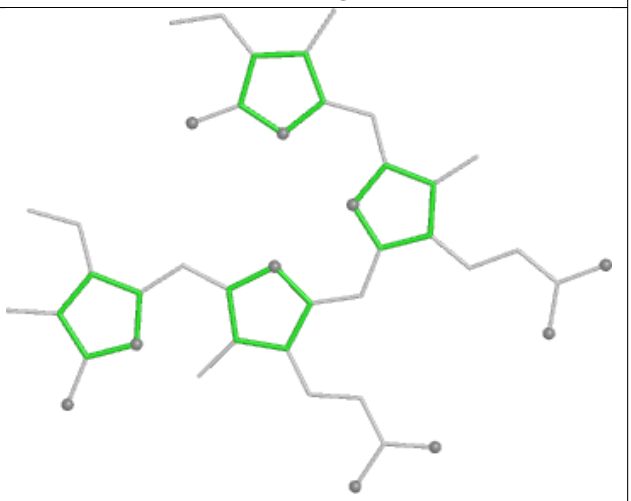
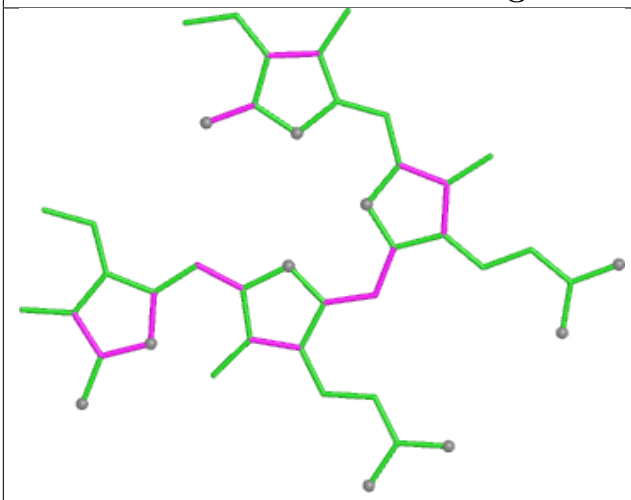


Rings

Ligand PEB MB 201



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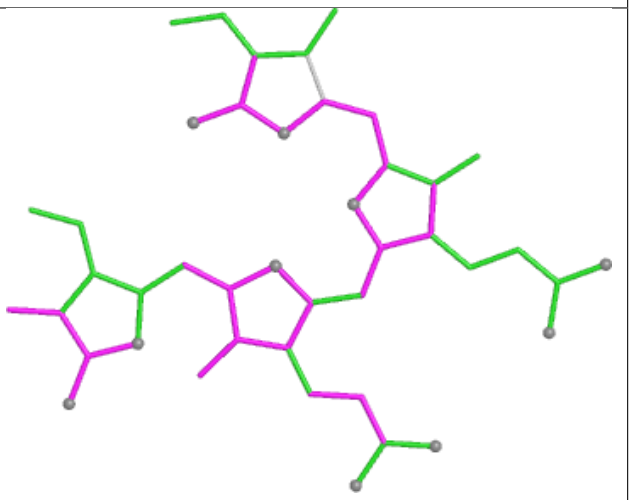

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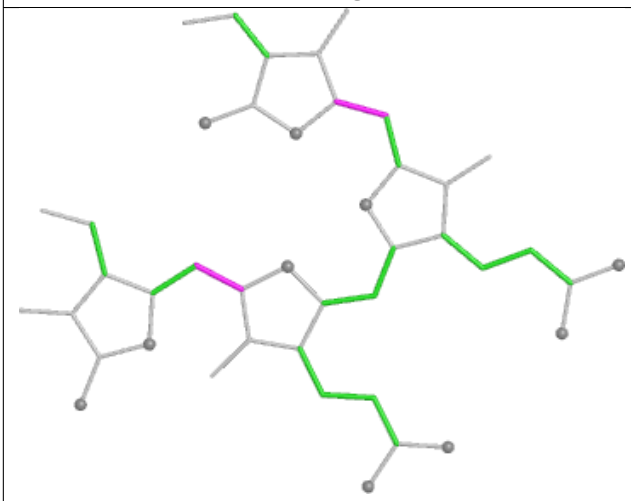

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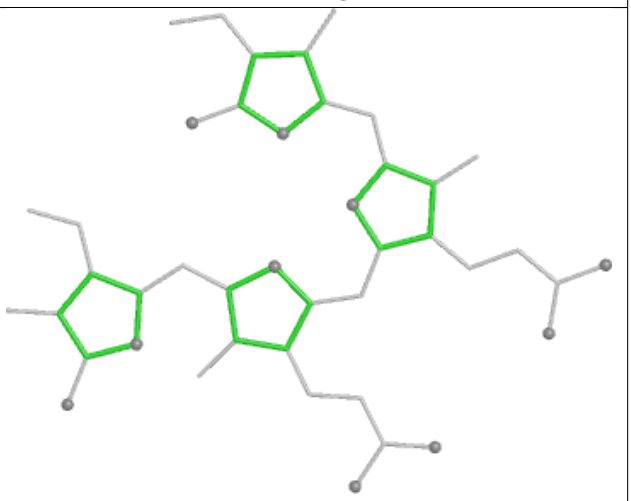

Rings

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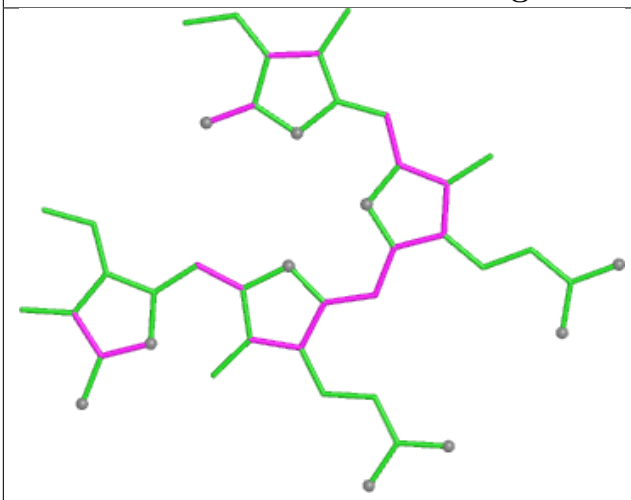

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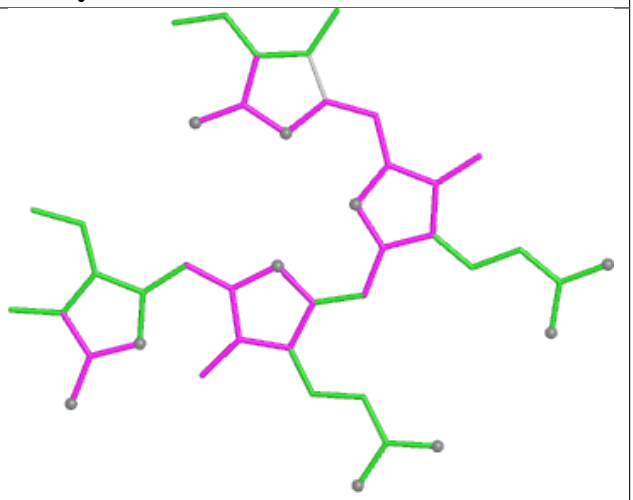

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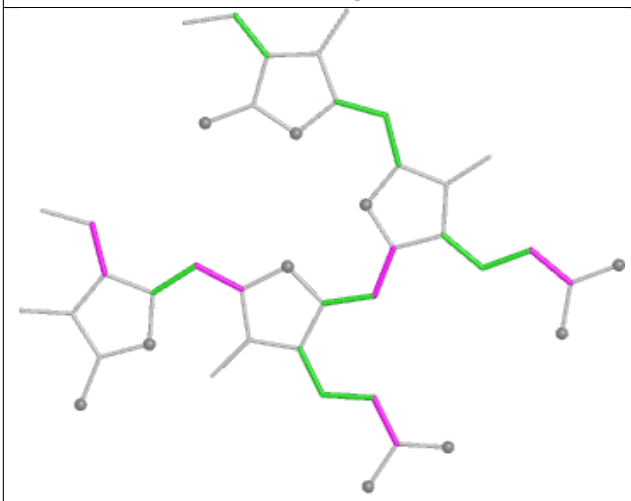

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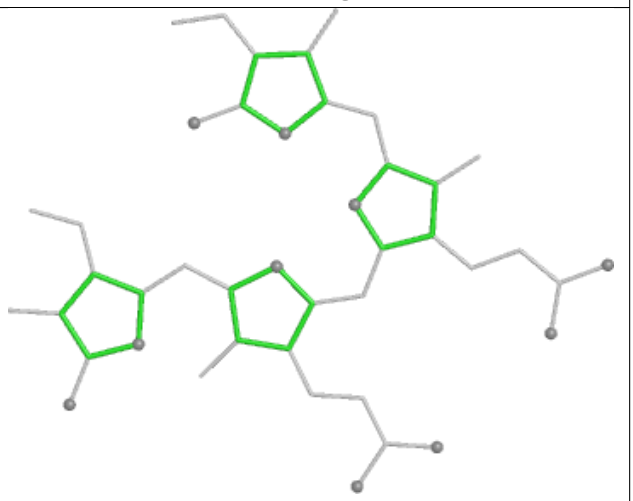
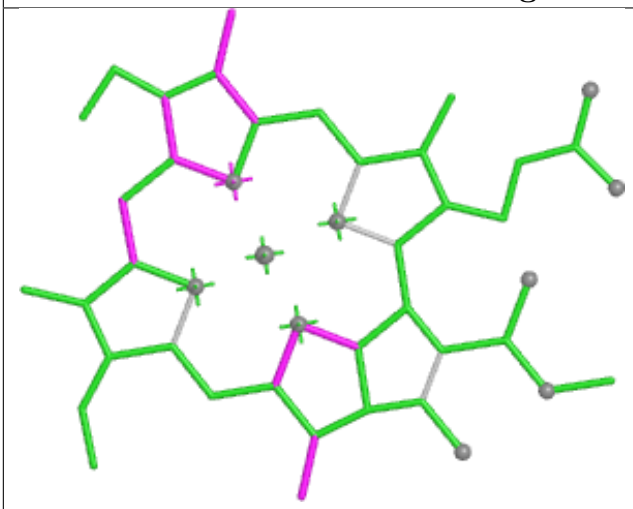


Rings

Ligand CLA 62 307



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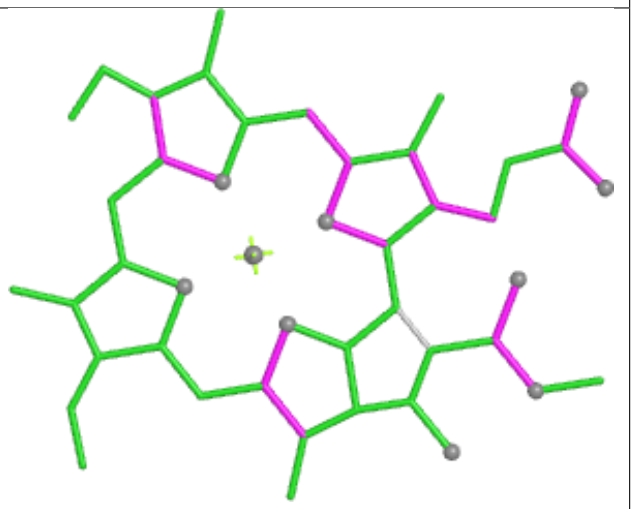

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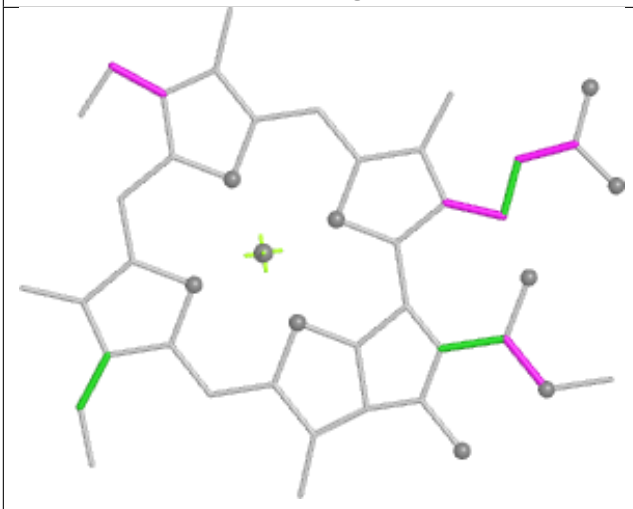
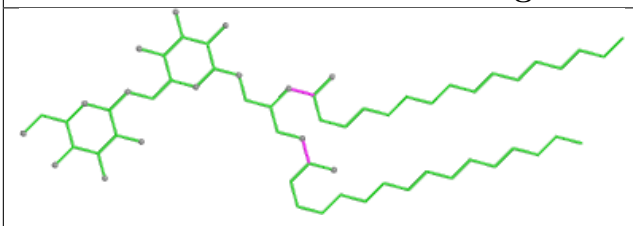


Torsions



Rings

Ligand DGD J6 101



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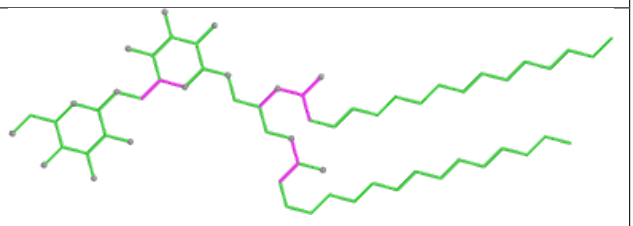

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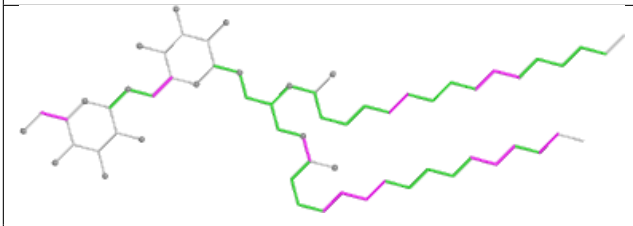

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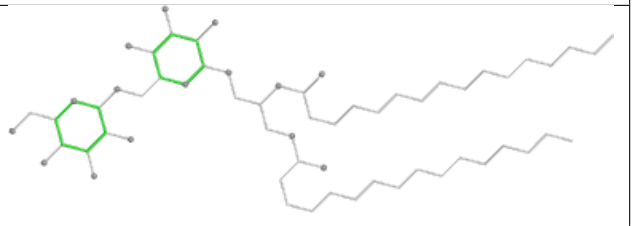
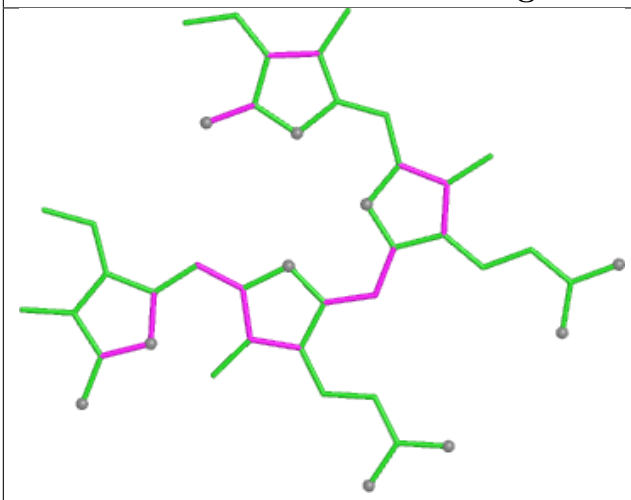


Rings

Ligand PEB aF 203



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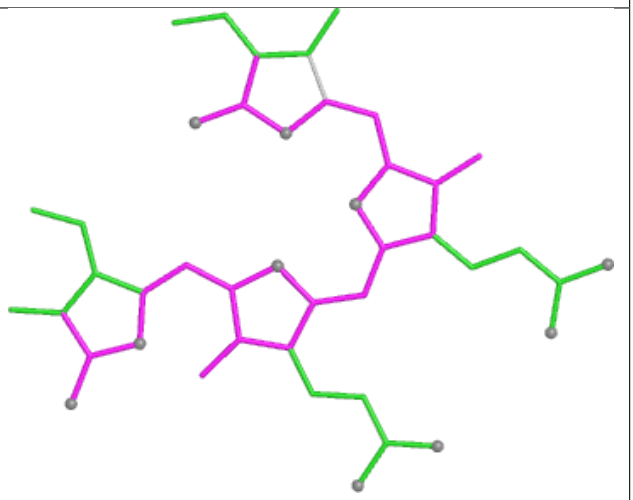

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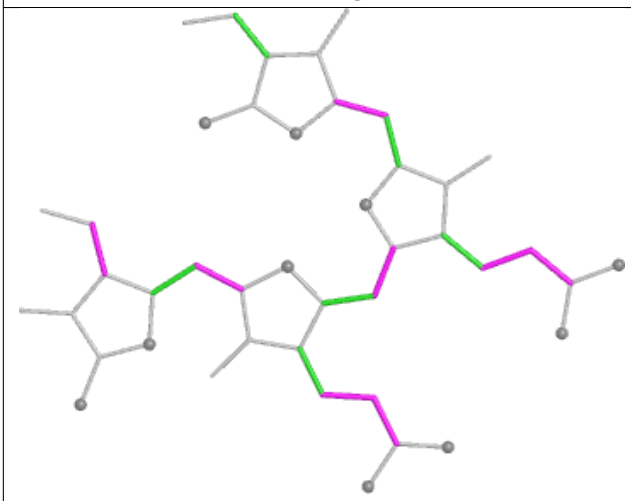

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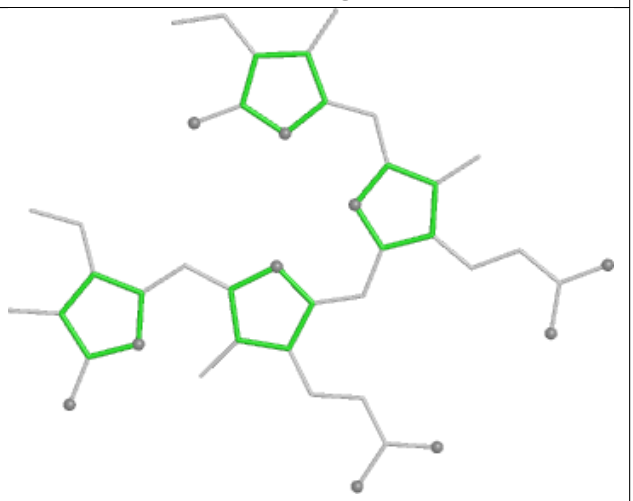
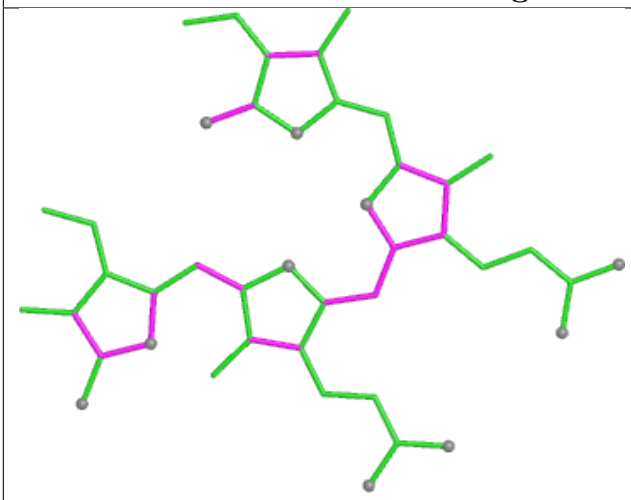


Rings

Ligand PEB RO 201



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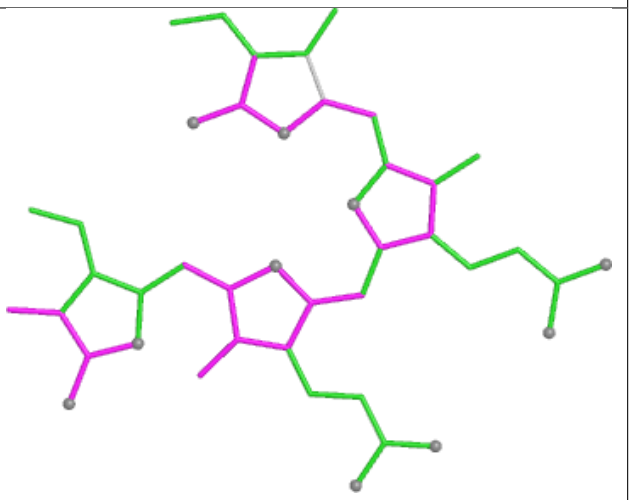

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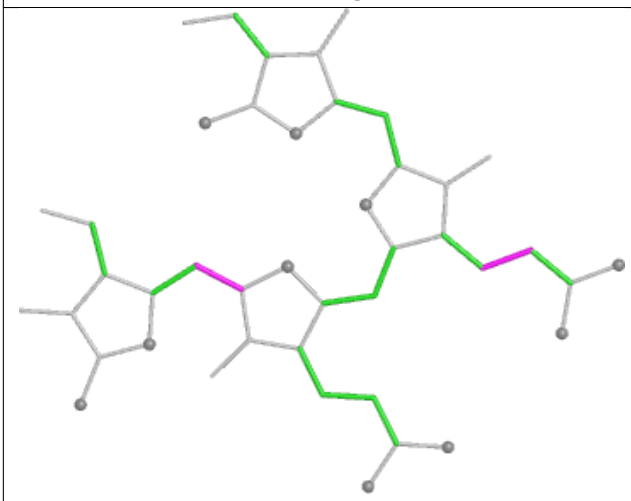

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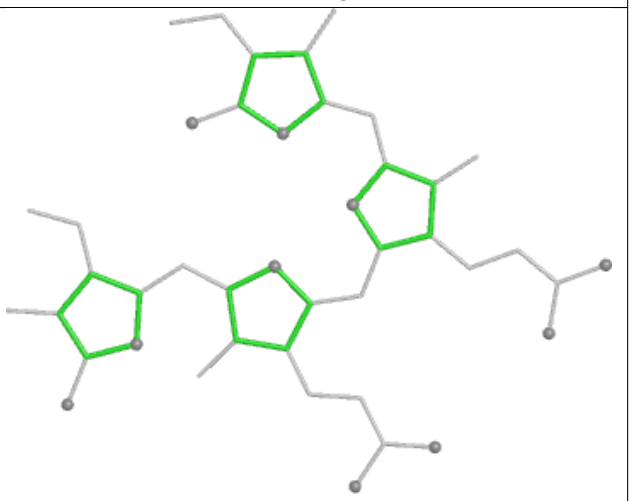
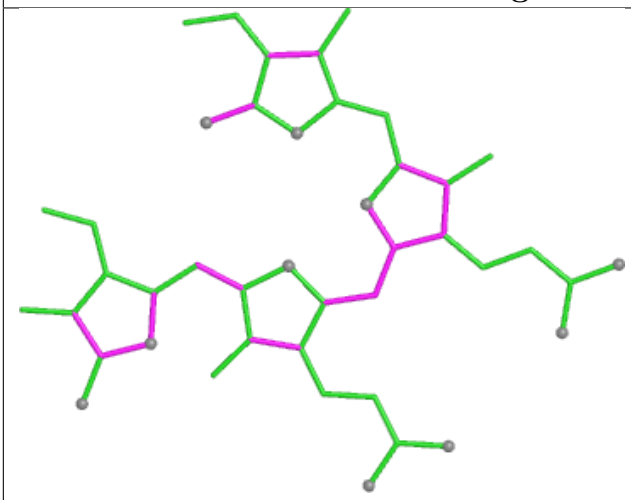


Rings

Ligand PEB QB 202



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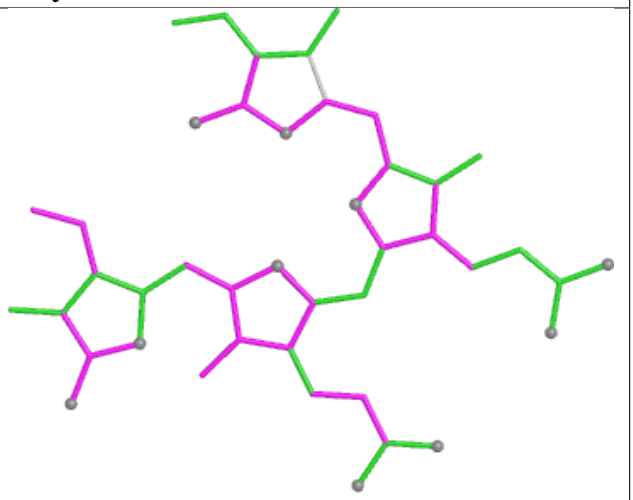

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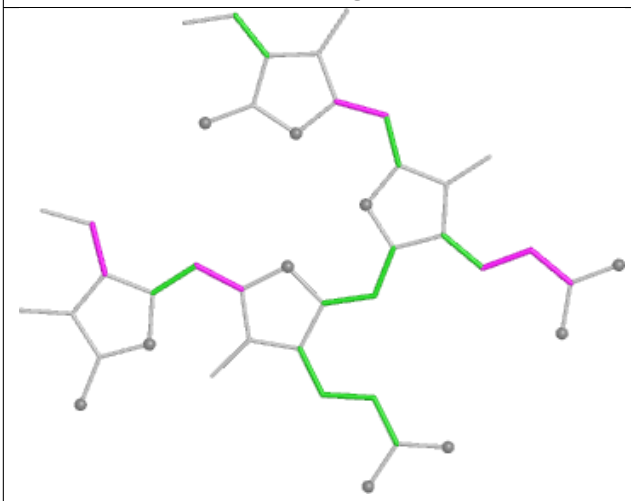

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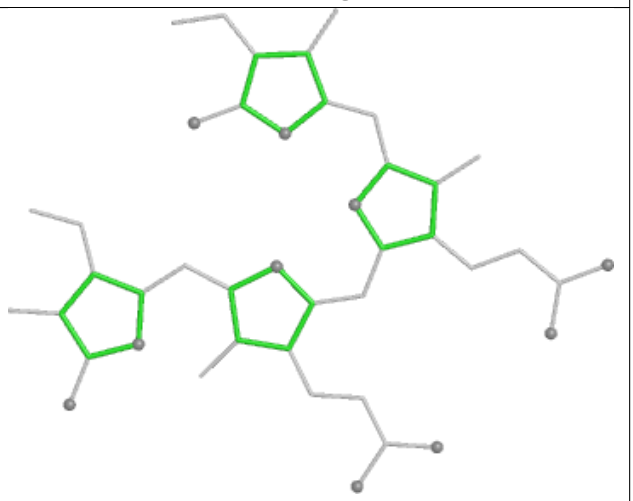
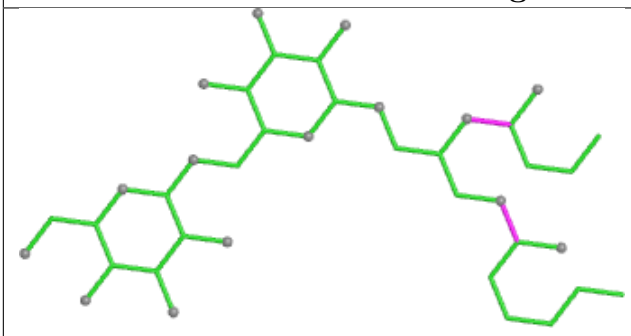


Rings

Ligand DGD BL 607



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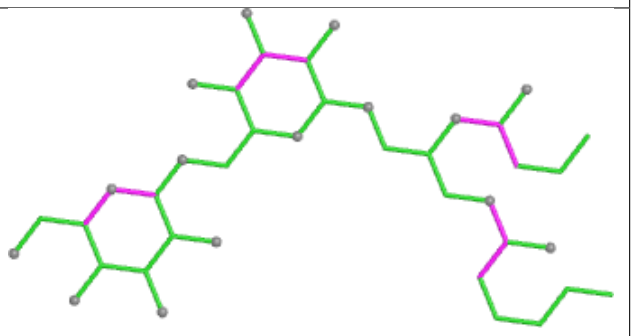
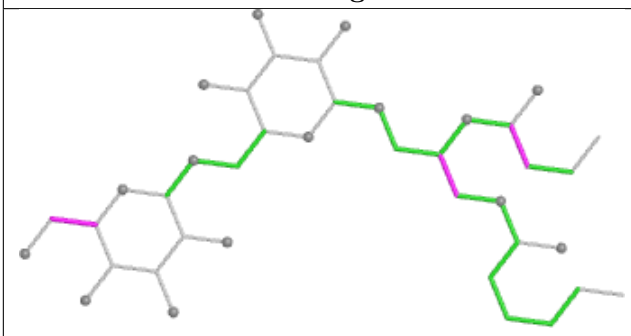


Bond angles



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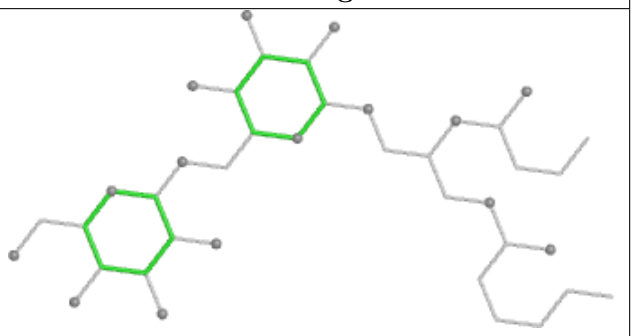
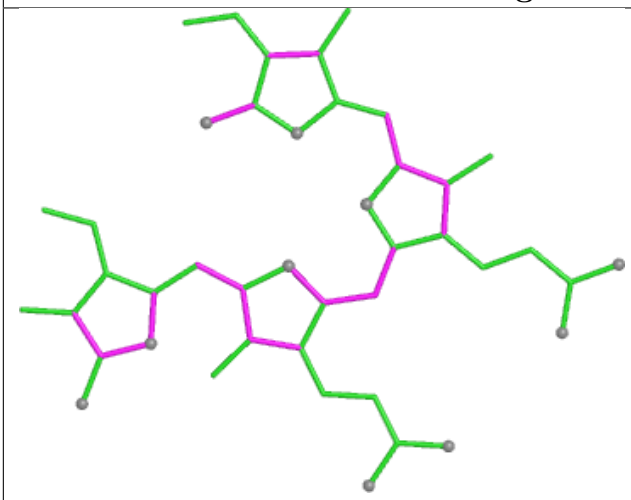


Rings

Ligand PEB C7 201



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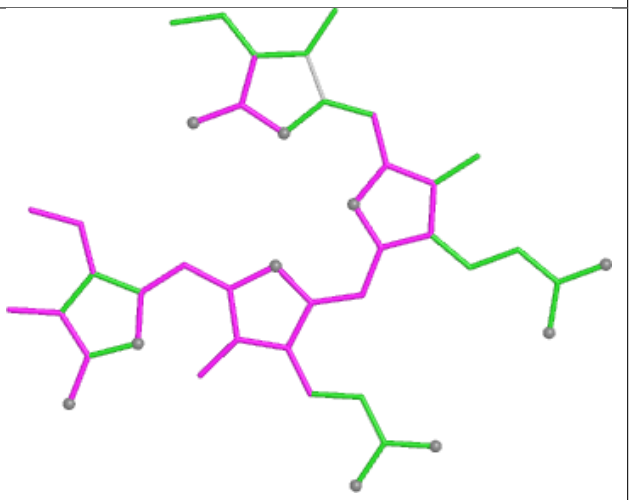
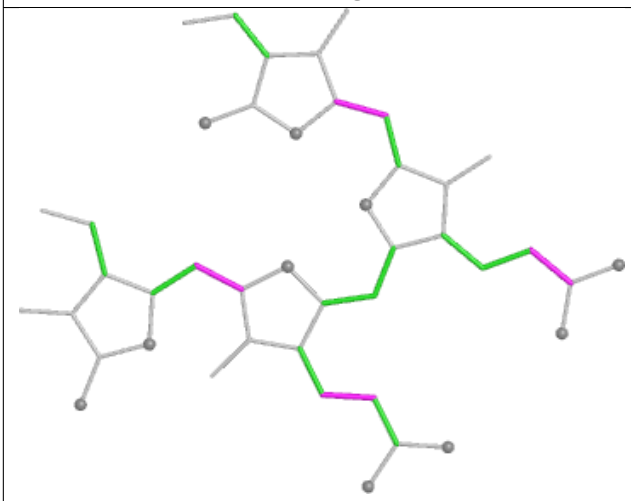


Bond angles



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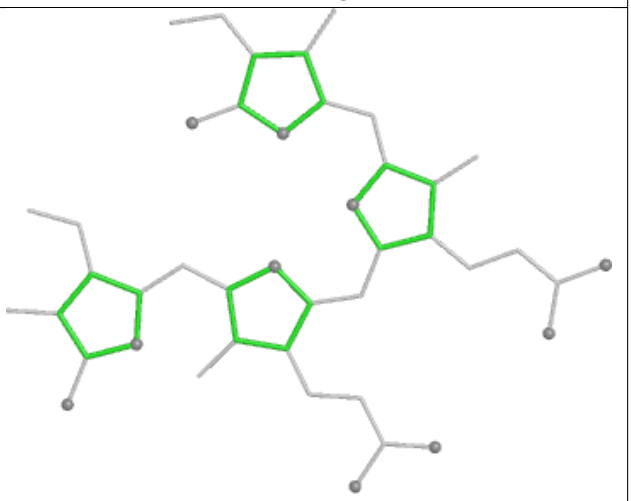
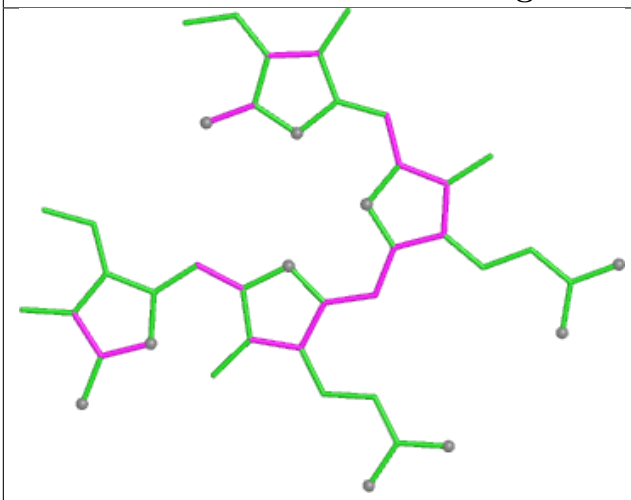


Rings

Ligand PEB B7 202



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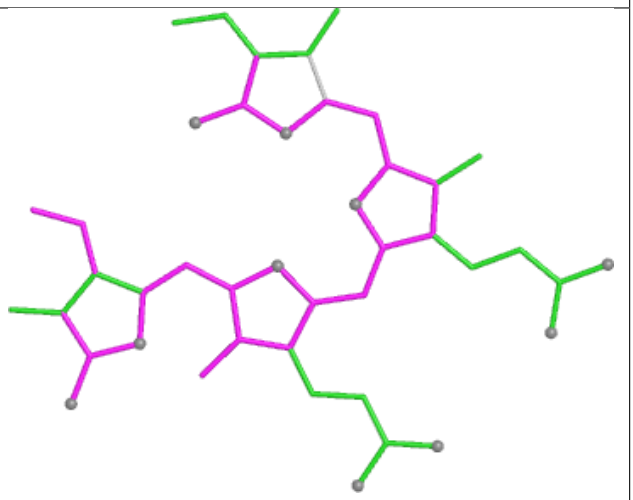
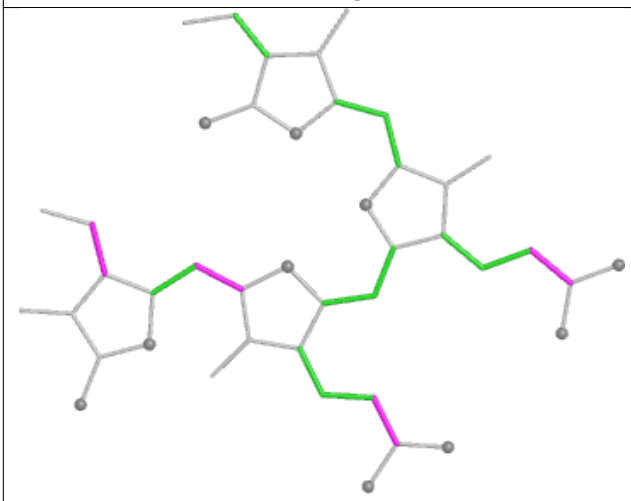


Bond angles



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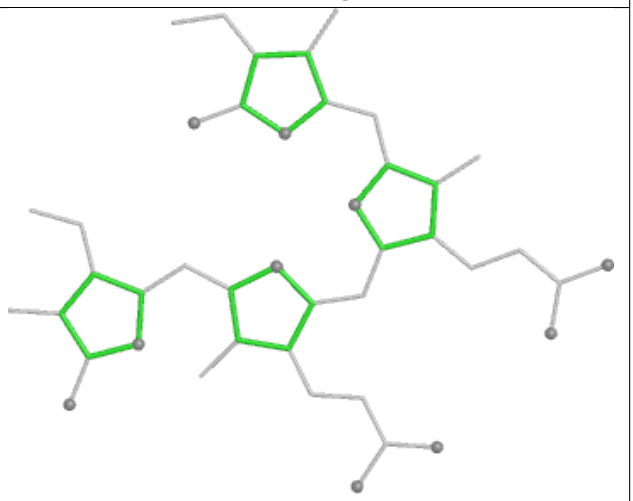

Rings

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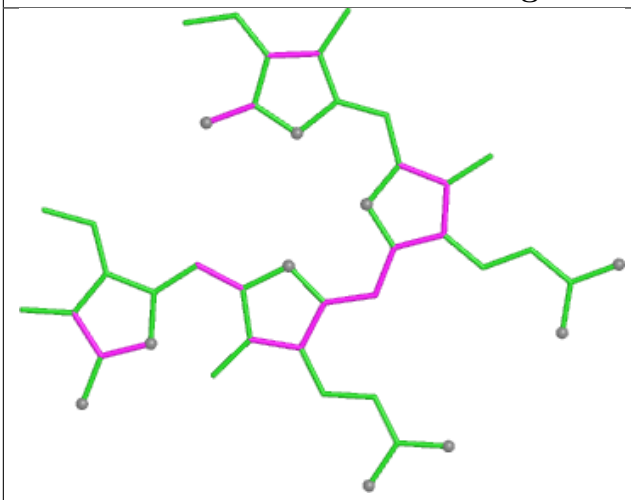

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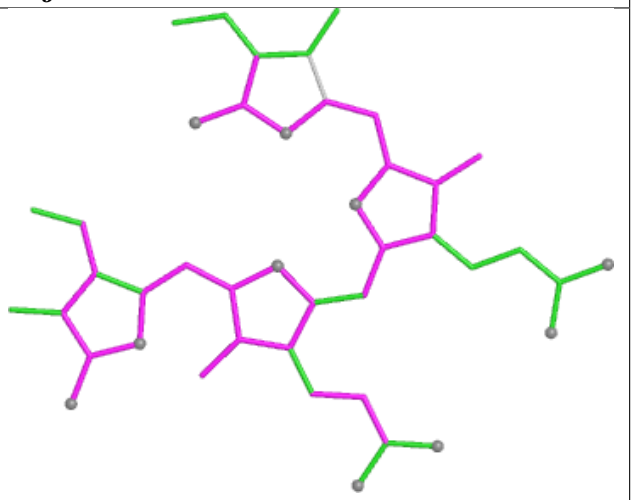
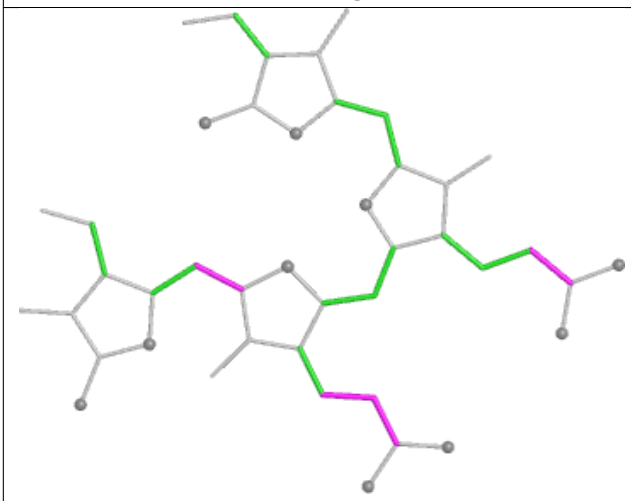


Bond angles



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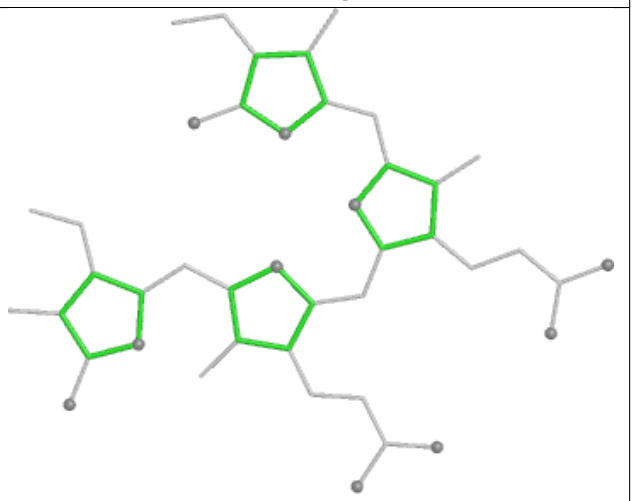
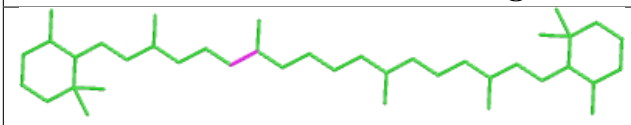


Rings

Ligand BCR KN 101



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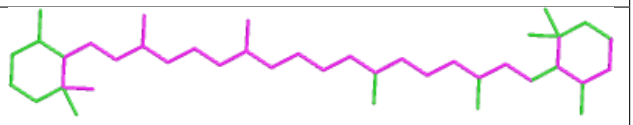
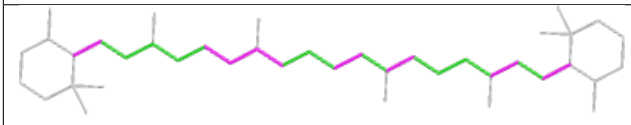


Bond angles



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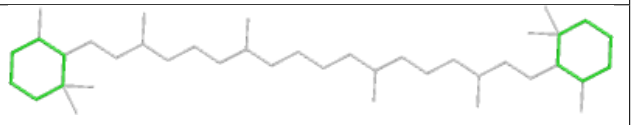
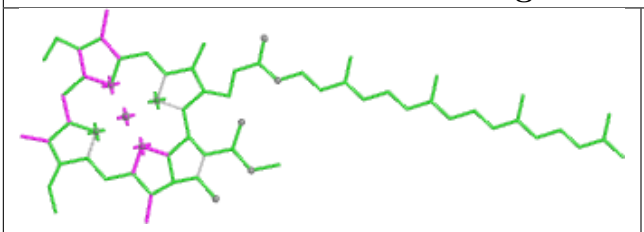


Rings

Ligand CLA B6 616



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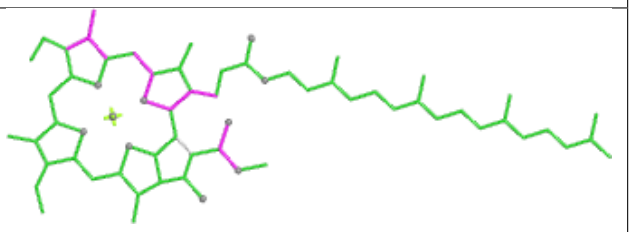

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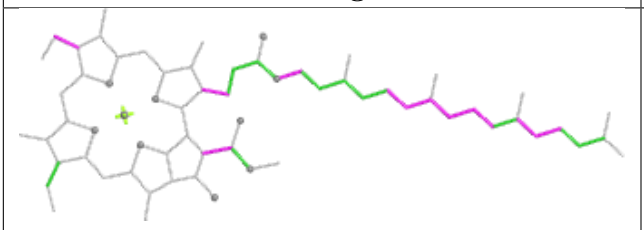

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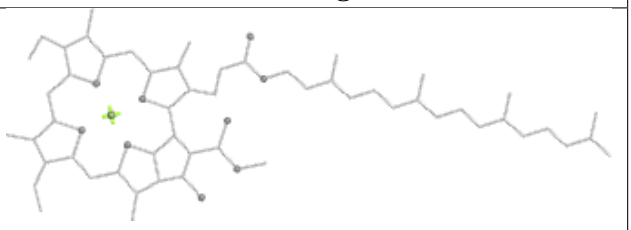
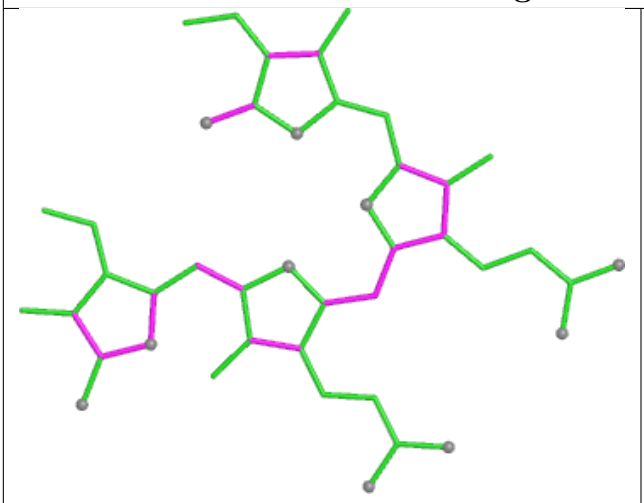


Rings

Ligand PEB ZB 202



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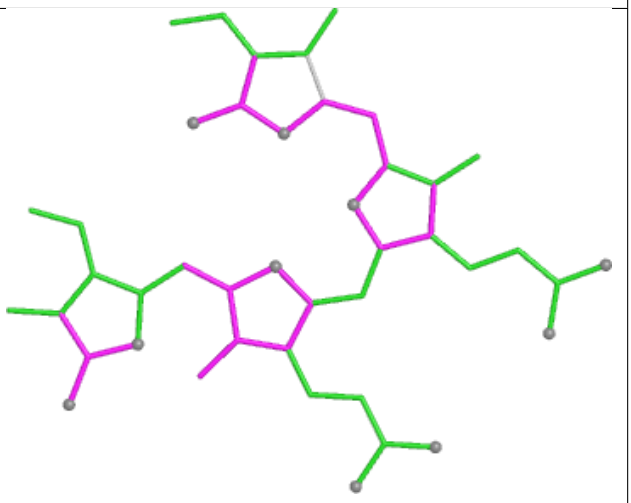

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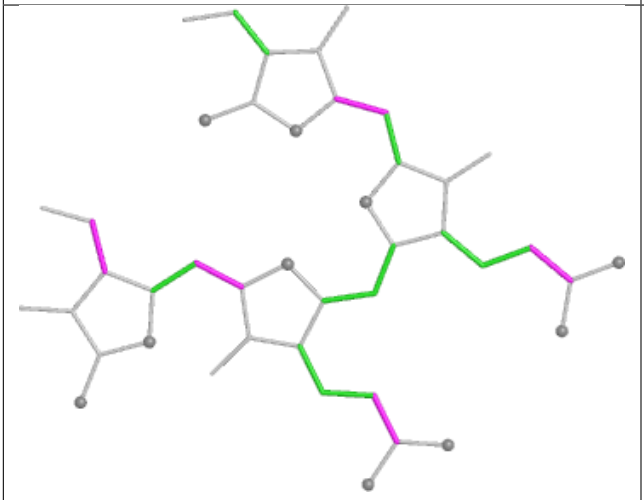

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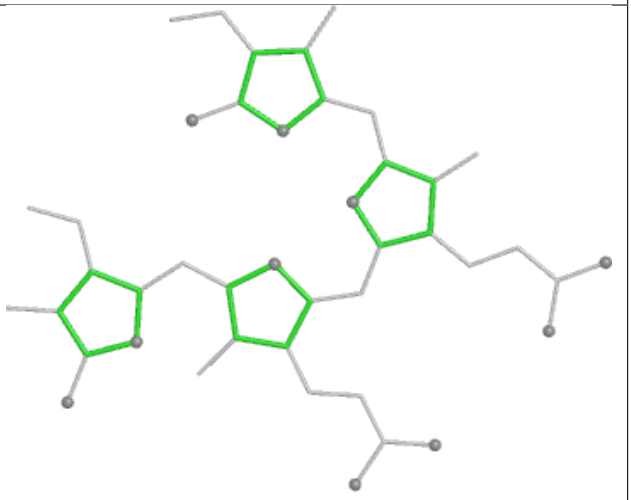
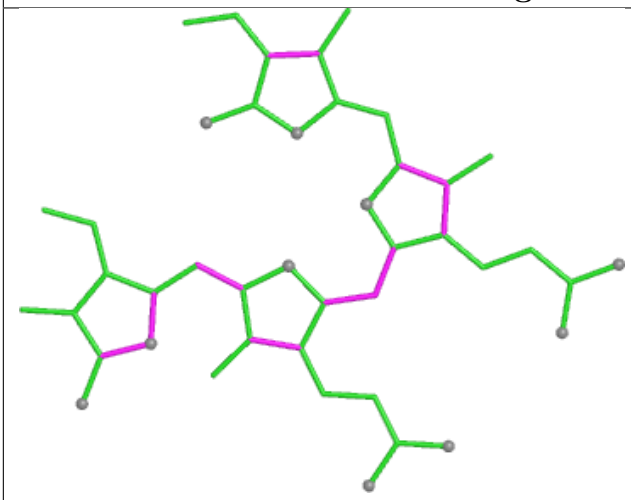


Rings

Ligand PEB G7 201



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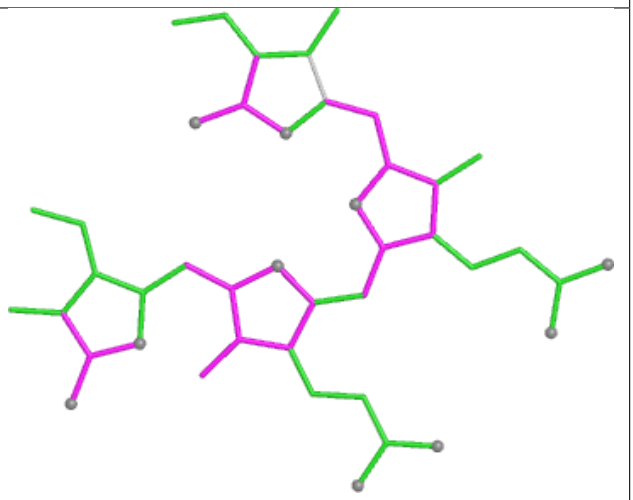

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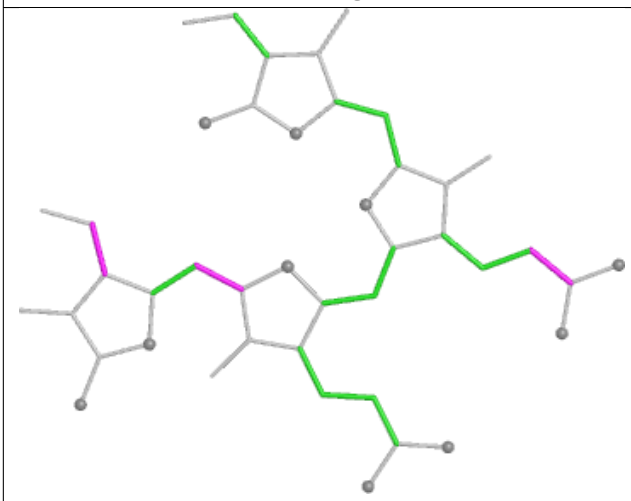

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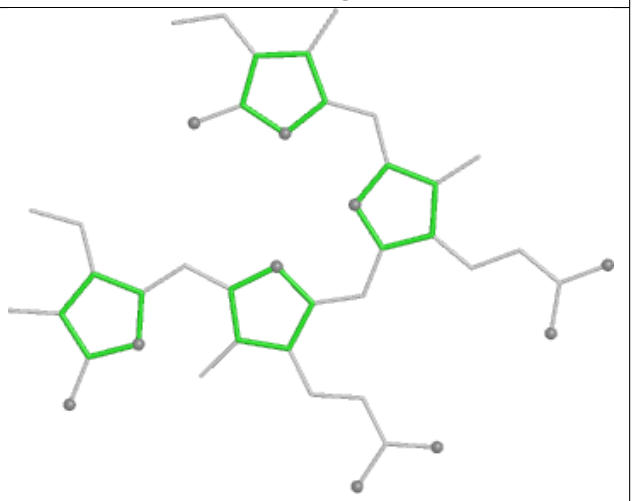
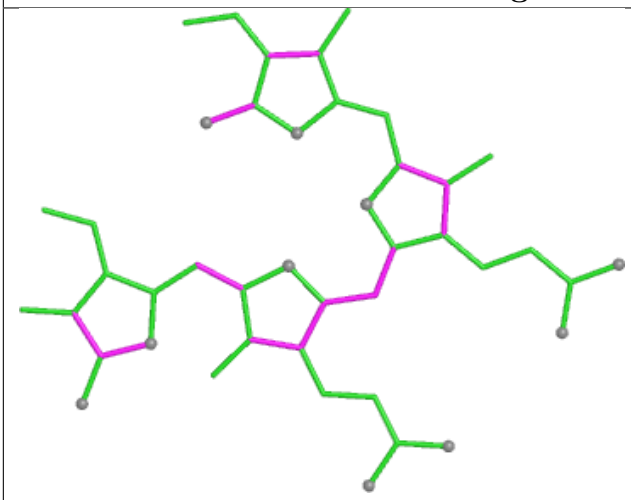


Rings

Ligand PEB RA 202



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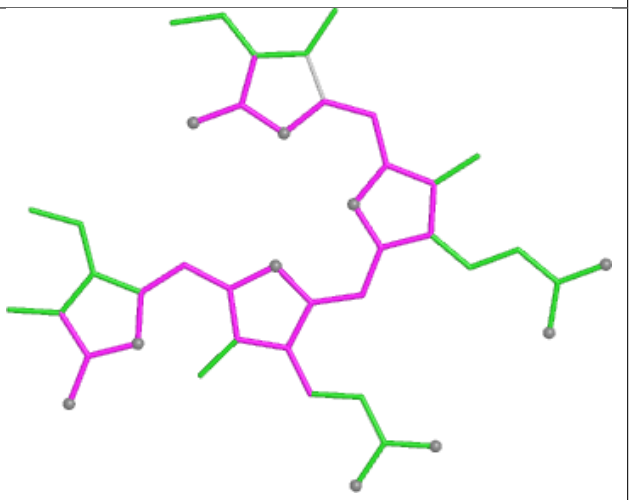

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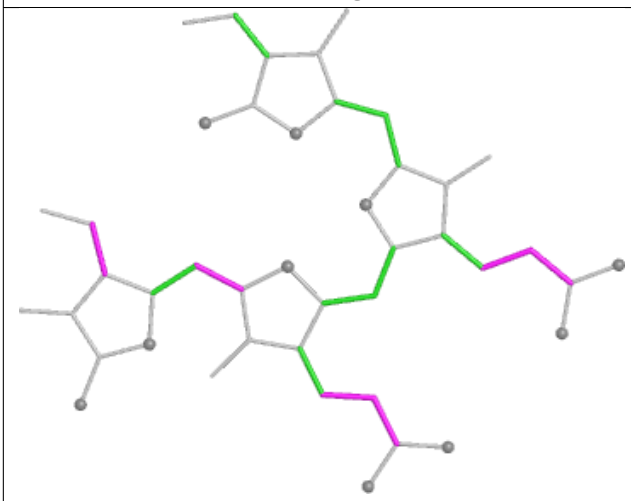

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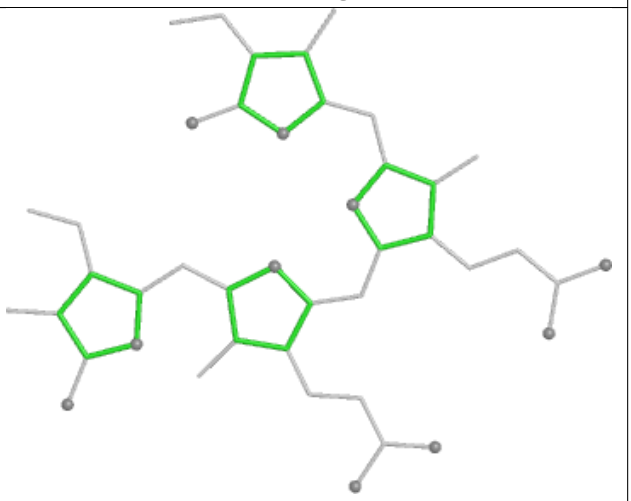

Rings

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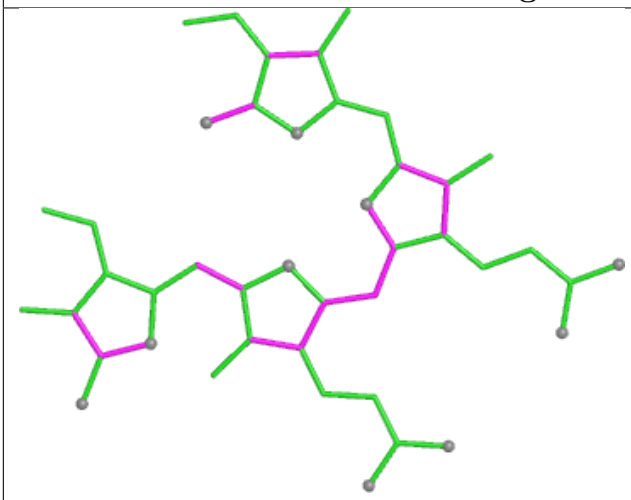

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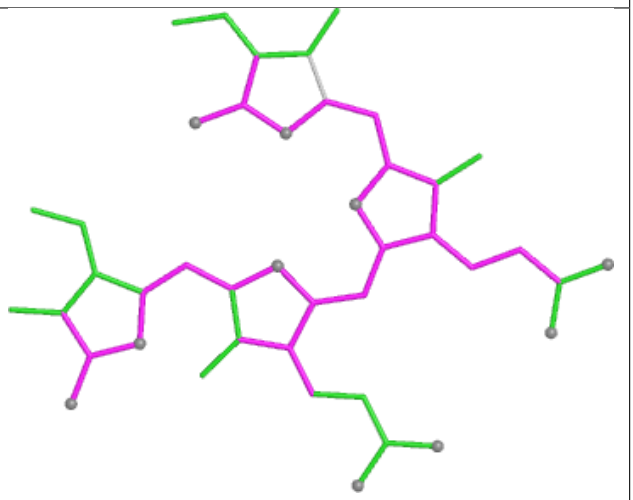

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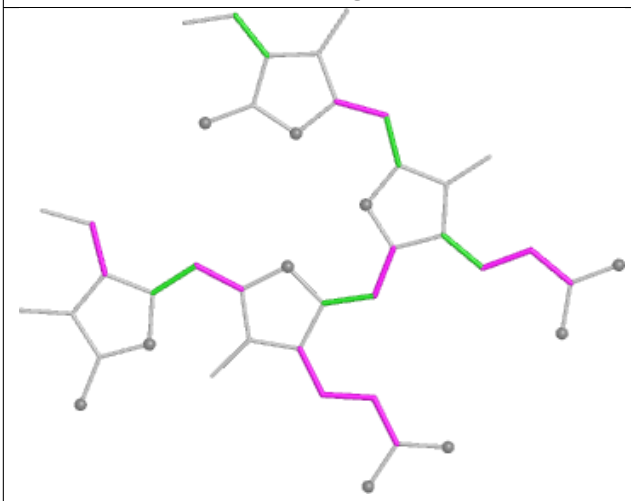

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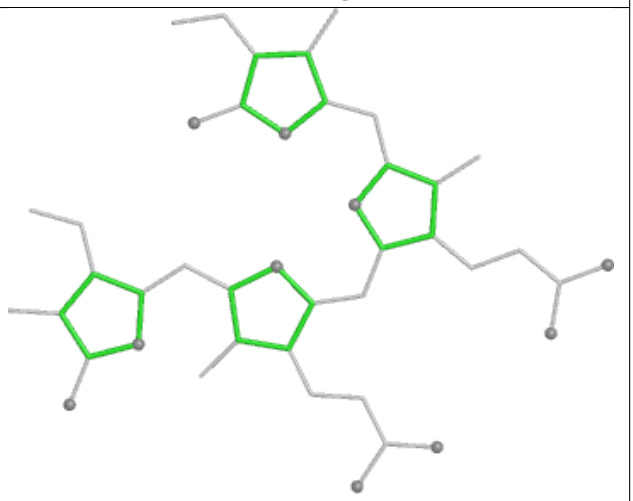
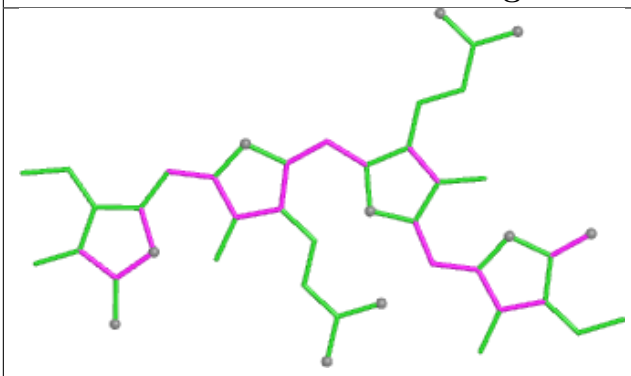


Rings

Ligand CYC D1 1003



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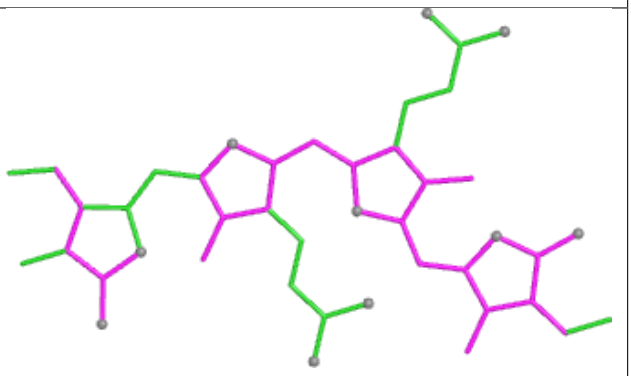

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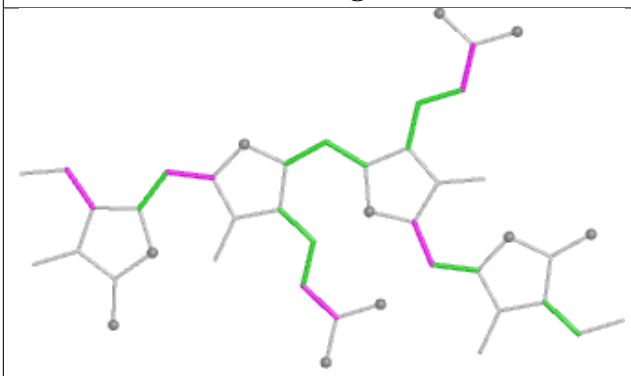

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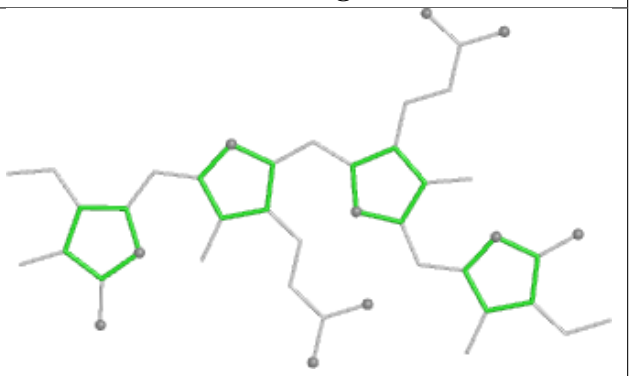

Rings

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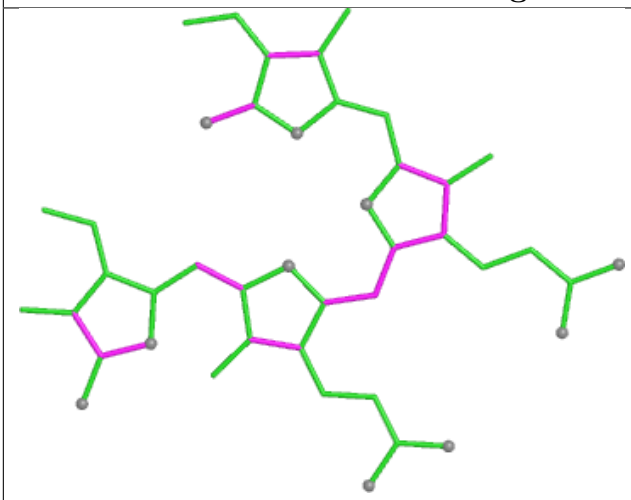

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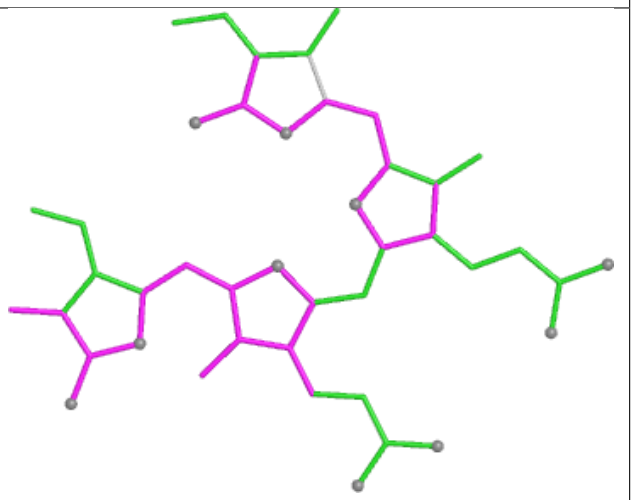

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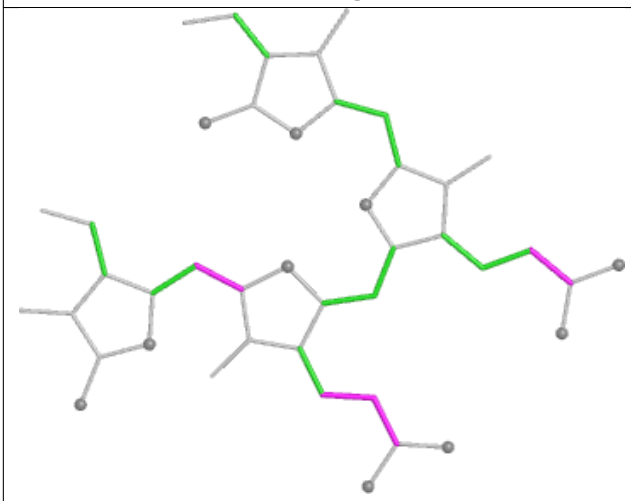

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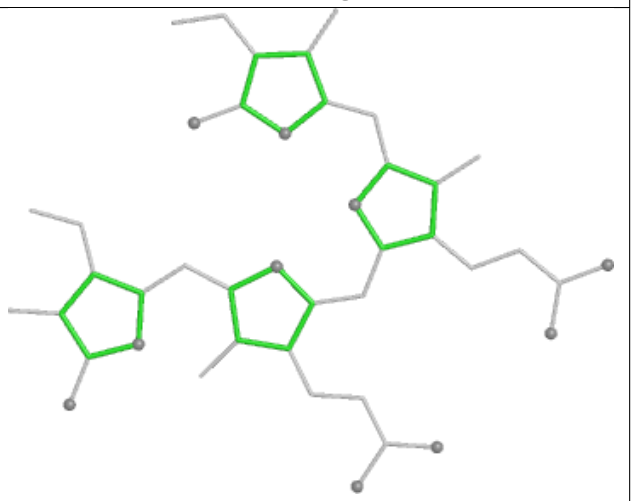

Rings

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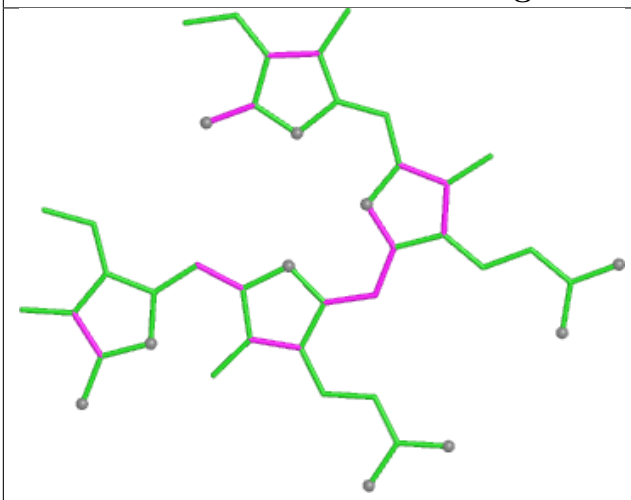

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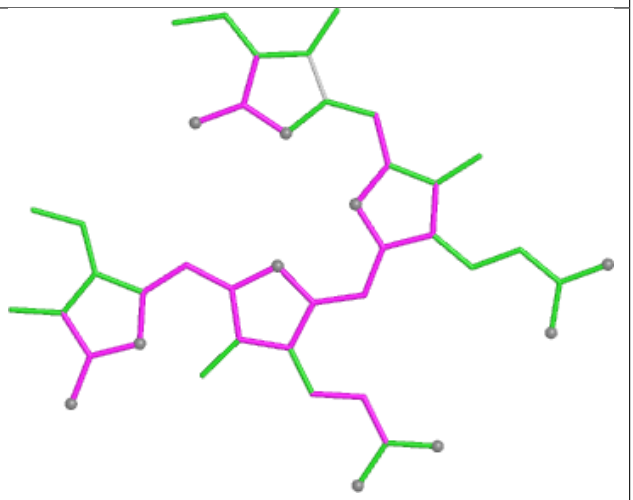

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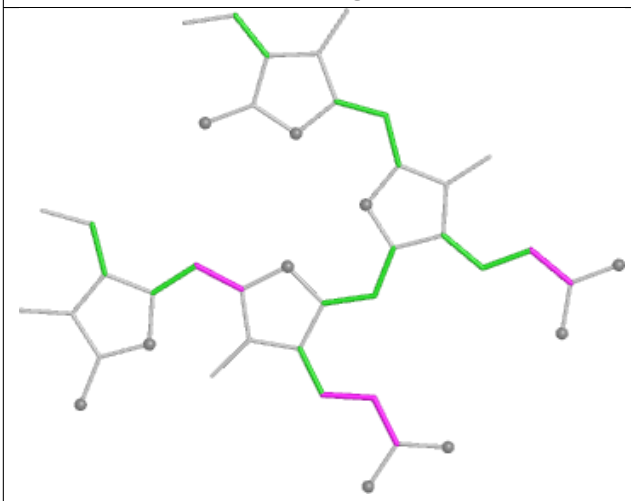

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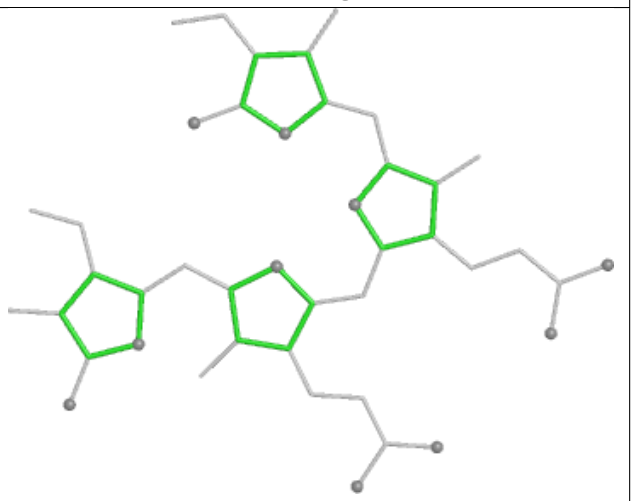

Rings

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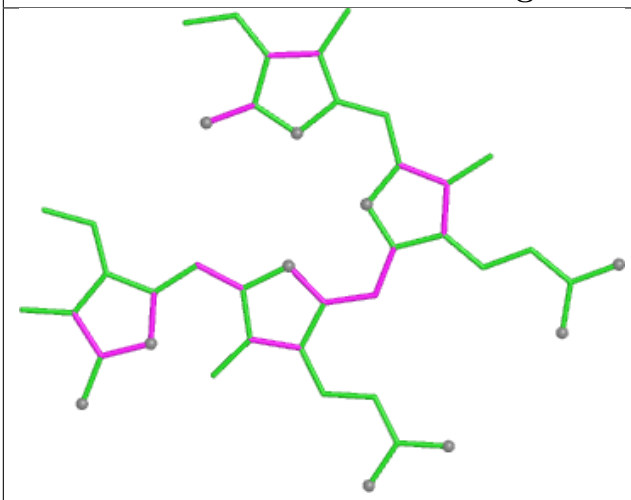

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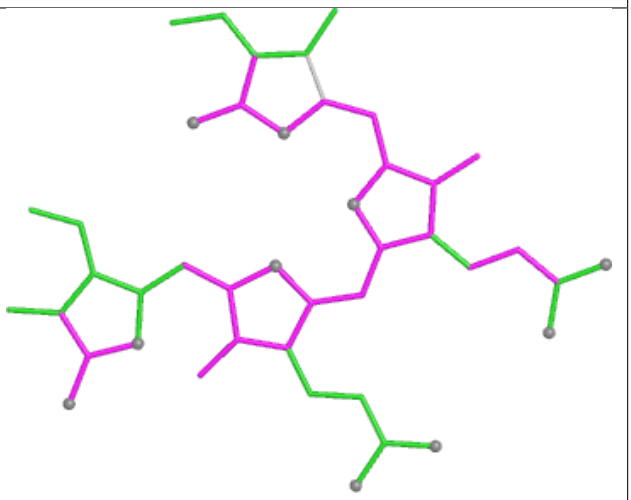

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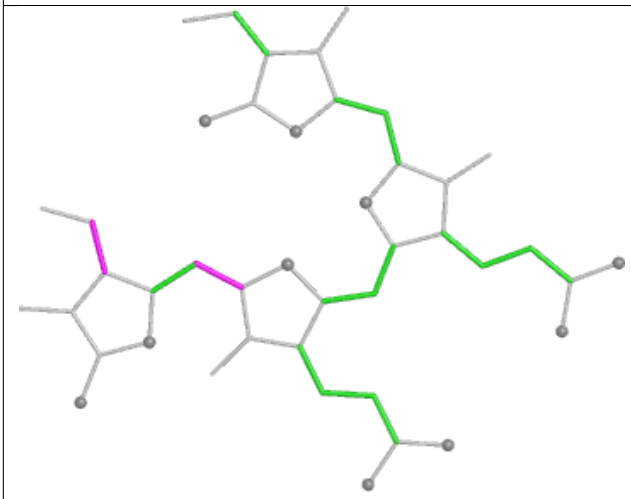

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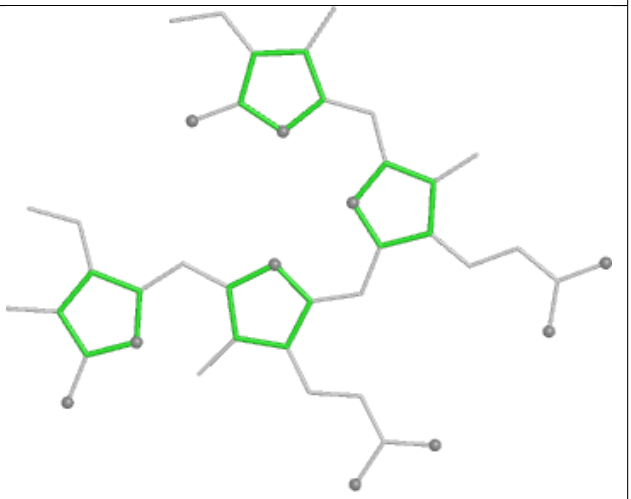
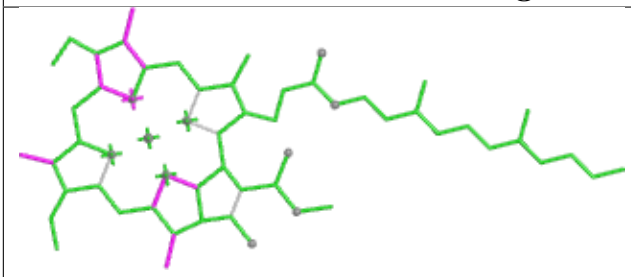


Rings

Ligand CLA B2 801



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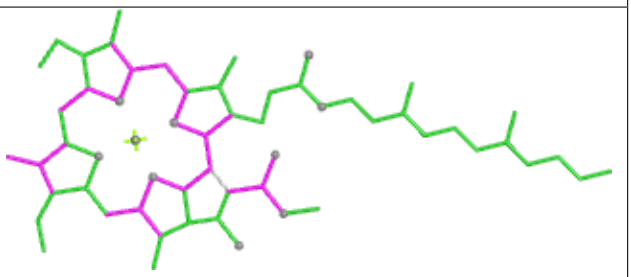

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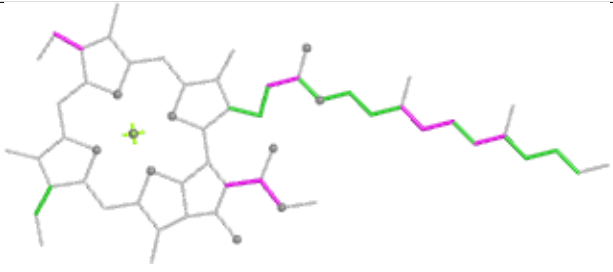

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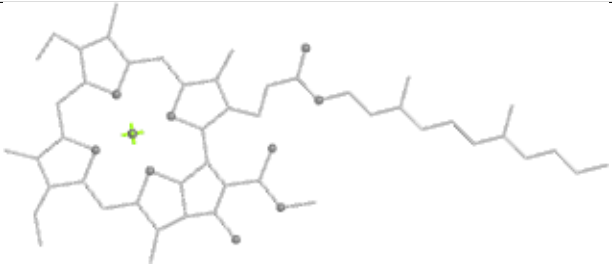
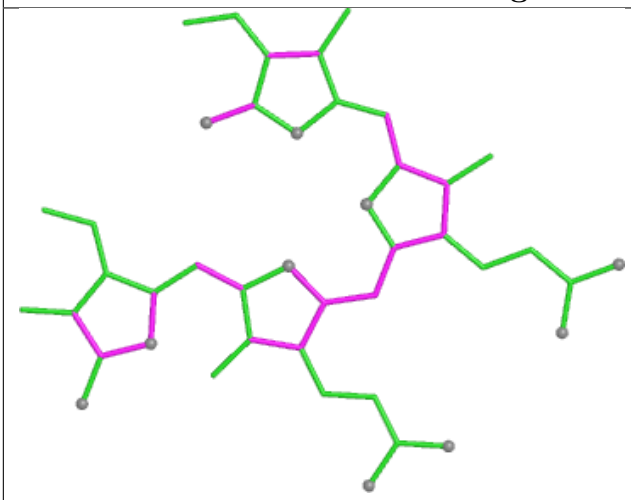


Rings

Ligand PEB VD 203



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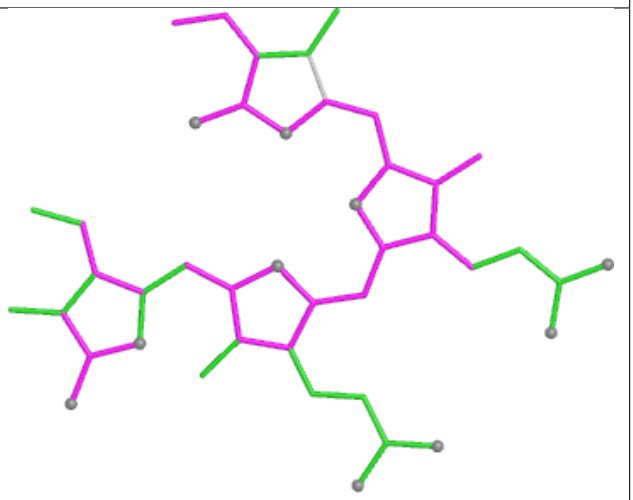

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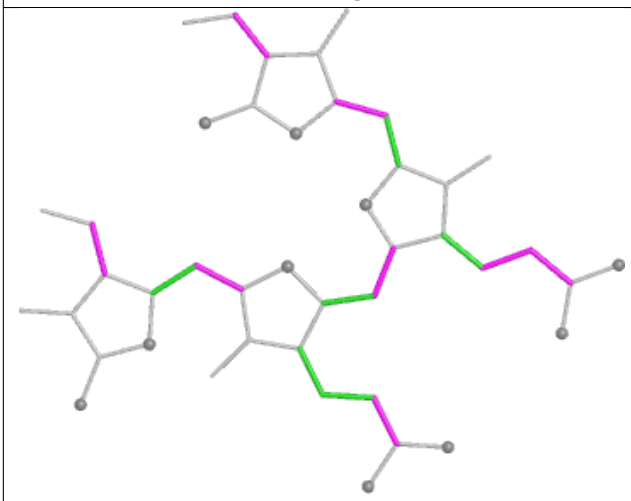

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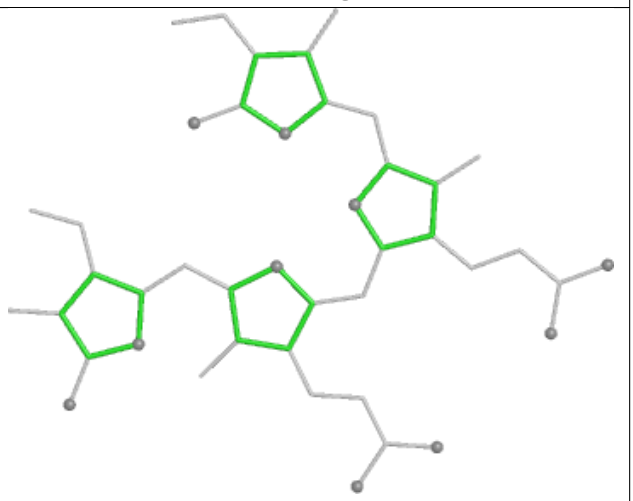
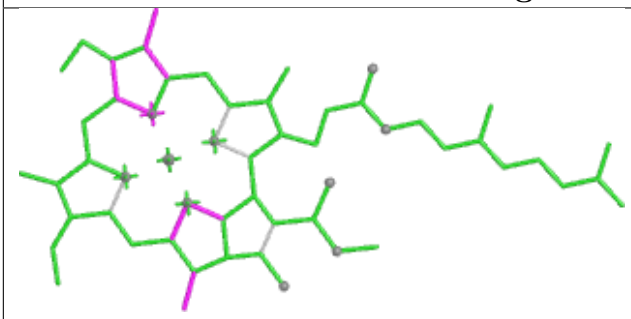


Rings

Ligand CLA B2 815



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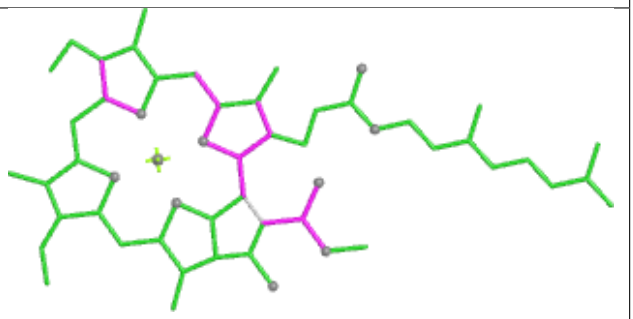
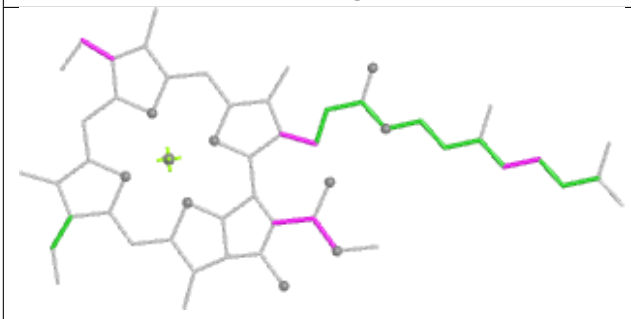


Bond angles



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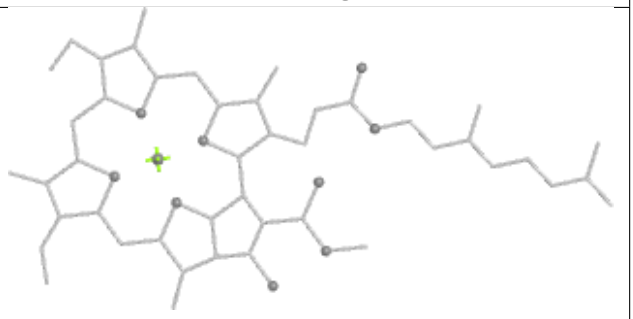
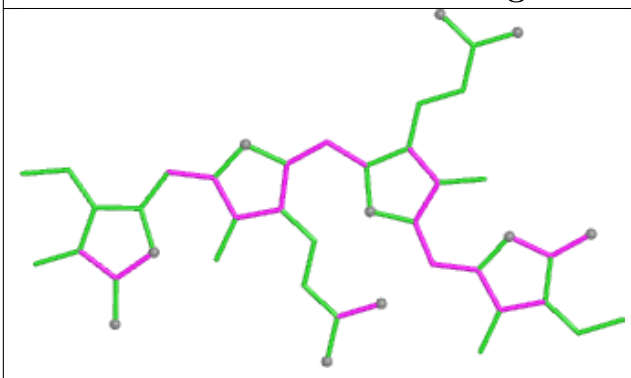


Rings

Ligand CYC k3 1001



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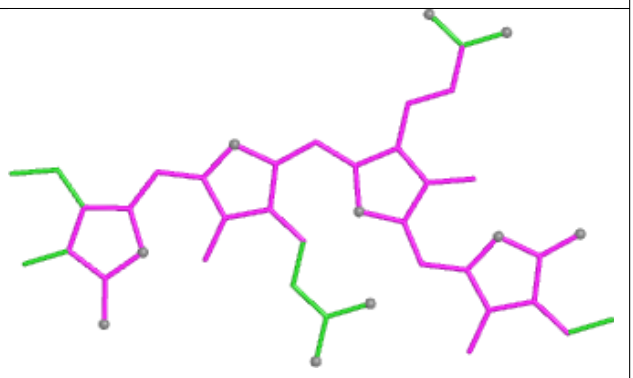
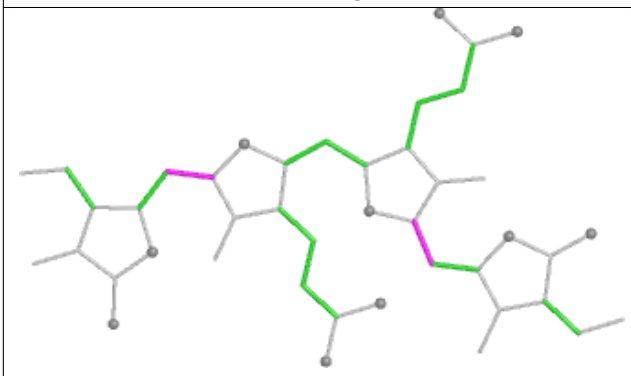


Bond angles



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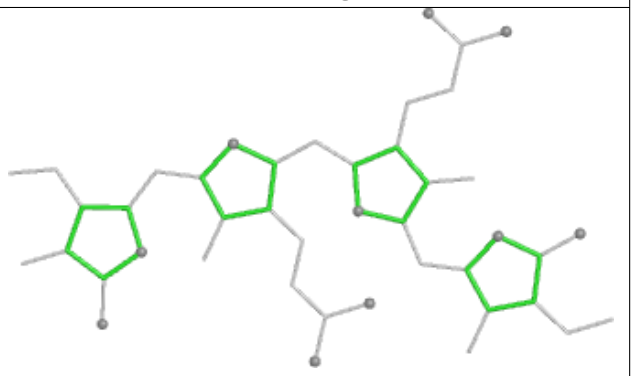
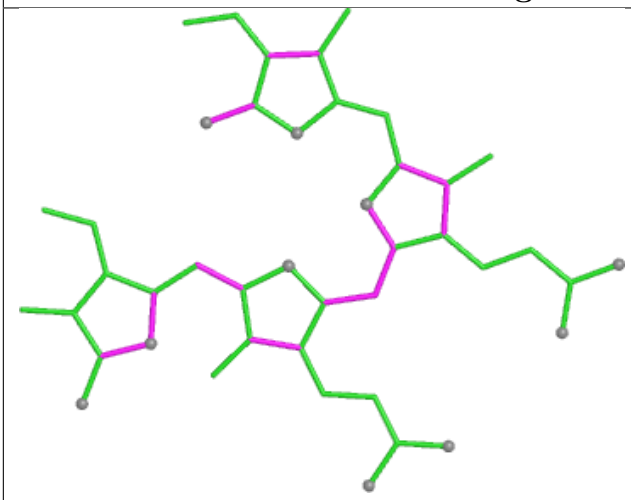
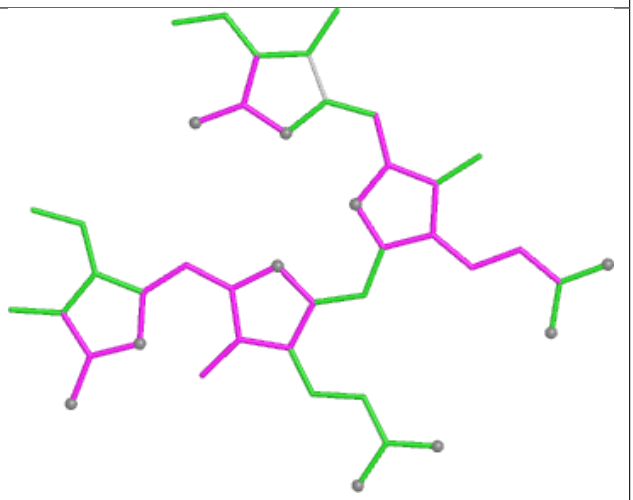


Rings

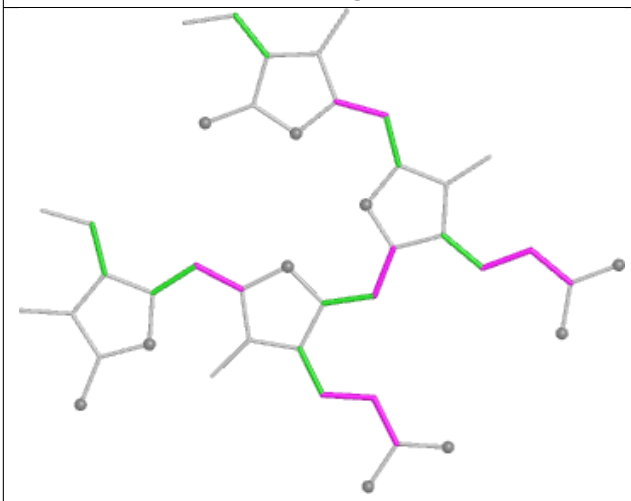
Ligand PEB D5 203



Bond lengths



Bond angles



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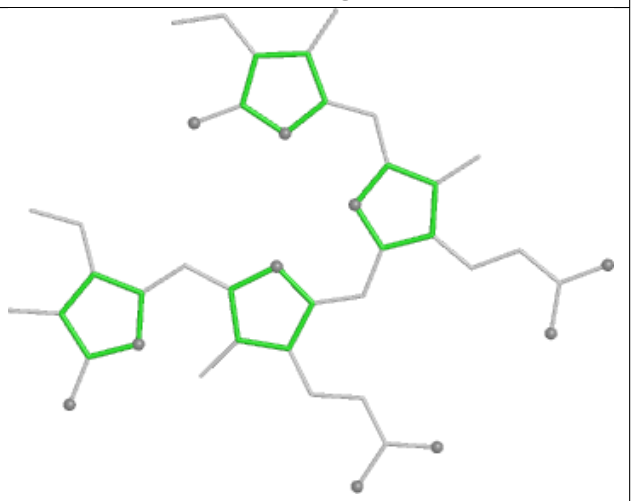
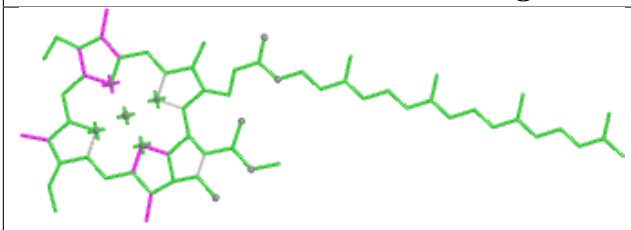


Rings

Ligand CLA A2 813



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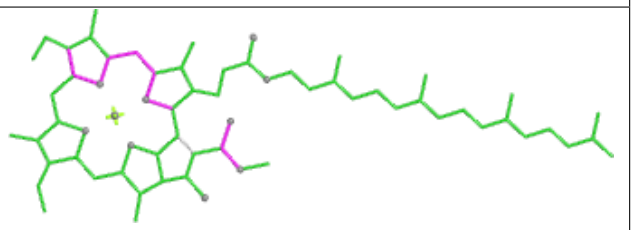
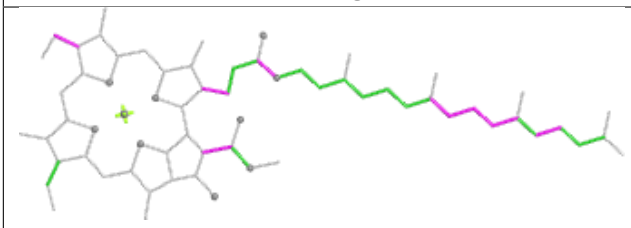
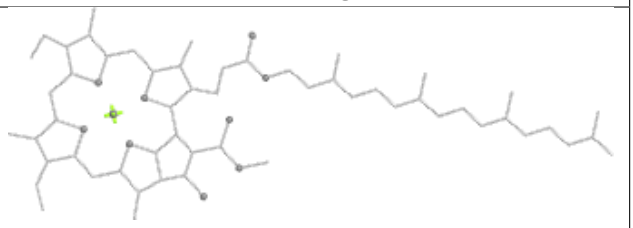


Bond angles

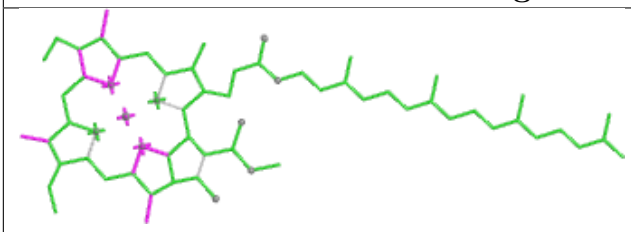


Torsions



Rings

Ligand CLA CL 510



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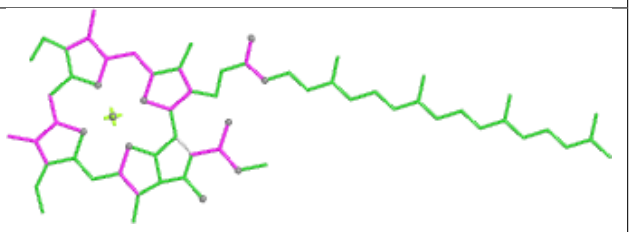

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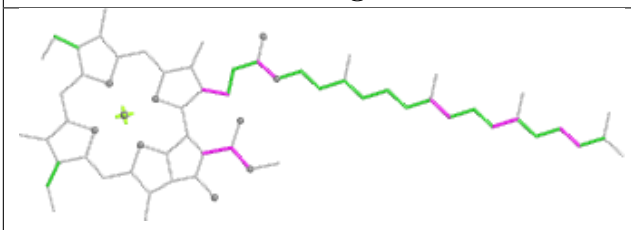

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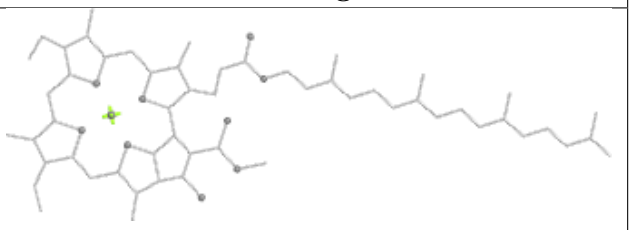
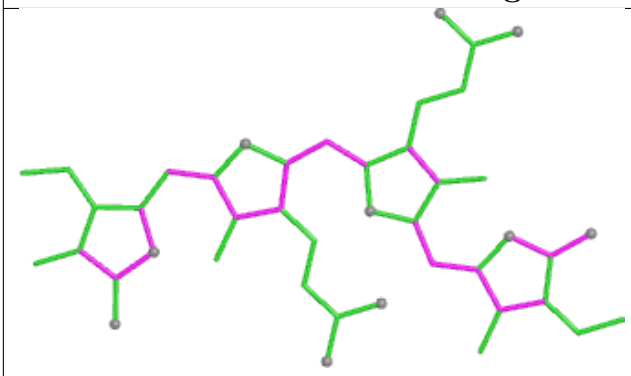


Rings

Ligand CYC A3 1001



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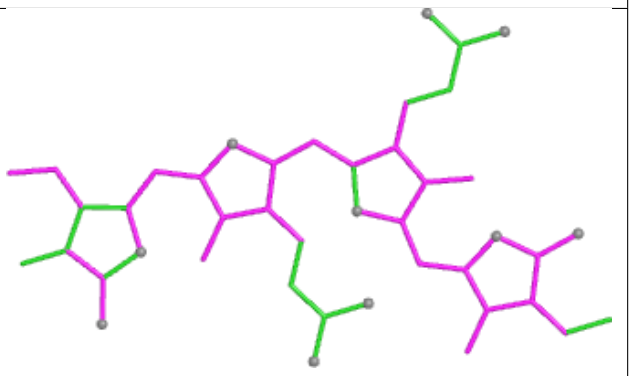

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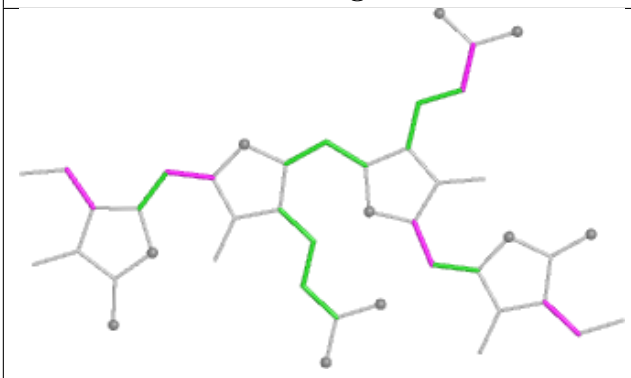

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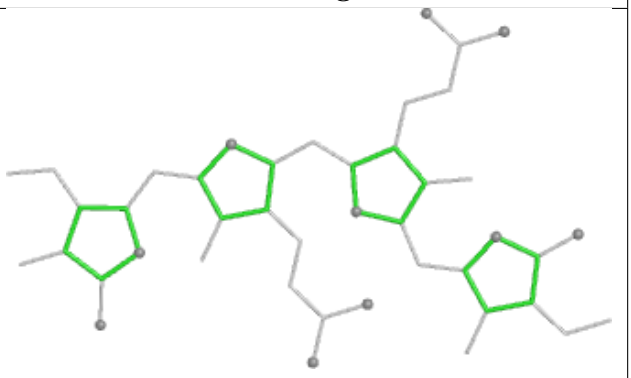
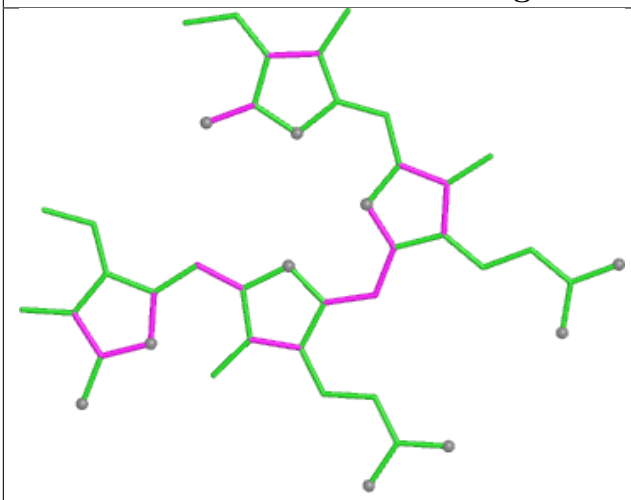


Rings

Ligand PEB PP 201



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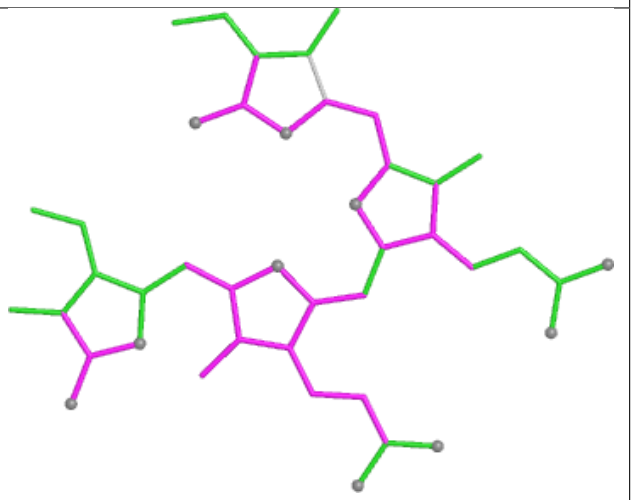
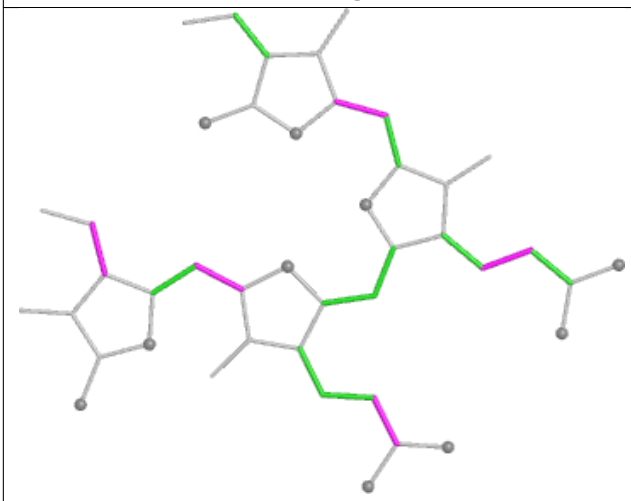


Bond angles



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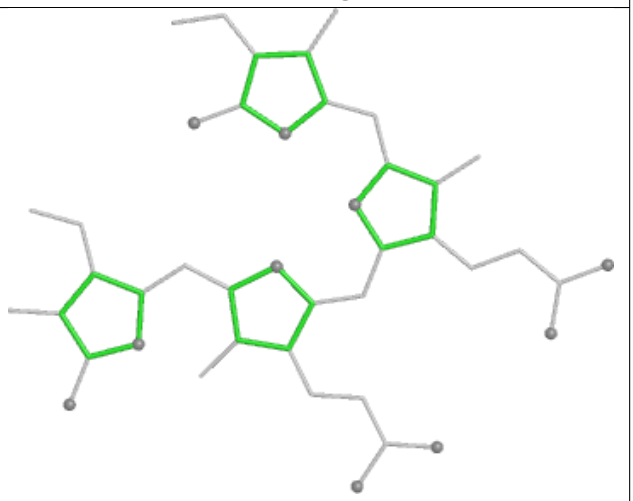
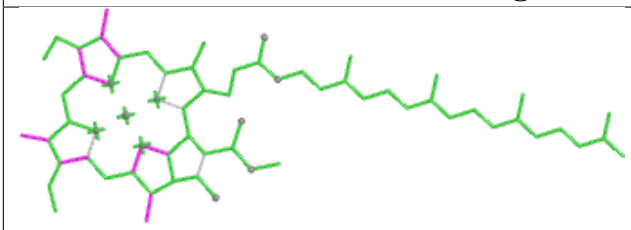


Rings

Ligand CLA FN 205



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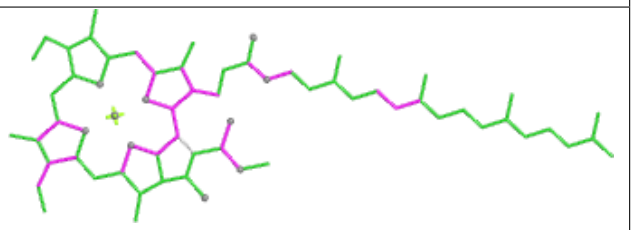

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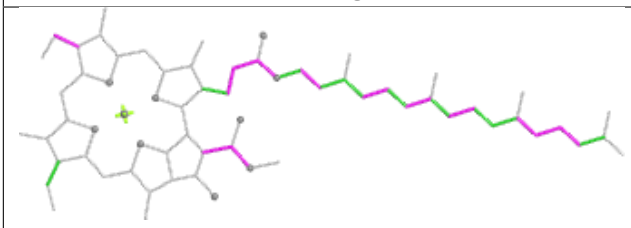

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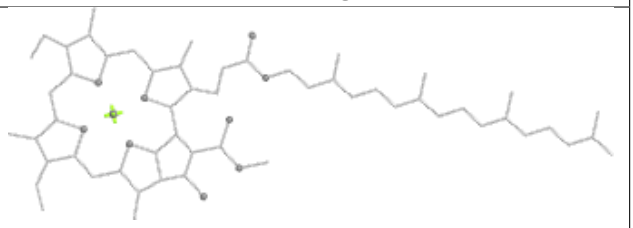
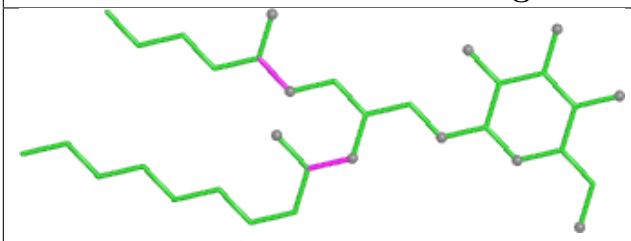
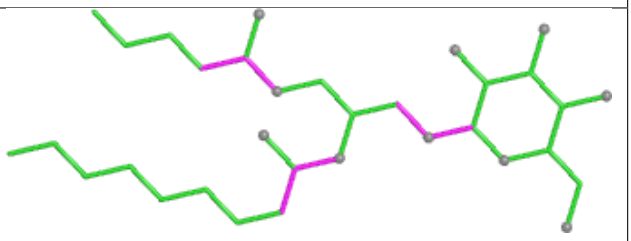
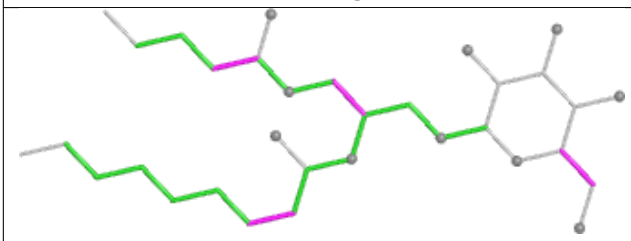
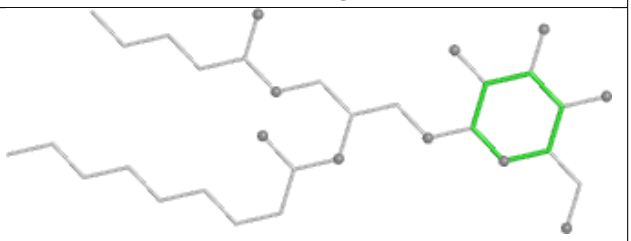


Rings

Ligand LMG JL 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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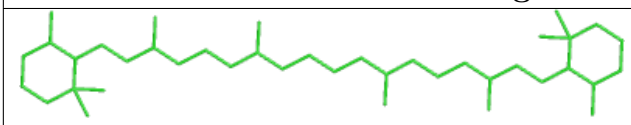
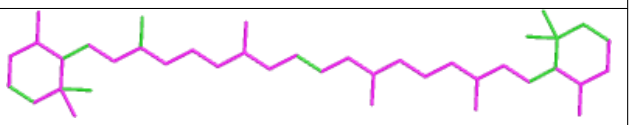
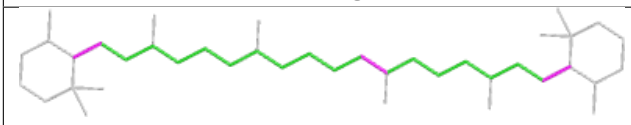
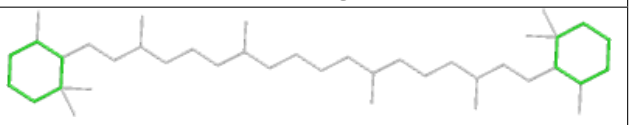
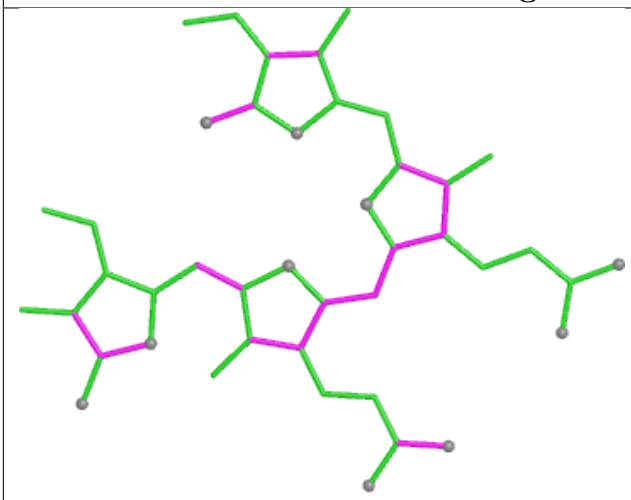
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEB fB 301



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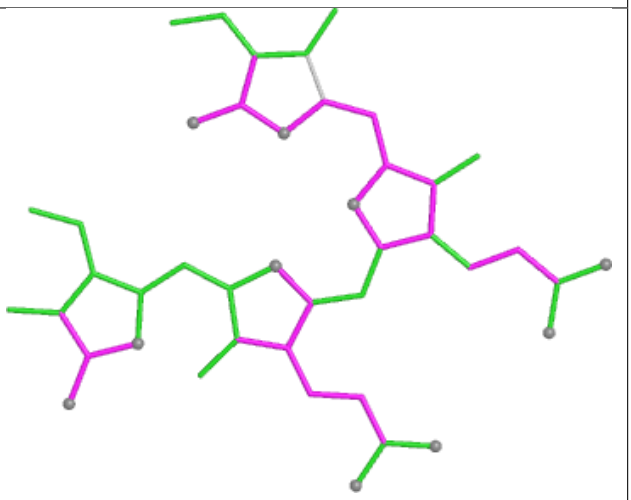
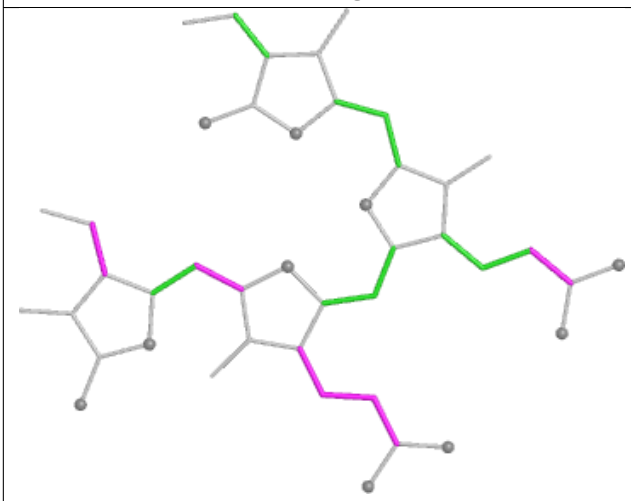


Bond angles



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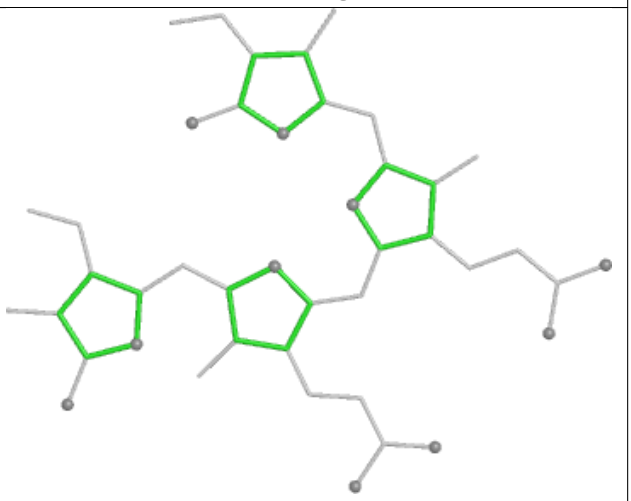
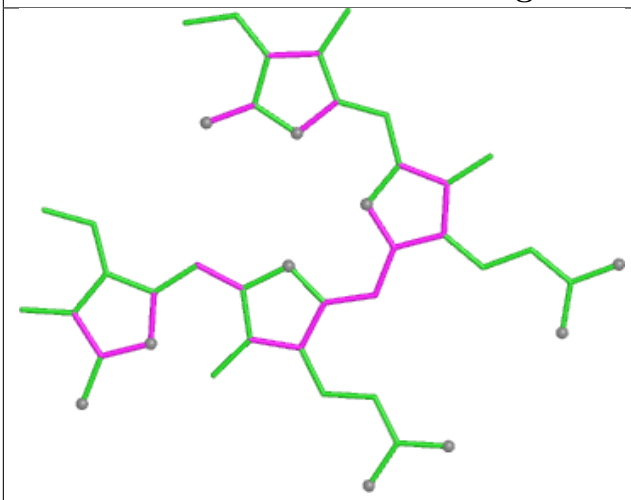


Rings

Ligand PEB C9 201



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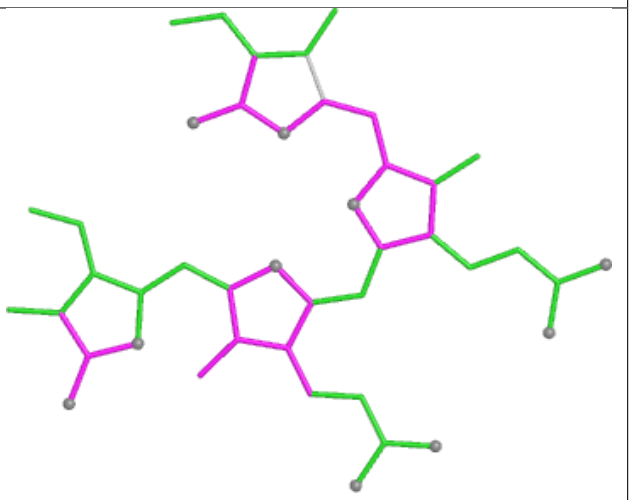
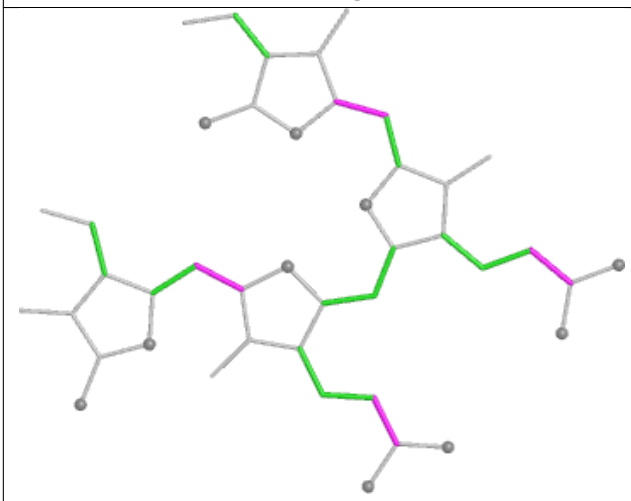


Bond angles



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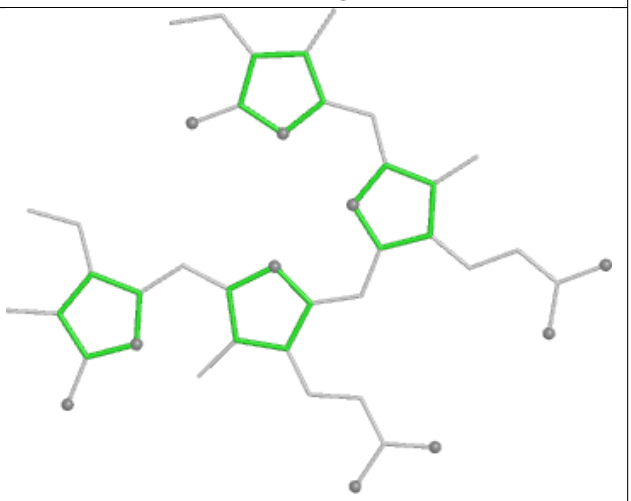
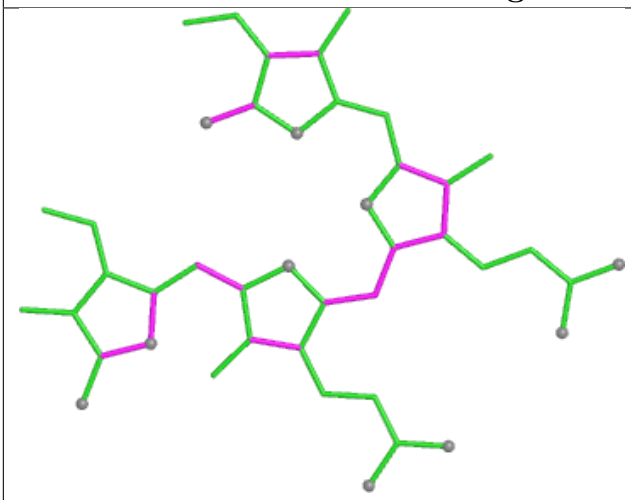


Rings

Ligand PEB MD 202



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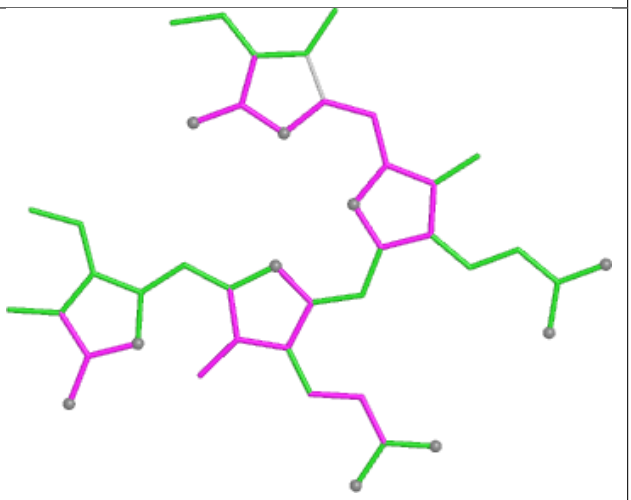
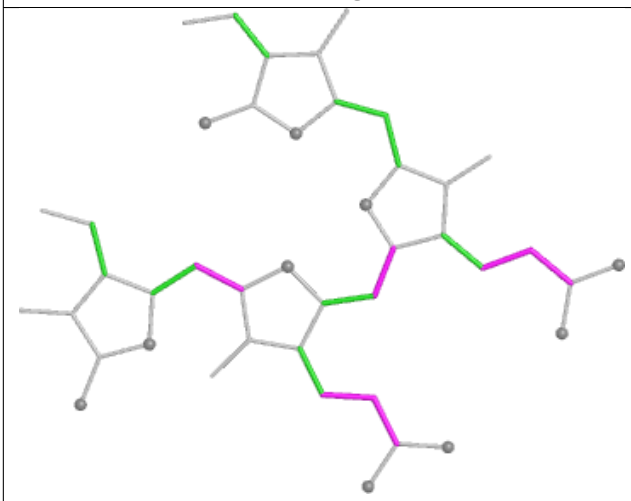


Bond angles



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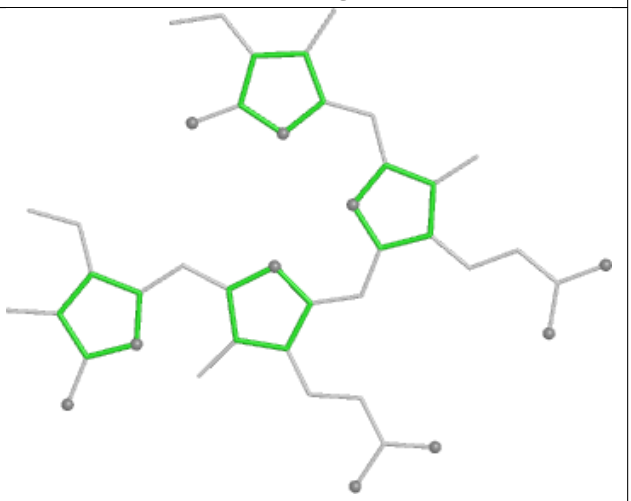
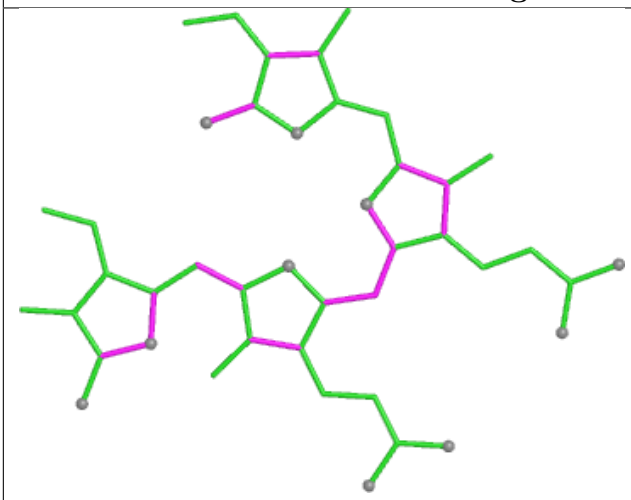


Rings

Ligand PEB QG 203



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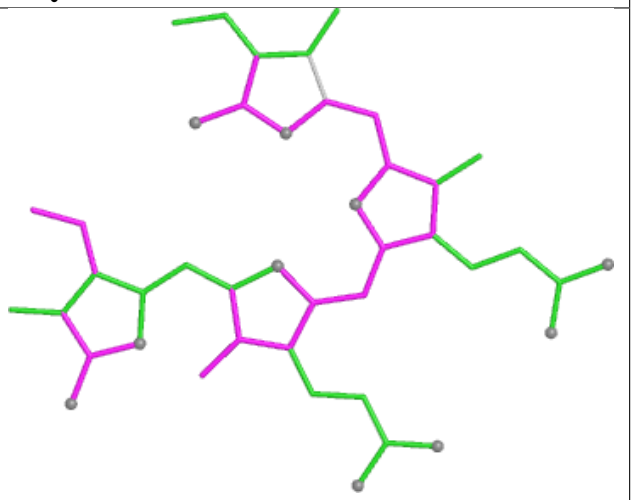
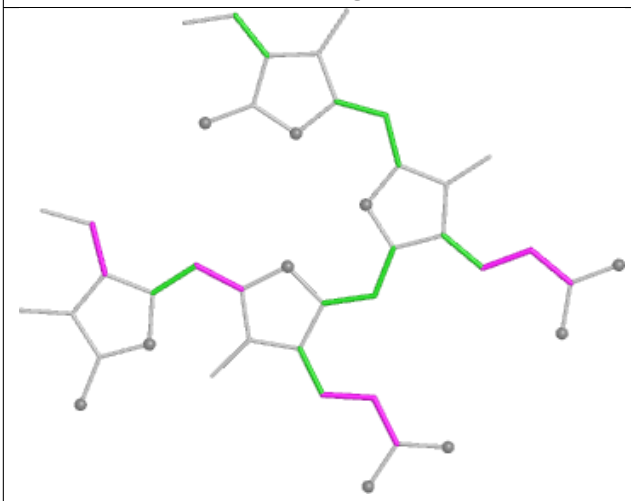


Bond angles



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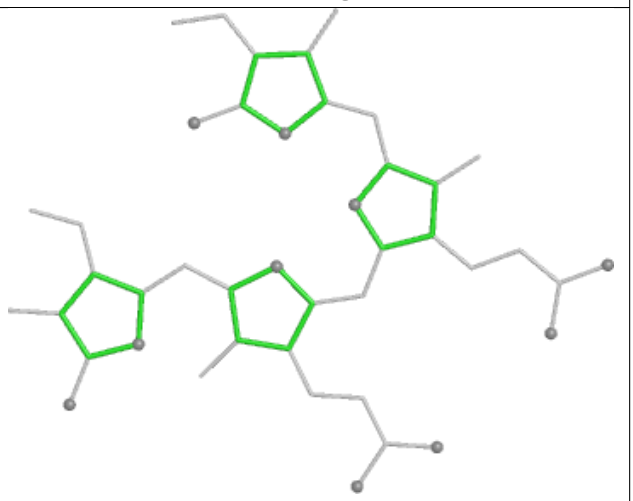
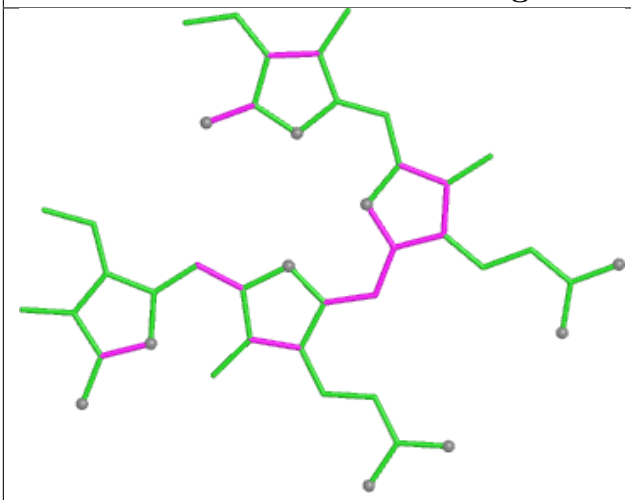


Rings

Ligand PEB TD 203



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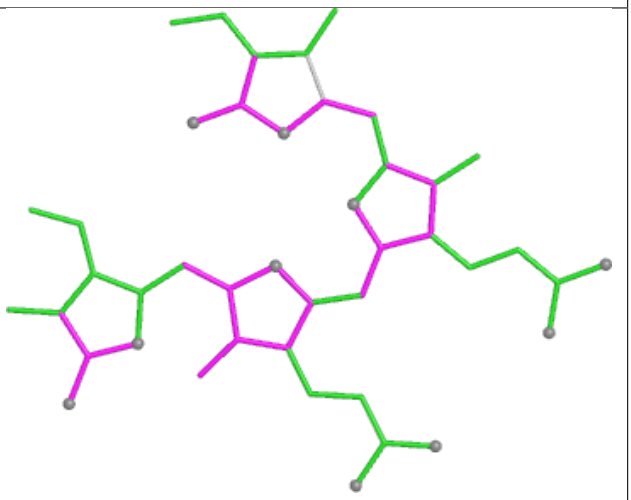

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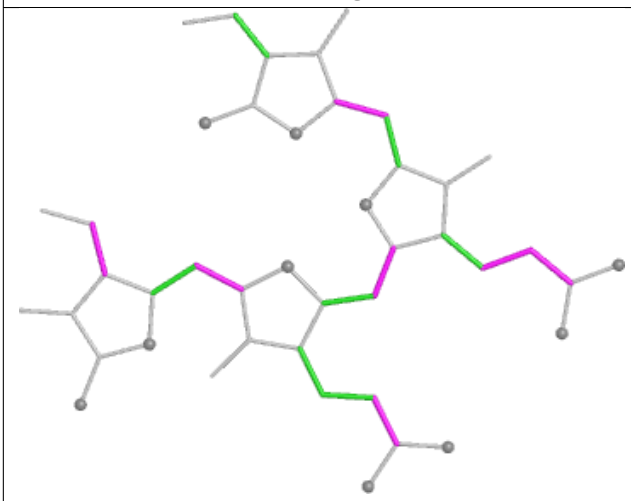

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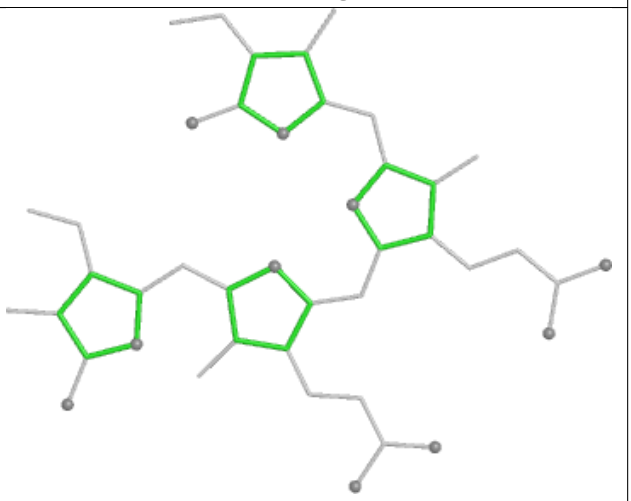
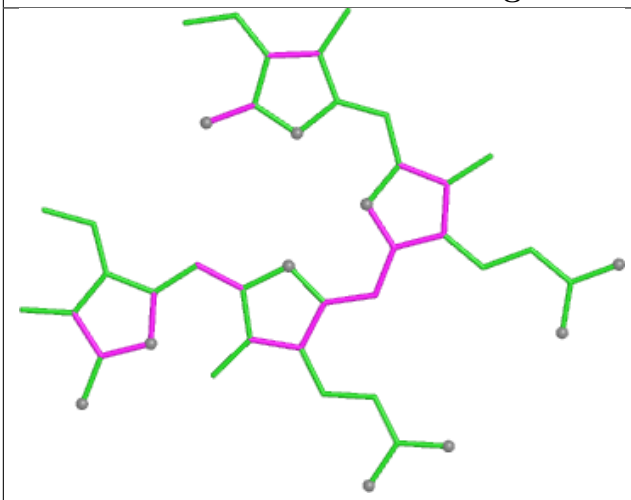


Rings

Ligand PEB MM 203



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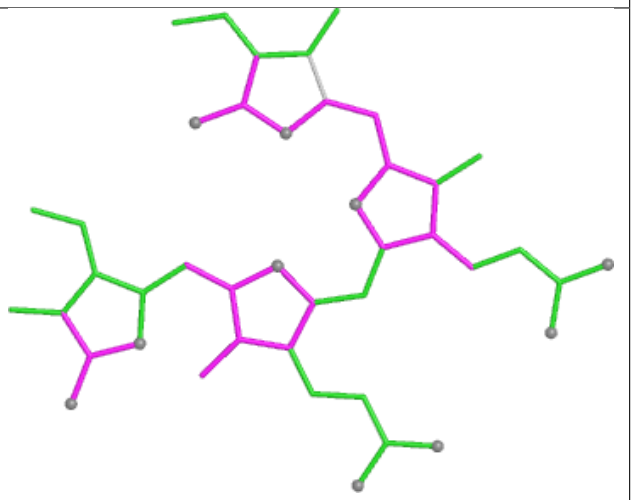
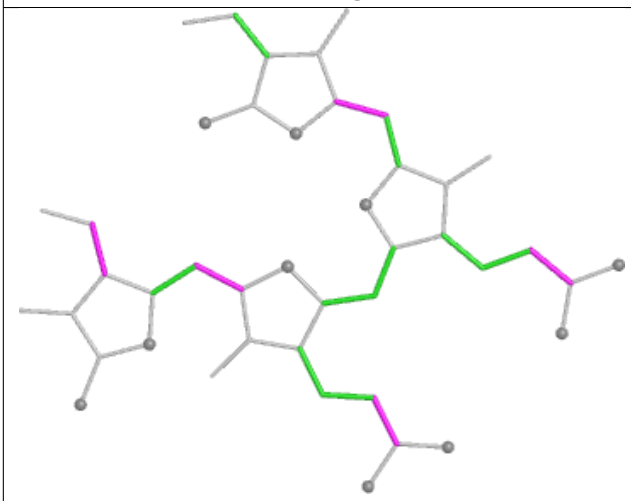


Bond angles



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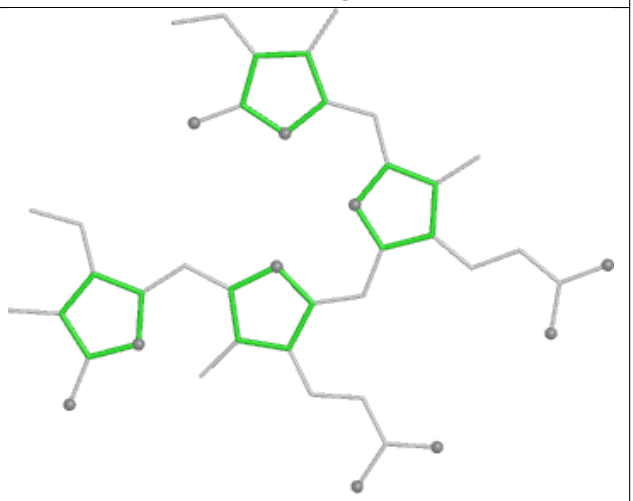
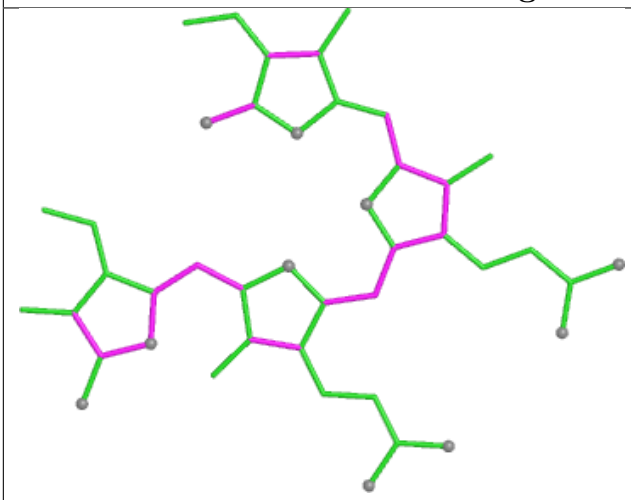
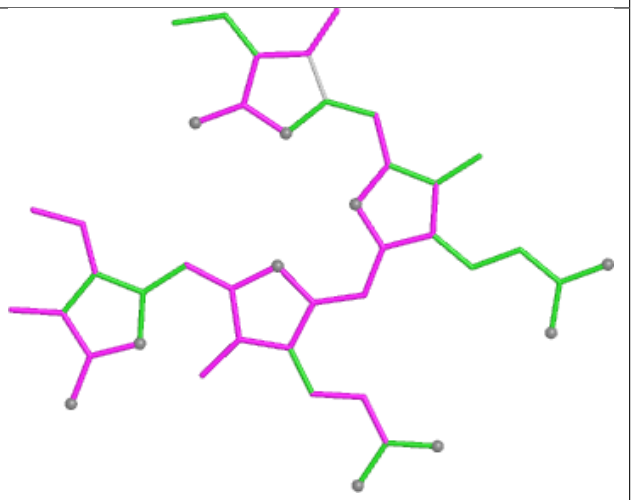


Rings

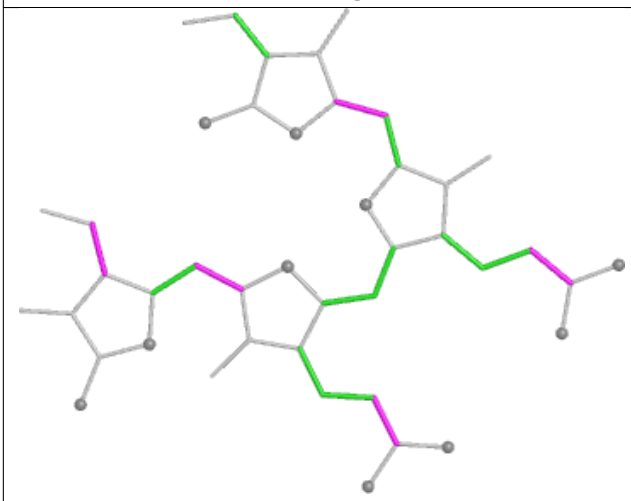
Ligand PEB h4 201



Bond lengths



Bond angles



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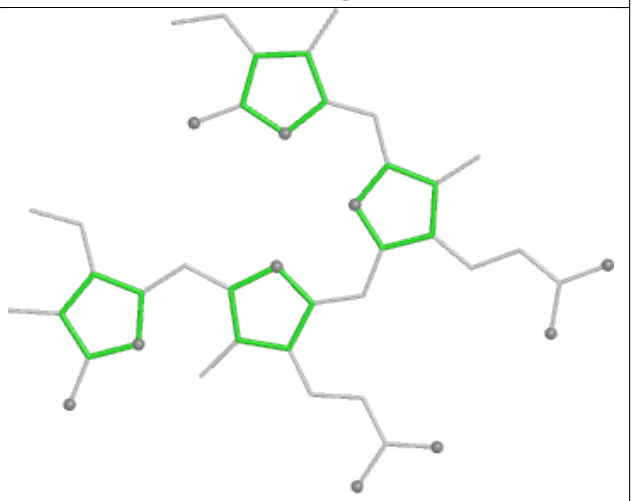
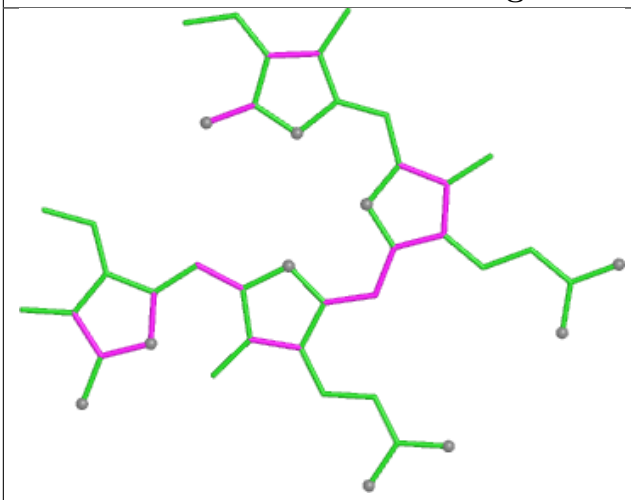
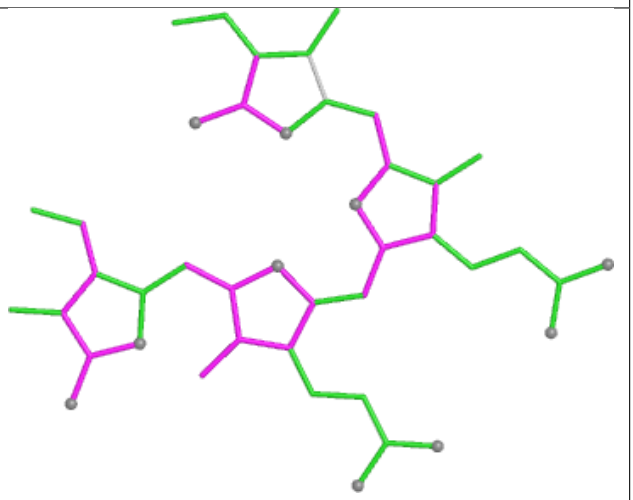


Rings

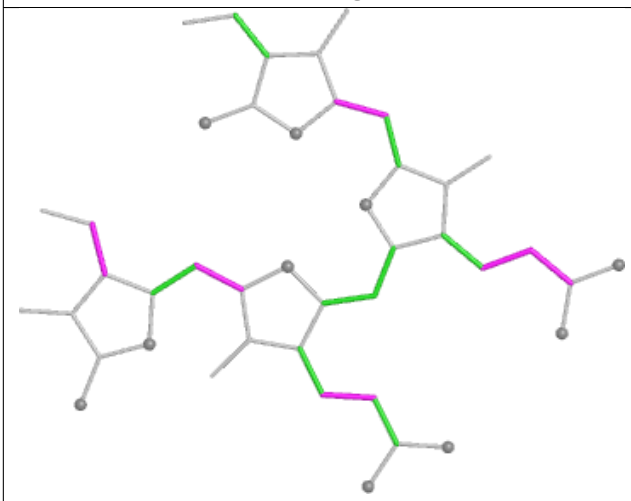
Ligand PEB KM 201



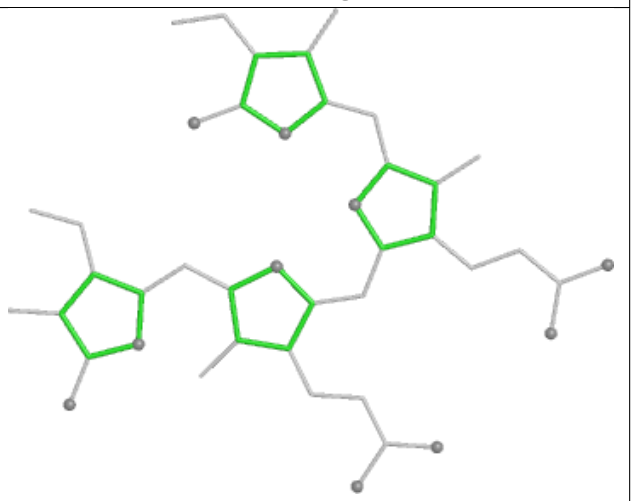
Bond lengths



Bond angles

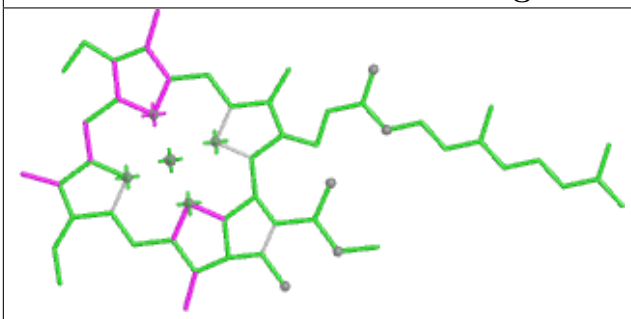


Torsions



Rings

Ligand CLA CL 514



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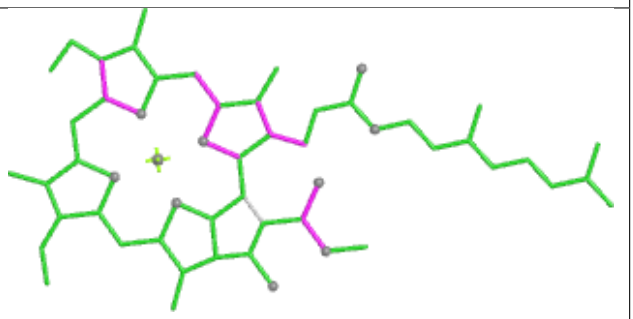
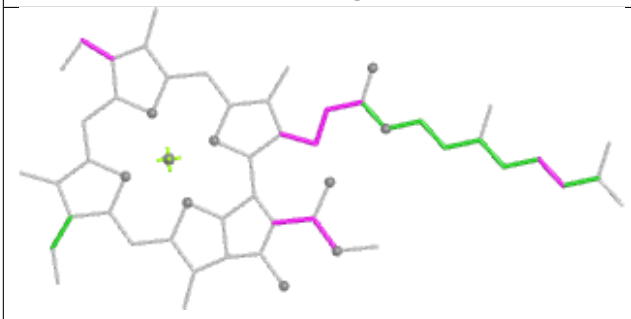


Bond angles



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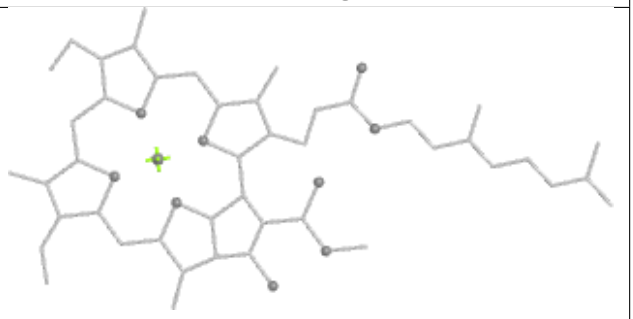
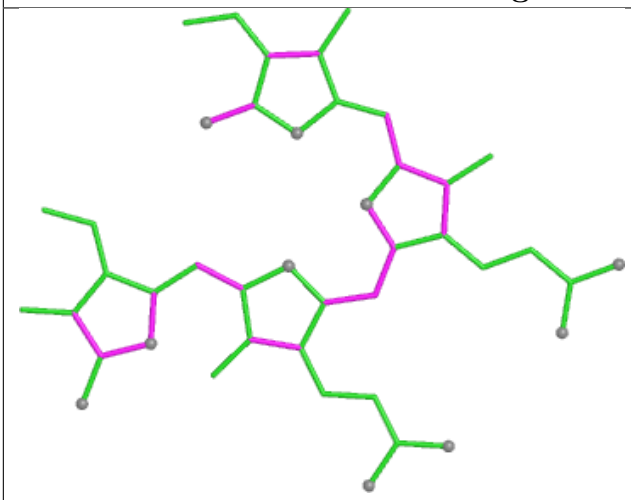


Rings

Ligand PEB UP 203



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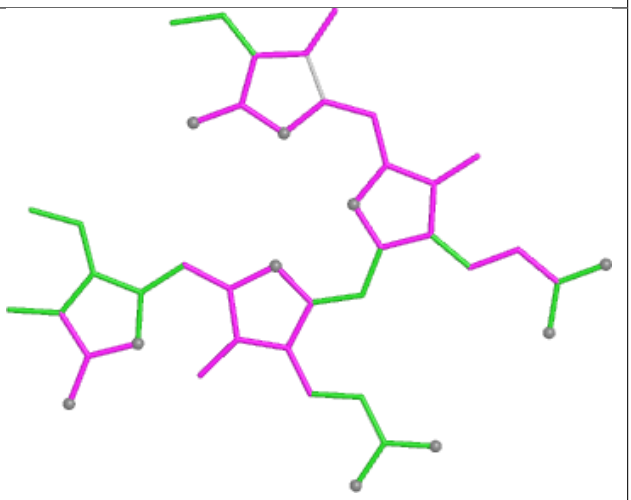

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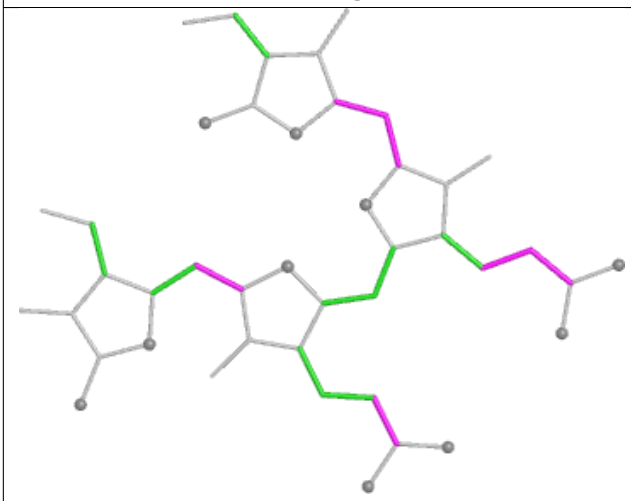

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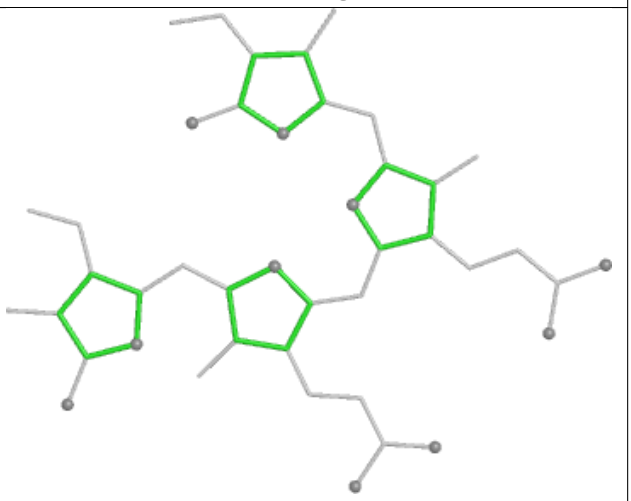
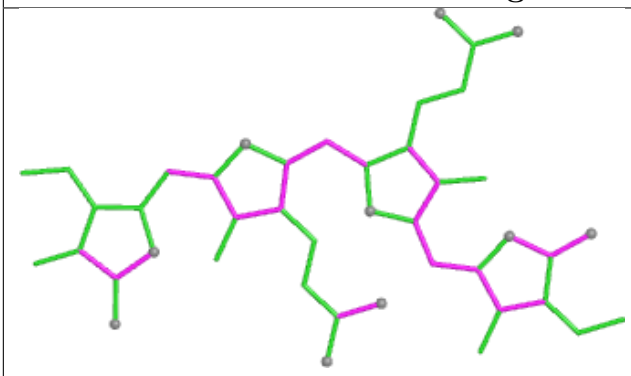


Rings

Ligand CYC S3 1001



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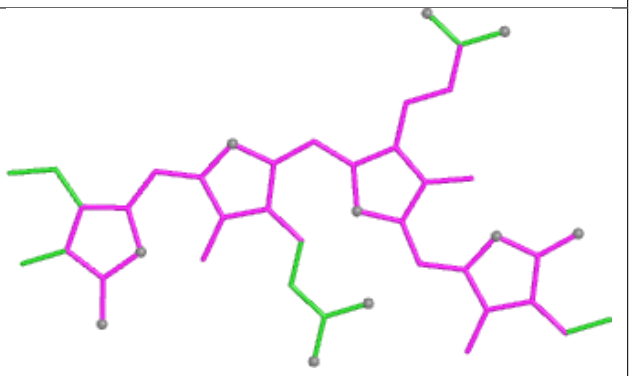

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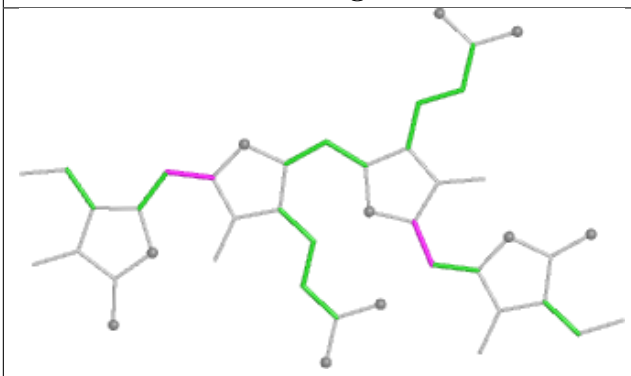

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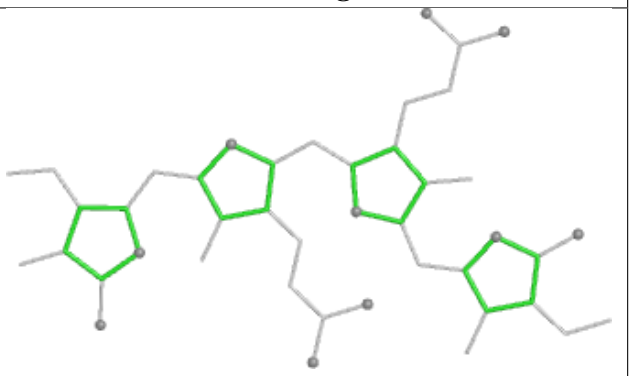
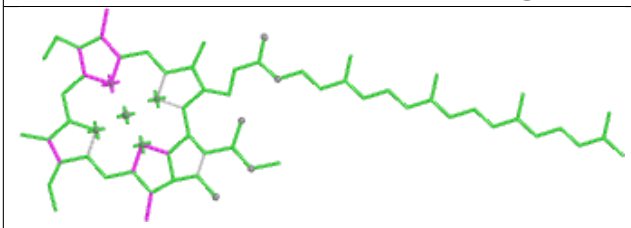


Rings

Ligand CLA cL 509



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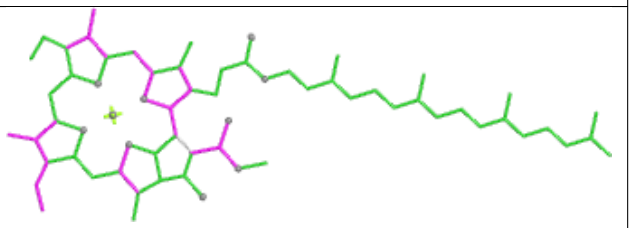

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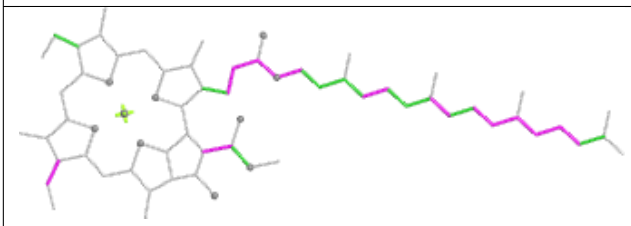

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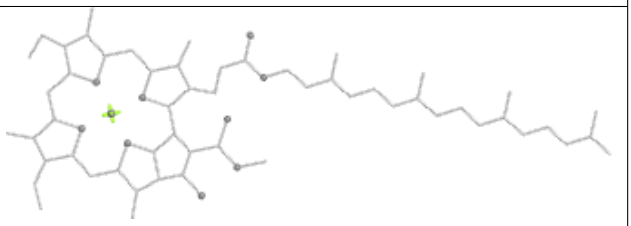
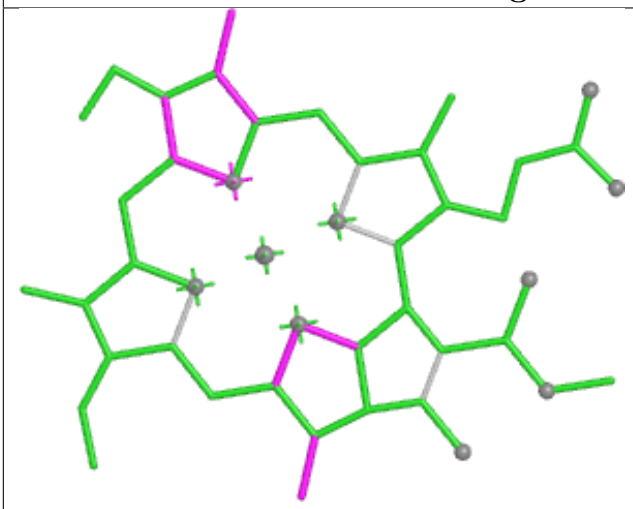


Rings

Ligand CLA RN 202



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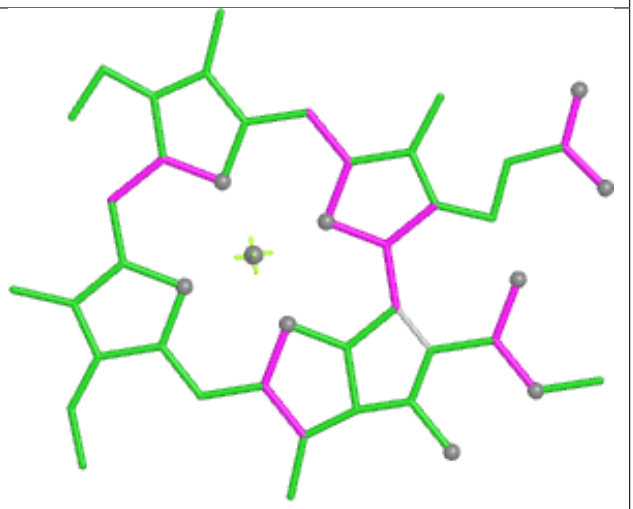
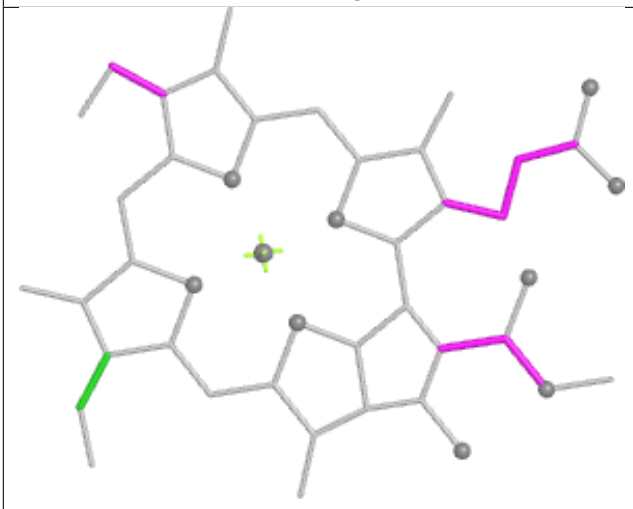


Bond angles

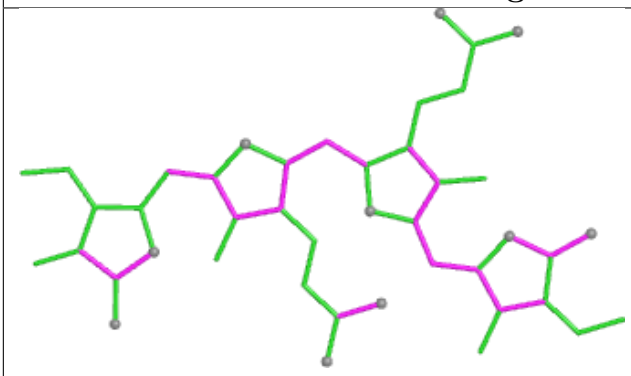


Torsions



Rings

Ligand CYC n3 1001



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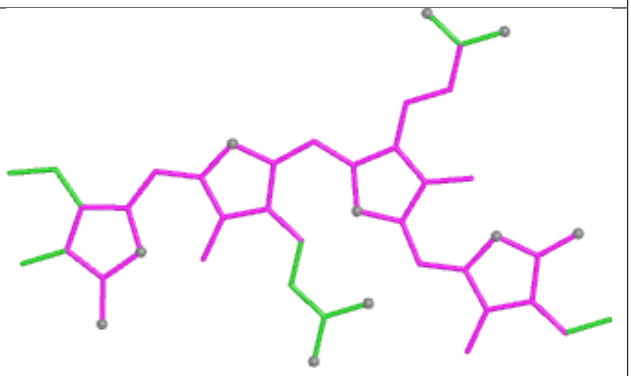

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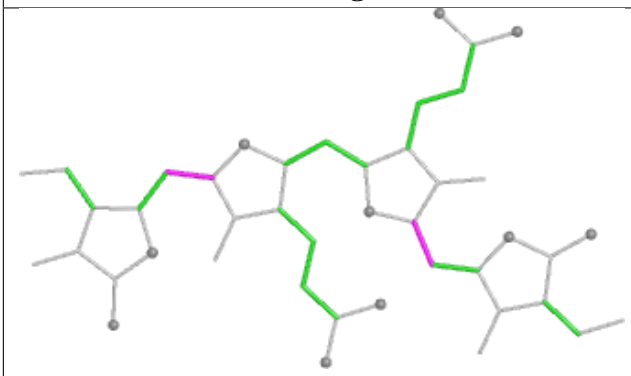

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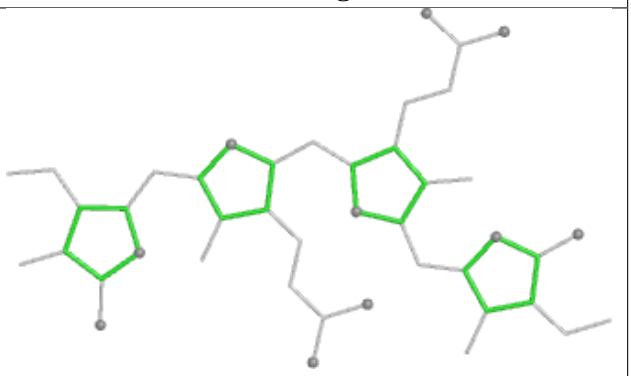
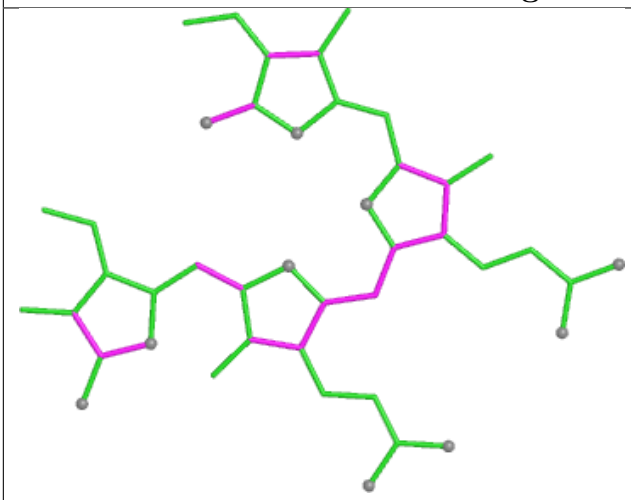


Rings

Ligand PEB s8 203



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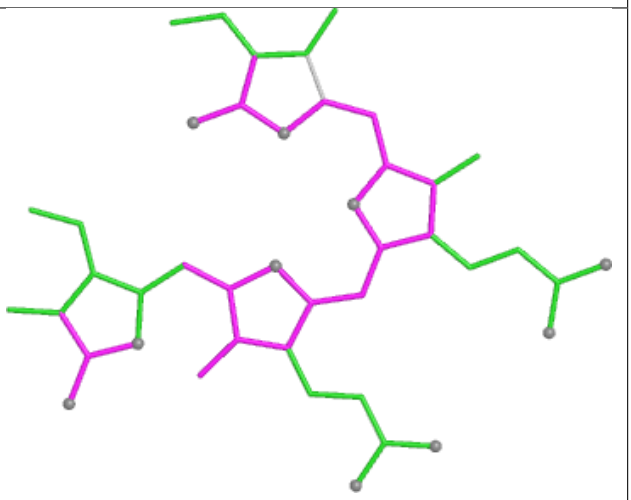
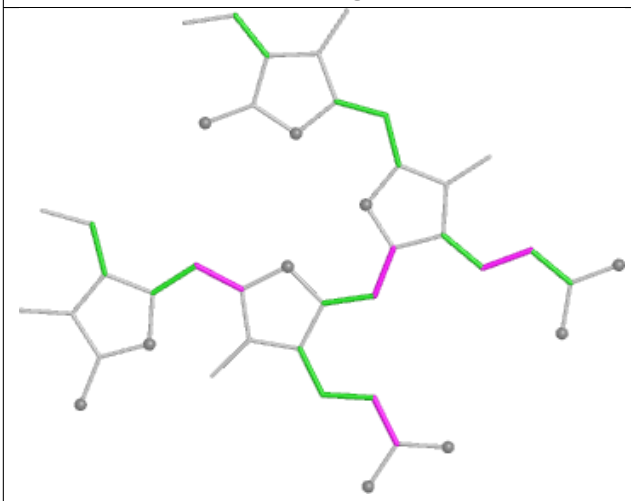


Bond angles



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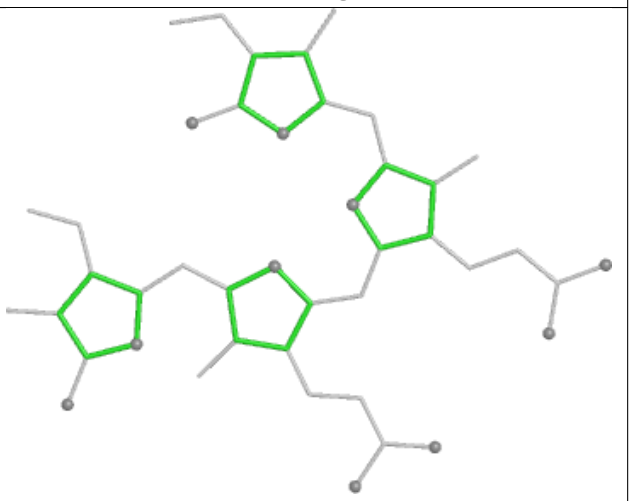
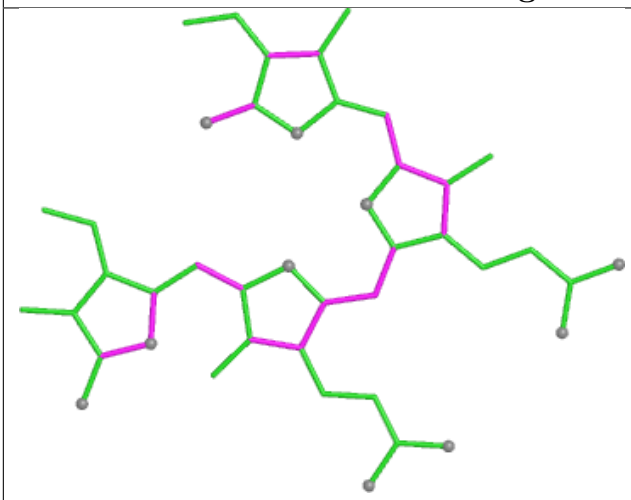


Rings

Ligand PEB cF 201



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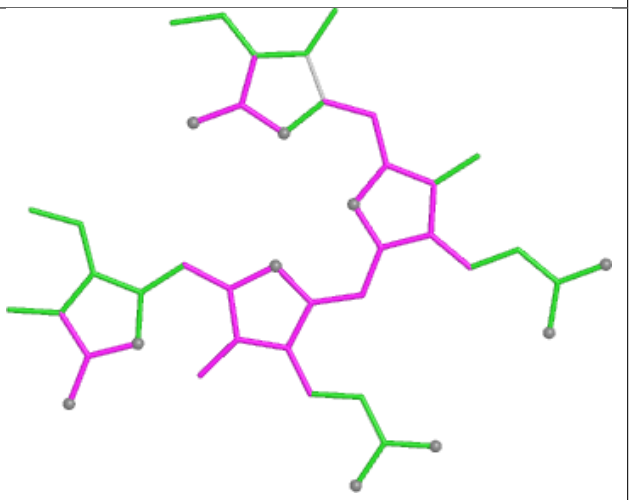

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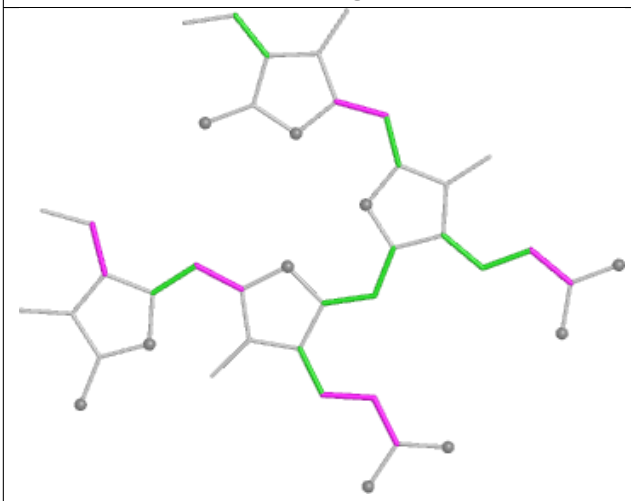

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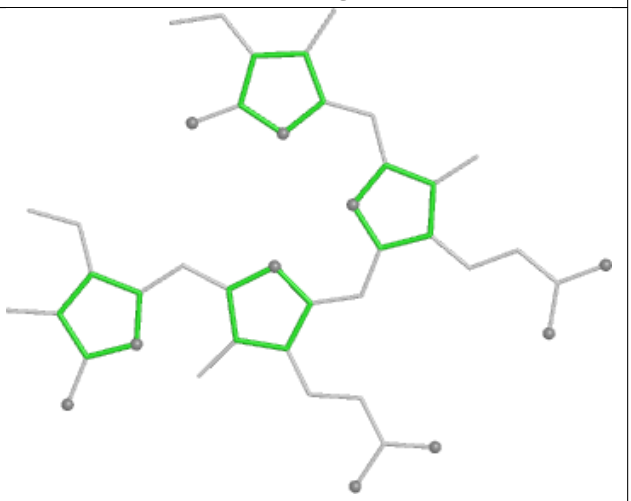
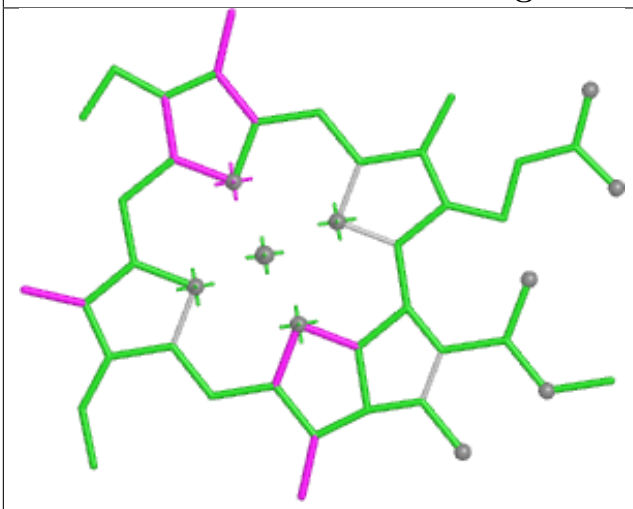


Rings

Ligand CLA B2 813



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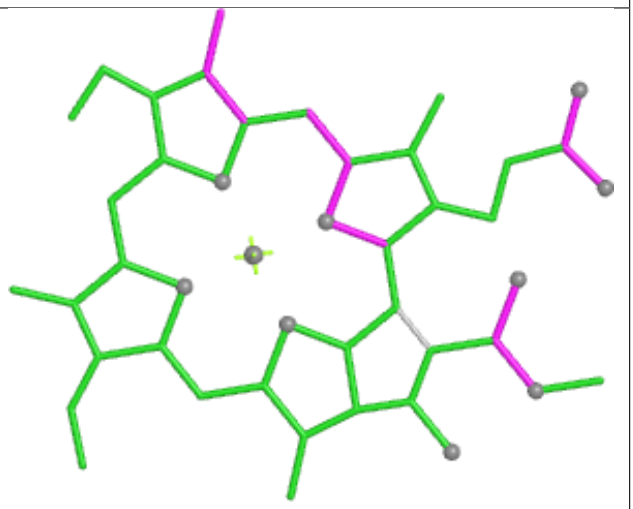

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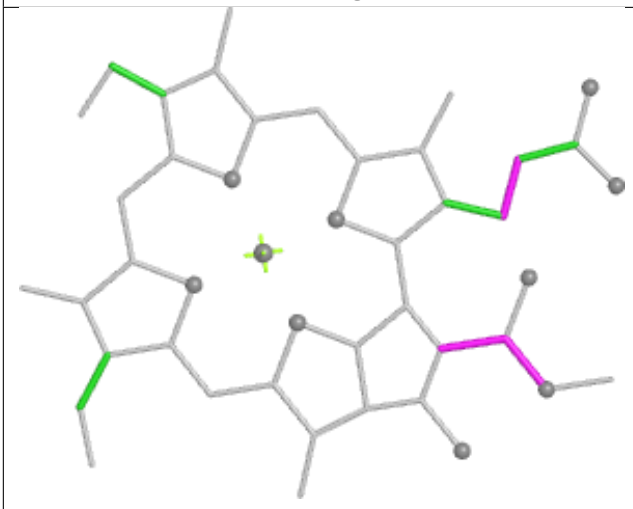
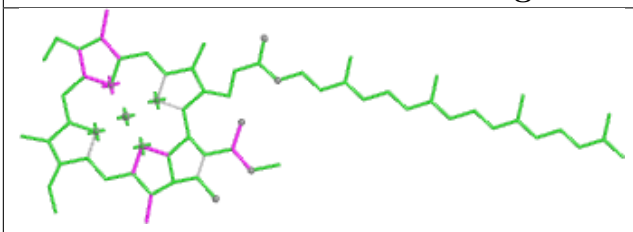


Torsions



Rings

Ligand CLA 3N 305



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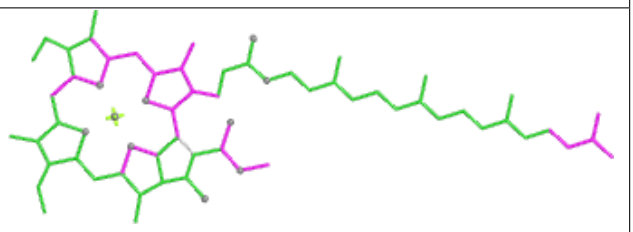

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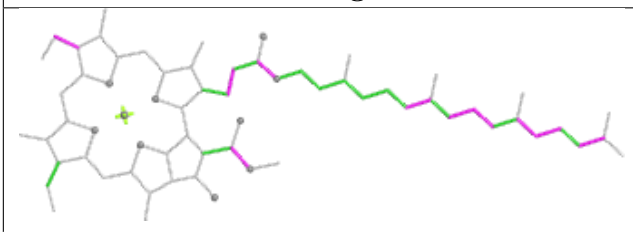

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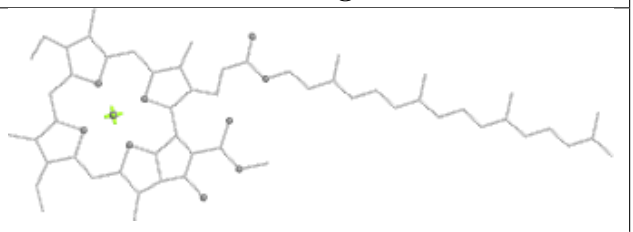
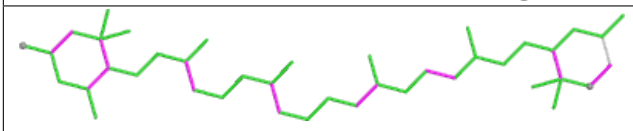


Rings

Ligand ZEX 8N 310



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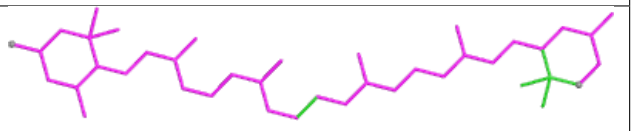
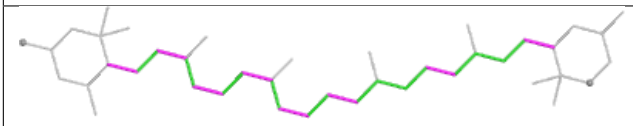


Bond angles



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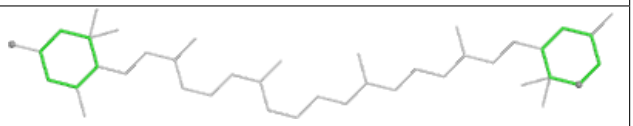
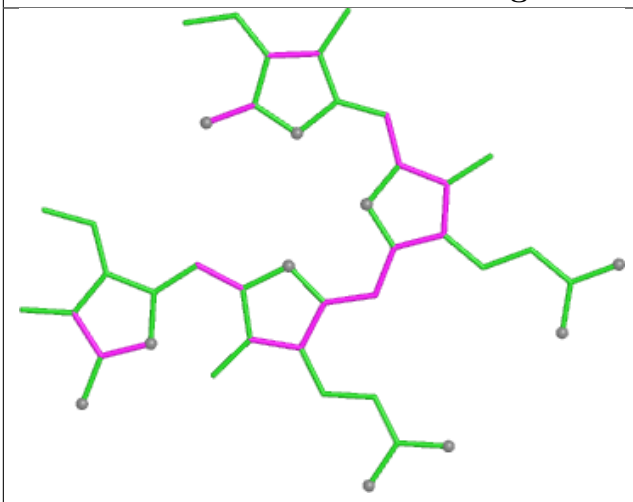


Rings

Ligand PEB W9 202



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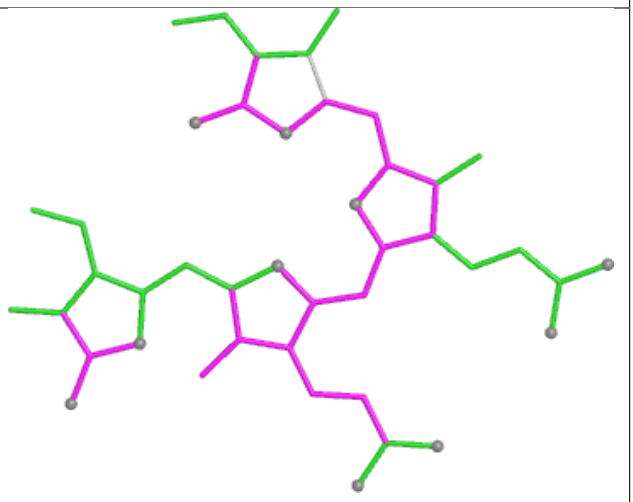

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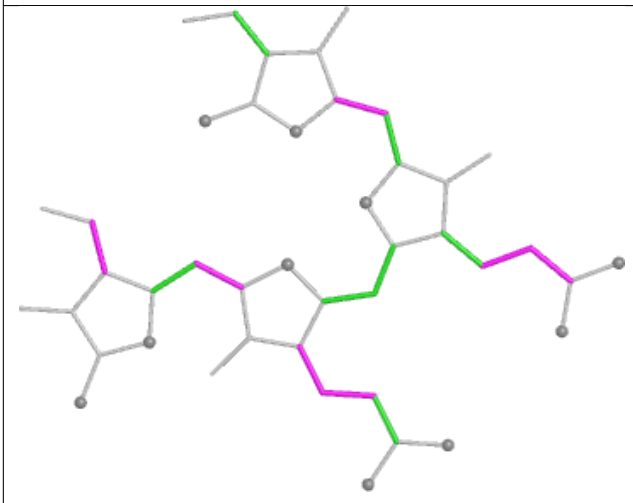

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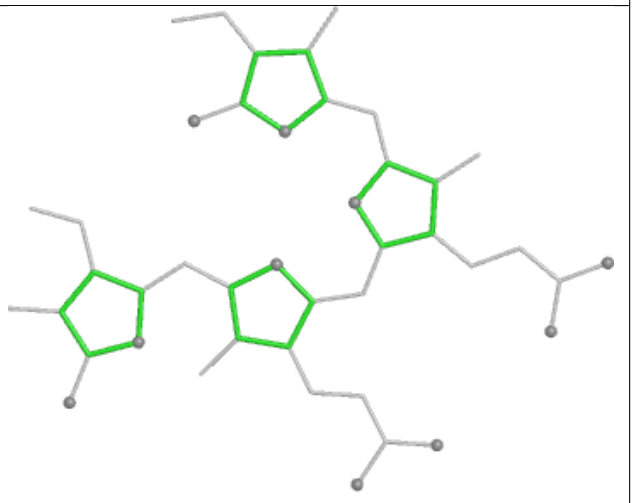
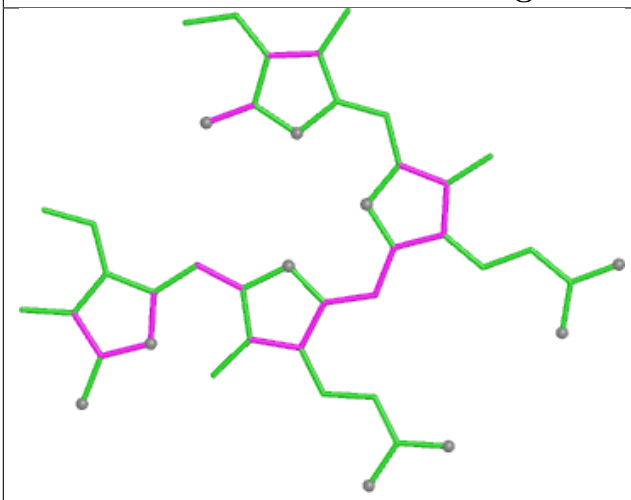


Rings

Ligand PEB Y9 202



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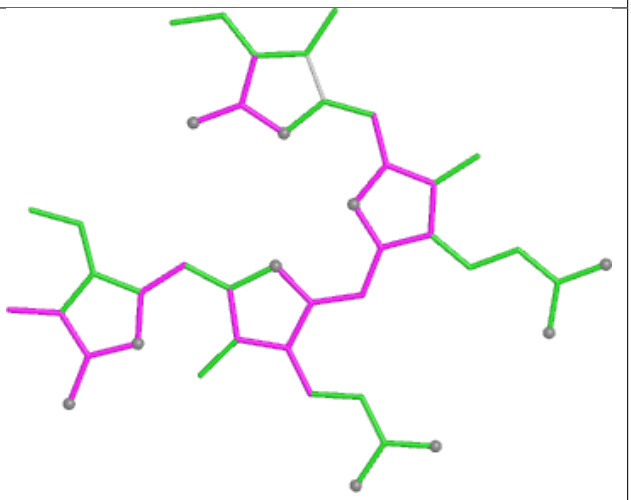
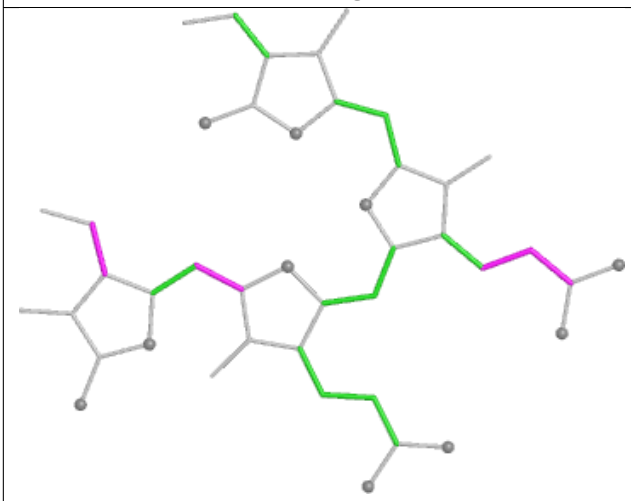


Bond angles



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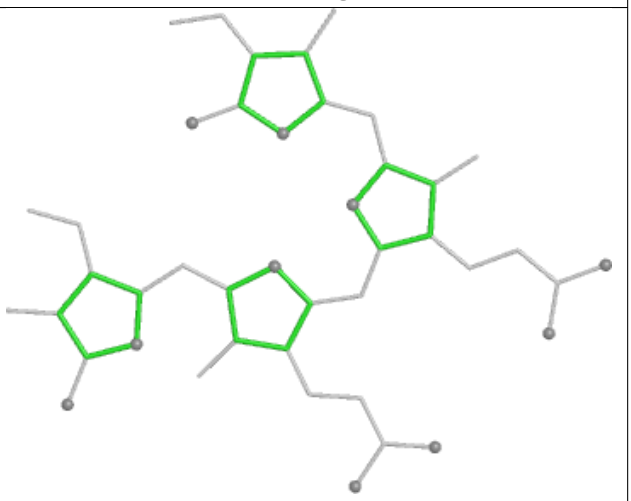

Rings

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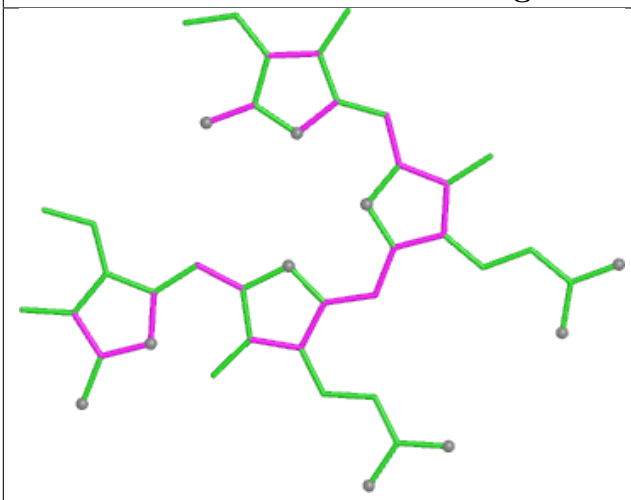

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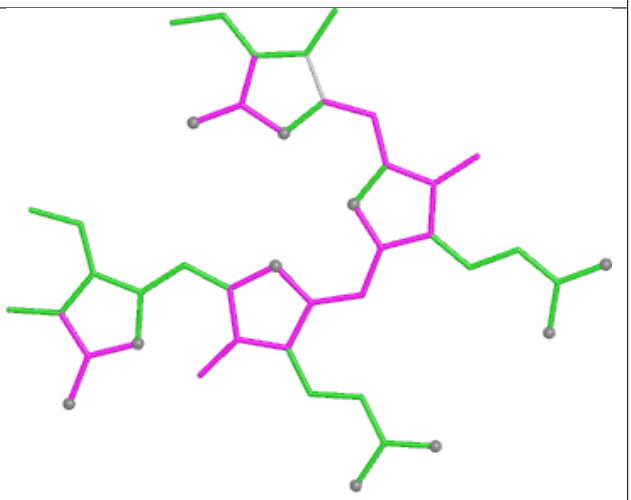
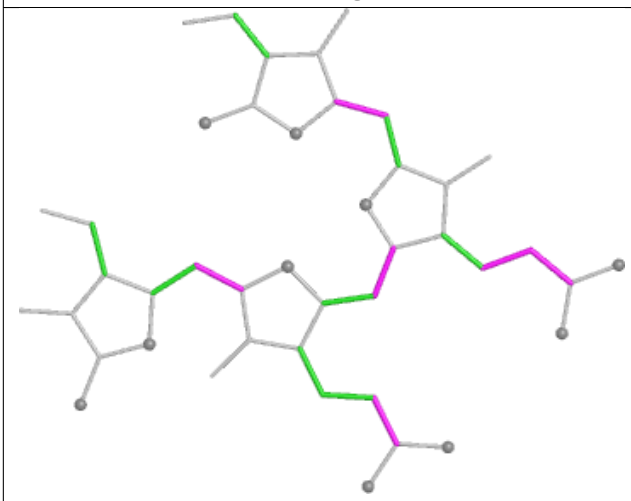


Bond angles



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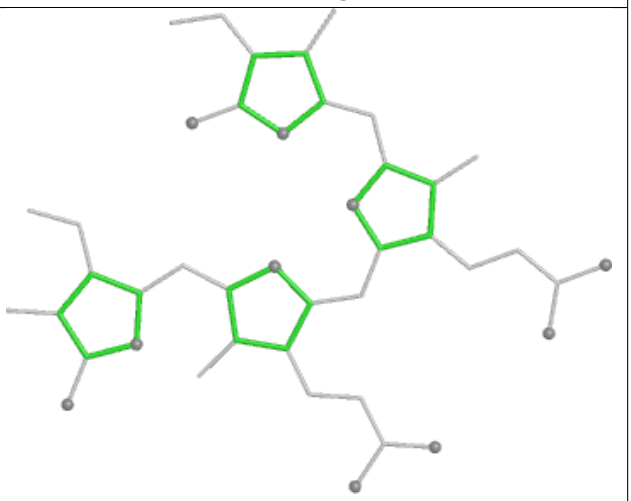
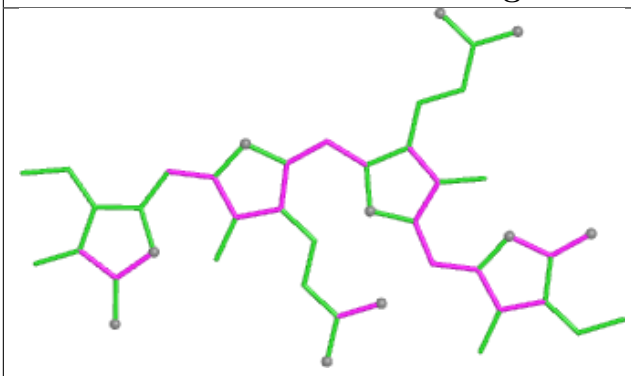


Rings

Ligand CYC D3 1001



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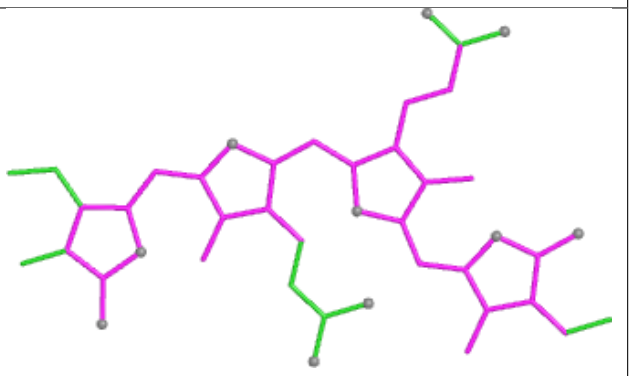
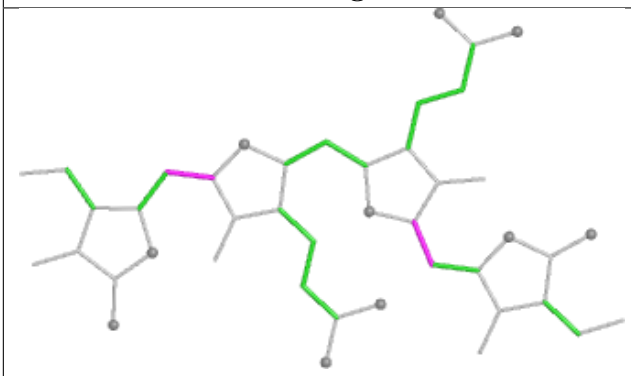
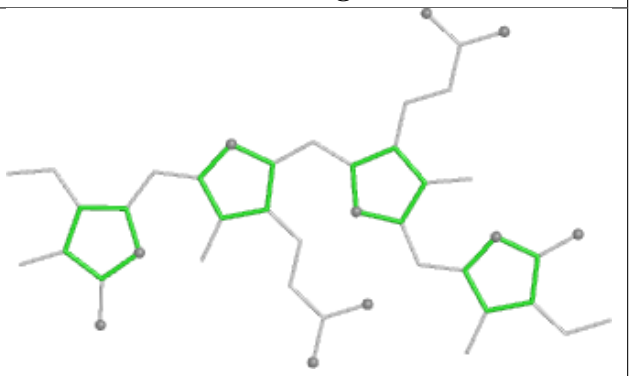


Bond angles

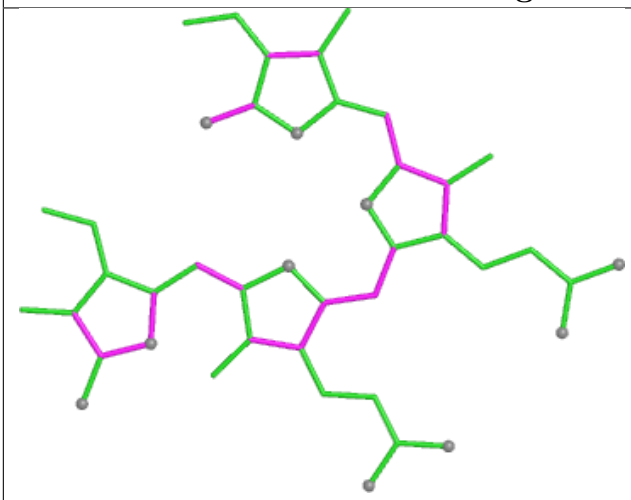


Torsions



Rings

Ligand PEB w8 204



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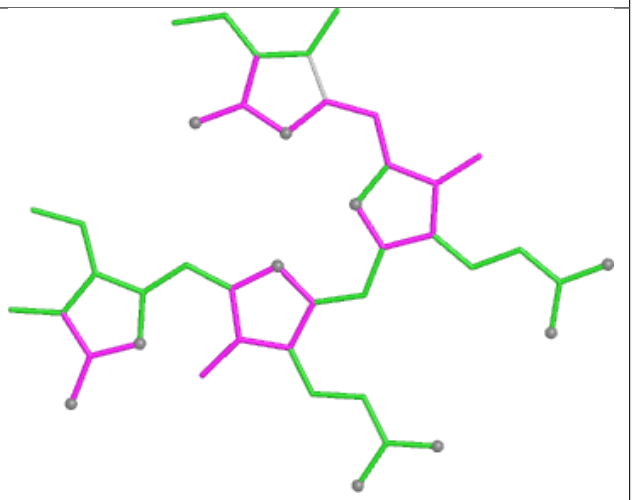
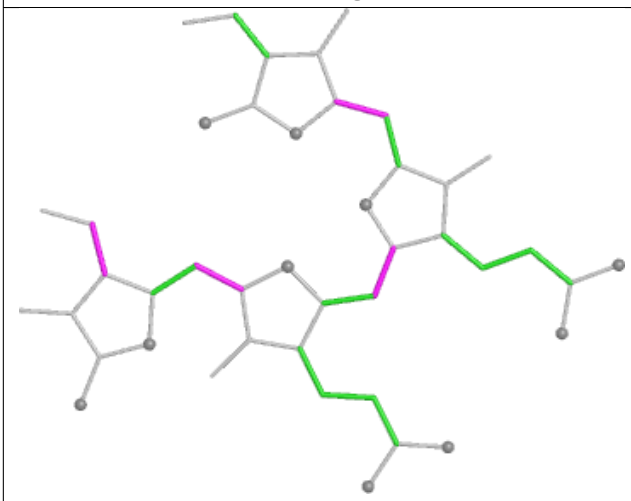


Bond angles



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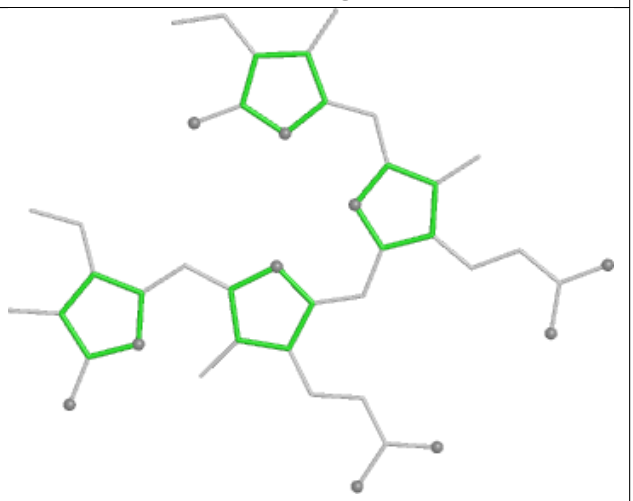
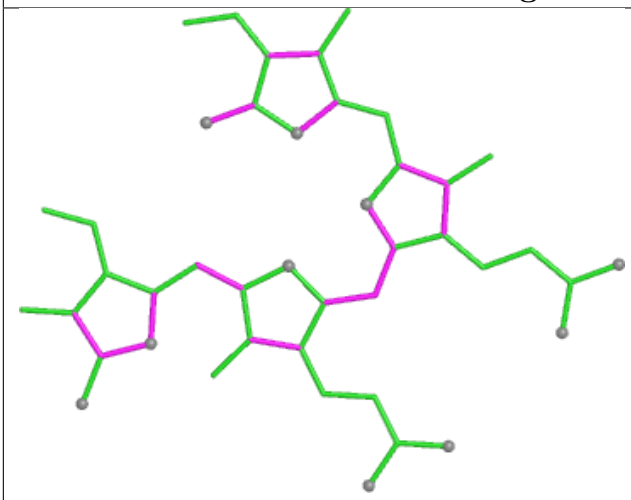


Rings

Ligand PEB aJ 201



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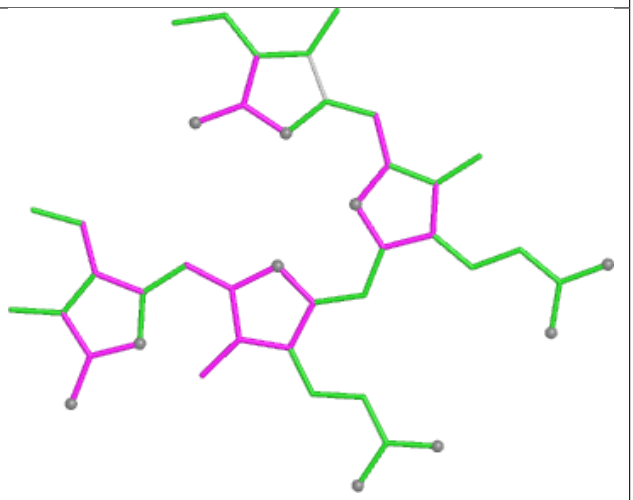

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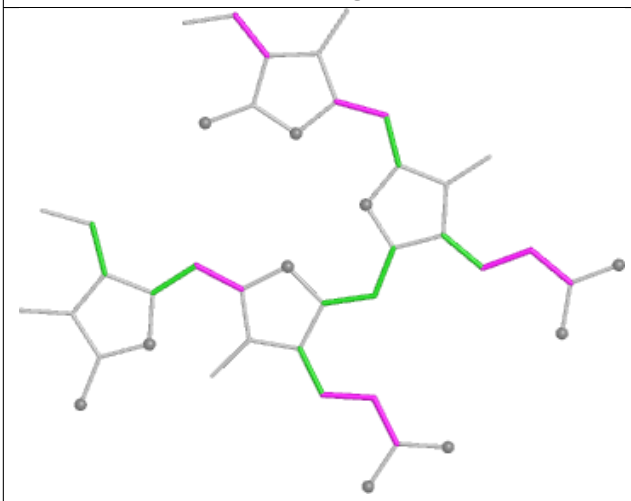

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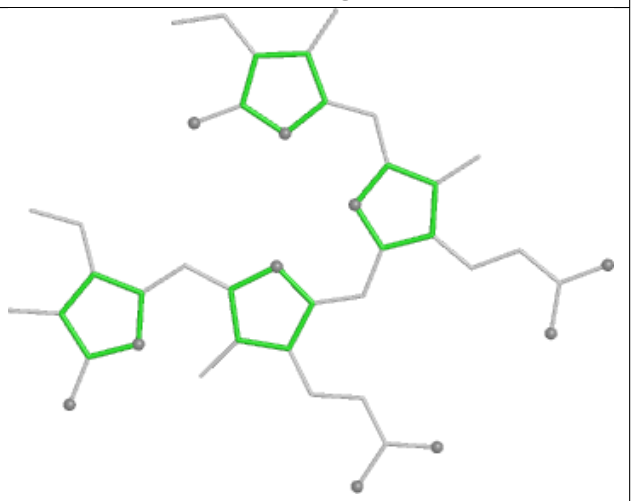
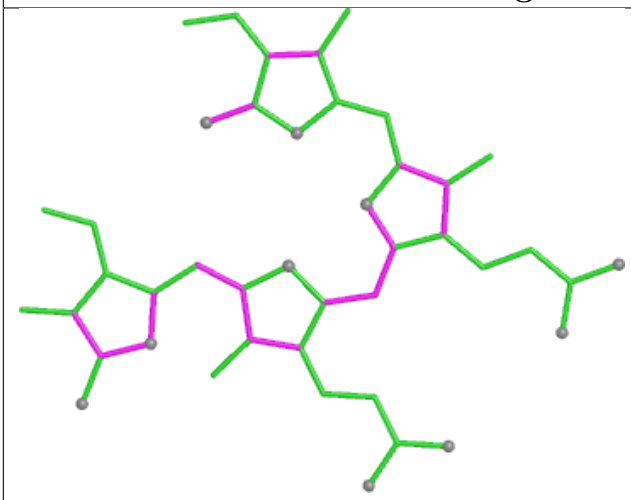


Rings

Ligand PEB Q5 201



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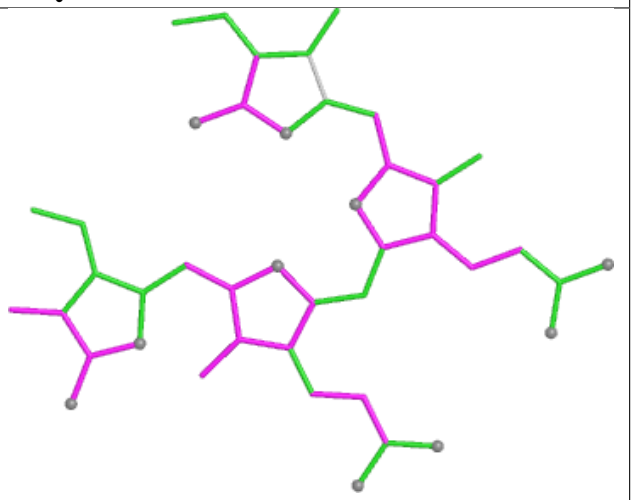

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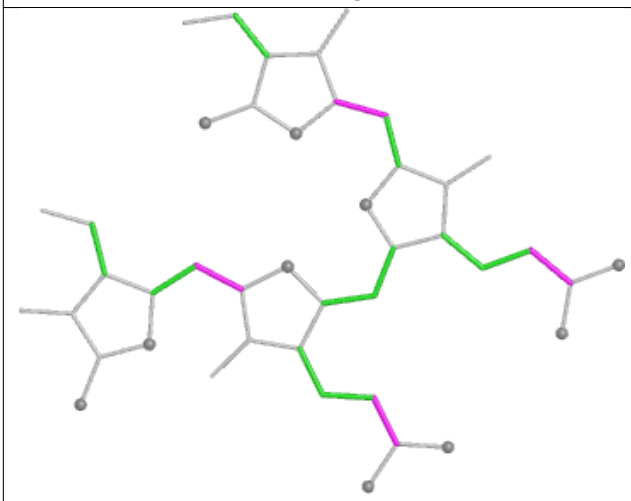

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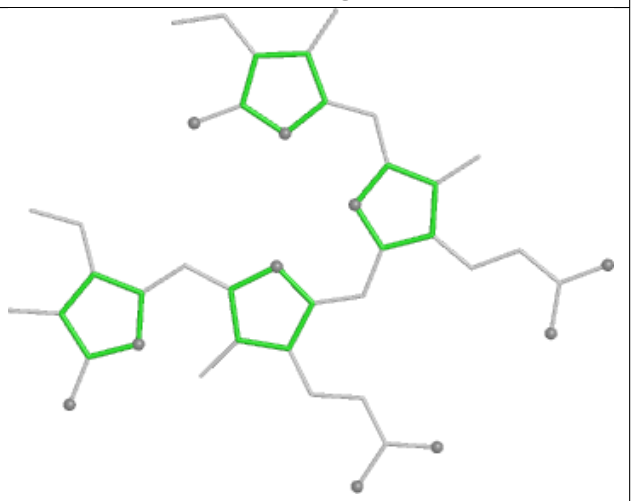
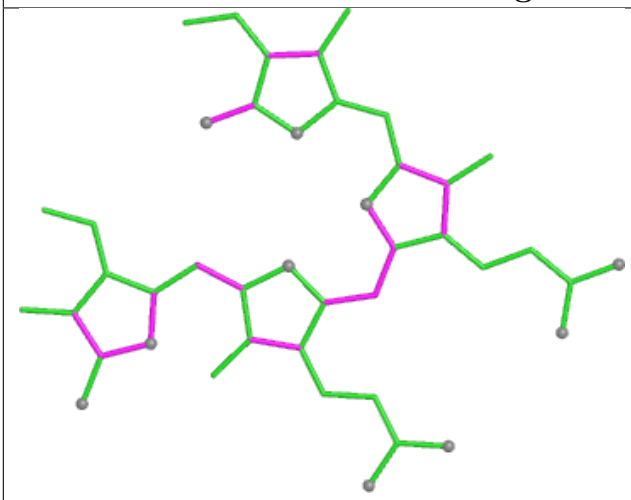


Rings

Ligand PEB N7 201



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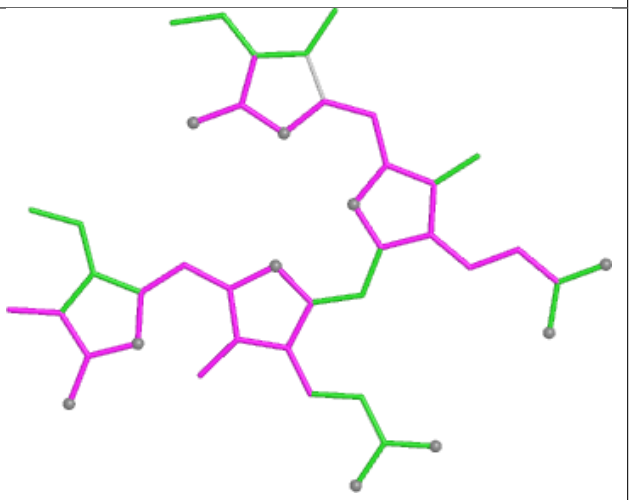

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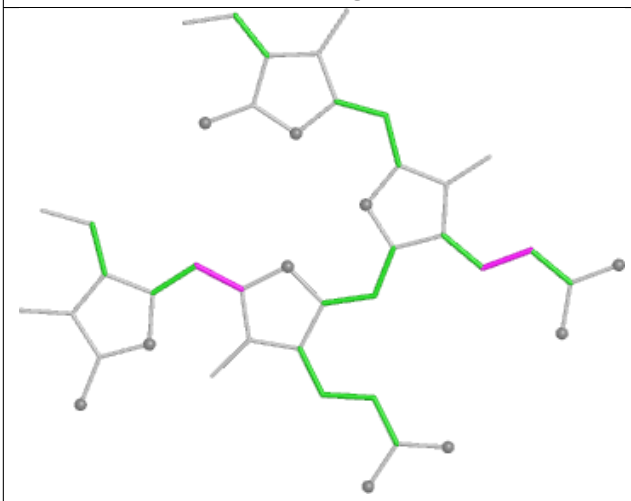

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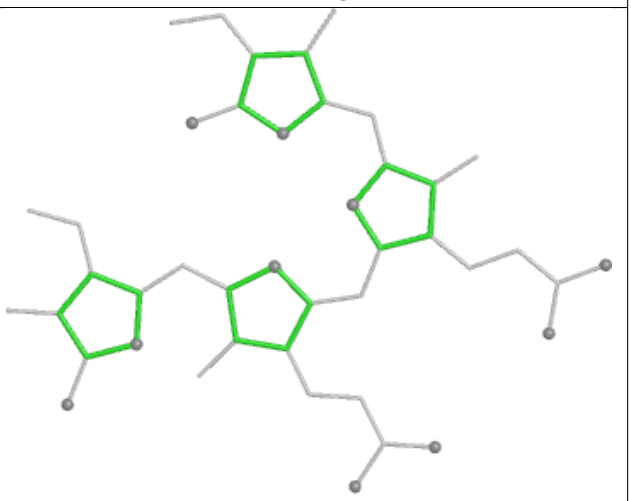
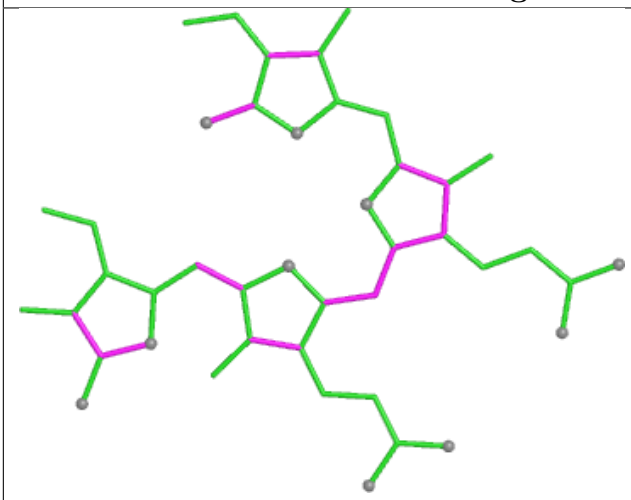


Rings

Ligand PEB VK 201



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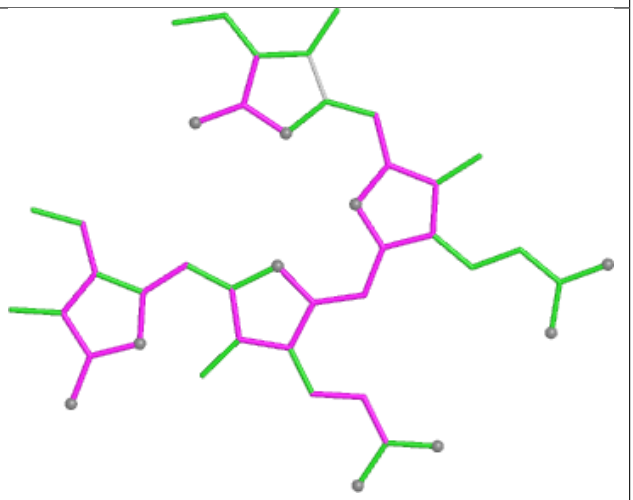

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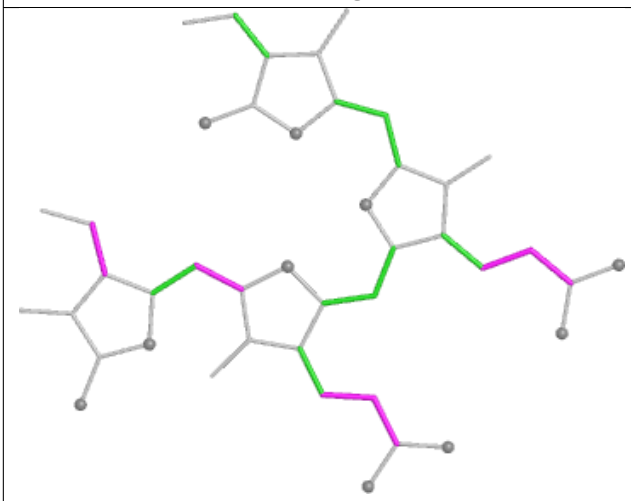

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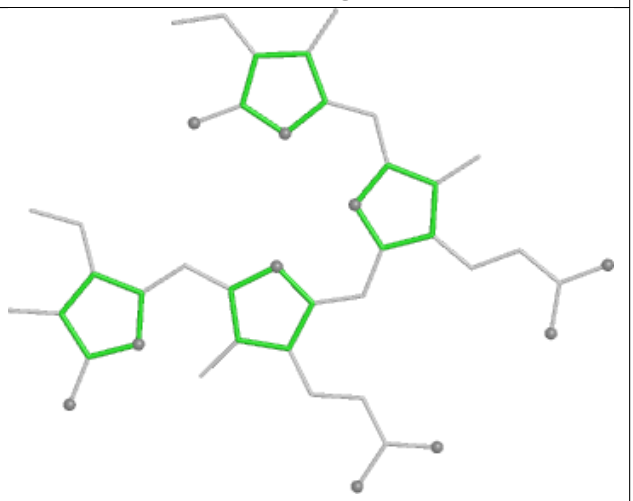
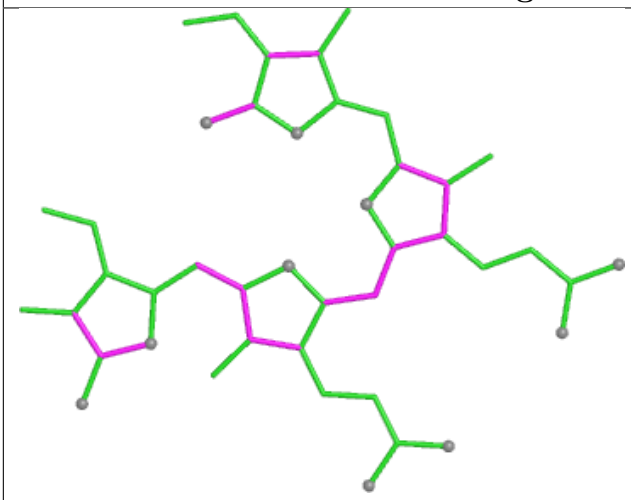


Rings

Ligand PEB hF 201



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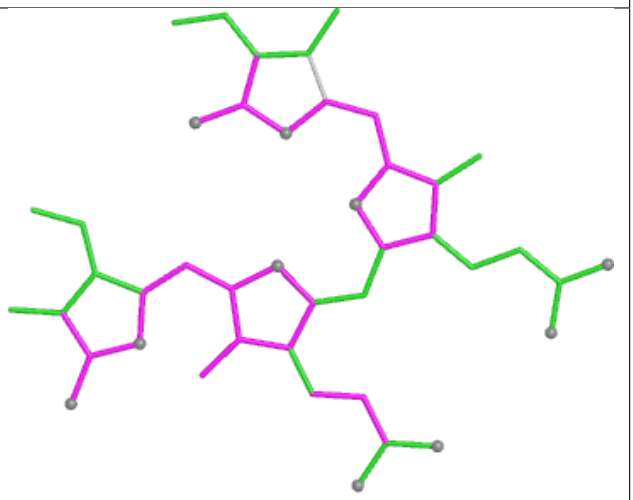

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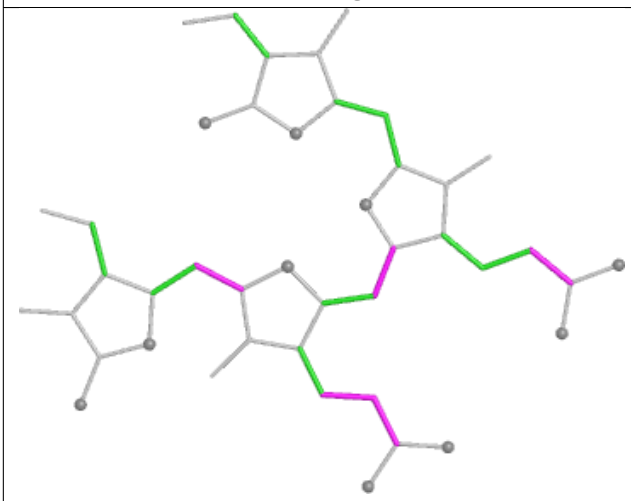

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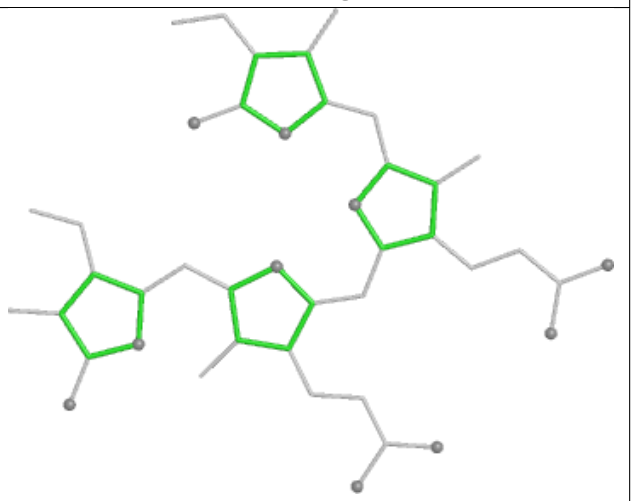
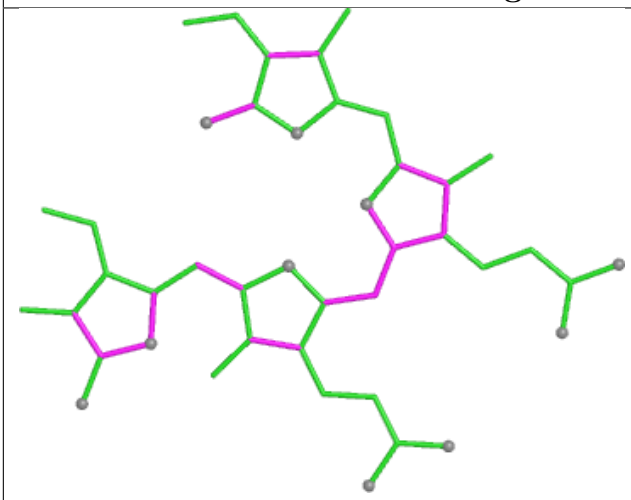


Rings

Ligand PEB FO 1002



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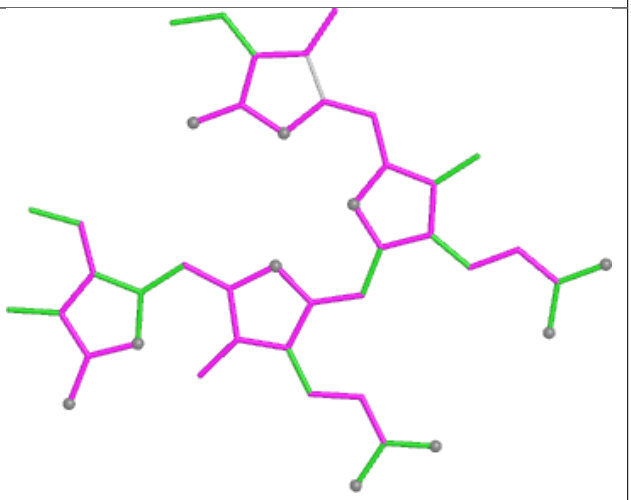

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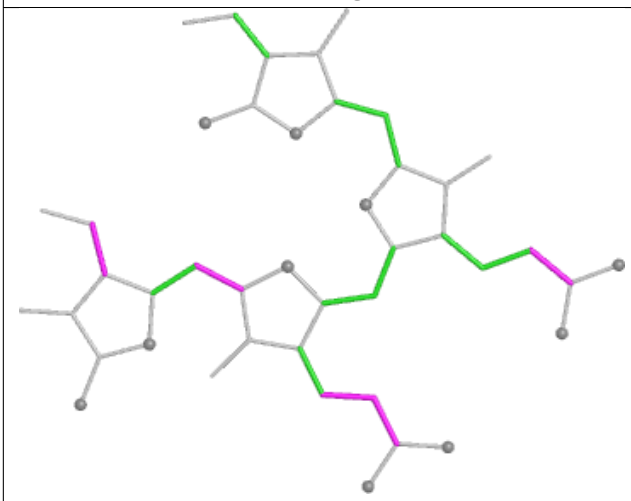

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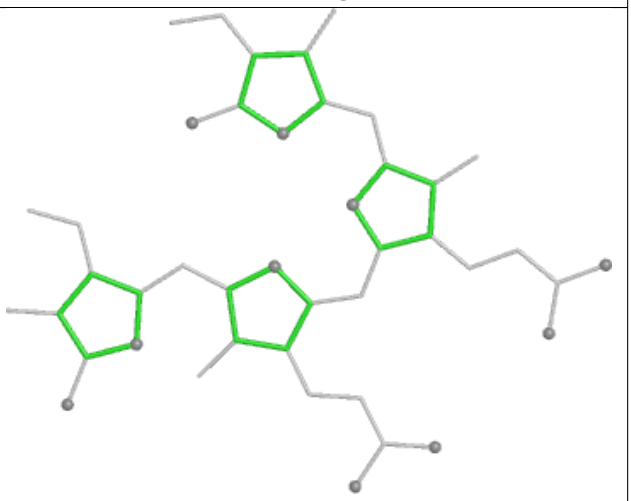
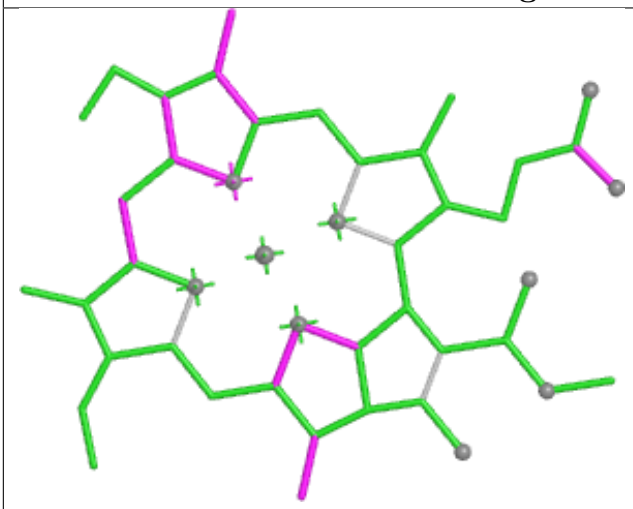


Rings

Ligand CLA 62 301



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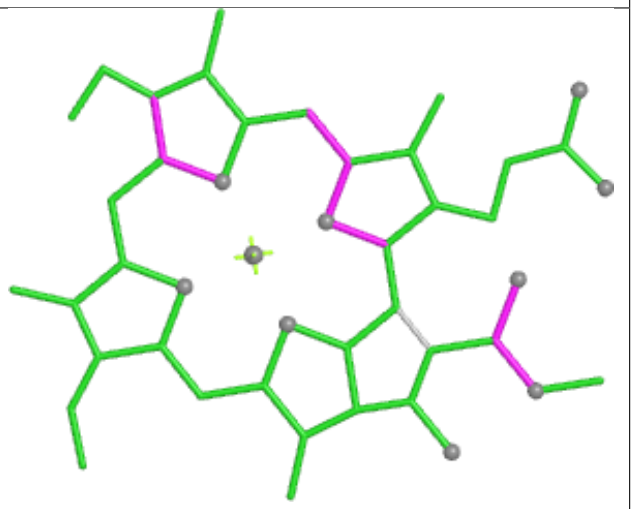

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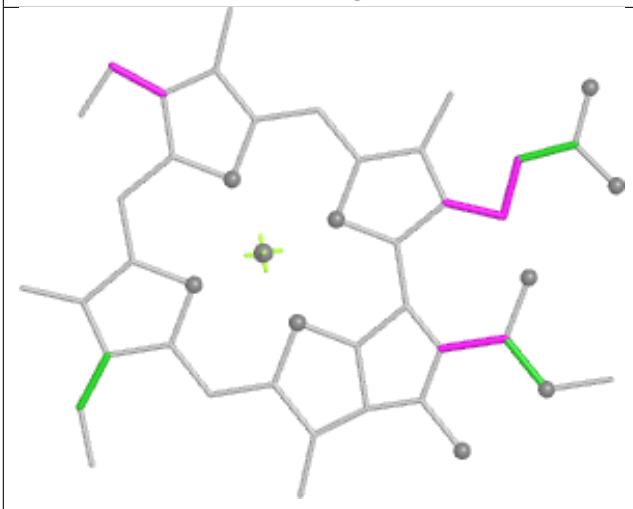
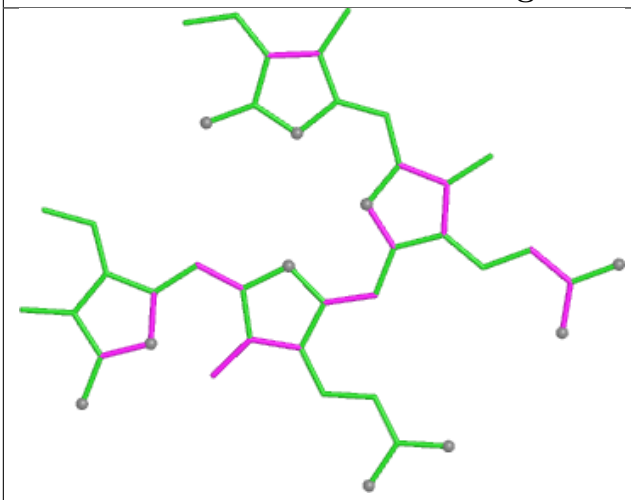


Torsions



Rings

Ligand PEB IK 201



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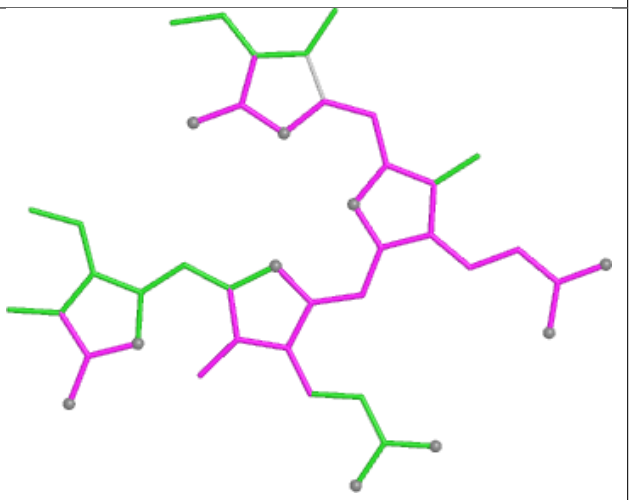

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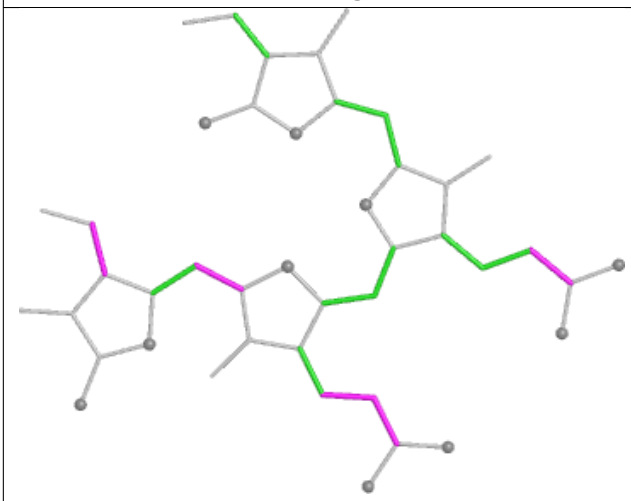

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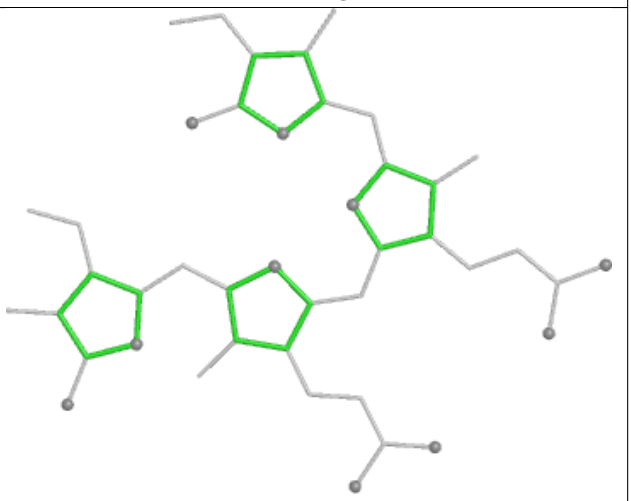
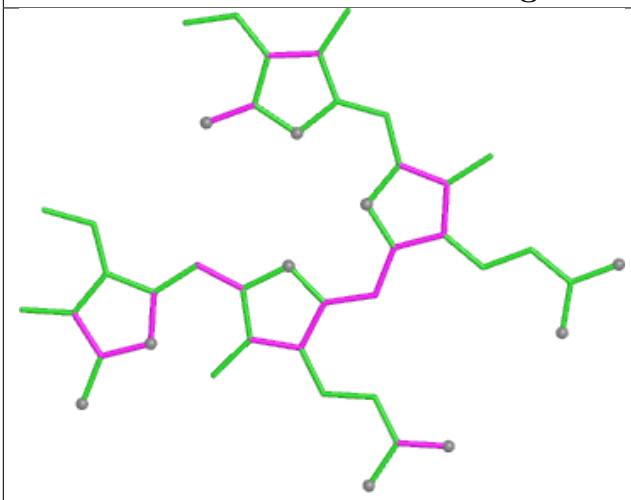


Rings

Ligand PEB a4 203



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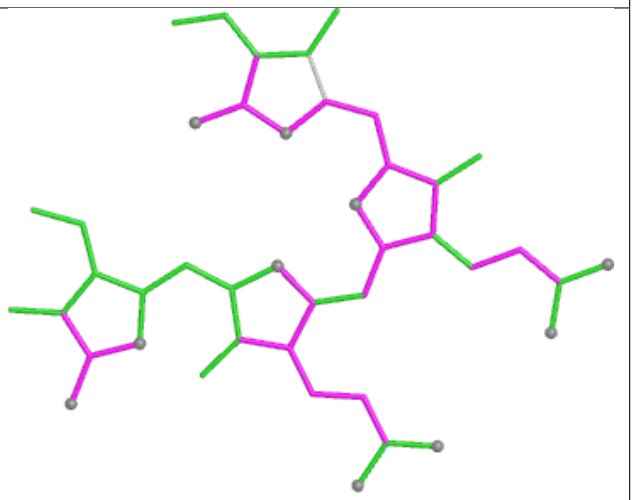

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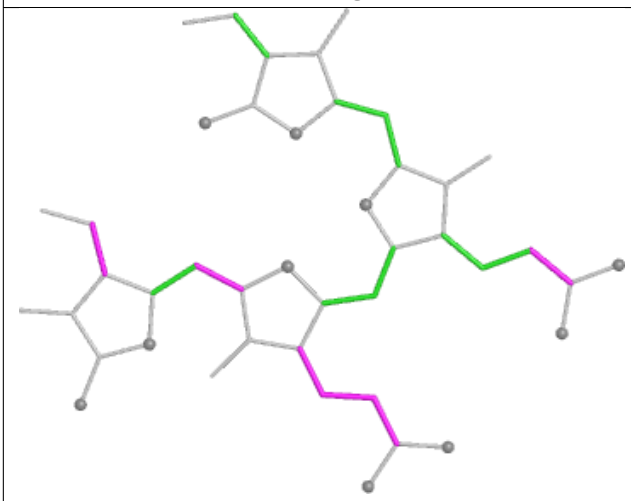

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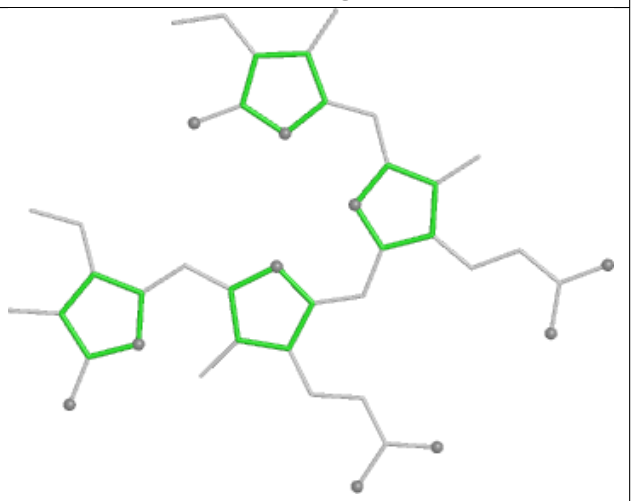
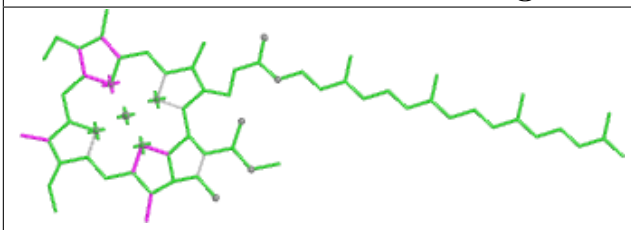


Rings

Ligand CLA bL 621



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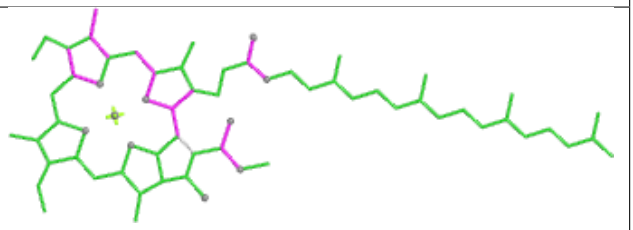
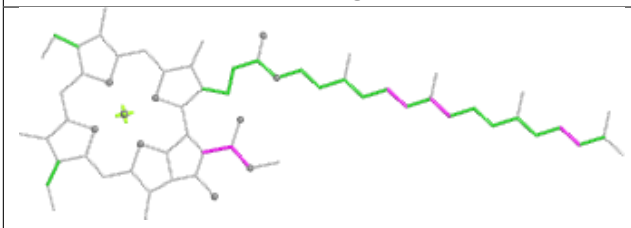


Bond angles



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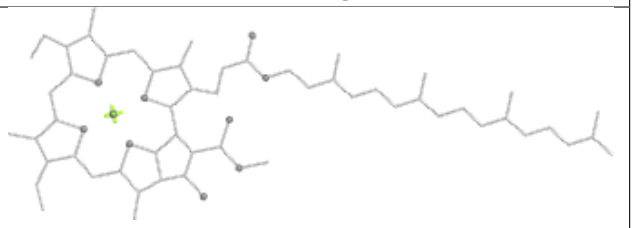
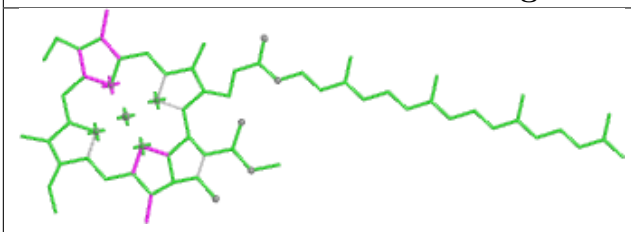


Rings

Ligand CLA c6 607



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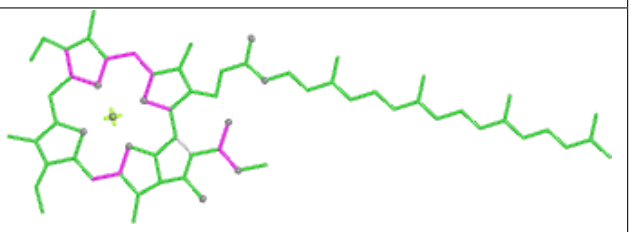
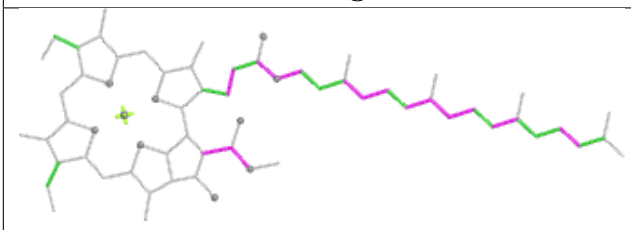


Bond angles



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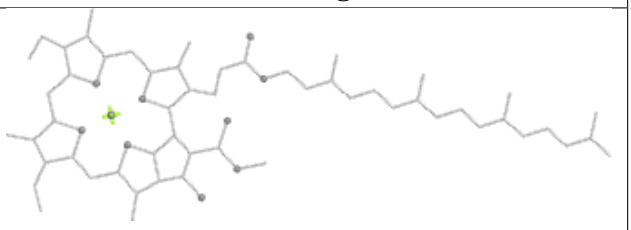
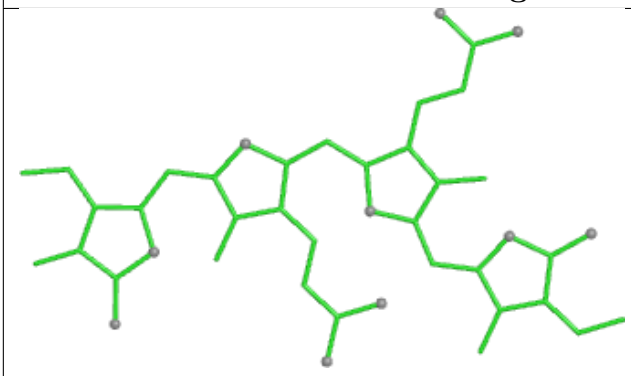


Rings

Ligand CYC r3 1001



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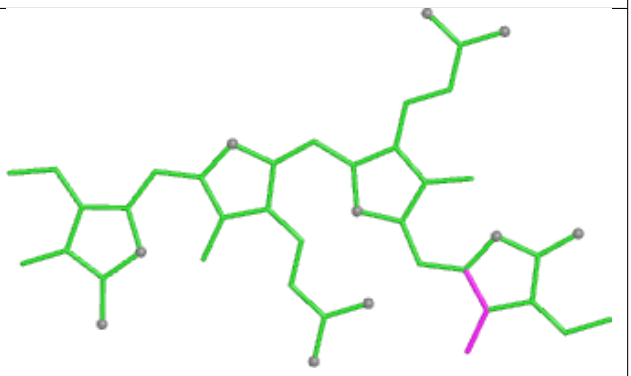
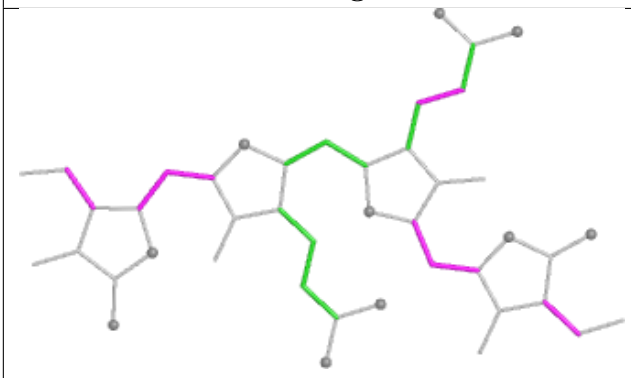


Bond angles



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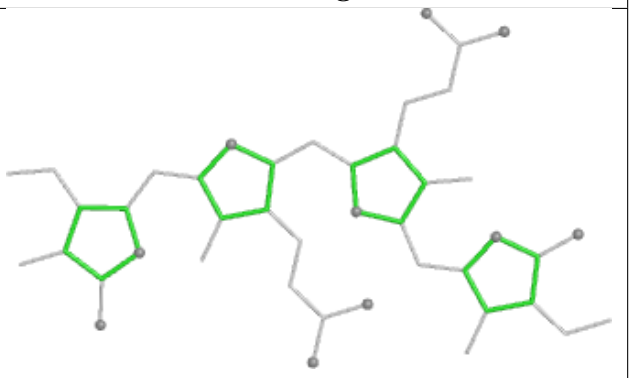
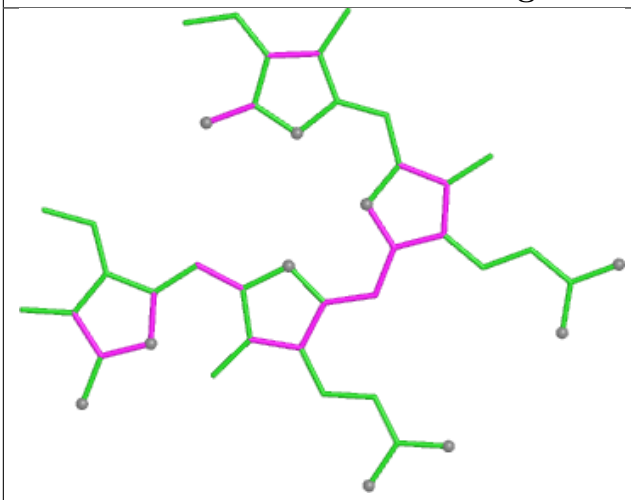


Rings

Ligand PEB IQ 201



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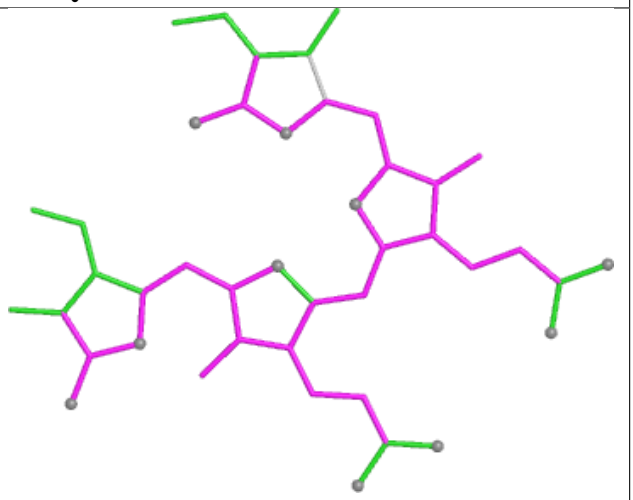
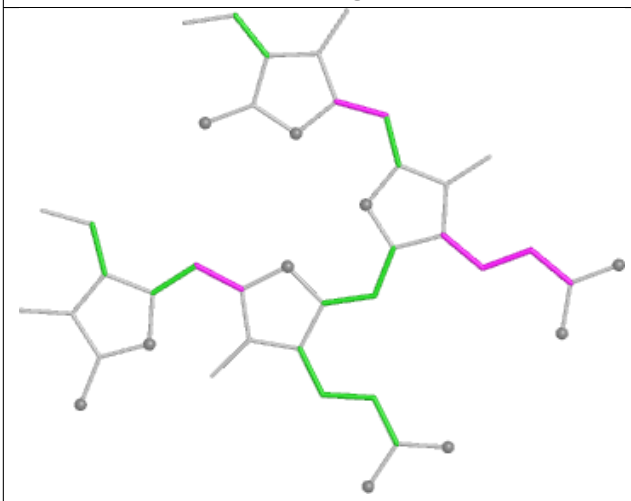


Bond angles



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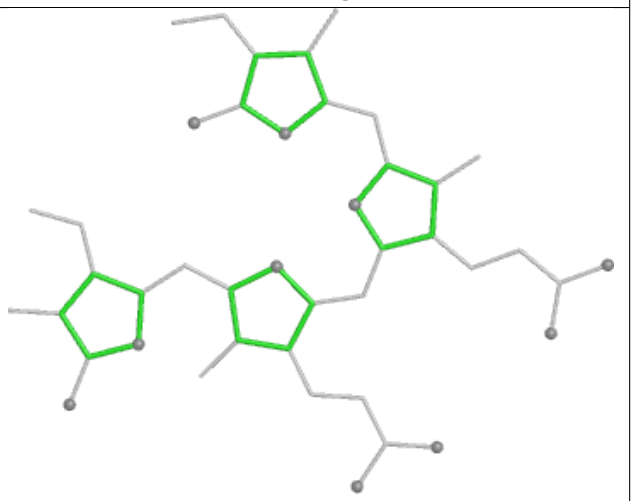
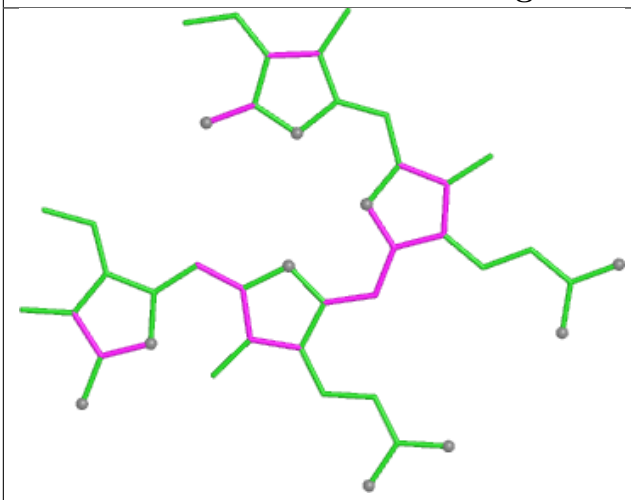


Rings

Ligand PEB cH 202



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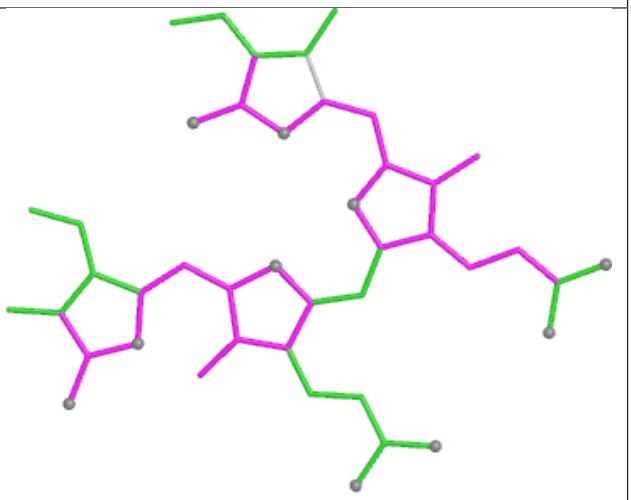
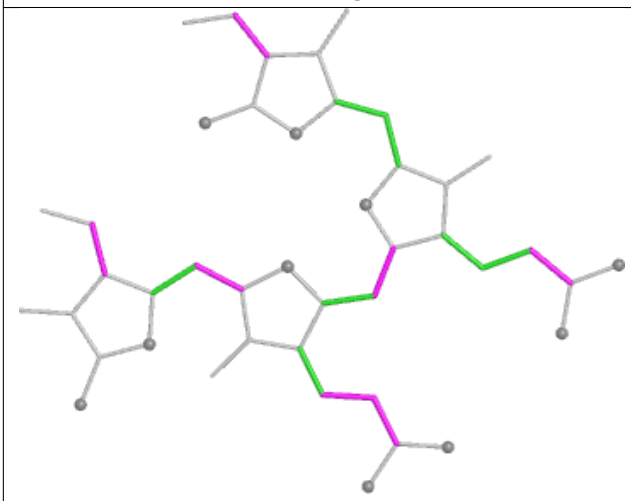
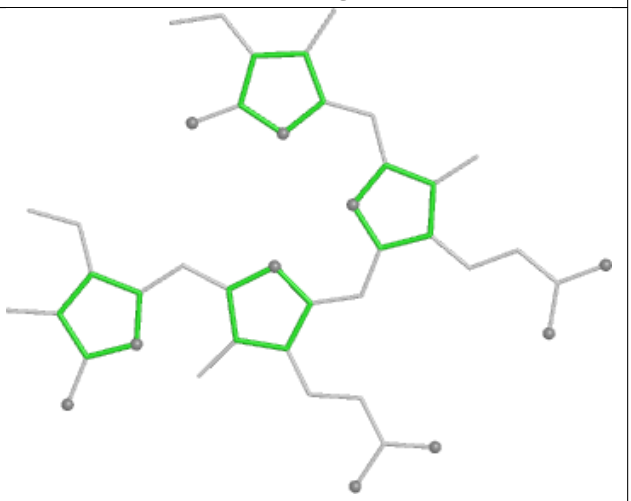


Bond angles



Torsions

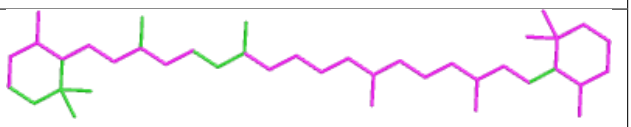


Rings

Ligand BCR Z6 101



Bond lengths



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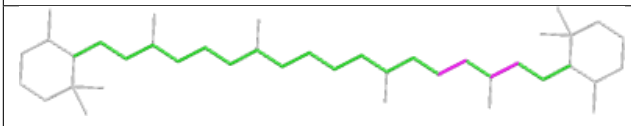

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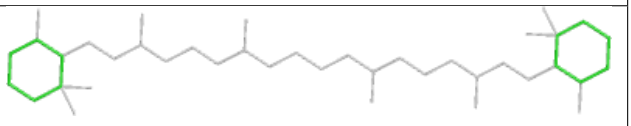
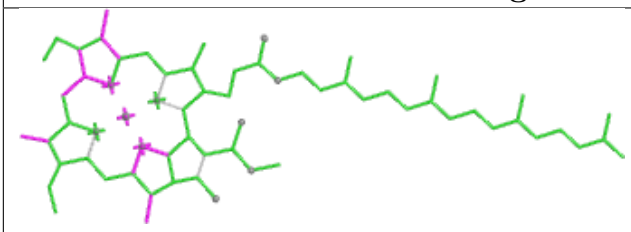


Rings

Ligand CLA AN 811



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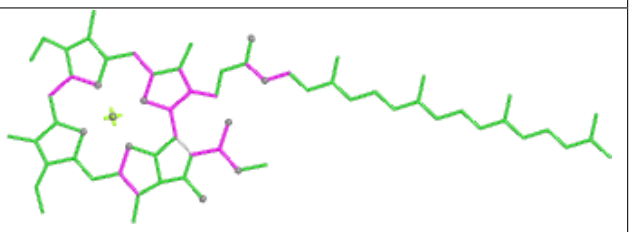

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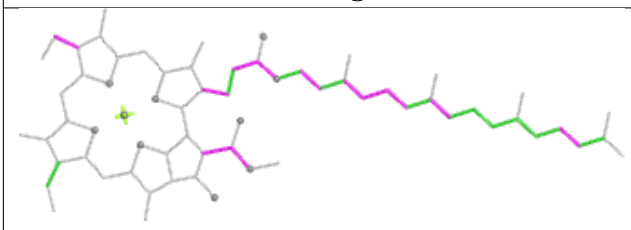

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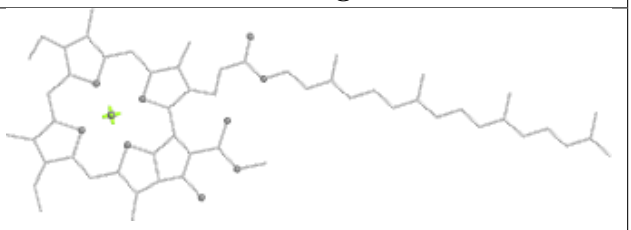
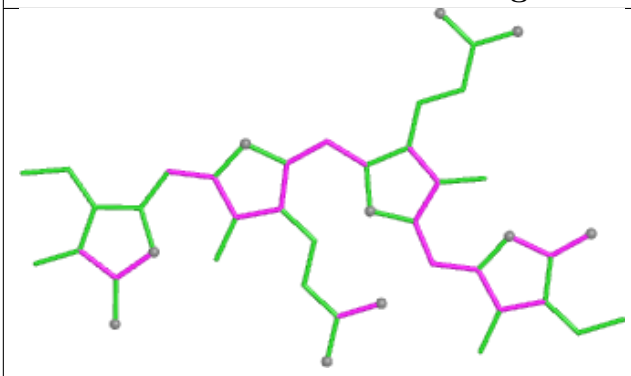


Rings

Ligand CYC I3 1001



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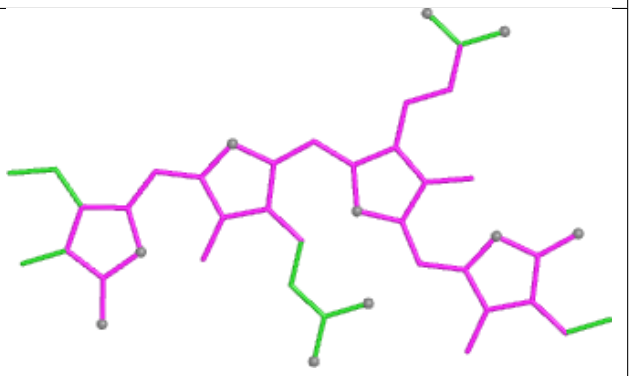

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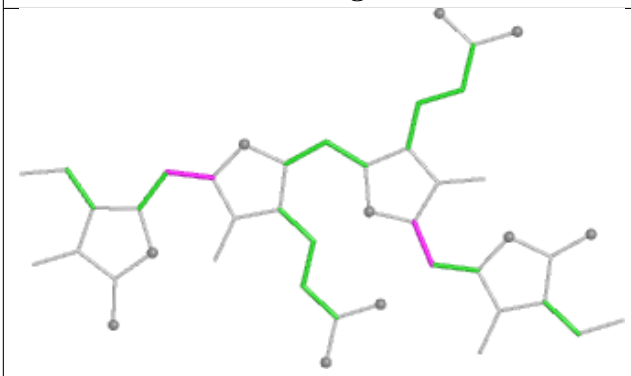

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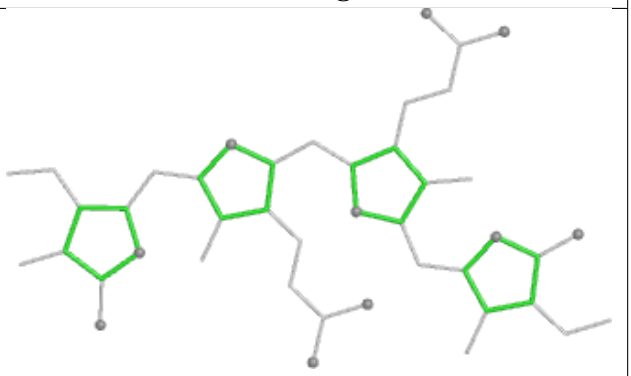
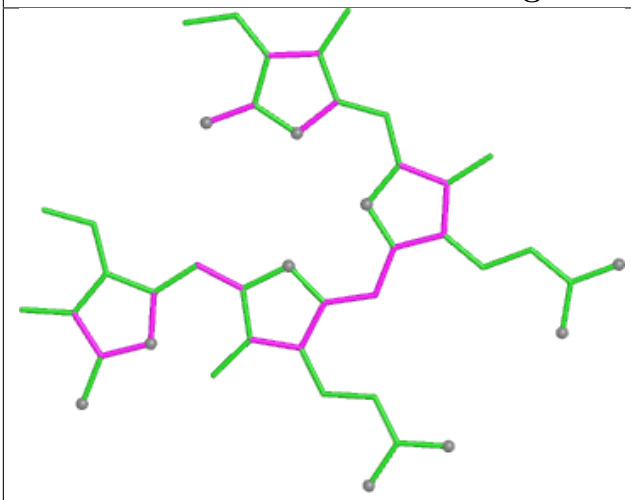


Rings

Ligand PEB j1 202



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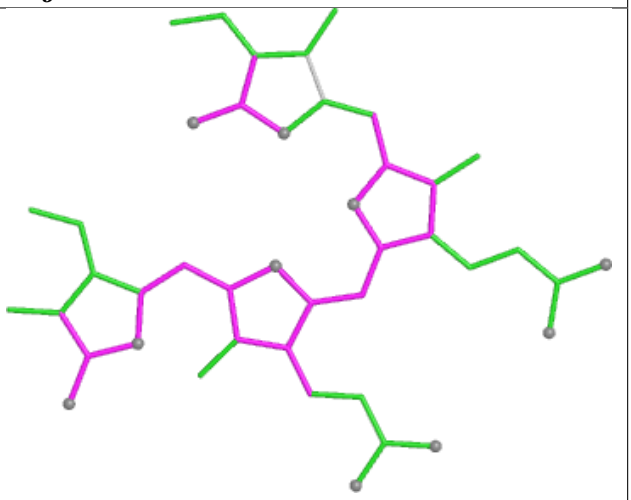

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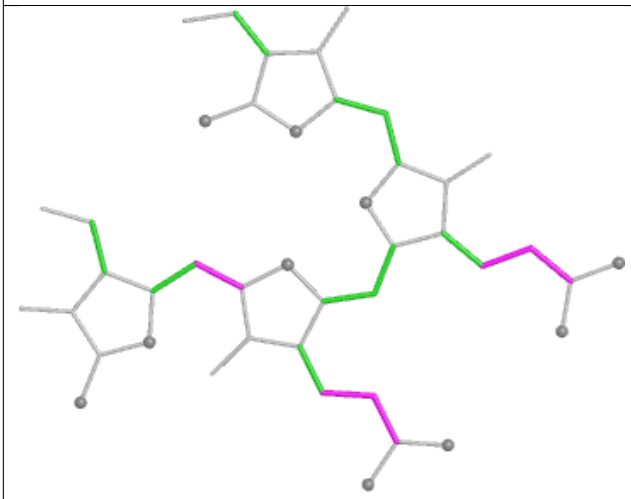

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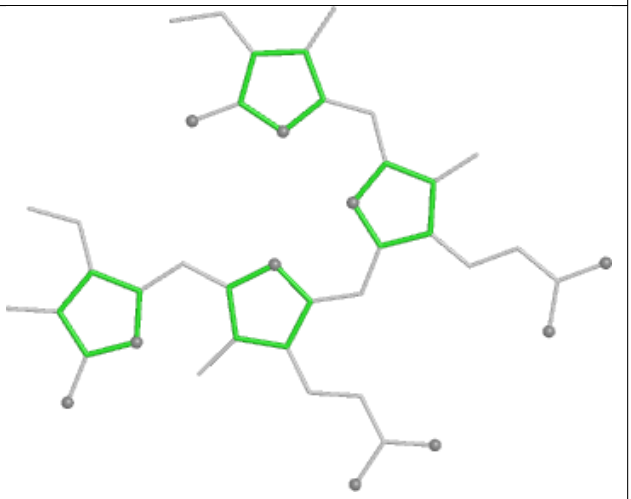
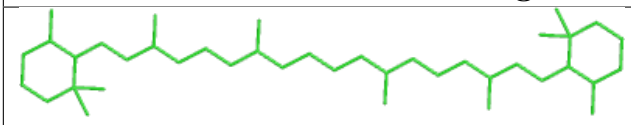


Rings

Ligand BCR F2 204



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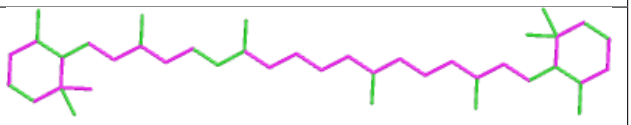

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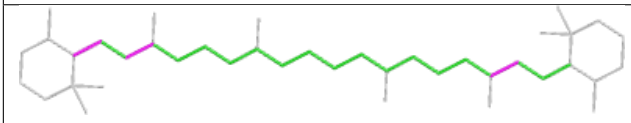

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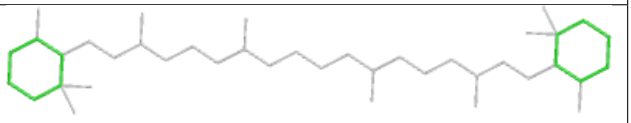
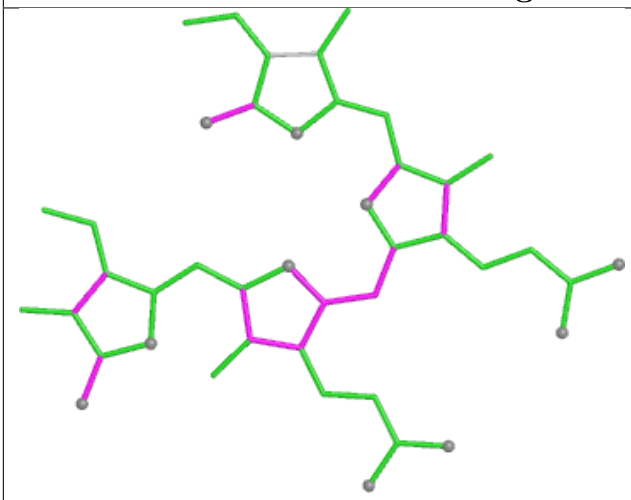


Rings

Ligand PUB Z5 303



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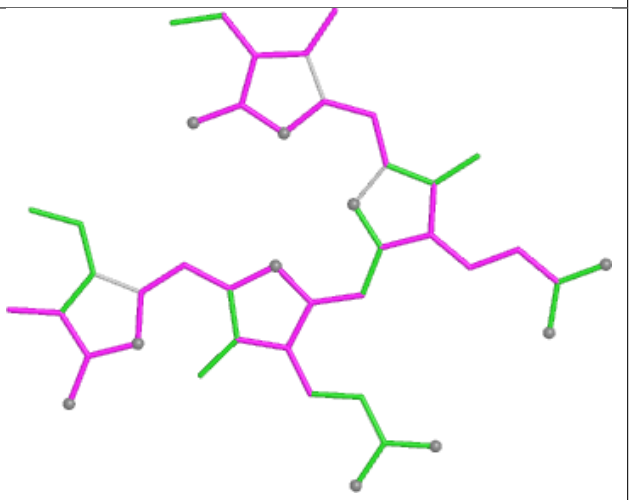
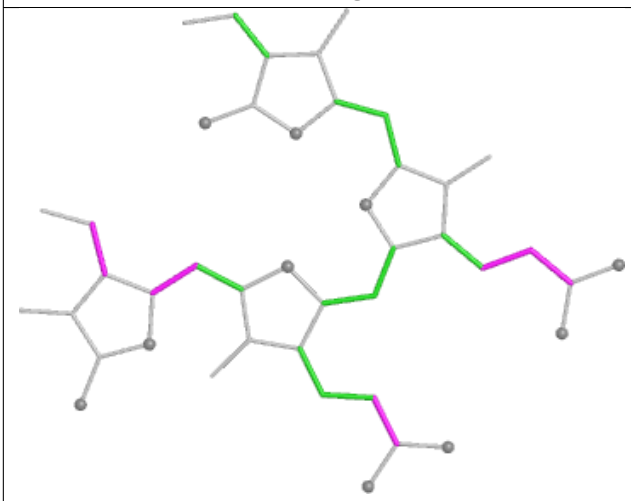


Bond angles



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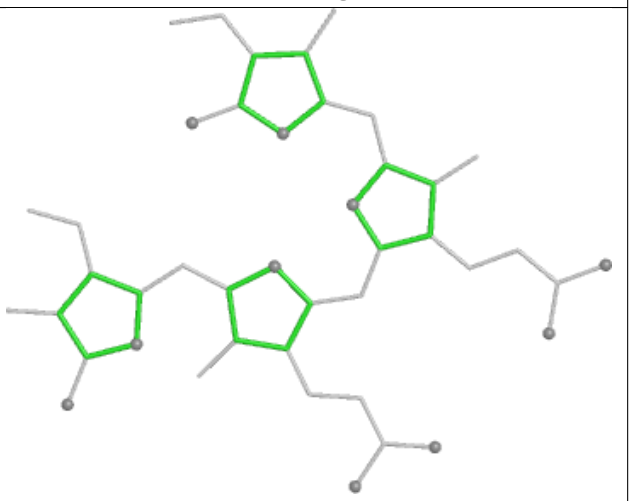
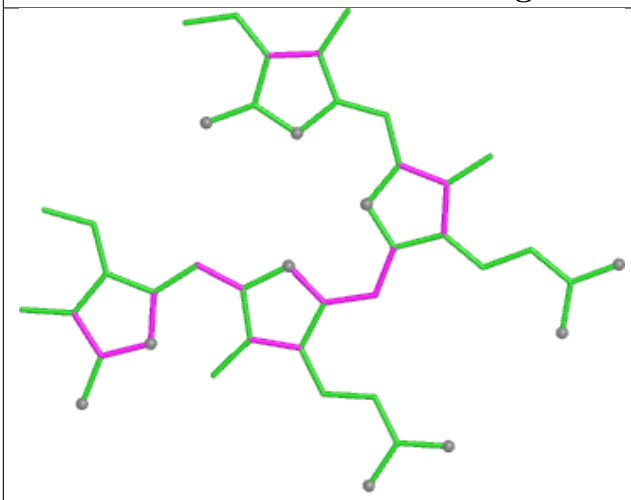


Rings

Ligand PEB U7 201



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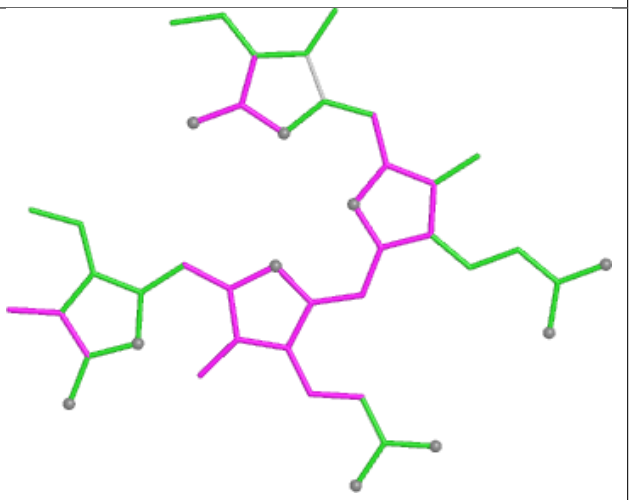

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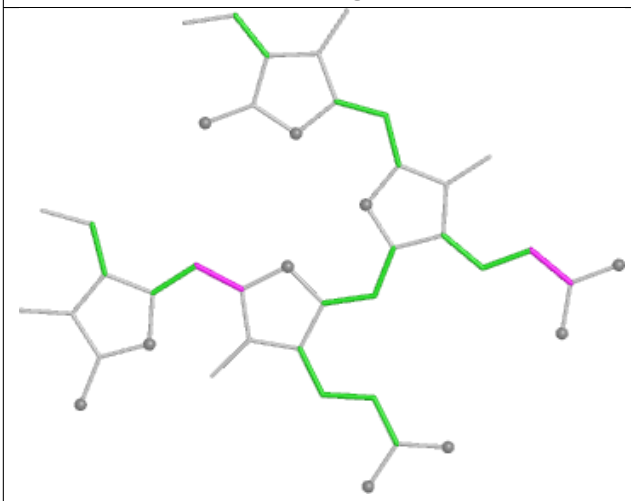

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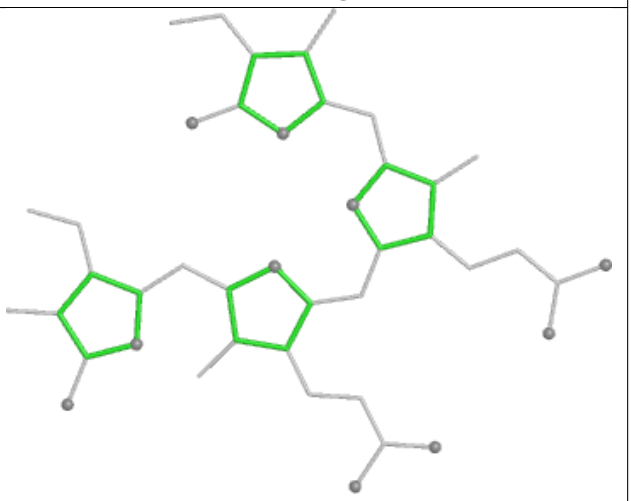
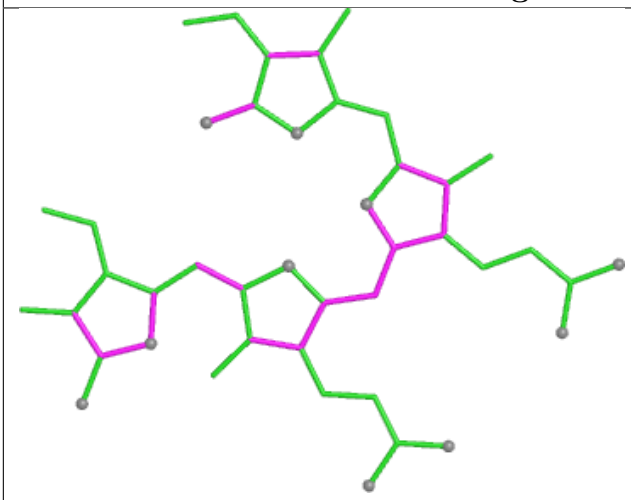


Rings

Ligand PEB HP 201



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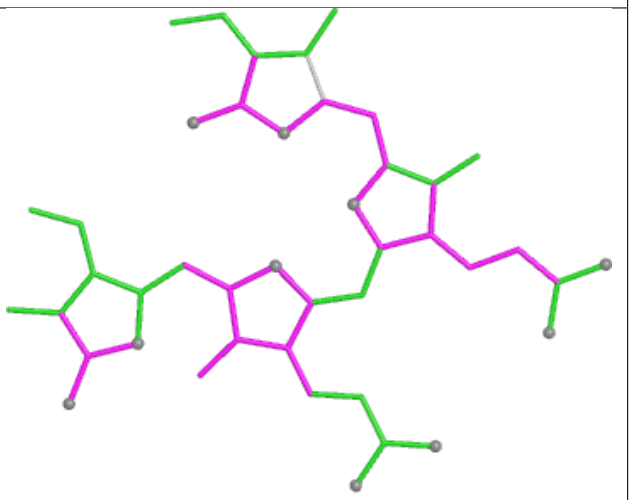

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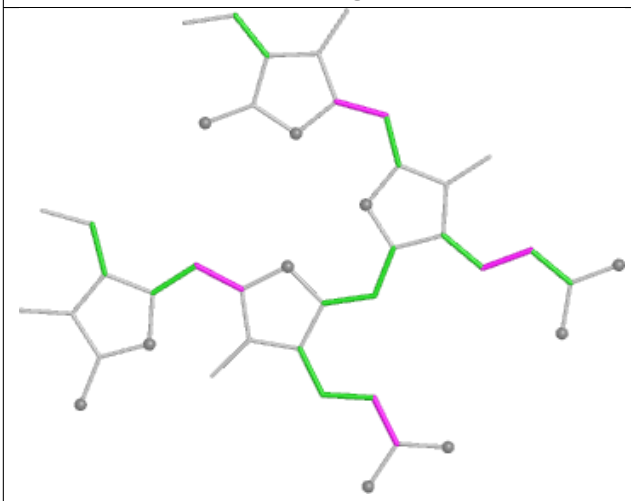

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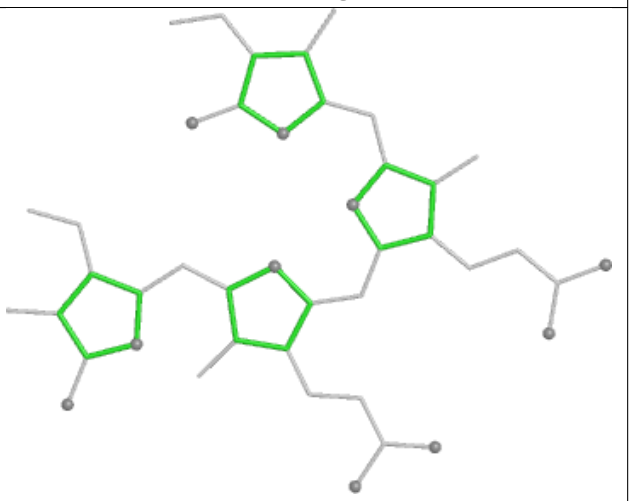
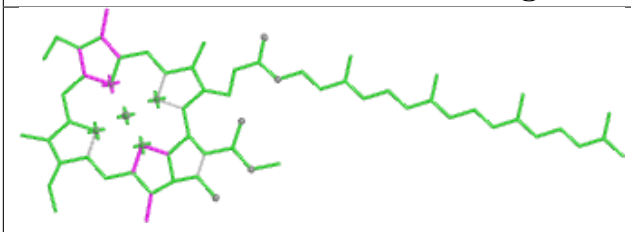


Rings

Ligand CLA c6 605



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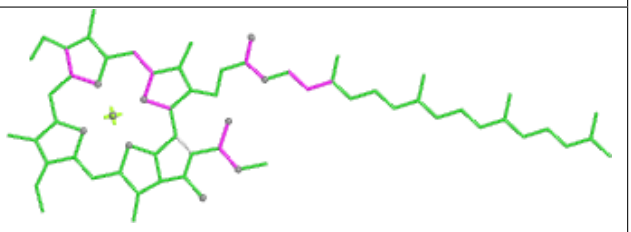

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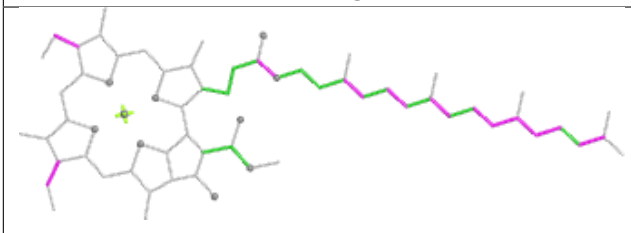

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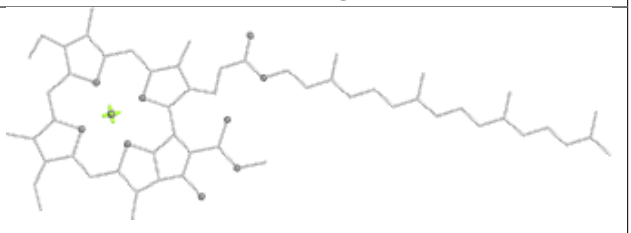
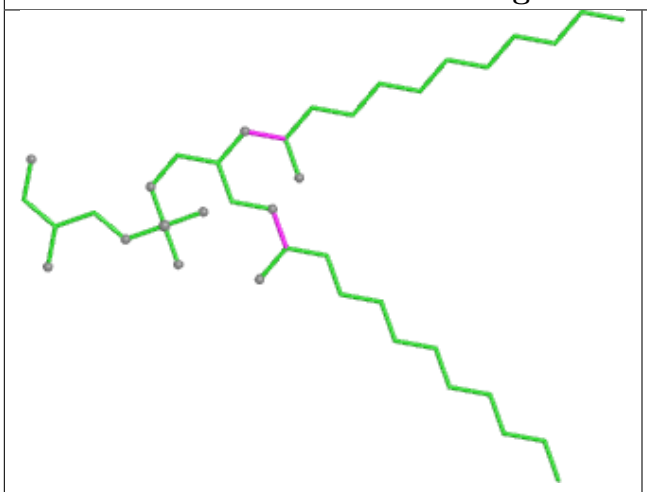


Rings

Ligand LHG m6 102



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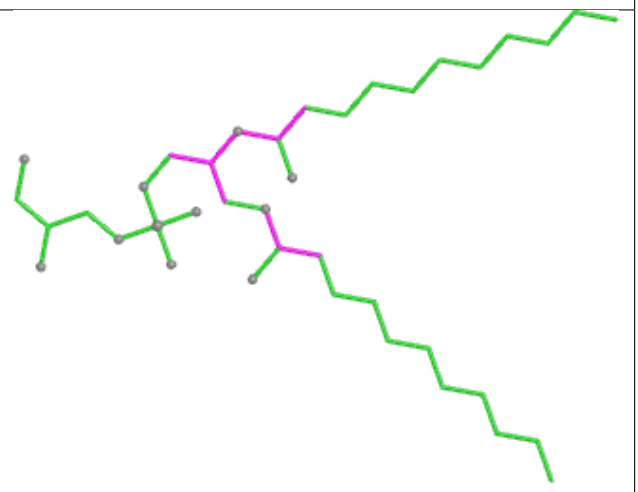
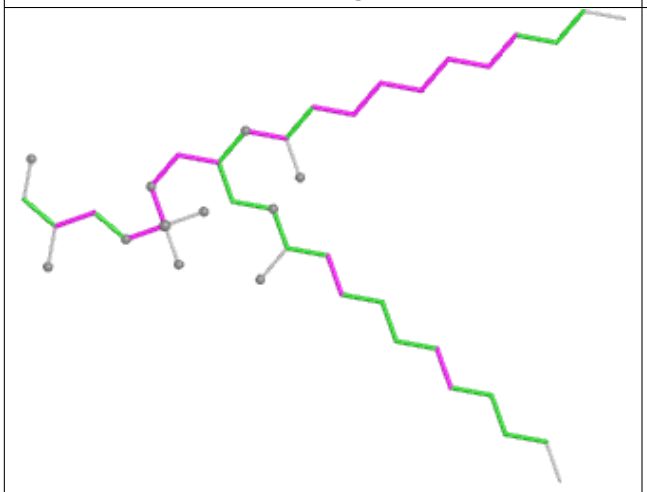


Bond angles



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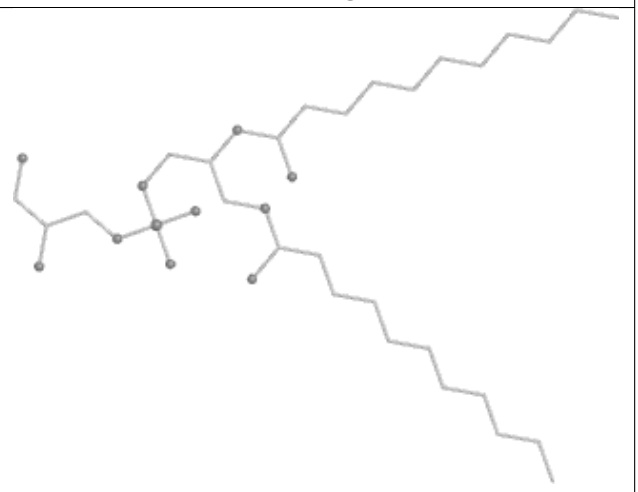
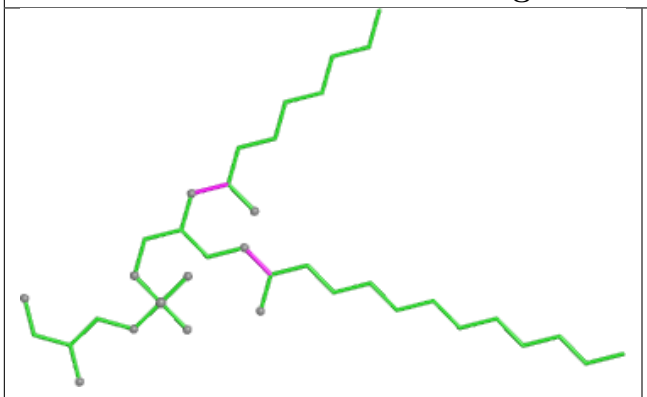


Rings

Ligand LHG CL 521



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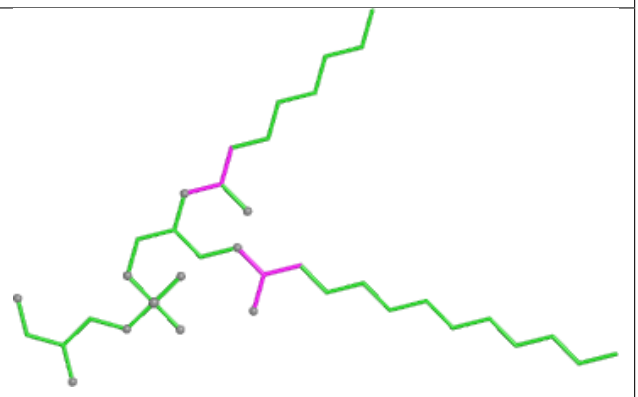

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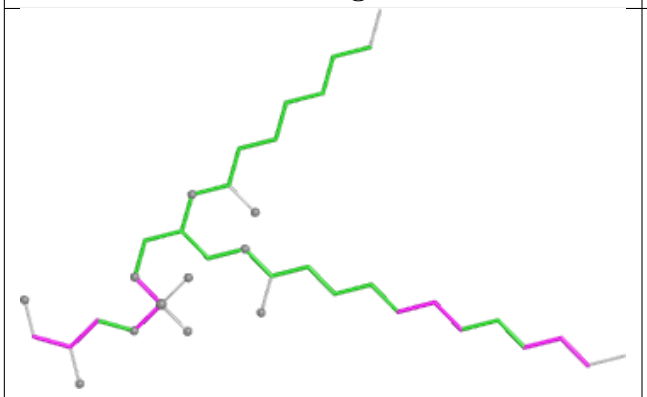

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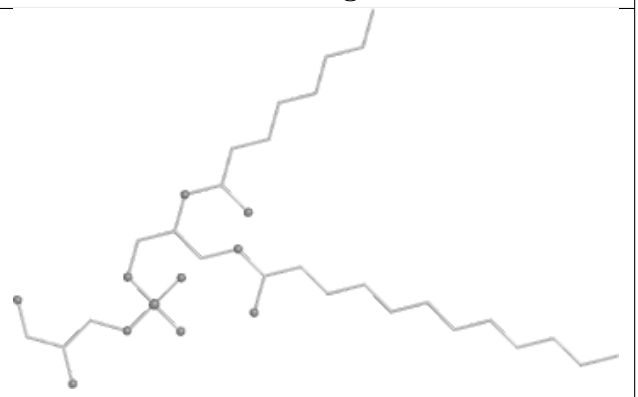
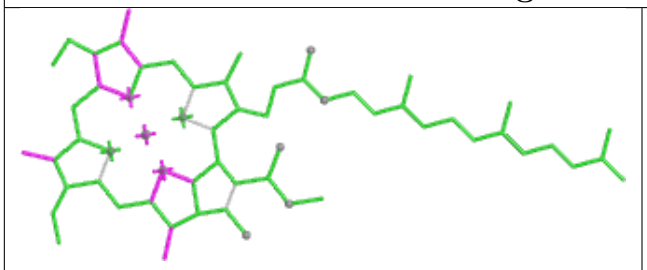


Rings

Ligand CLA B2 831



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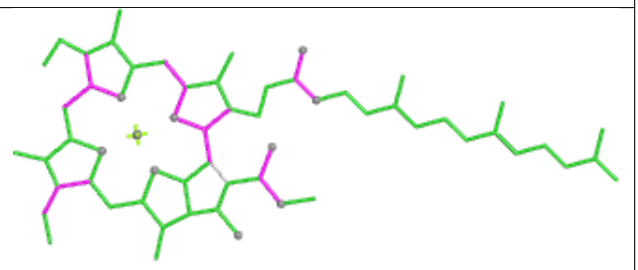
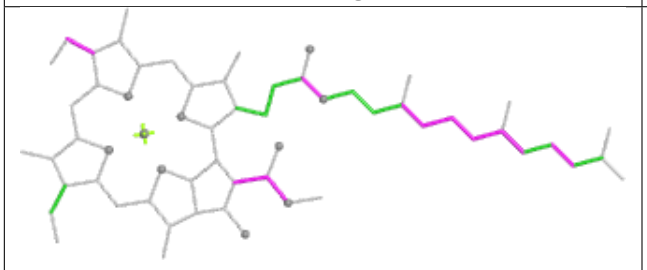


Bond angles



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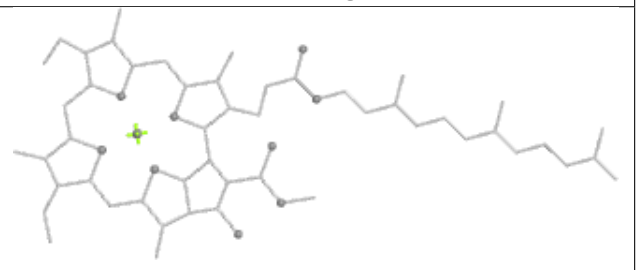
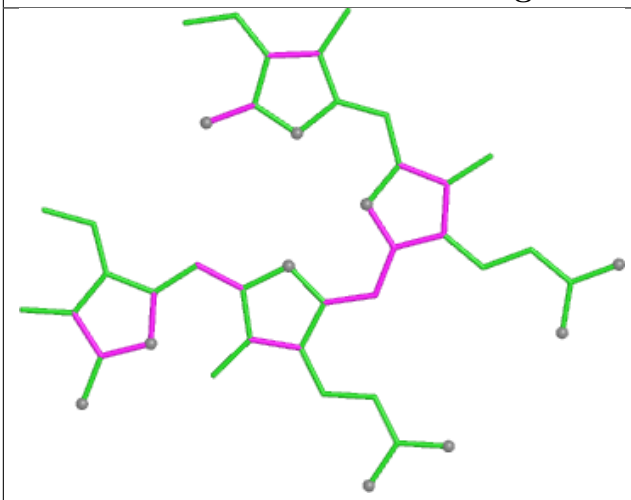


Rings

Ligand PEB LP 201



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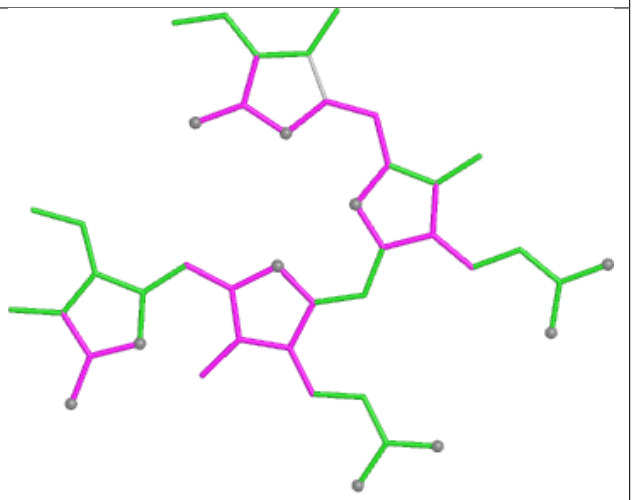
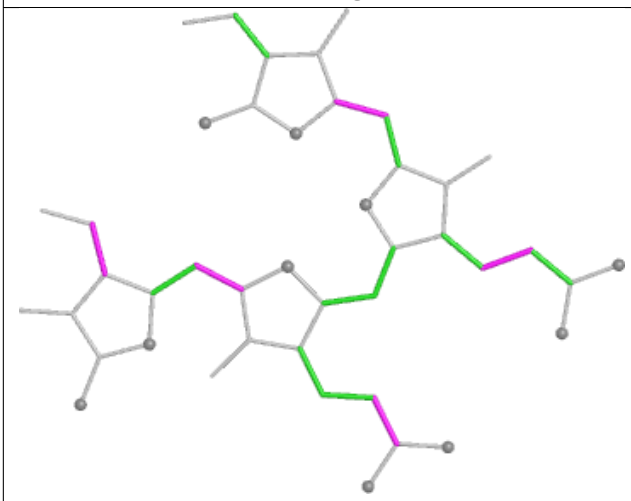


Bond angles



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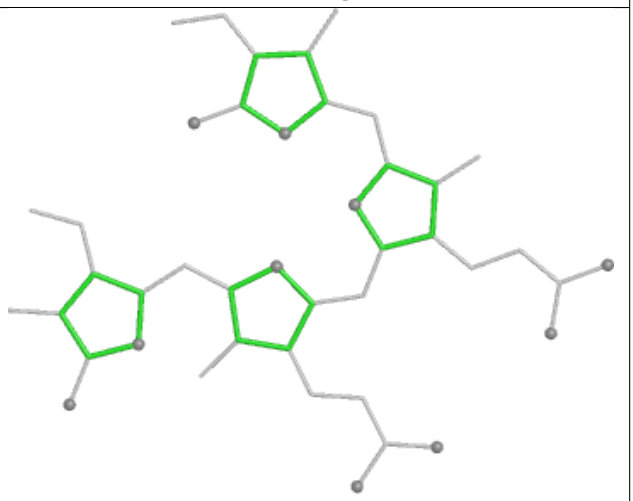
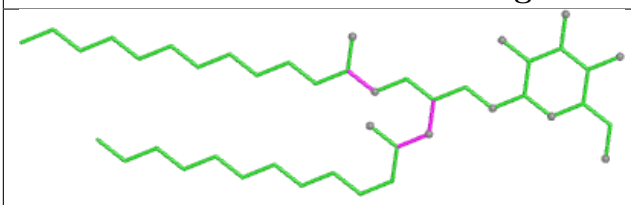


Rings

Ligand LMG J6 102



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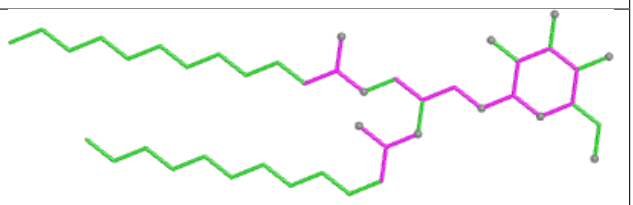
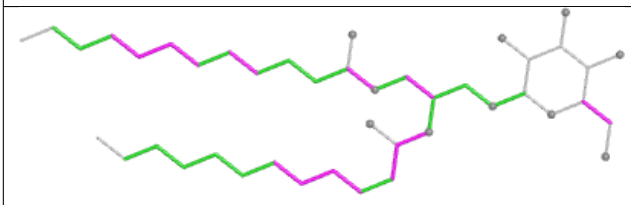


Bond angles



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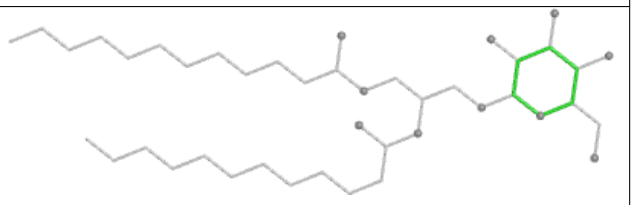
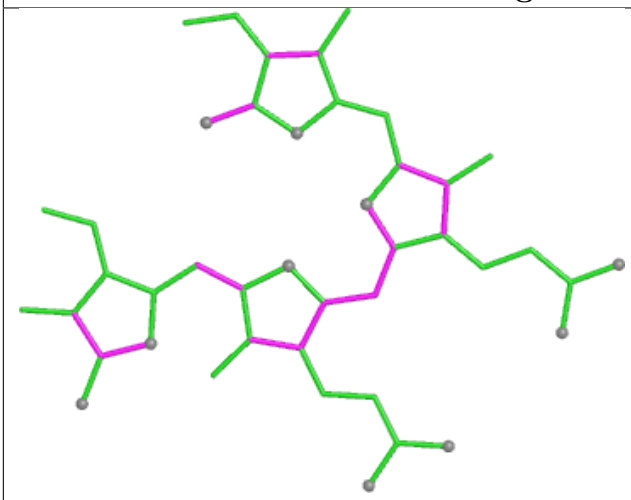
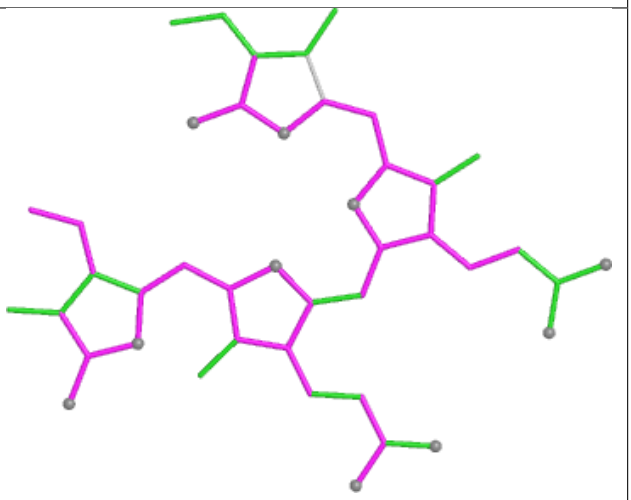


Rings

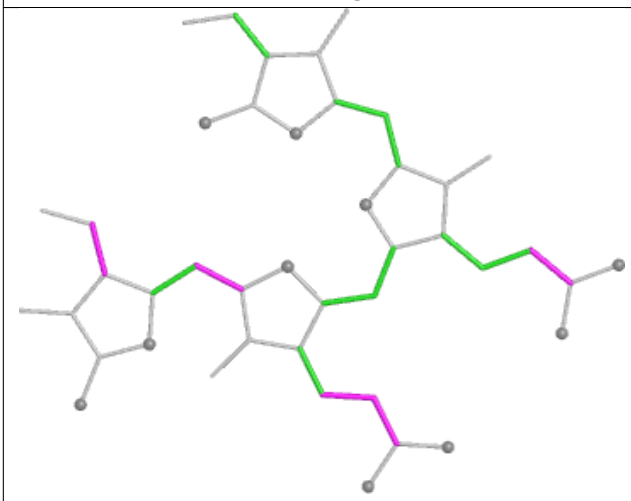
Ligand PEB LF 201



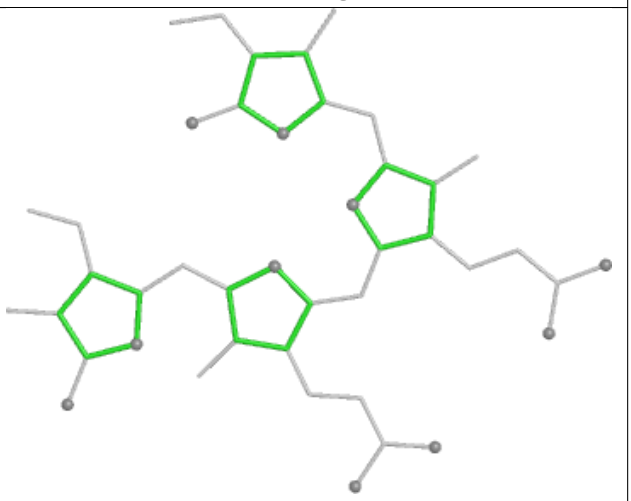
Bond lengths



Bond angles

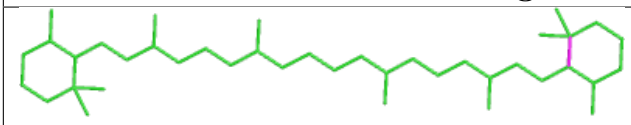


Torsions



Rings

Ligand BCR cL 504



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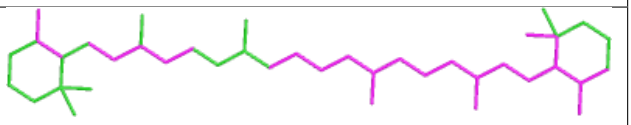

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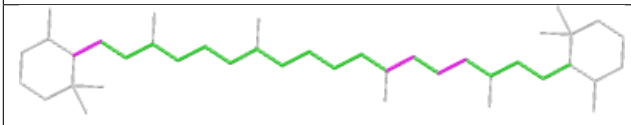

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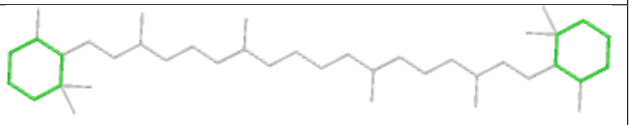
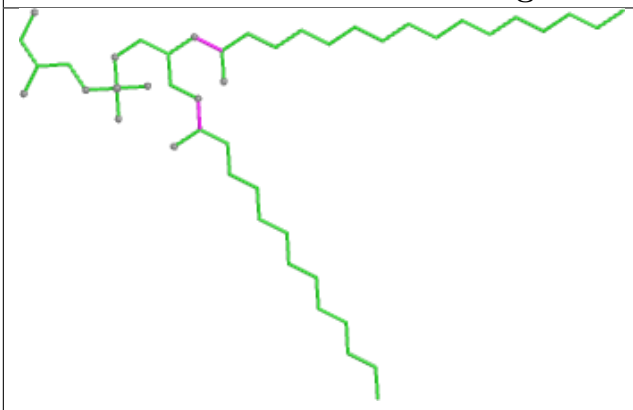


Rings

Ligand LHG d6 402



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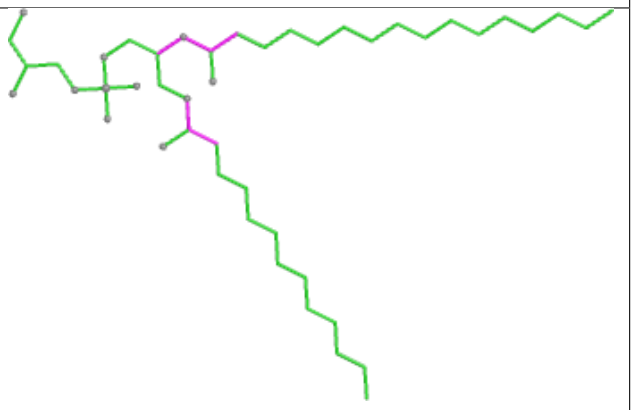

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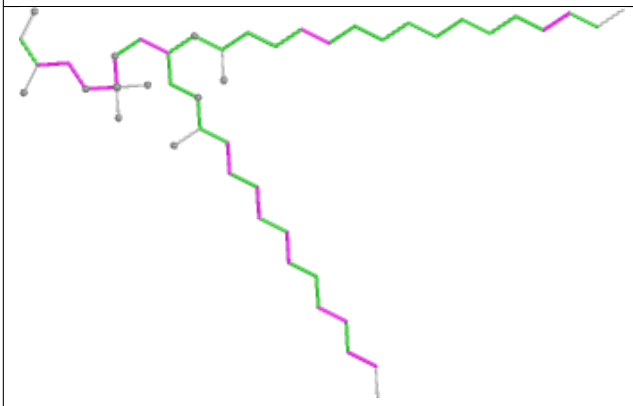

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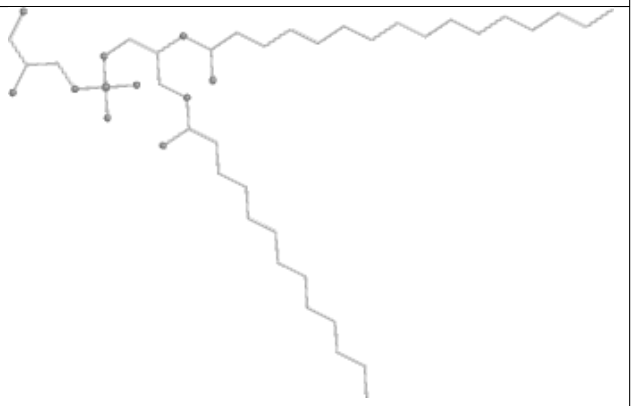
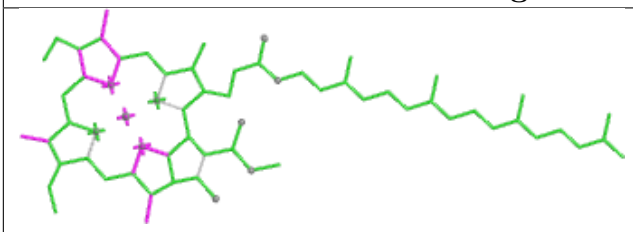


Rings

Ligand CLA BN 811



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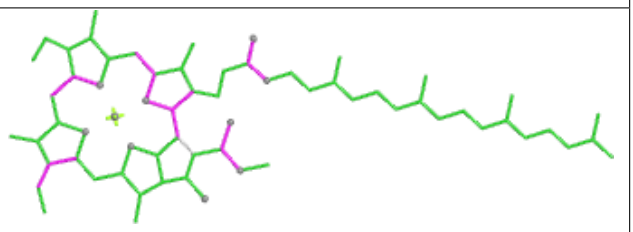

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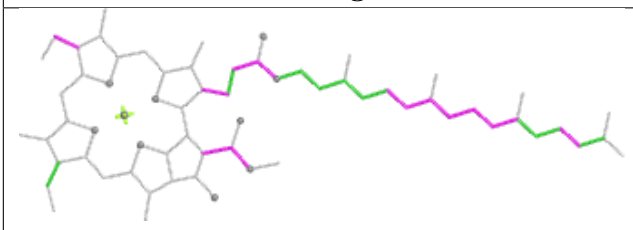

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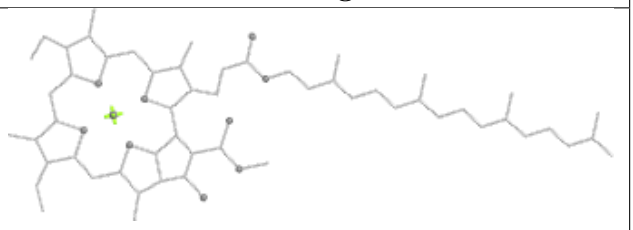
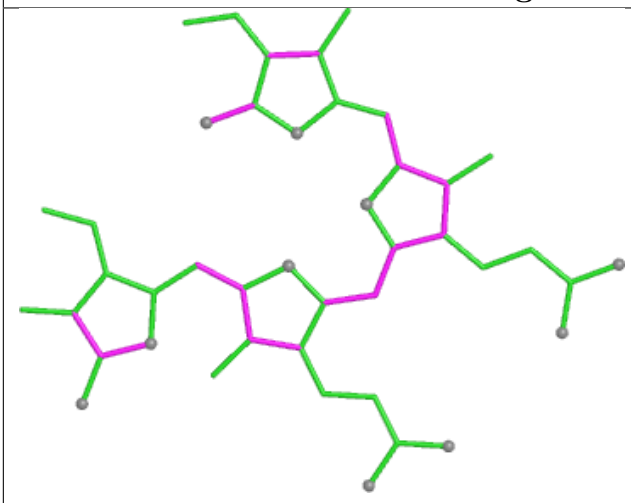


Rings

Ligand PEB V1 203



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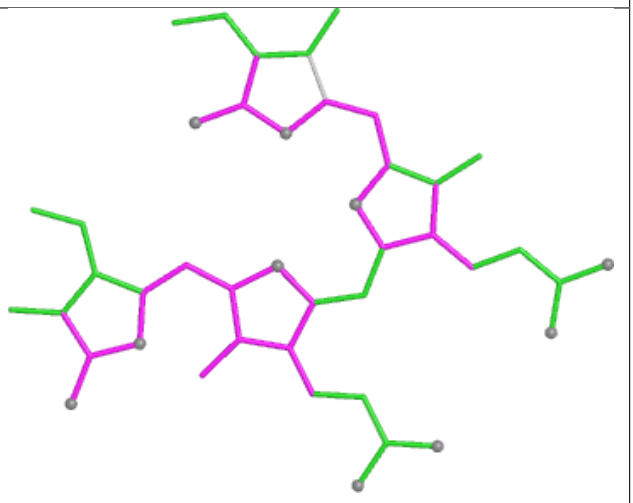

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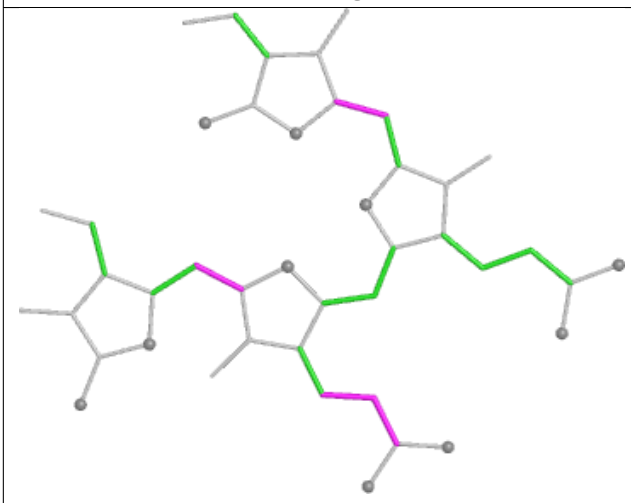

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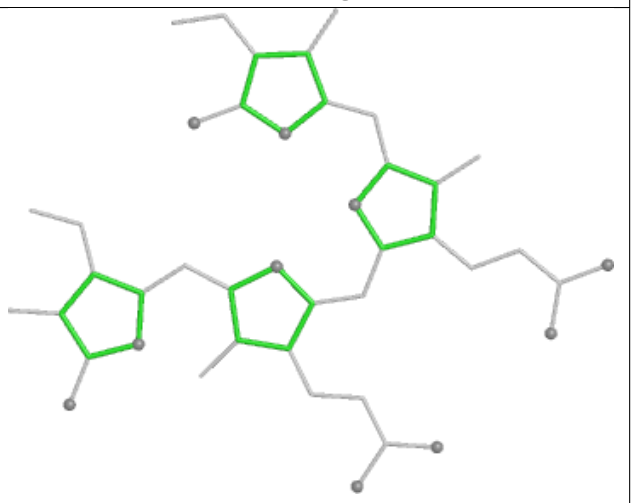
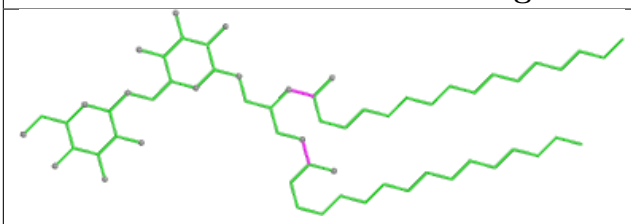


Rings

Ligand DGD h6 101



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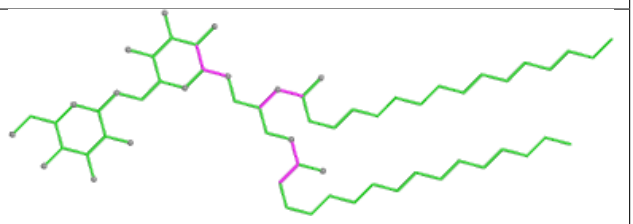

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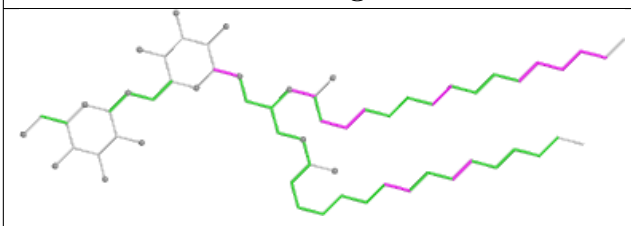

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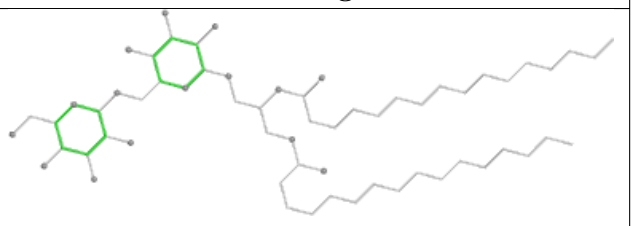
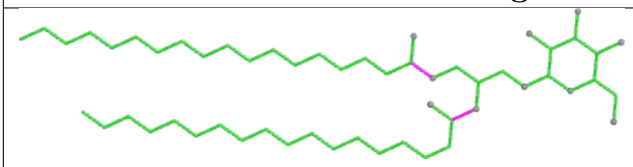


Rings

Ligand LMG C6 501



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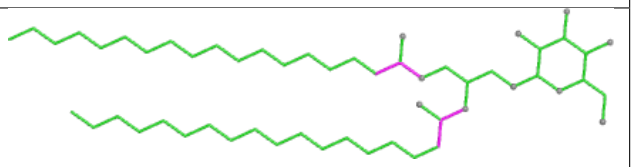

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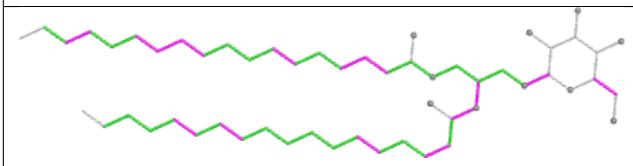

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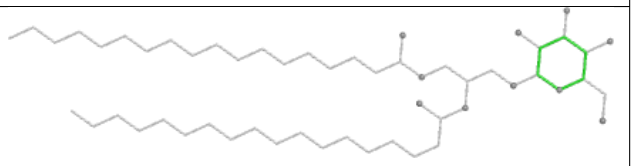
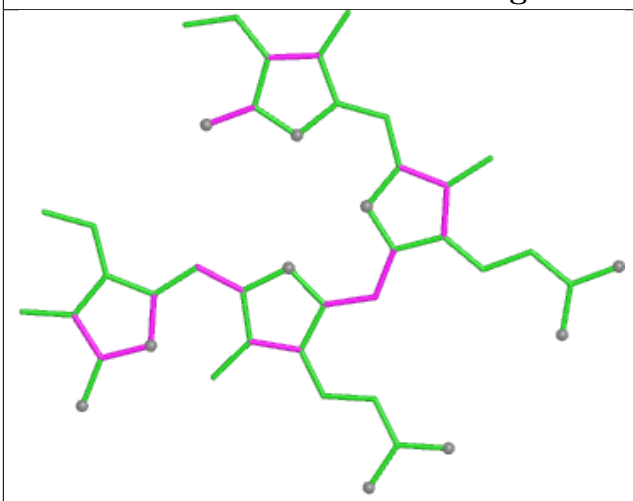


Rings

Ligand PEB UG 201



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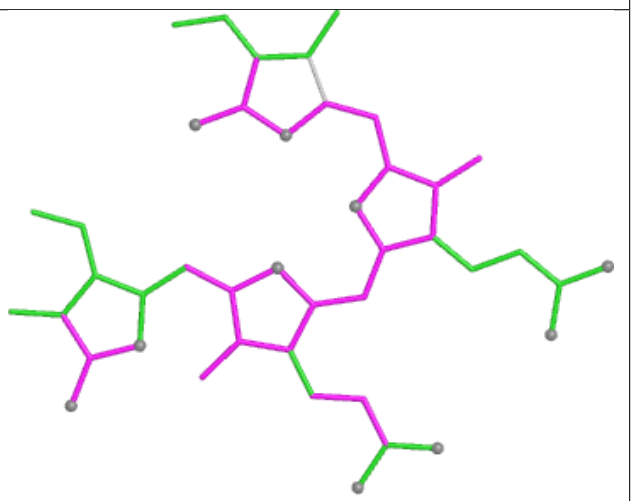

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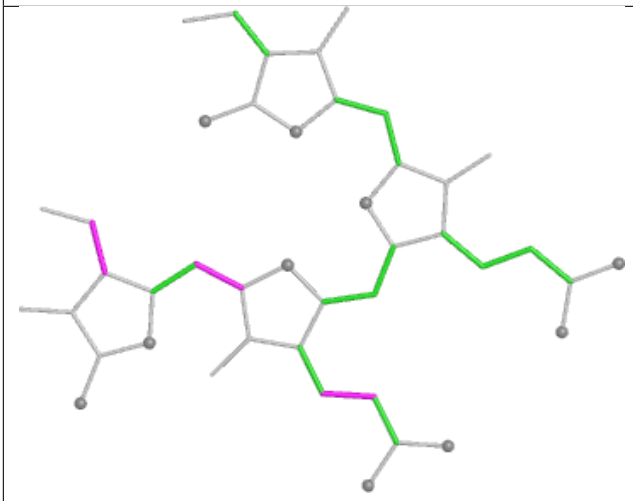

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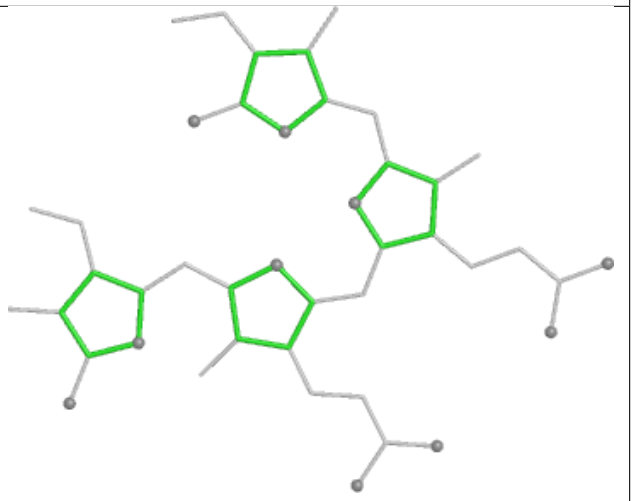
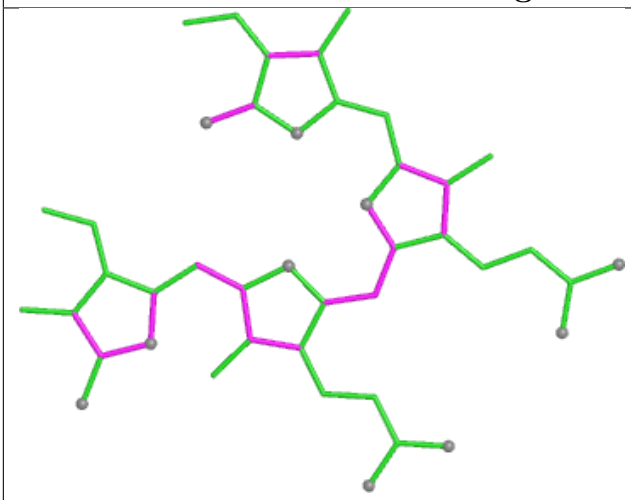


Rings

Ligand PEB K5 201



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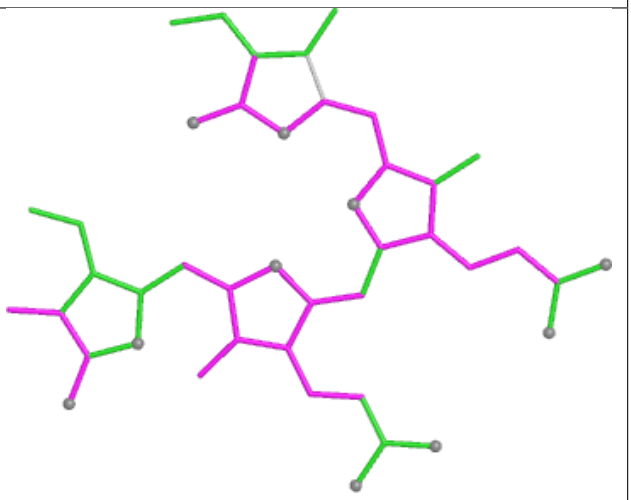
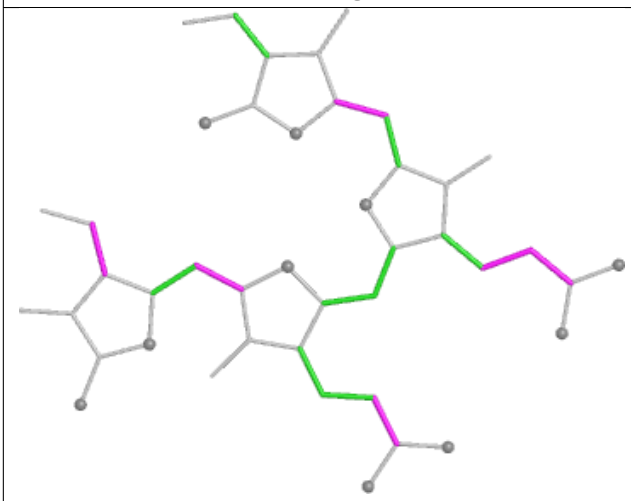


Bond angles



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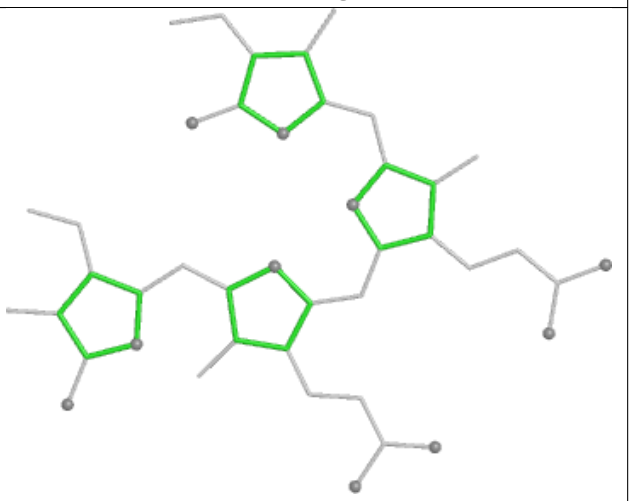
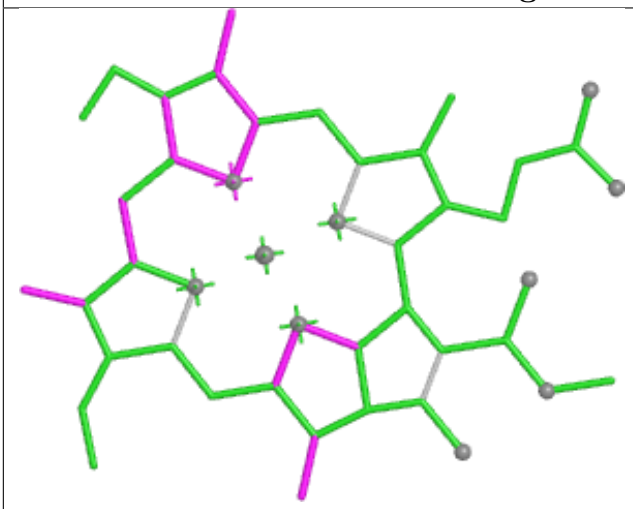


Rings

Ligand CLA 42 603



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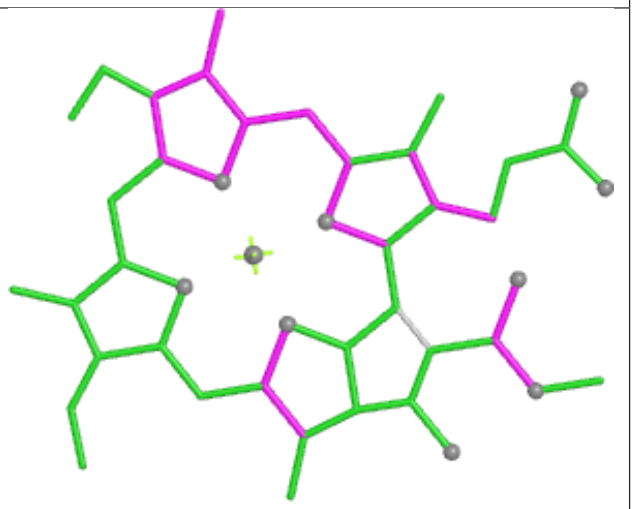
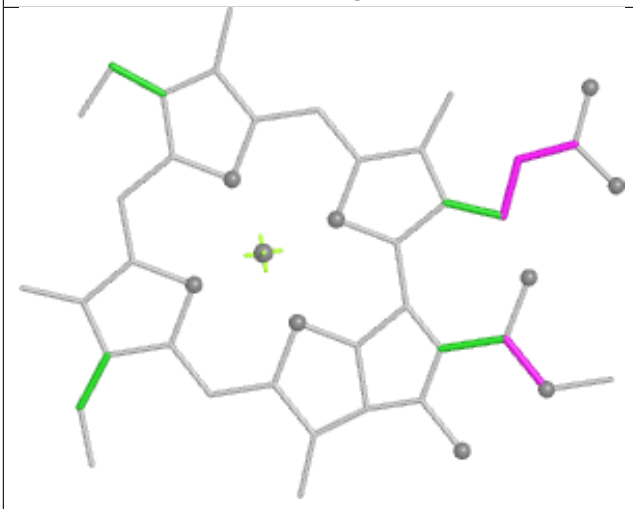


Bond angles

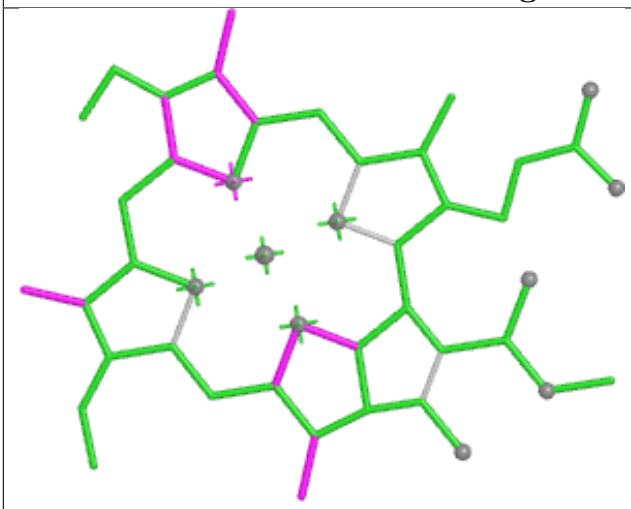


Torsions



Rings

Ligand CLA 12 611



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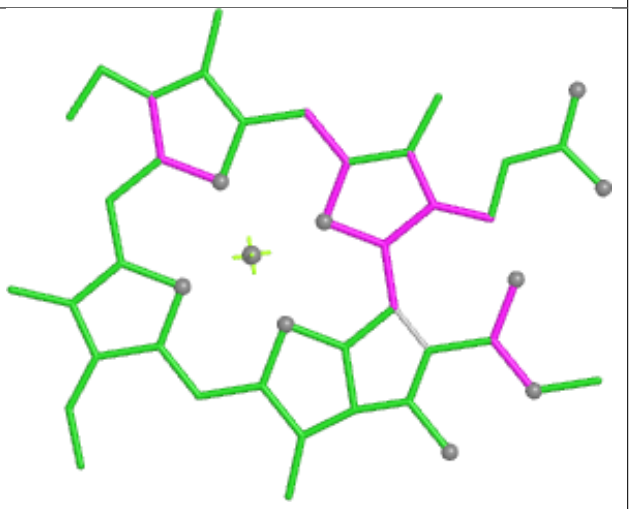
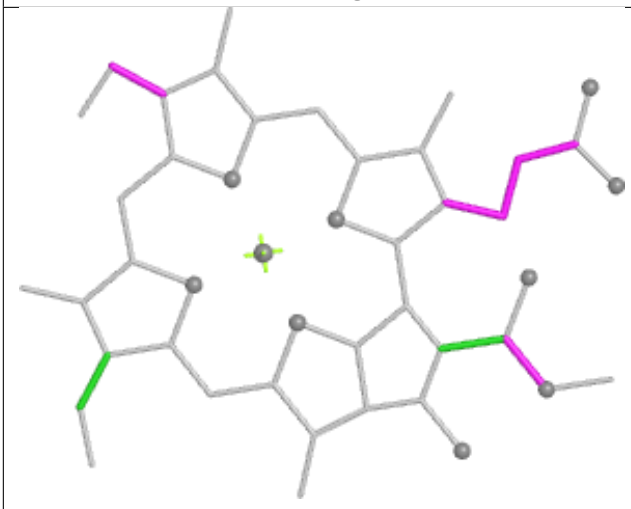


Bond angles

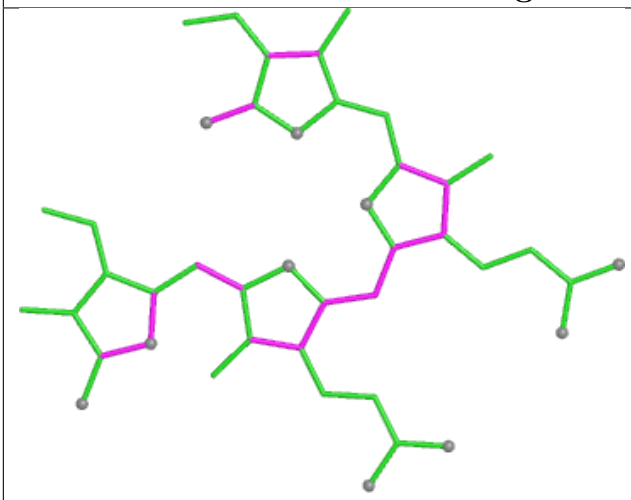


Torsions



Rings

Ligand PEB fM 202



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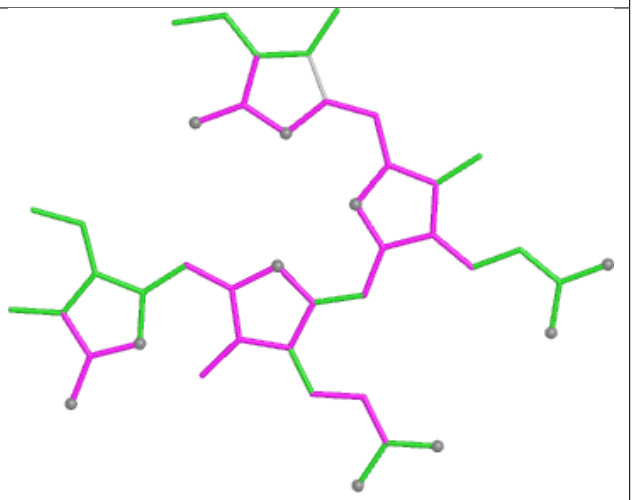
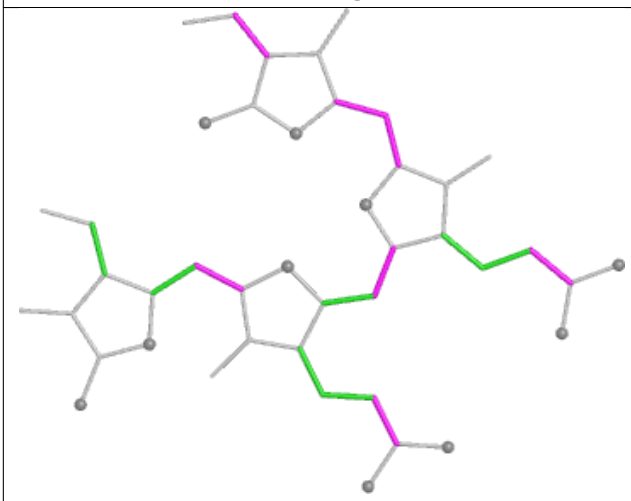


Bond angles



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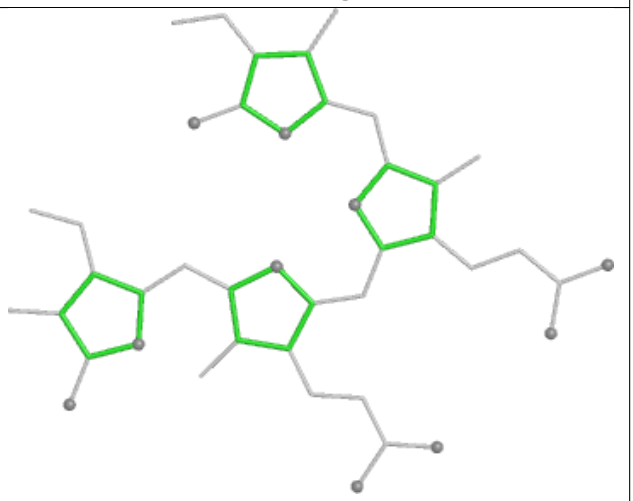
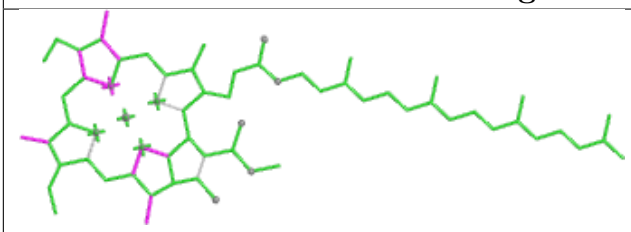


Rings

Ligand CLA b6 612



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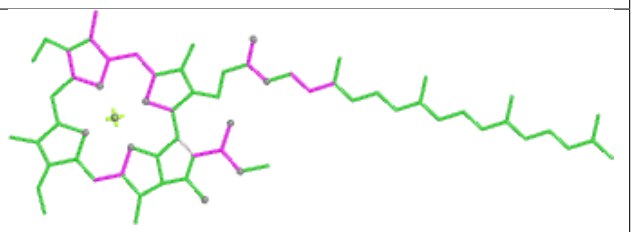
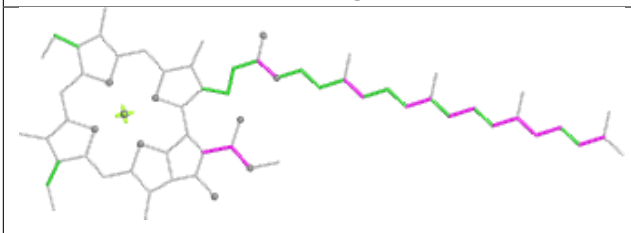


Bond angles



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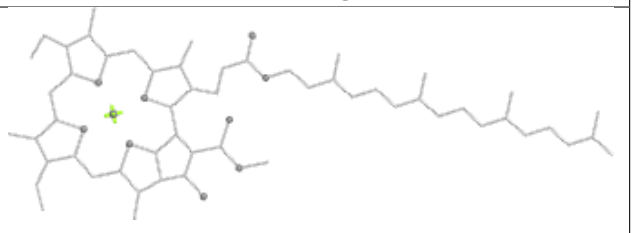
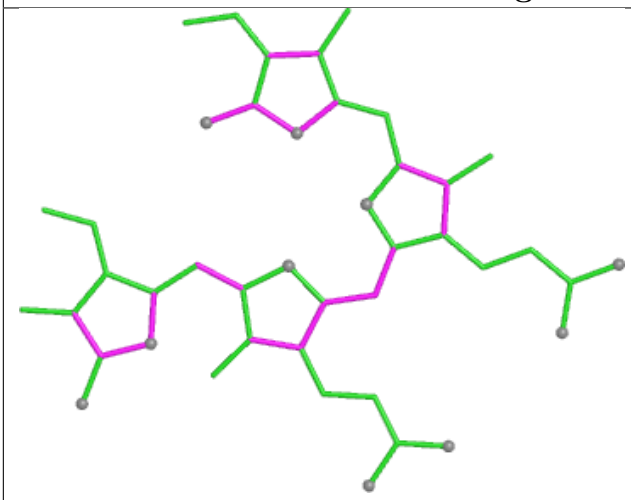


Rings

Ligand PEB U5 201



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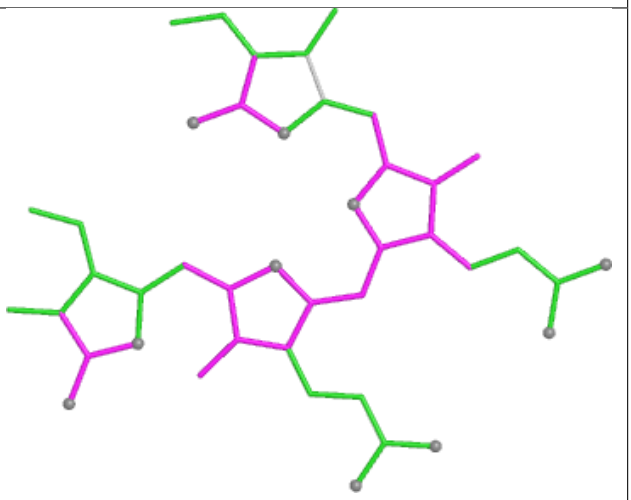
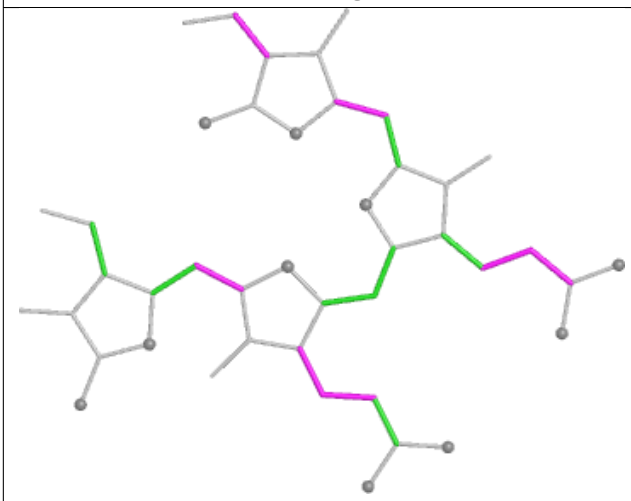


Bond angles



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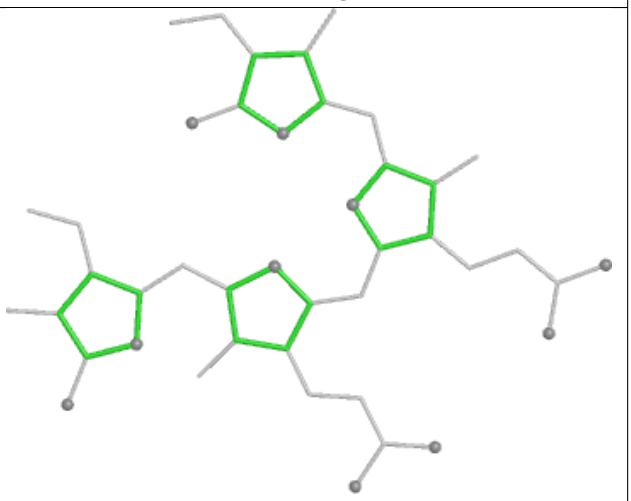
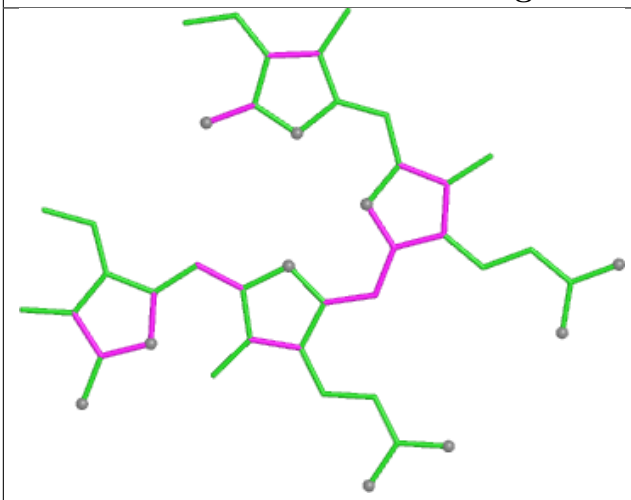


Rings

Ligand PEB U7 202



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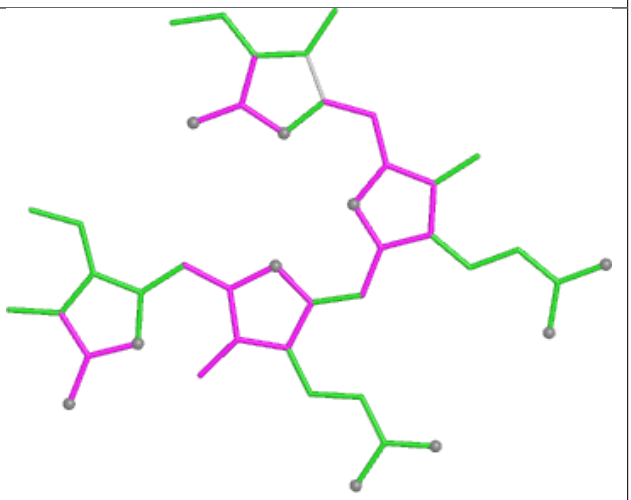
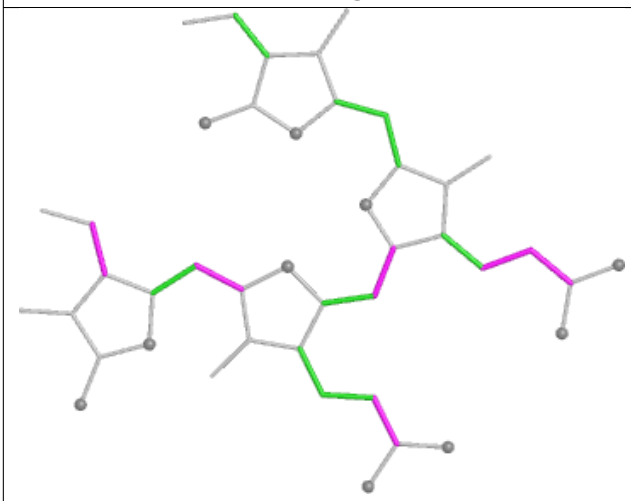


Bond angles



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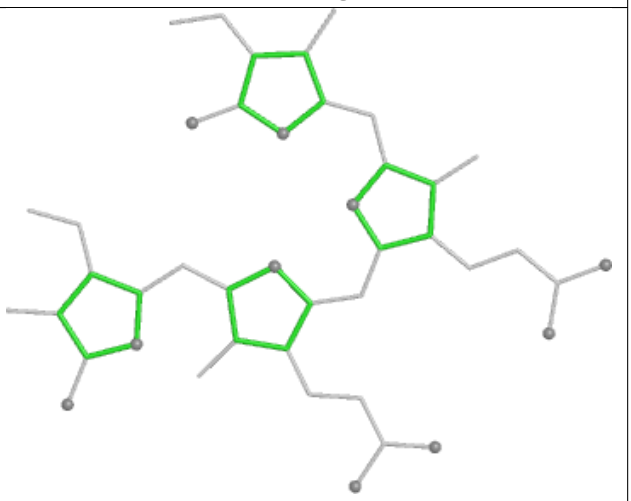

Rings

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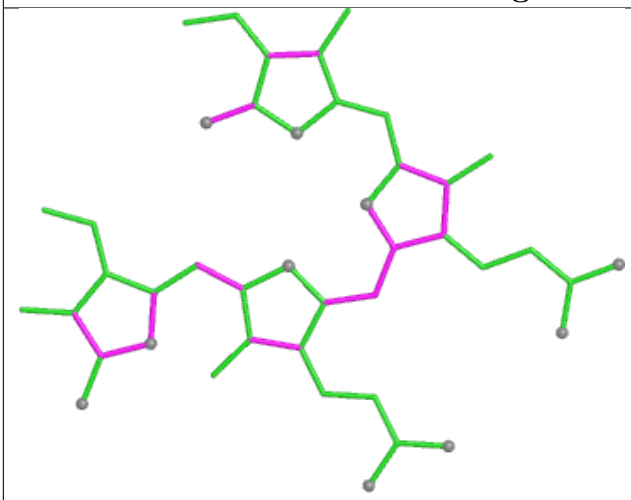
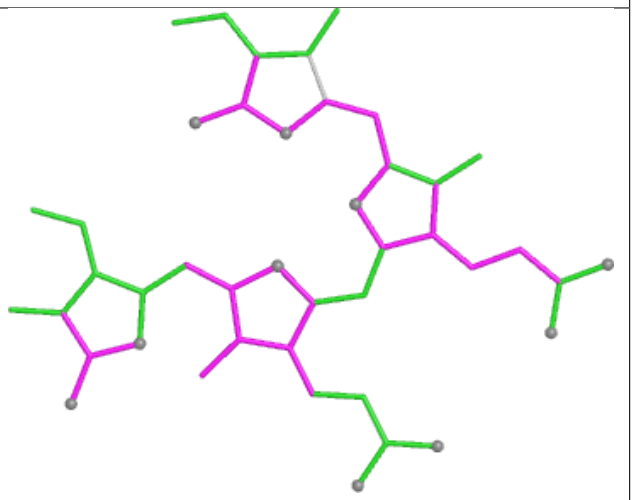


Bond lengths



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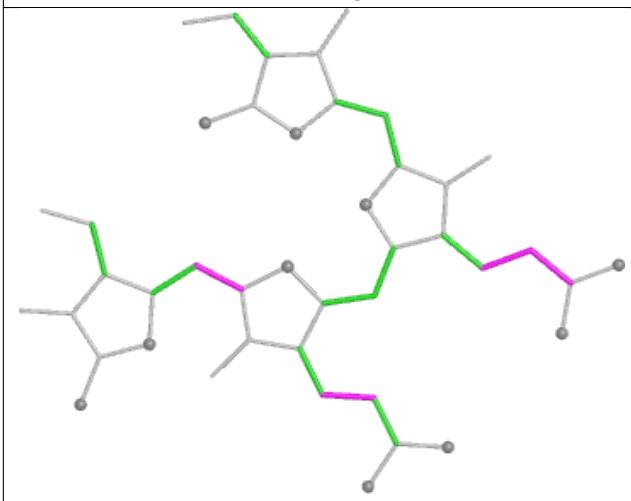

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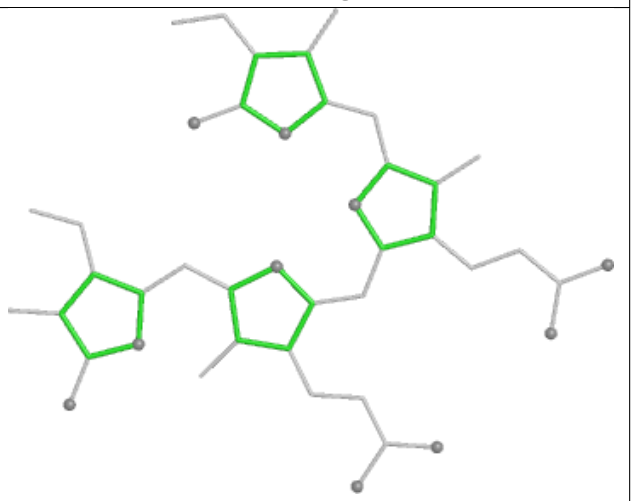
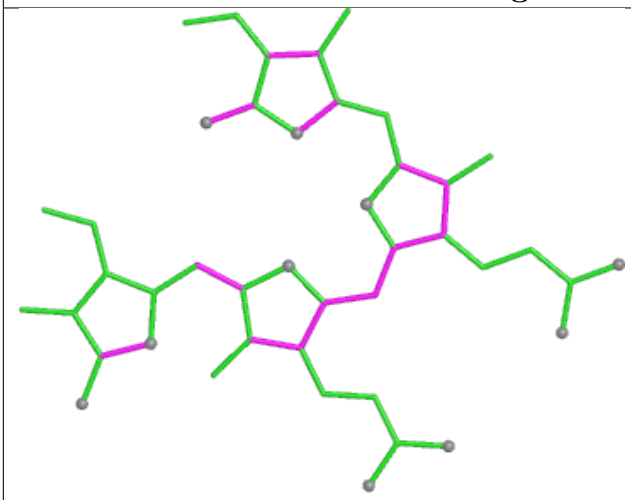


Rings

Ligand PEB DA 202



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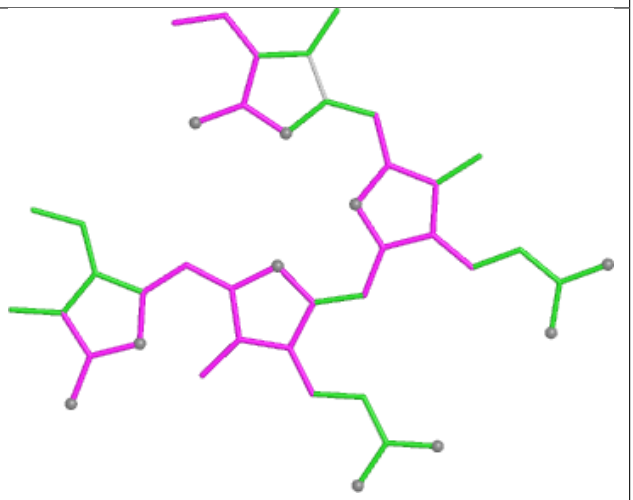

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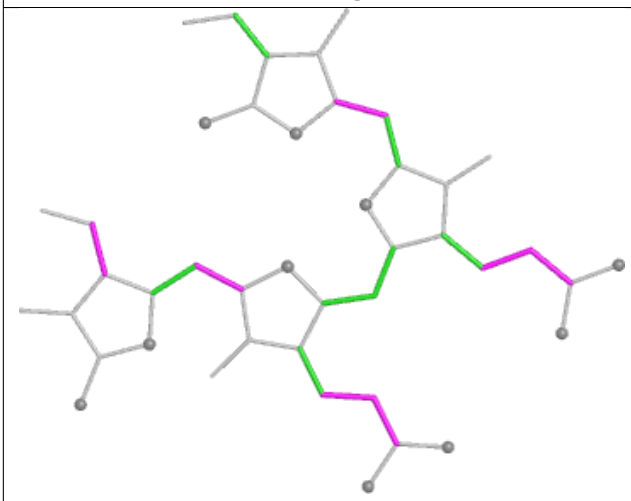

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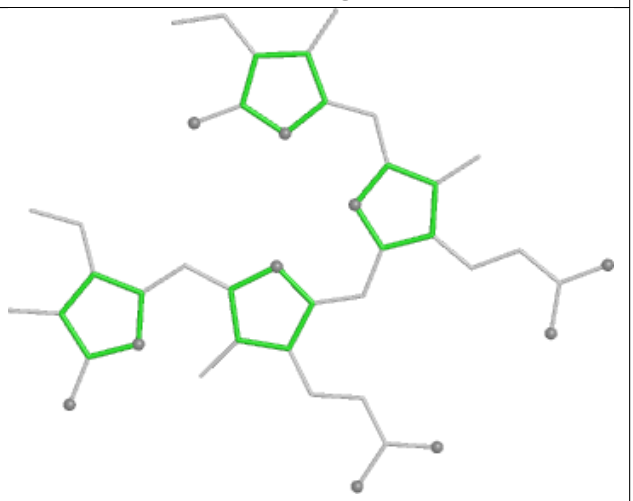

Rings

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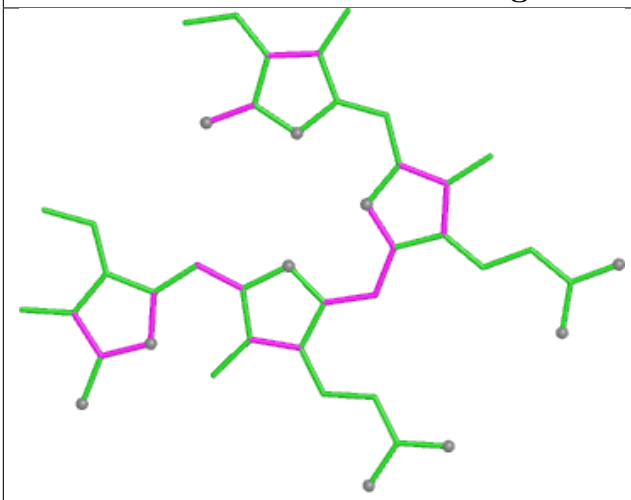

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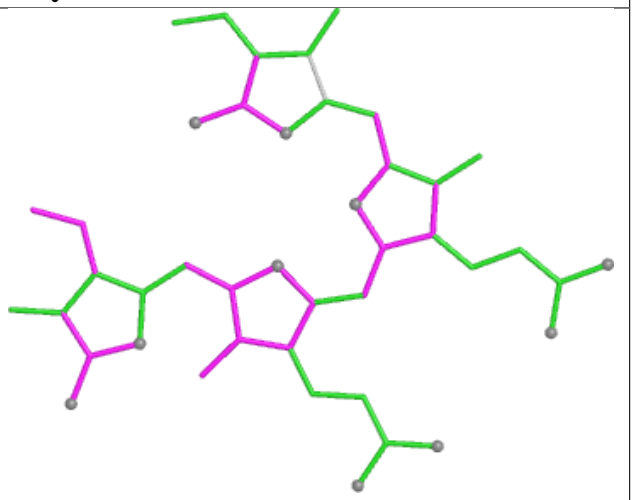

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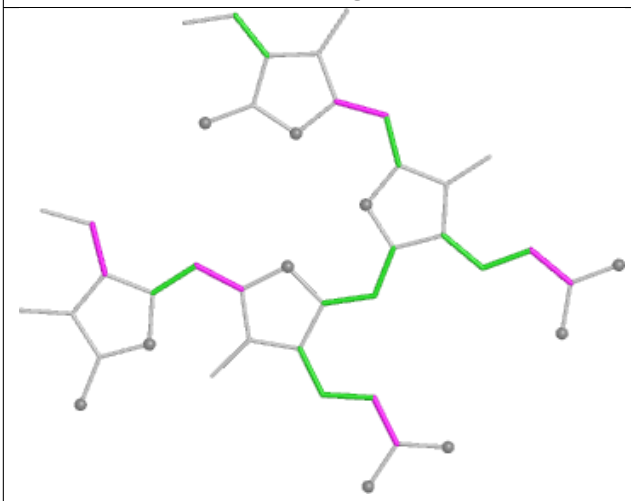

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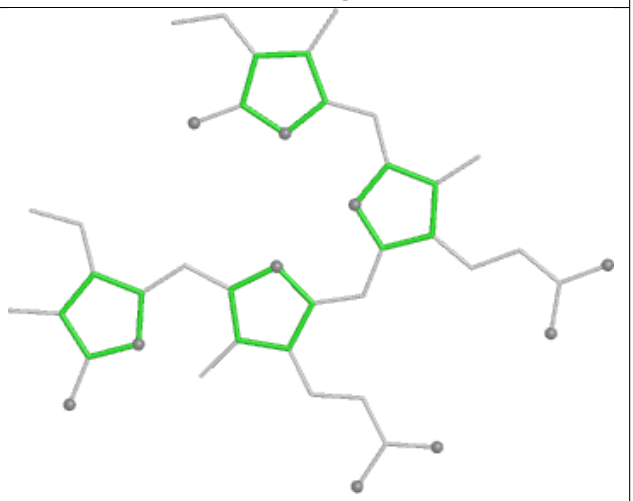

Rings

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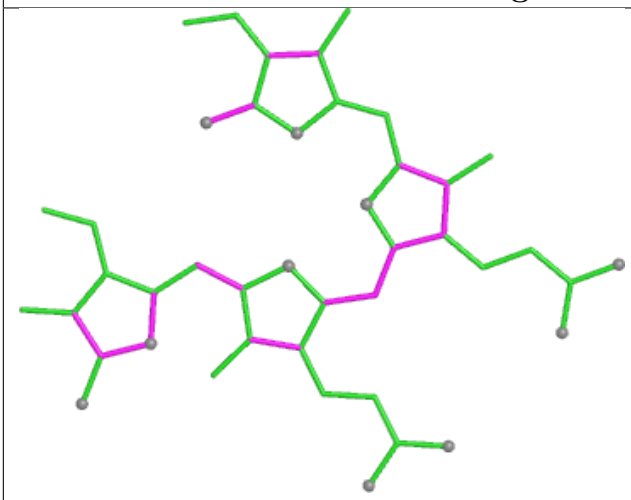

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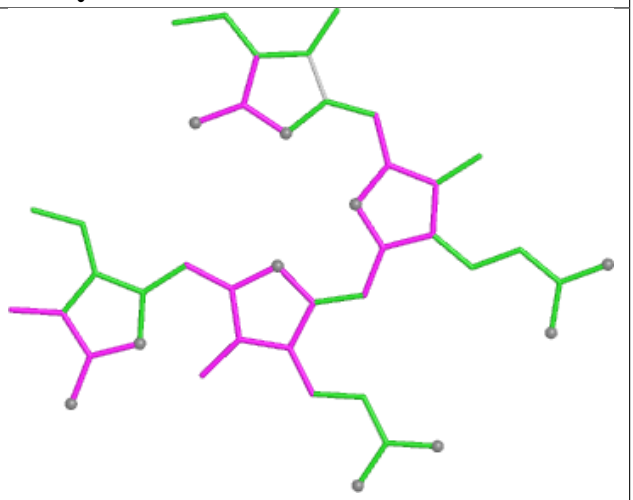

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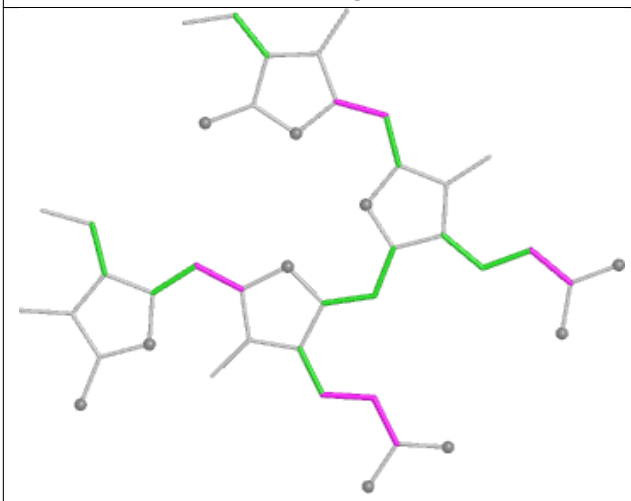

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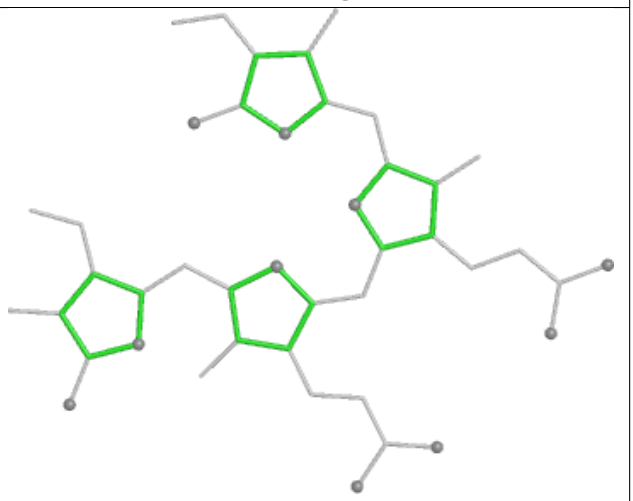
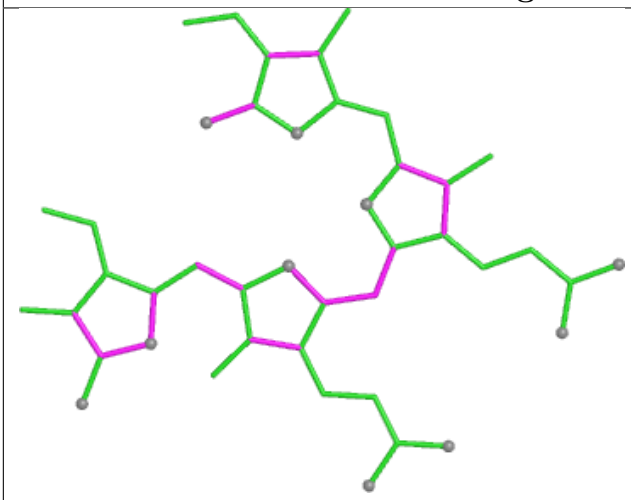


Rings

Ligand PEB IK 203



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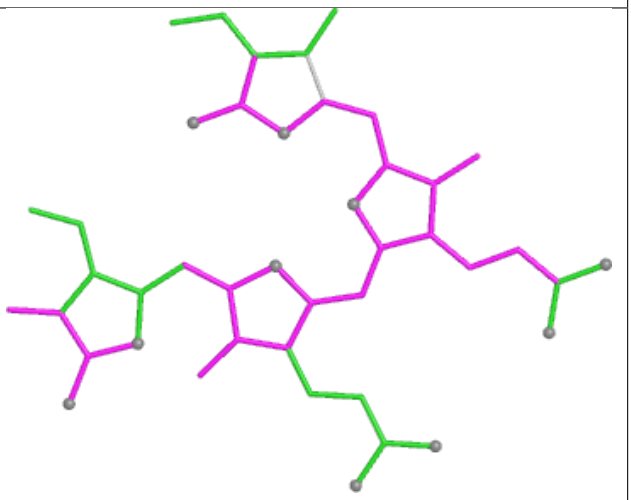

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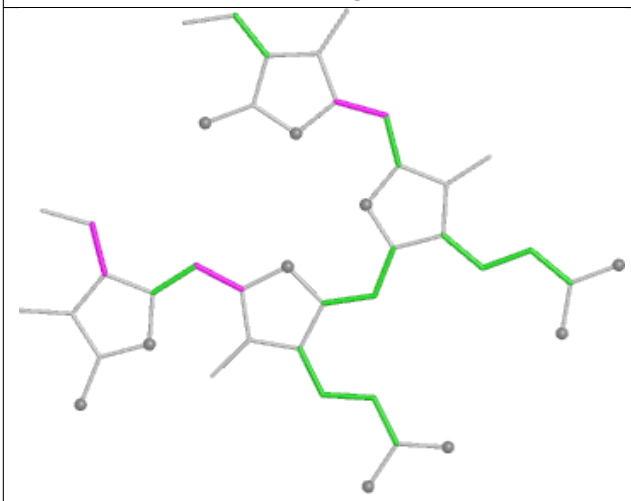

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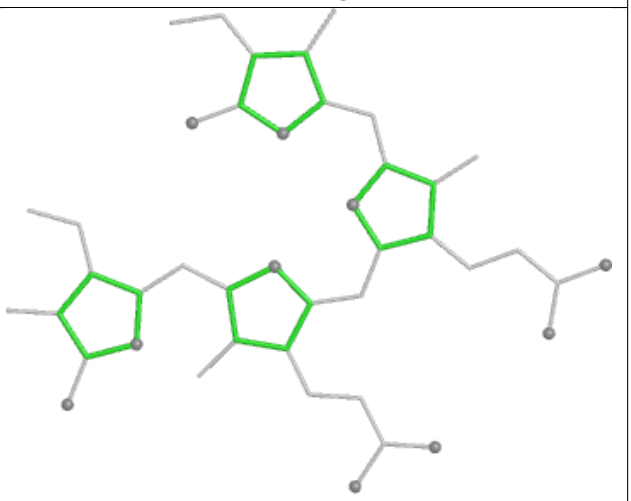

Rings

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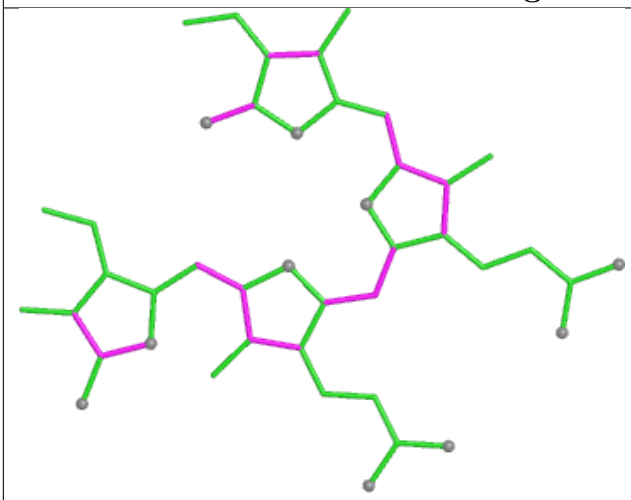

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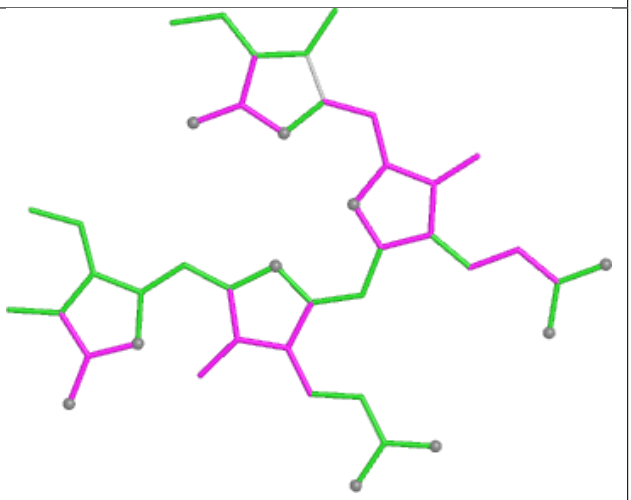

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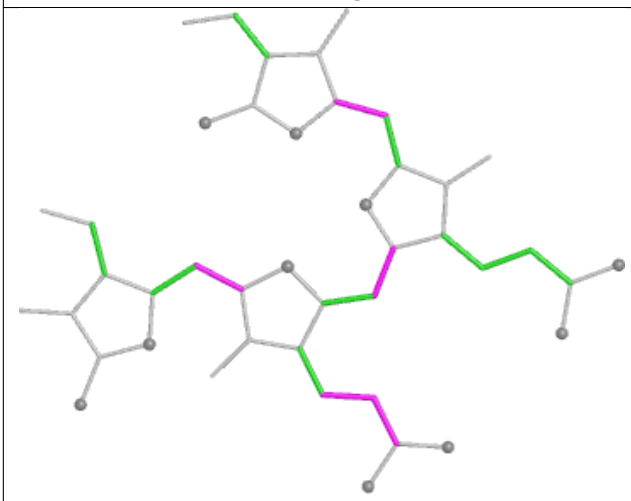

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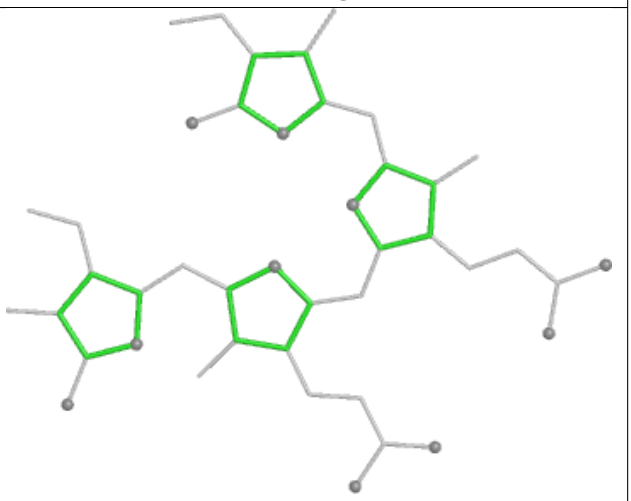

Rings

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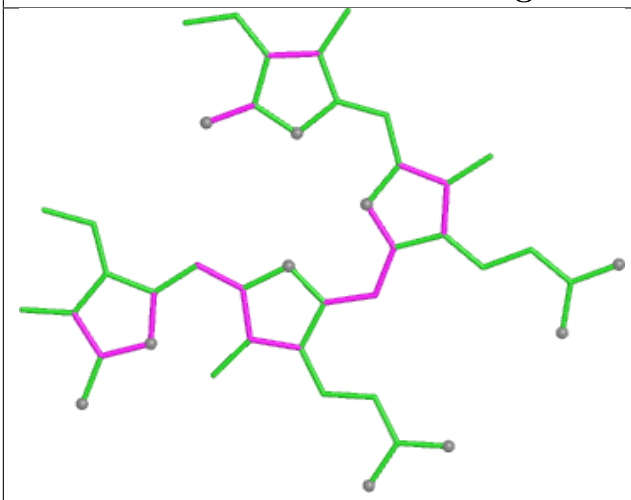

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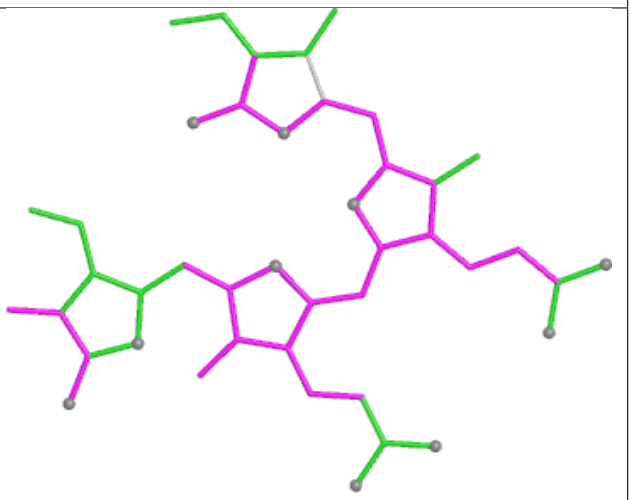
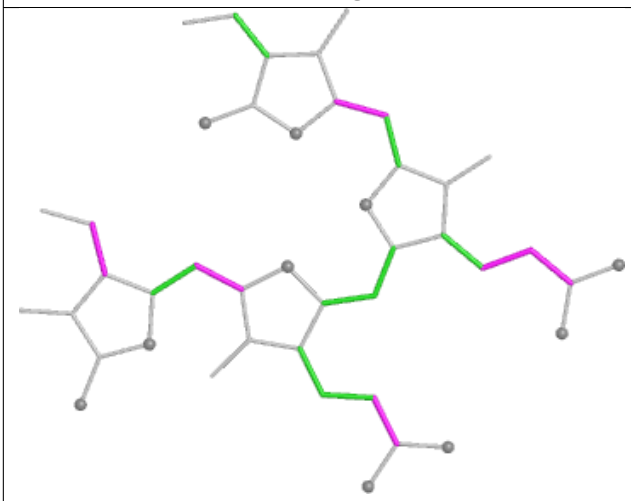


Bond angles



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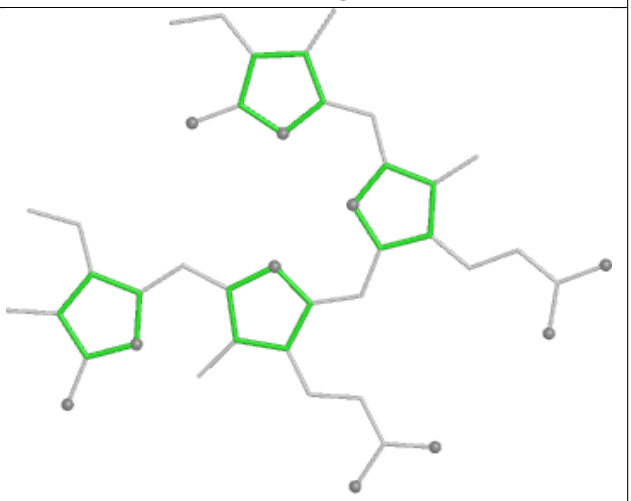
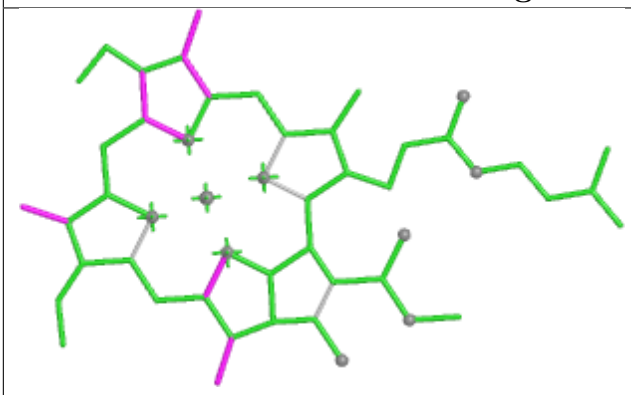


Rings

Ligand CLA O2 202



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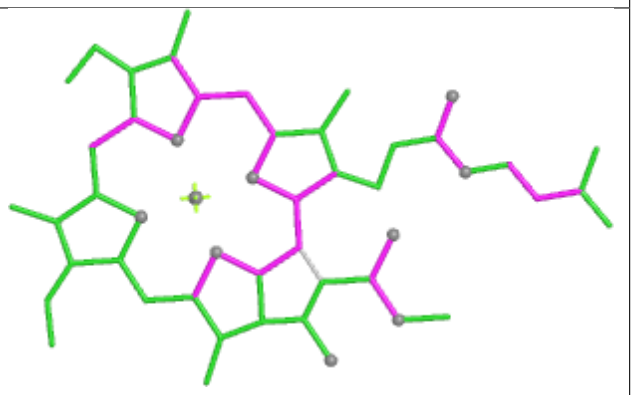

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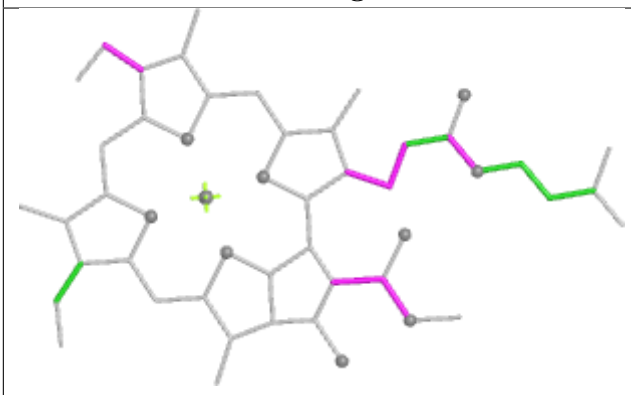

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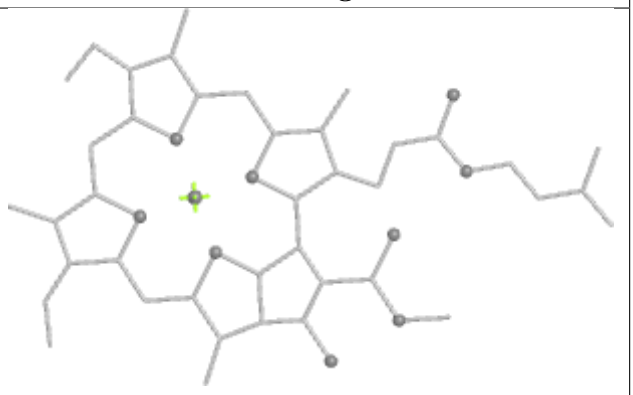
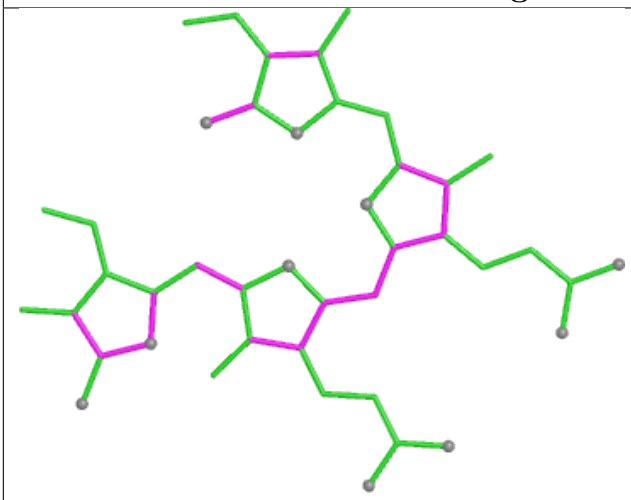


Rings

Ligand PEB dM 202



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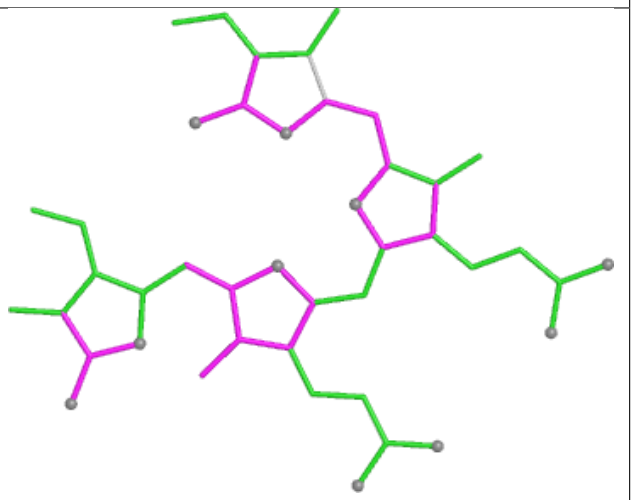

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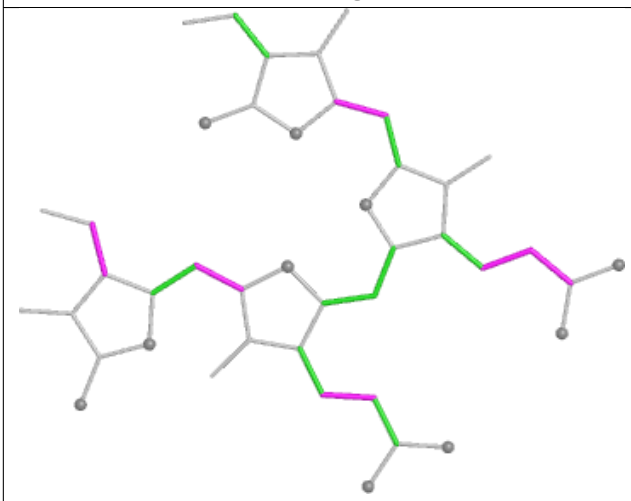

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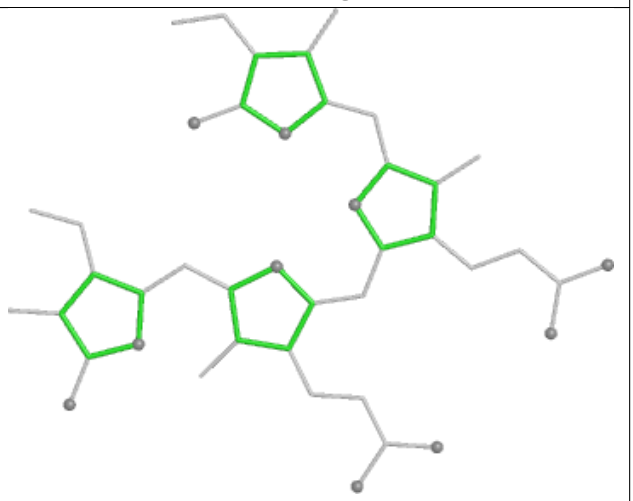
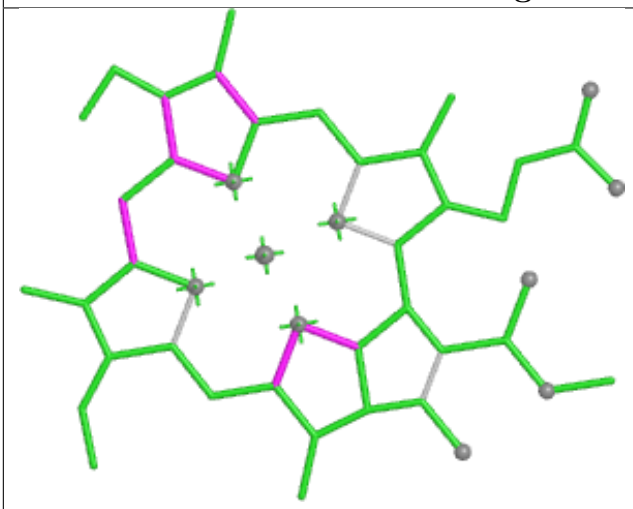


Rings

Ligand CLA 6N 611



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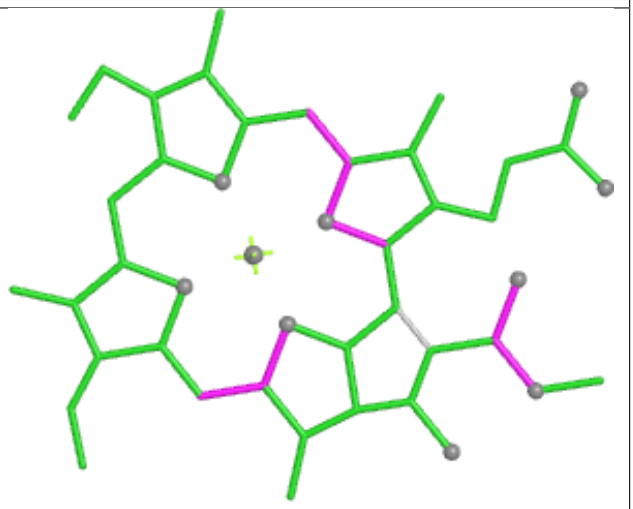

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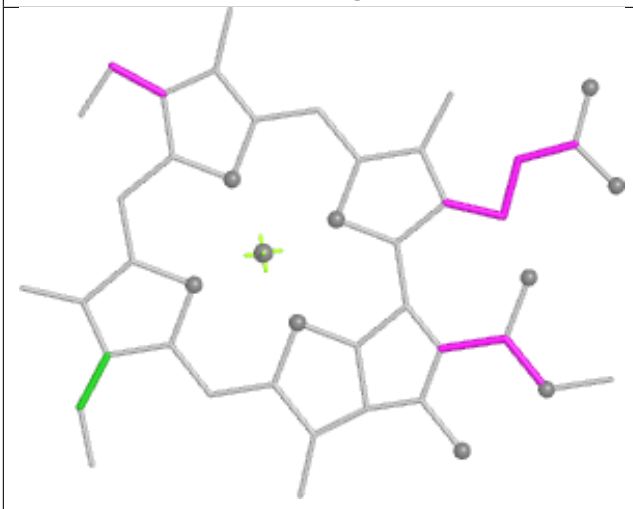
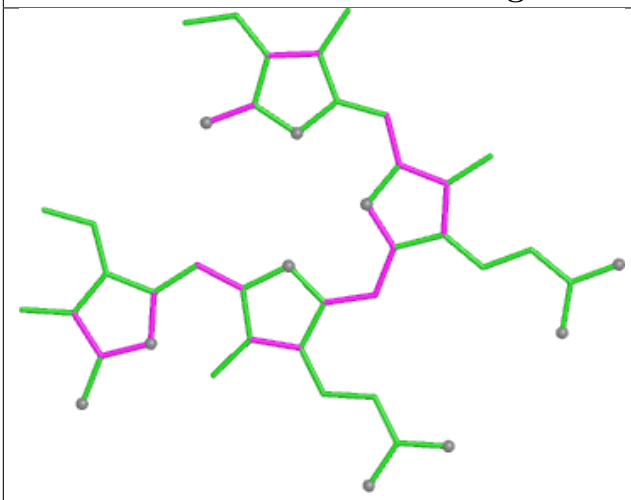


Torsions



Rings

Ligand PEB XM 201



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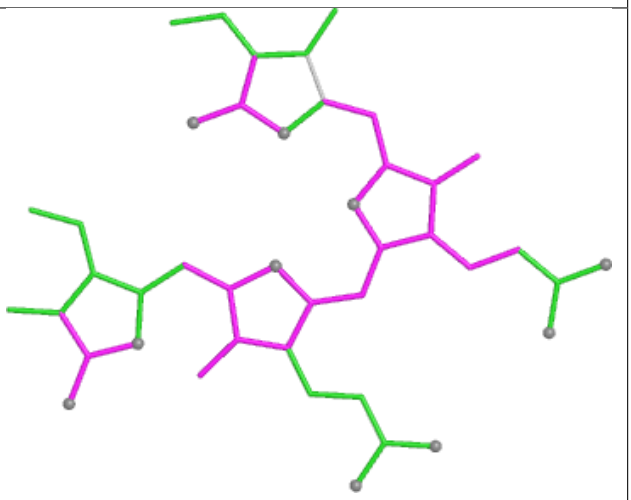

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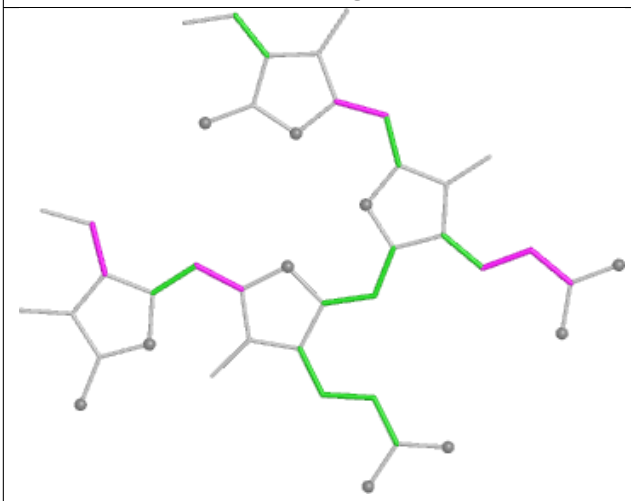

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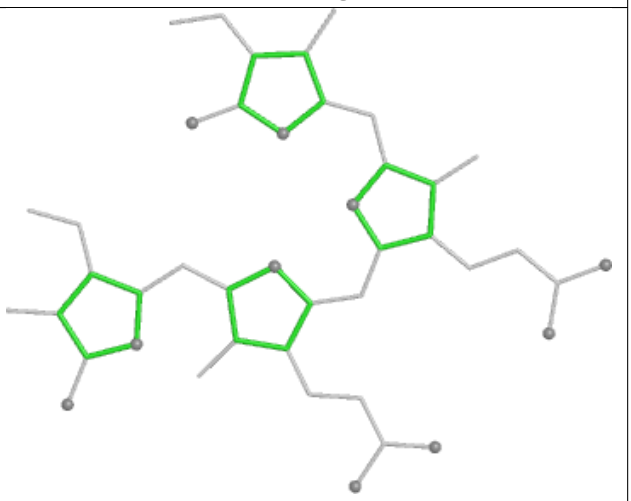
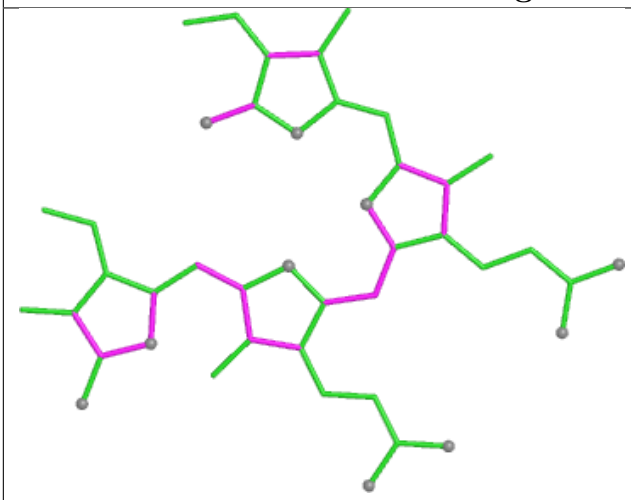


Rings

Ligand PEB XJ 202



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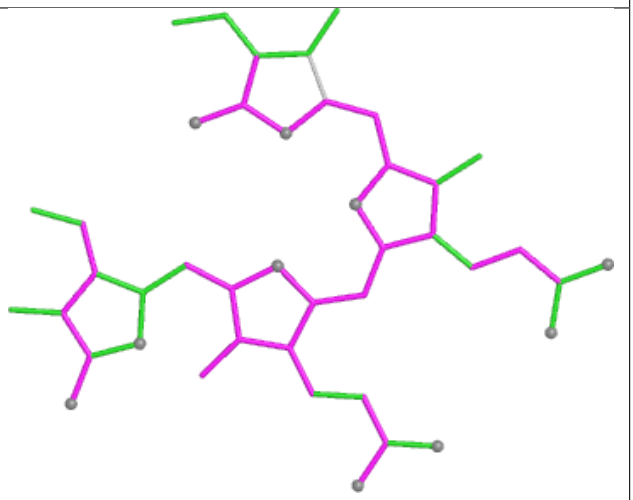

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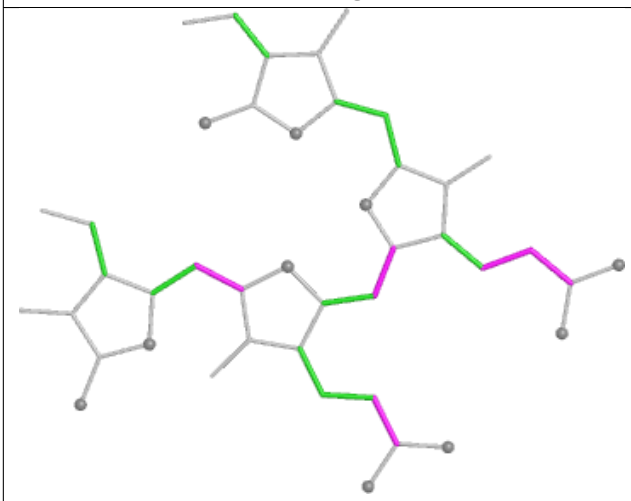

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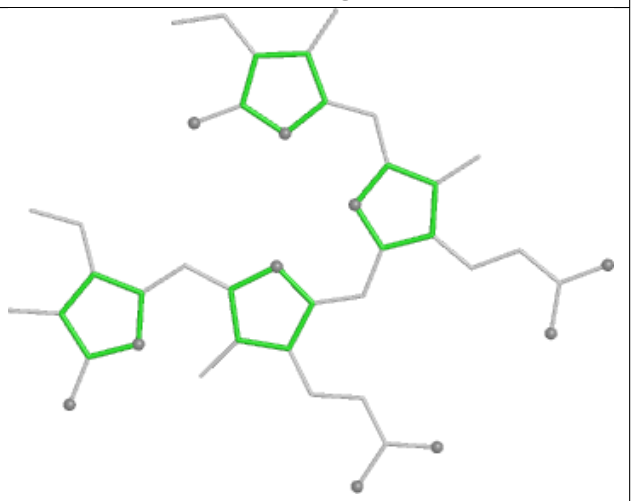
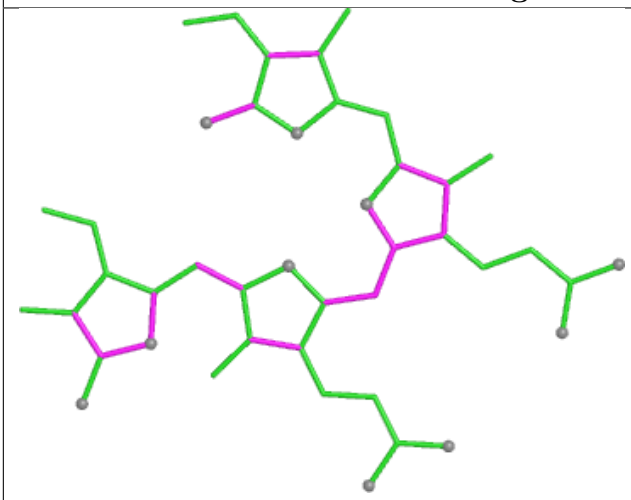


Rings

Ligand PEB RA 203



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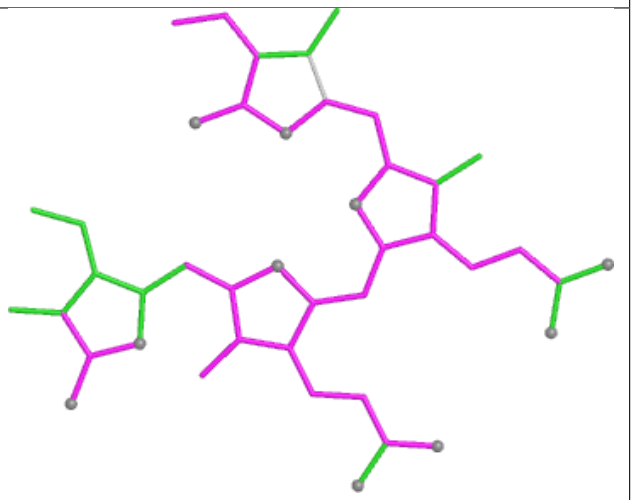
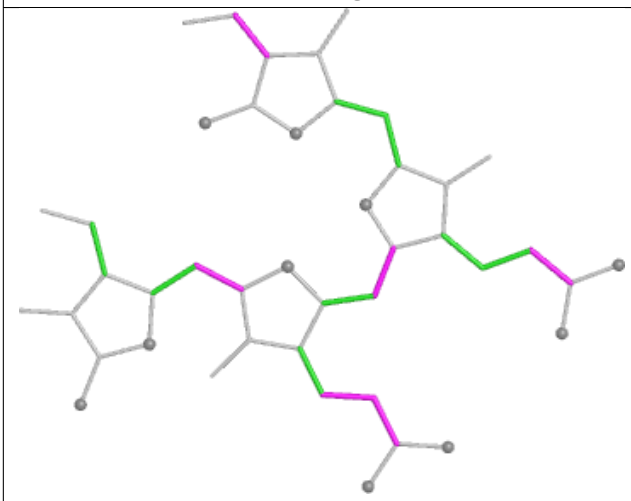


Bond angles



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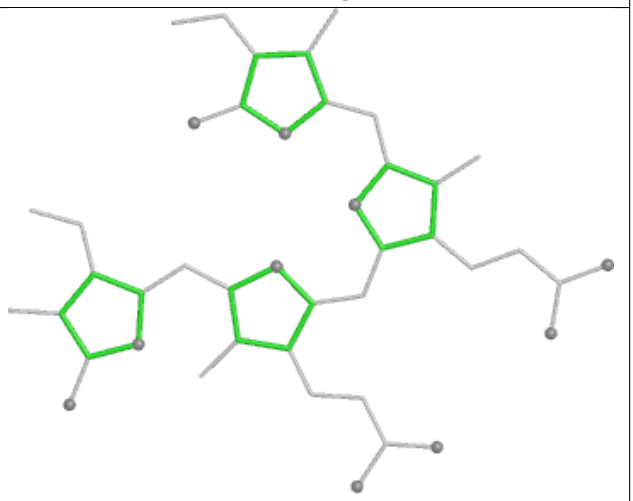

Rings

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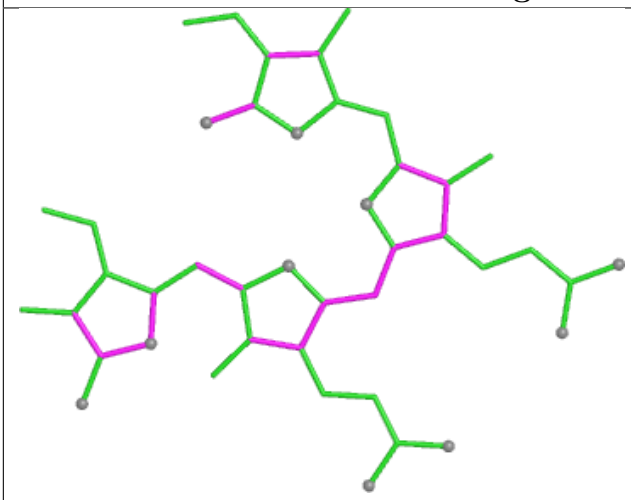

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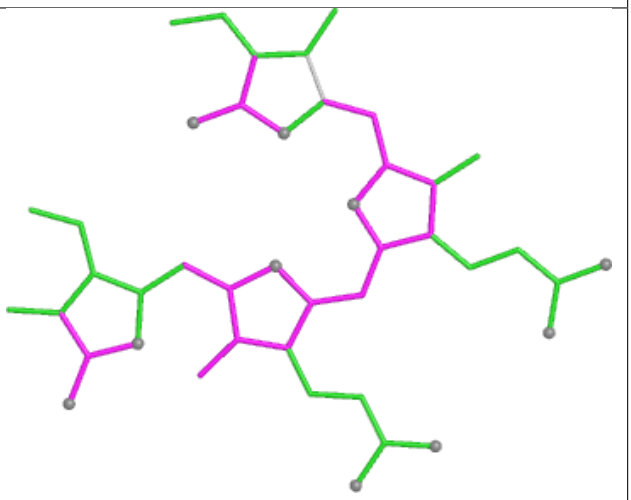
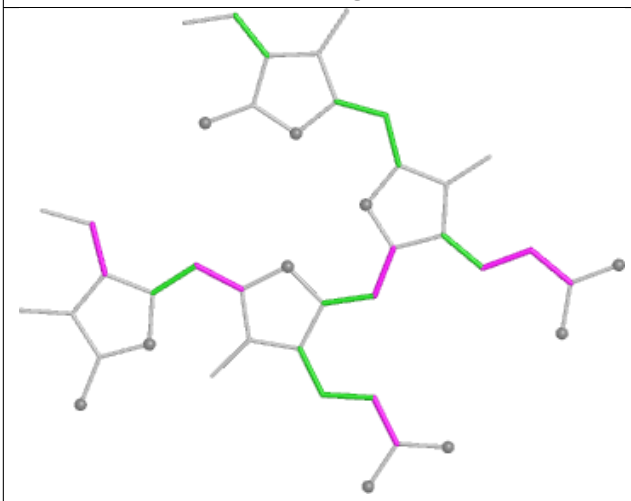


Bond angles



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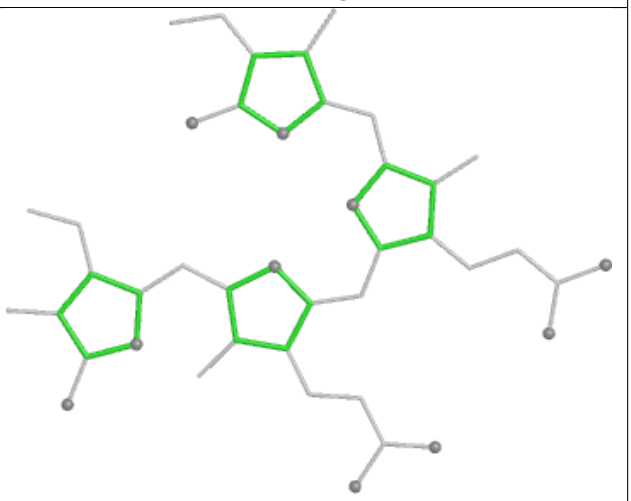
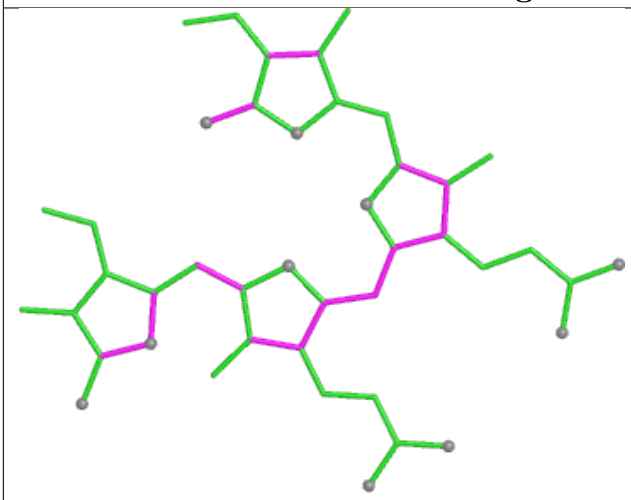


Rings

Ligand PEB O1 202



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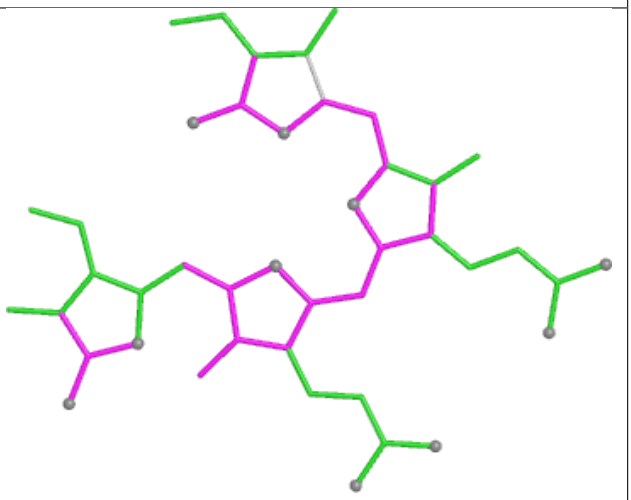
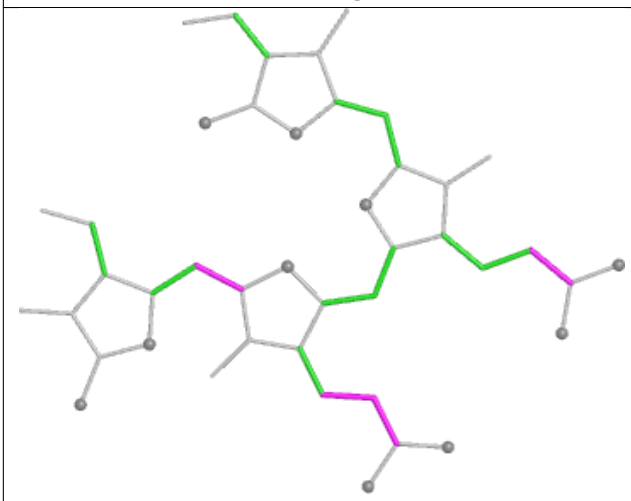


Bond angles



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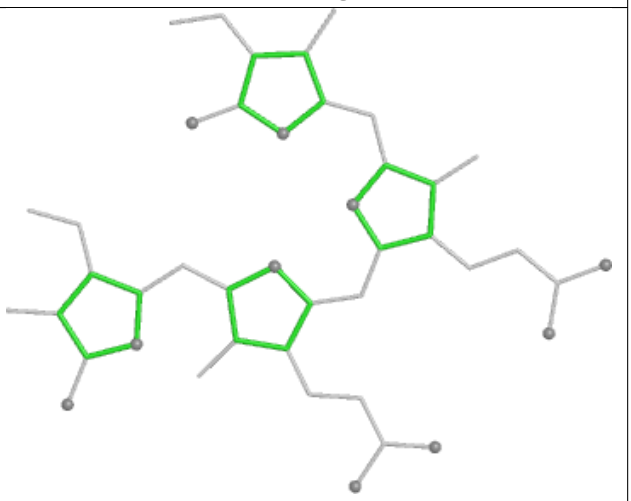
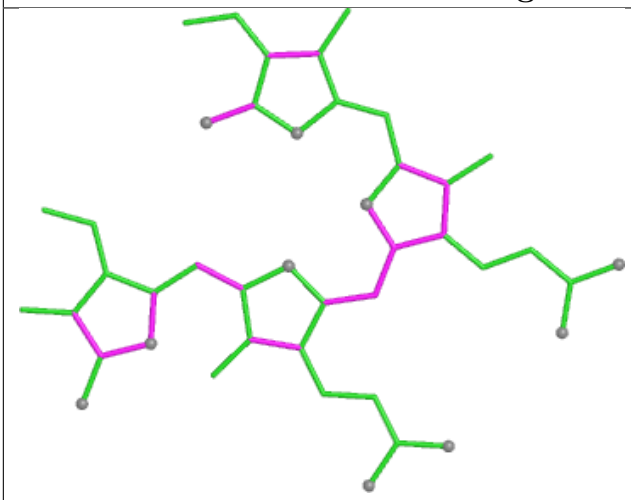


Rings

Ligand PEB yF 301



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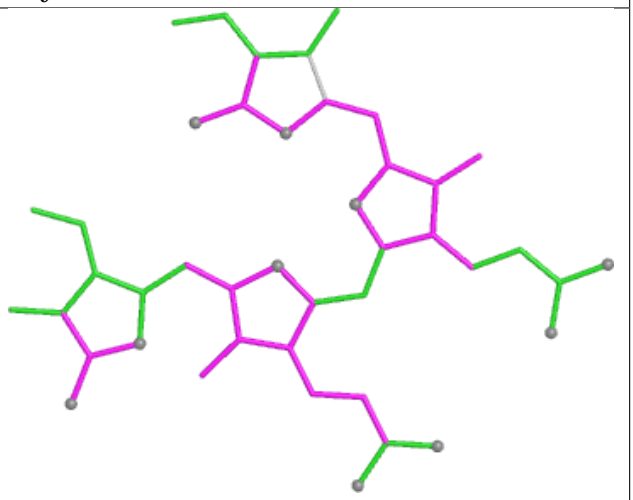

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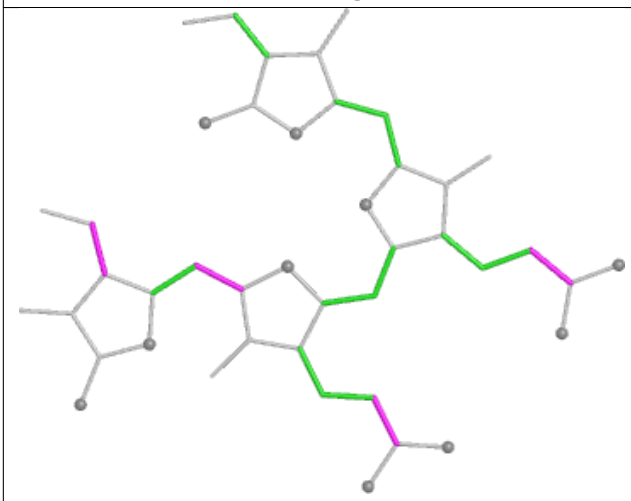

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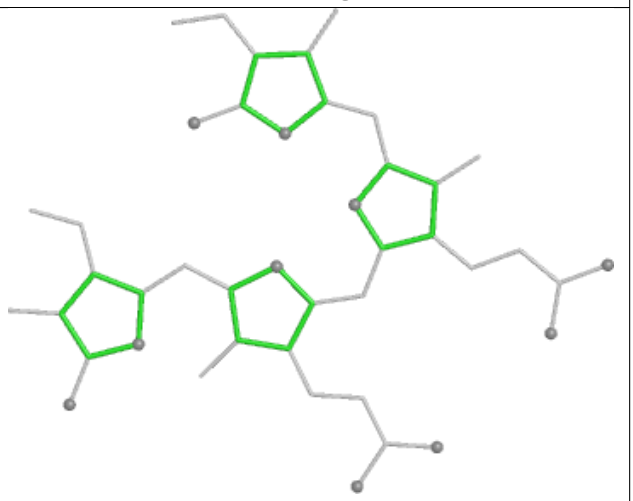
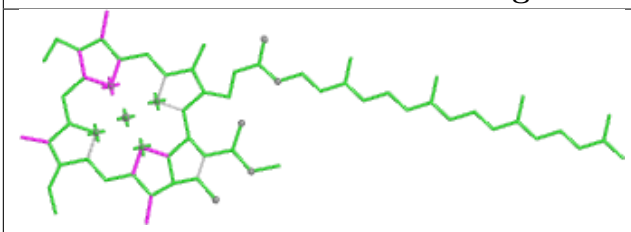


Rings

Ligand CLA HL 101



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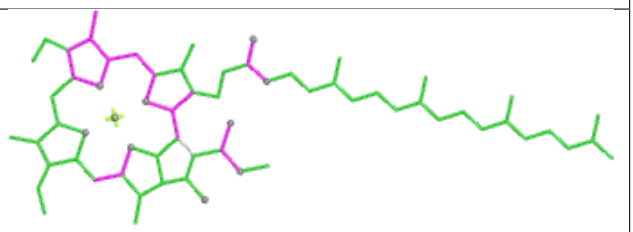

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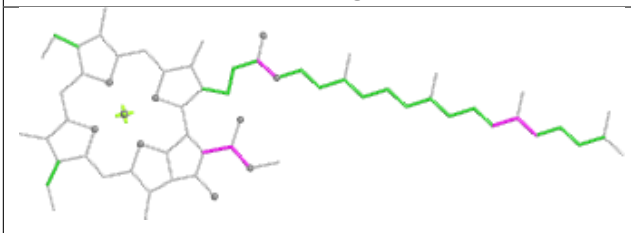

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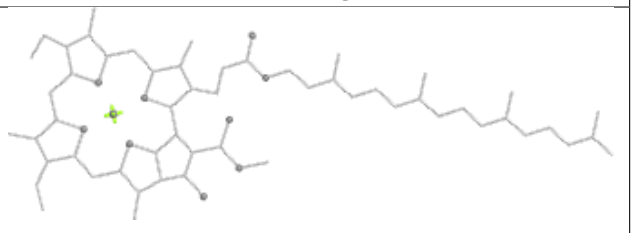
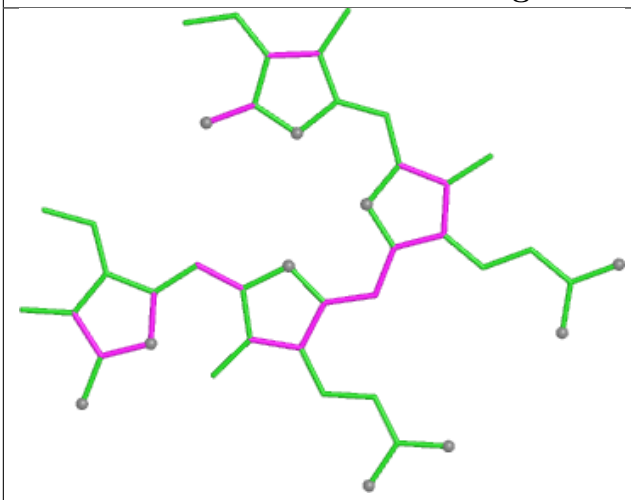


Rings

Ligand PEB OE 203



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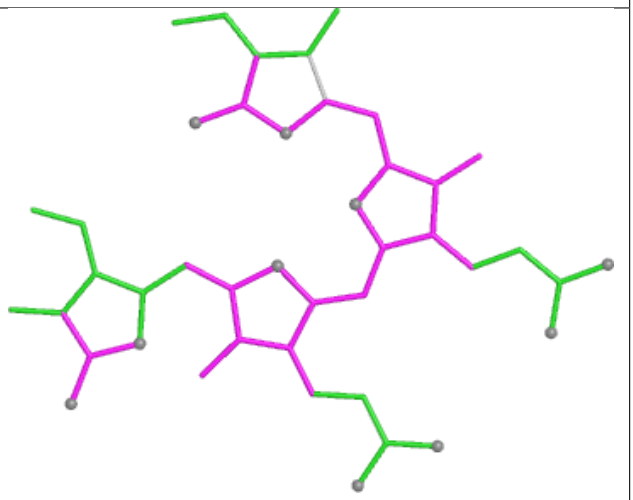

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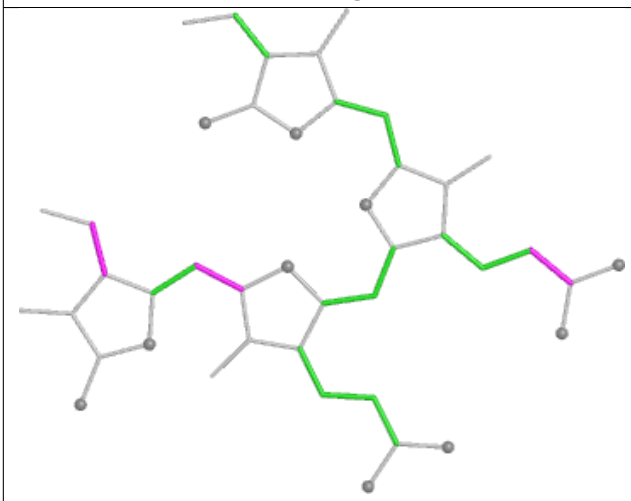

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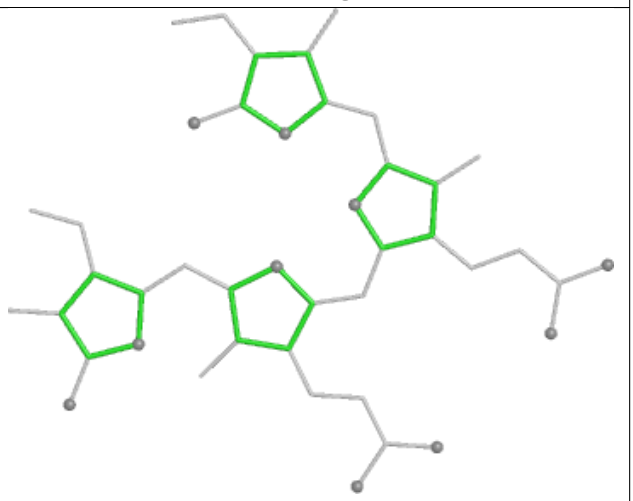
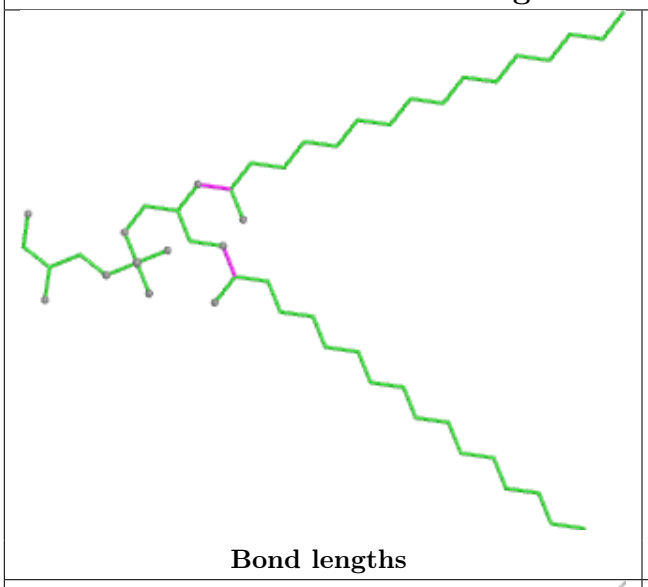


Rings

Ligand LHG BL 610



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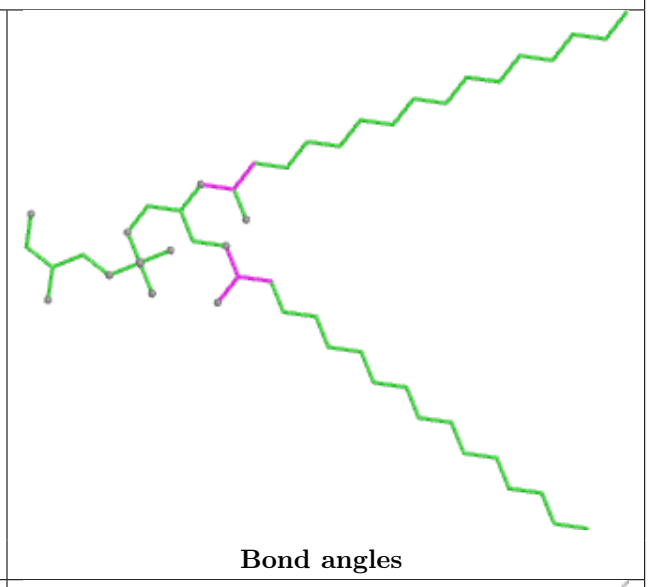

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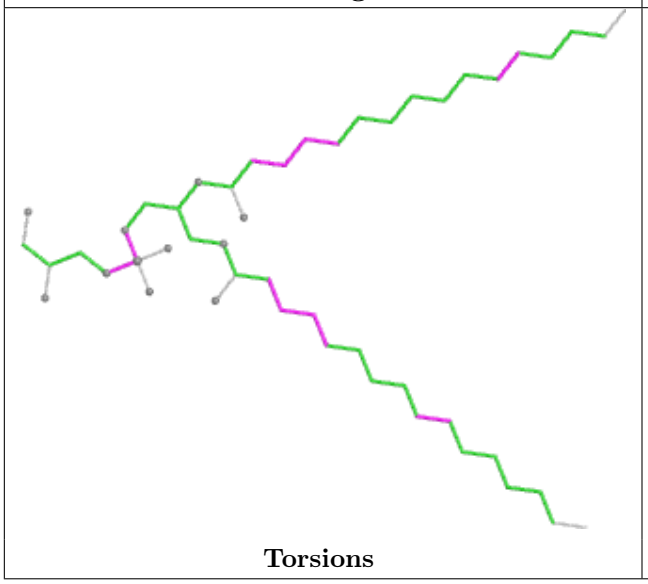

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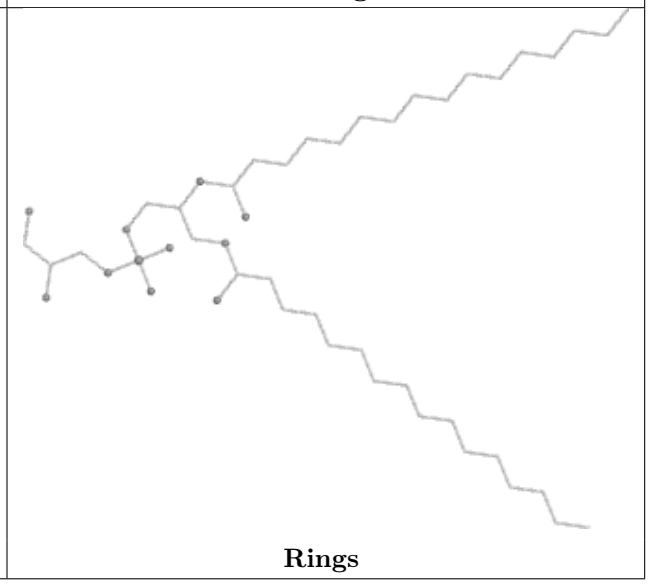
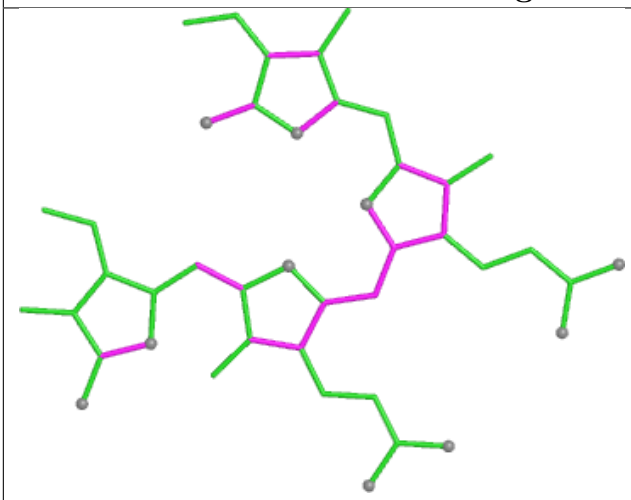


Rings

Ligand PEB A9 201



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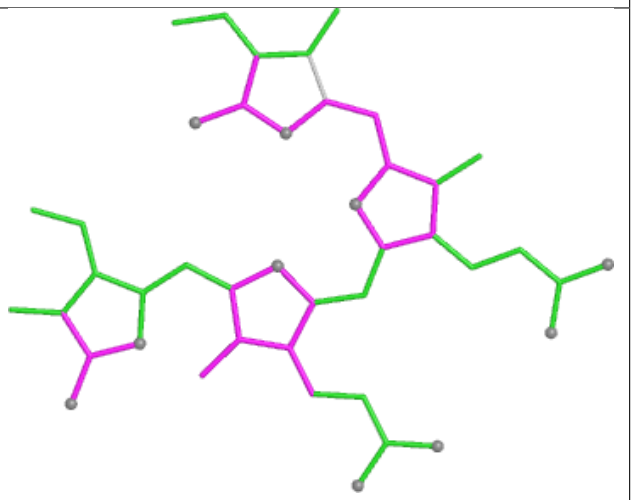

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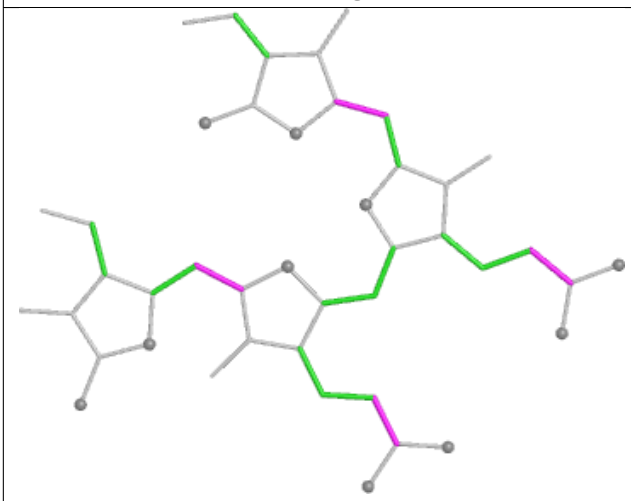

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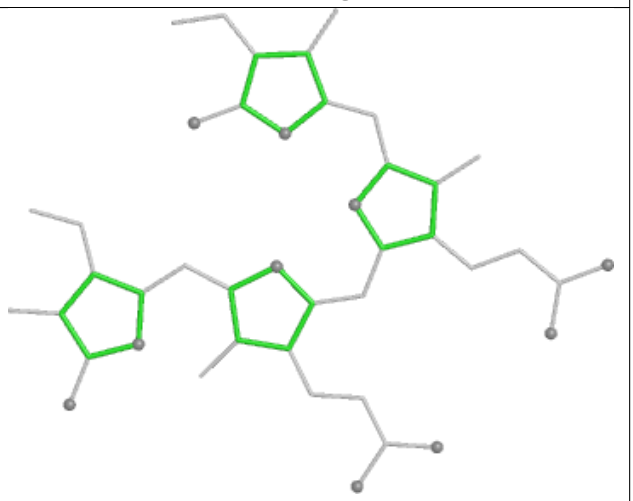
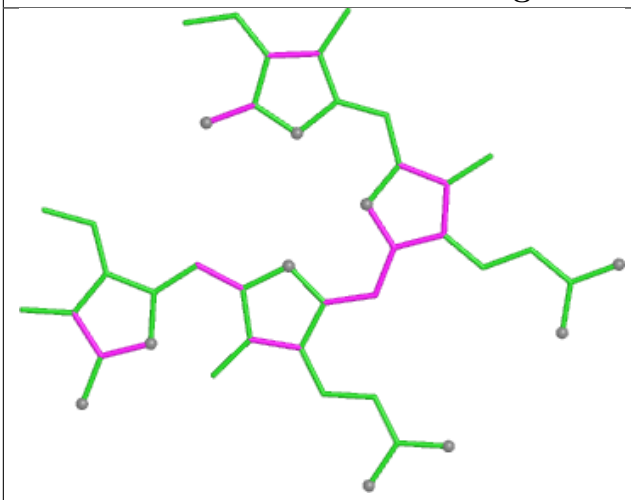


Rings

Ligand PEB wF 301



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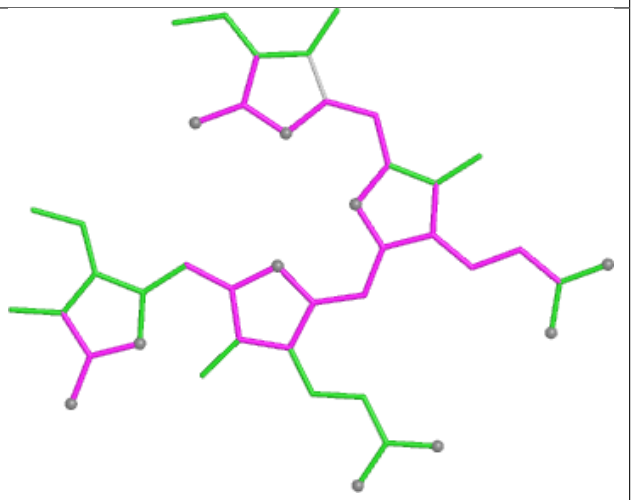

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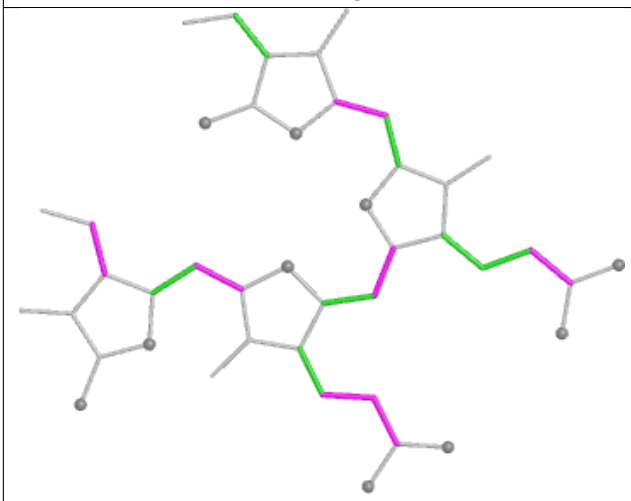

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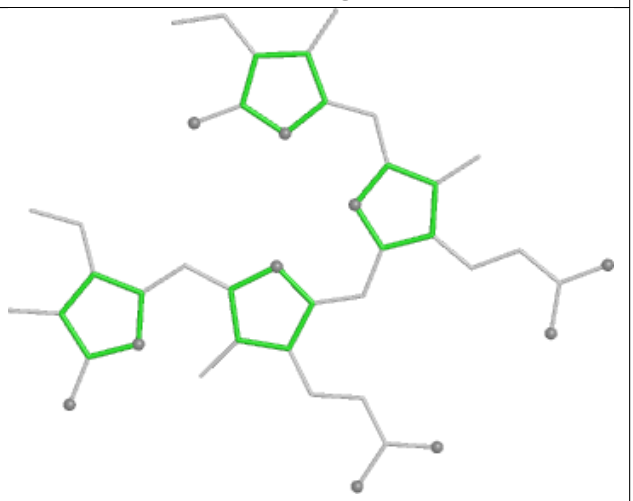
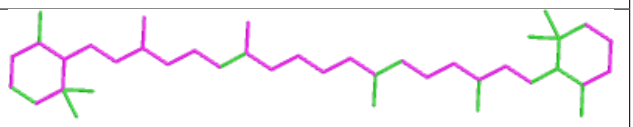


Rings

Ligand BCR FN 202



Bond lengths



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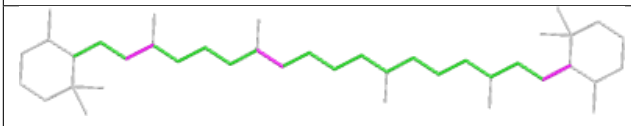

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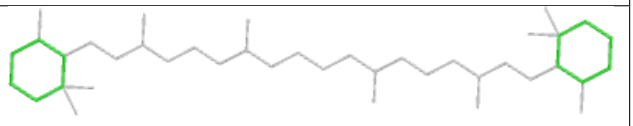
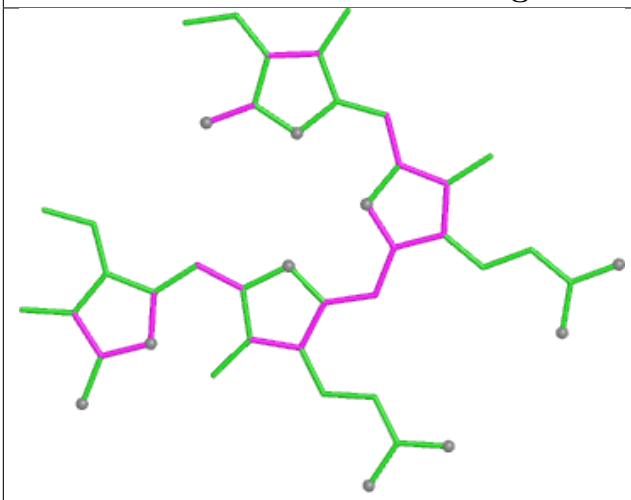


Rings

Ligand PEB PK 202



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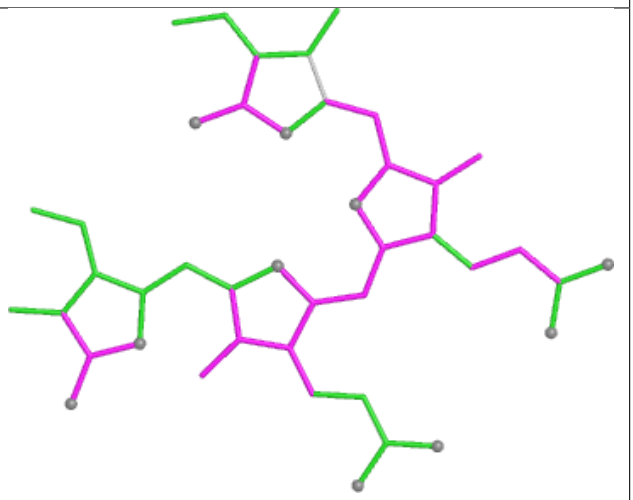

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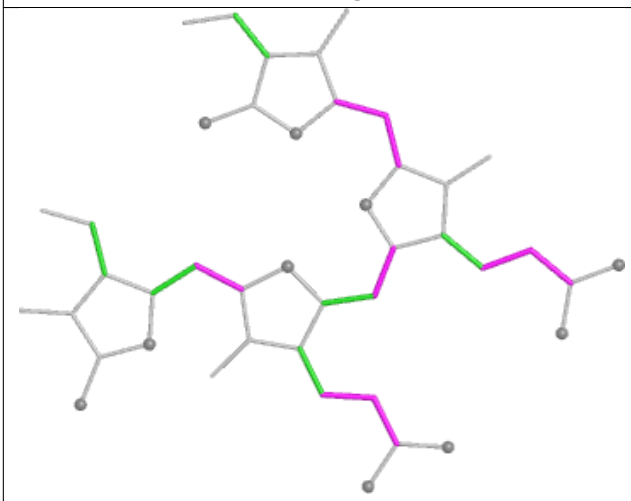

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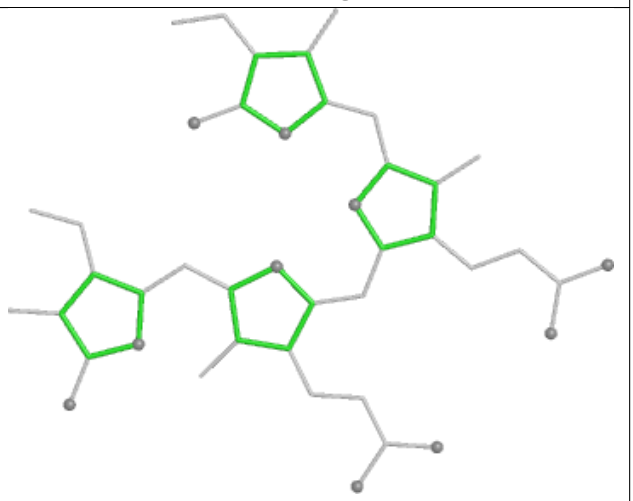
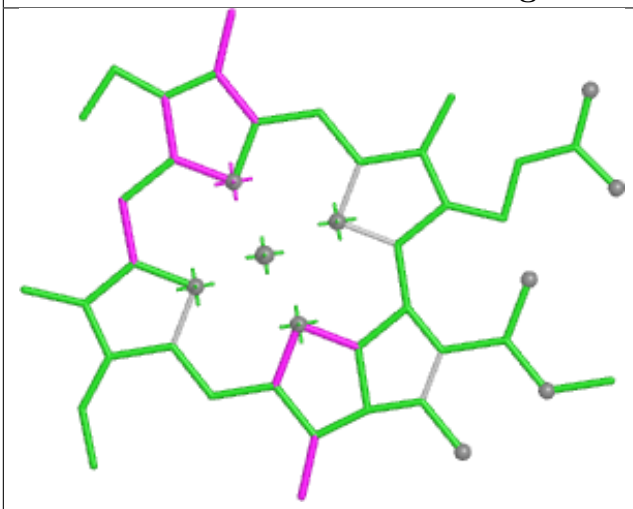


Rings

Ligand CLA 62 308



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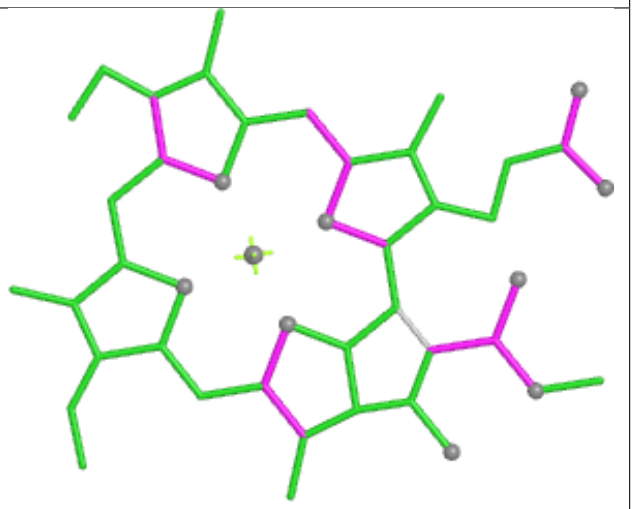

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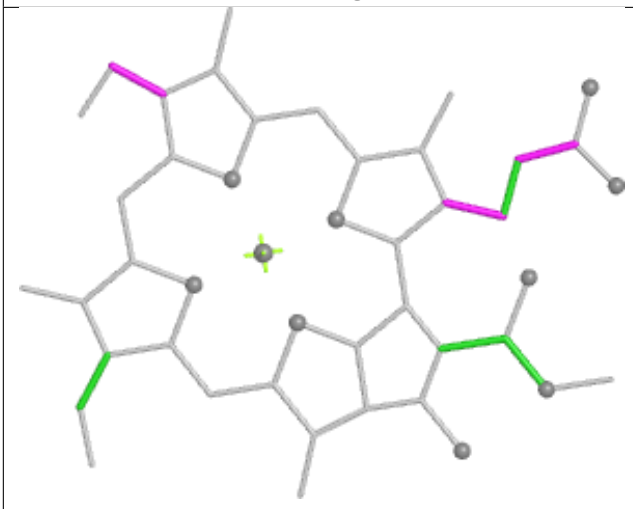
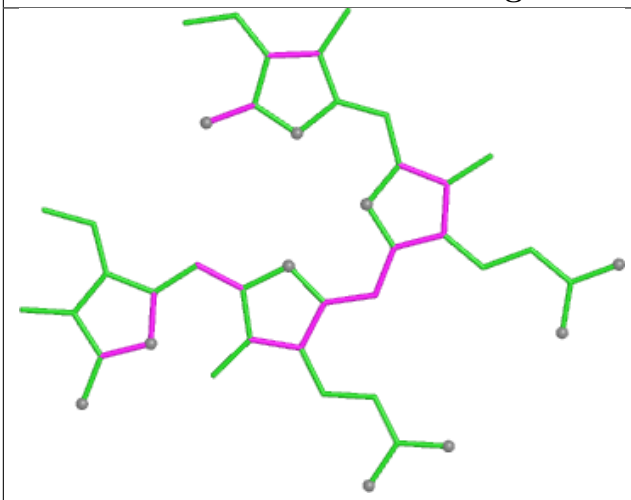


Torsions



Rings

Ligand PEB WK 203



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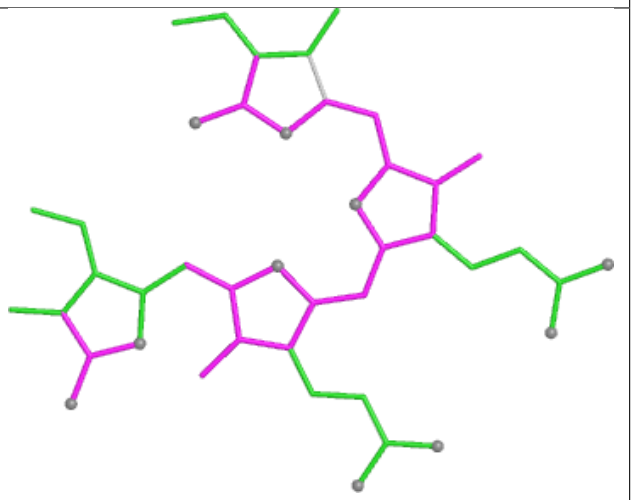

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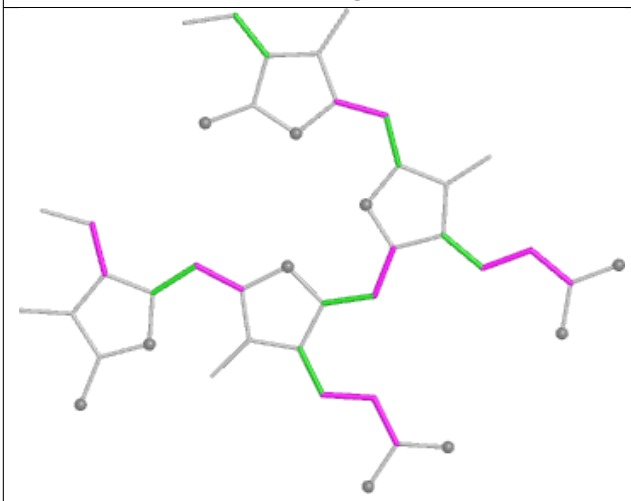

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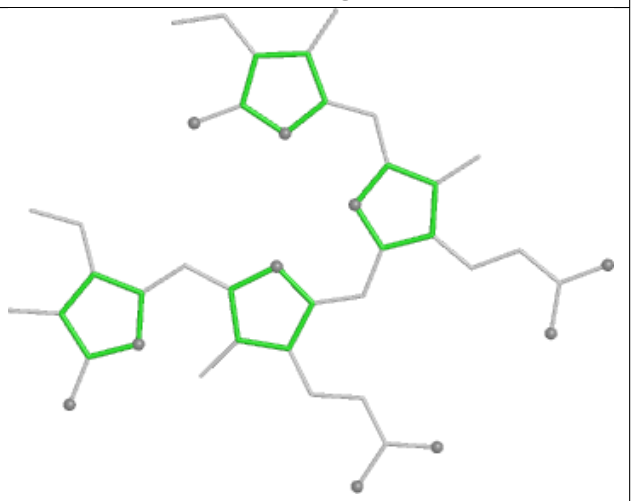
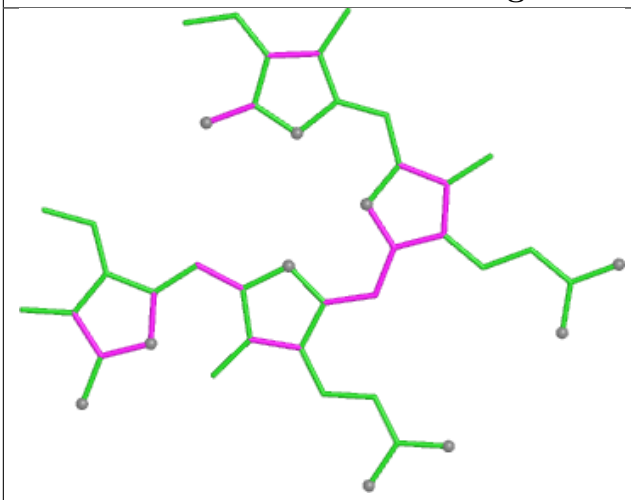


Rings

Ligand PEB MQ 201



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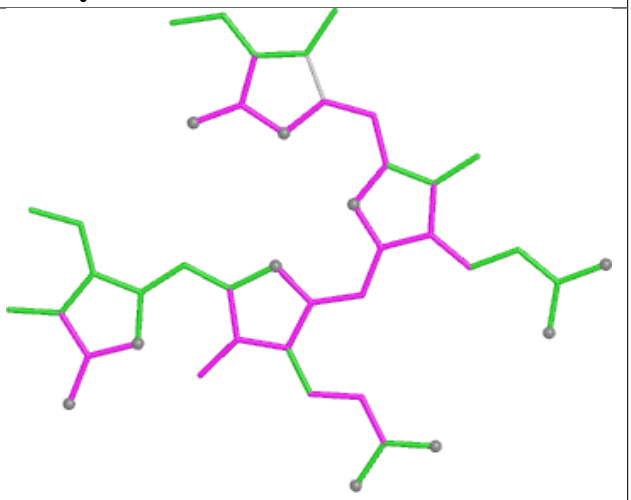

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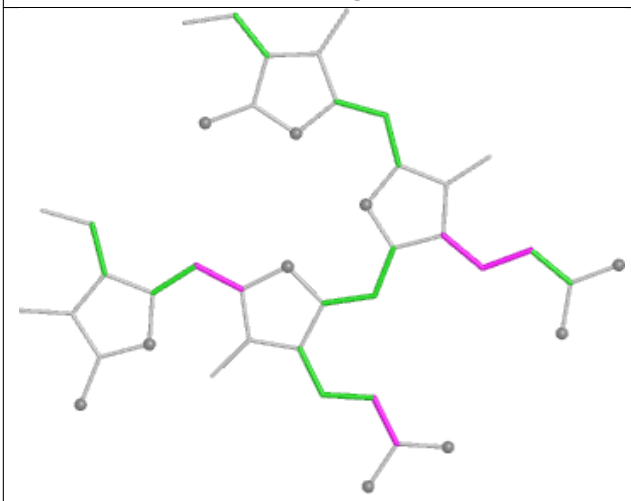

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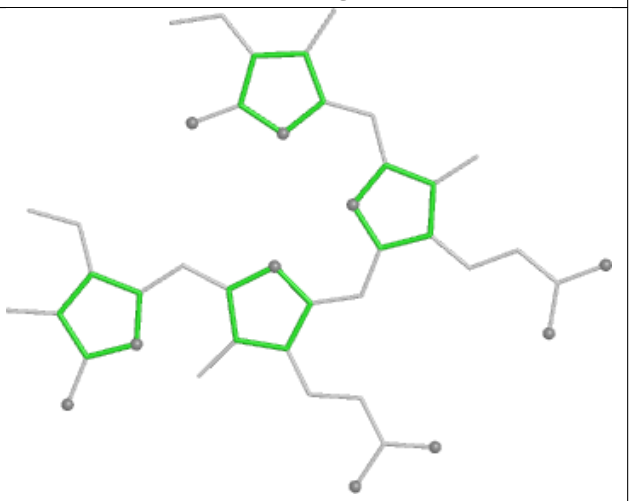
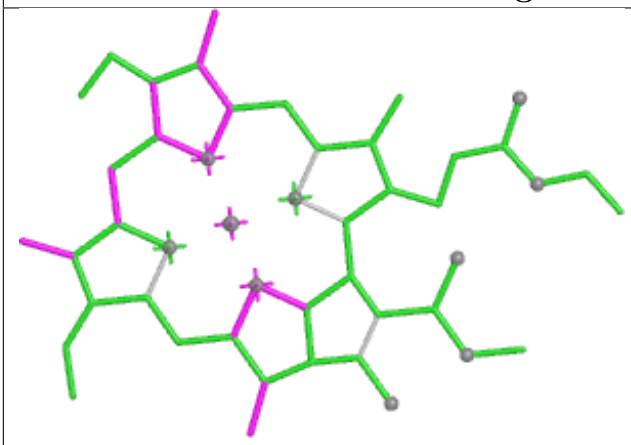


Rings

Ligand CLA B2 833



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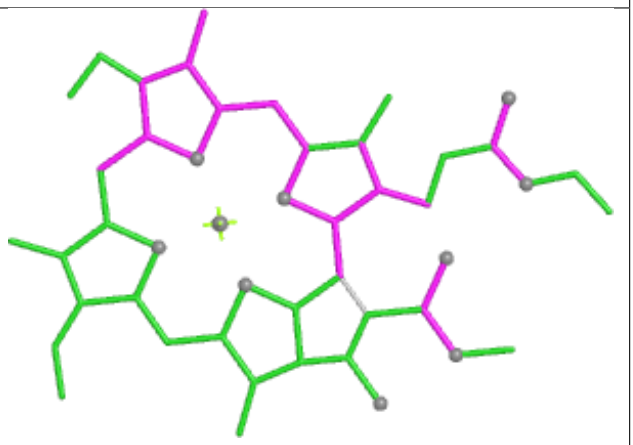

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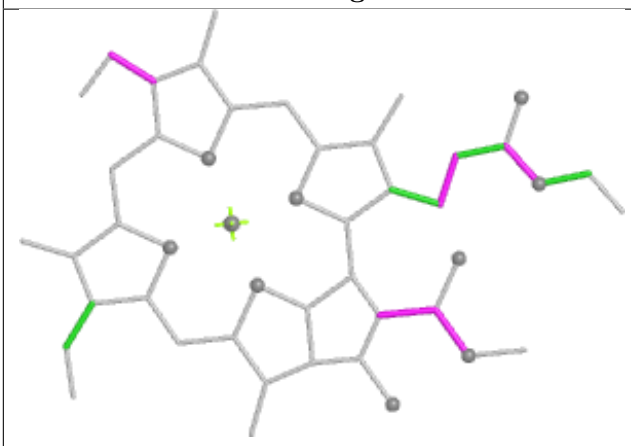

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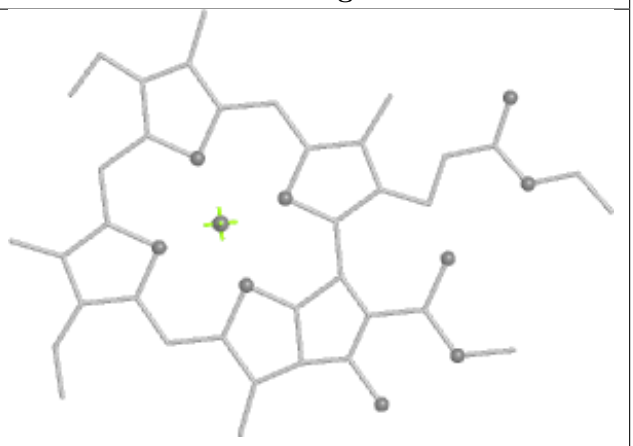
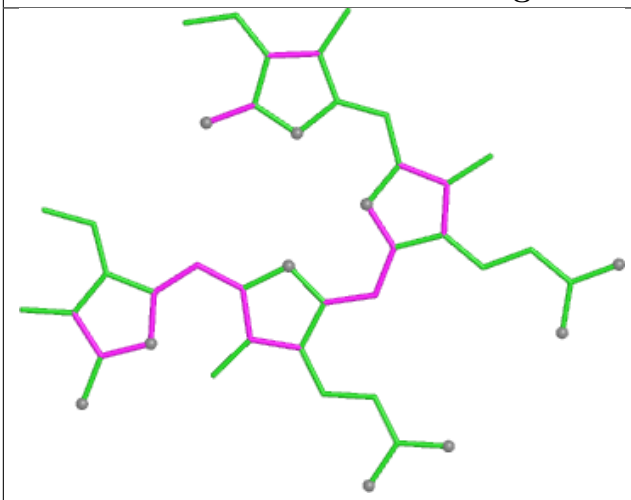


Rings

Ligand PEB ZO 201



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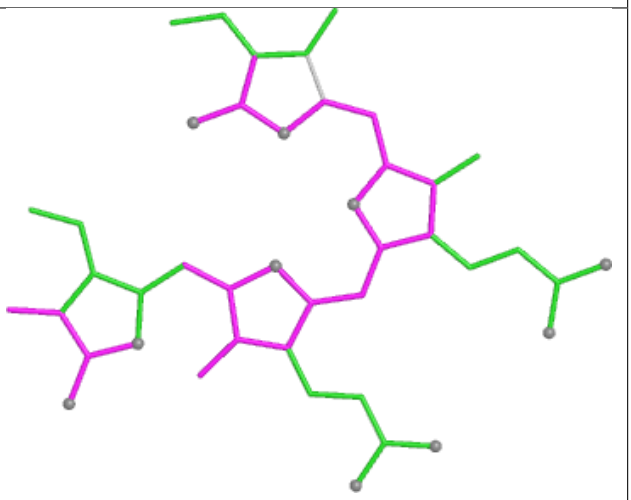
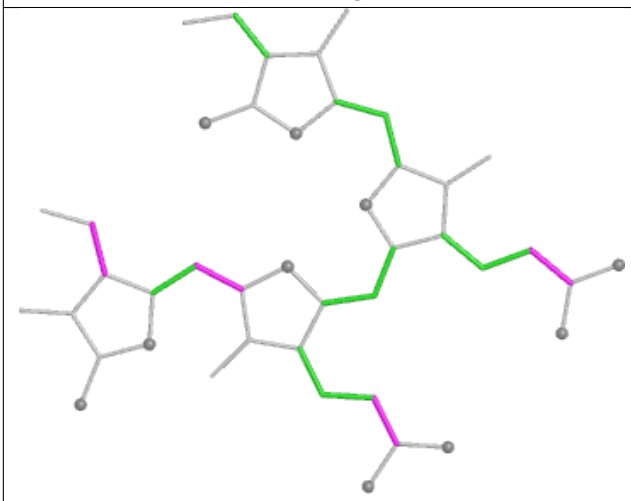


Bond angles



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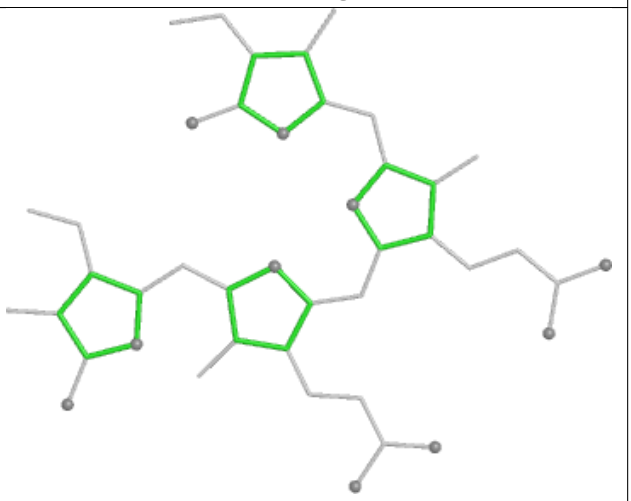
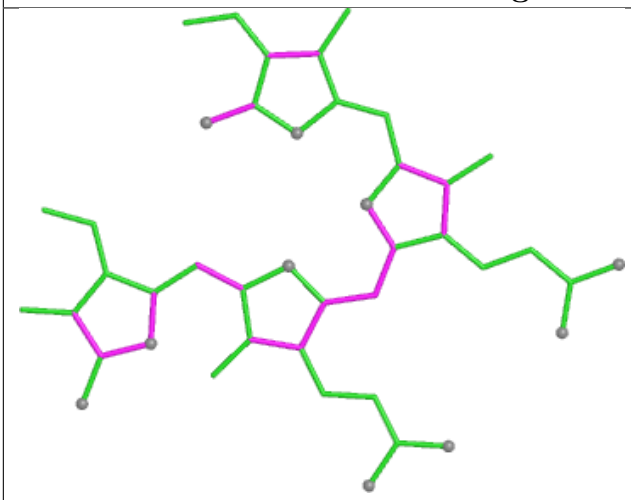


Rings

Ligand PEB M5 305



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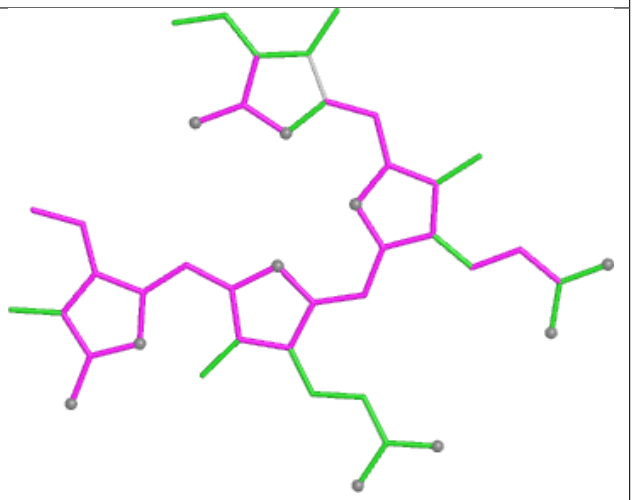
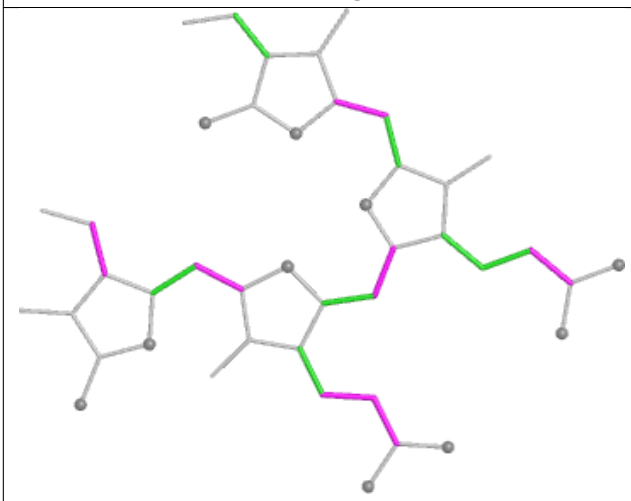


Bond angles



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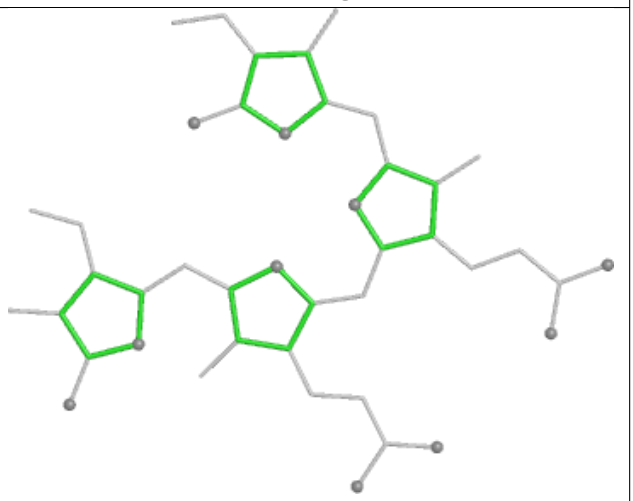
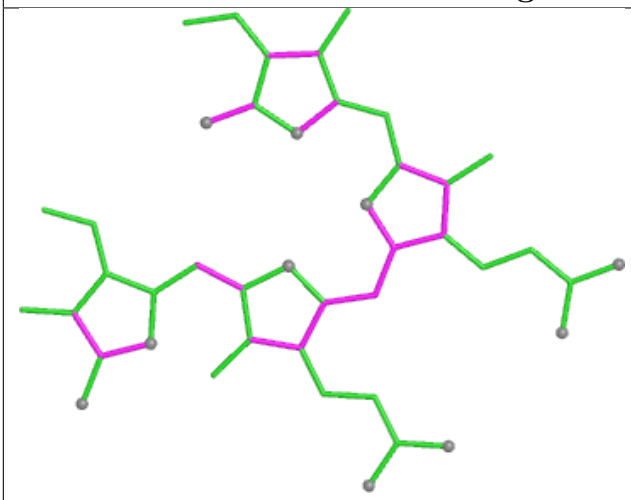


Rings

Ligand PEB E9 202



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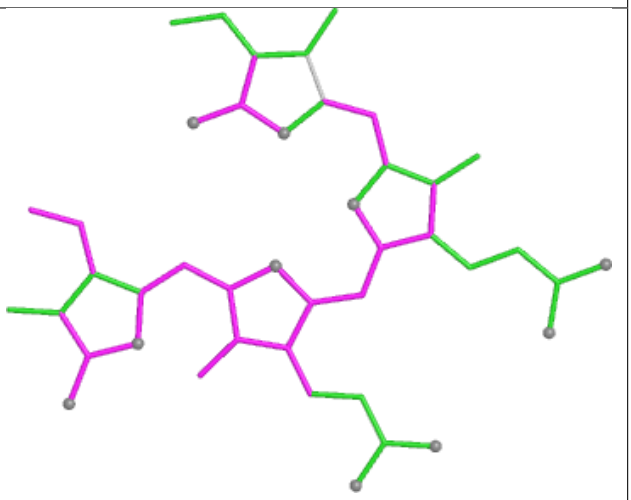

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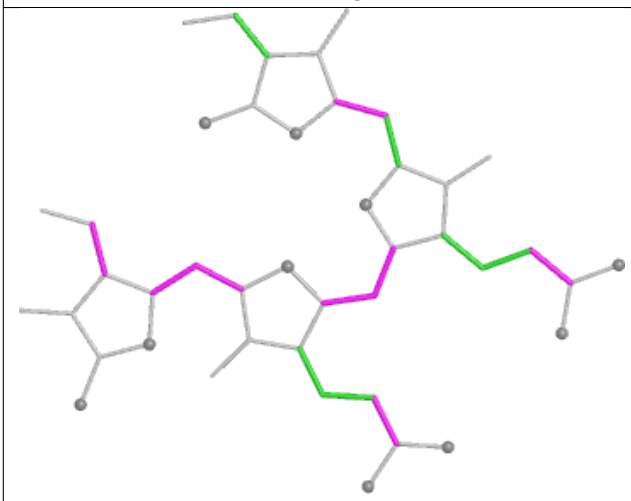

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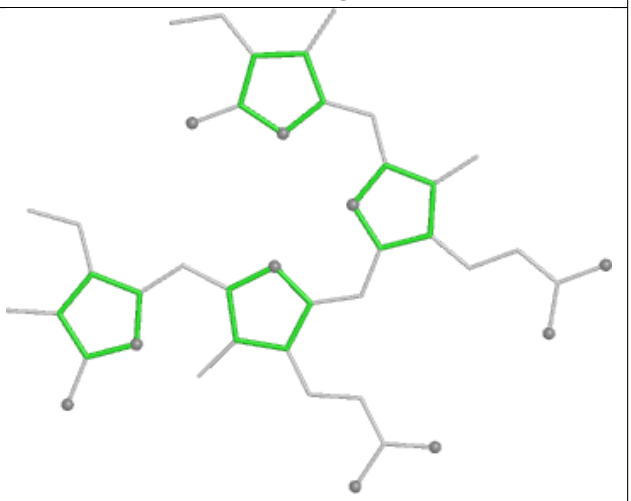
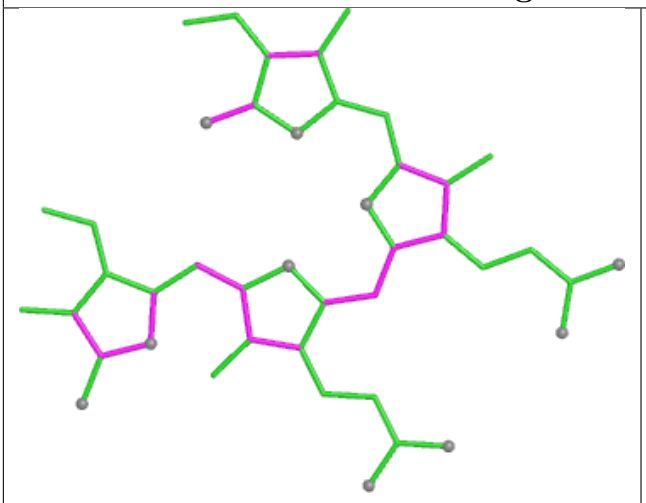
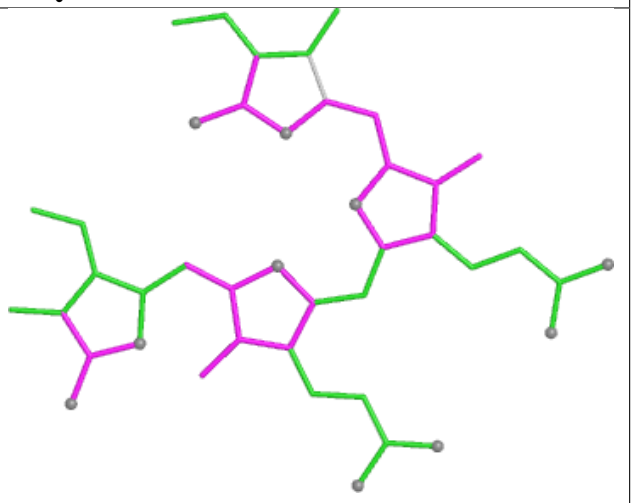


Rings

Ligand PEB Q1 203



Bond lengths



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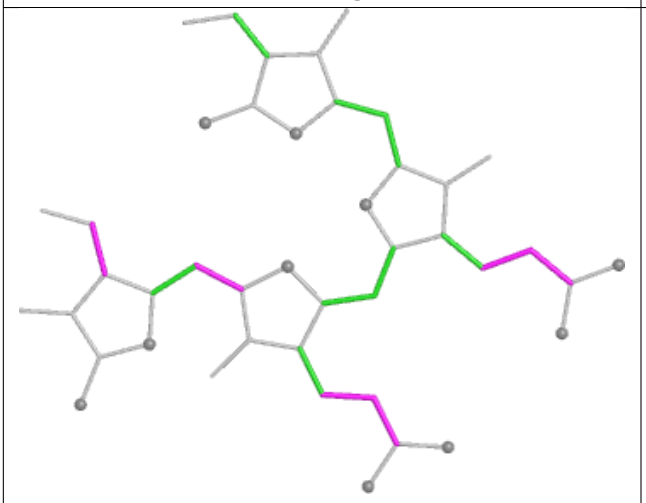
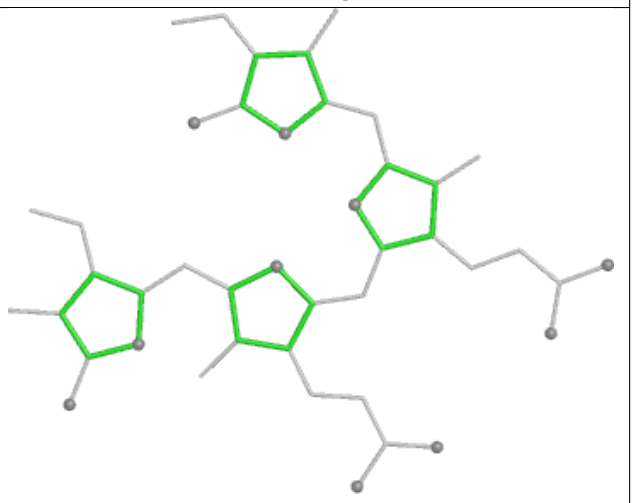
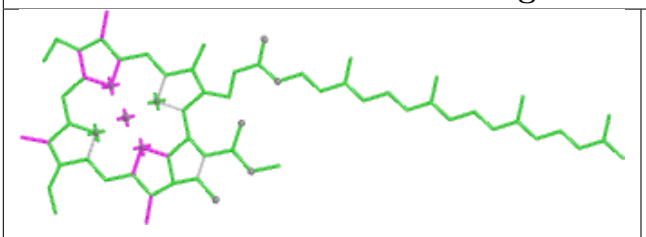


Torsions



Rings

Ligand CLA cL 512



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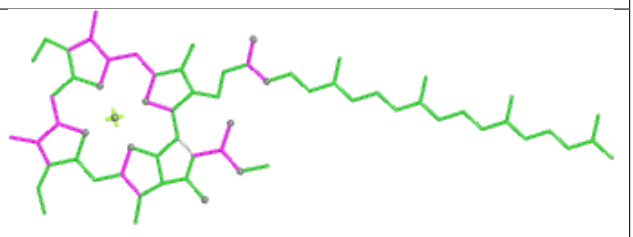

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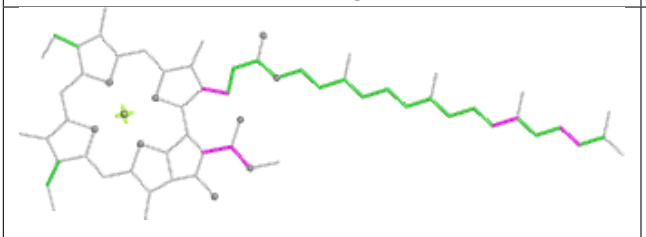

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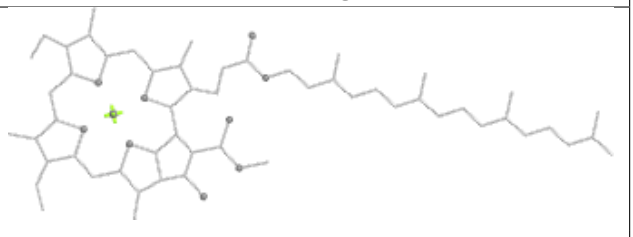
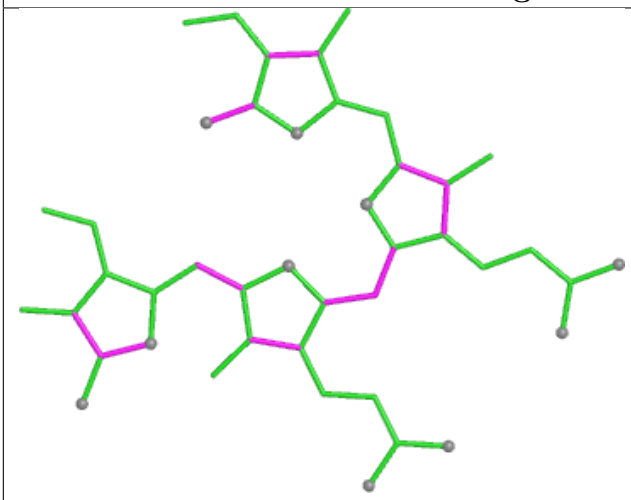


Rings

Ligand PEB LD 203



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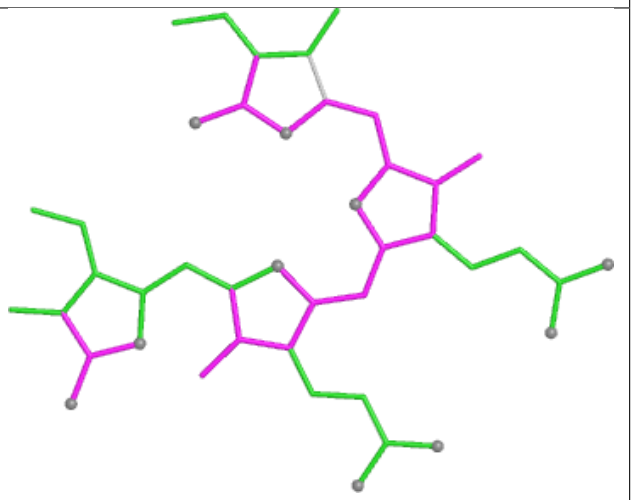

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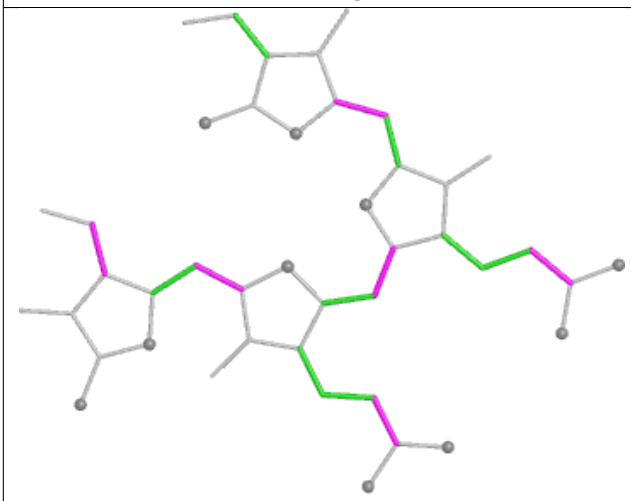

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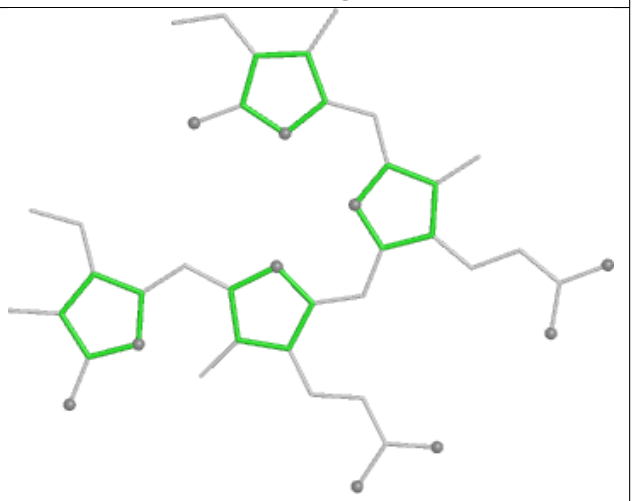
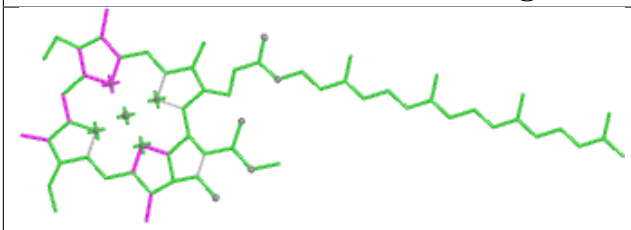


Rings

Ligand CLA cL 506



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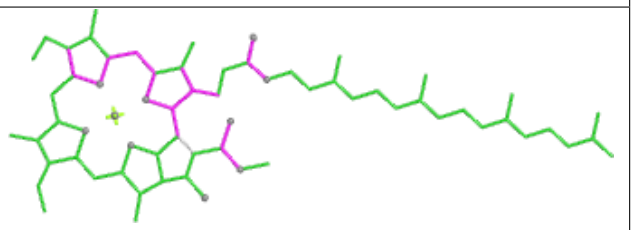

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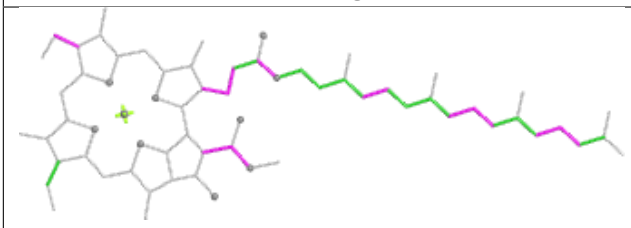

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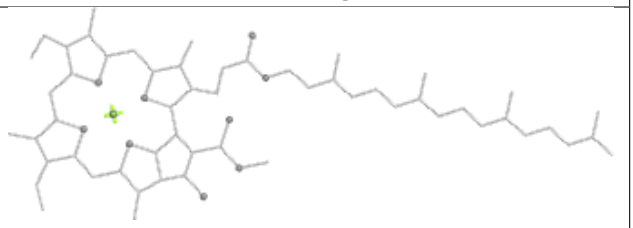
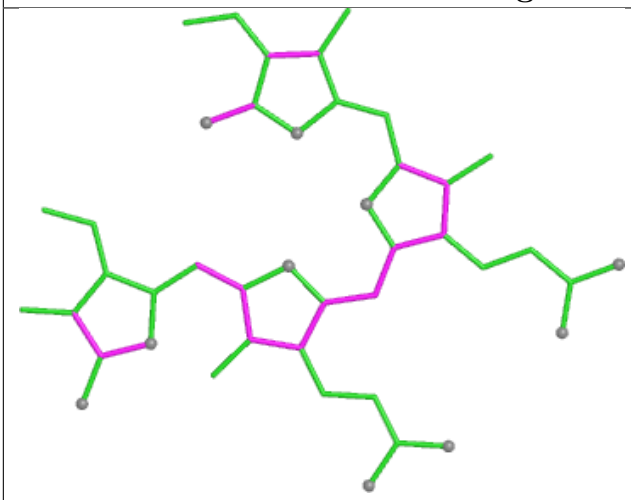


Rings

Ligand PEB uF 203



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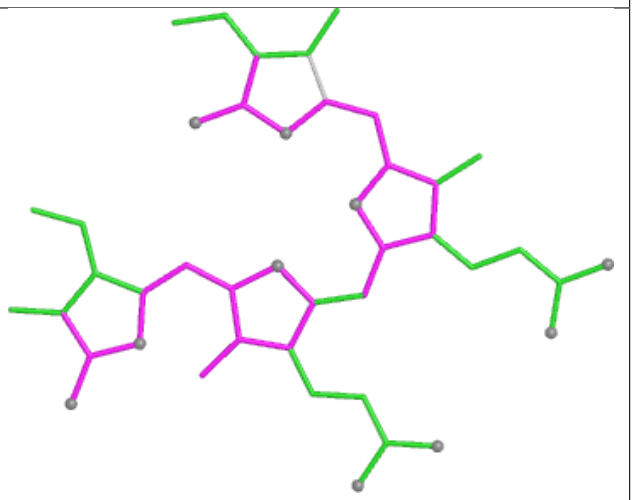

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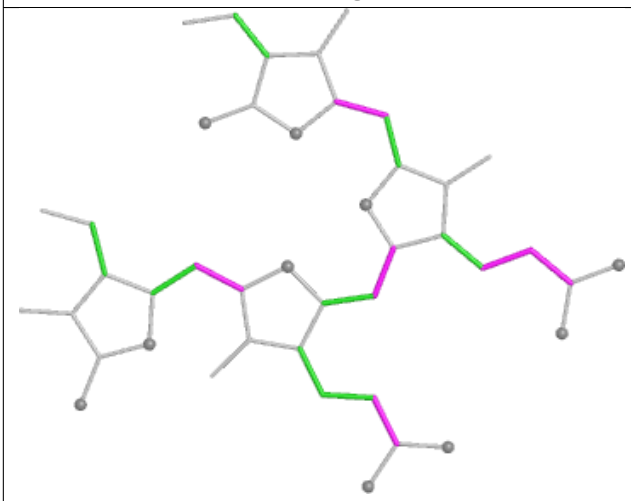

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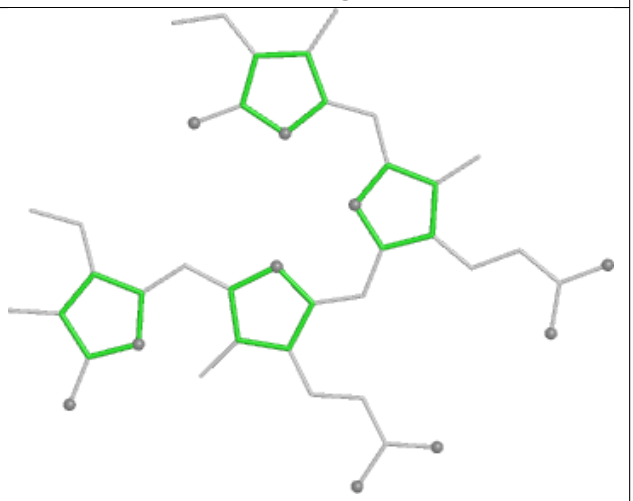
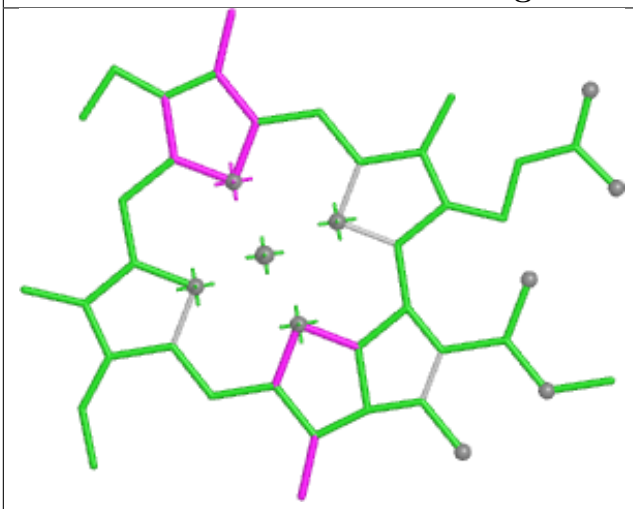


Rings

Ligand CLA 4N 605



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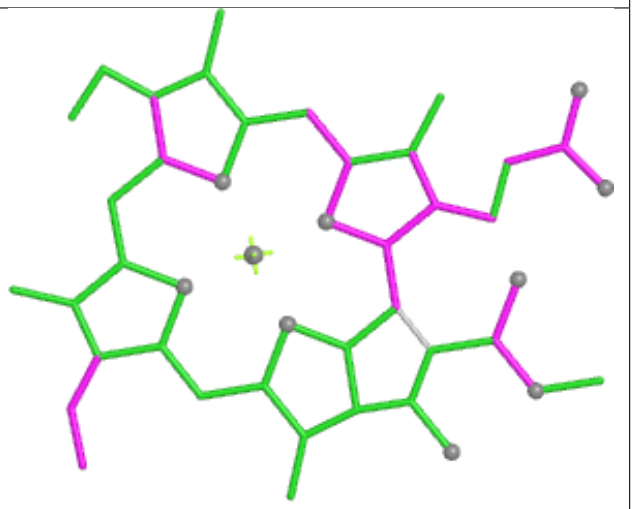

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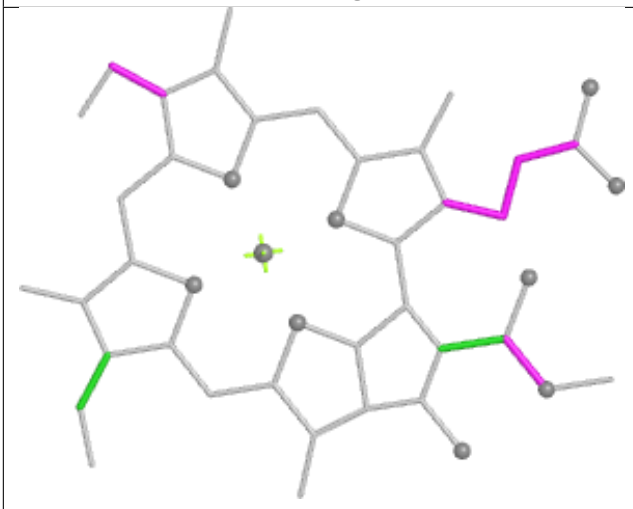
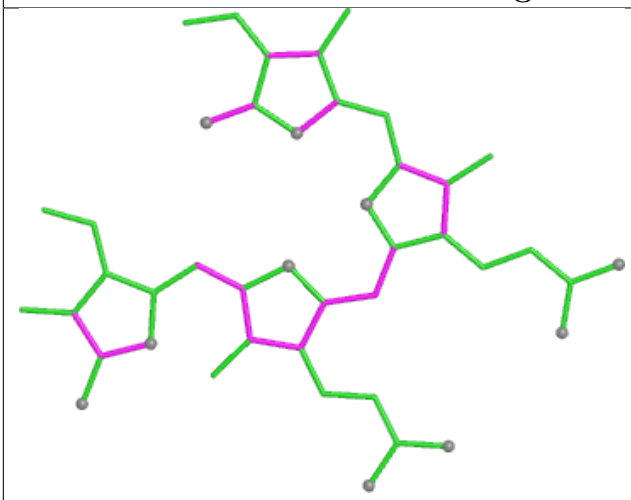


Torsions



Rings

Ligand PEB qK 203



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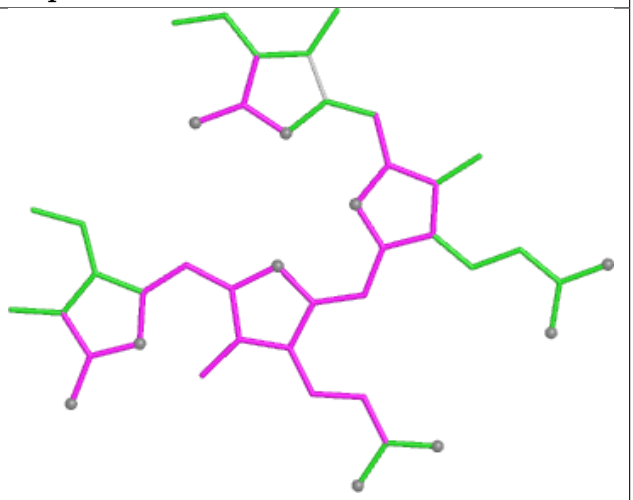

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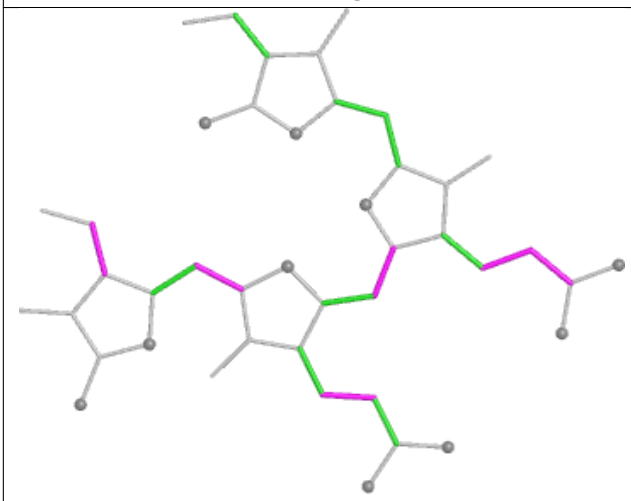

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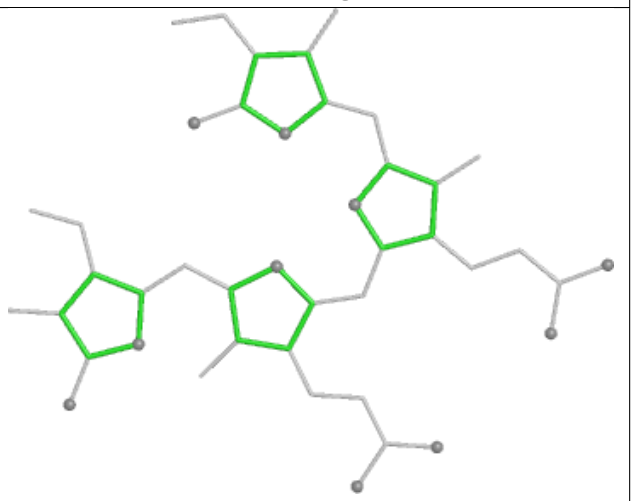

Rings

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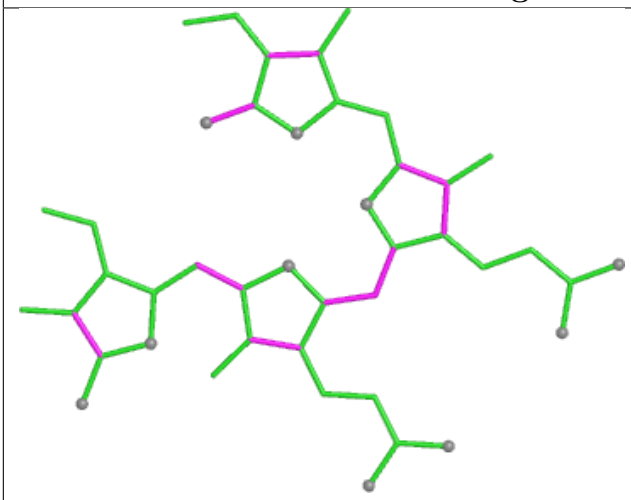

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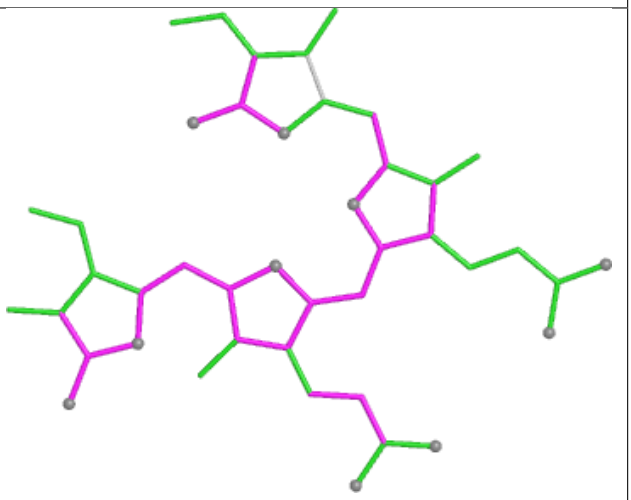

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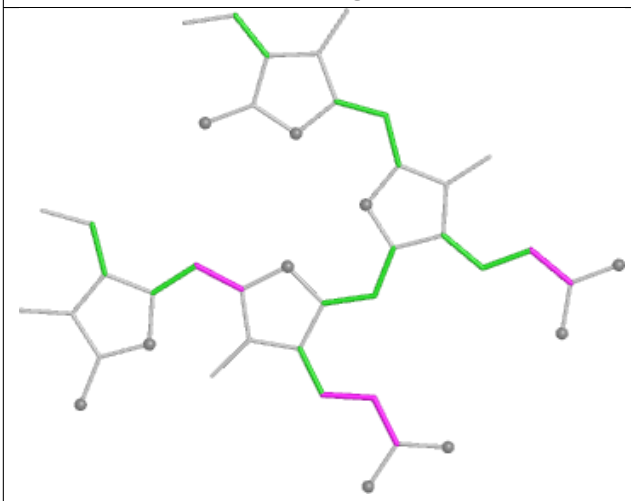

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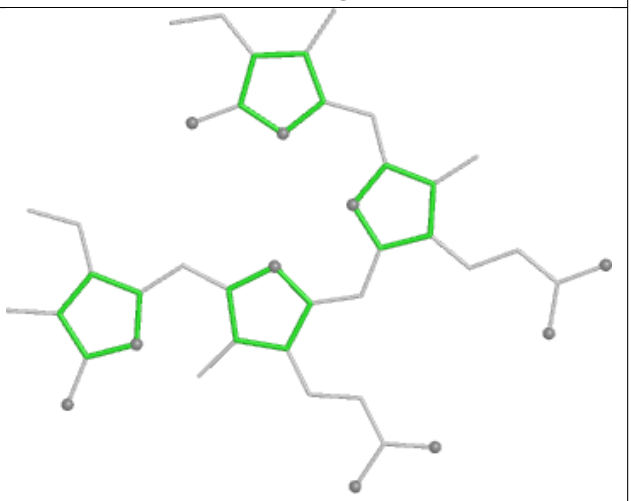
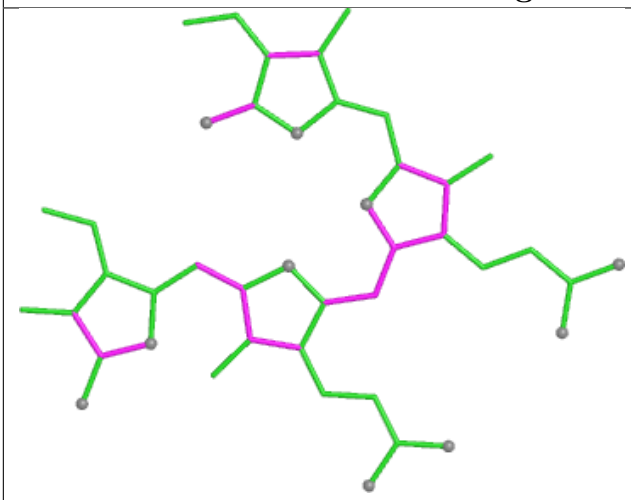


Rings

Ligand PEB Y1 202



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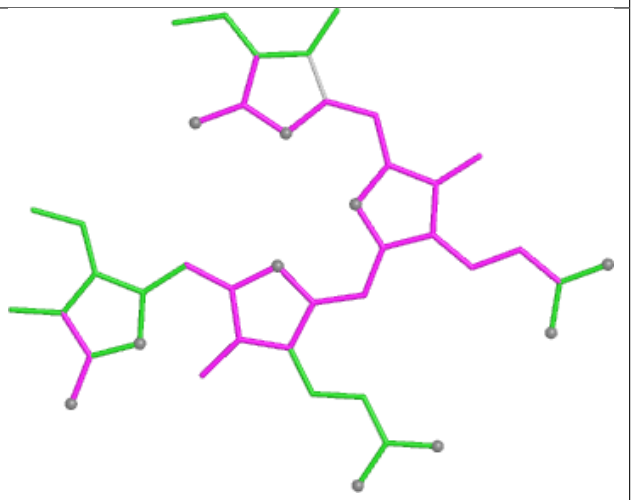

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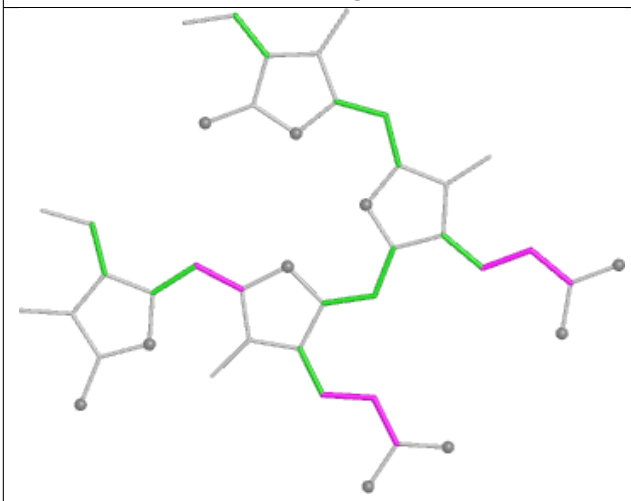

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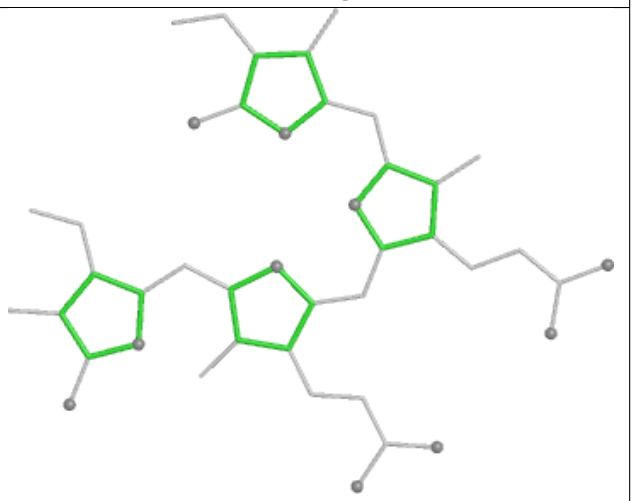
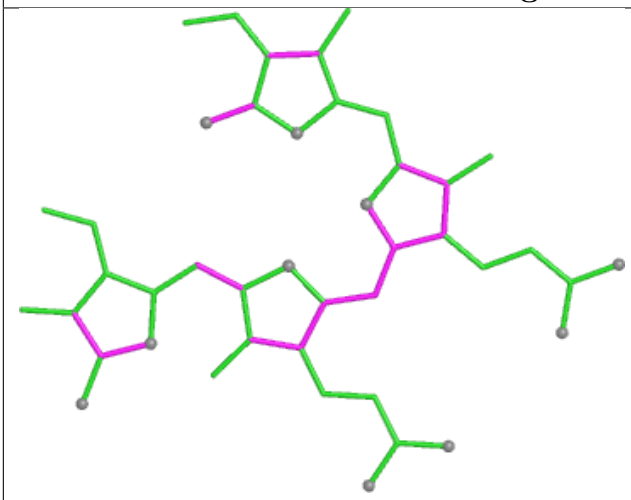


Rings

Ligand PEB e1 201



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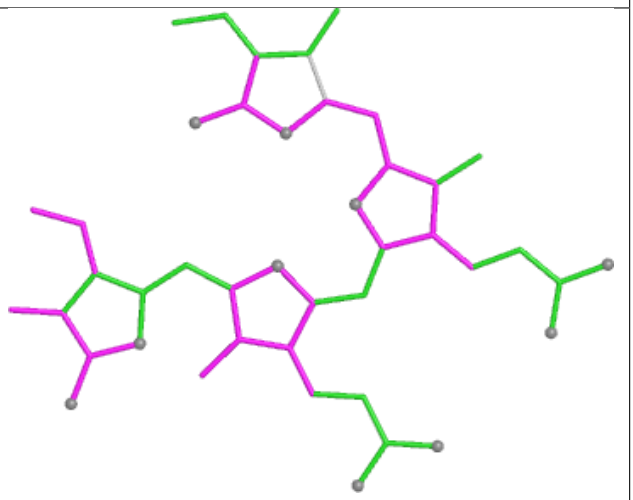
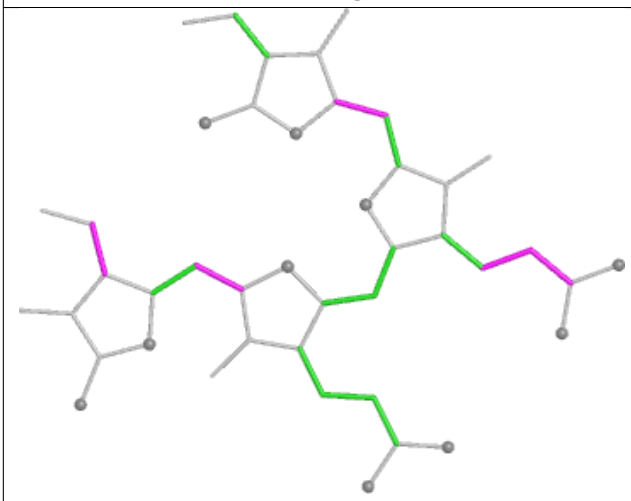


Bond angles



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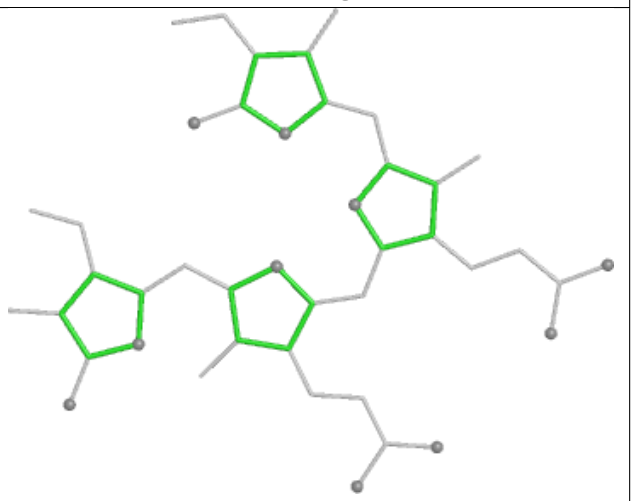
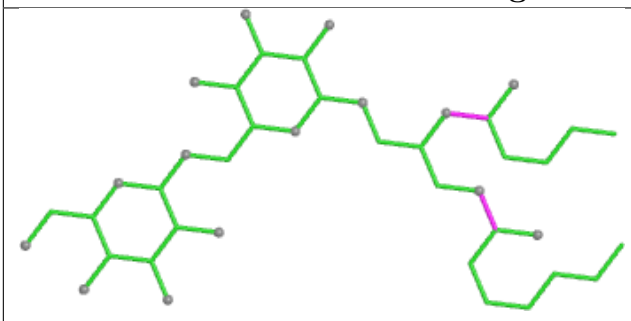


Rings

Ligand DGD CL 520



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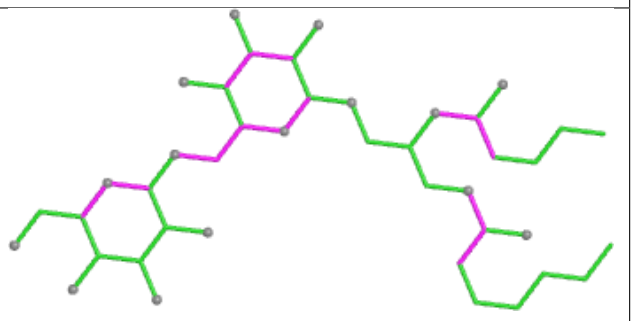
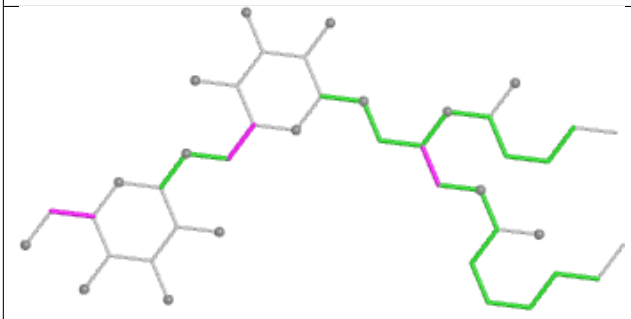


Bond angles



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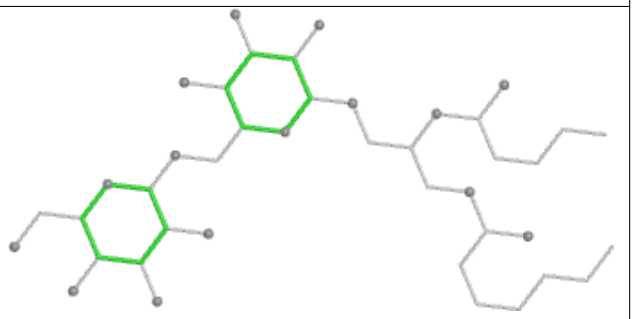
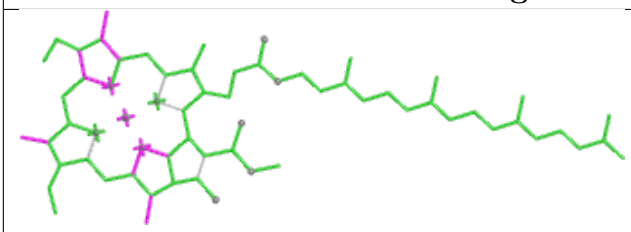


Rings

Ligand CLA BN 832



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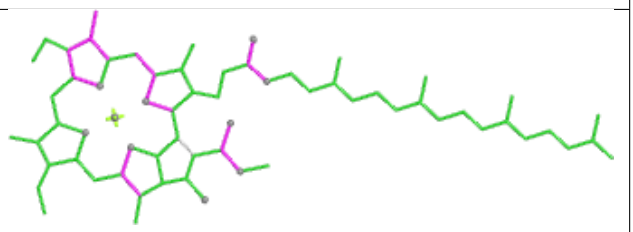

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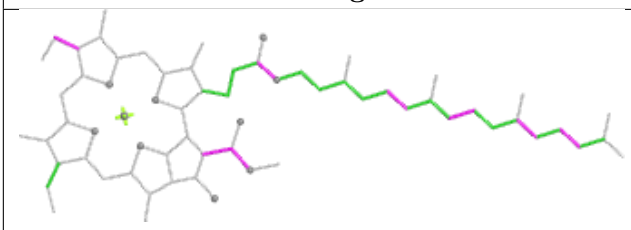

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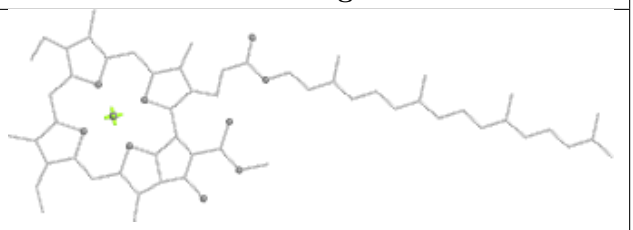
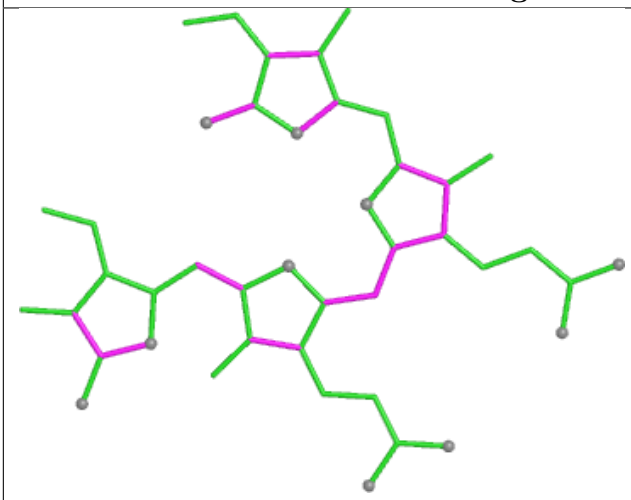


Rings

Ligand PEB OD 201



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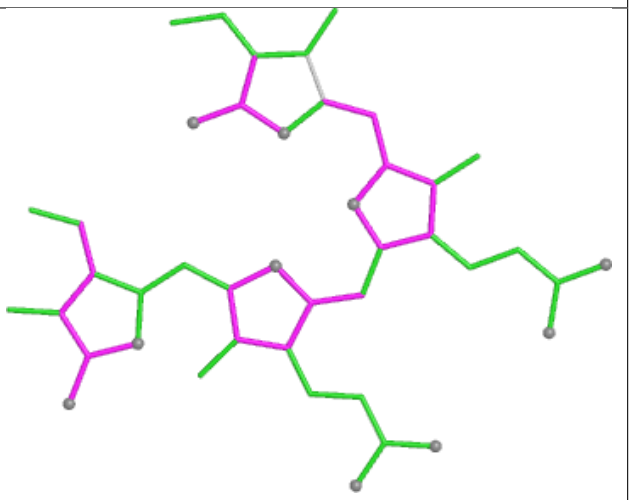
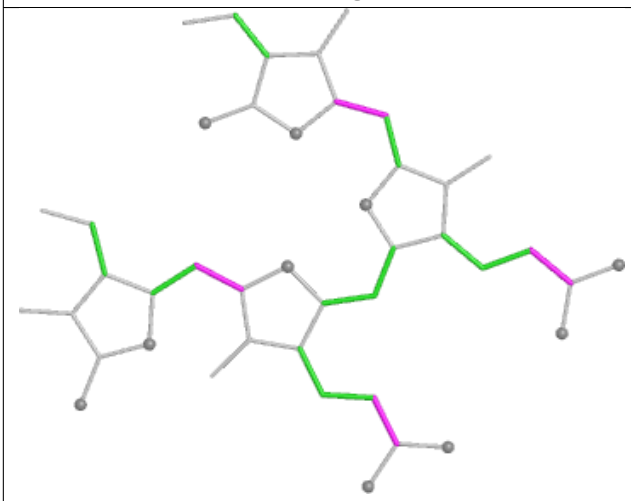


Bond angles



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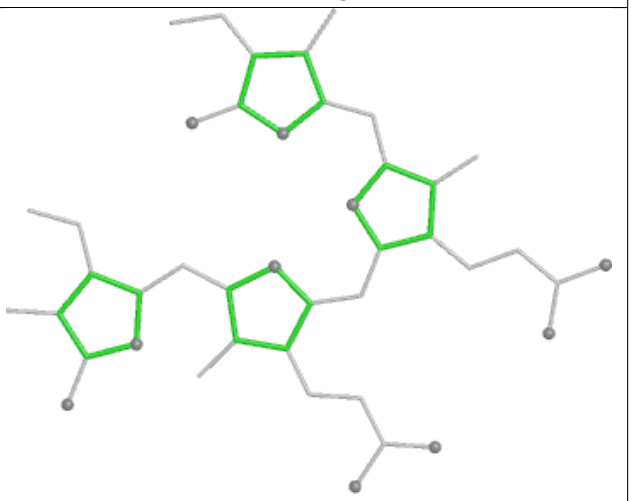
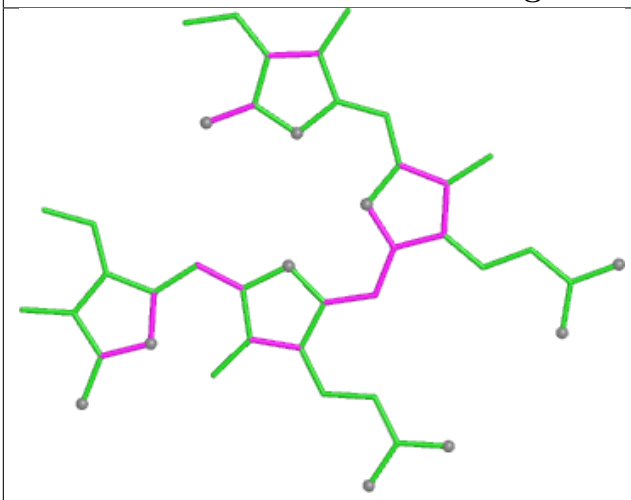


Rings

Ligand PEB II 201



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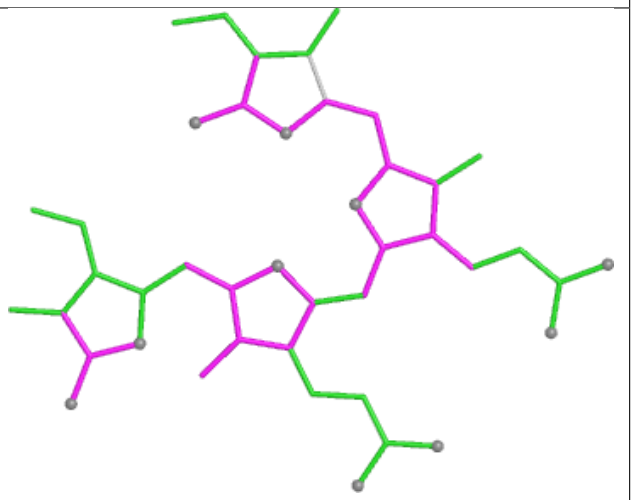
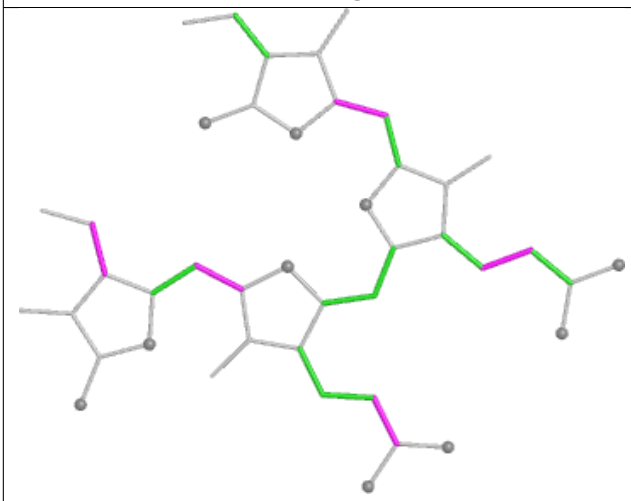


Bond angles



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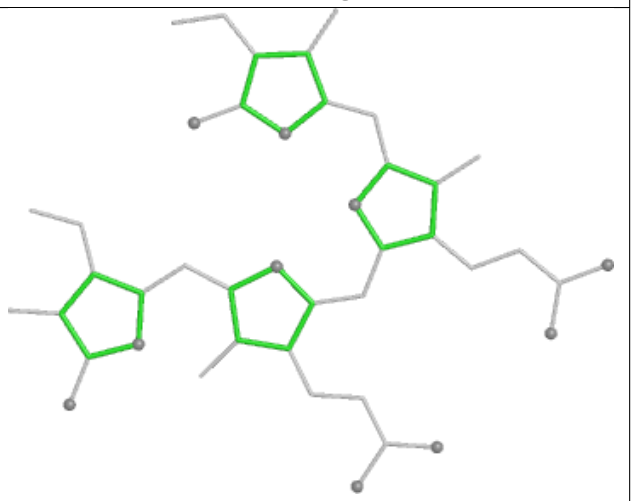
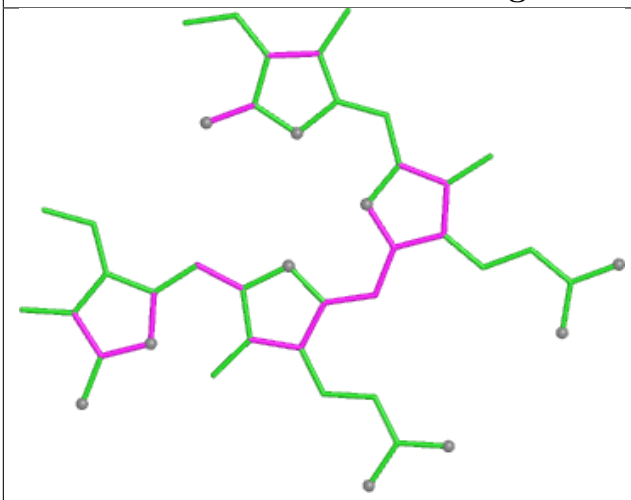


Rings

Ligand PEB mG 203



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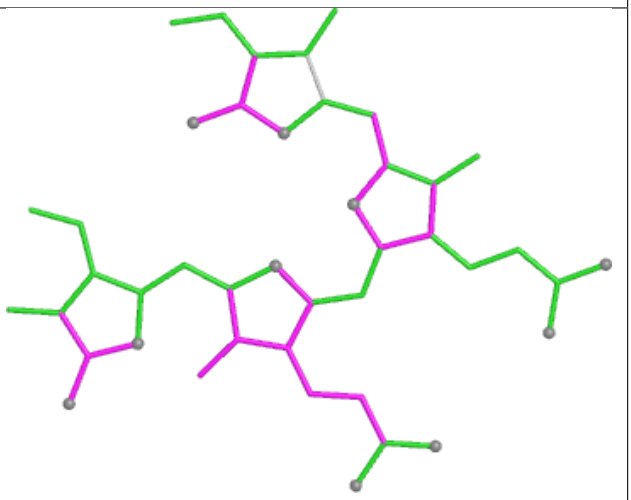
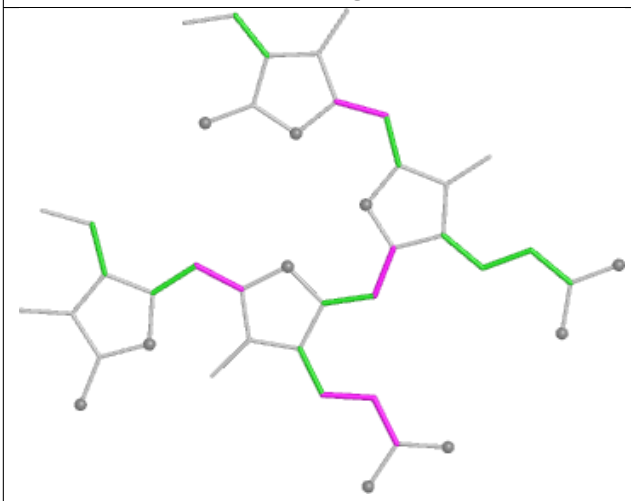


Bond angles



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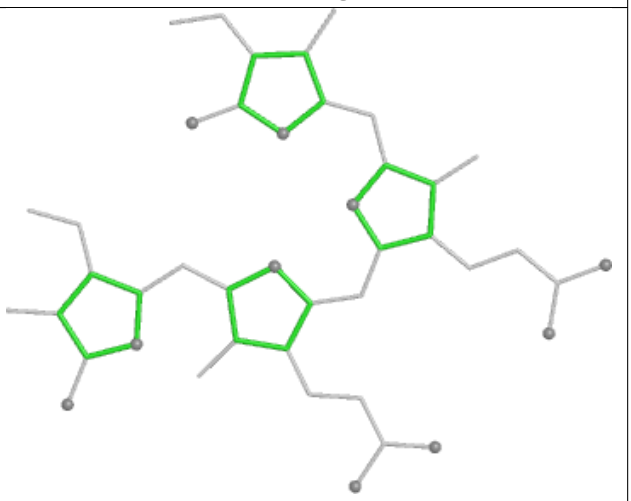
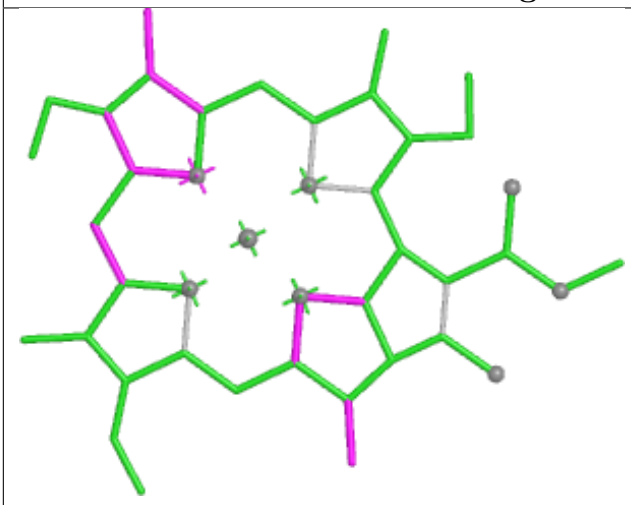


Rings

Ligand CLA 22 611



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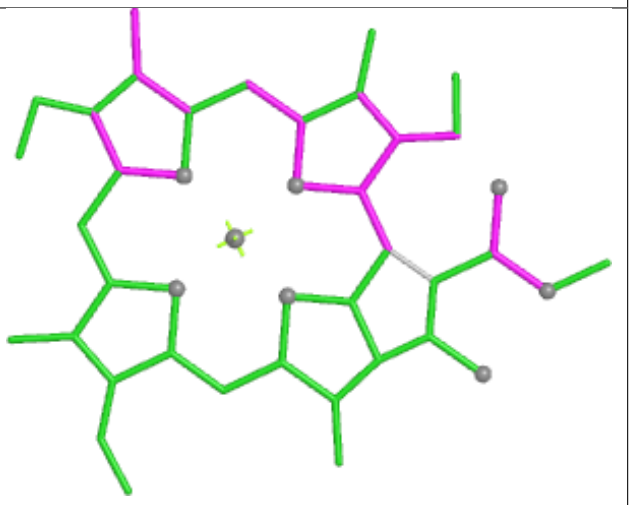

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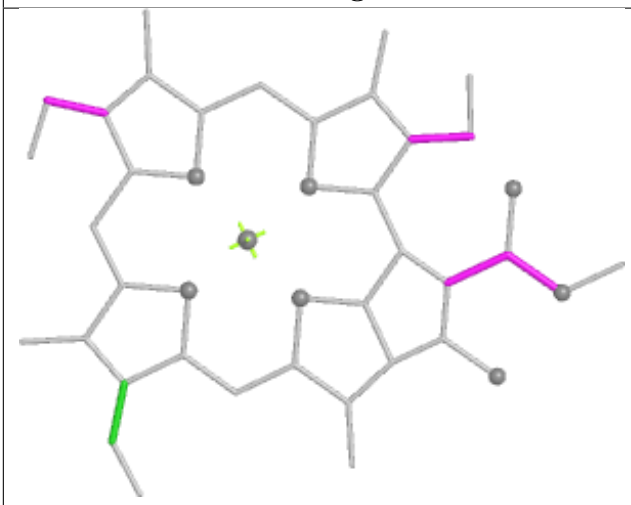
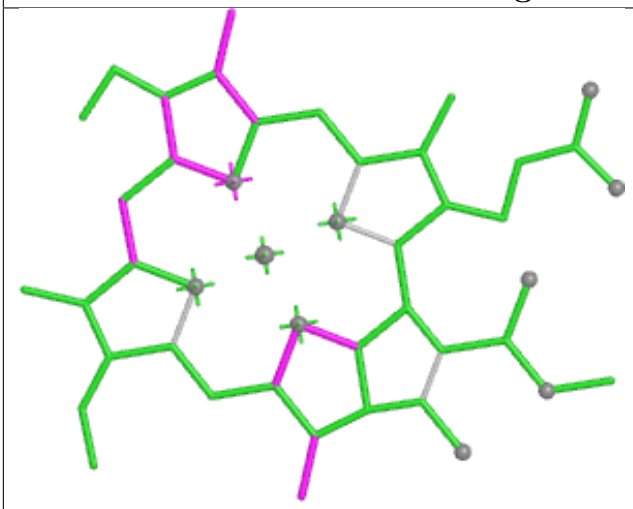


Torsions



Rings

Ligand CLA 6N 603



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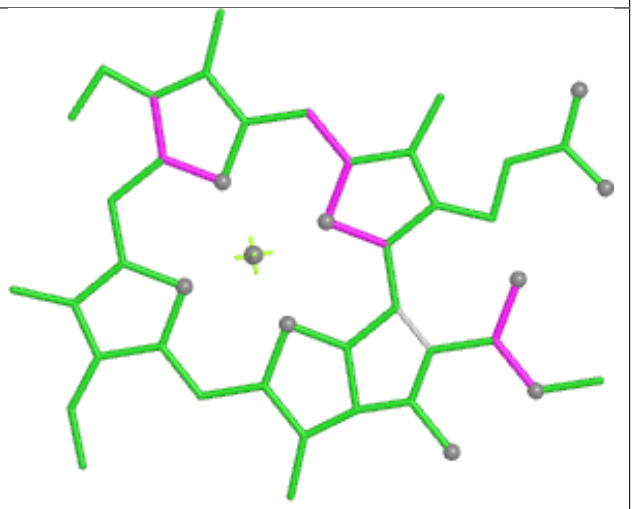

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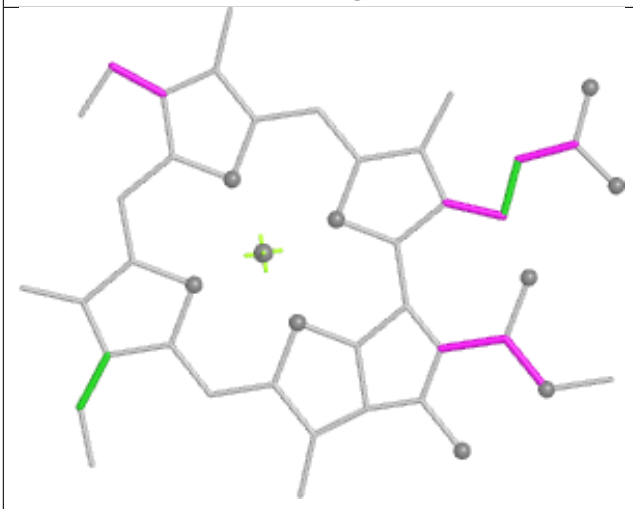
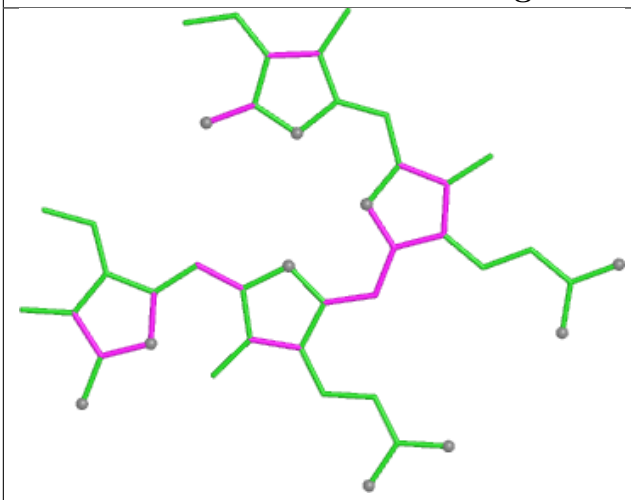


Torsions



Rings

Ligand PEB yK 301



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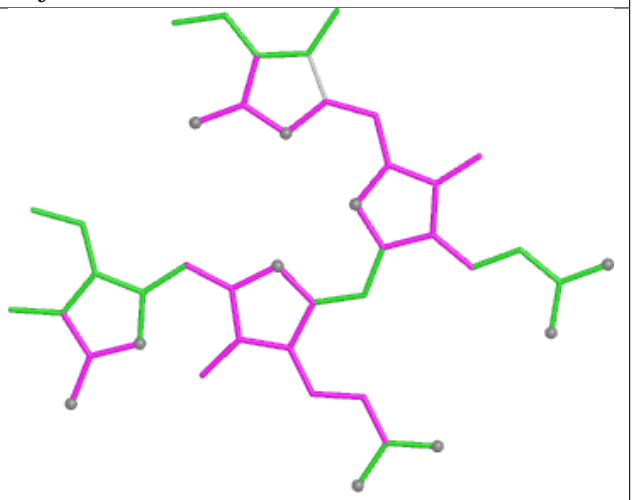

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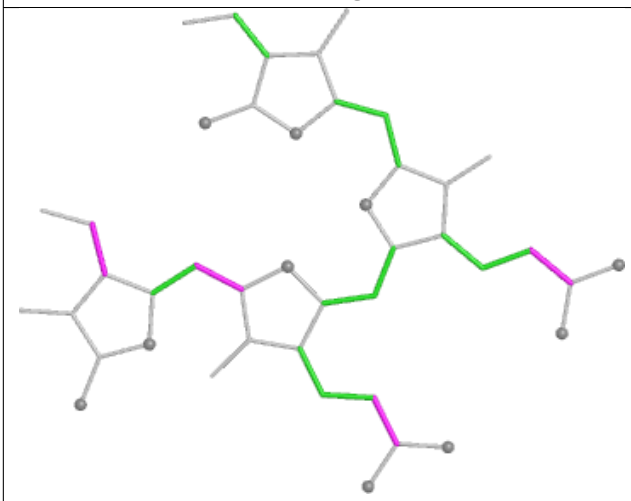

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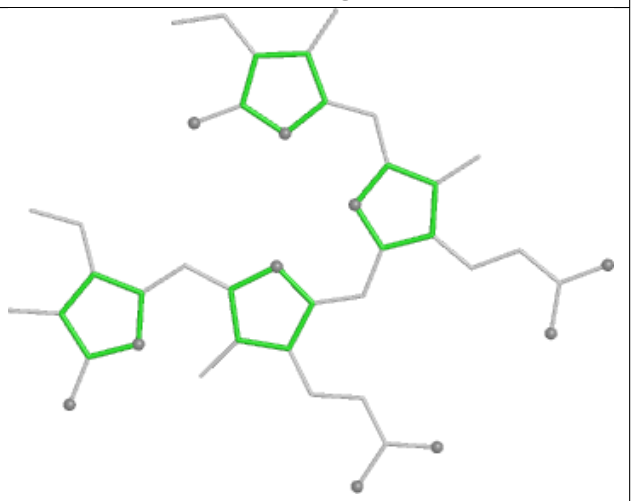
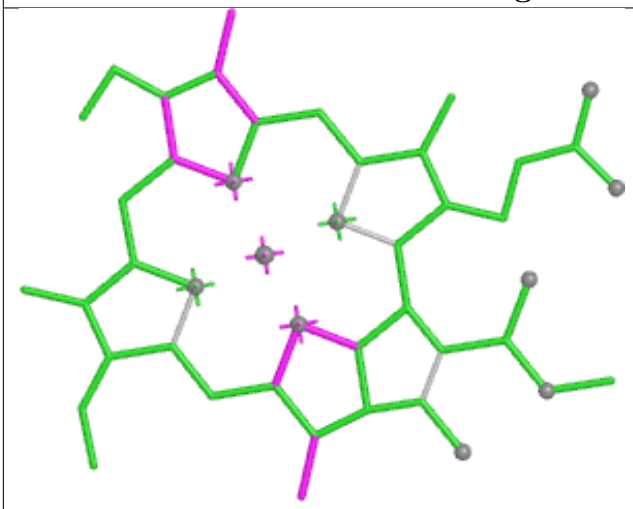


Rings

Ligand CLA 4N 606



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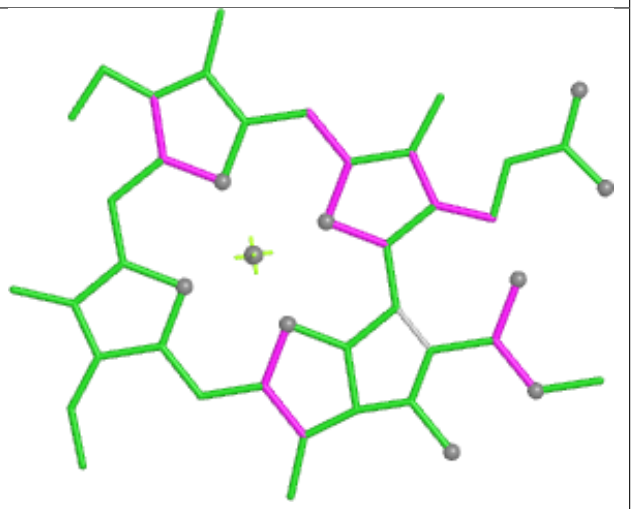

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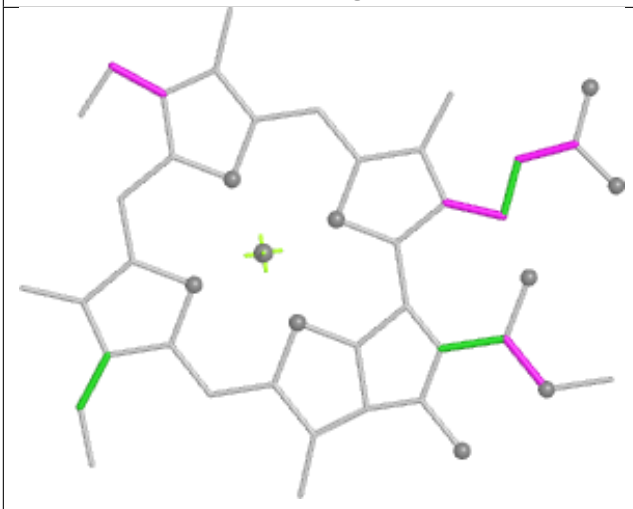

Torsions



Rings

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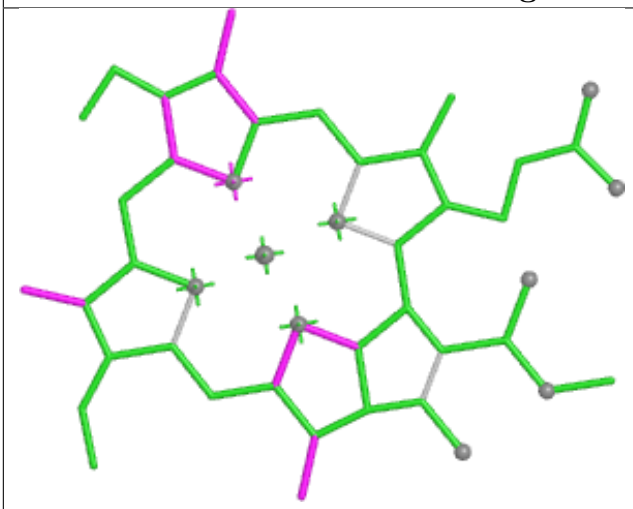

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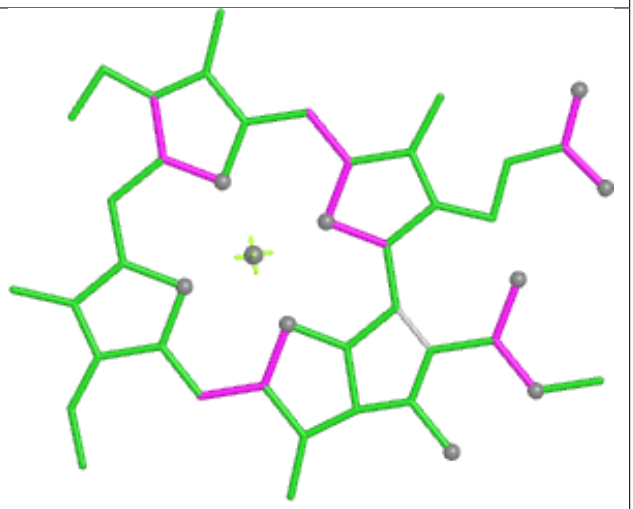

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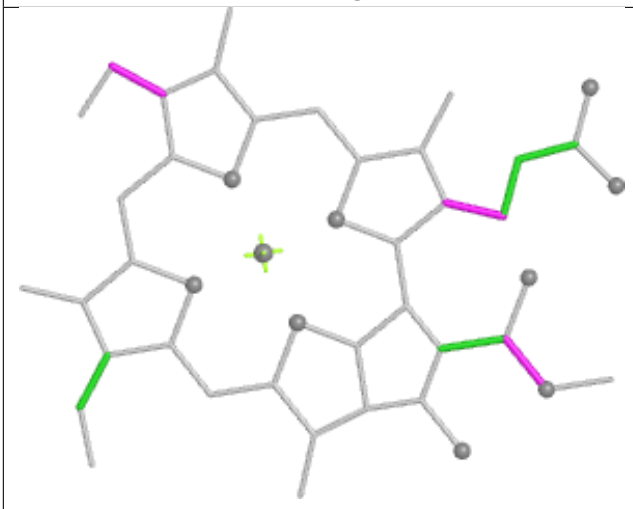
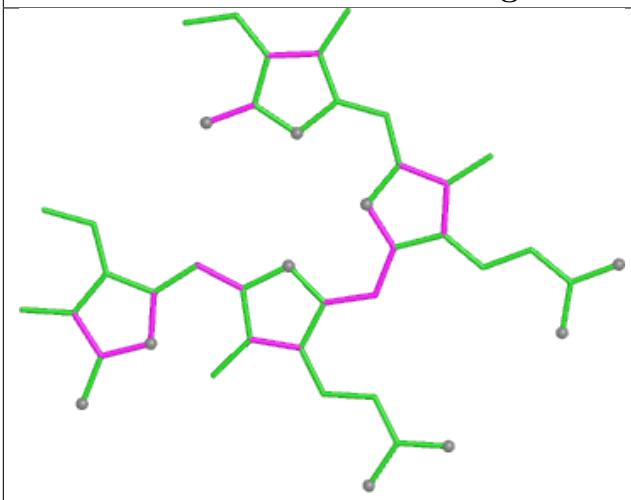


Torsions



Rings

Ligand PEB GG 1002



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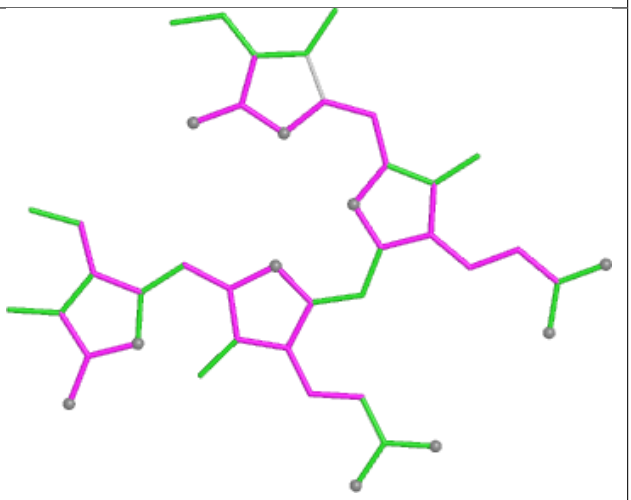

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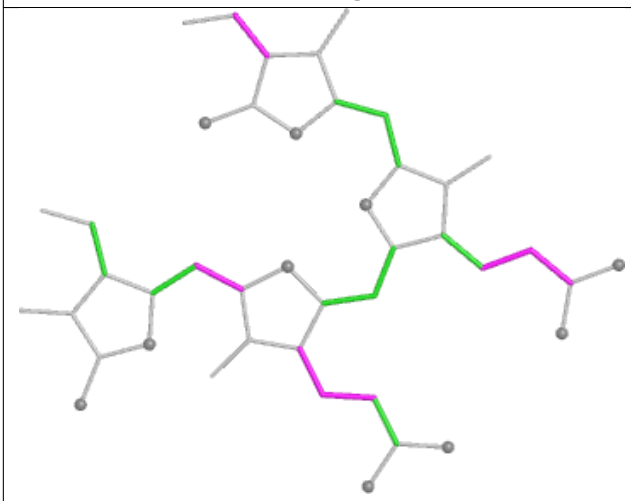

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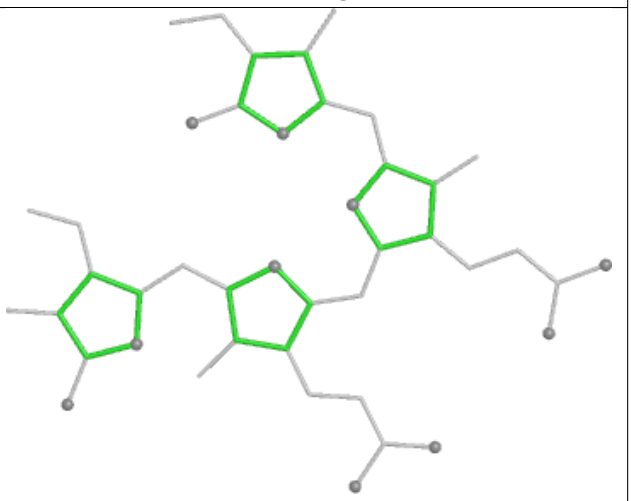
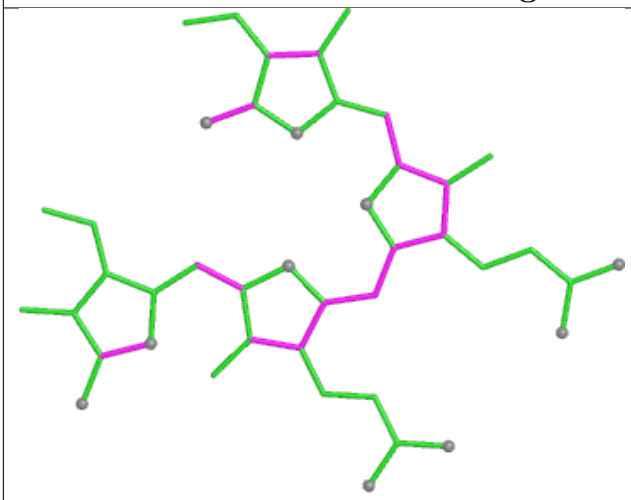


Rings

Ligand PEB J7 202



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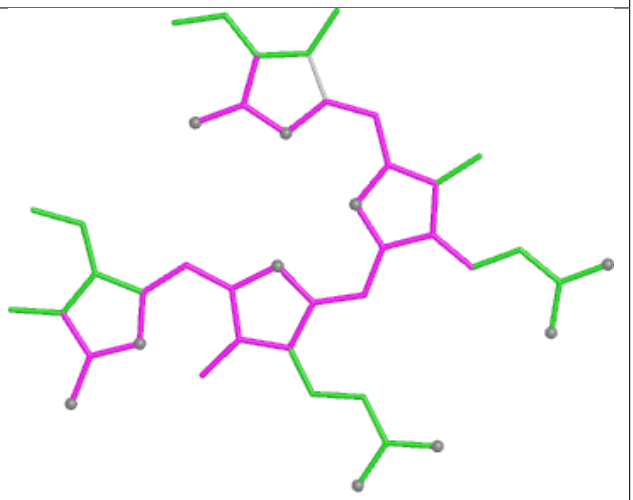

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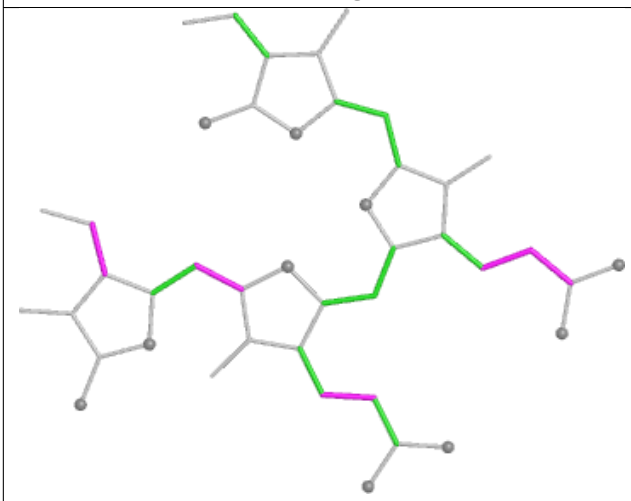

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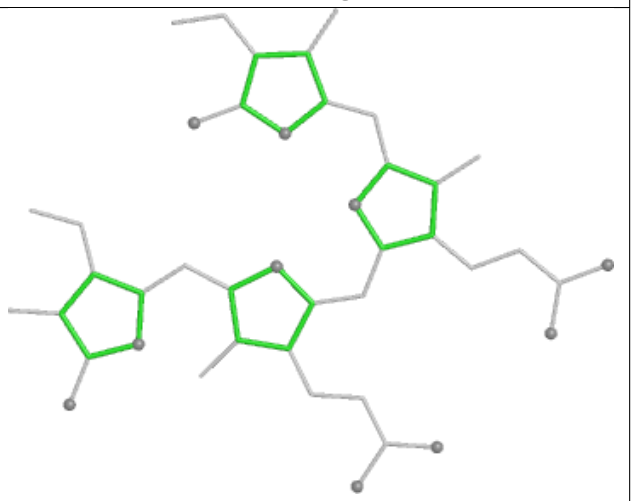

Rings

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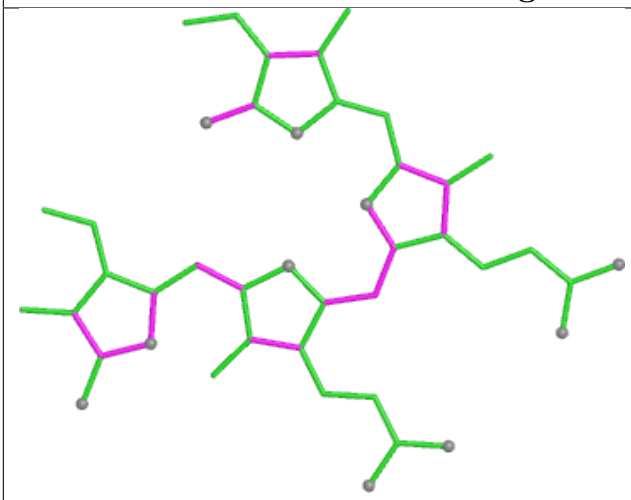

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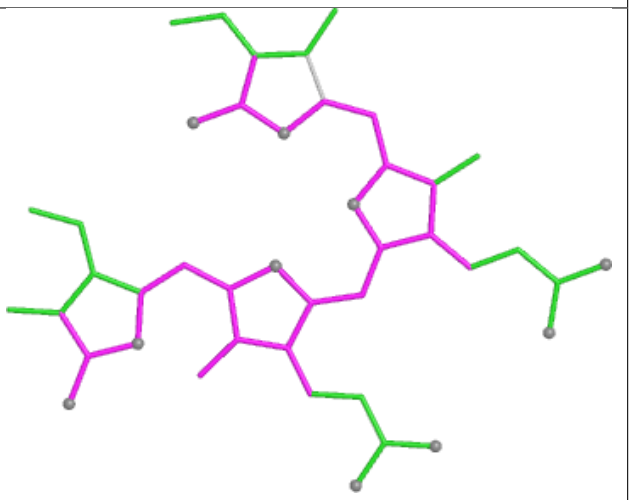

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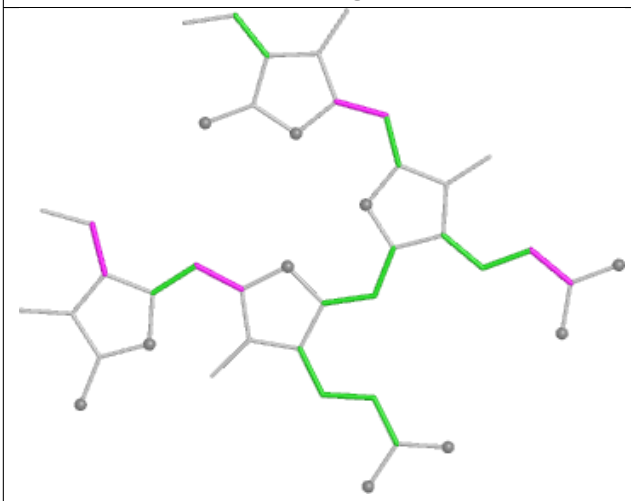

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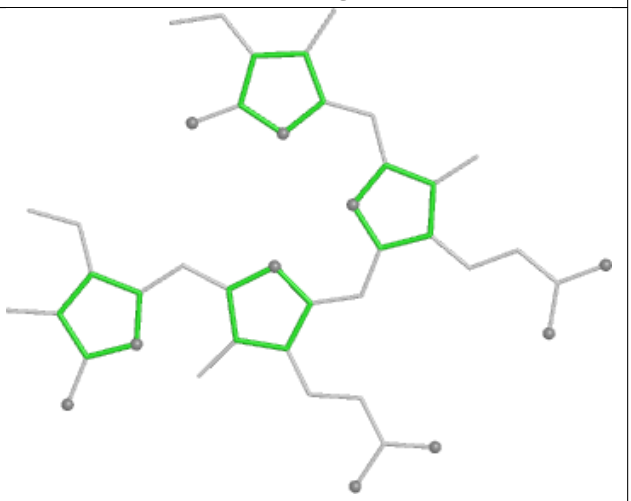
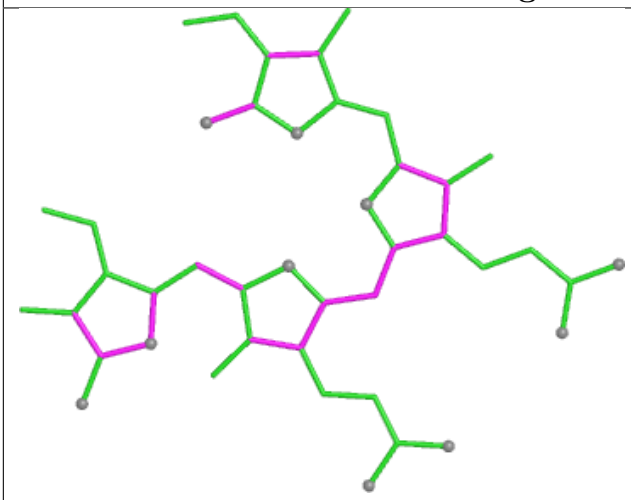


Rings

Ligand PEB lG 201



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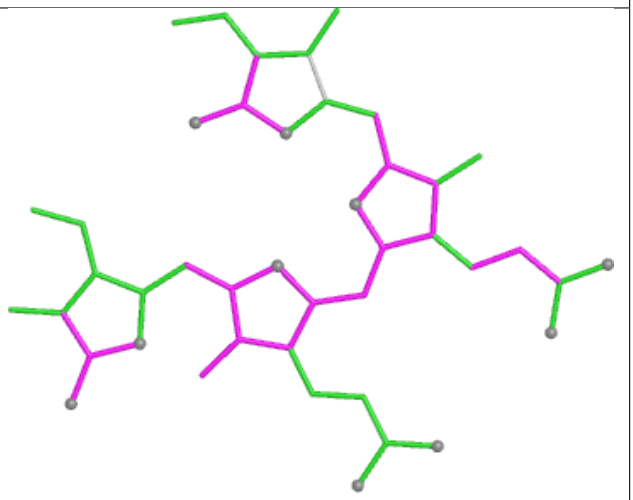

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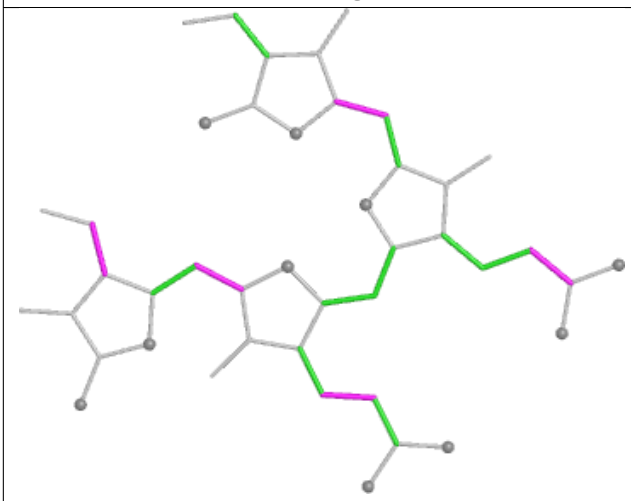

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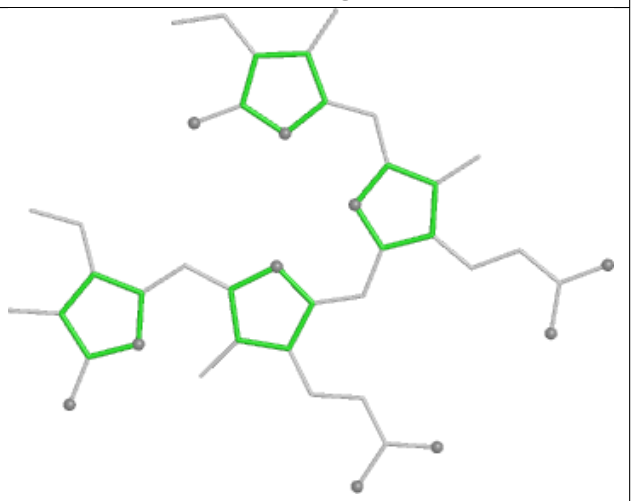
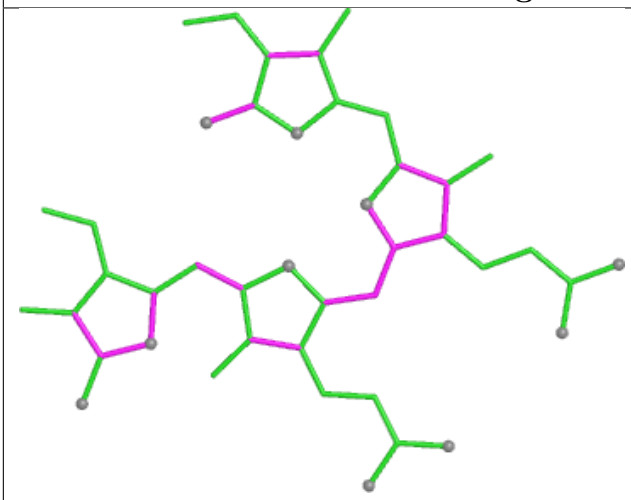


Rings

Ligand PEB R7 201



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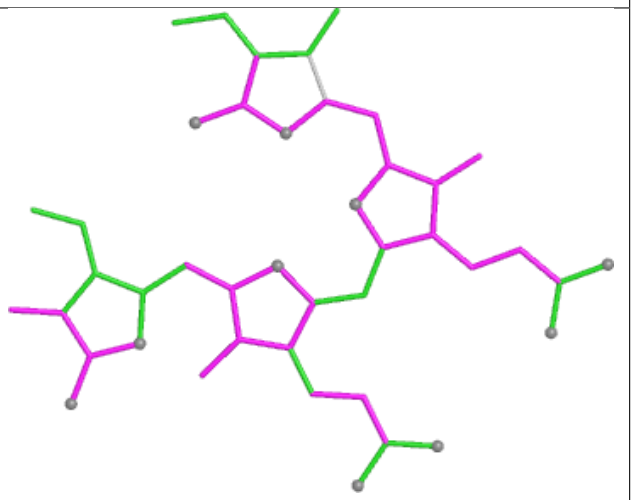

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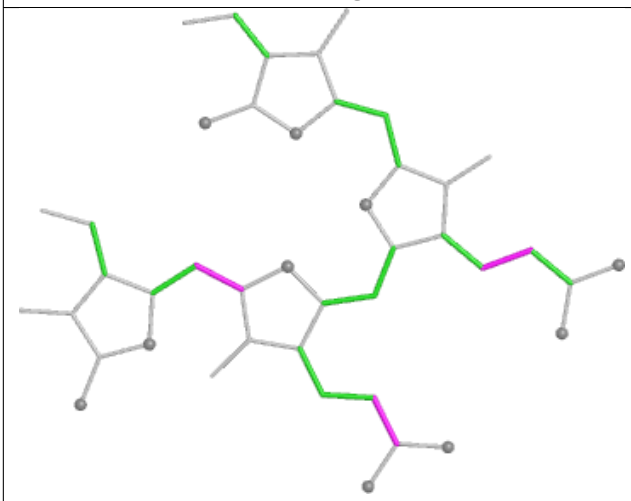

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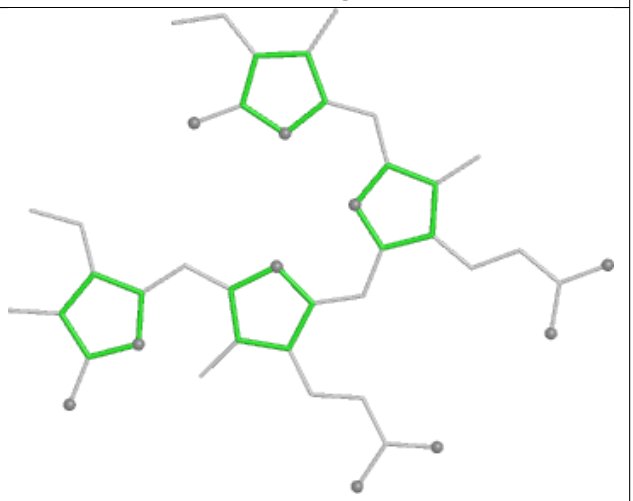
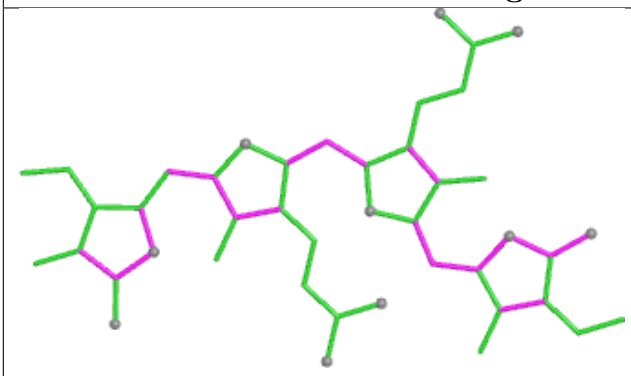


Rings

Ligand CYC F4 1001



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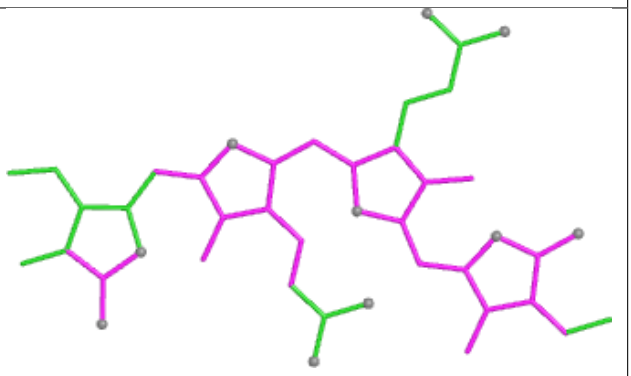

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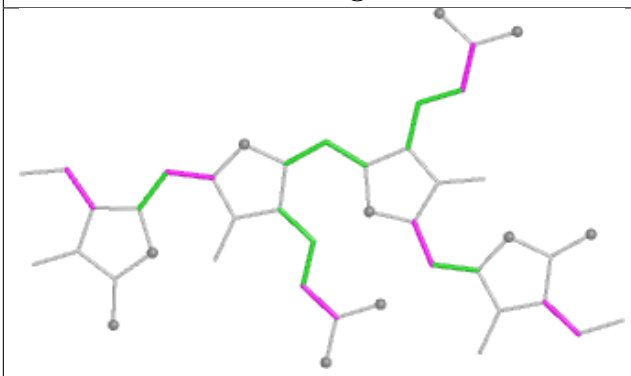

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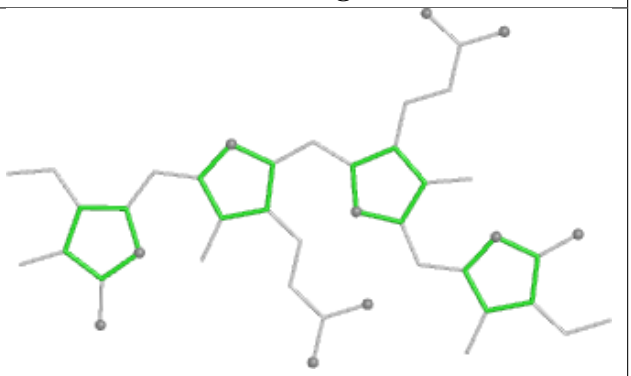
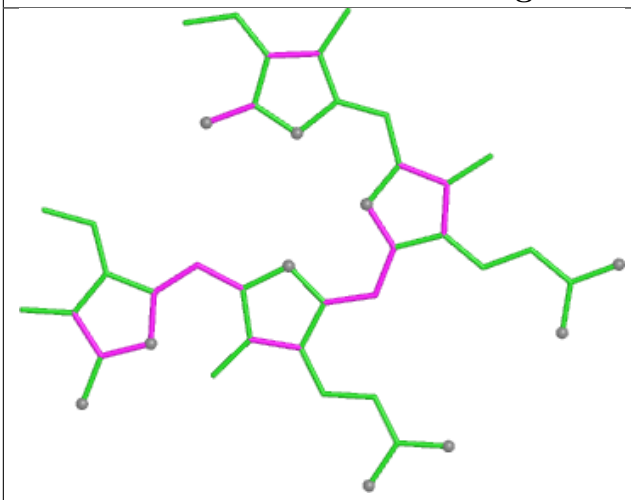


Rings

Ligand PEB Q4 201



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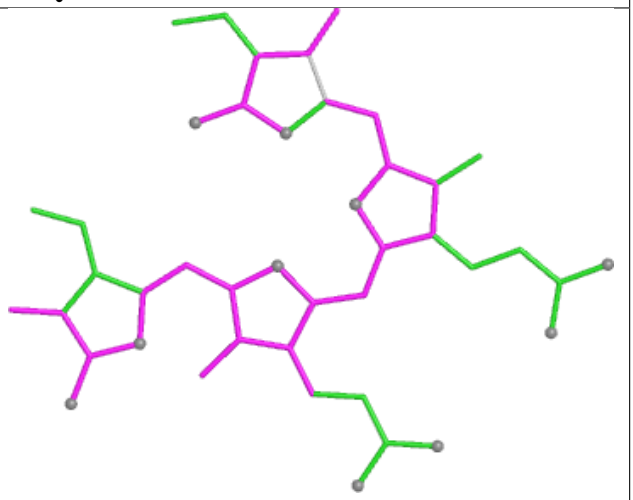

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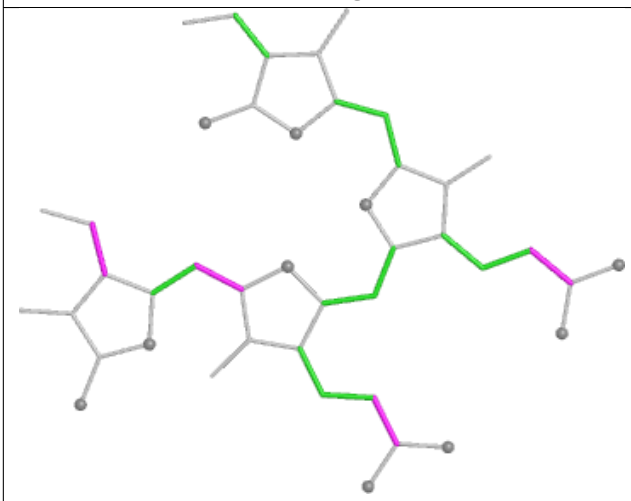

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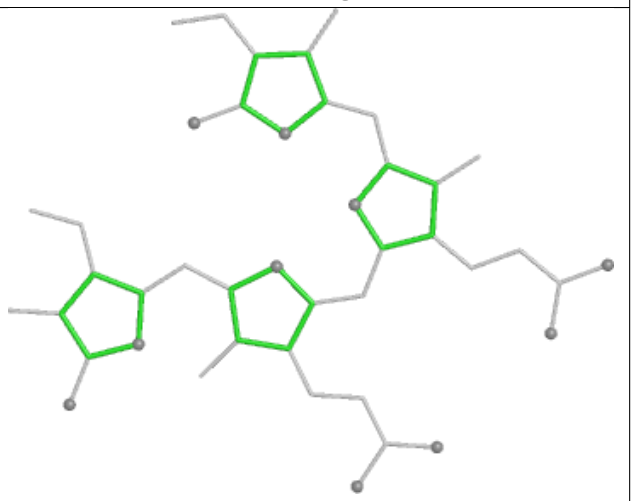
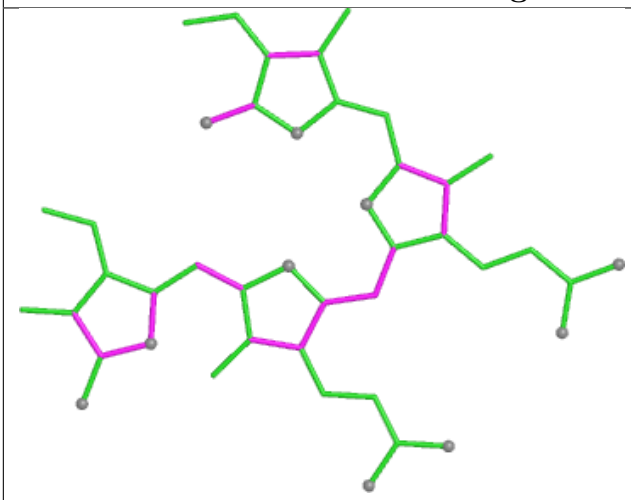


Rings

Ligand PEB HD 201



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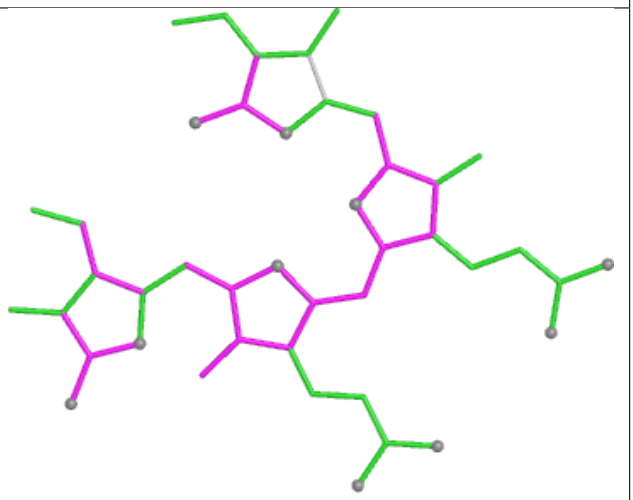

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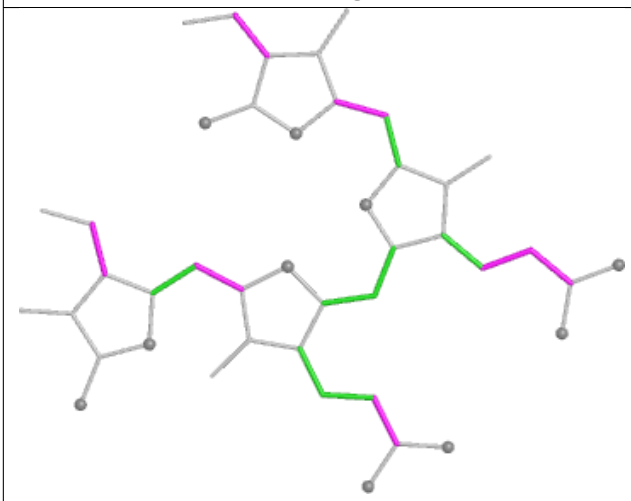

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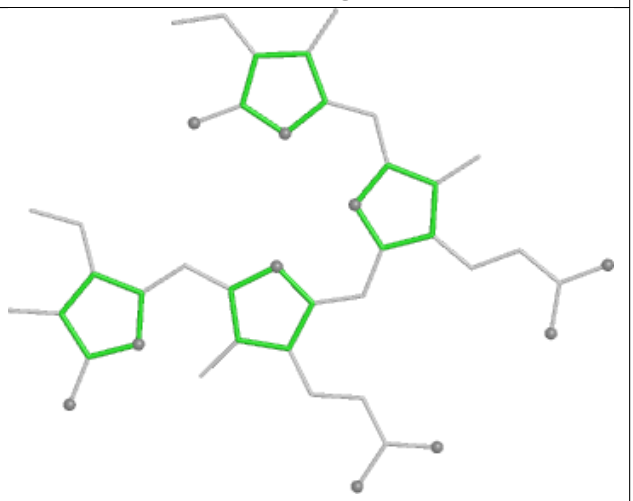

Rings

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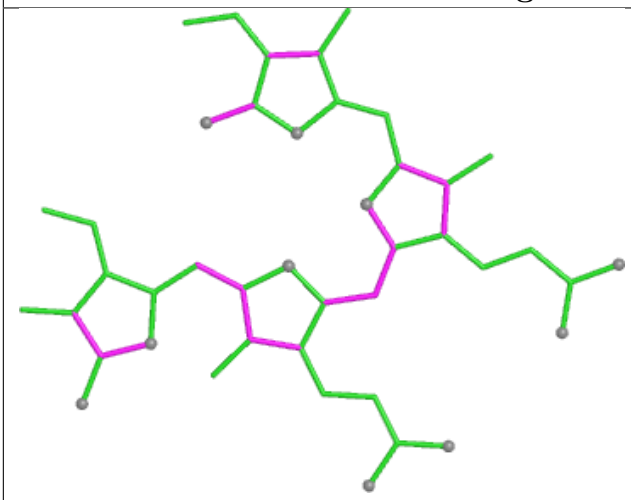

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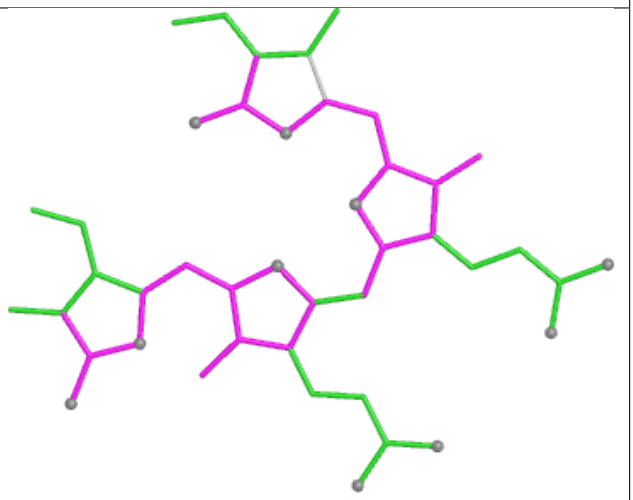
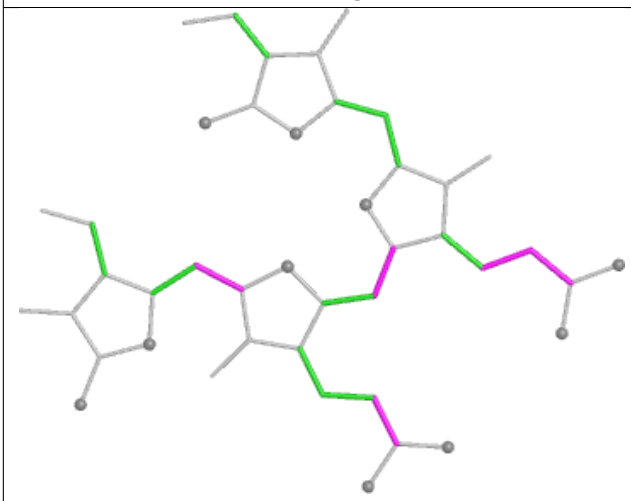


Bond angles



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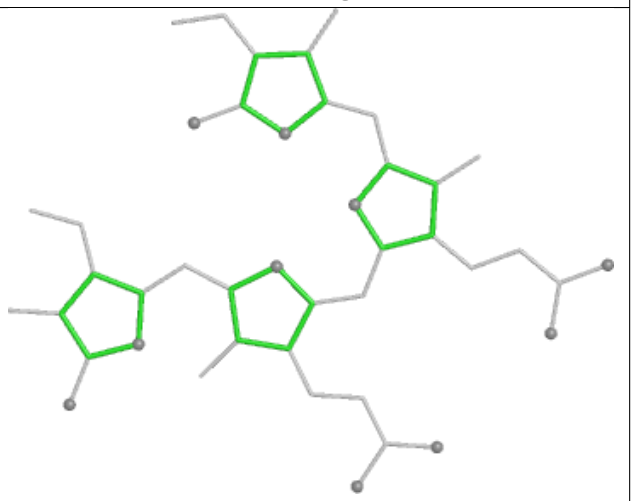
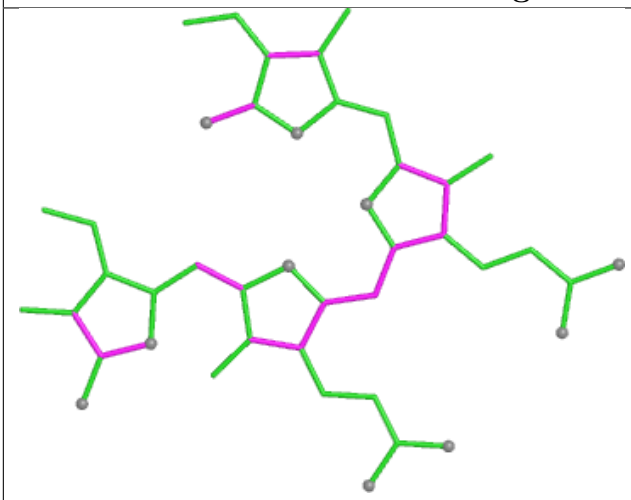


Rings

Ligand PEB FD 202



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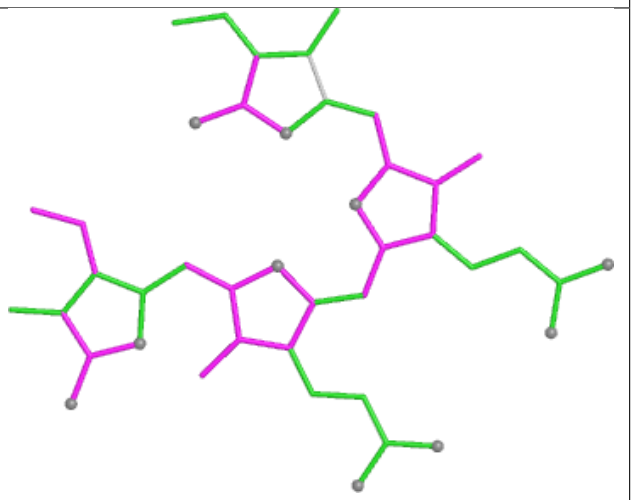
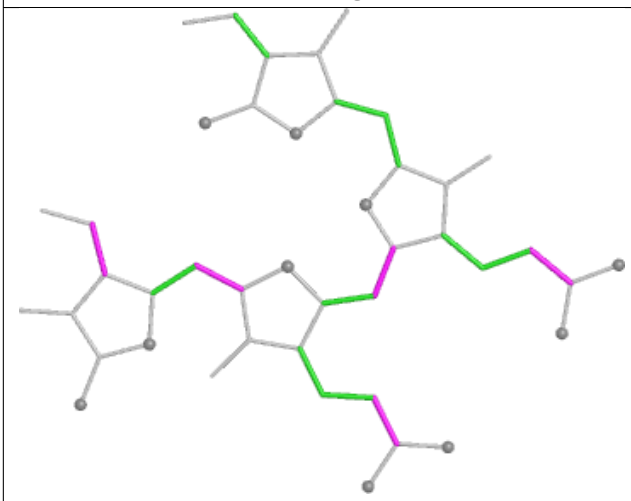


Bond angles



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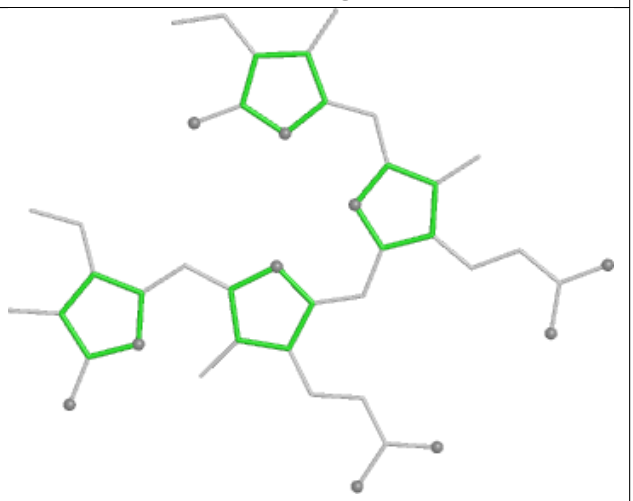

Rings

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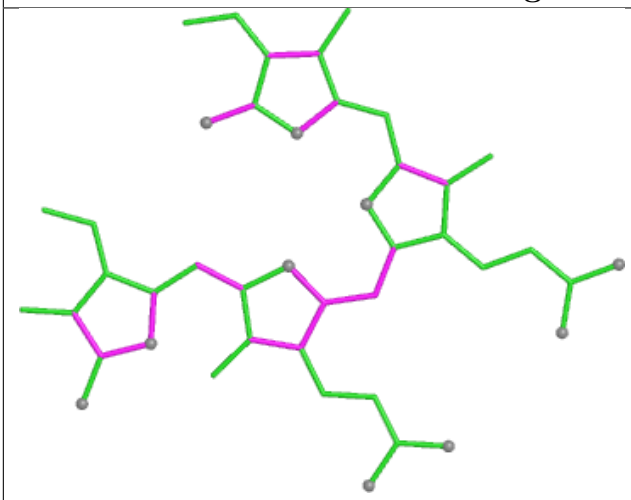

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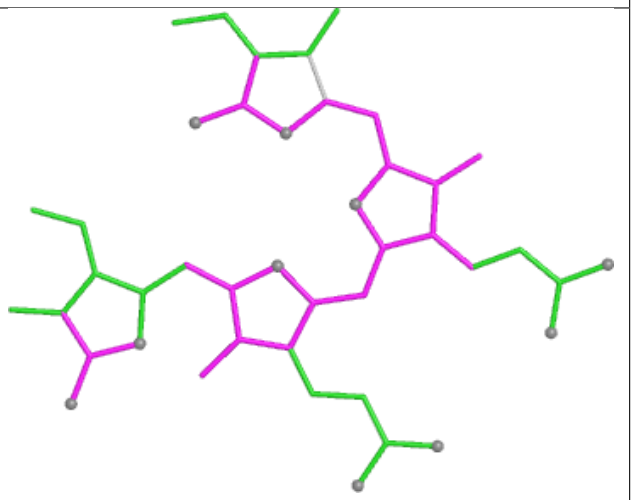
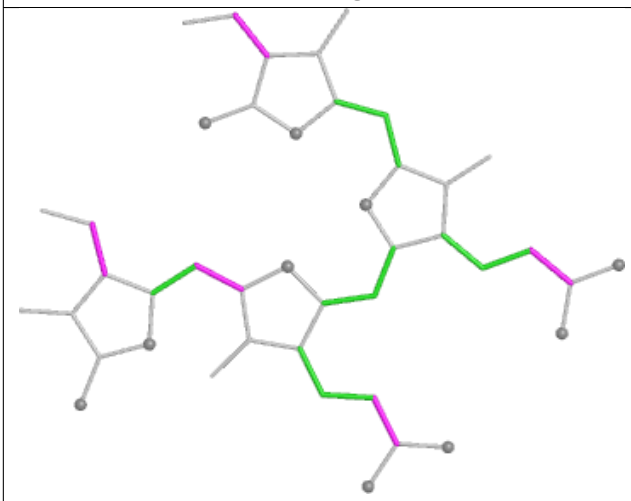
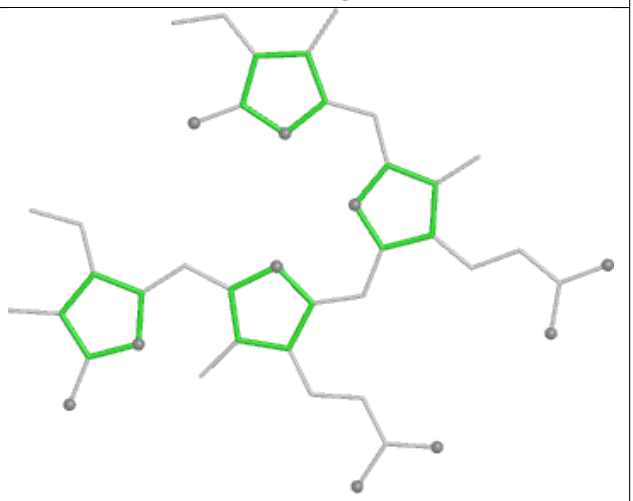


Bond angles

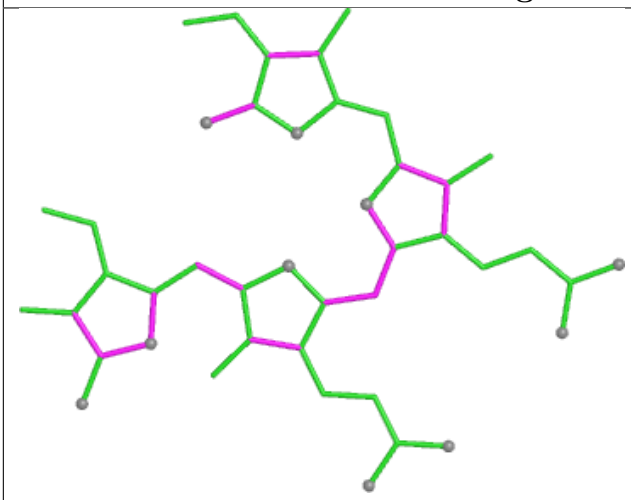


Torsions



Rings

Ligand PEB TJ 202



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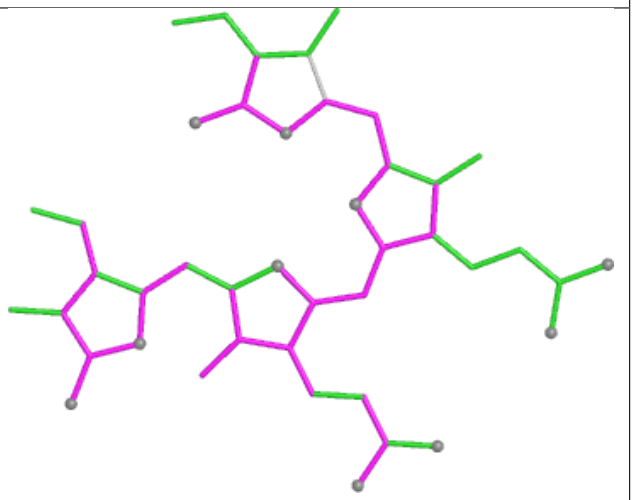
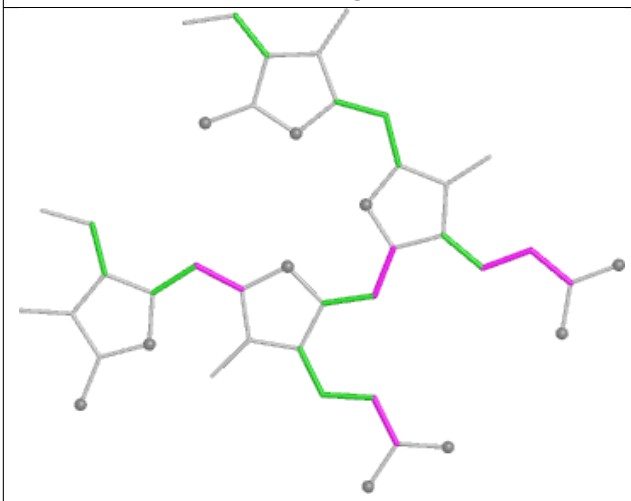


Bond angles



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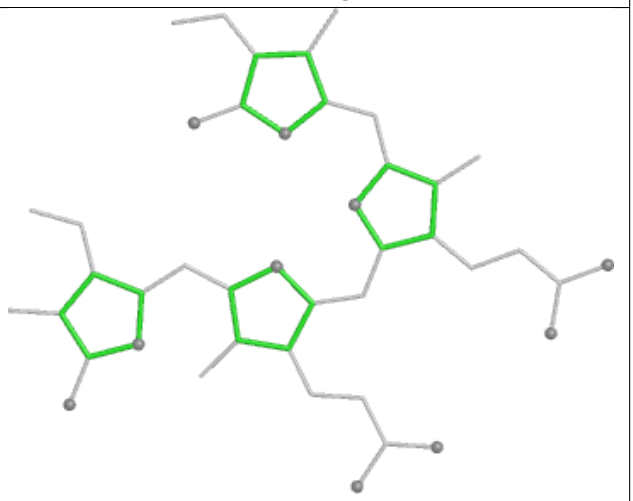
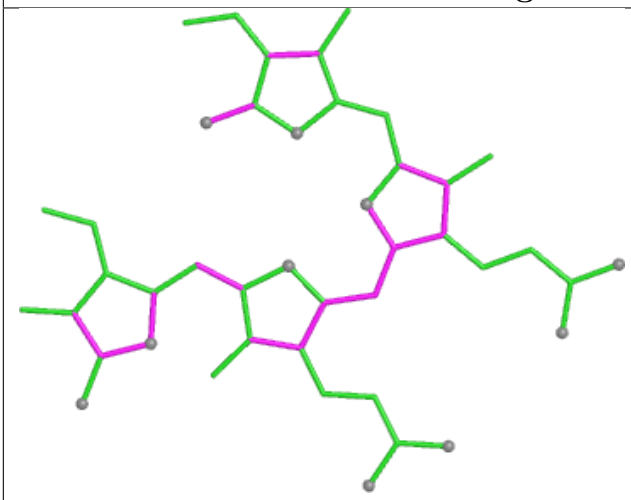


Rings

Ligand PEB dE 203



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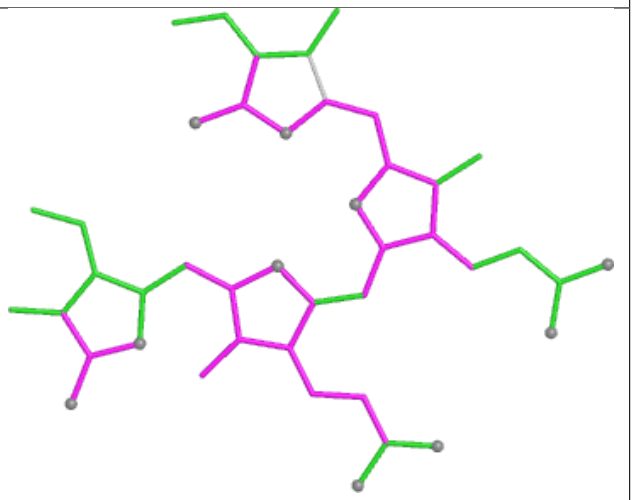

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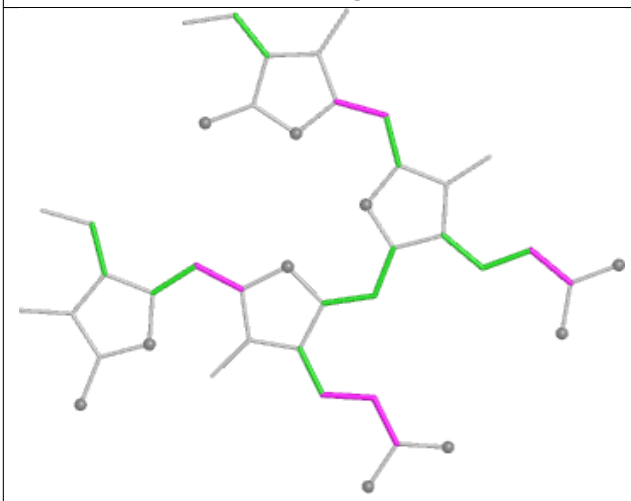

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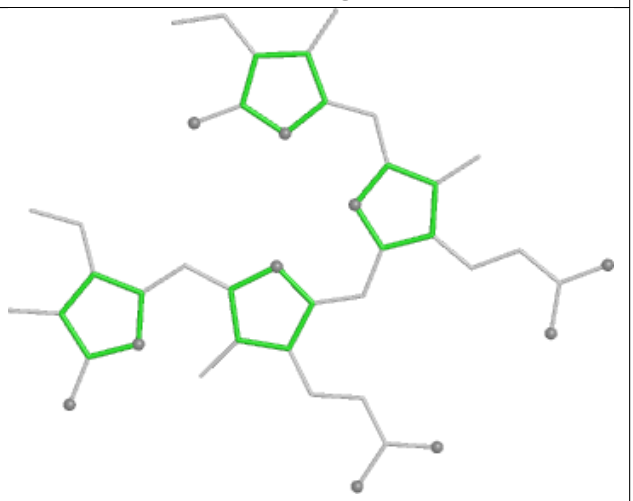
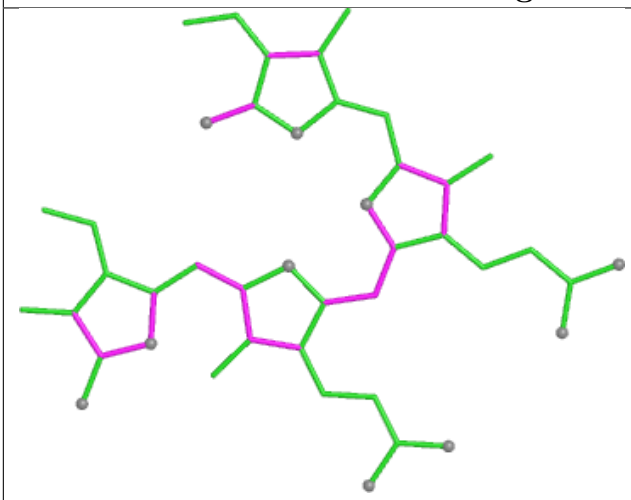


Rings

Ligand PEB JB 201



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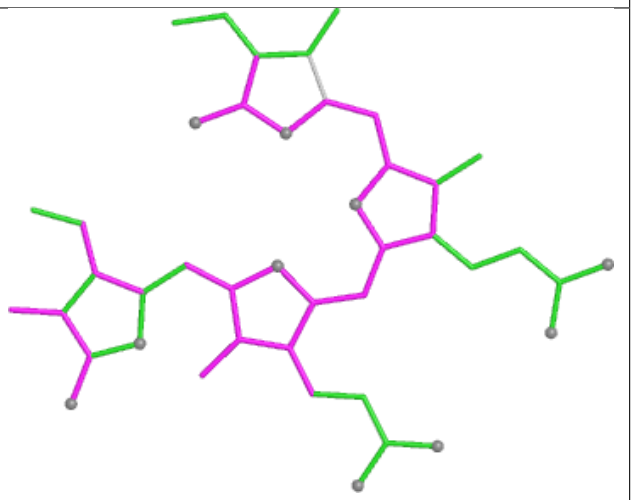

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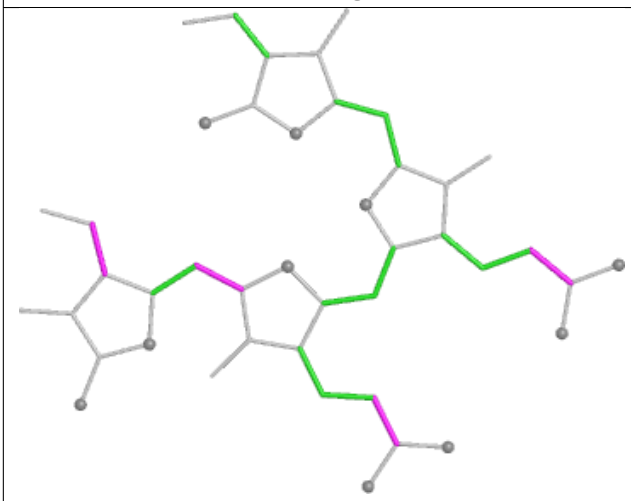

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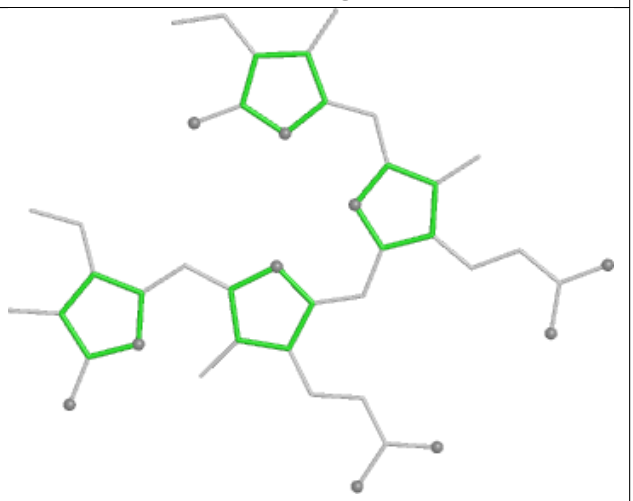

Rings

Ligand BCR C6 507



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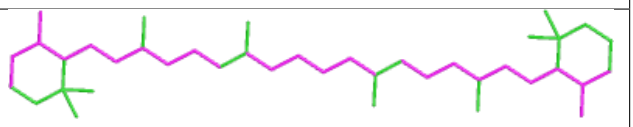

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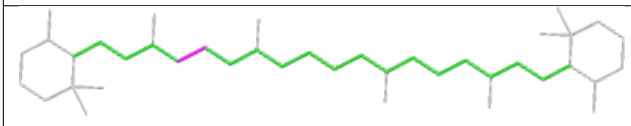

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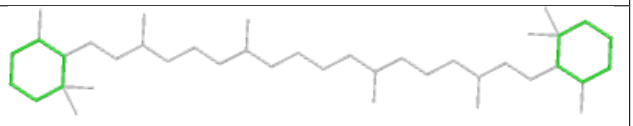
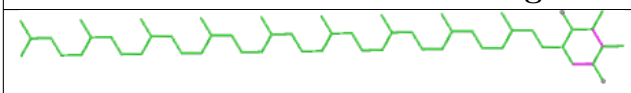


Rings

Ligand PL9 a6 601



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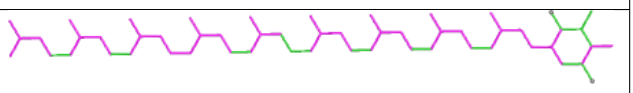

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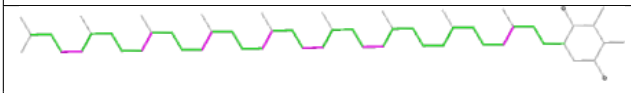

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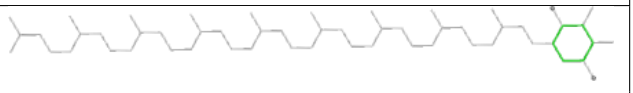
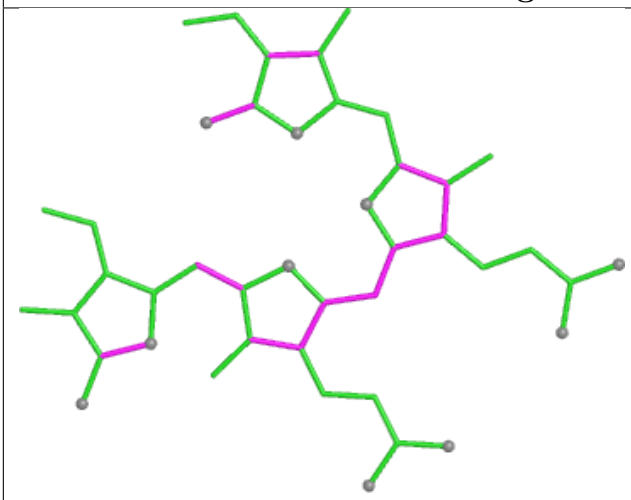


Rings

Ligand PEB xF 304



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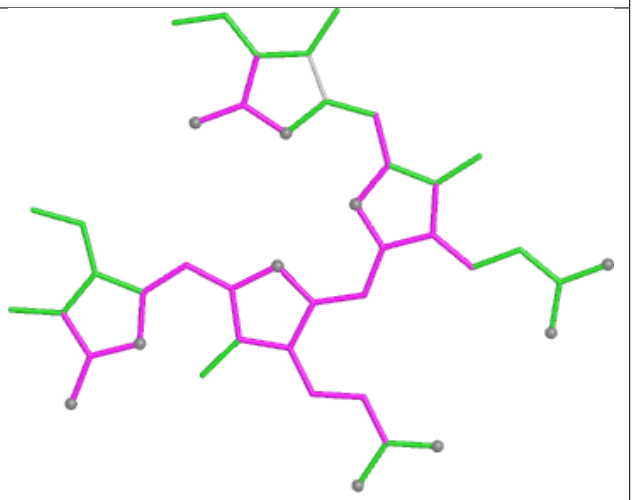
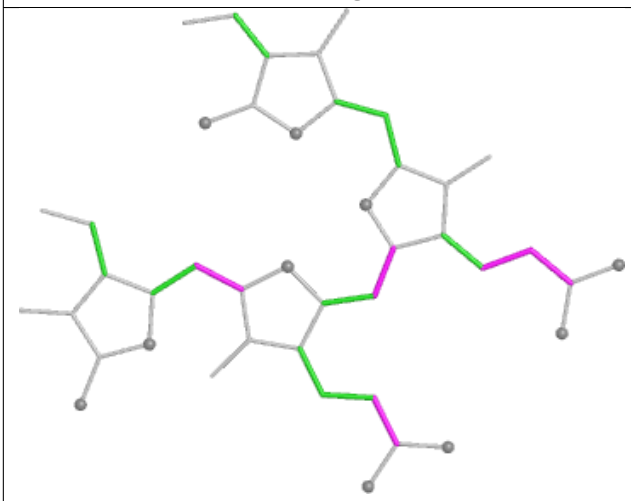


Bond angles



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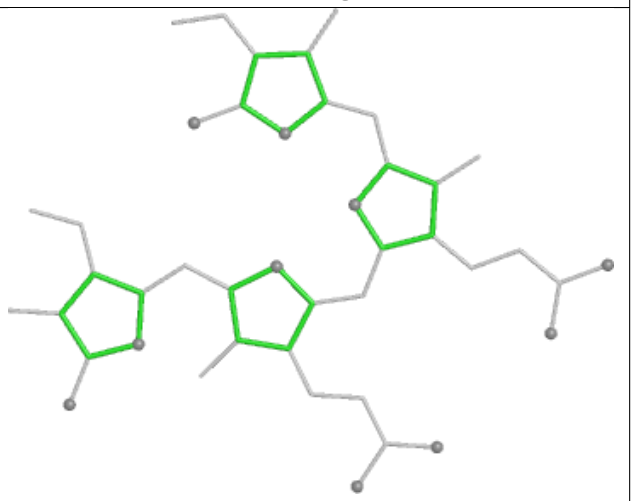
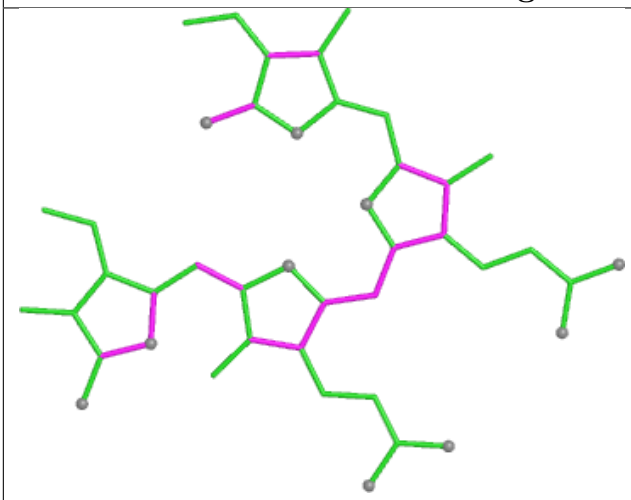


Rings

Ligand PEB sC 203



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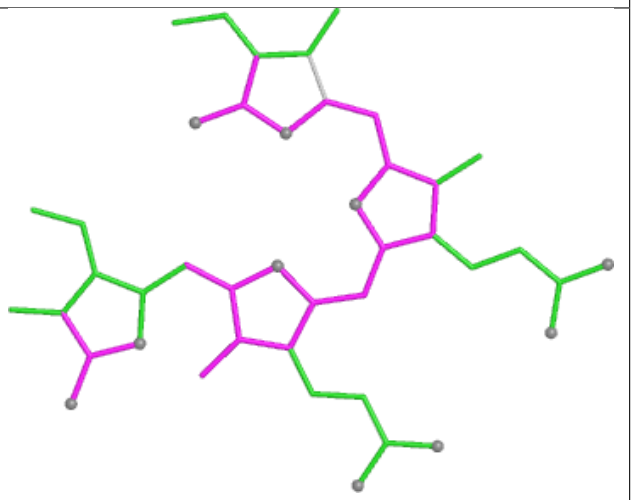

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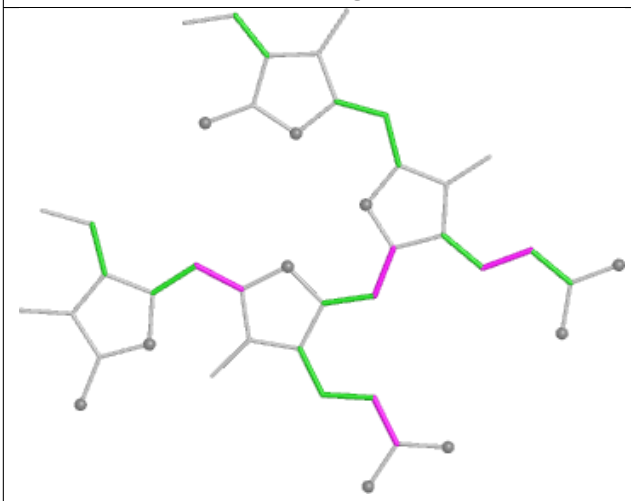

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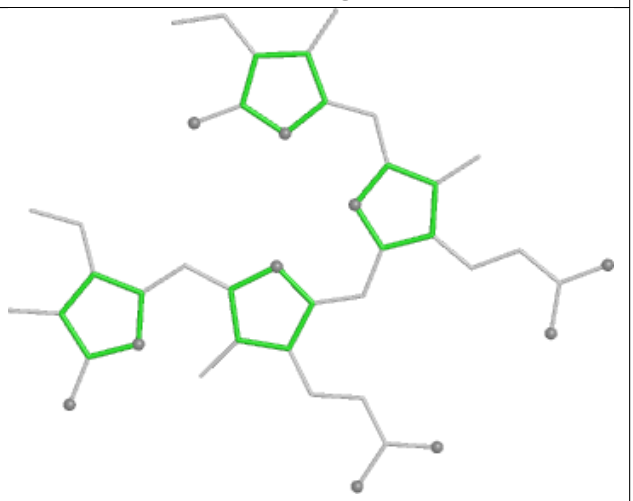
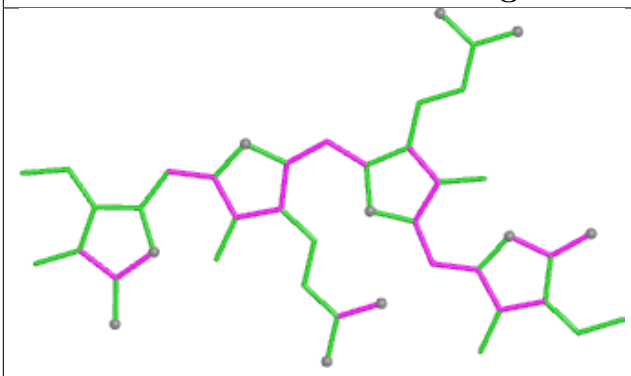


Rings

Ligand CYC M3 1001



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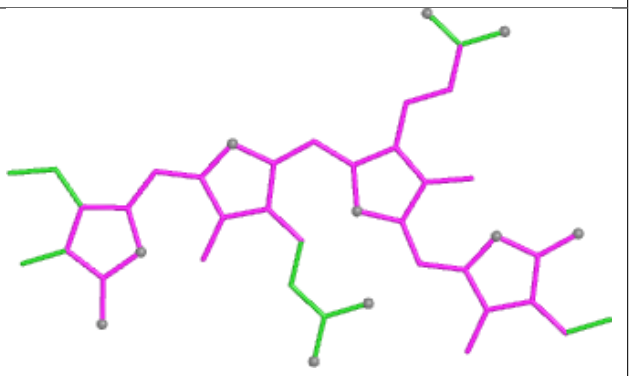

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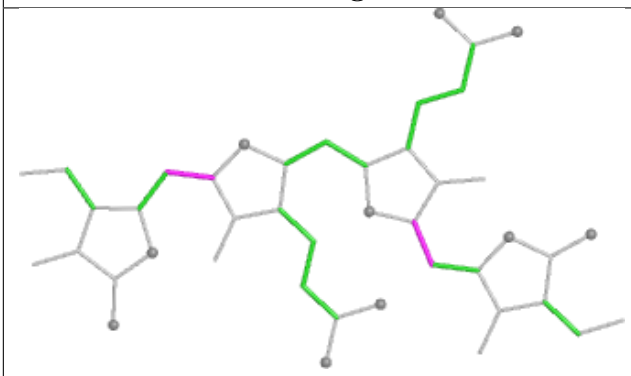

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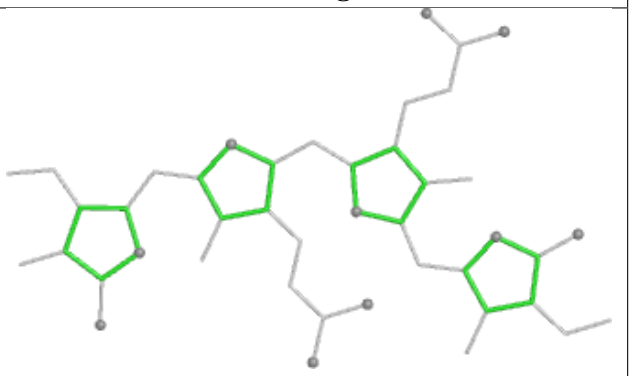
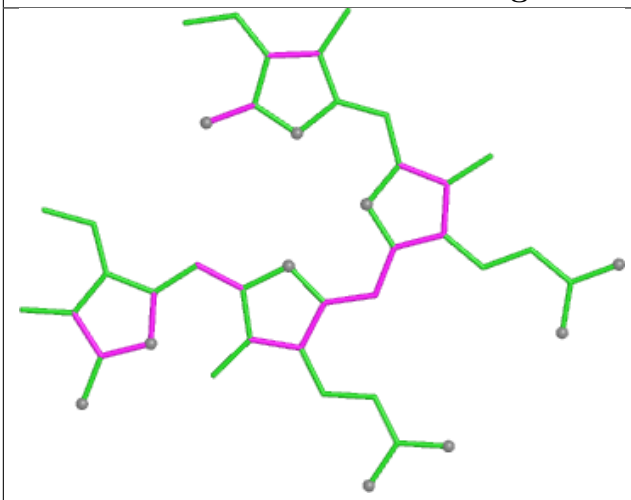


Rings

Ligand PEB CK 203



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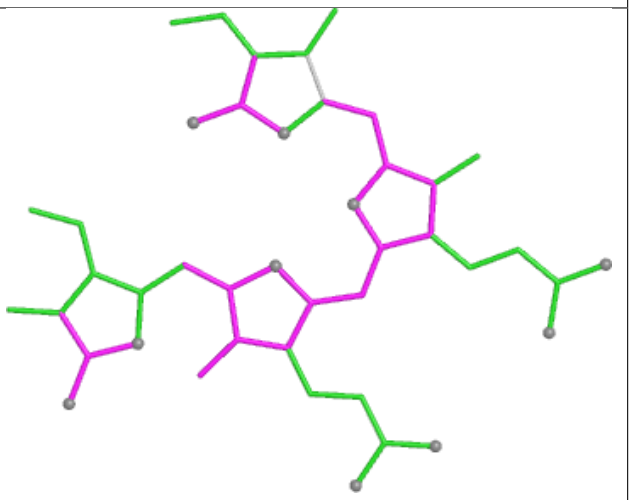

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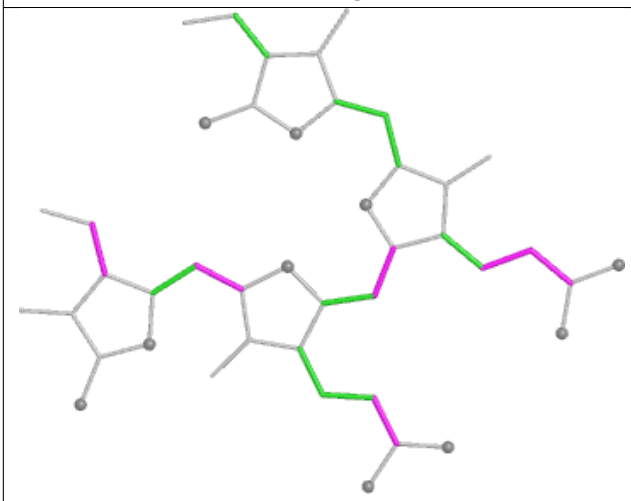

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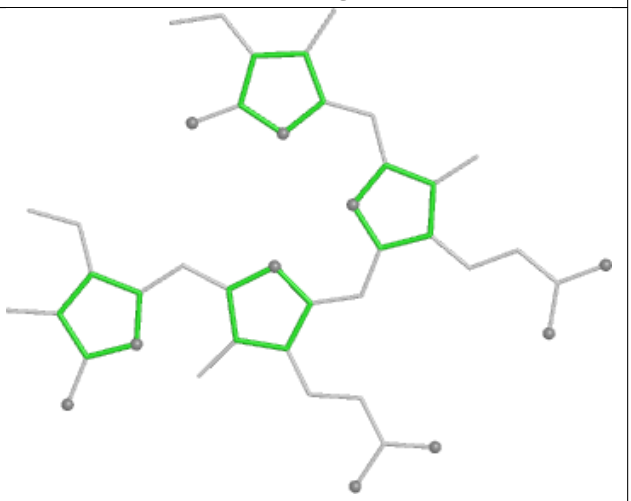
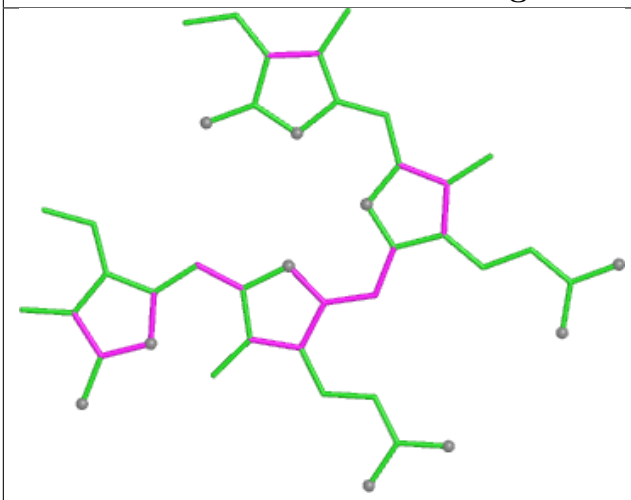


Rings

Ligand PEB GK 201



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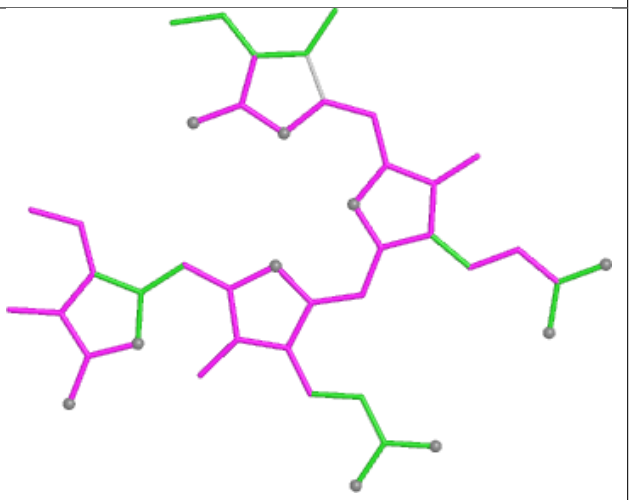

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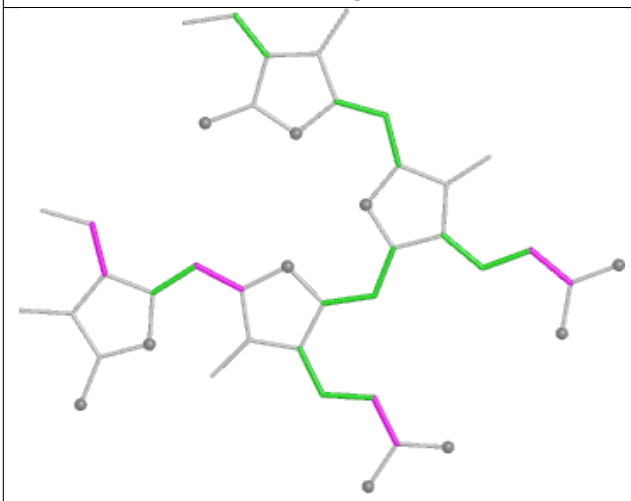

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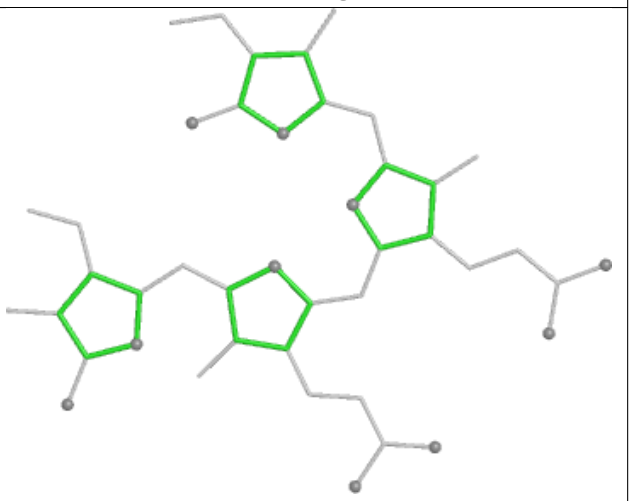
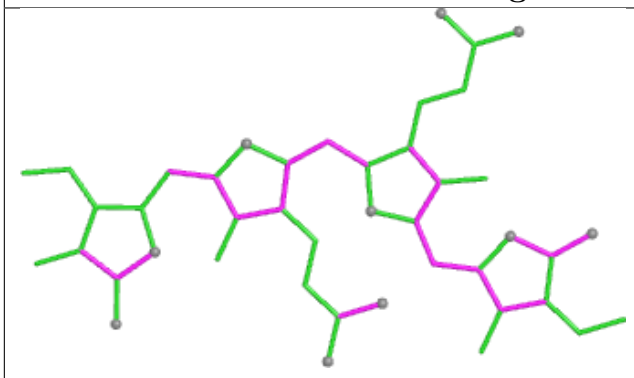


Rings

Ligand CYC o3 1001



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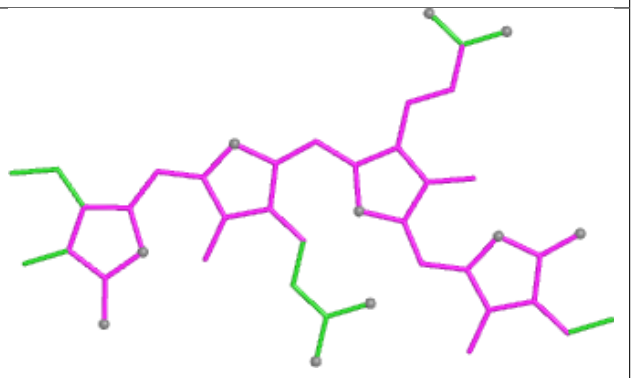

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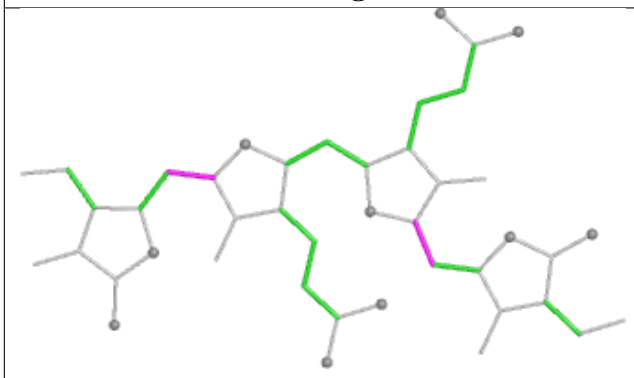

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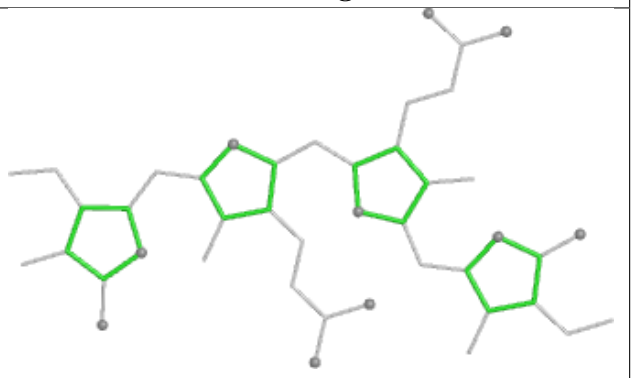
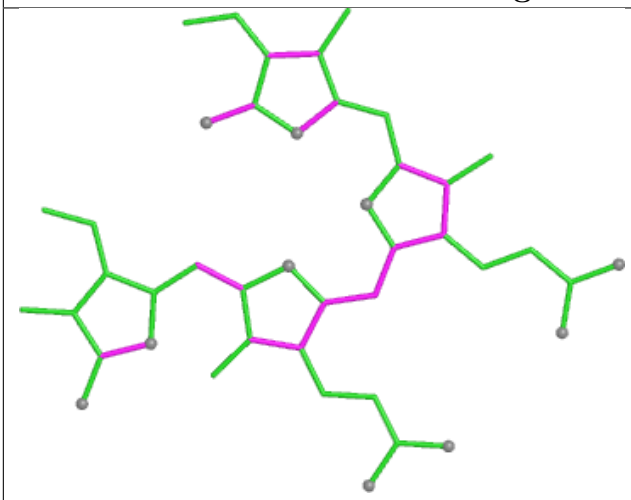


Rings

Ligand PEB bH 201



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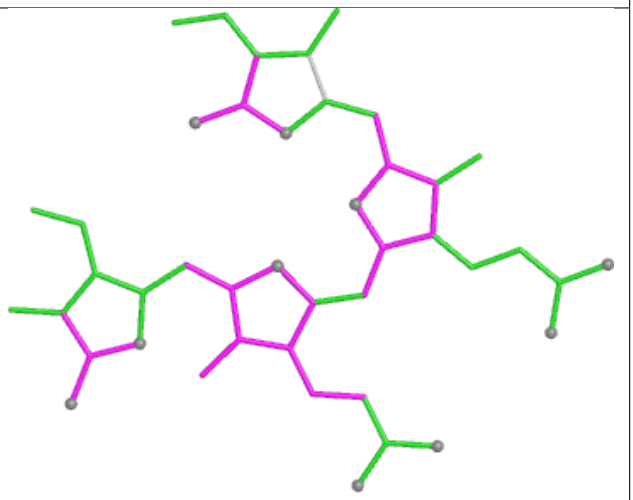
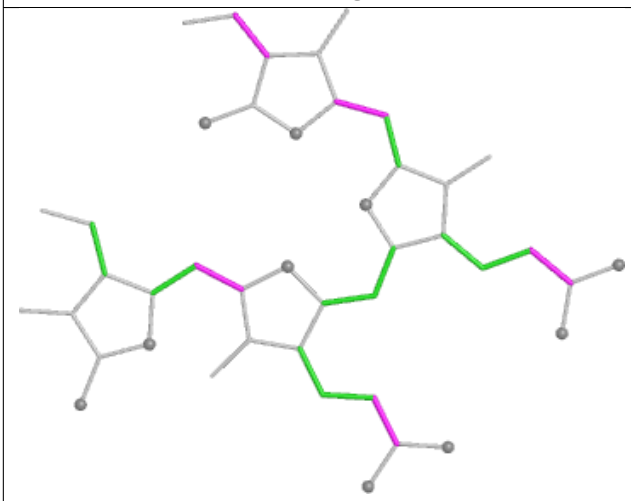


Bond angles



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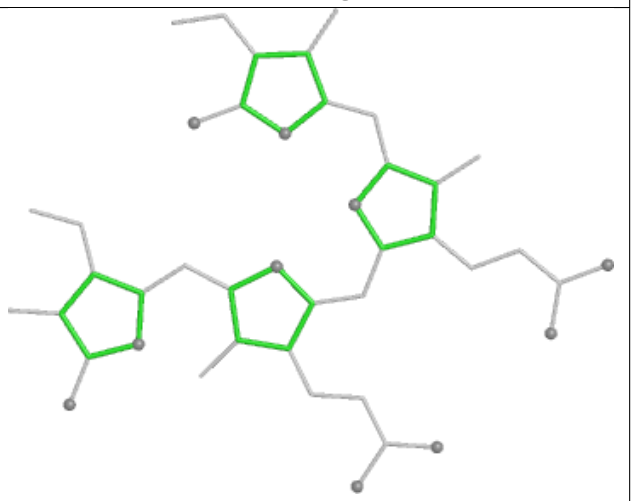
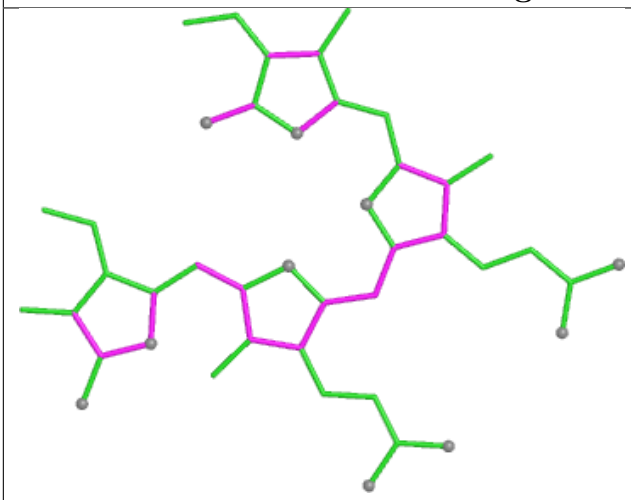


Rings

Ligand PEB uC 201



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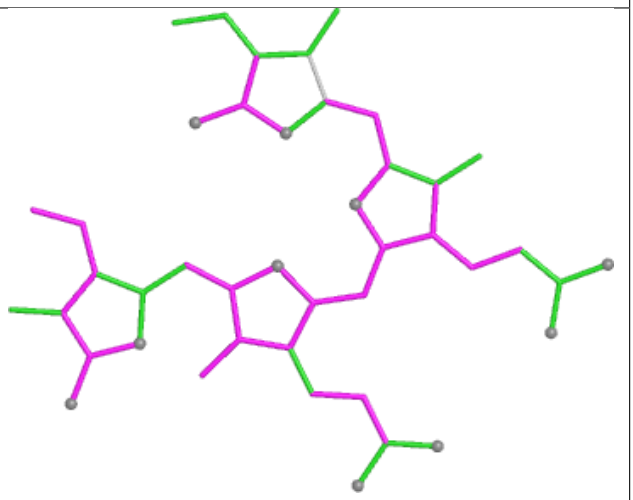
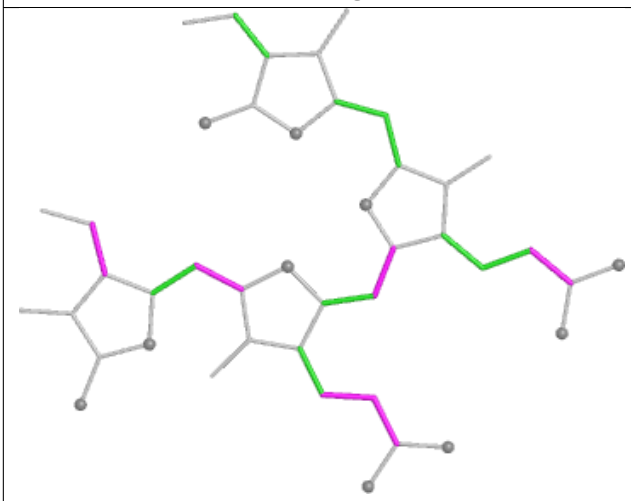


Bond angles



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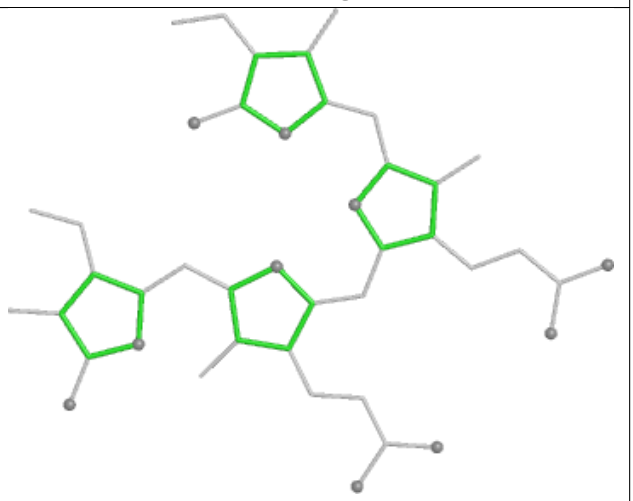
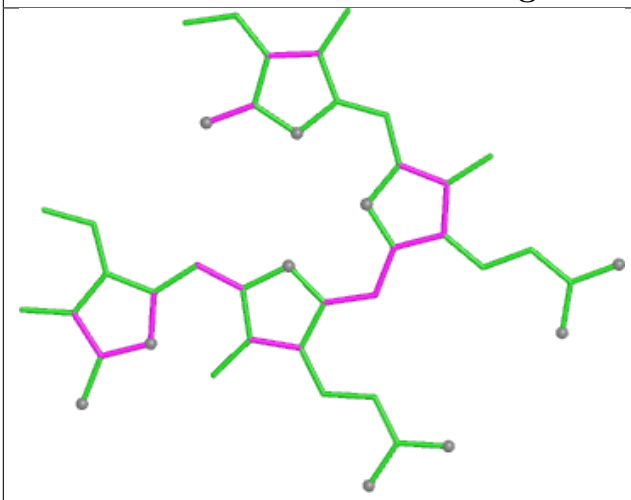


Rings

Ligand PEB S1 202



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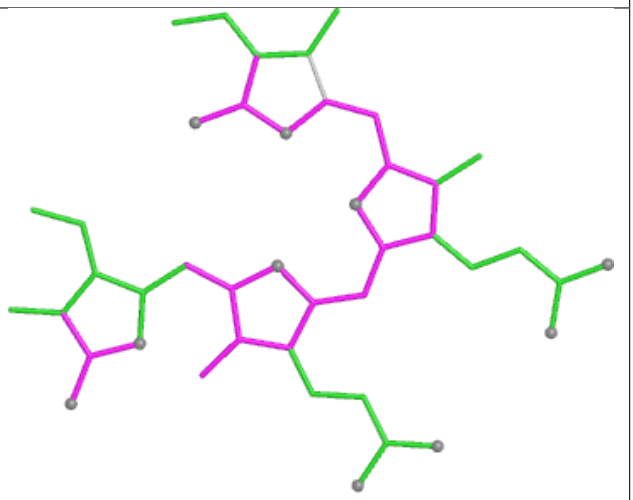
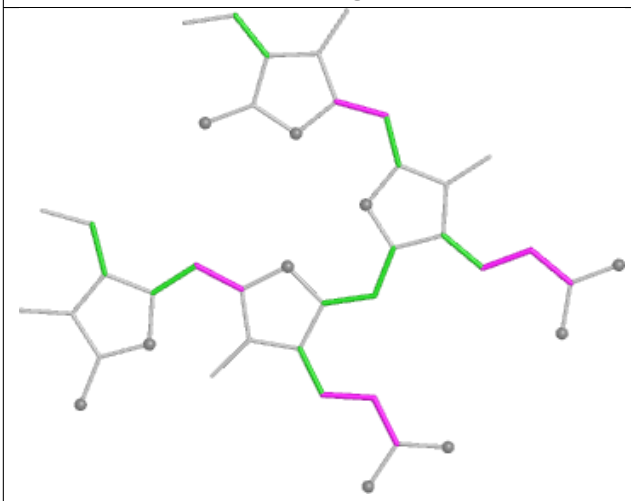


Bond angles



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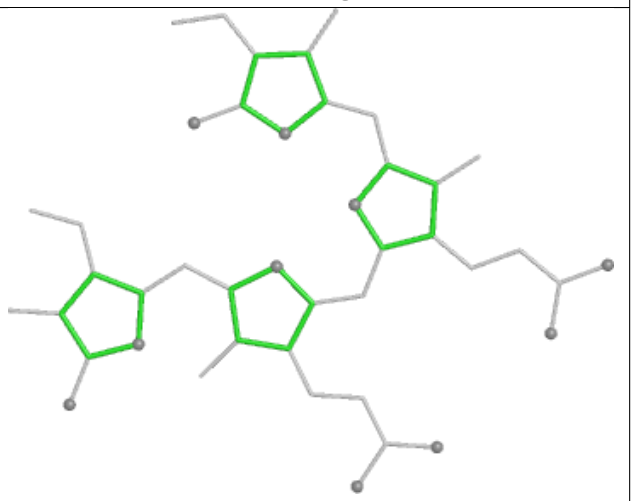
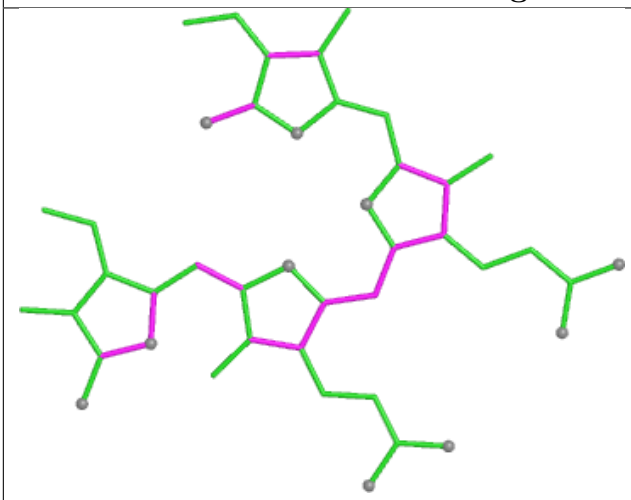


Rings

Ligand PEB YK 202



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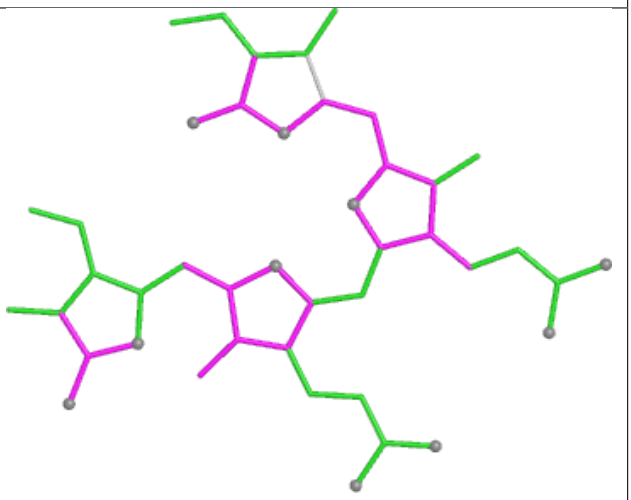
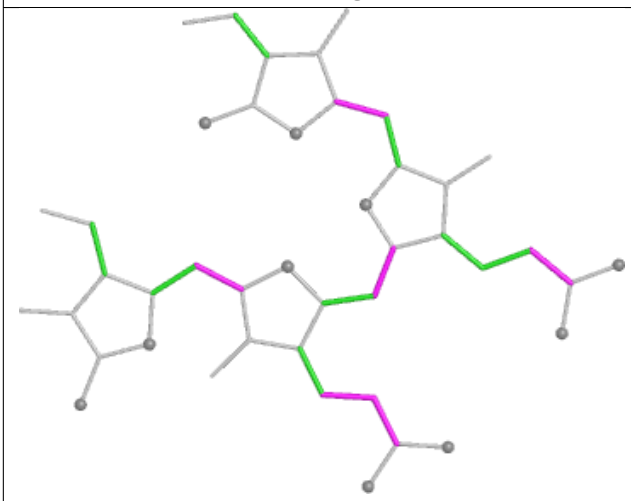
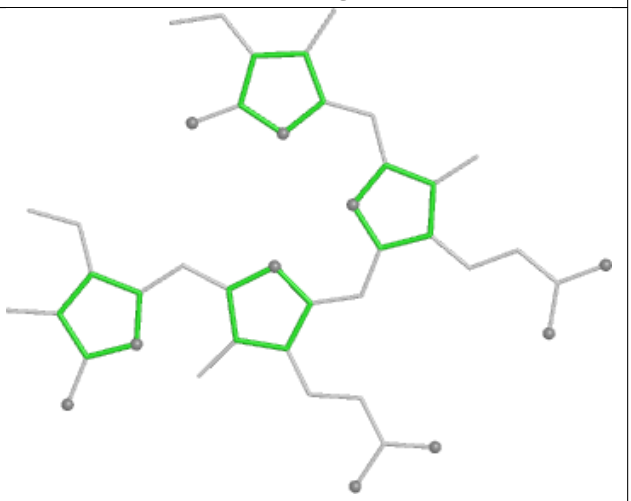


Bond angles

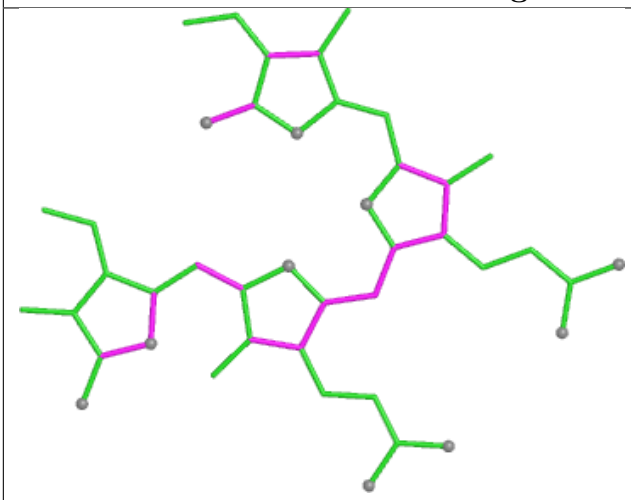


Torsions



Rings

Ligand PEB QH 201



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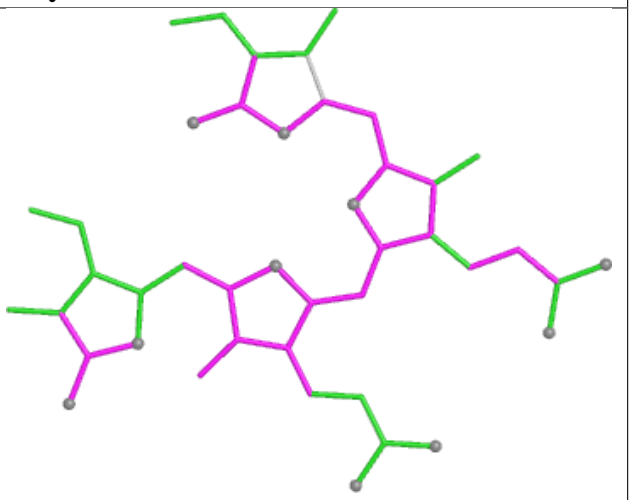

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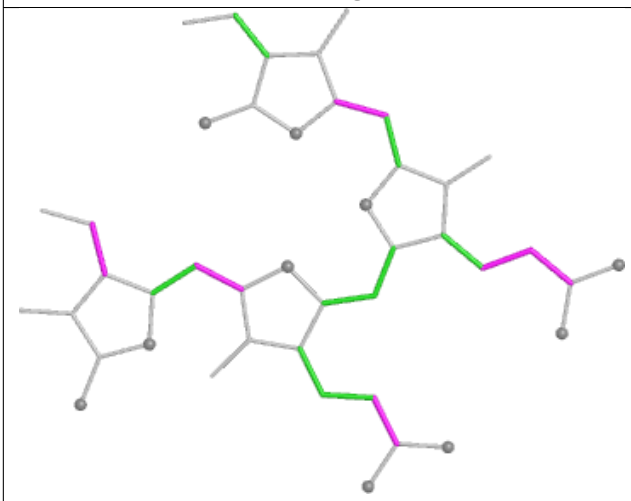

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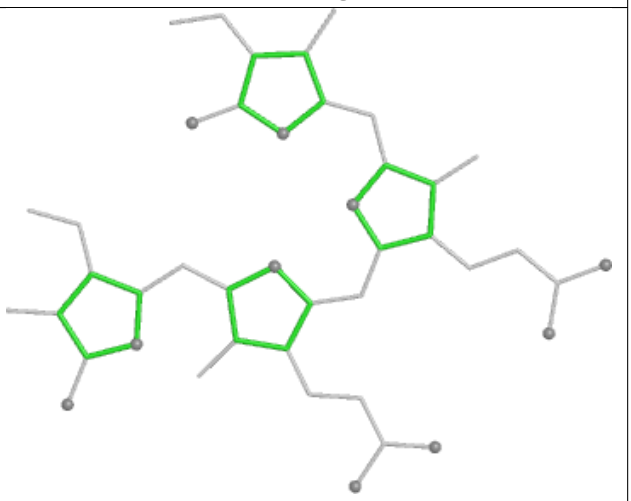
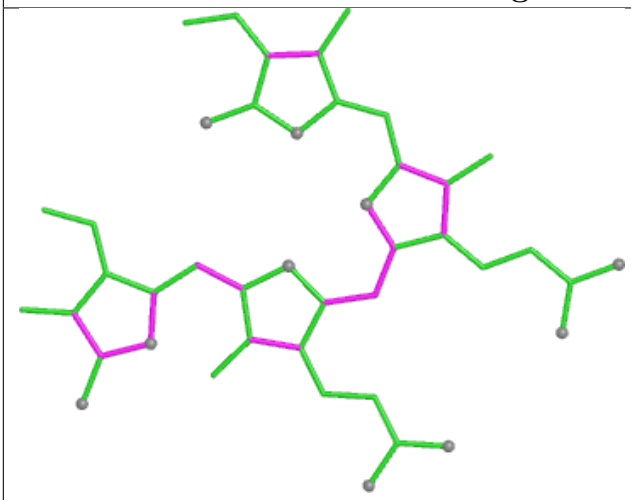


Rings

Ligand PEB MJ 202



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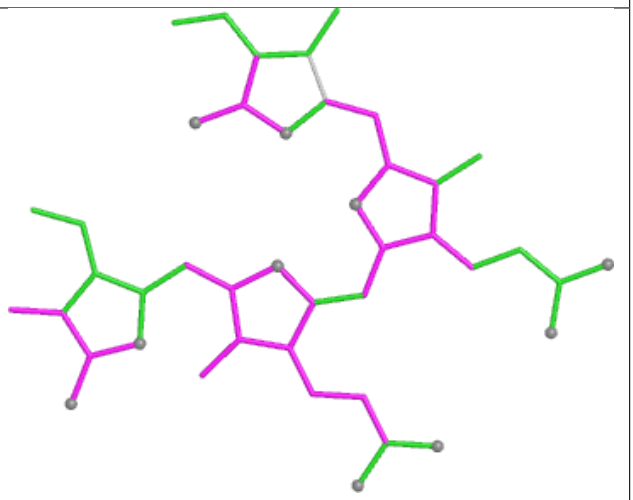

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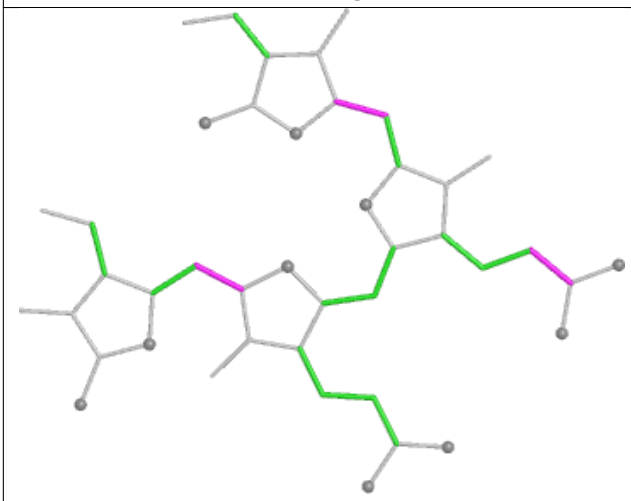

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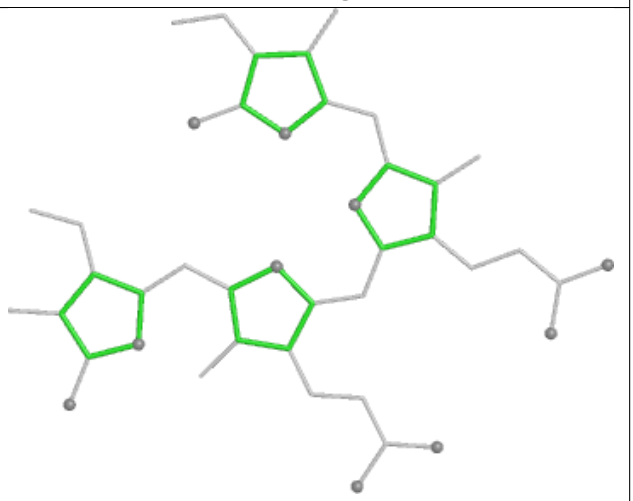
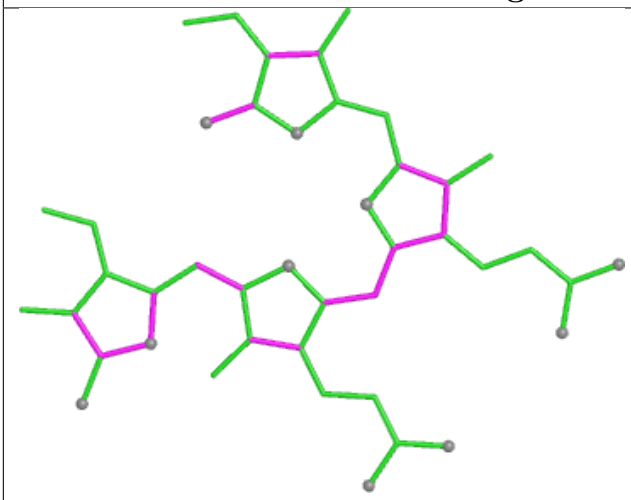


Rings

Ligand PEB MA 202



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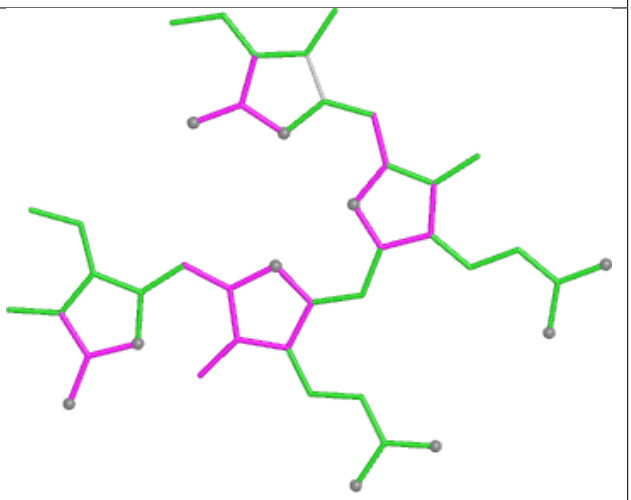

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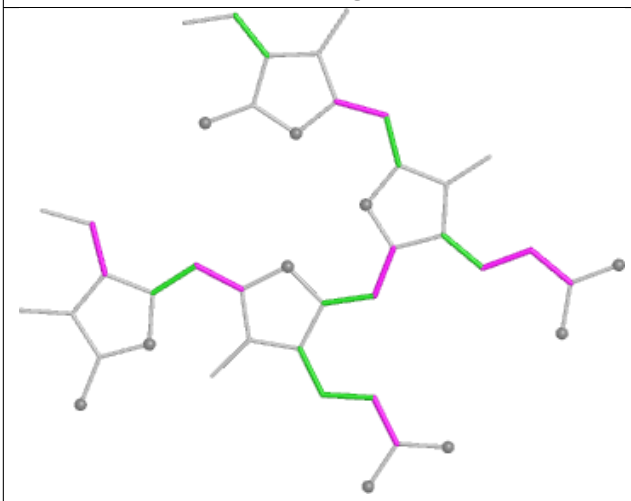

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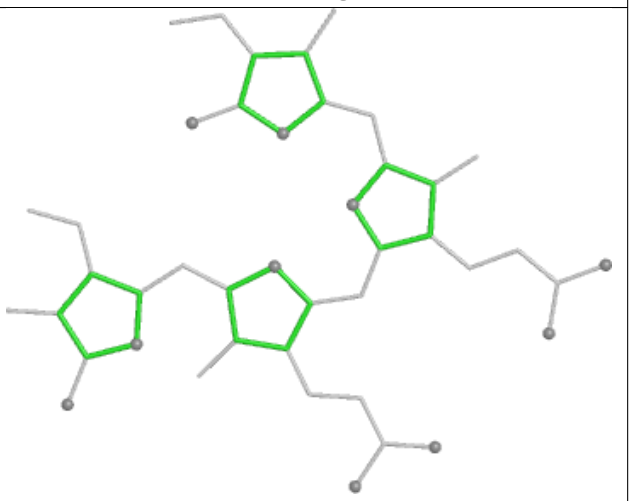
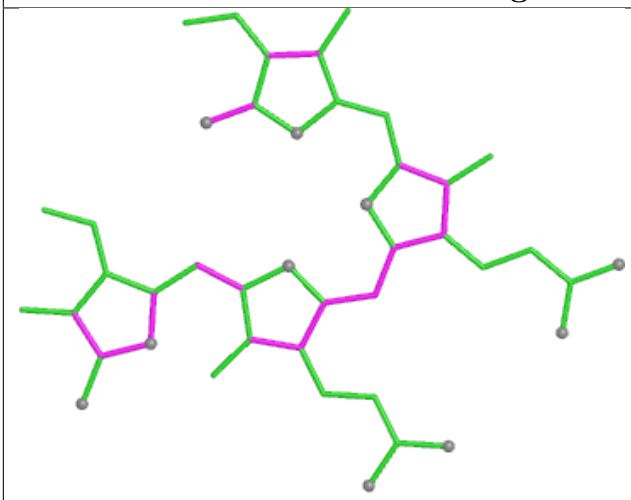


Rings

Ligand PEB YD 201



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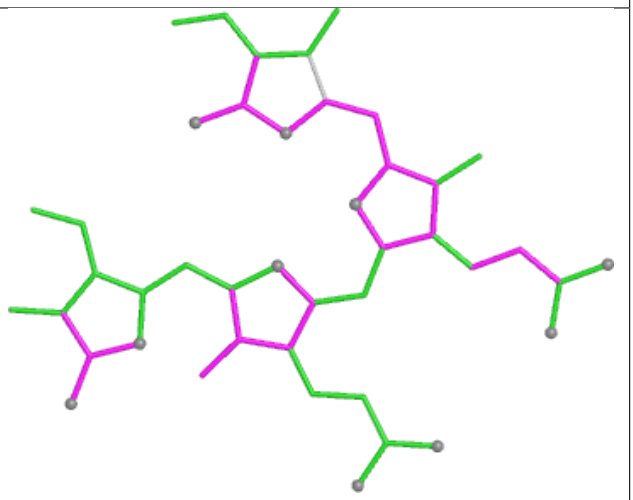
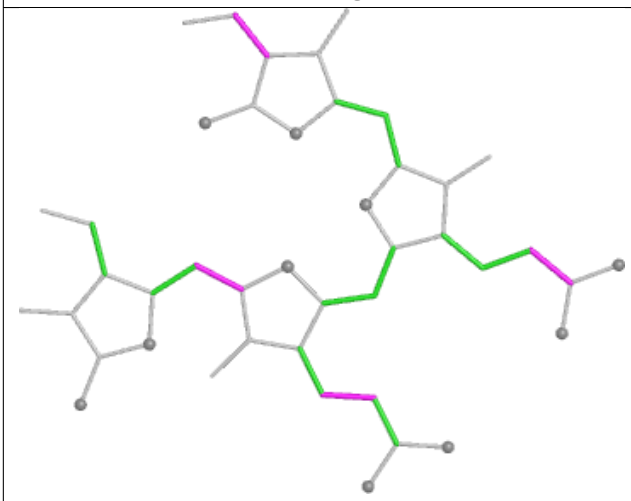


Bond angles



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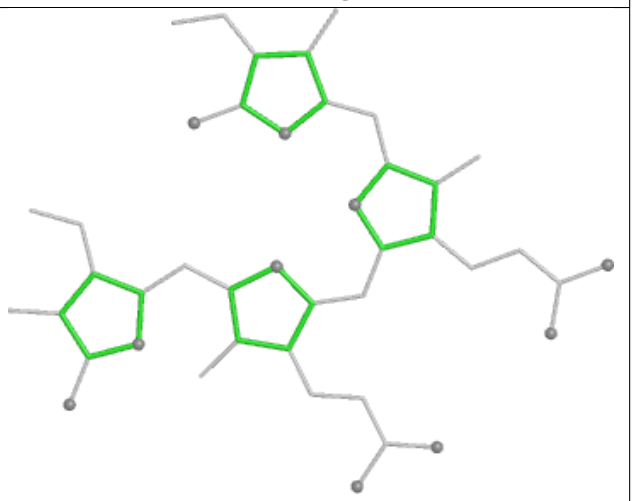
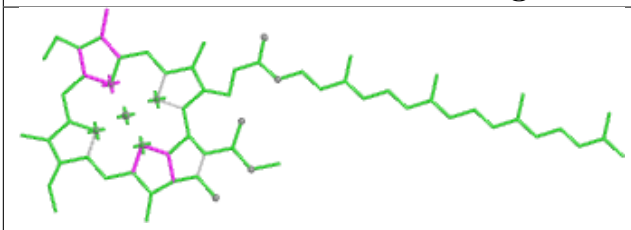


Rings

Ligand CLA BN 836



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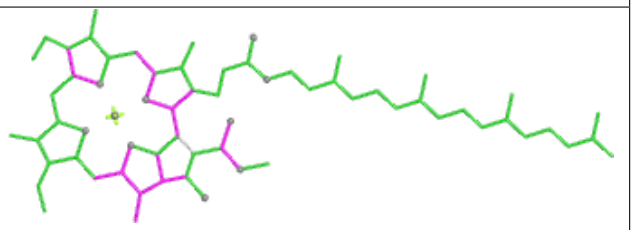

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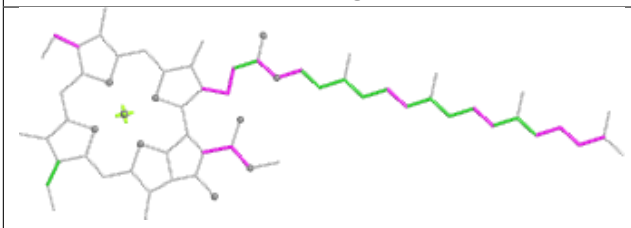

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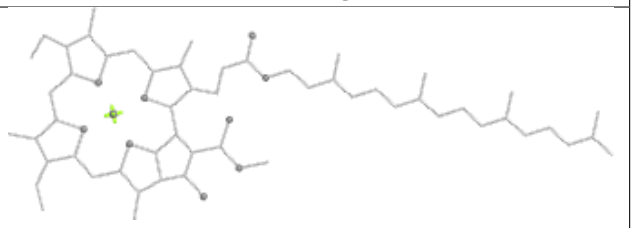
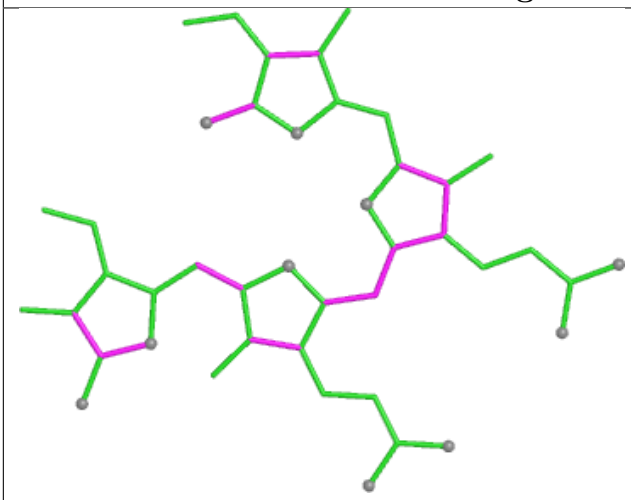


Rings

Ligand PEB pF 201



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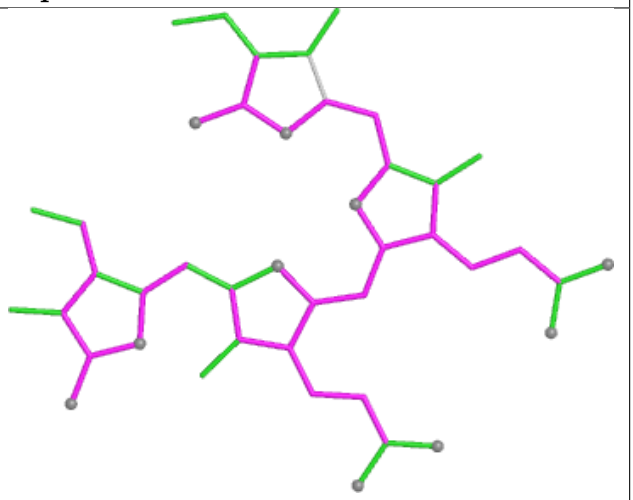
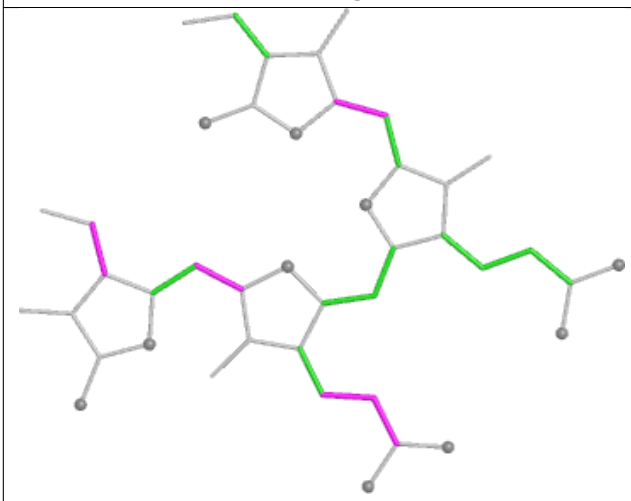


Bond angles



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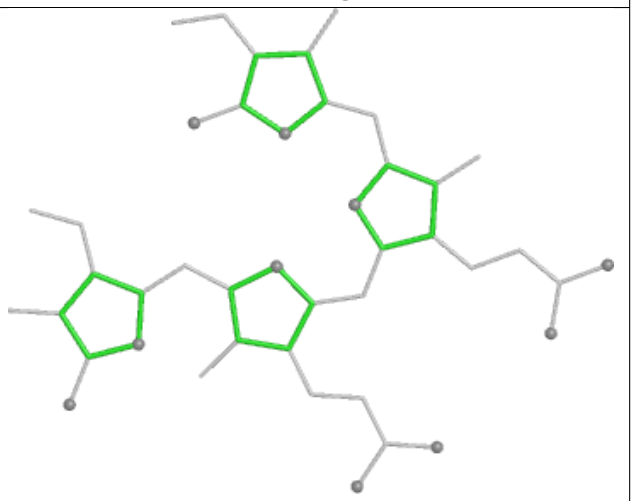
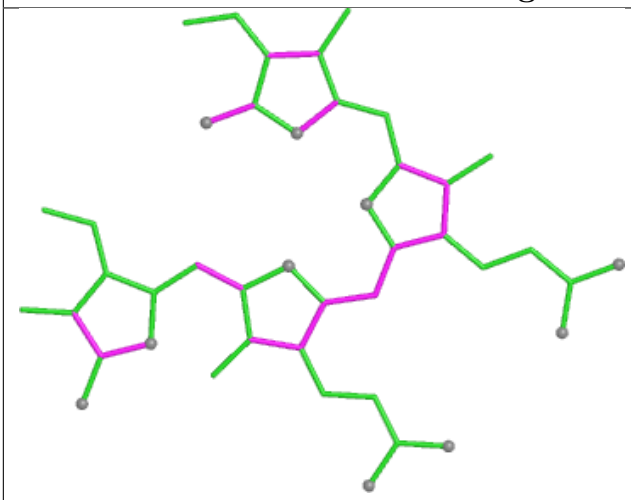


Rings

Ligand PEB jG 201



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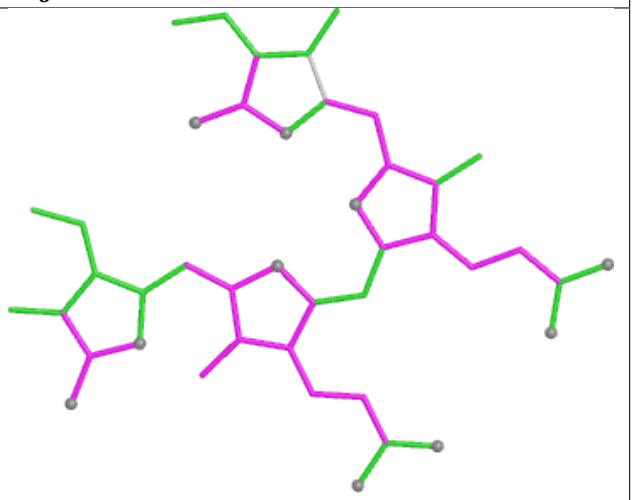

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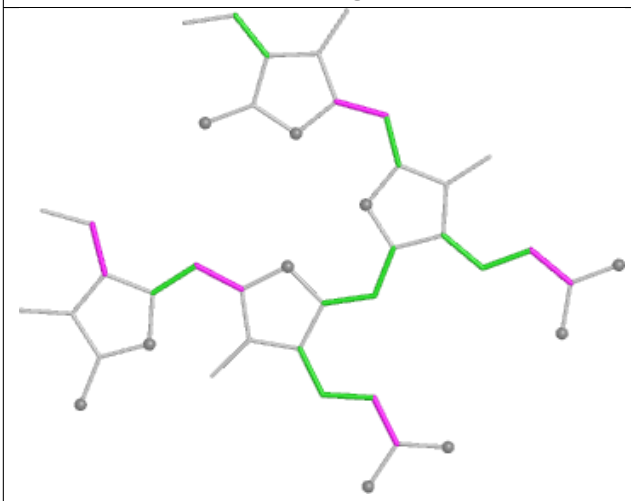

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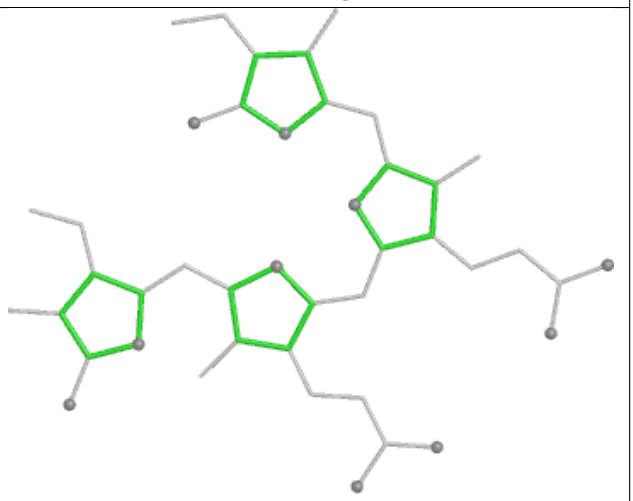
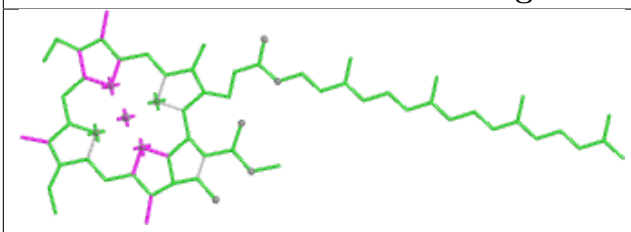


Rings

Ligand CLA B2 827



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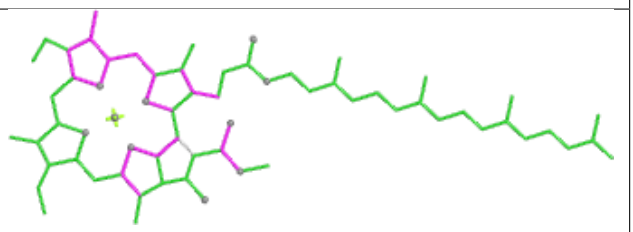

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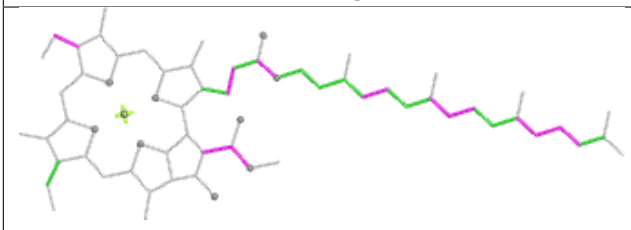

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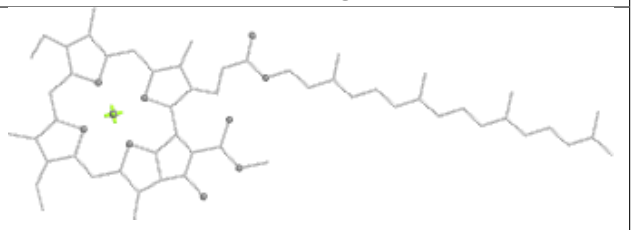
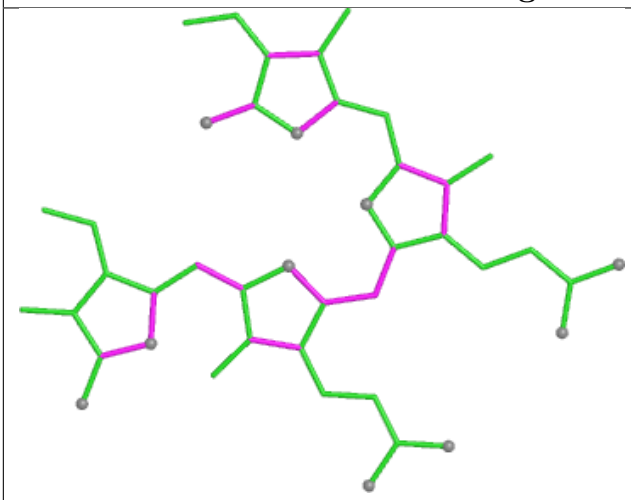


Rings

Ligand PEB BI 202



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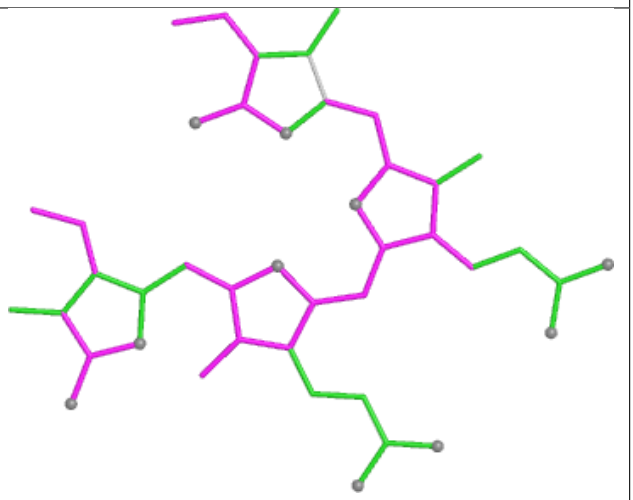
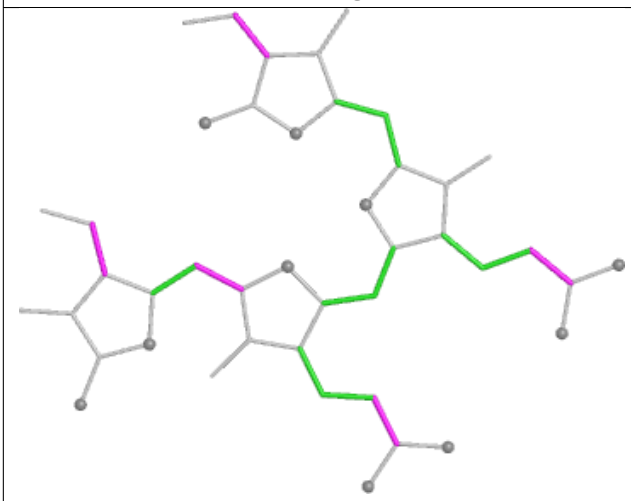


Bond angles



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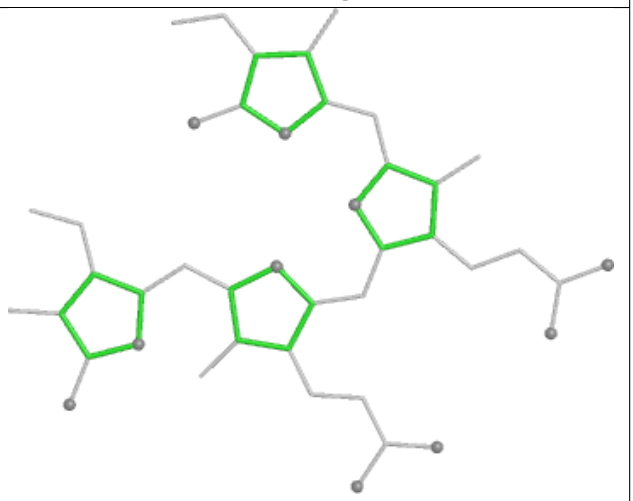
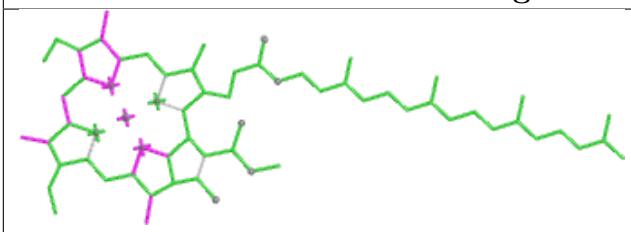


Rings

Ligand CLA AL 403



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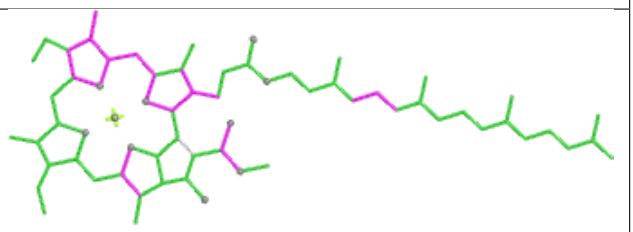
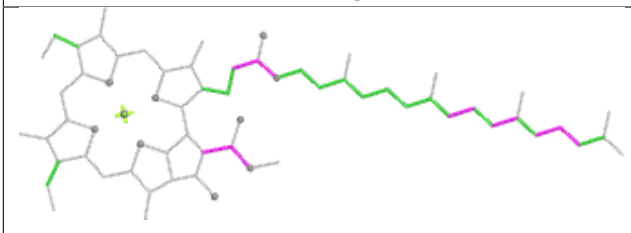


Bond angles



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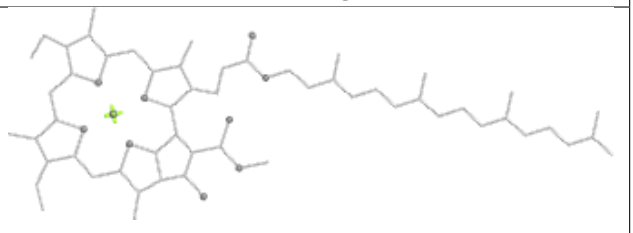
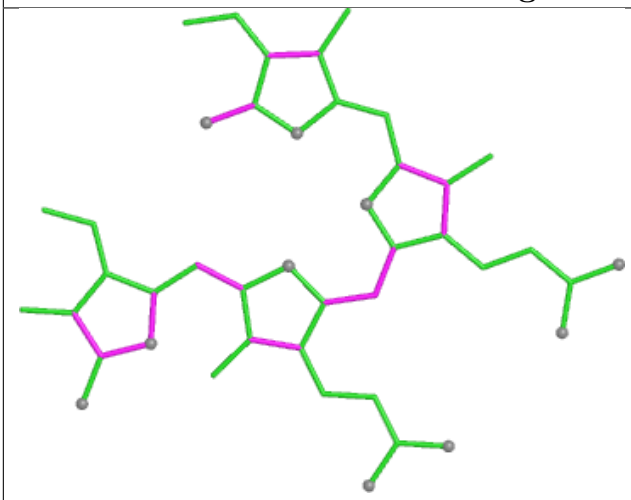


Rings

Ligand PEB b4 201



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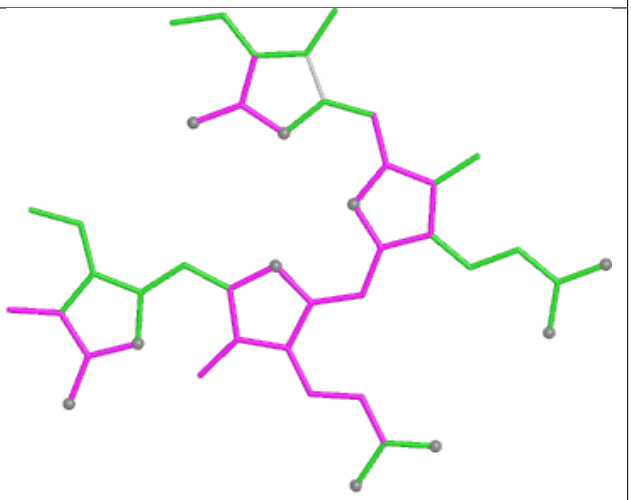
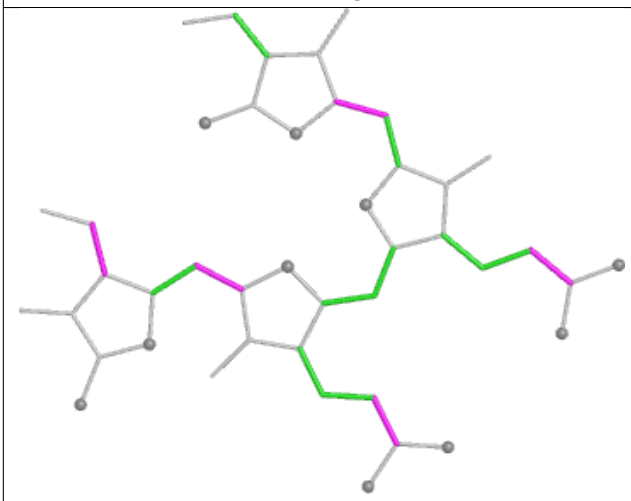


Bond angles



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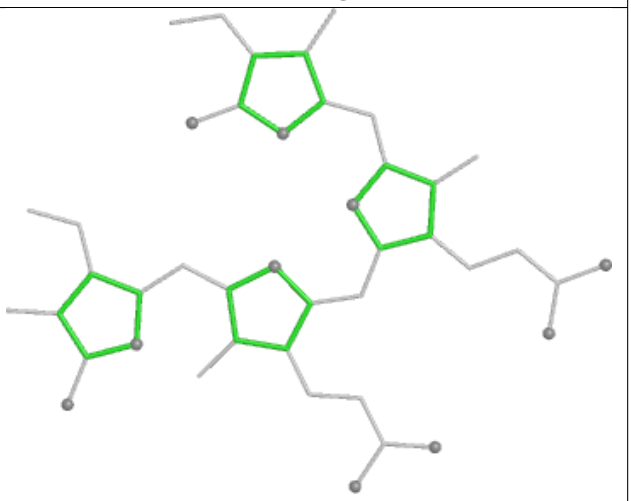
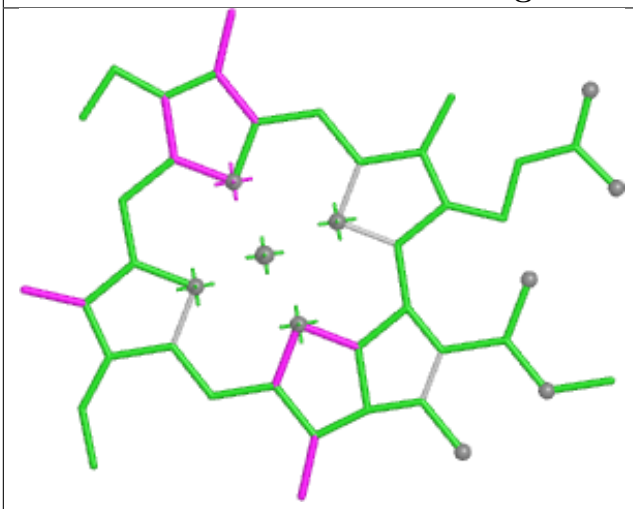


Rings

Ligand CLA A2 818



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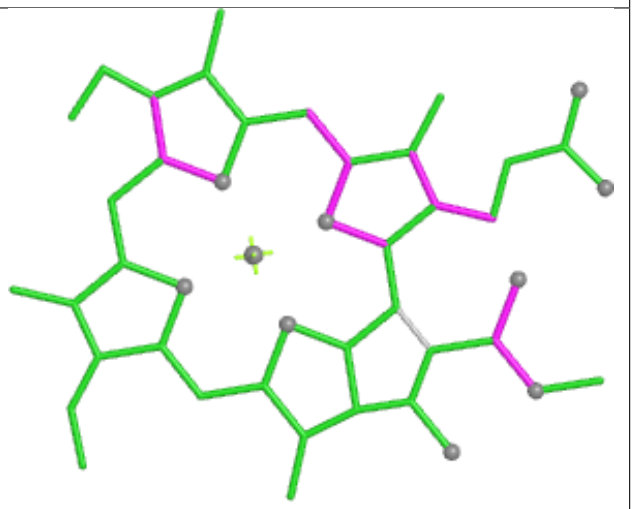

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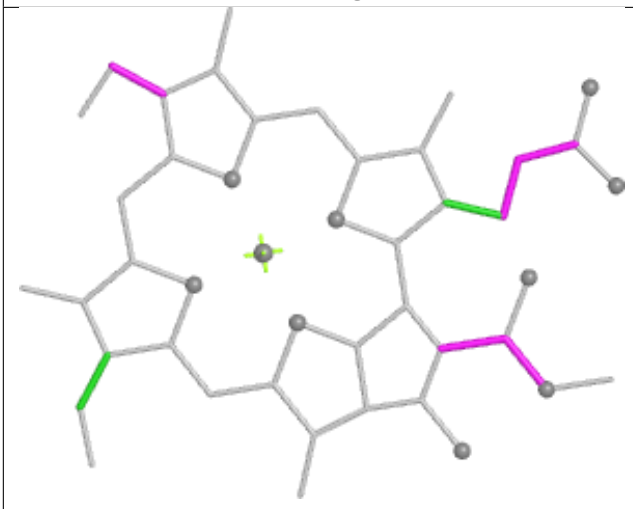
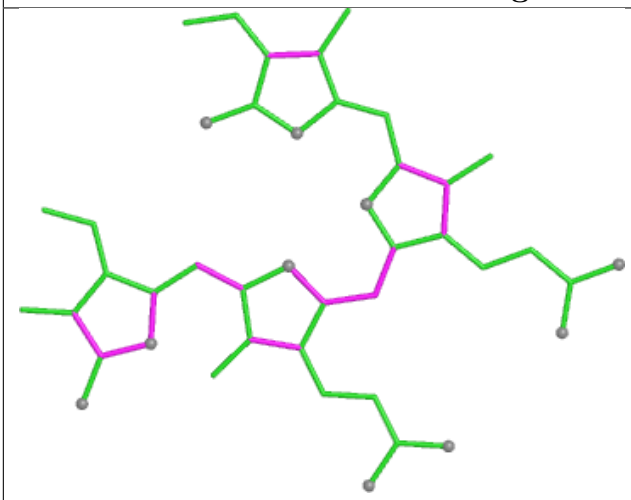


Torsions



Rings

Ligand PEB OA 201



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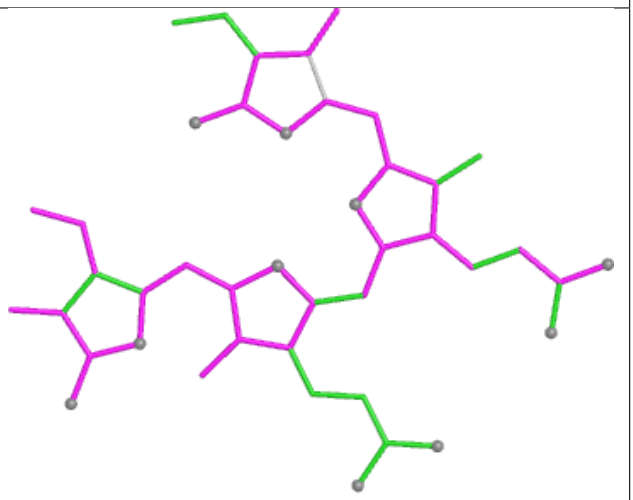
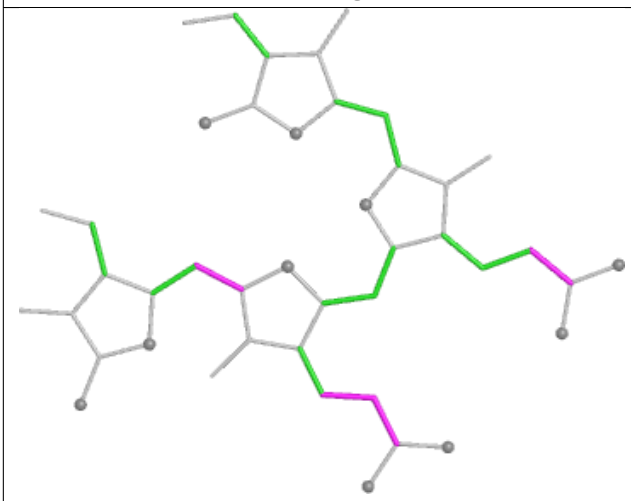


Bond angles



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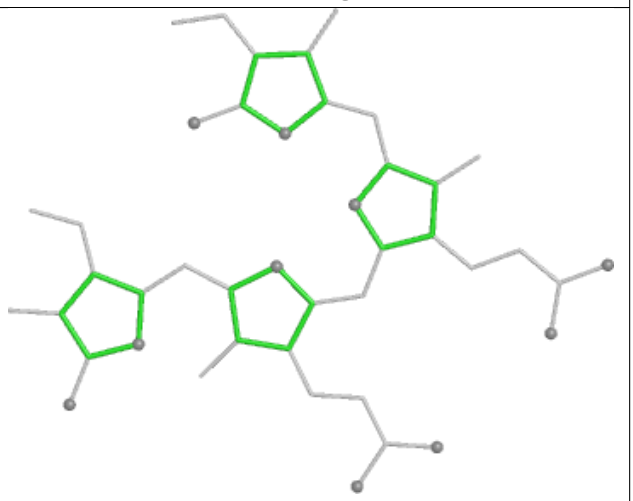
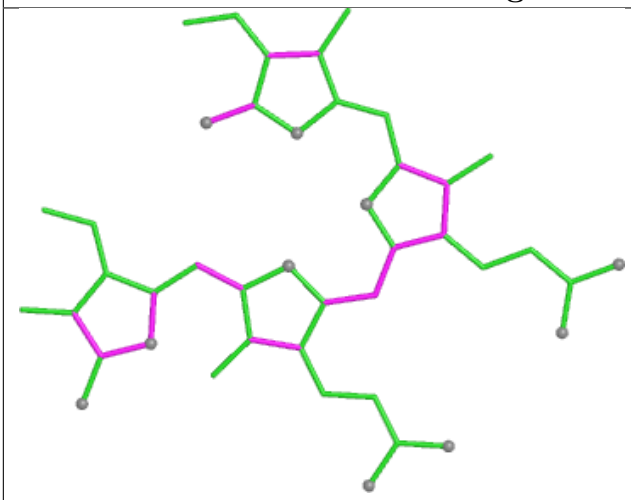
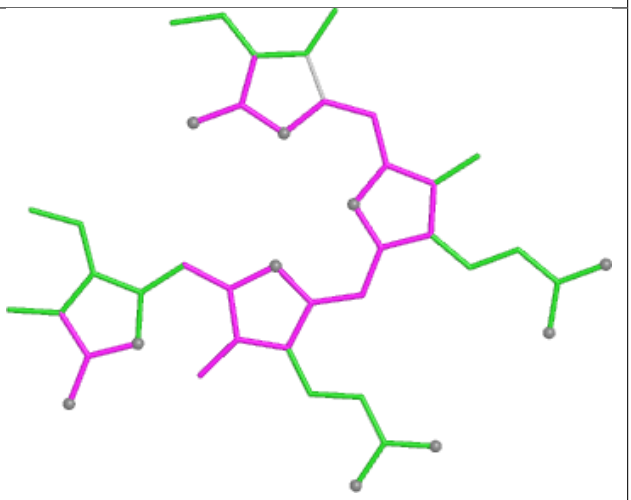


Rings

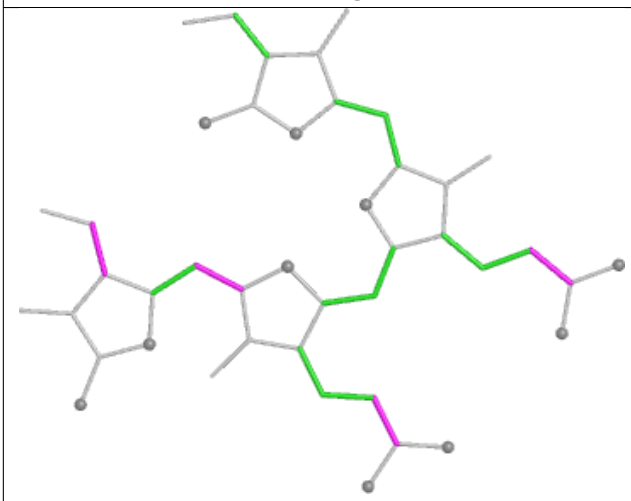
Ligand PEB GM 203



Bond lengths



Bond angles



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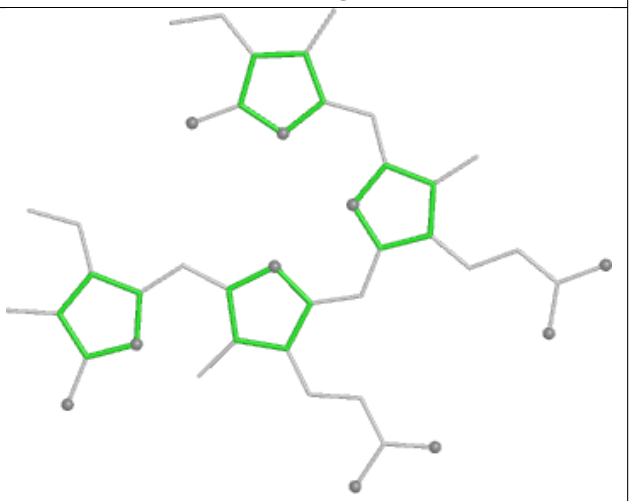
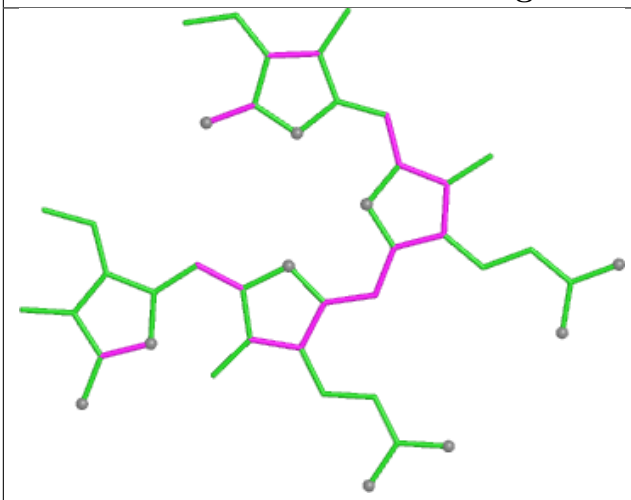
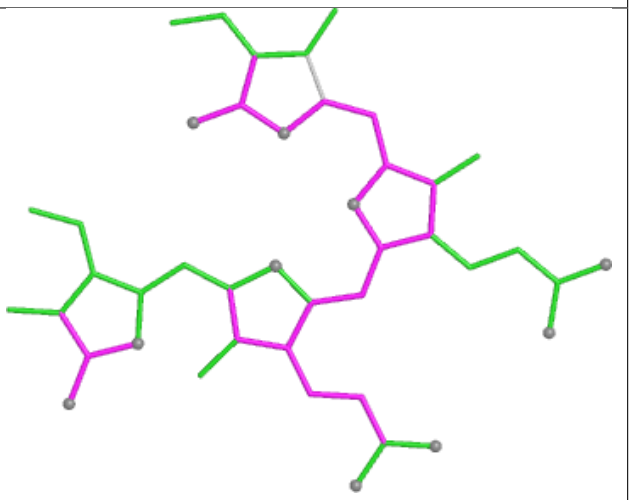


Rings

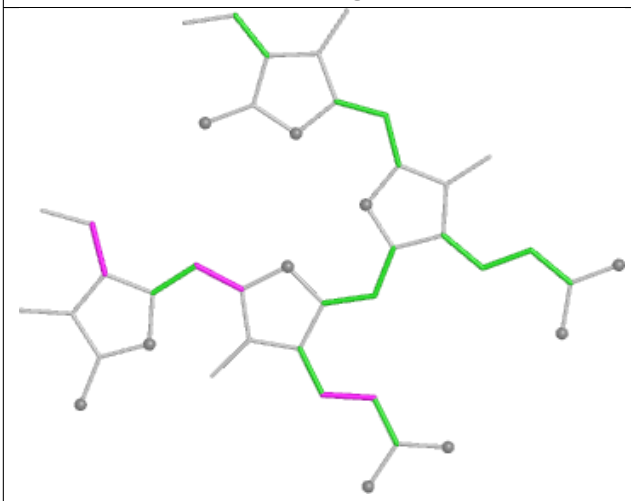
Ligand PEB w8 202



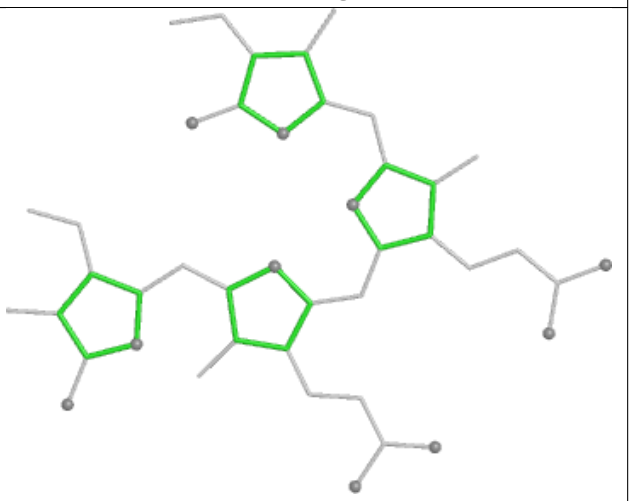
Bond lengths



Bond angles

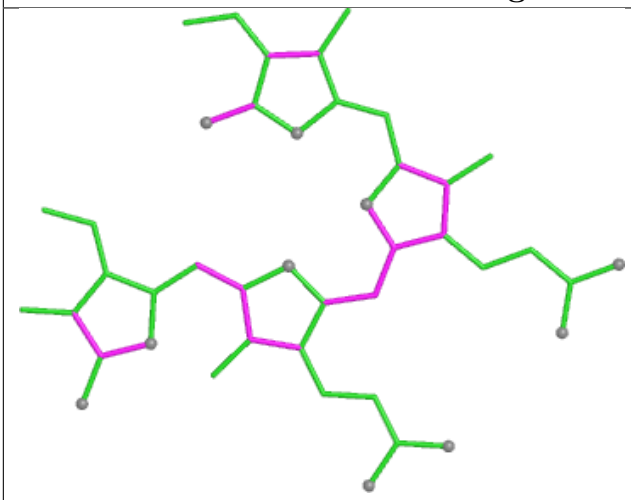


Torsions



Rings

Ligand PEB MB 202



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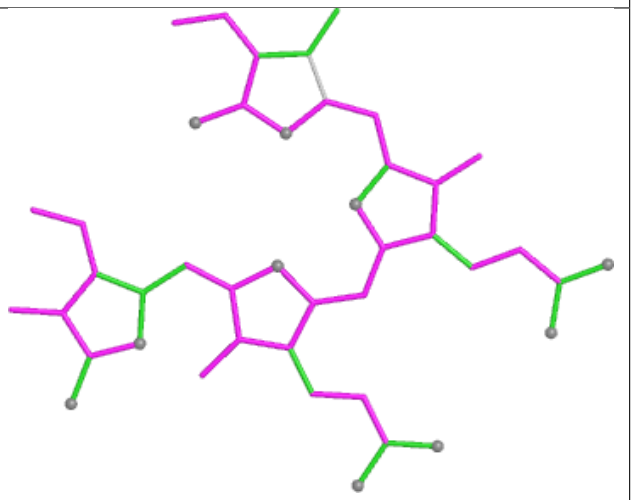

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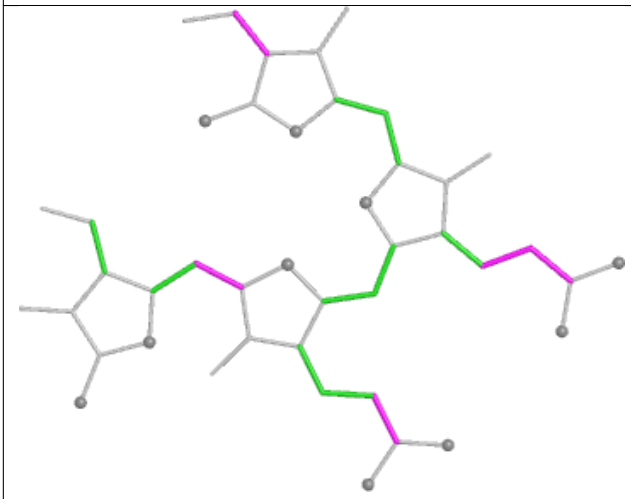

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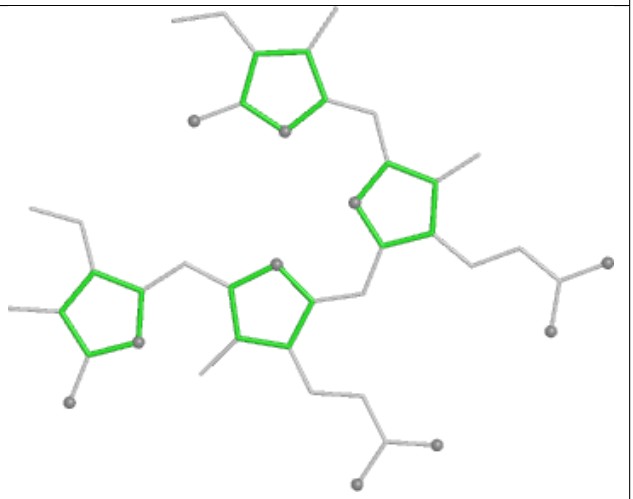
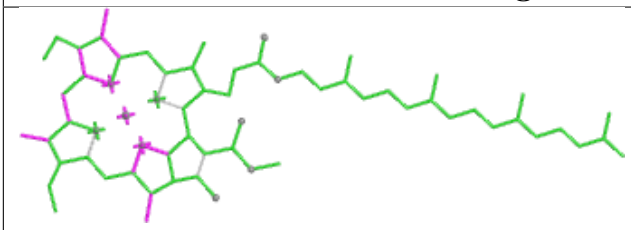


Rings

Ligand CLA A2 808



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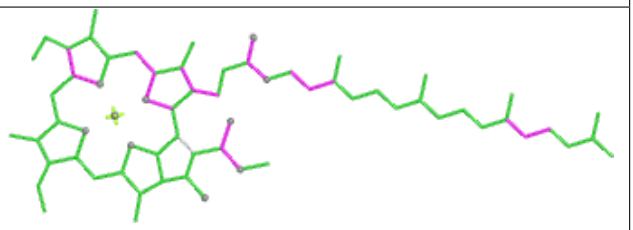

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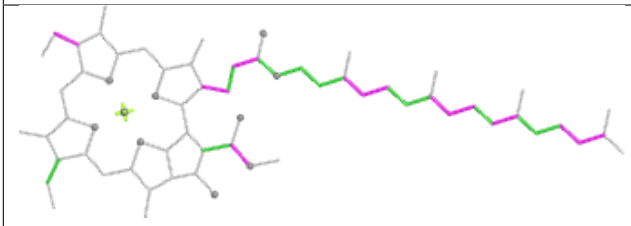

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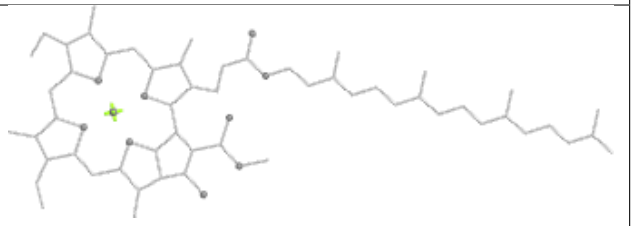
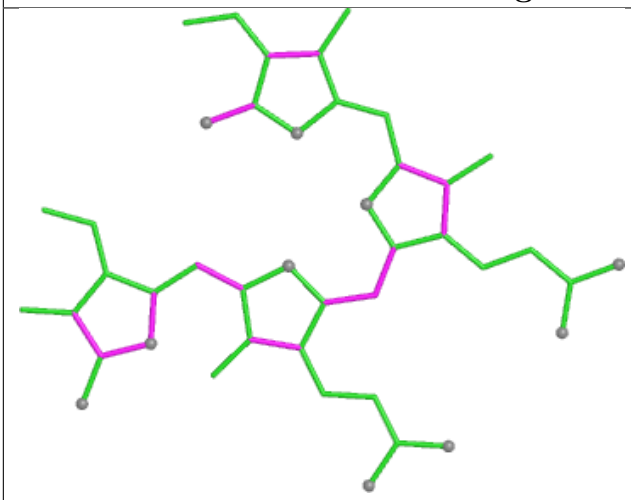


Rings

Ligand PEB YJ 201



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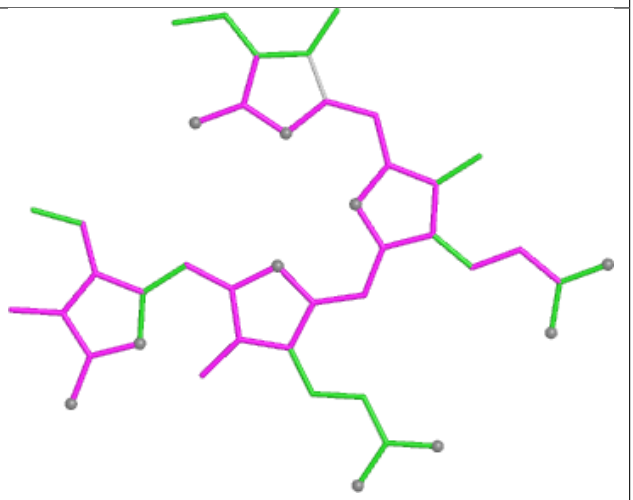
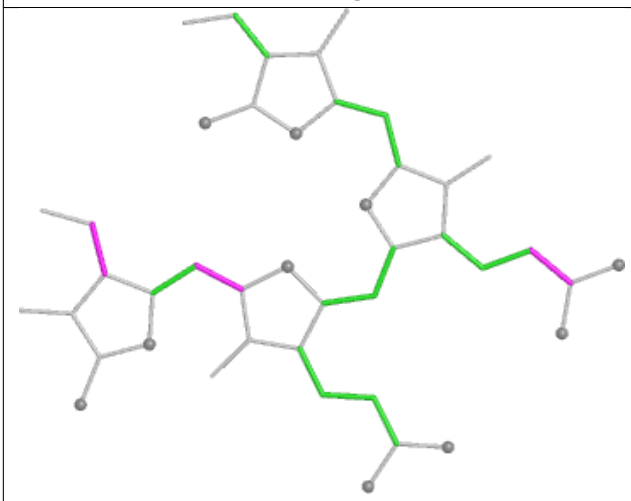


Bond angles



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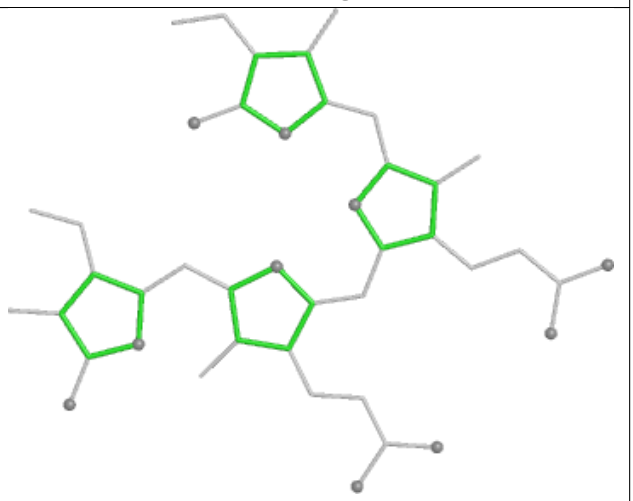
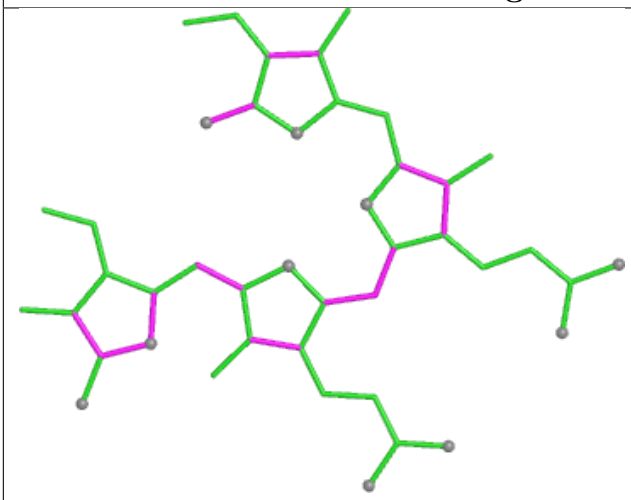


Rings

Ligand PEB WG 203



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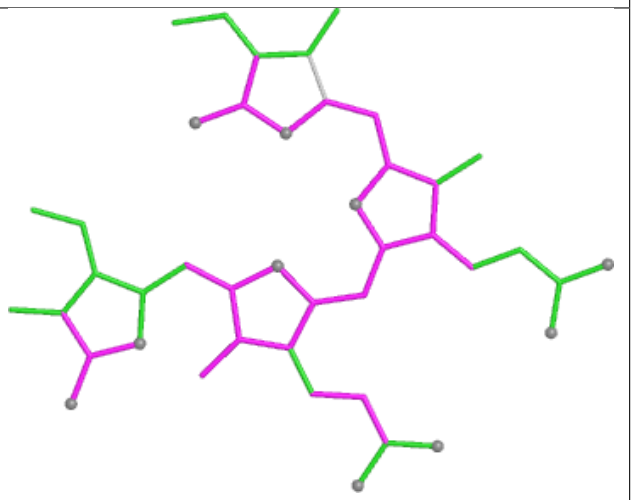
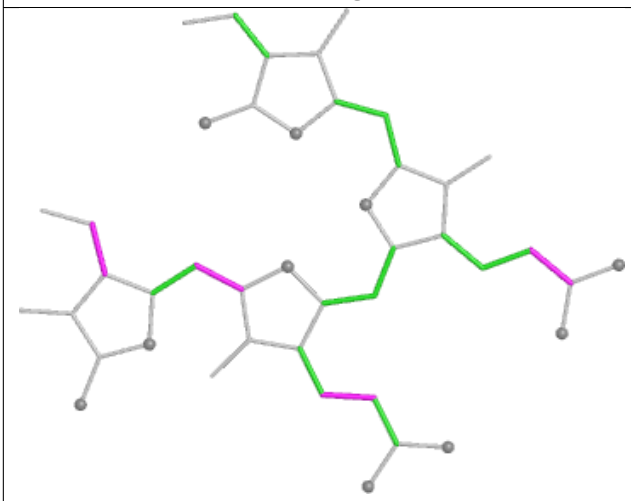


Bond angles



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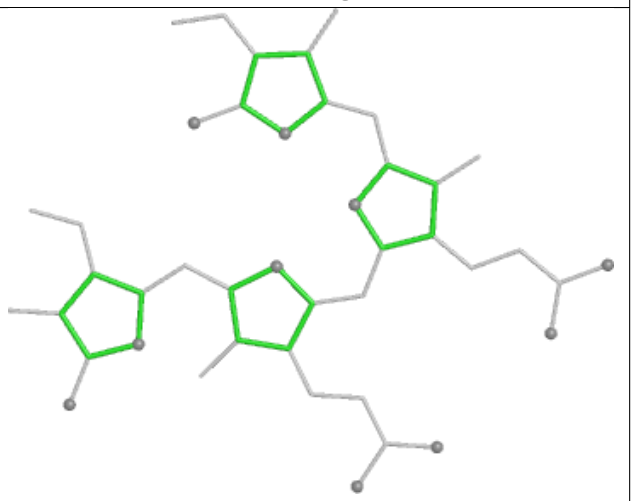
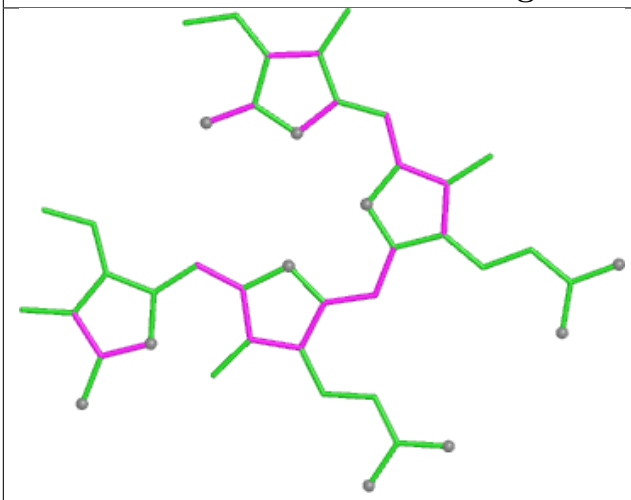


Rings

Ligand PEB qF 203



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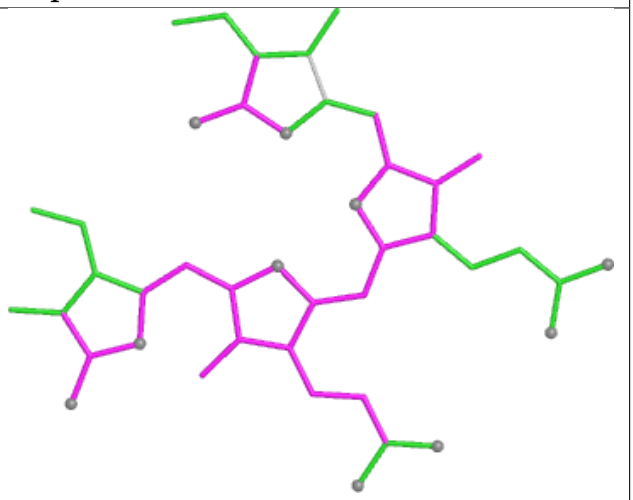
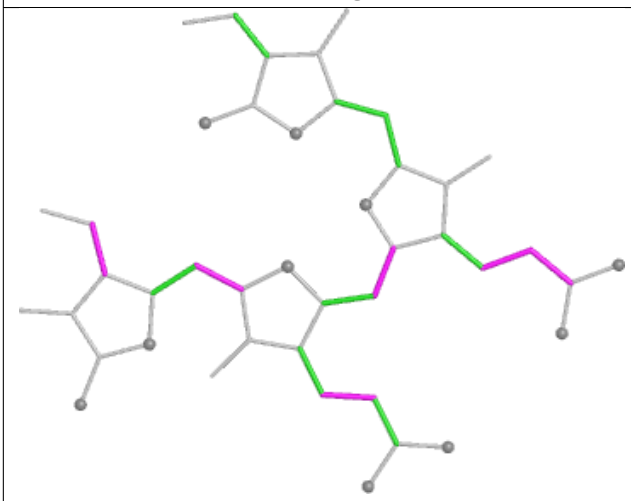


Bond angles



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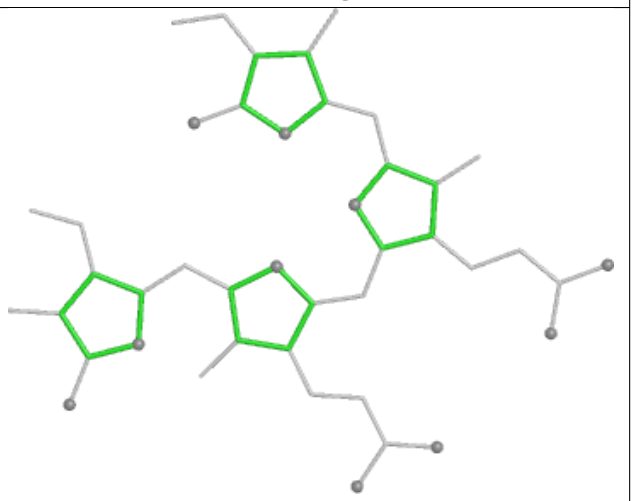
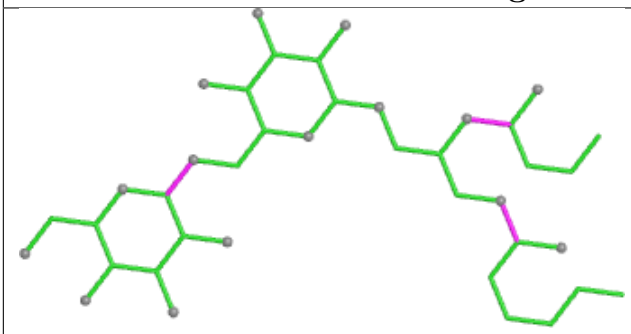


Rings

Ligand DGD AL 416



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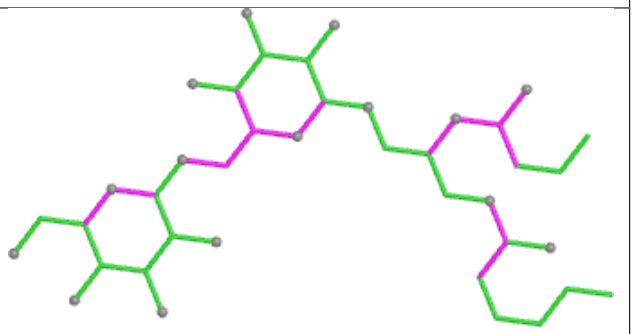
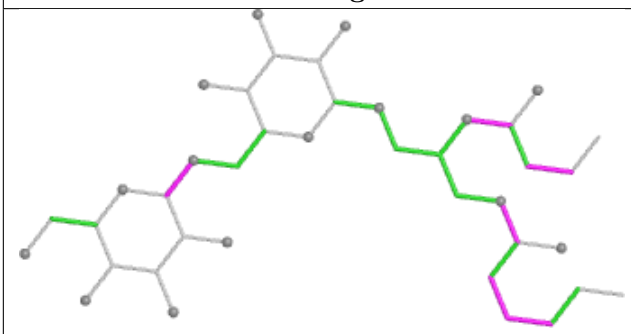


Bond angles



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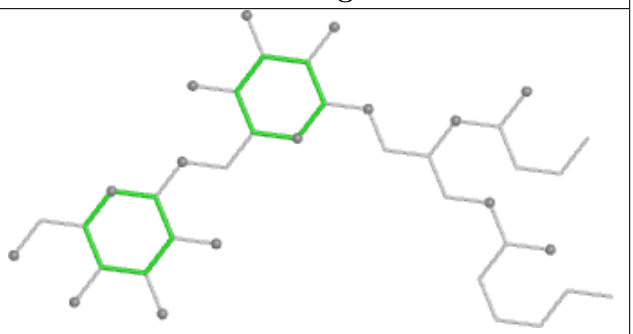
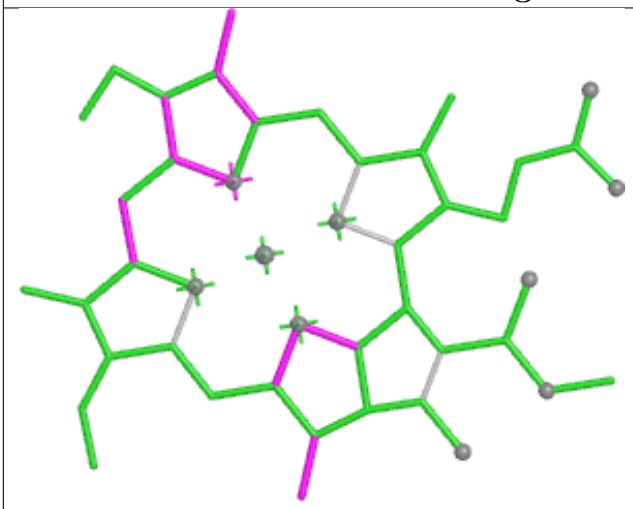


Rings

Ligand CLA 7N 605



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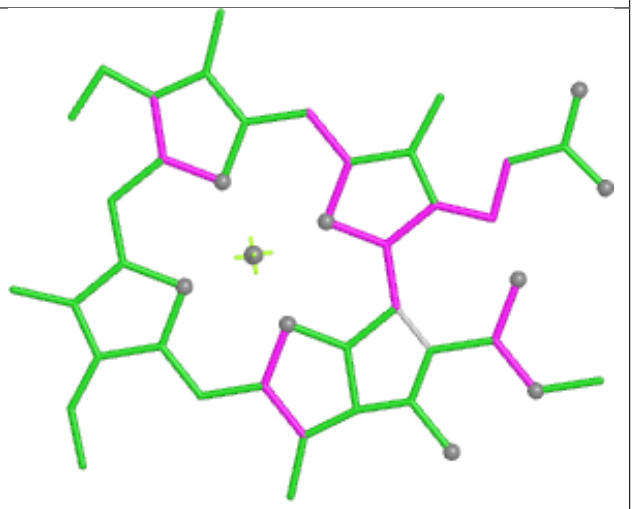

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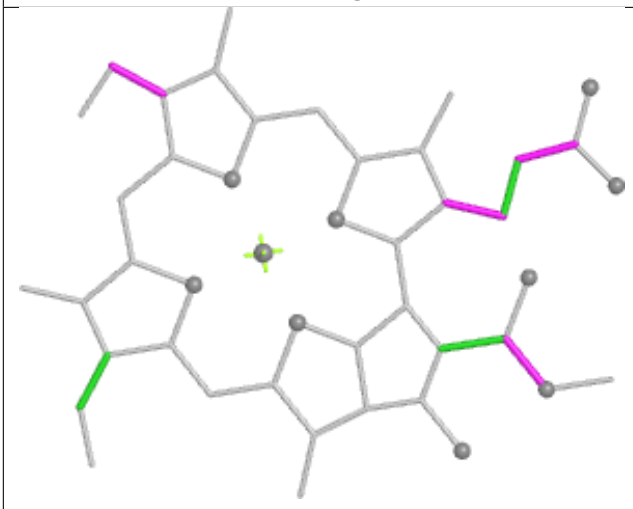
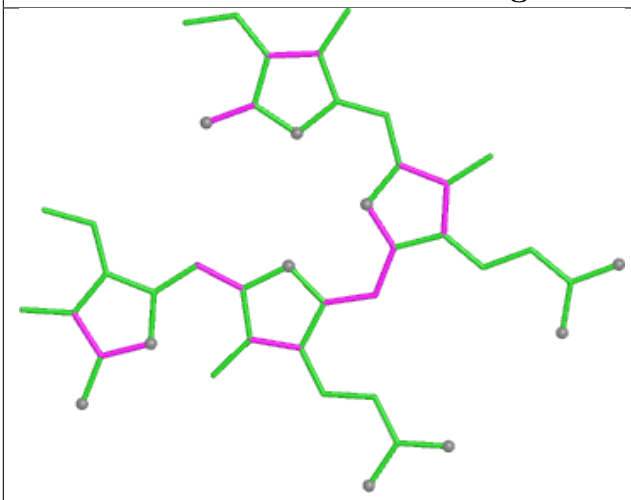


Torsions



Rings

Ligand PEB UO 202



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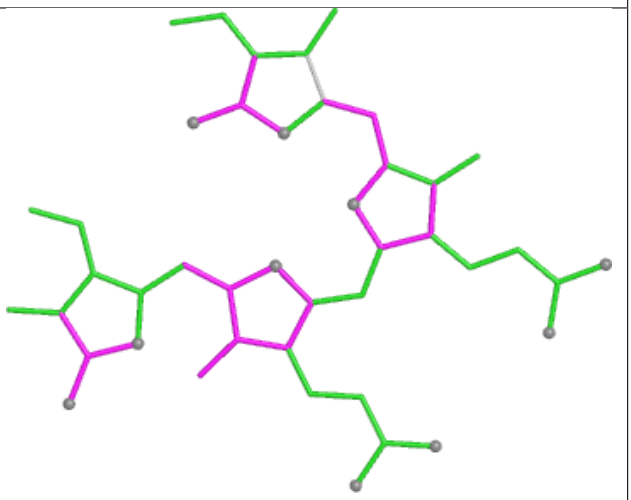
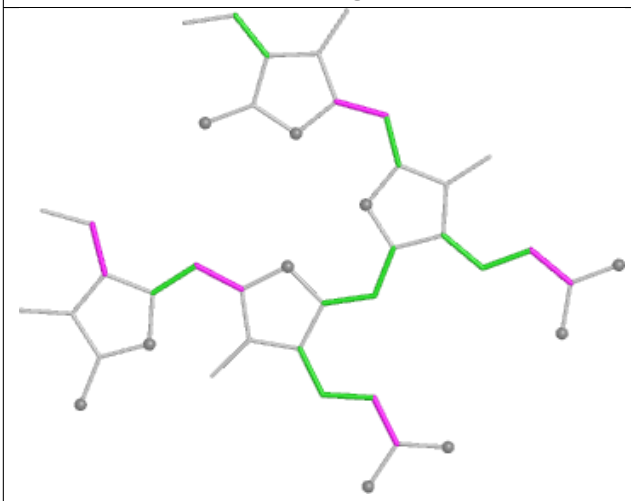


Bond angles



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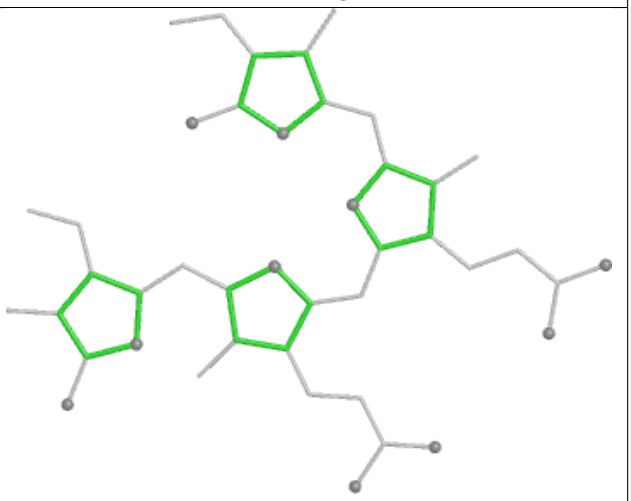
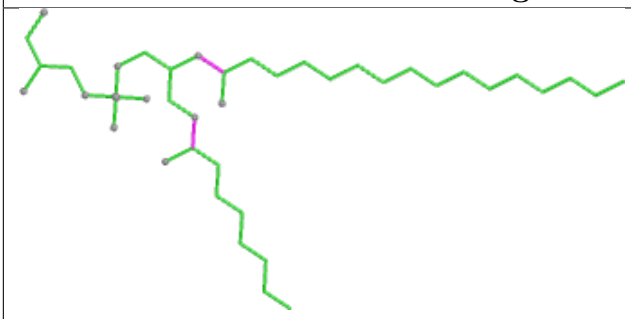


Rings

Ligand LHG BL 615



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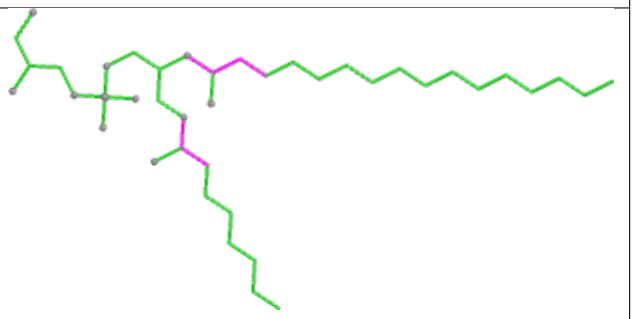
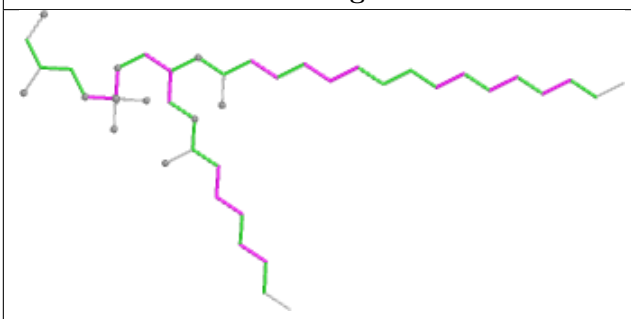


Bond angles



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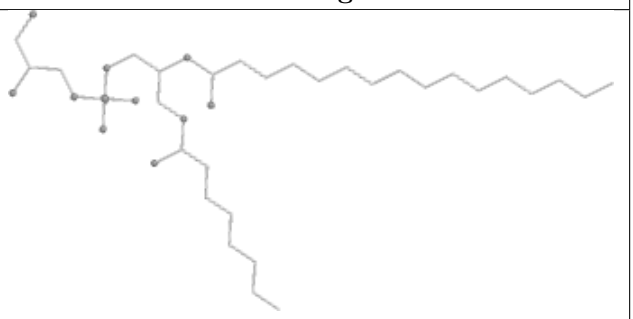
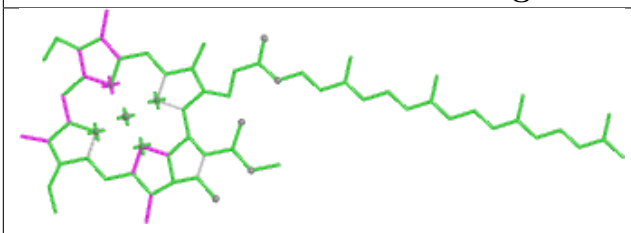


Rings

Ligand CLA DL 404



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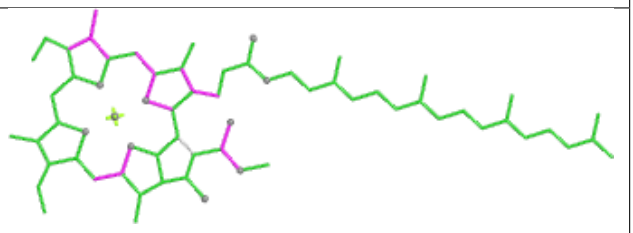
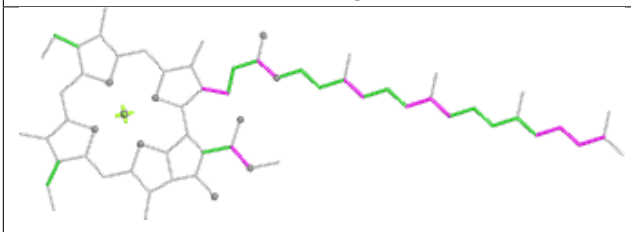


Bond angles



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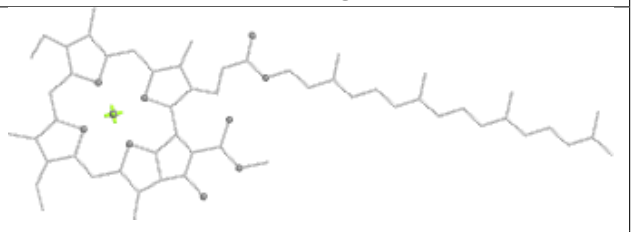
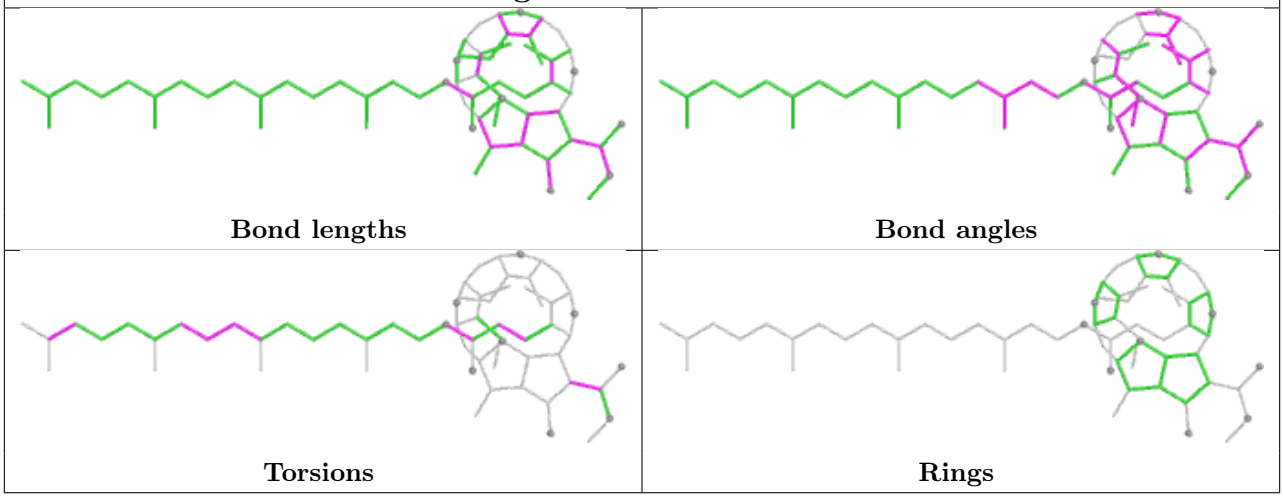
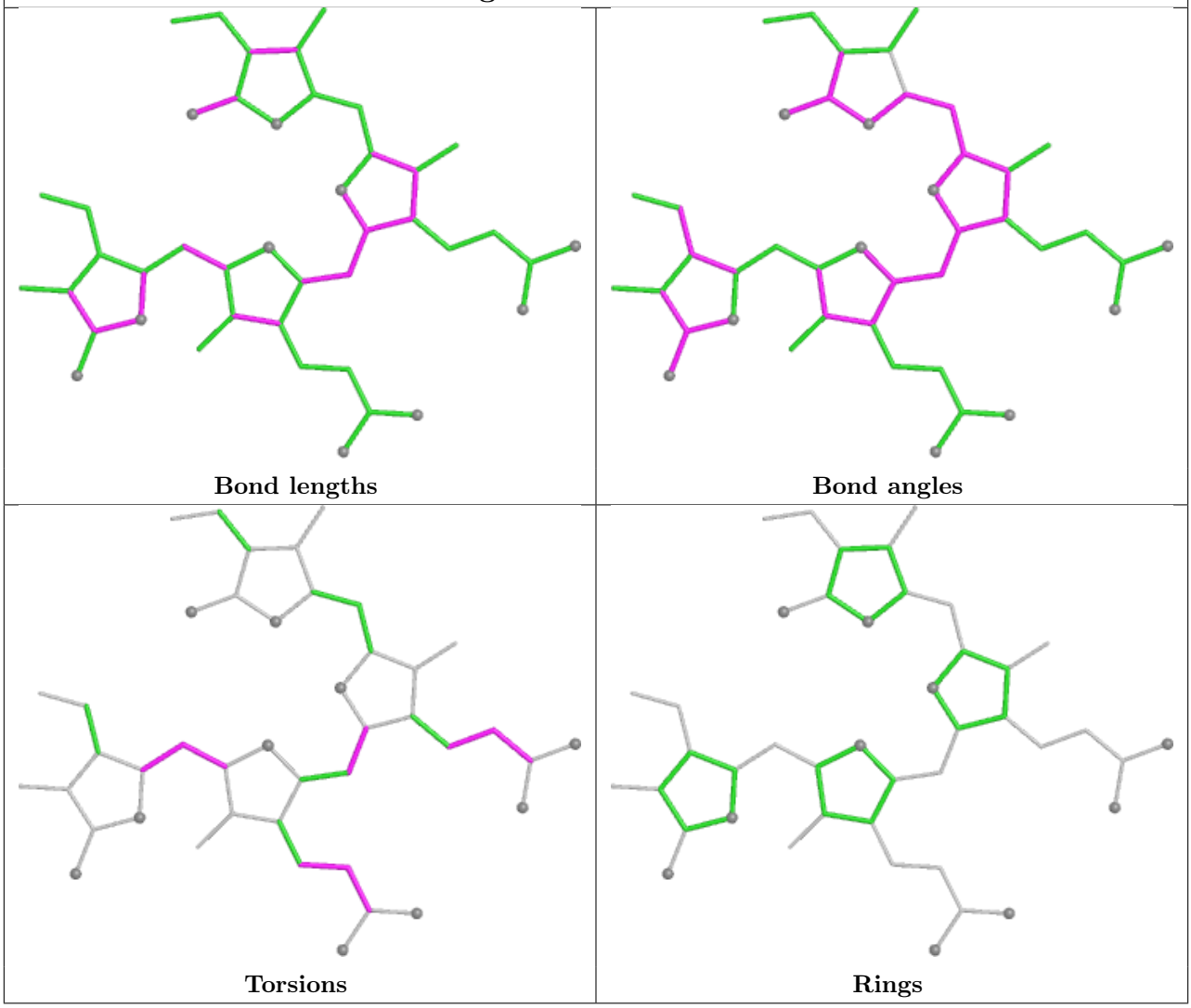


Rings

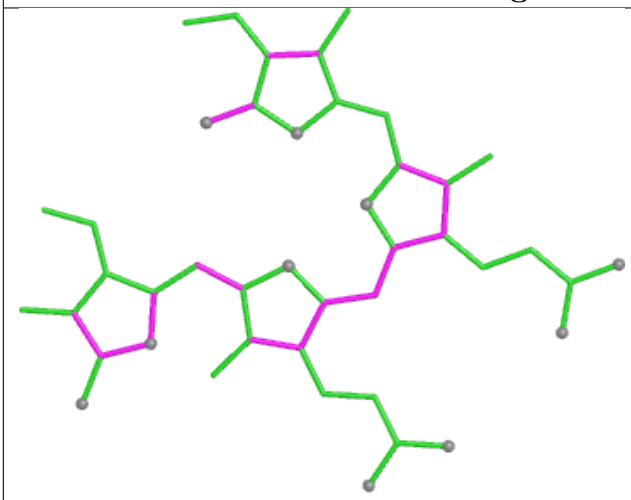
Ligand PHO A6 407



Ligand PEB X5 202



Ligand PEB DD 201



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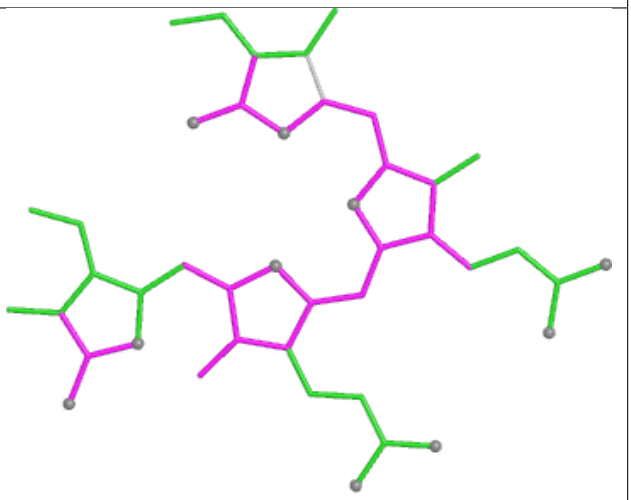
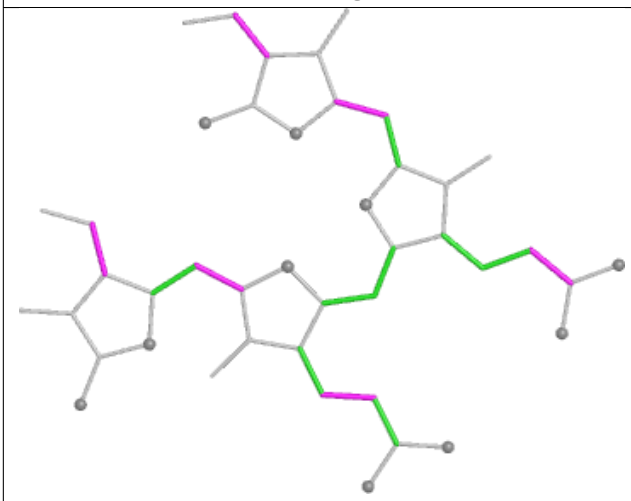


Bond angles



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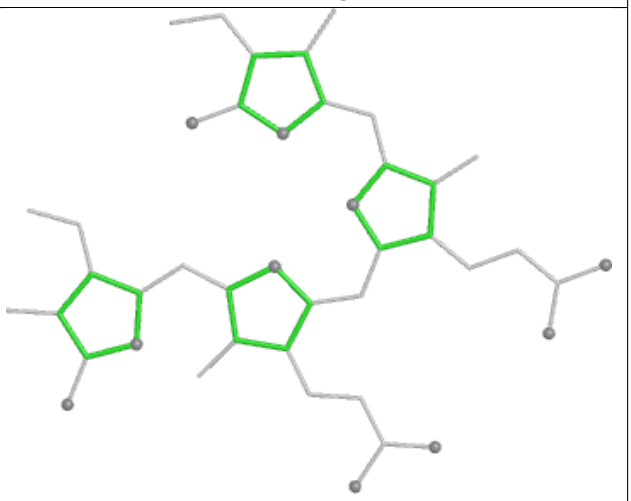
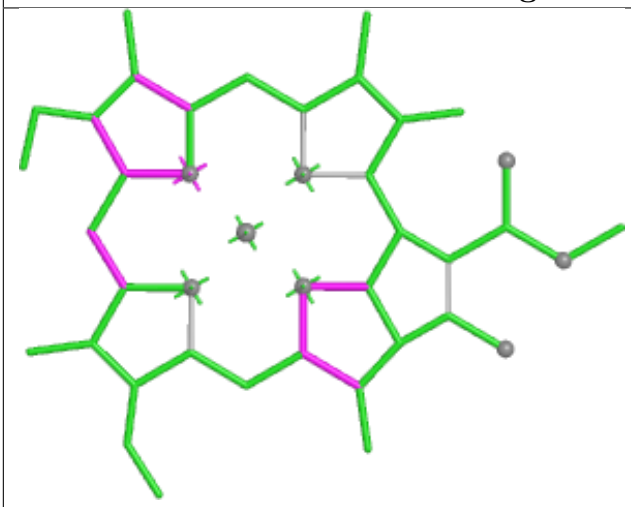


Rings

Ligand CLA 12 608



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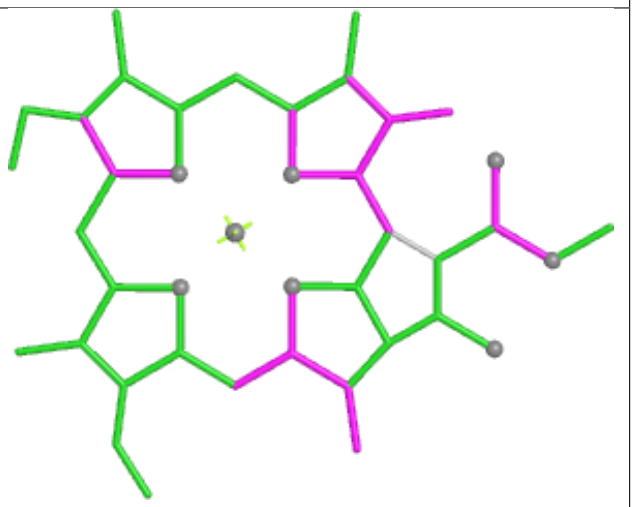
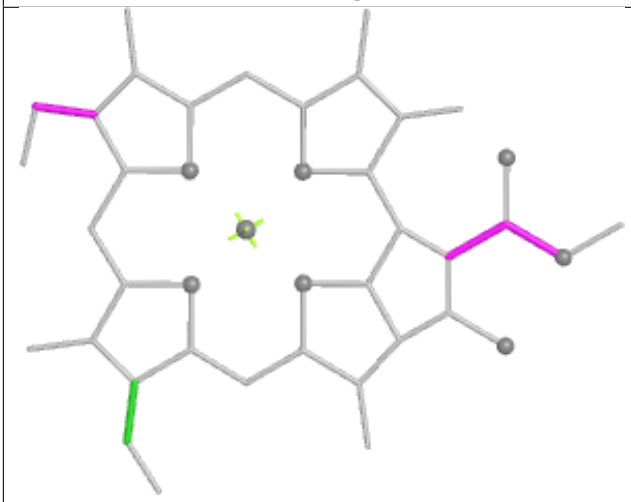


Bond angles



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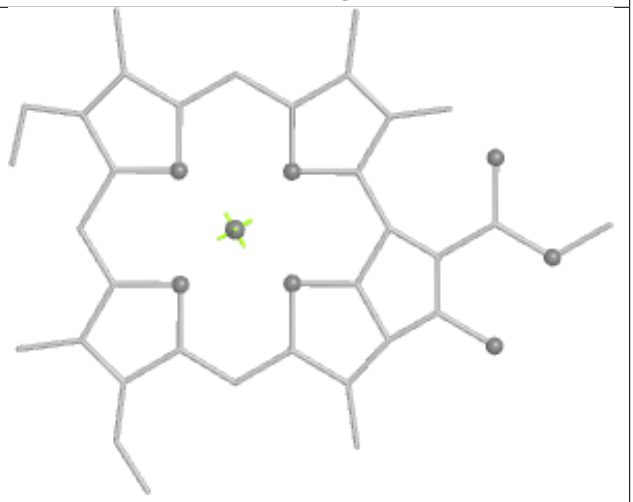
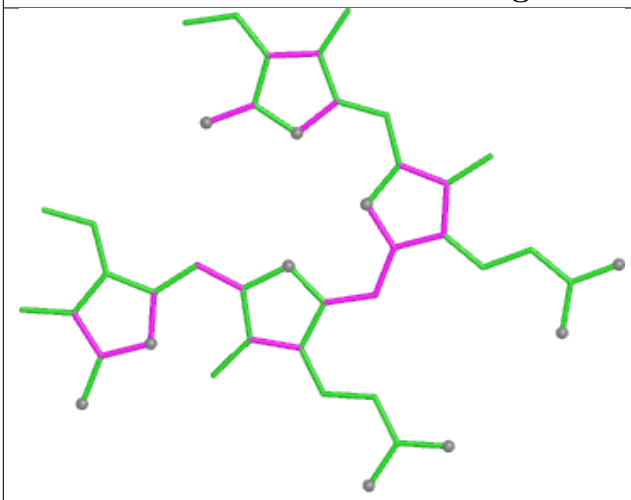


Rings

Ligand PEB YA 304



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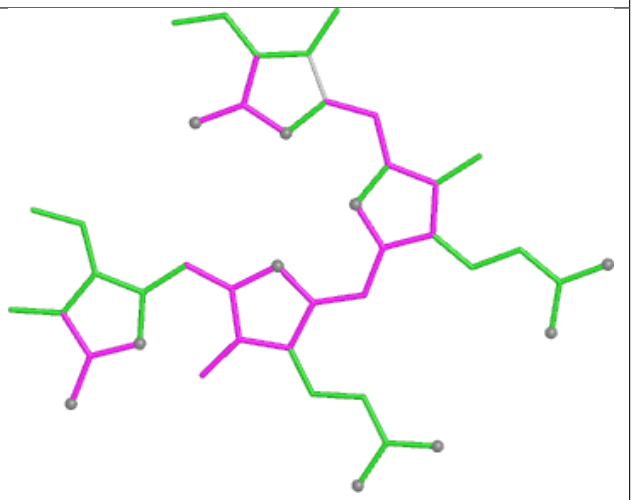
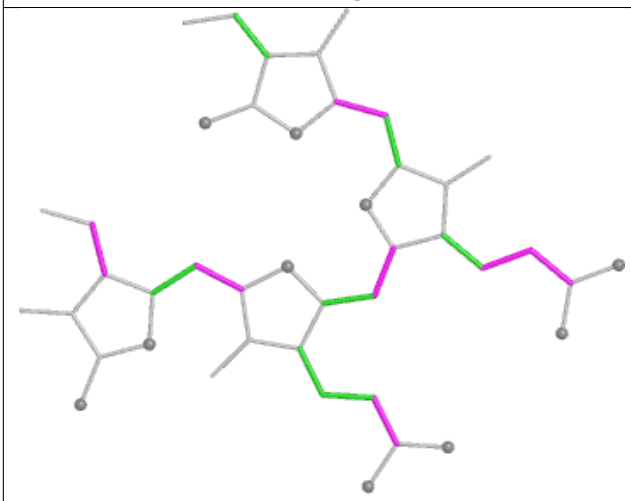


Bond angles



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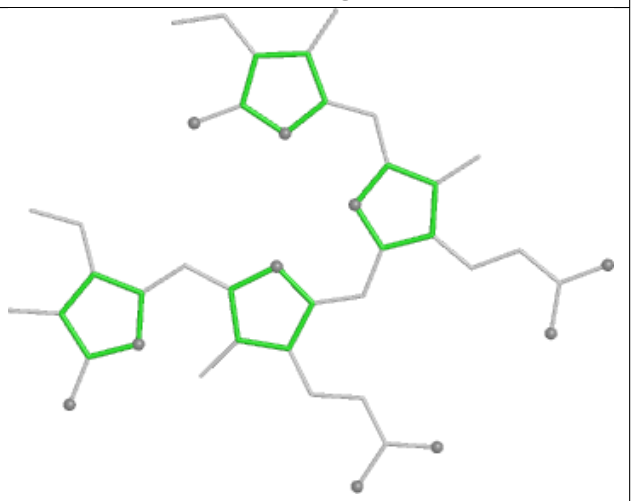
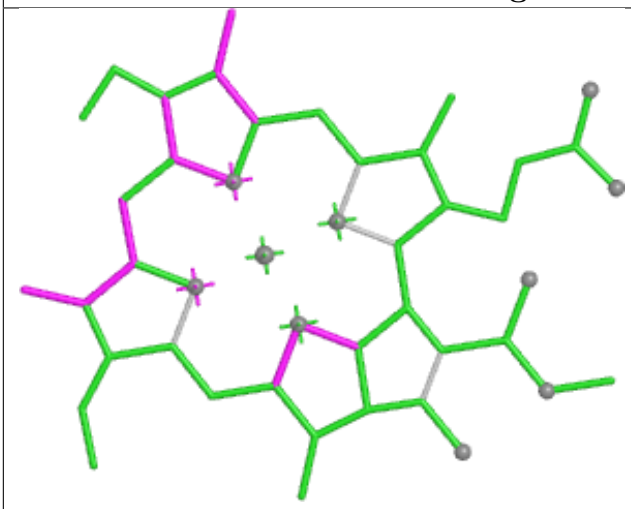
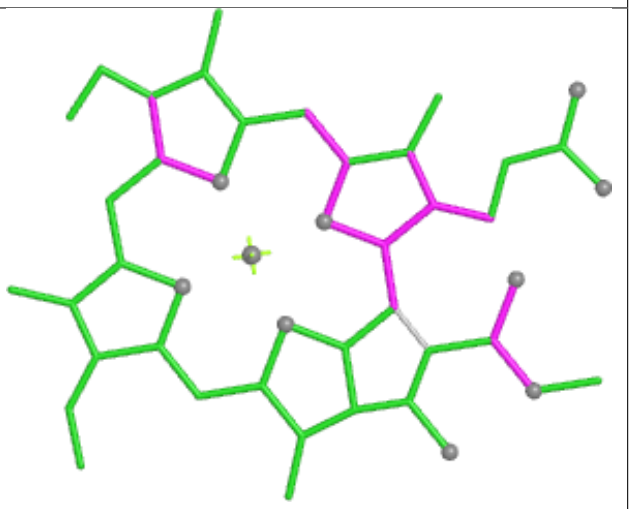


Rings

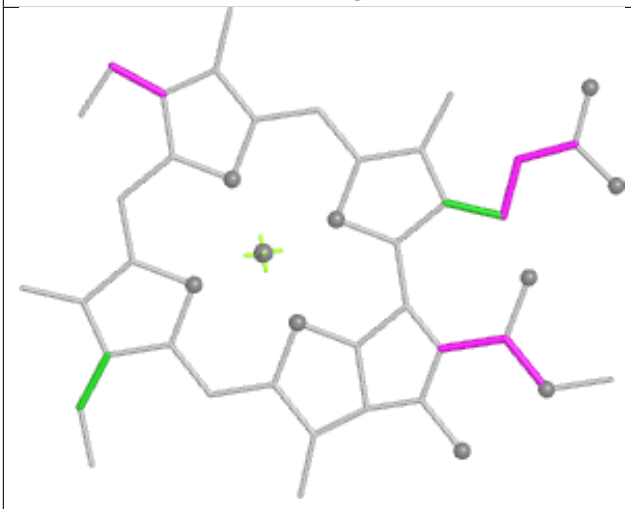
Ligand CLA ON 203



Bond lengths



Bond angles

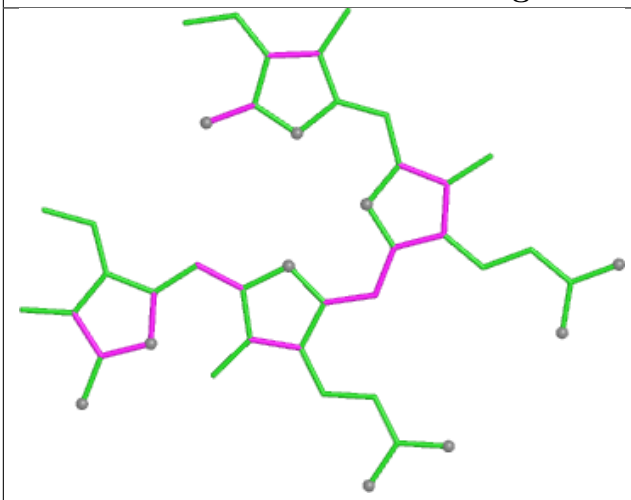


Torsions



Rings

Ligand PEB AE 304



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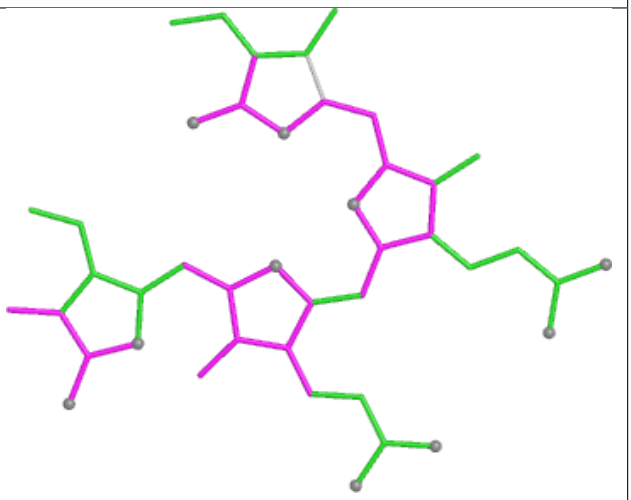

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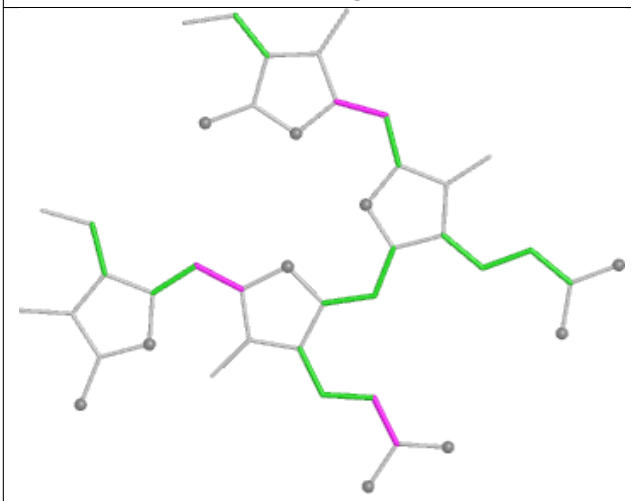

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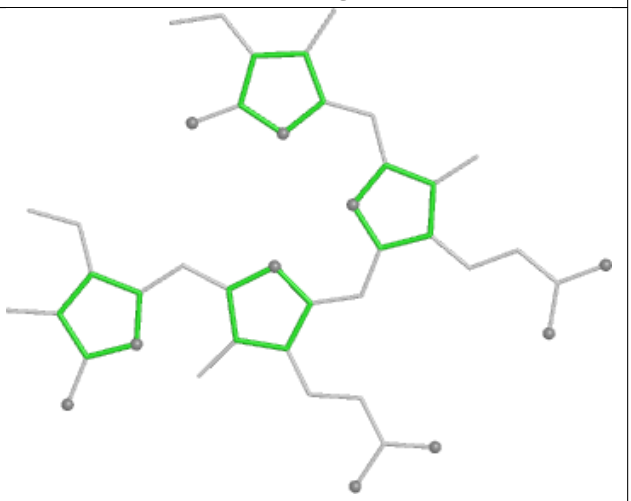
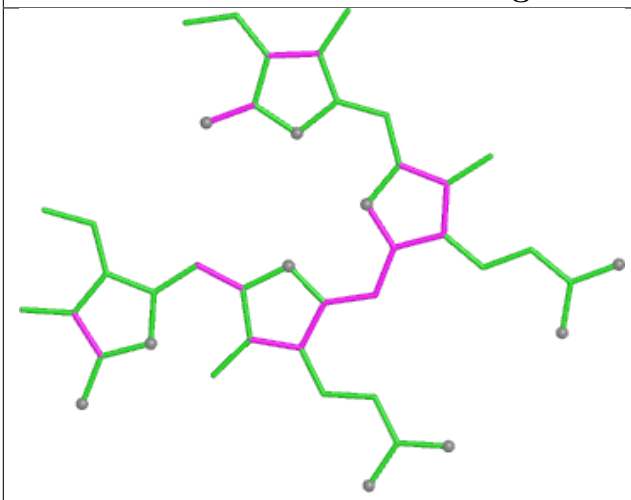


Rings

Ligand PEB FK 201



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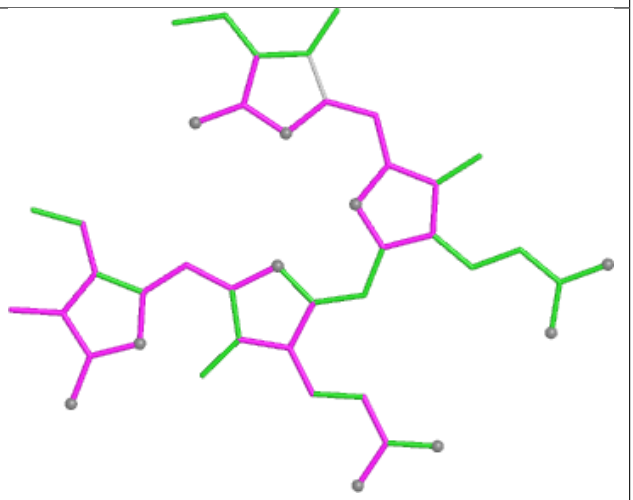

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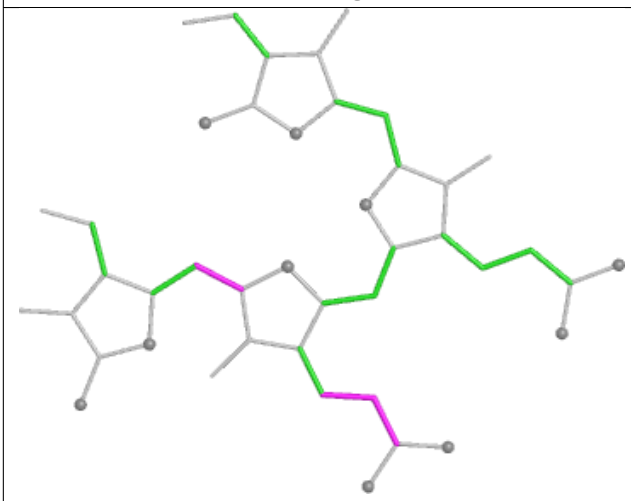

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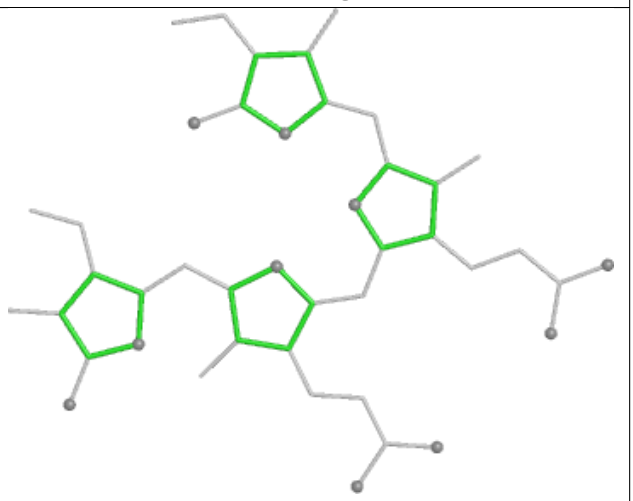

Rings

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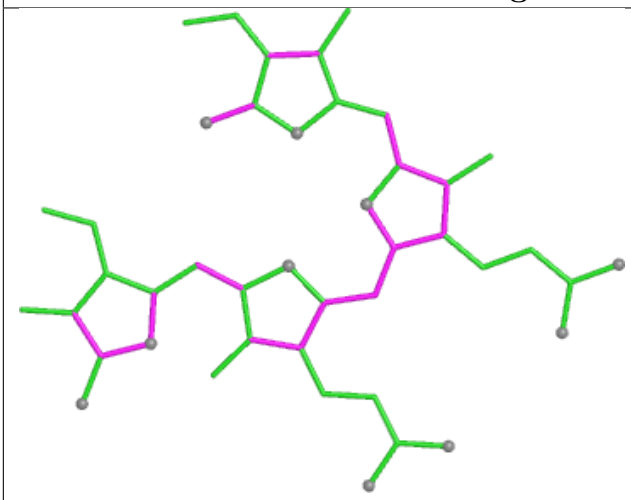

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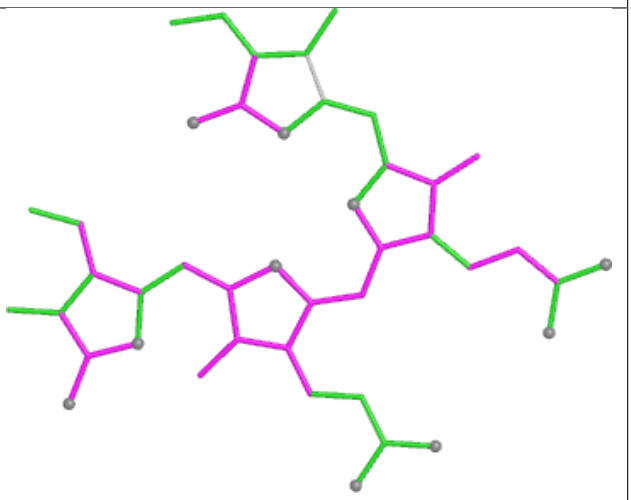

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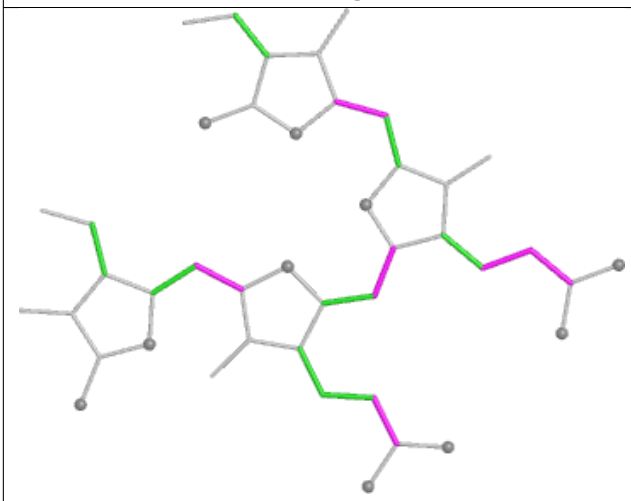

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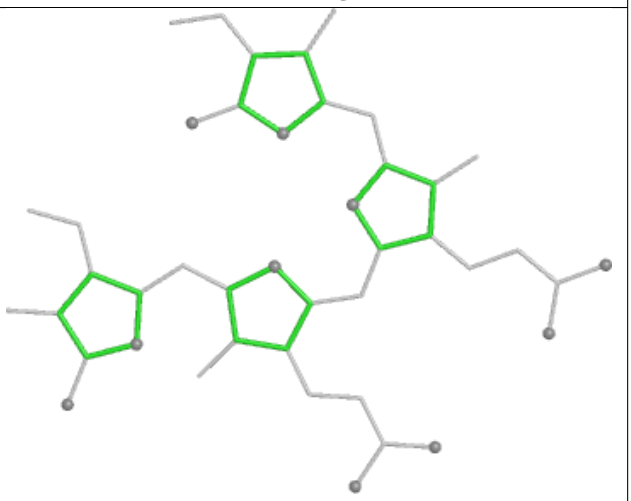
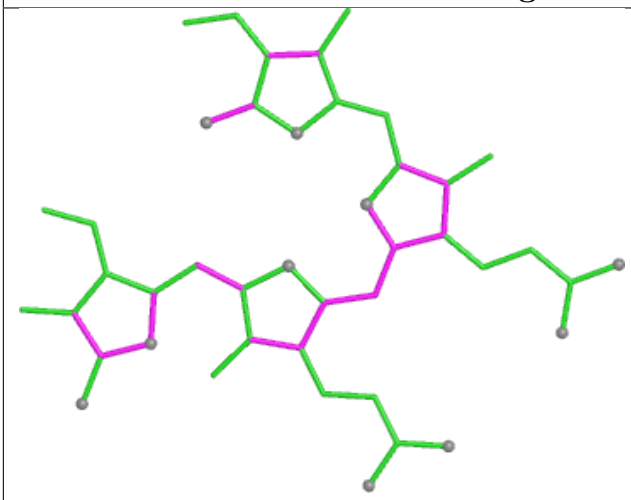


Rings

Ligand PEB lG 203



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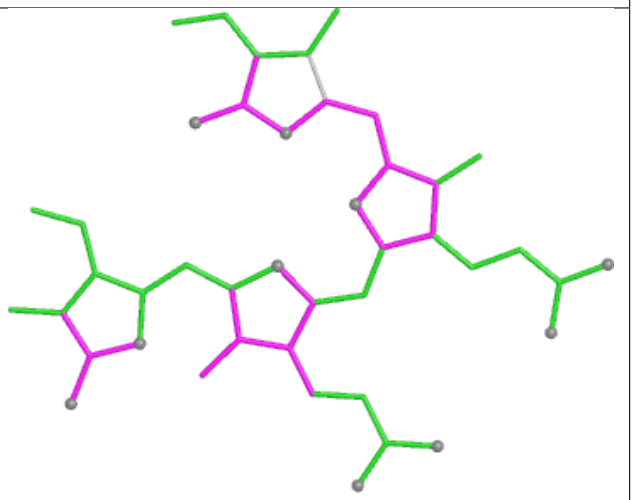

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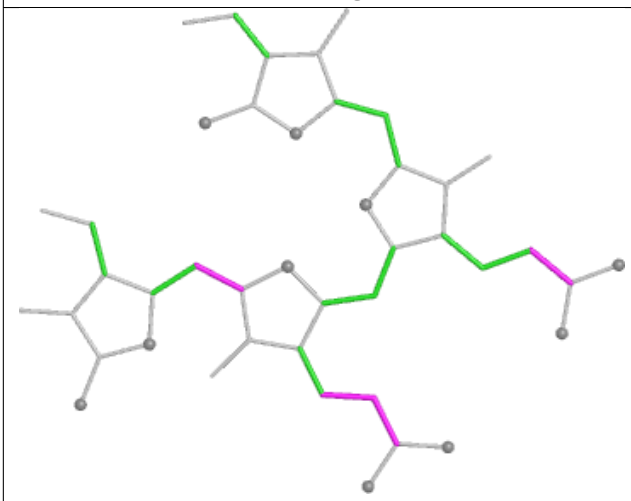

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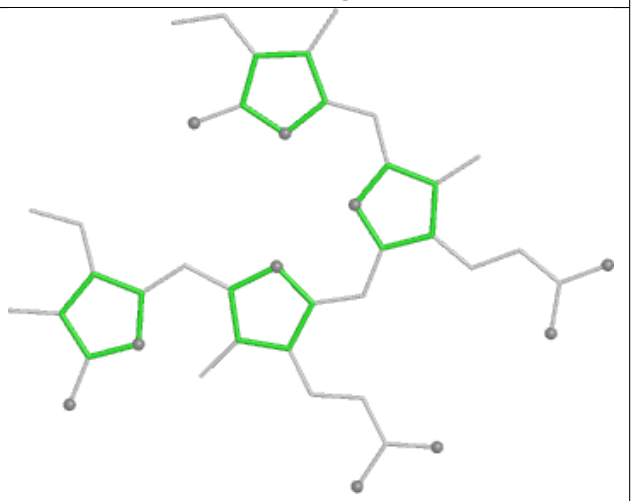
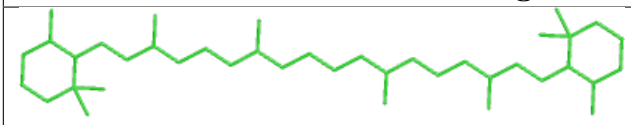


Rings

Ligand BCR kL 100



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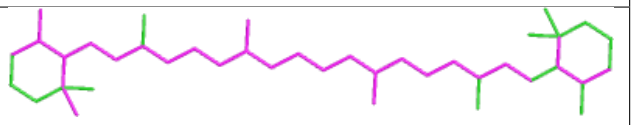

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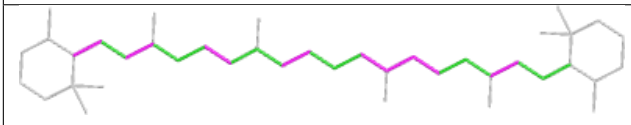

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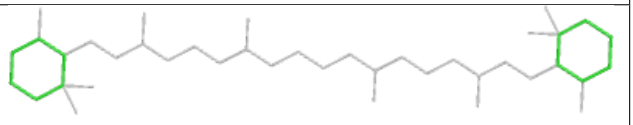
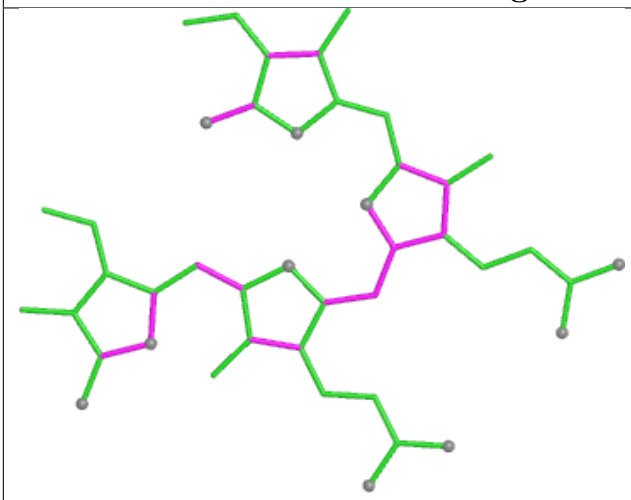


Rings

Ligand PEB AG 304



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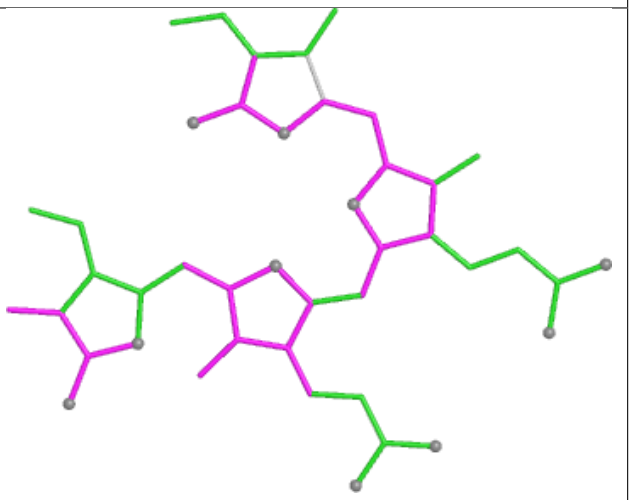

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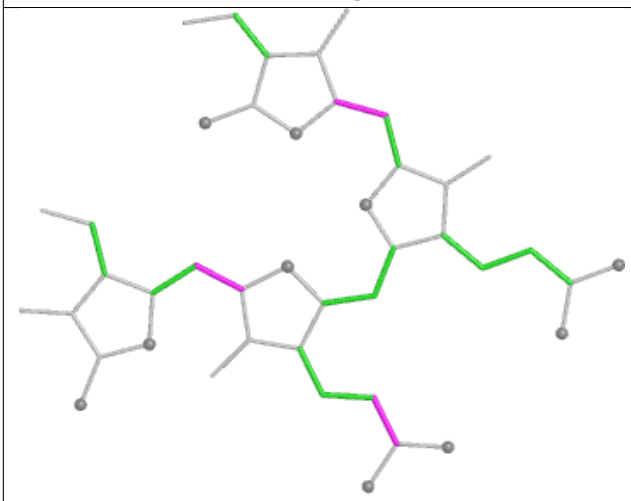

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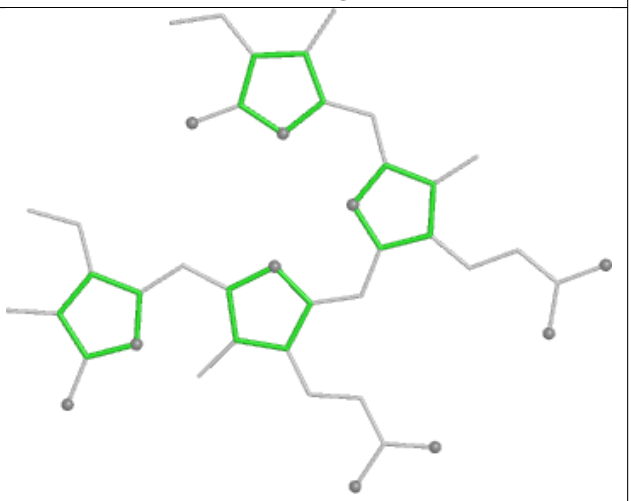
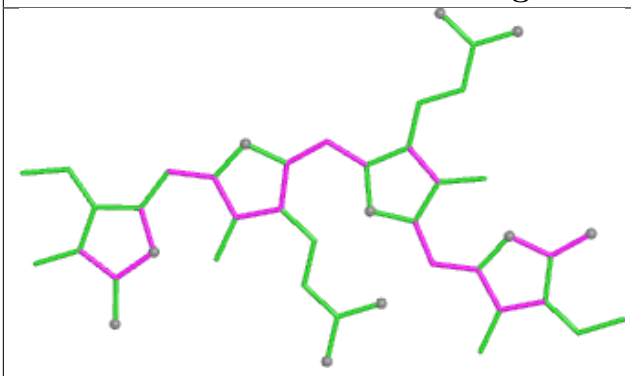


Rings

Ligand CYC l3 1001



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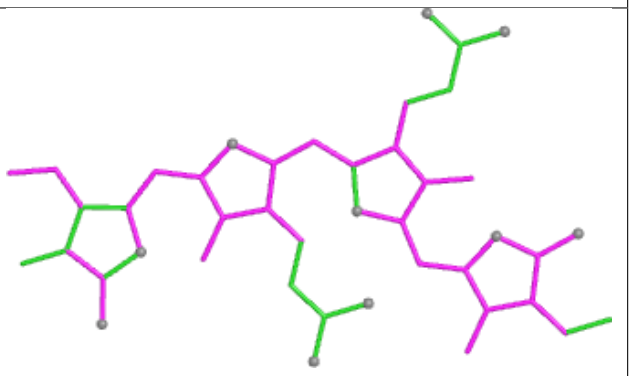

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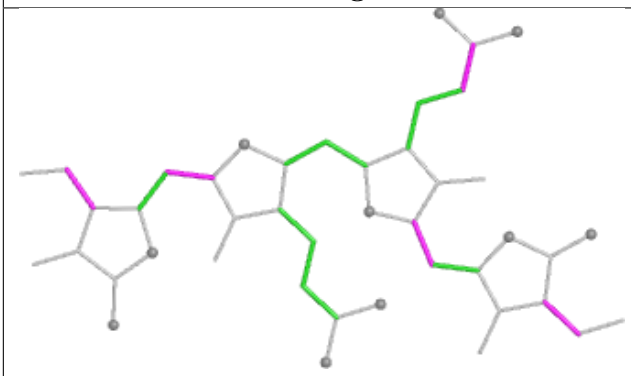

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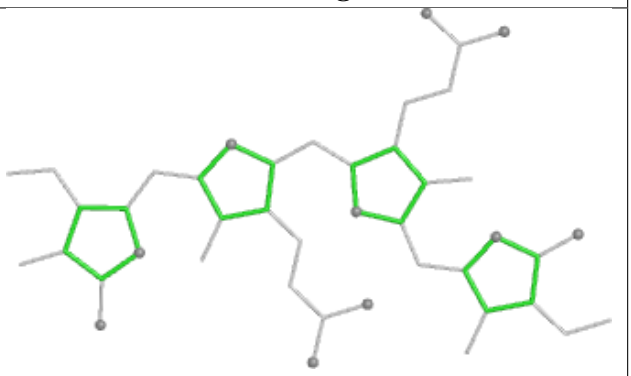
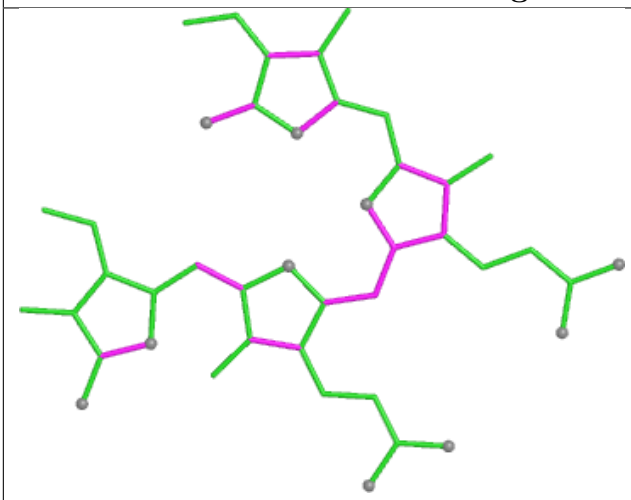


Rings

Ligand PEB KQ 202



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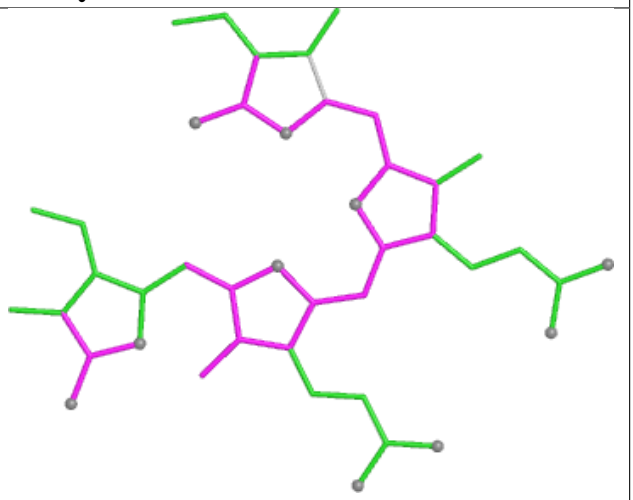

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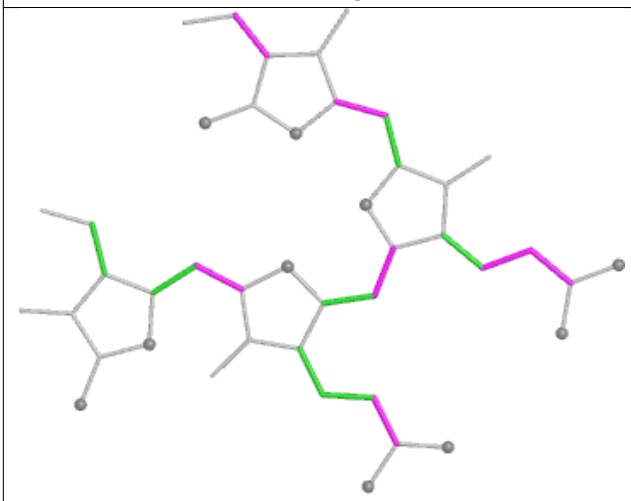

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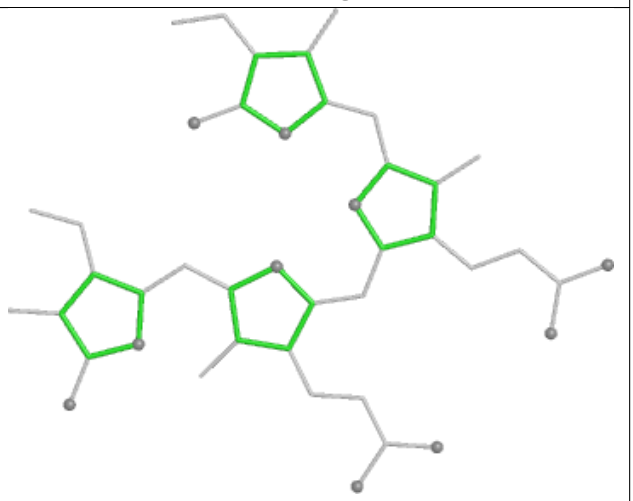
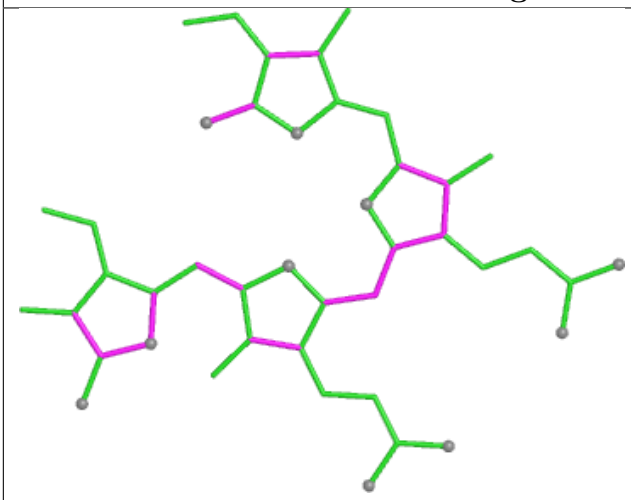


Rings

Ligand PEB HD 203



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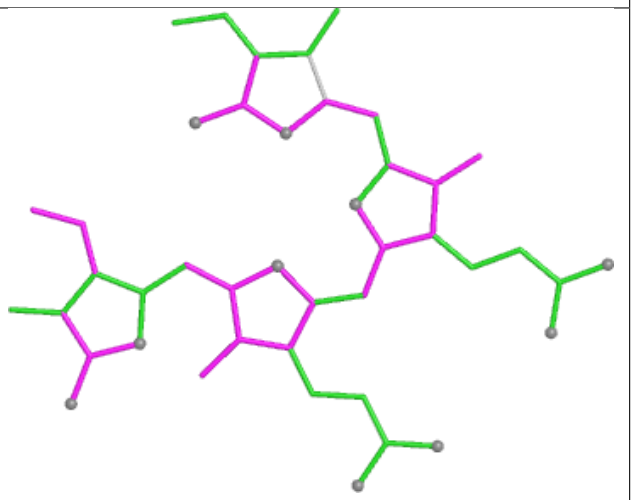

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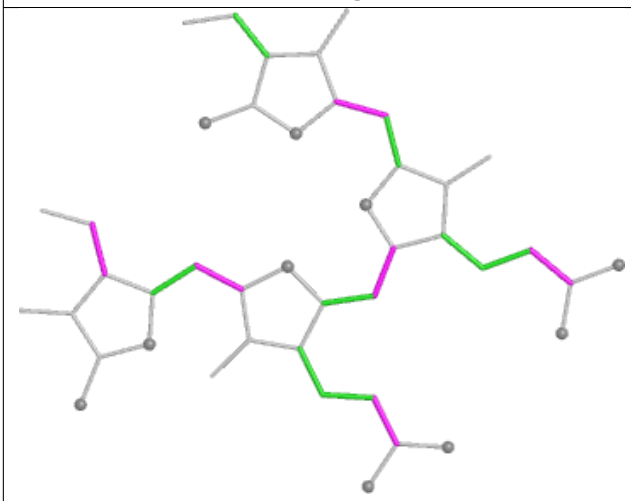

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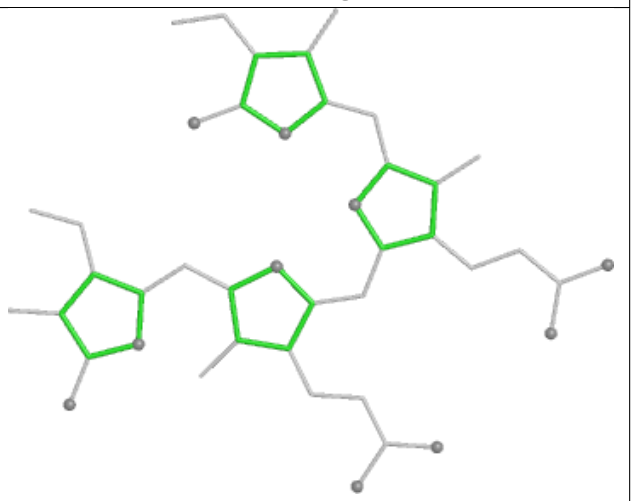
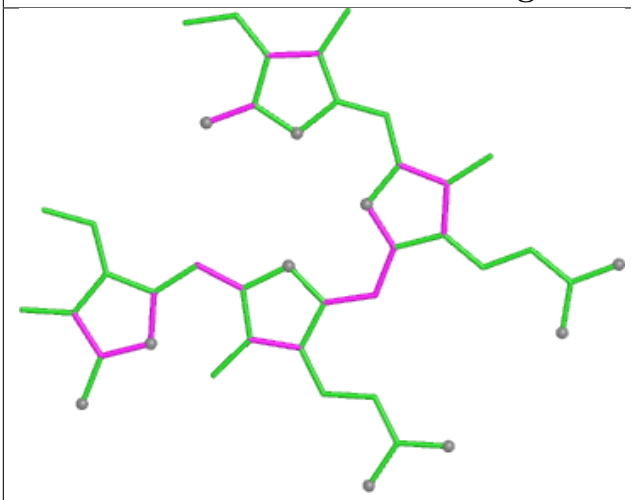


Rings

Ligand PEB YI 202



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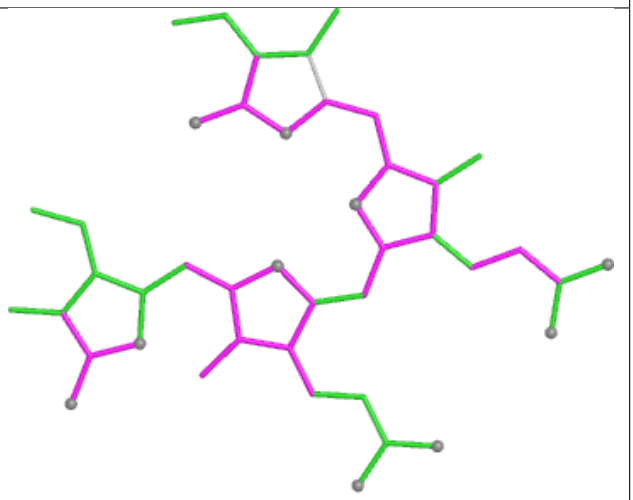

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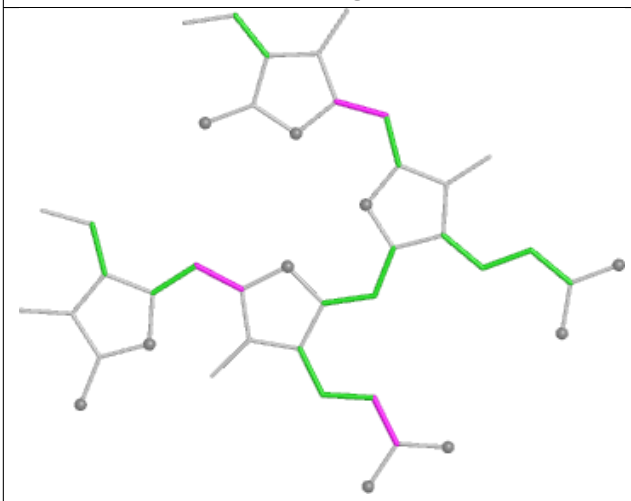

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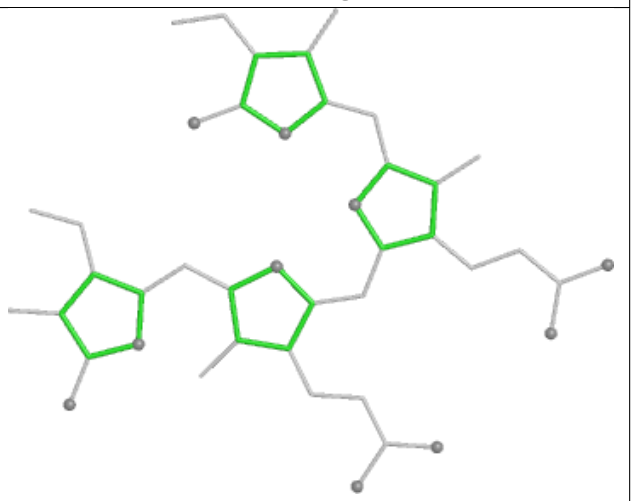
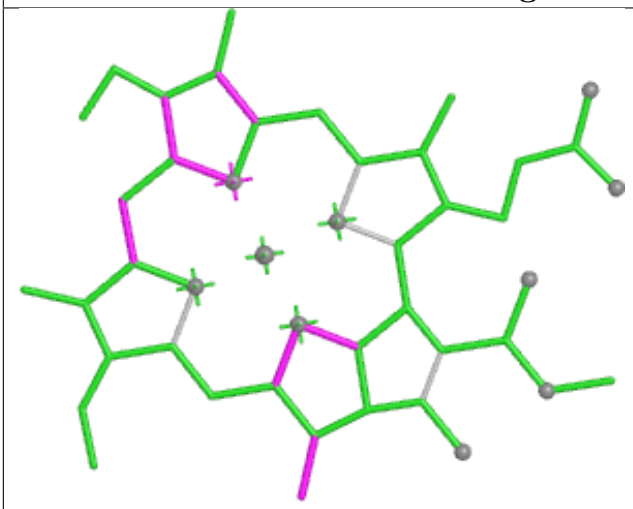


Rings

Ligand CLA 72 603



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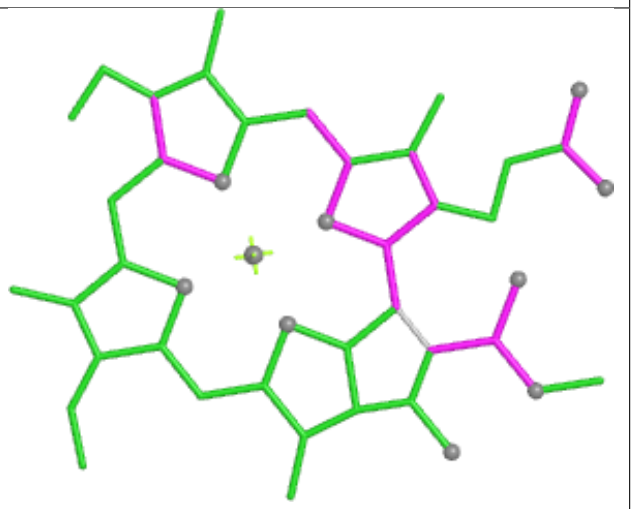

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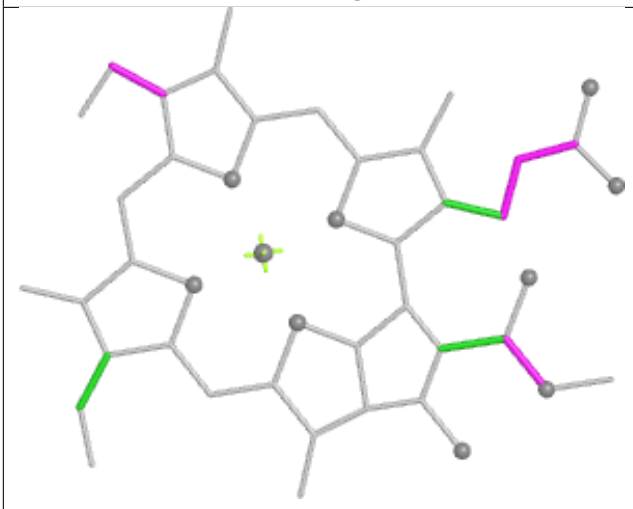
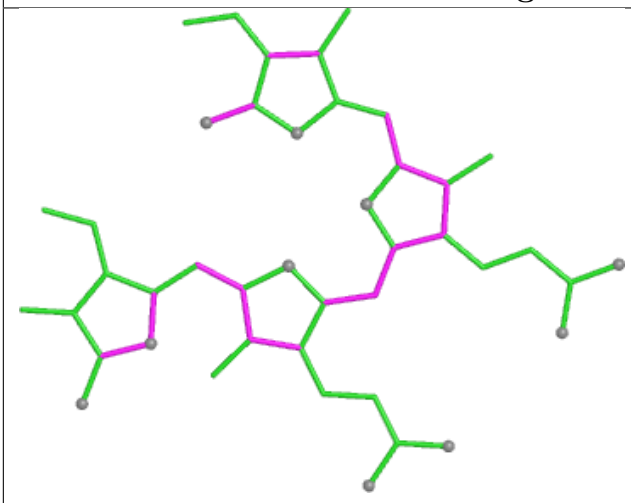


Torsions



Rings

Ligand PEB kF 201



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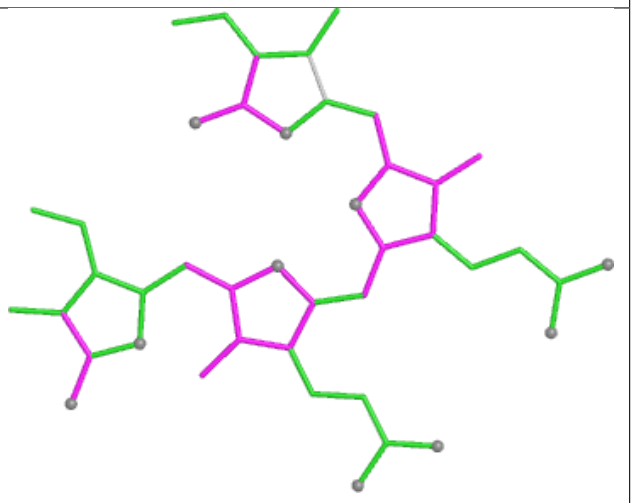

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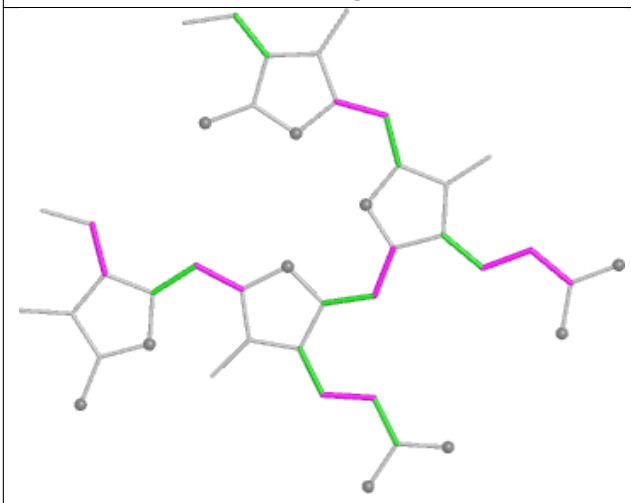

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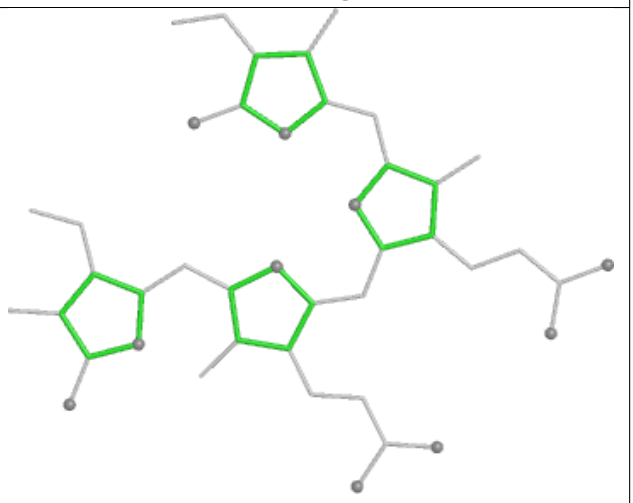
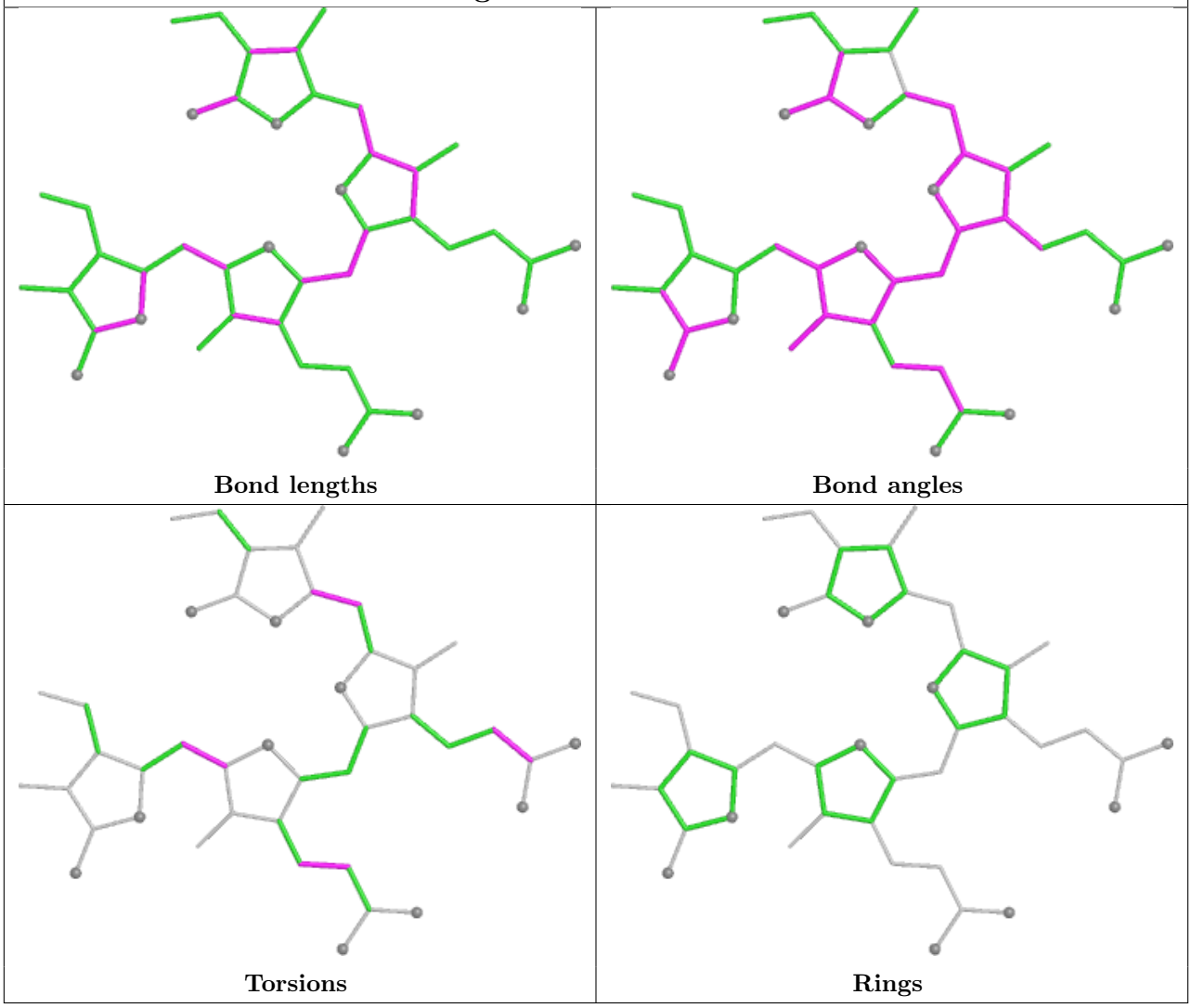
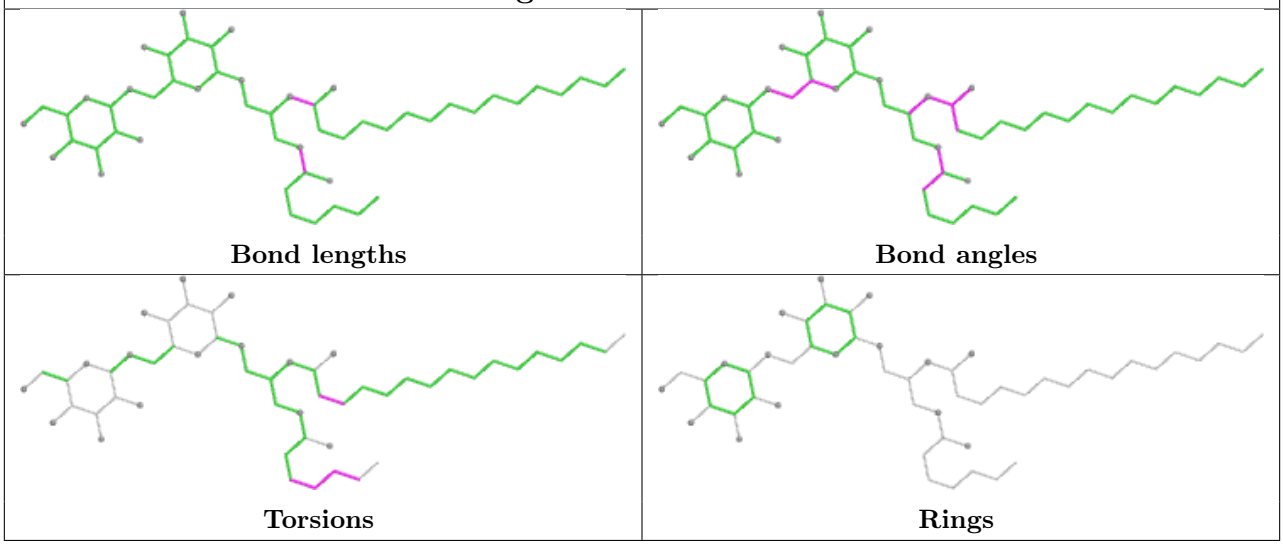


Rings

Ligand PEB YK 201



Ligand DGD a6 604



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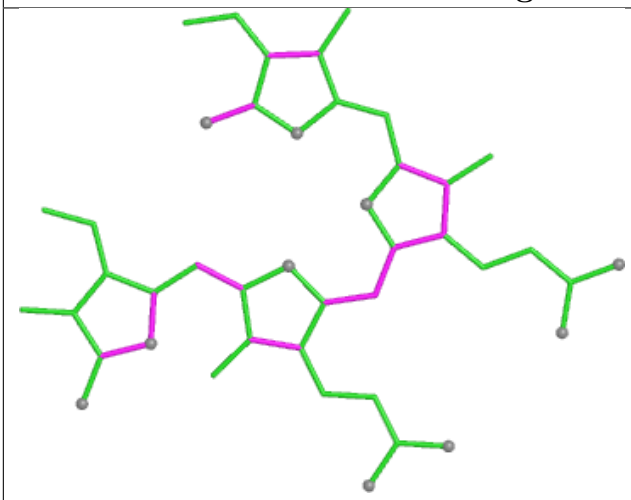

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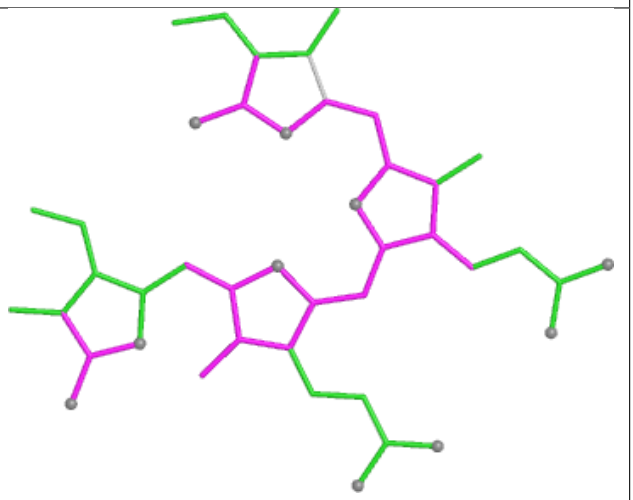
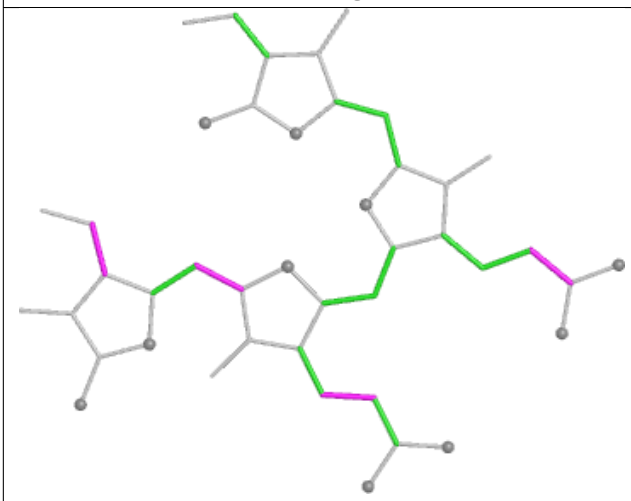


Bond angles



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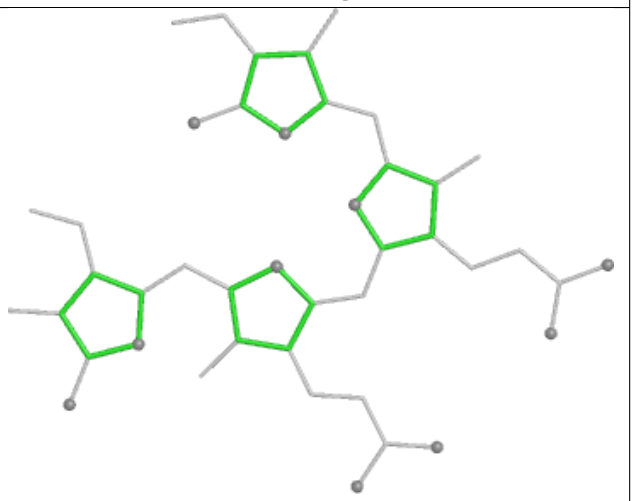
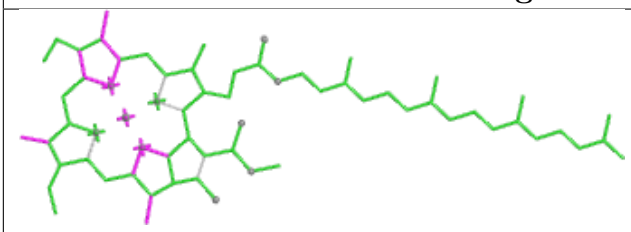


Rings

Ligand CLA B2 822



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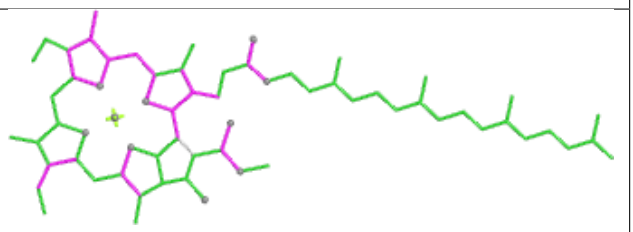
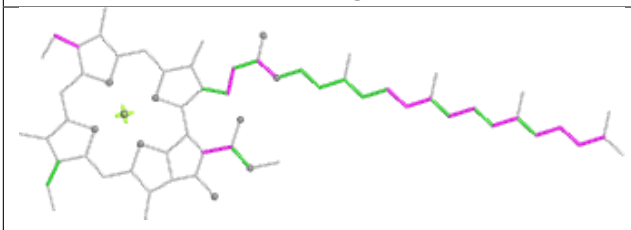


Bond angles



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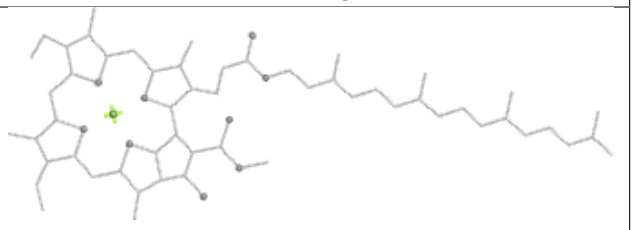
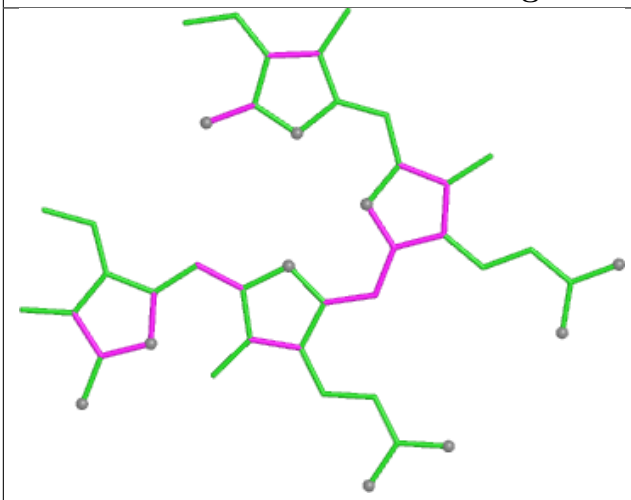


Rings

Ligand PEB JI 202



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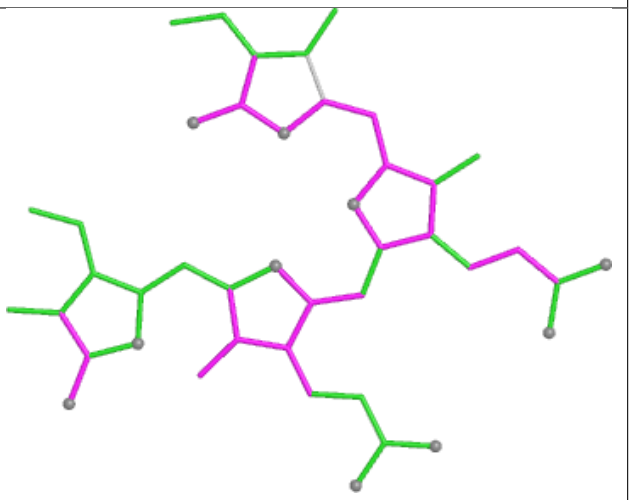

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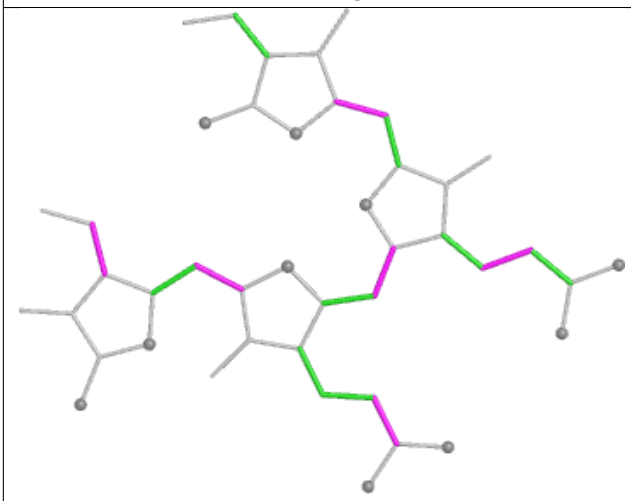
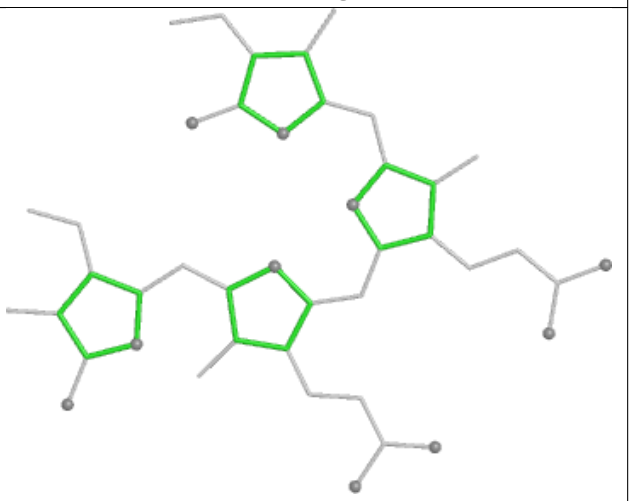
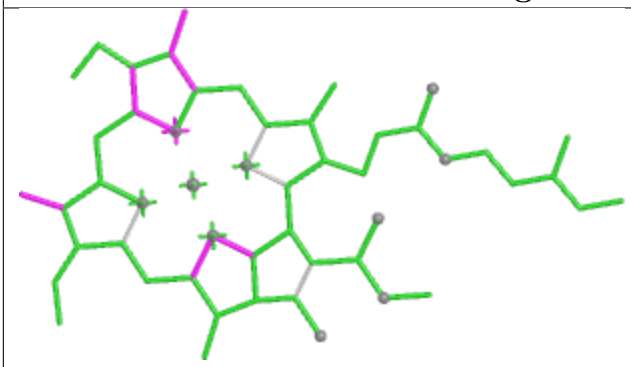


Torsions



Rings

Ligand CLA A2 824



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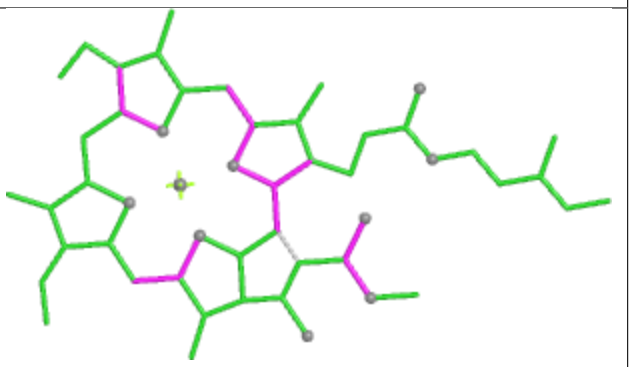

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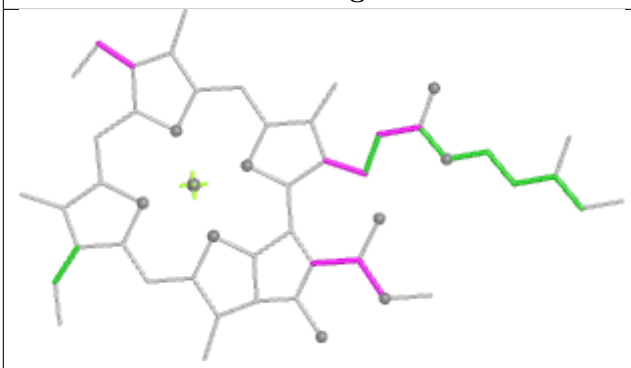

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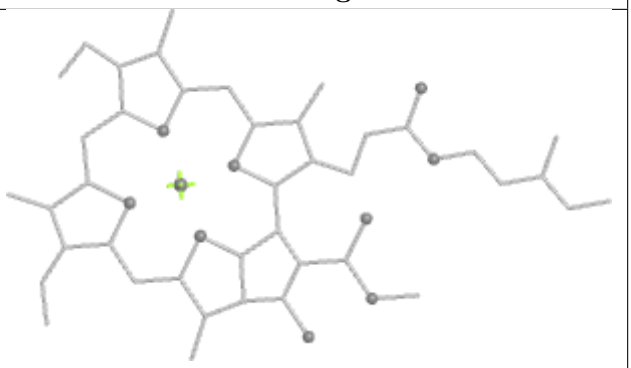
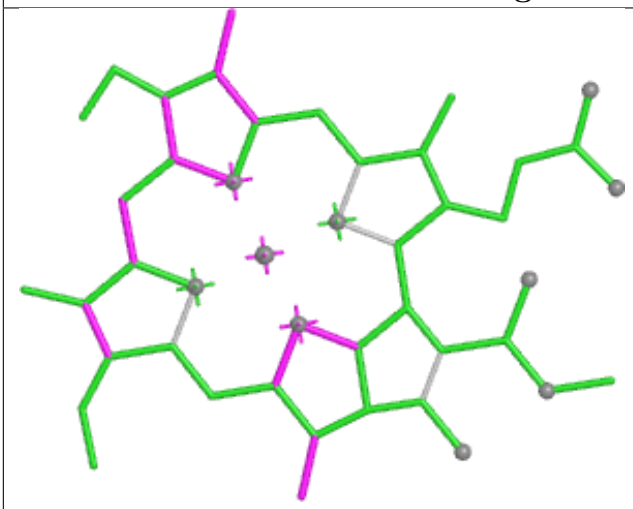


Rings

Ligand CLA 8N 308



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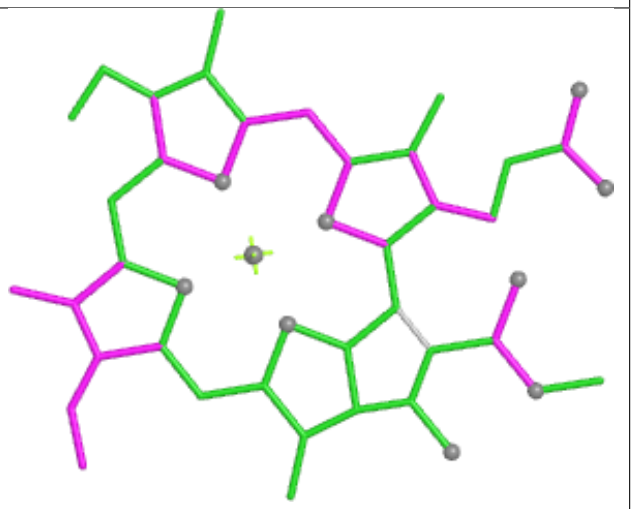

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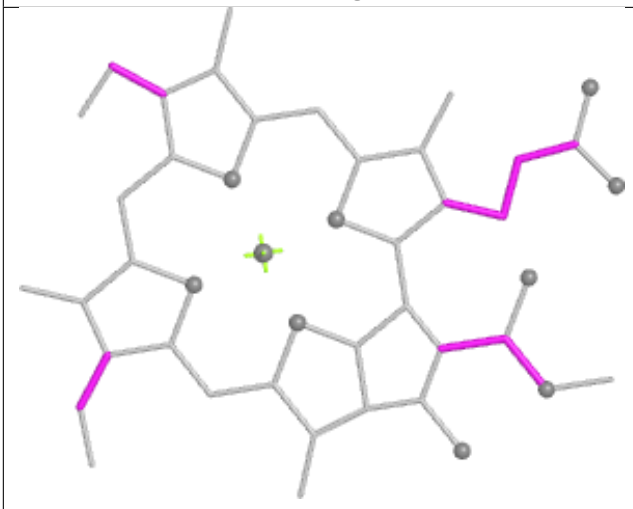
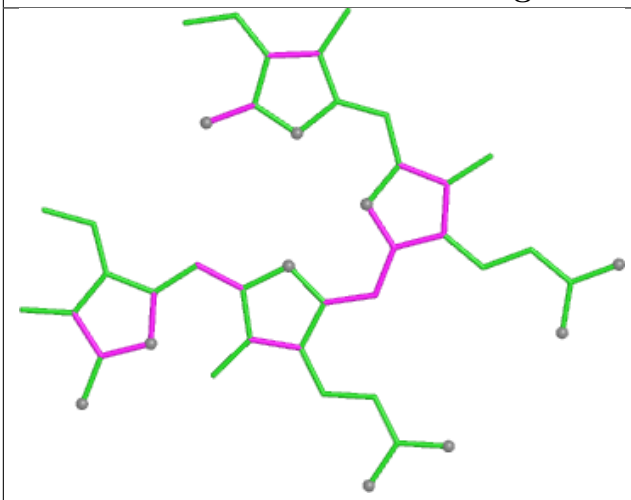


Torsions



Rings

Ligand PEB SD 201



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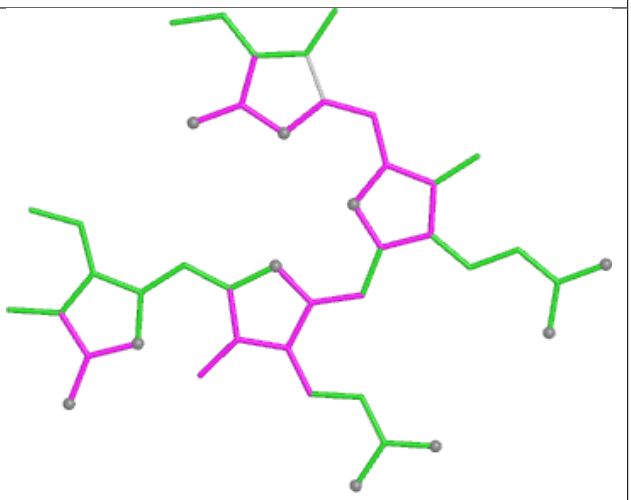

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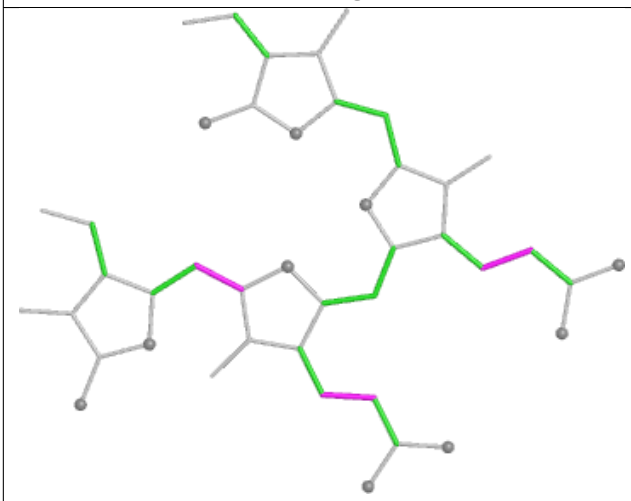

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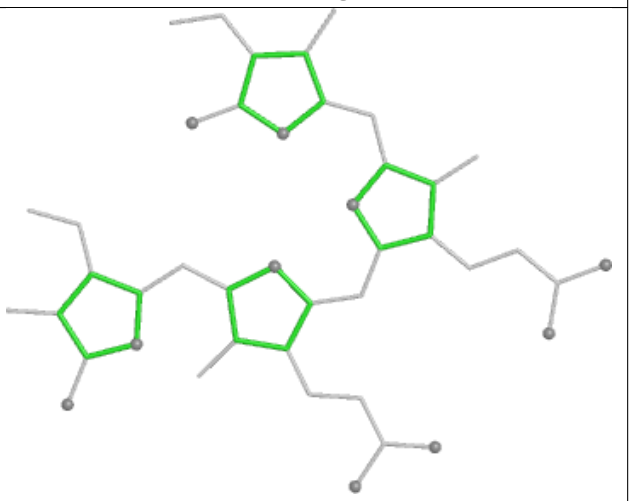
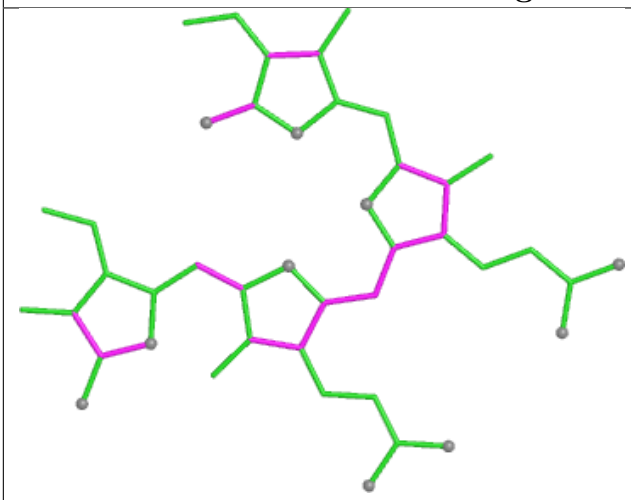


Rings

Ligand PEB Y4 203



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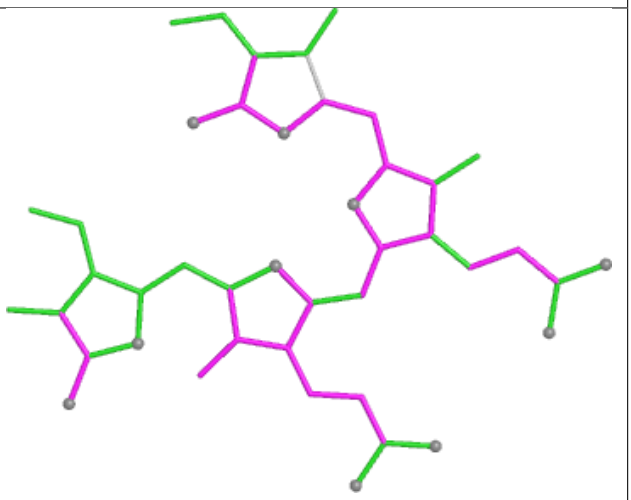

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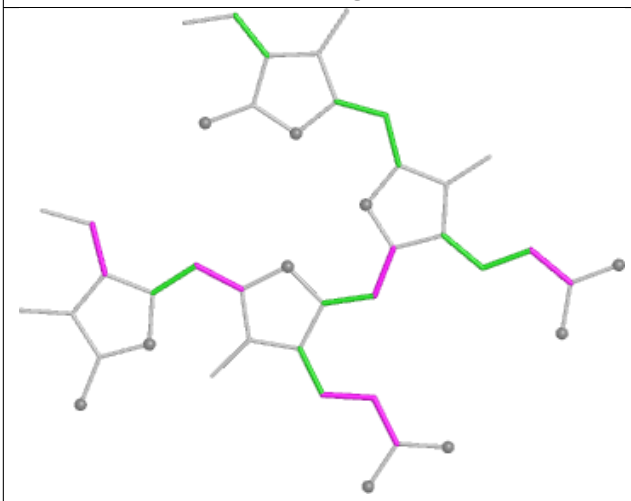

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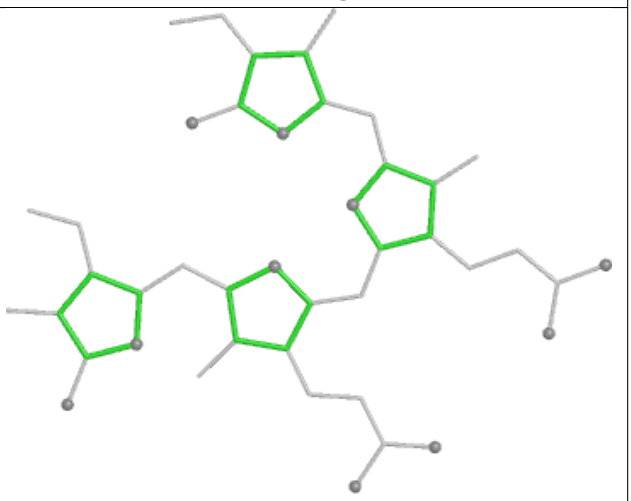

Rings

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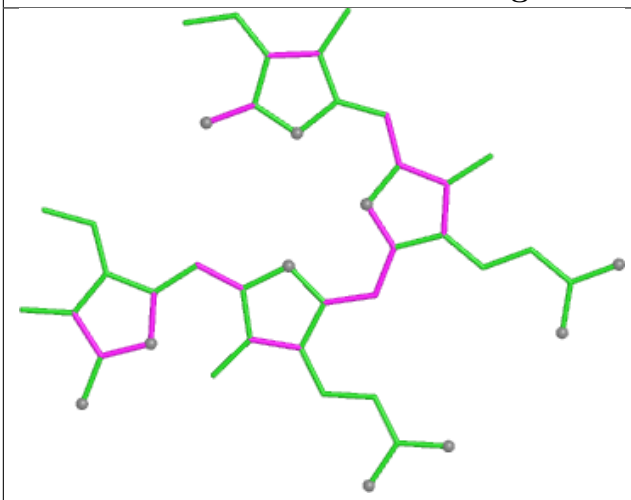

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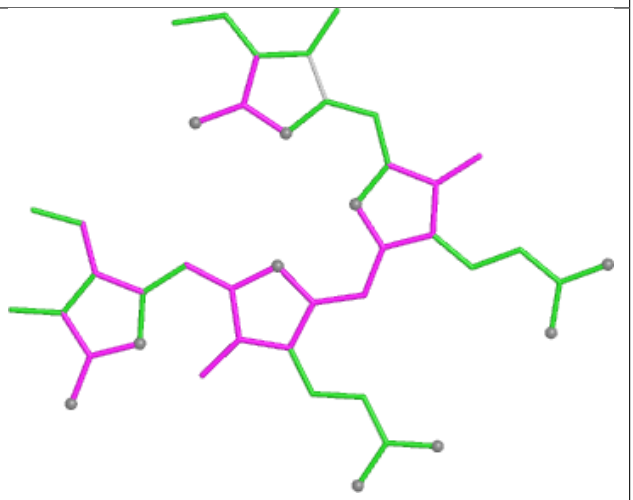

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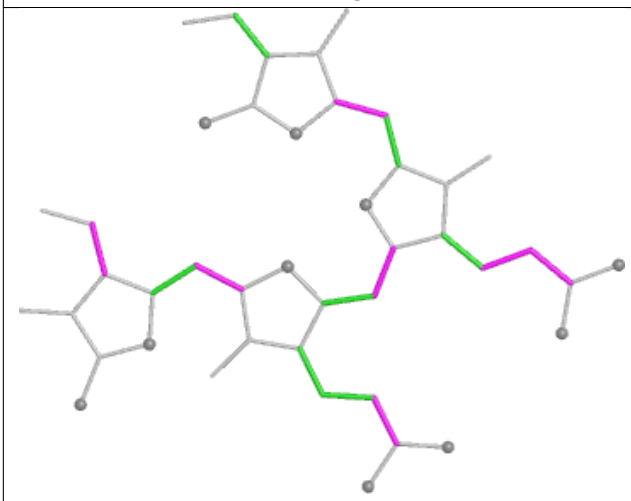

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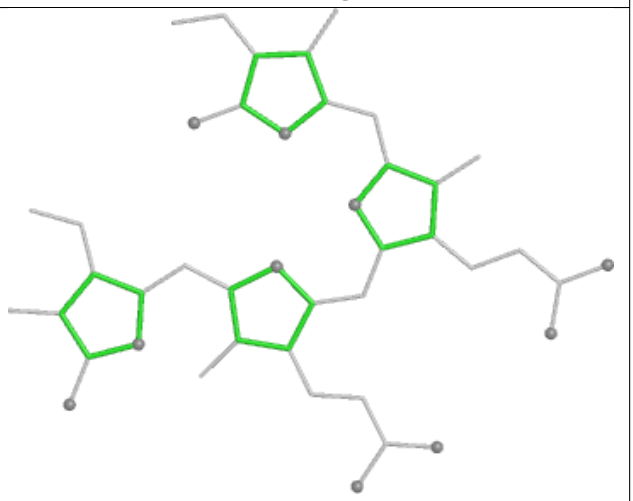

Rings

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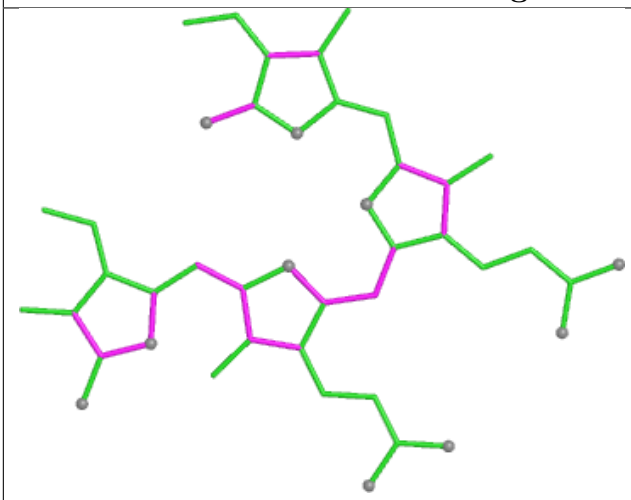

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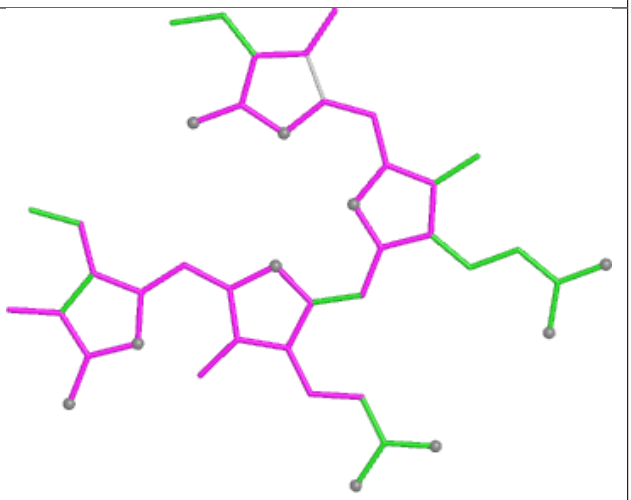

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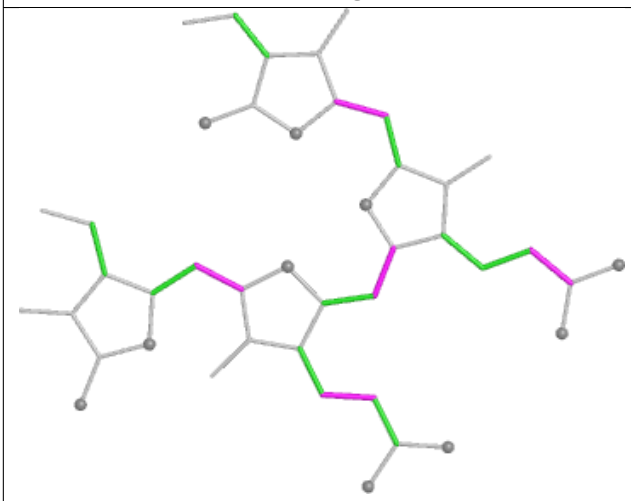

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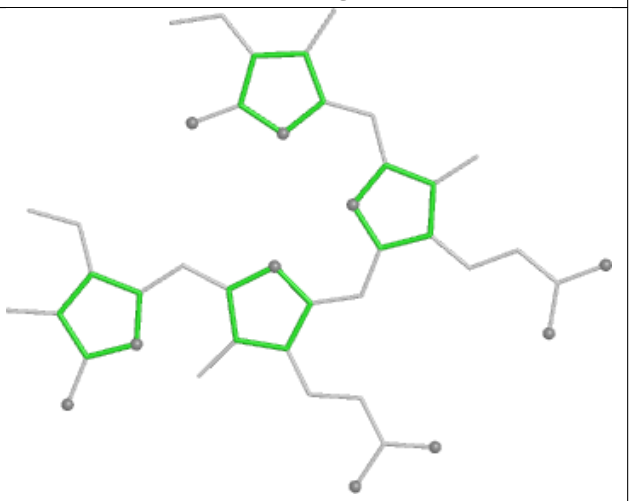

Rings

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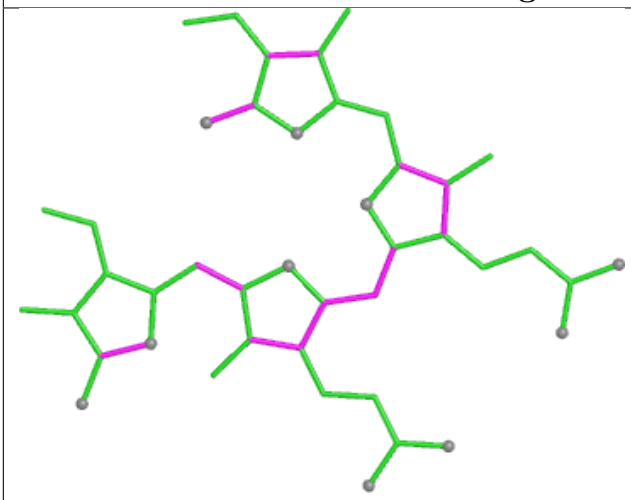

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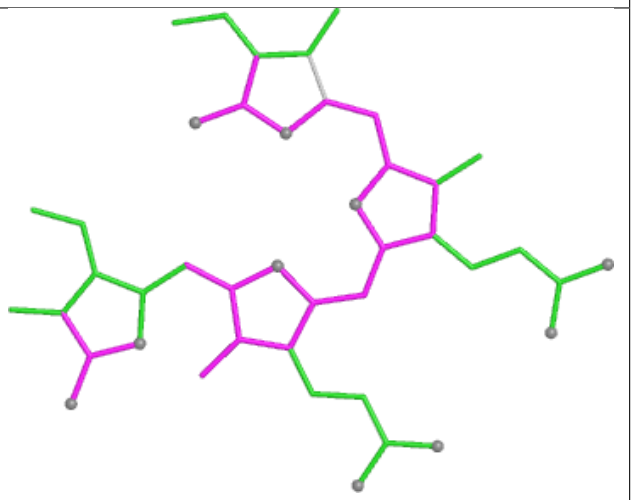

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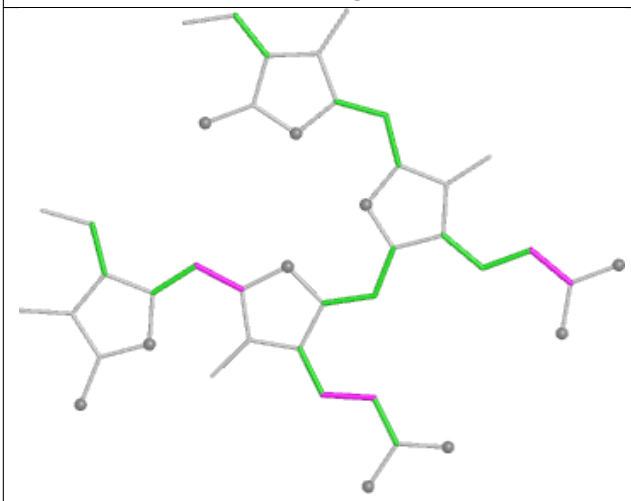

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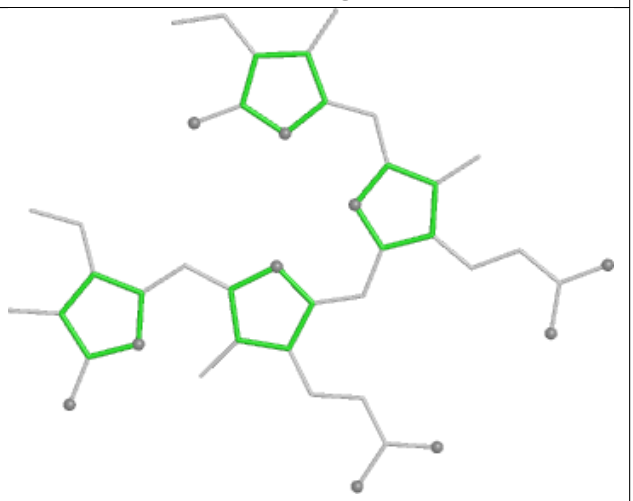
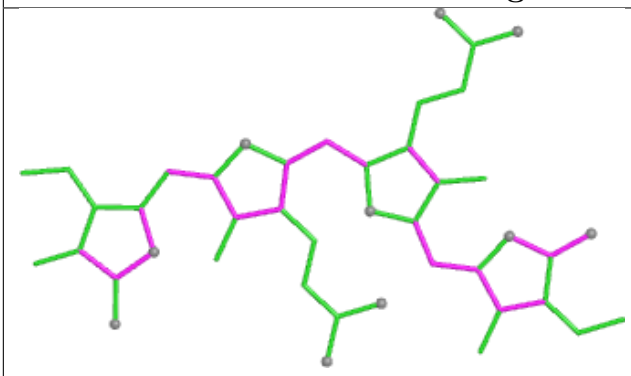


Rings

Ligand CYC p3 1001



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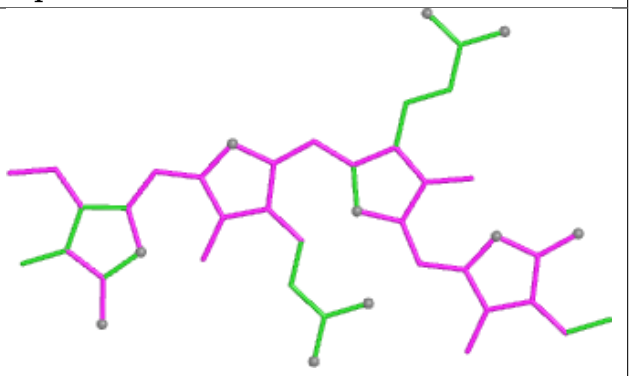

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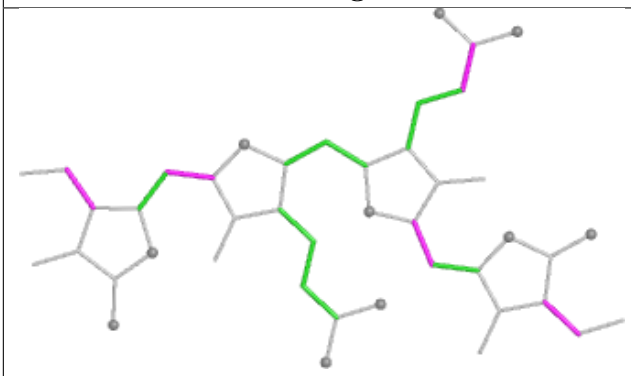

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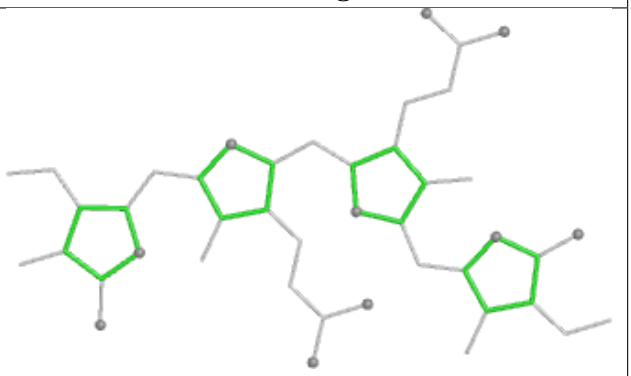
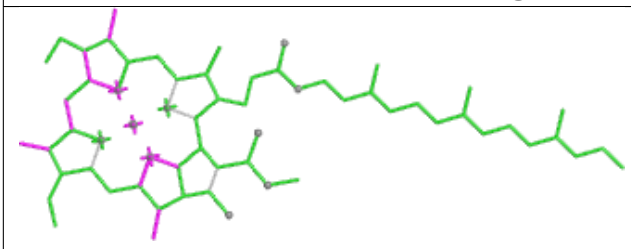


Rings

Ligand CLA AN 819



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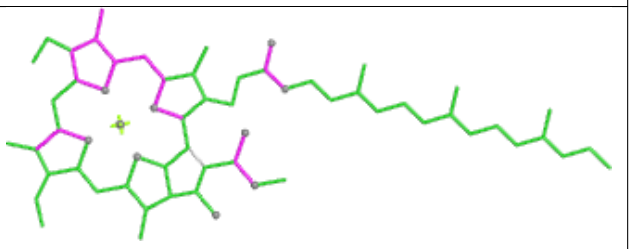

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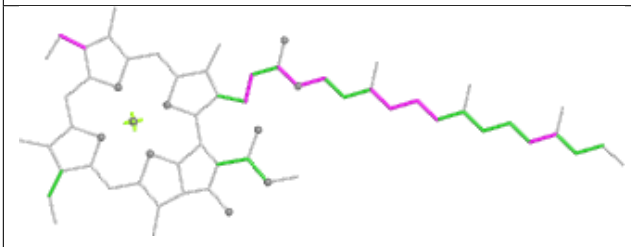

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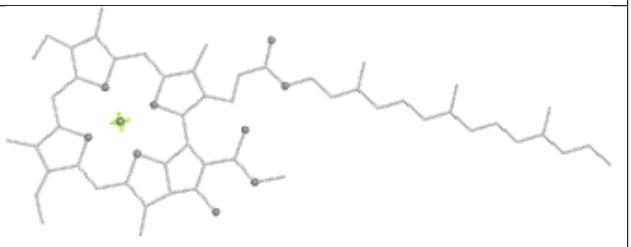
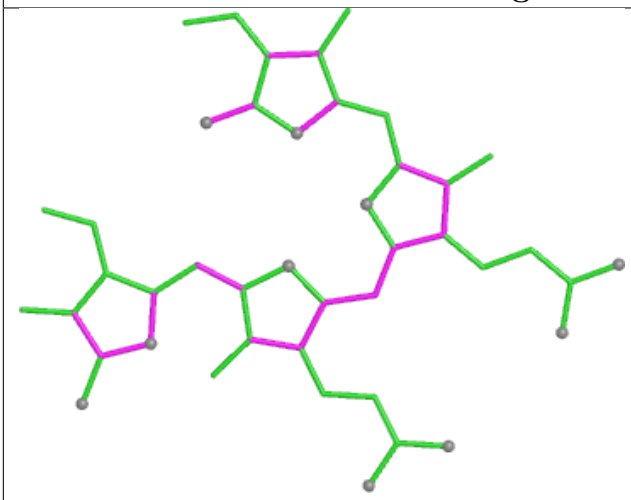


Rings

Ligand PEB EA 202



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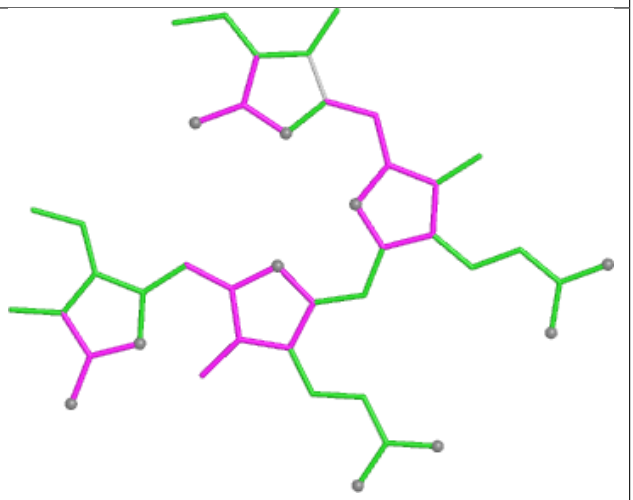

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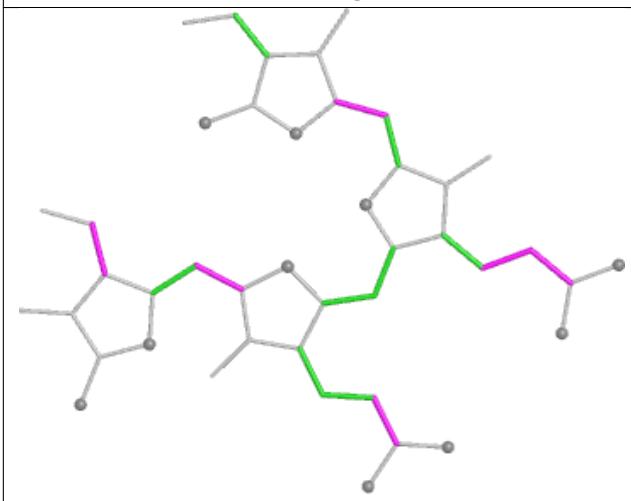

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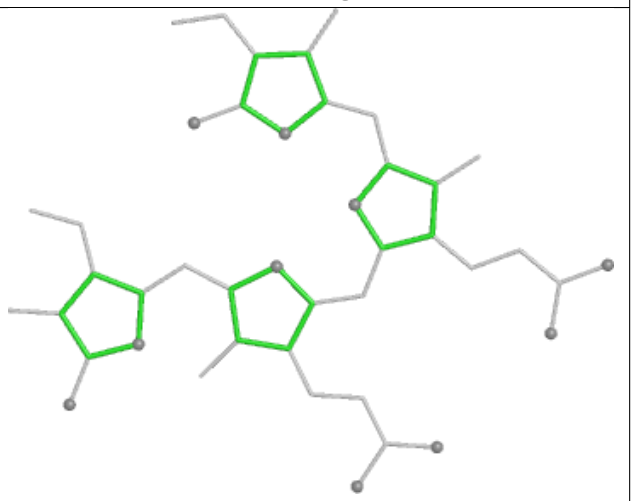
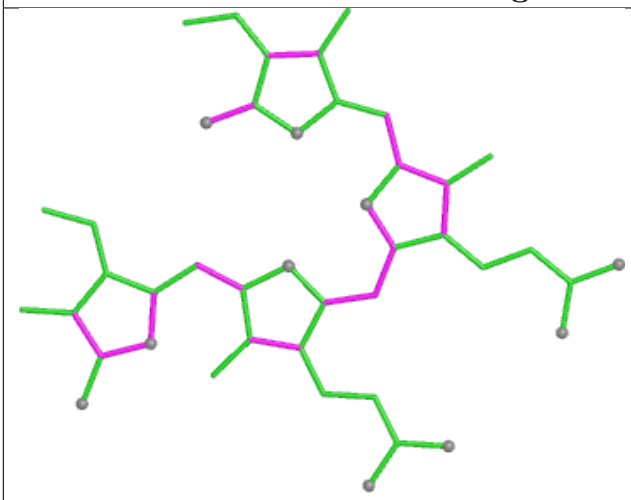


Rings

Ligand PEB GP 201



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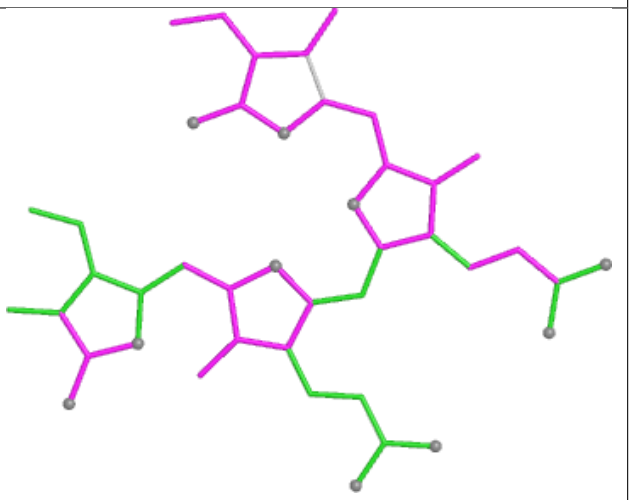

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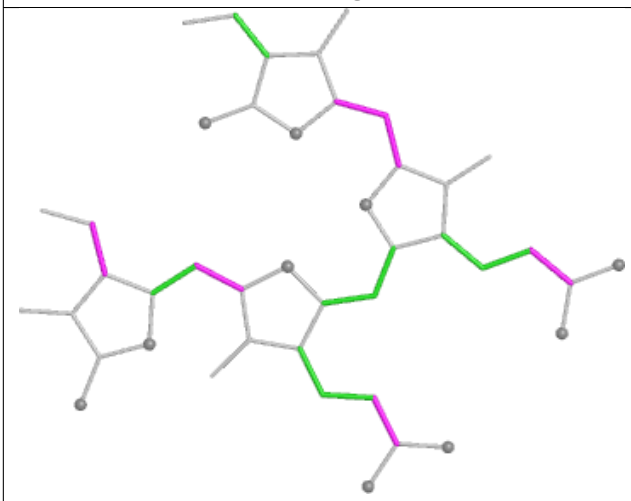

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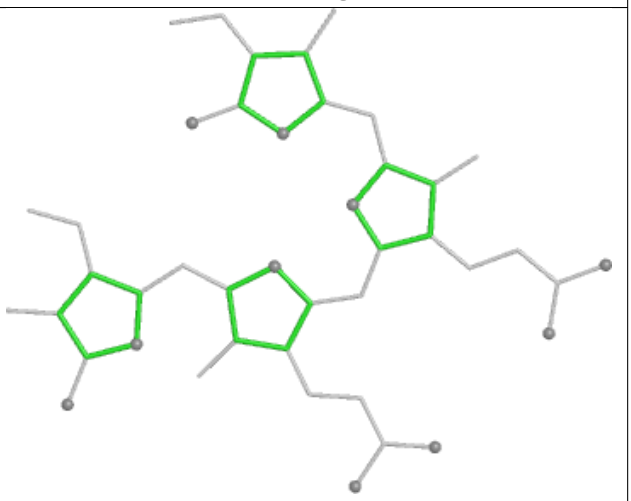
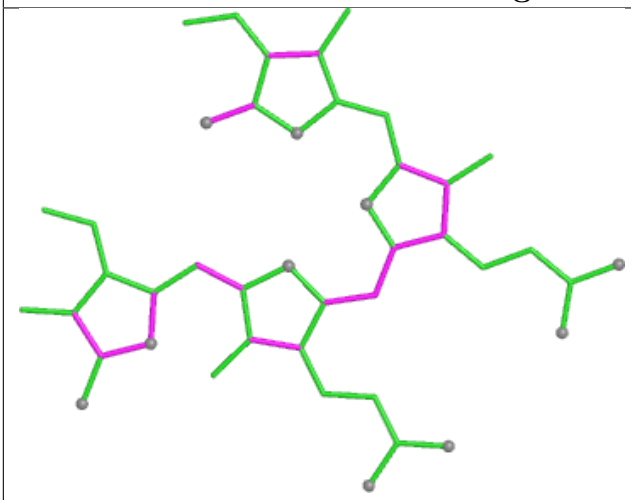


Rings

Ligand PEB PA 201



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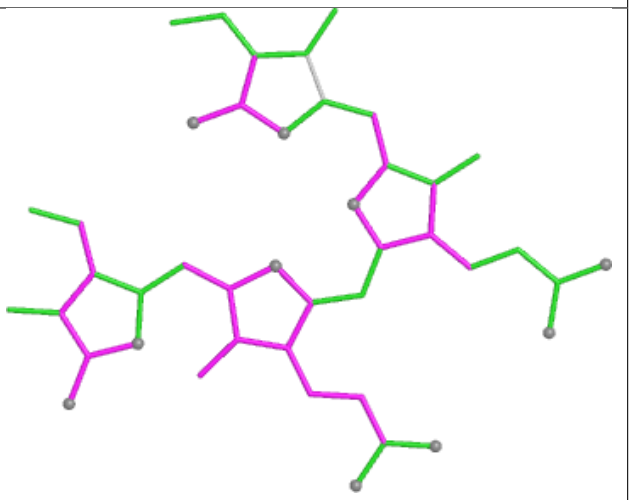

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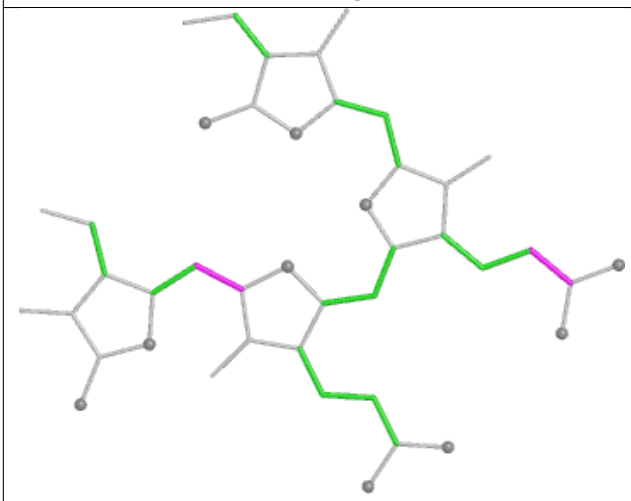

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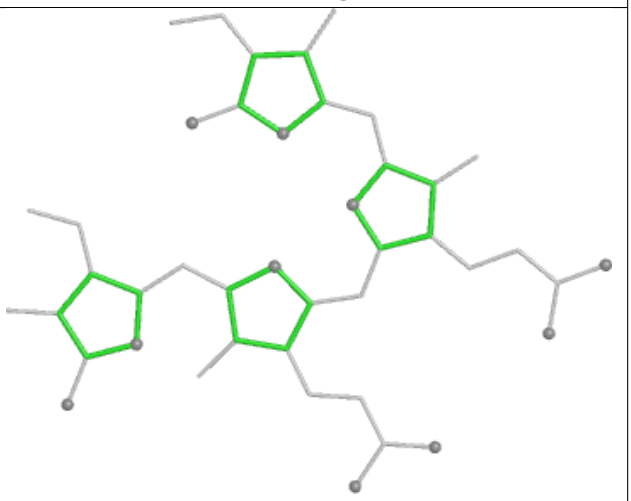
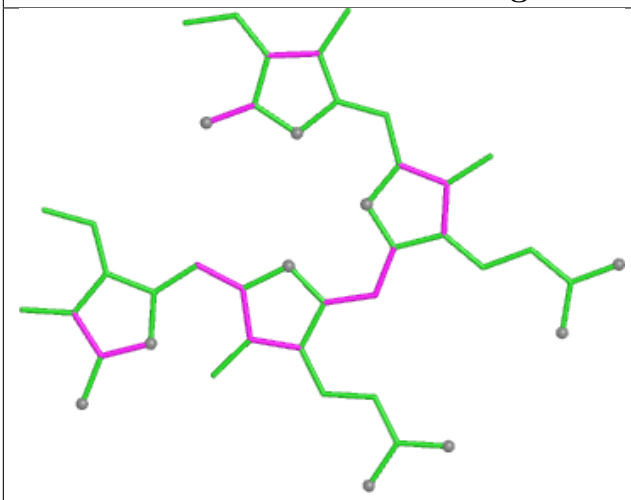


Rings

Ligand PEB QH 202



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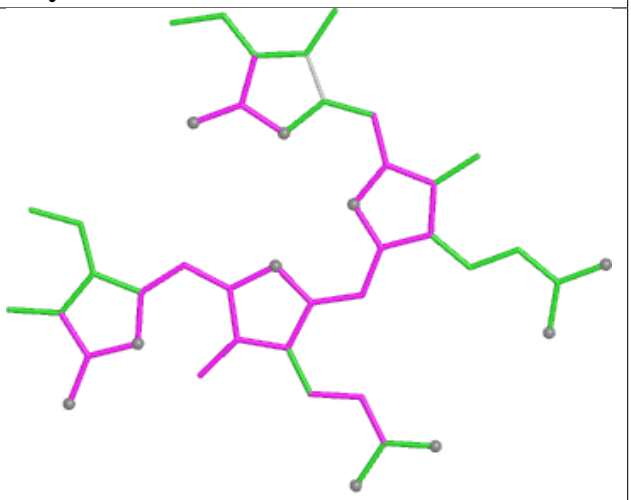

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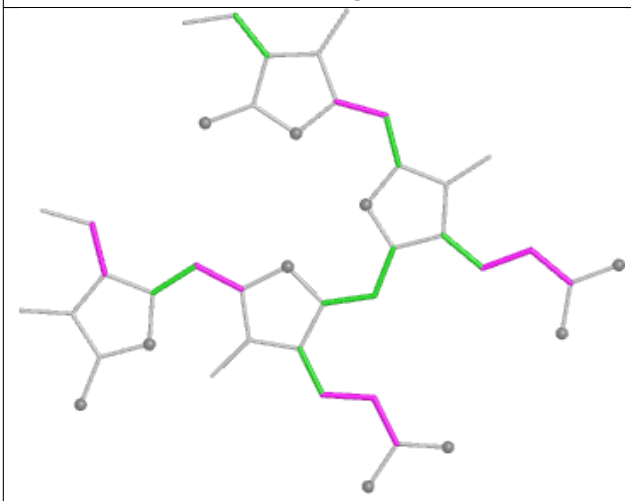

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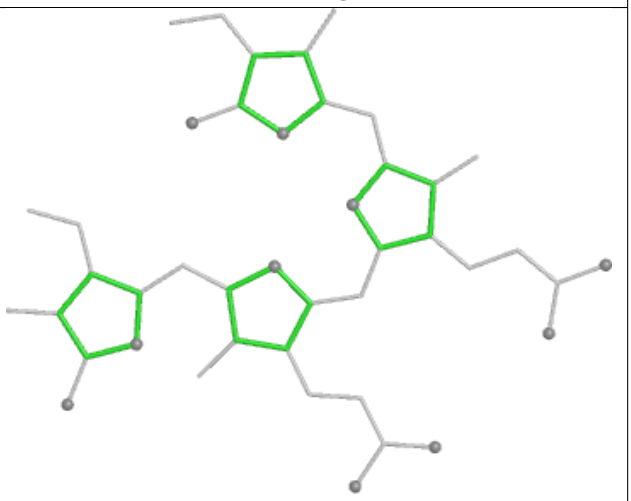
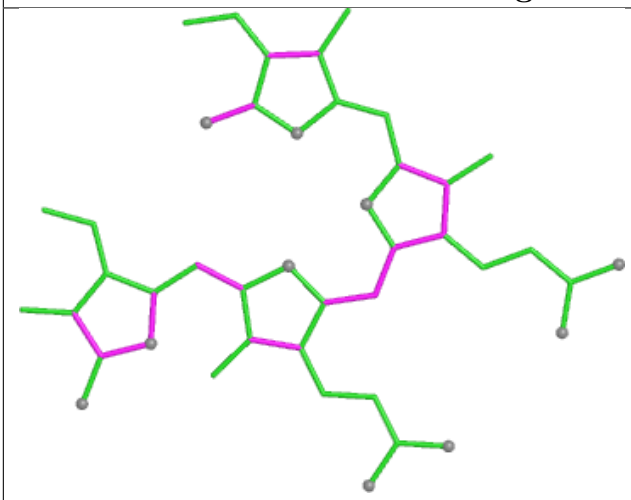


Rings

Ligand PEB A4 301



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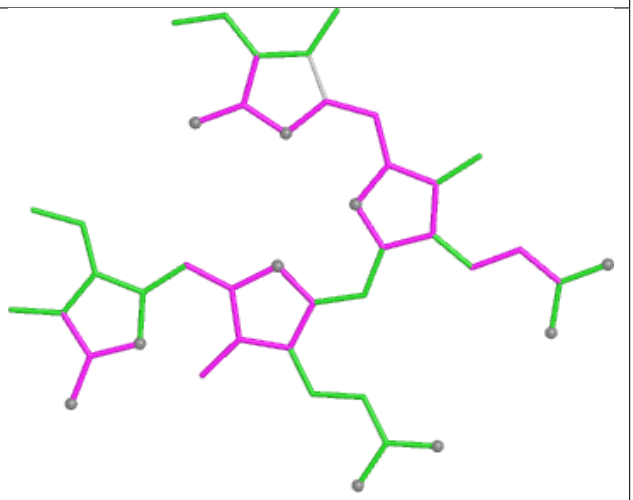
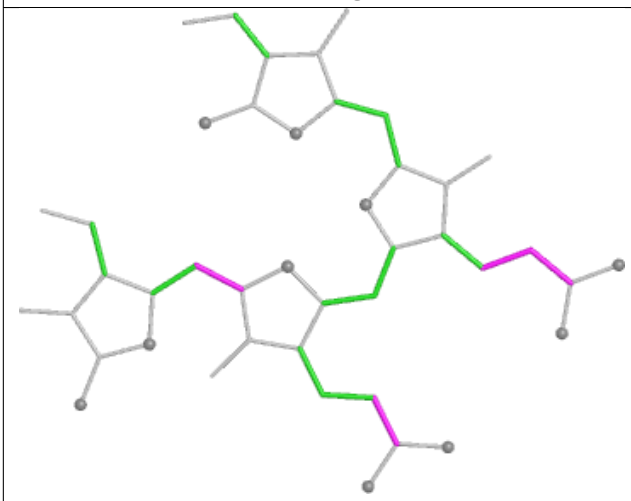


Bond angles



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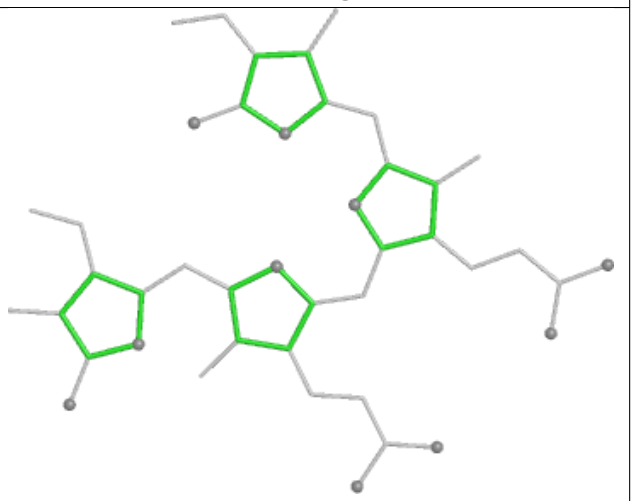
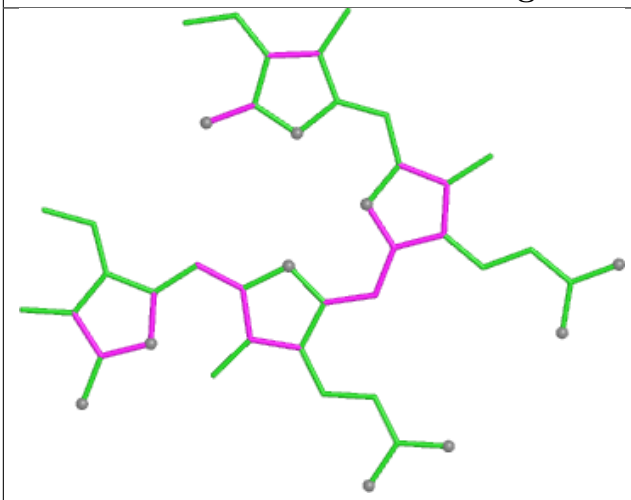


Rings

Ligand PEB eE 203



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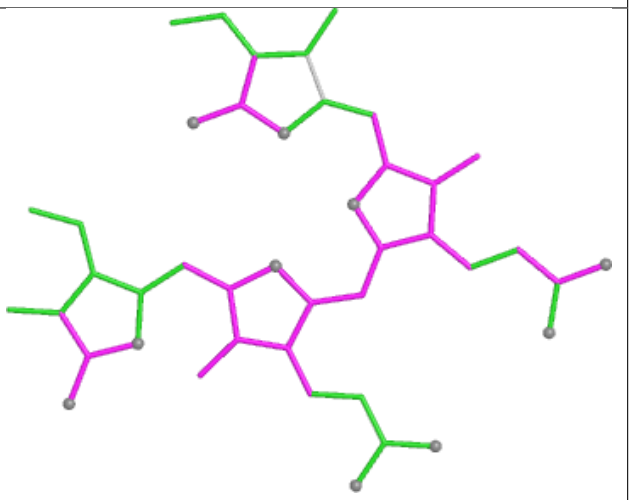

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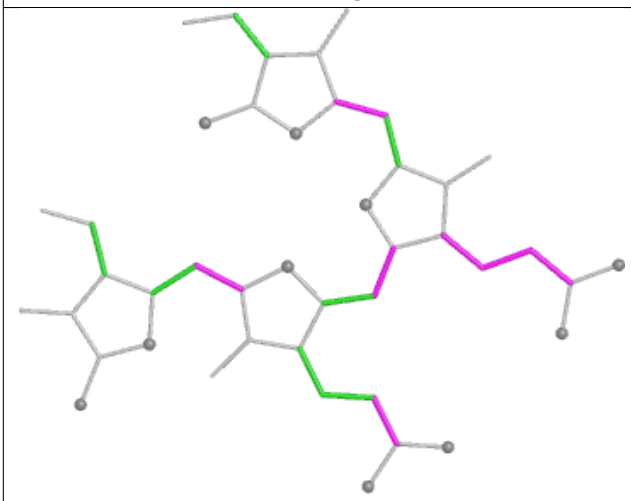

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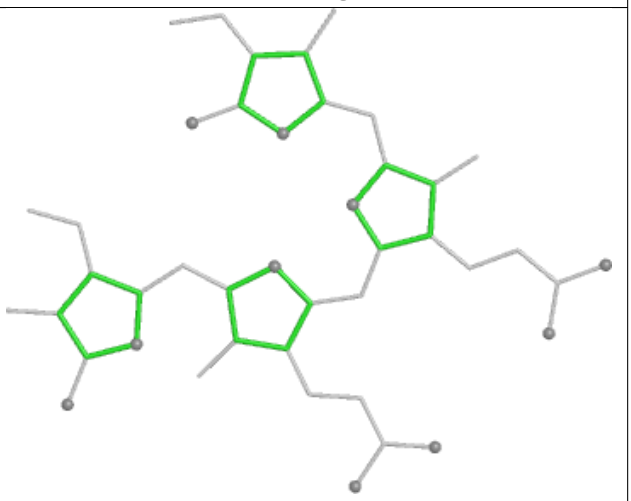
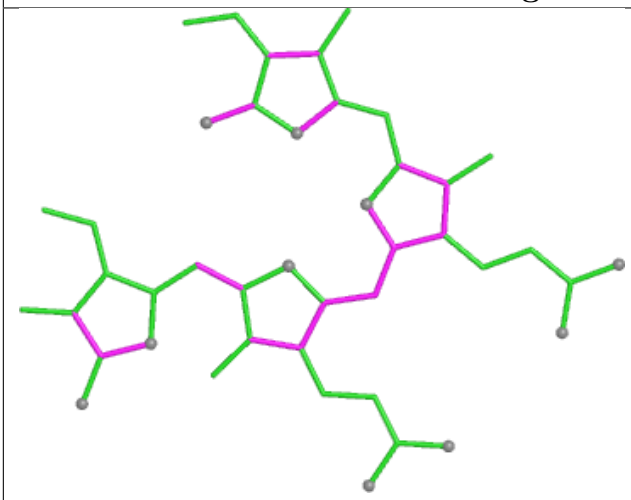


Rings

Ligand PEB I9 202



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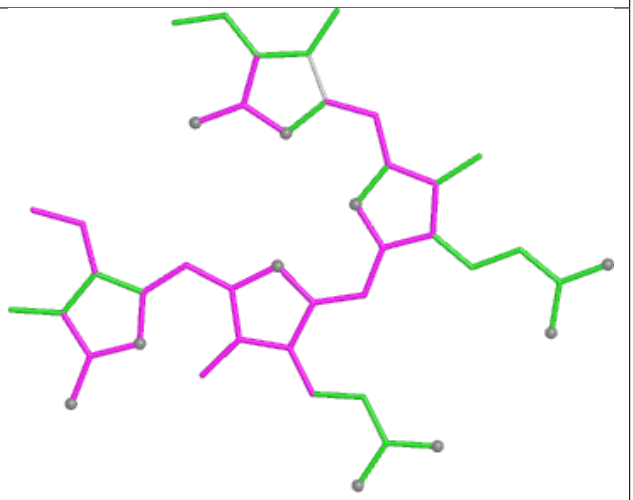

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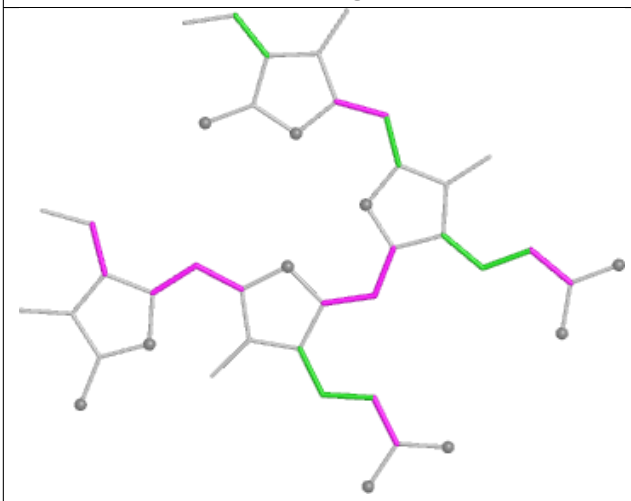

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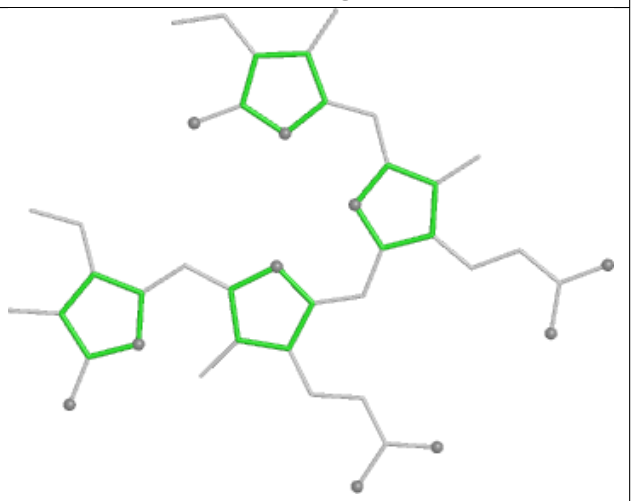
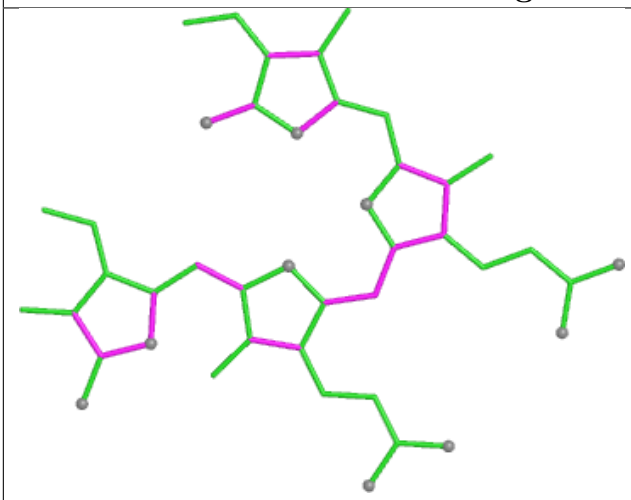


Rings

Ligand PEB A1 302



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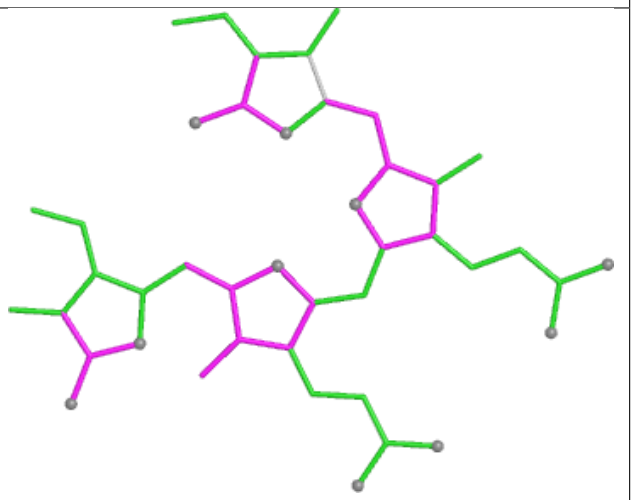

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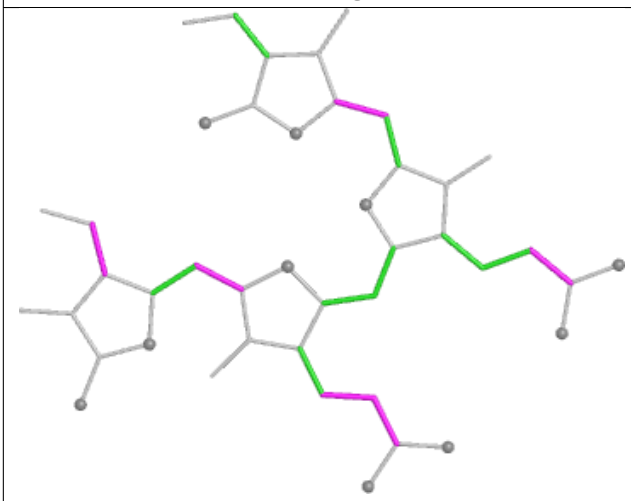

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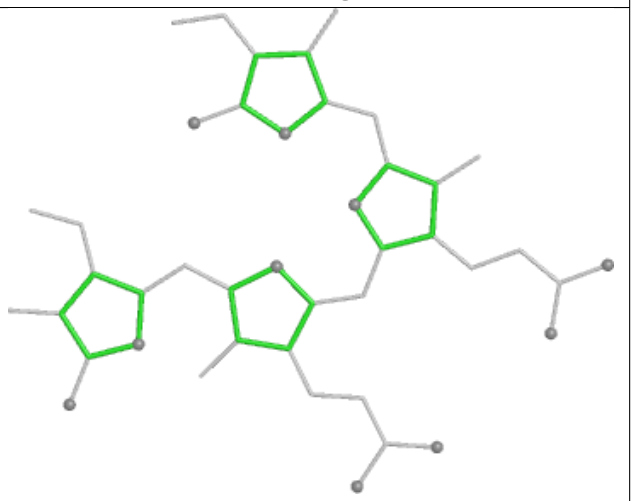
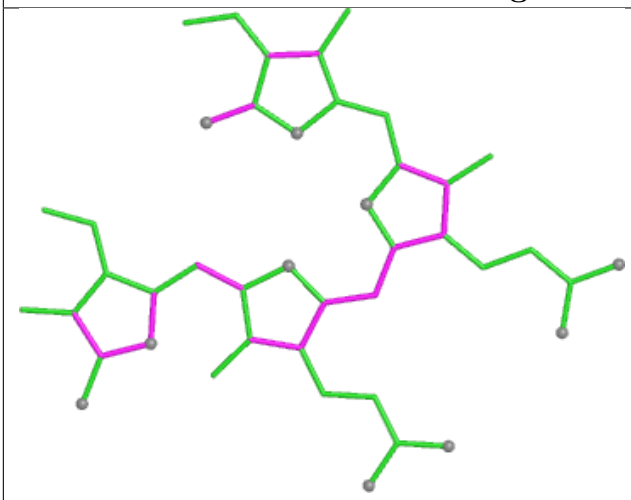


Rings

Ligand PEB KD 201



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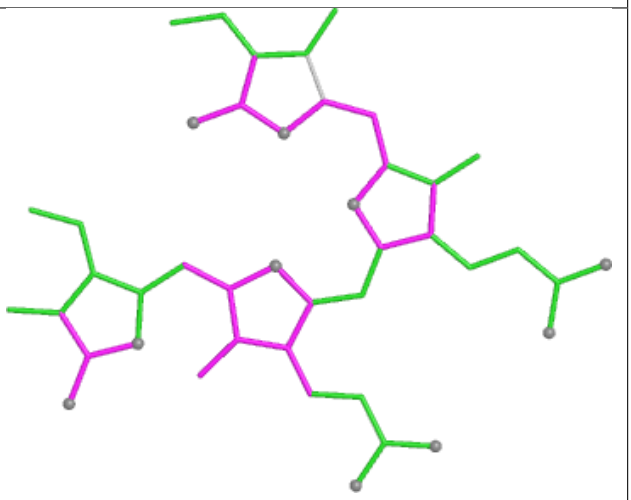

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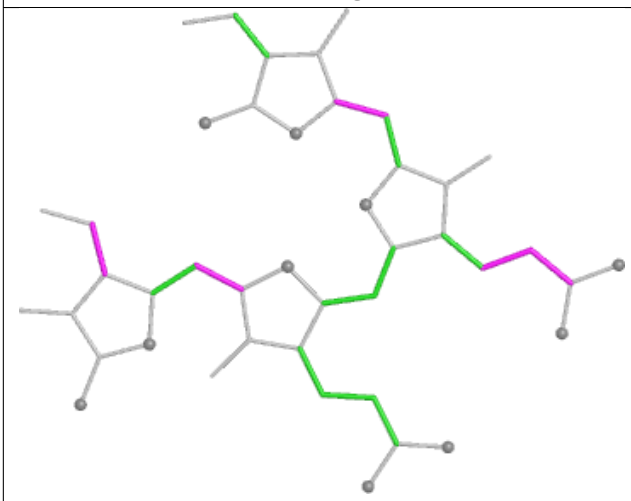

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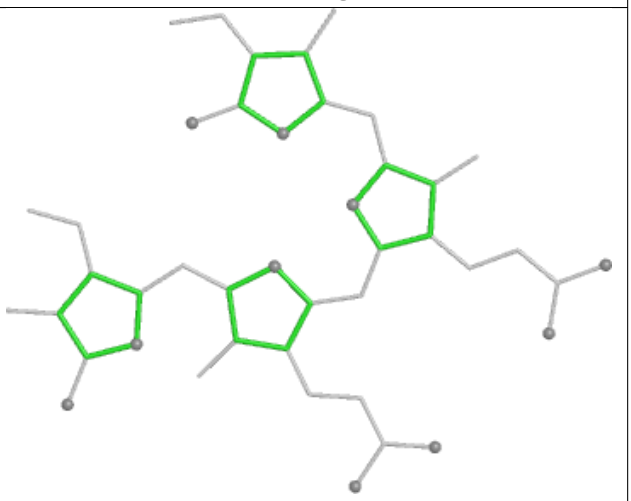

Rings

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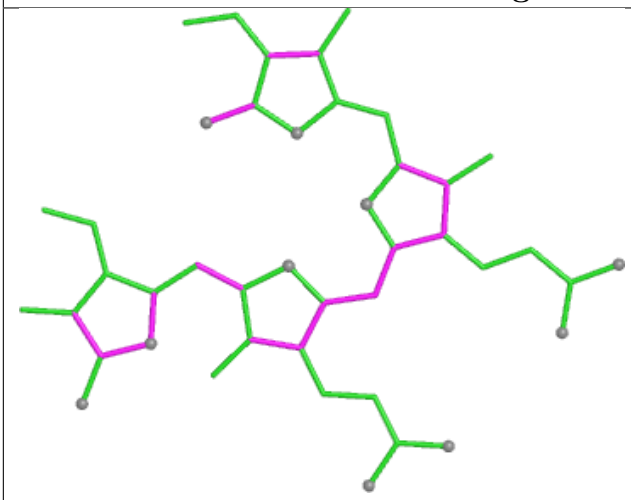

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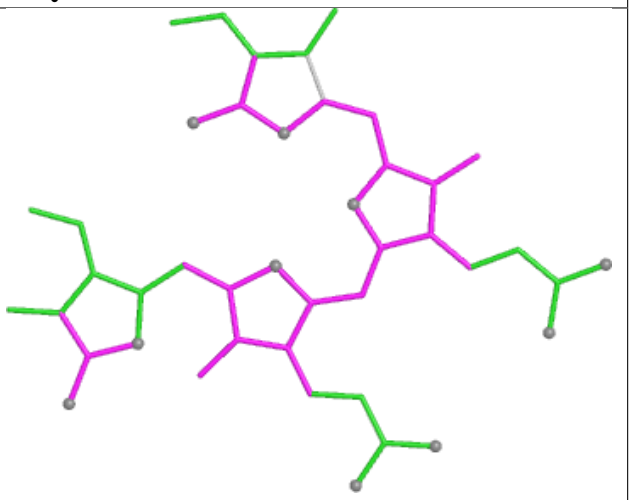

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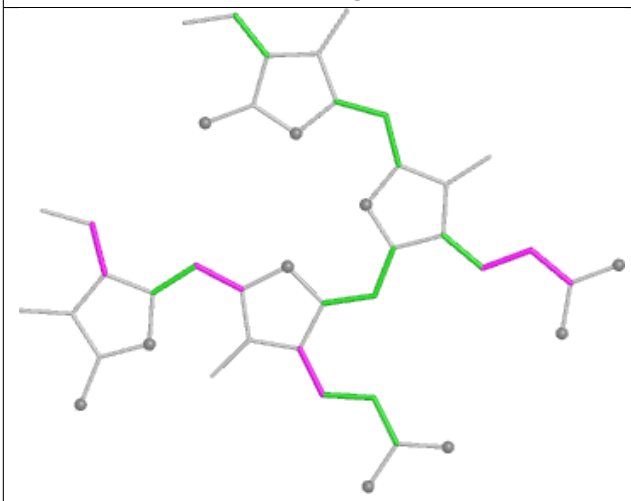

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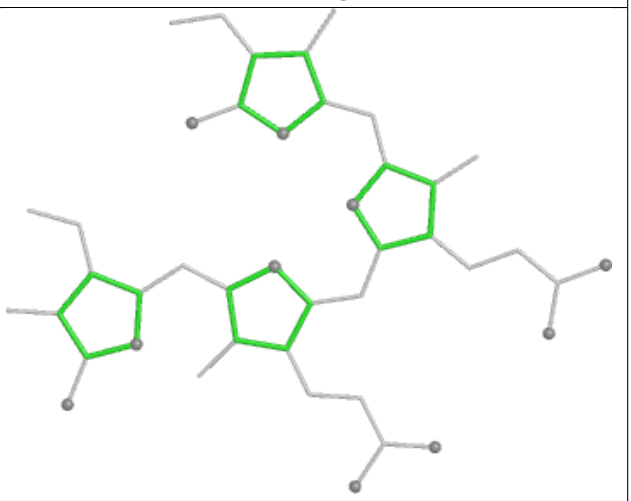
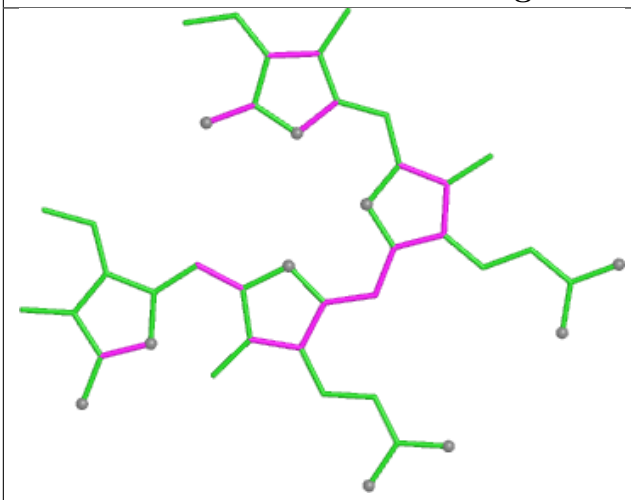


Rings

Ligand PEB kK 202



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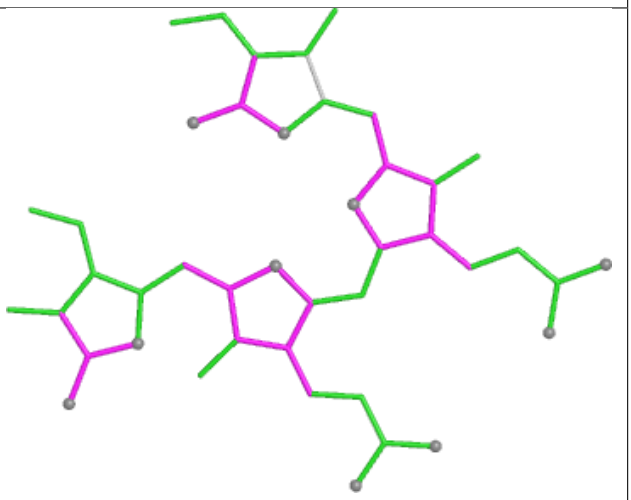

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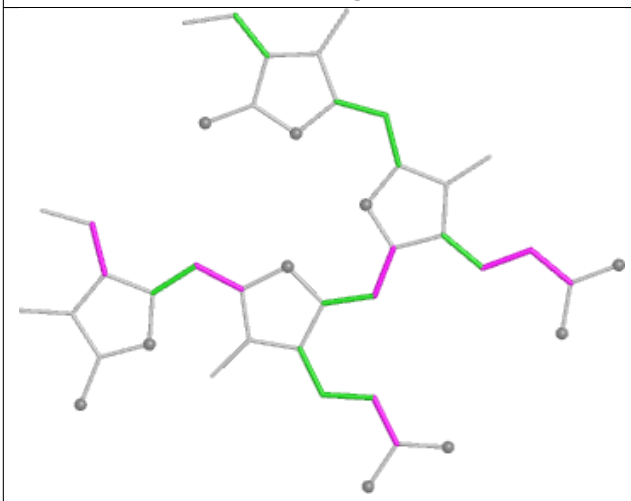

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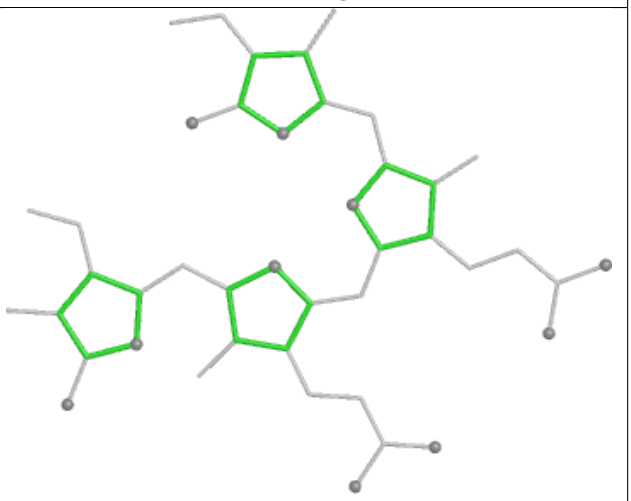

Rings

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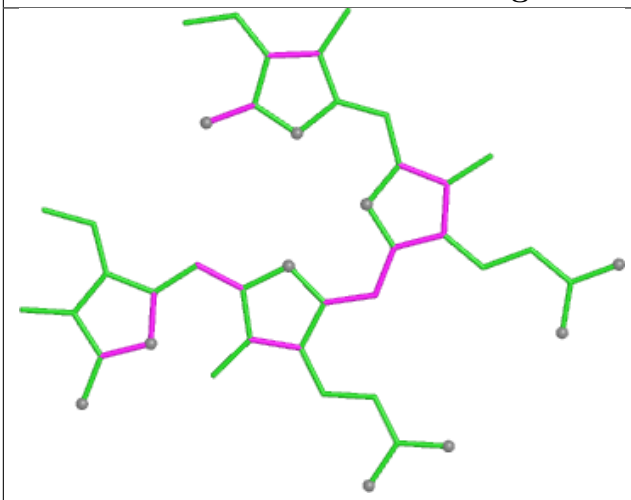

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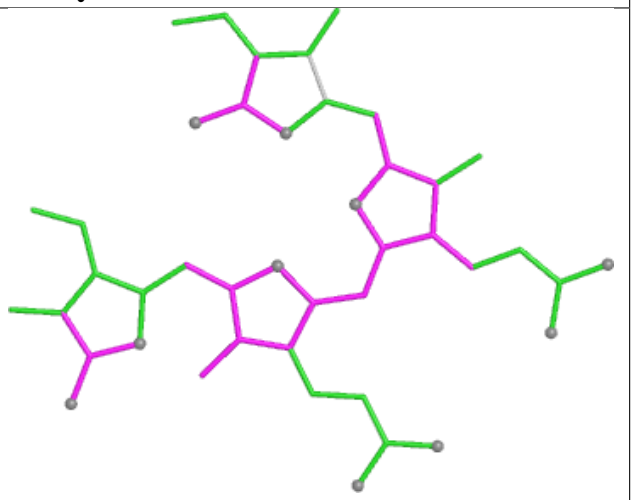

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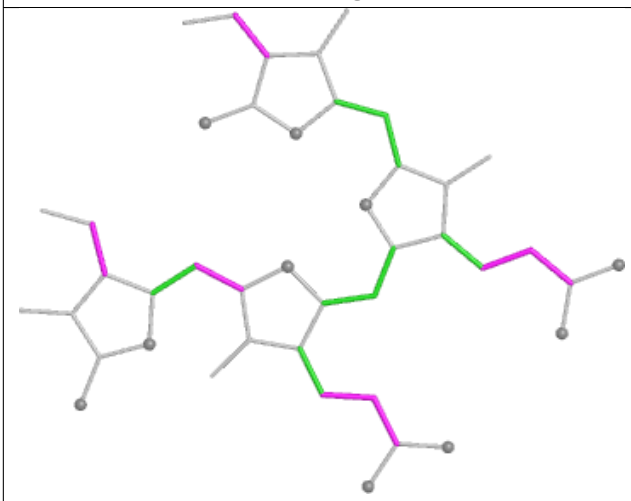

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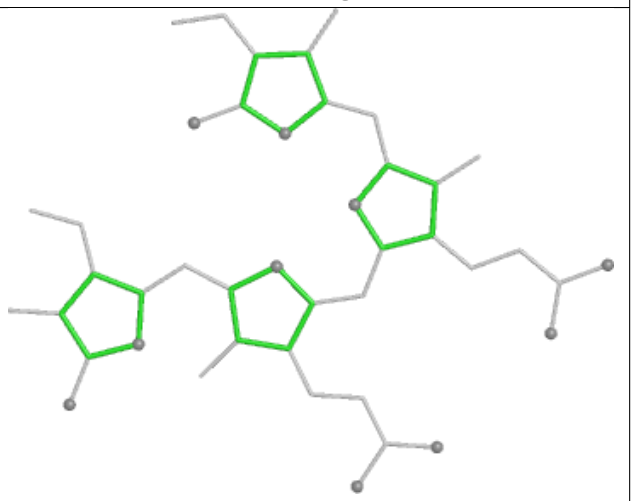
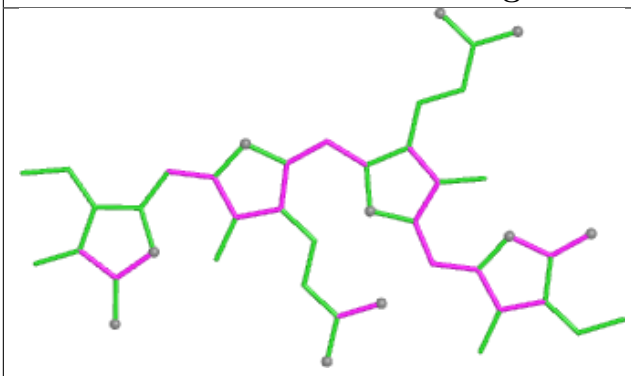


Rings

Ligand CYC H3 1001



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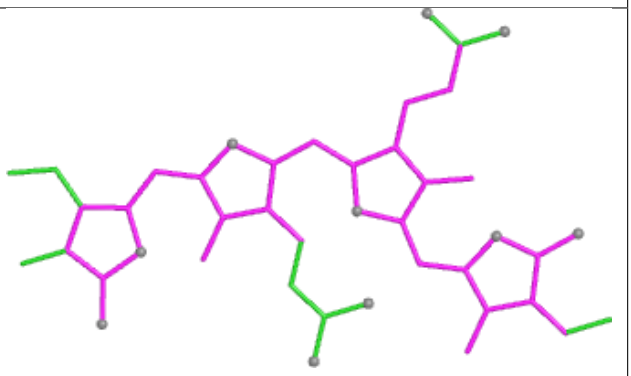

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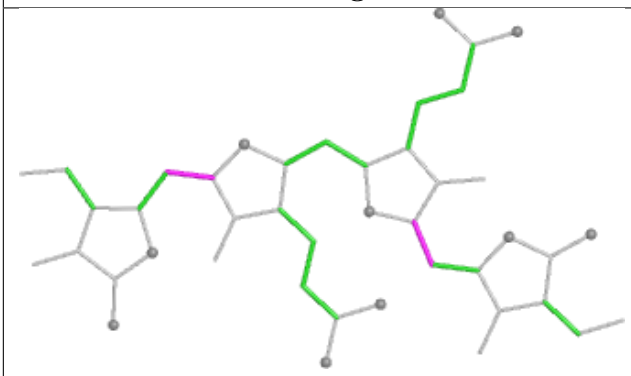

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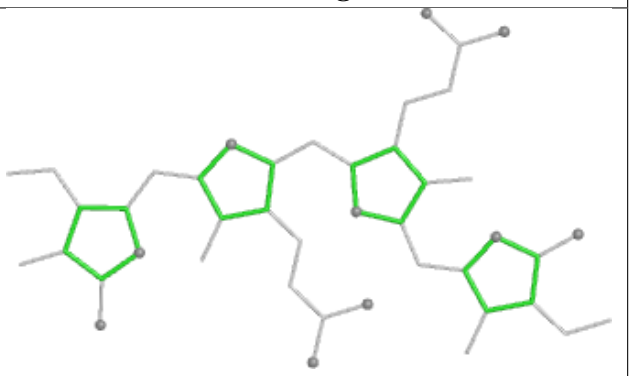
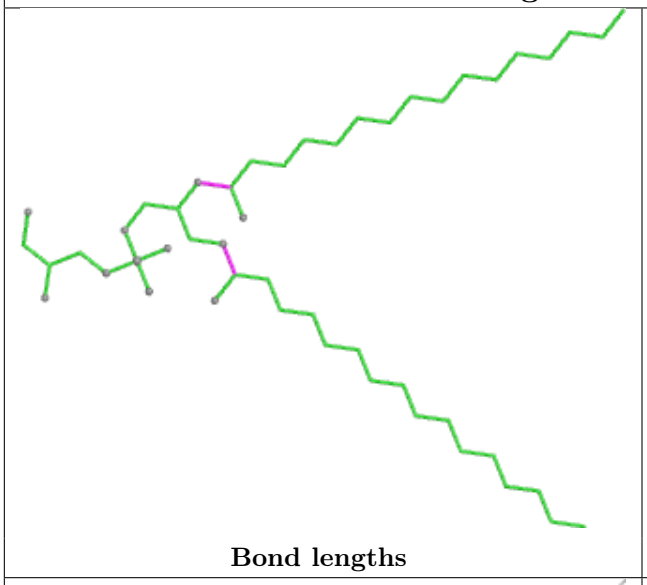


Rings

Ligand LHG I6 101



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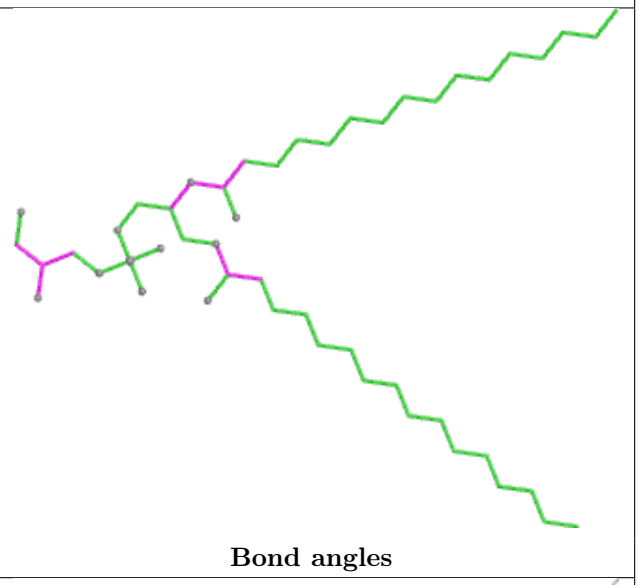

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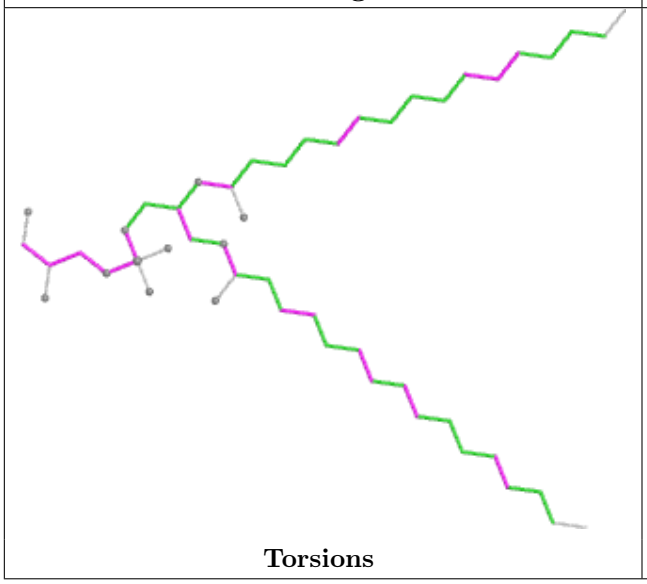

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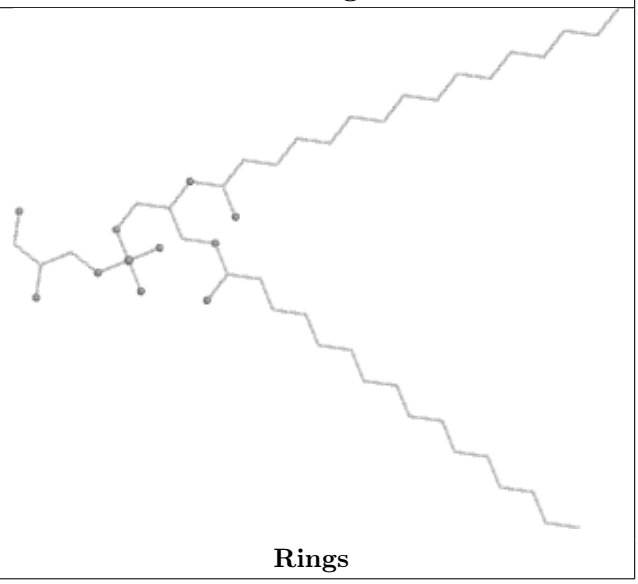
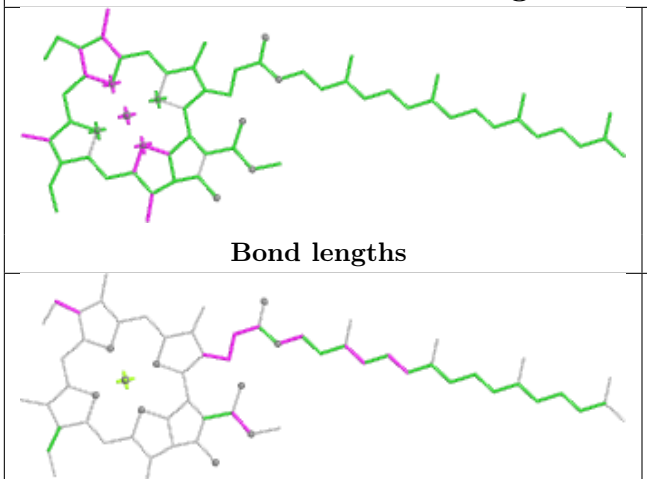


Rings

Ligand CLA AN 807



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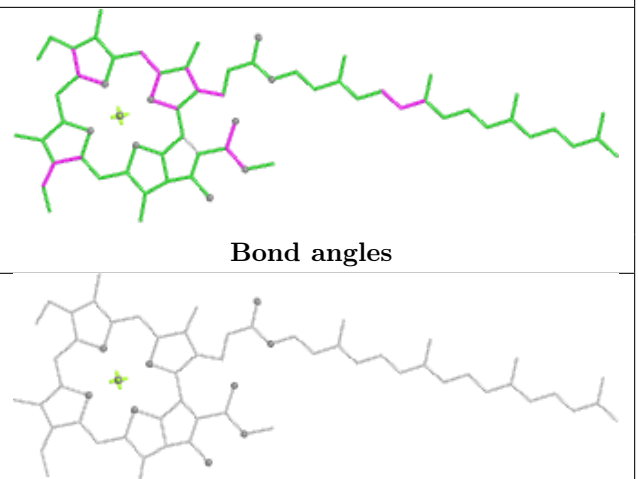
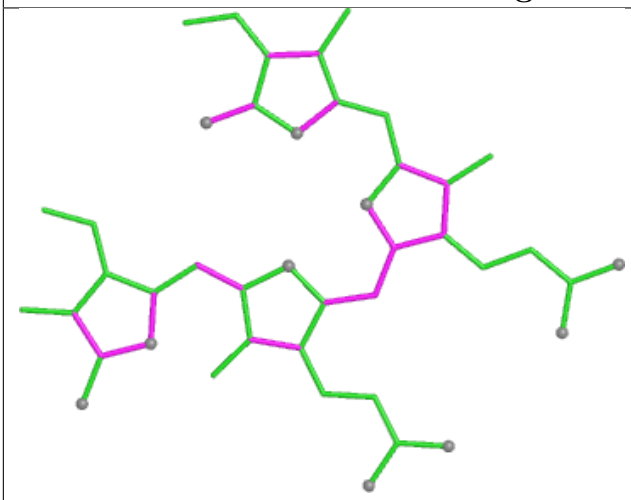


Bond angles

Torsions

Rings

Ligand PEB Y7 304



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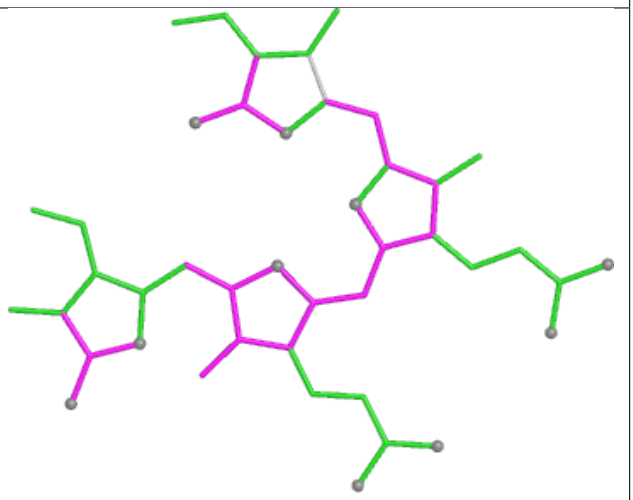

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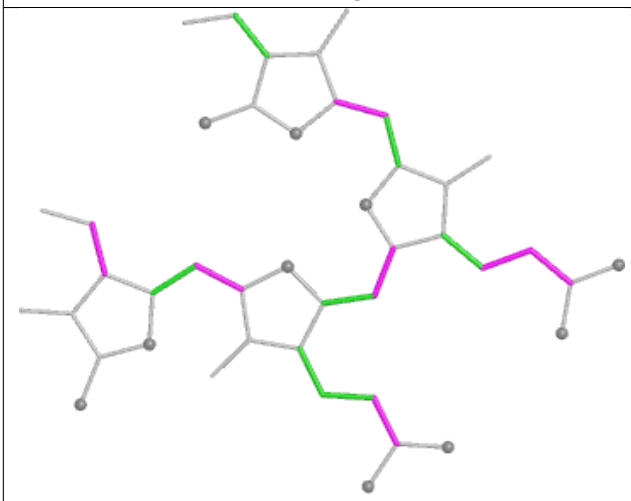

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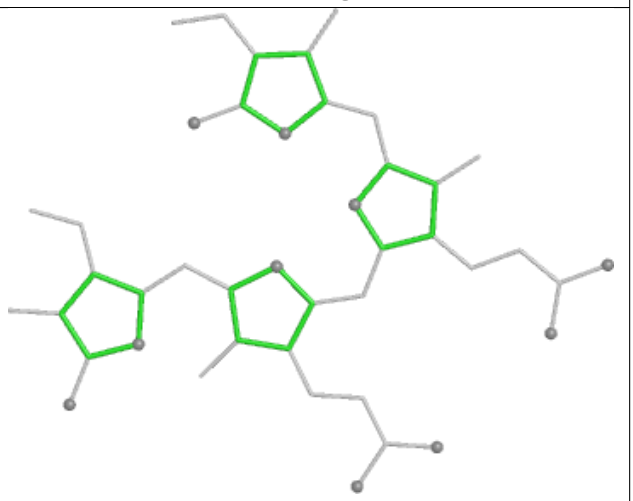
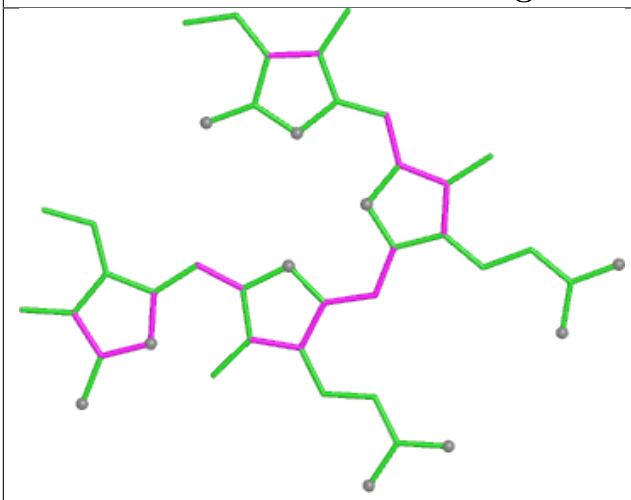


Rings

Ligand PEB Q5 202



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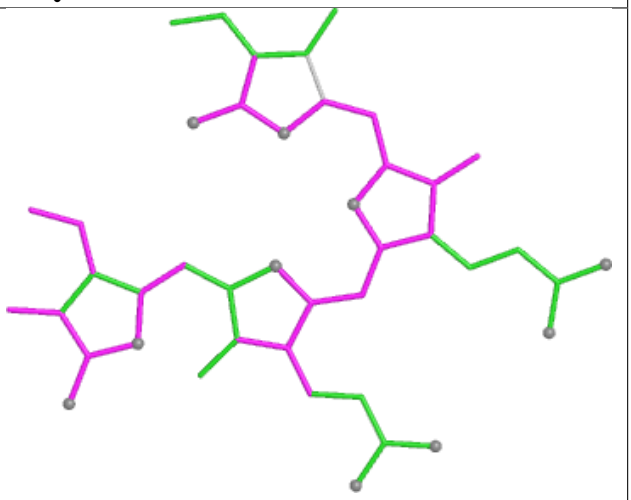

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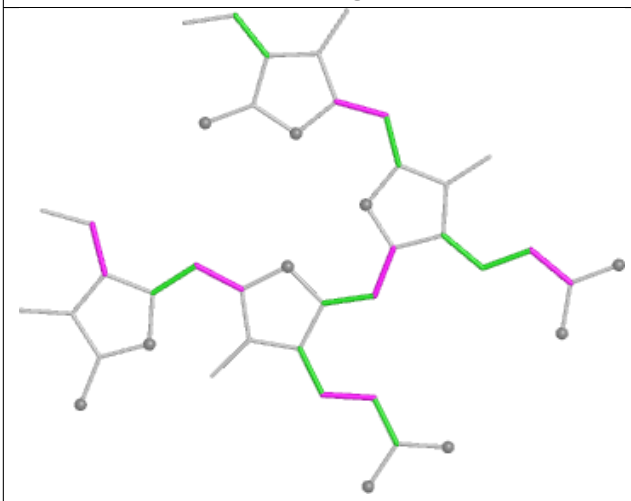

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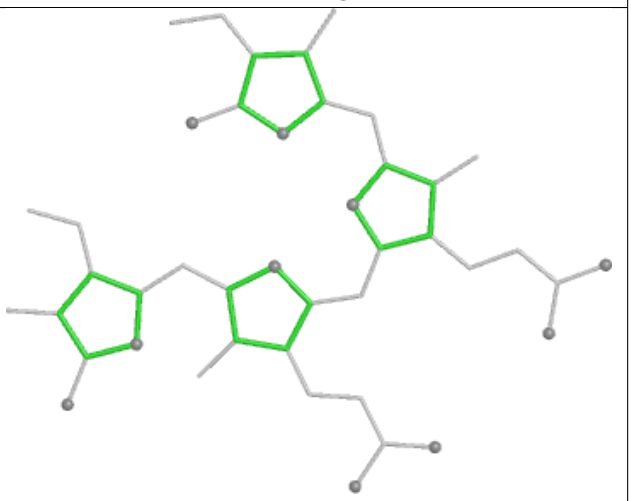
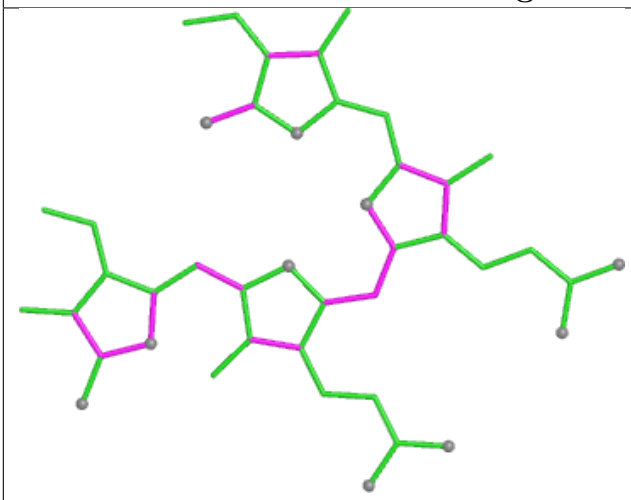


Rings

Ligand PEB aB 201



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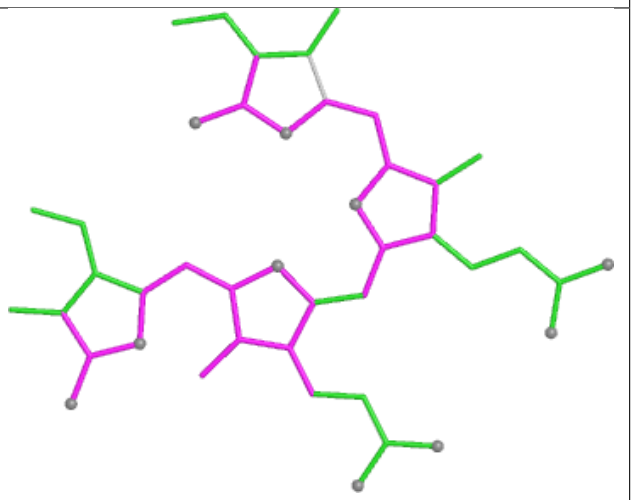

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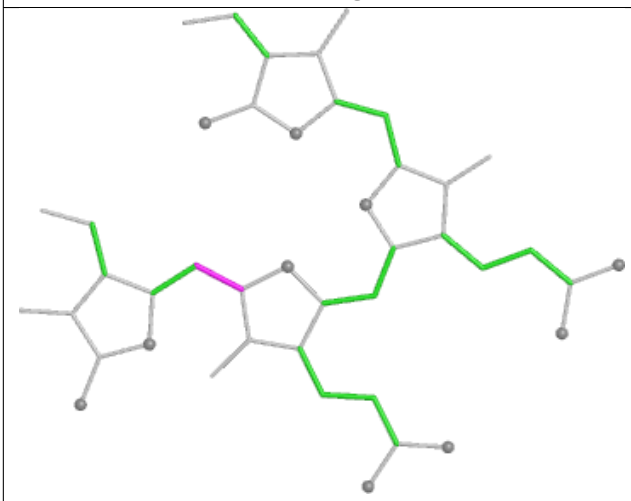

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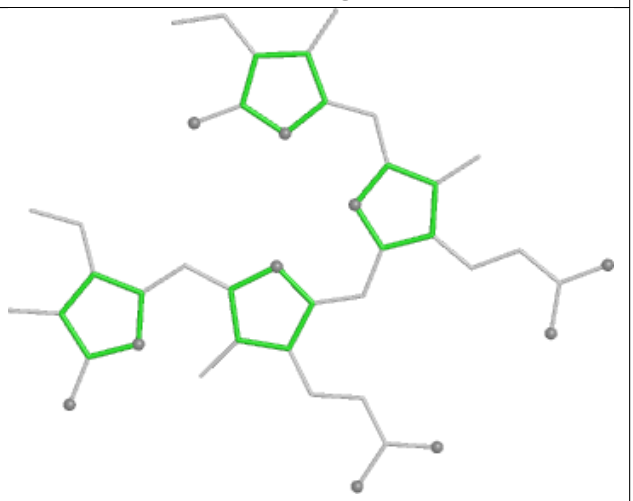
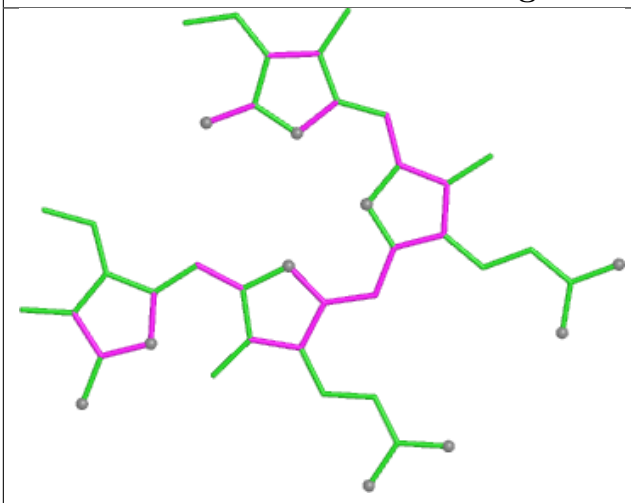


Rings

Ligand PEB lK 203



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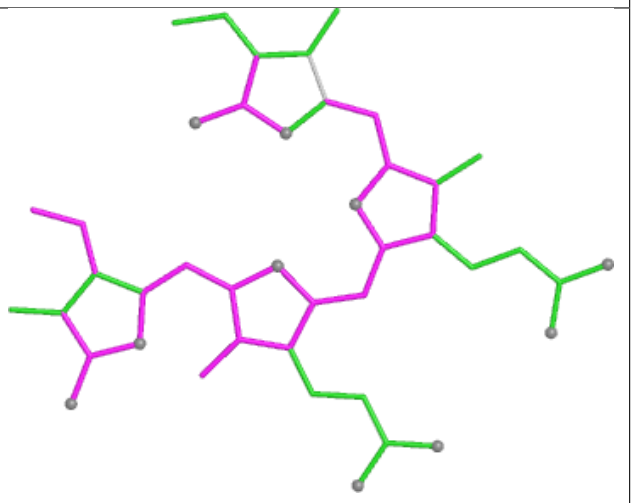

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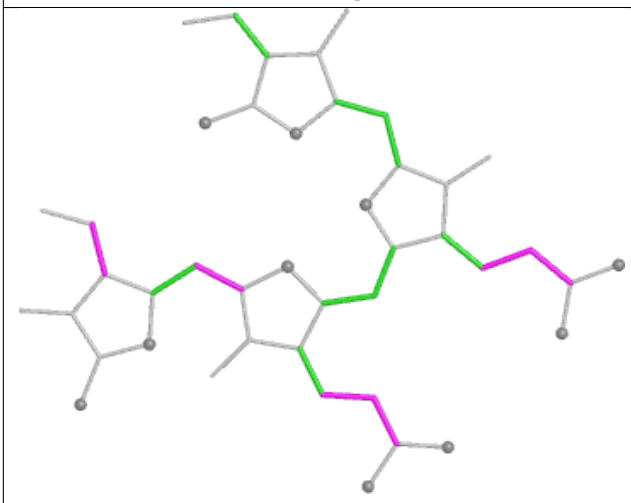

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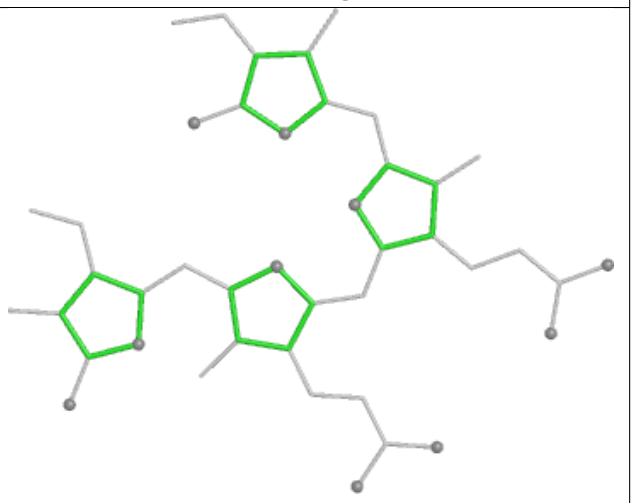
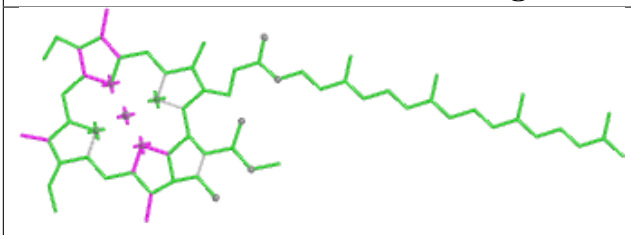


Rings

Ligand CLA AN 840



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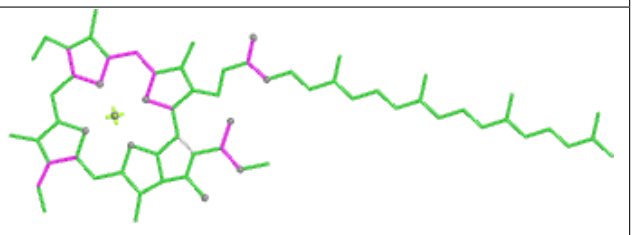

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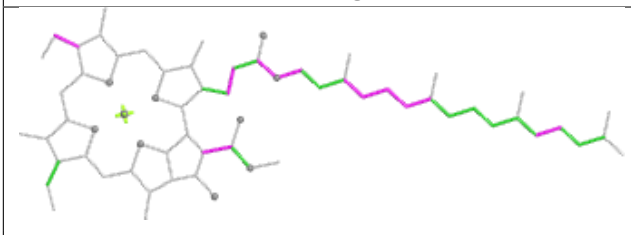

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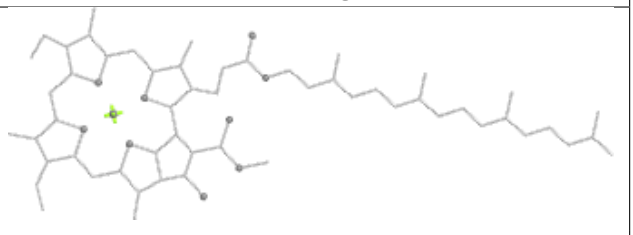

Rings

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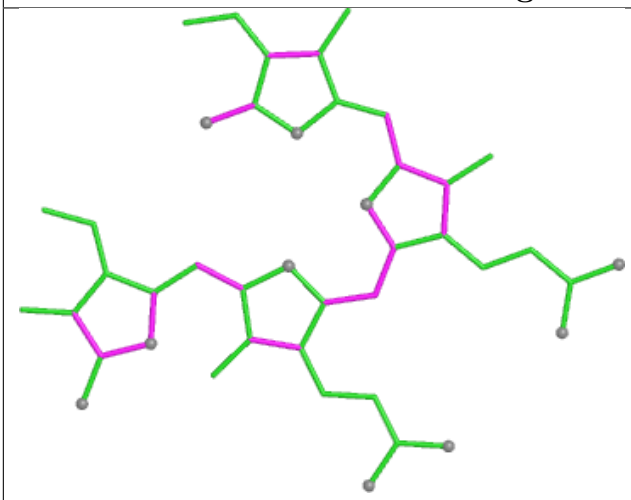

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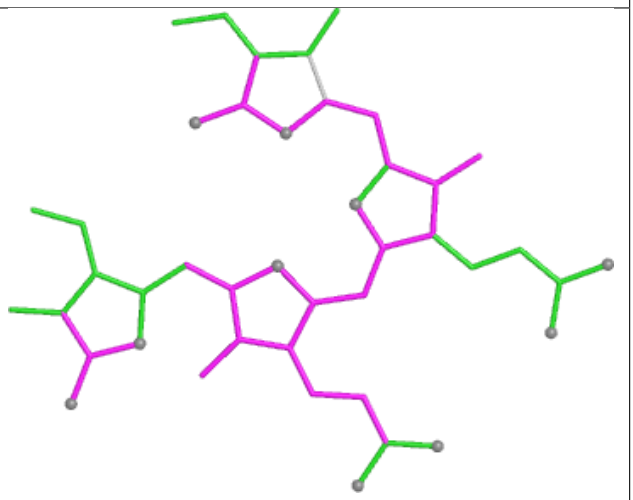
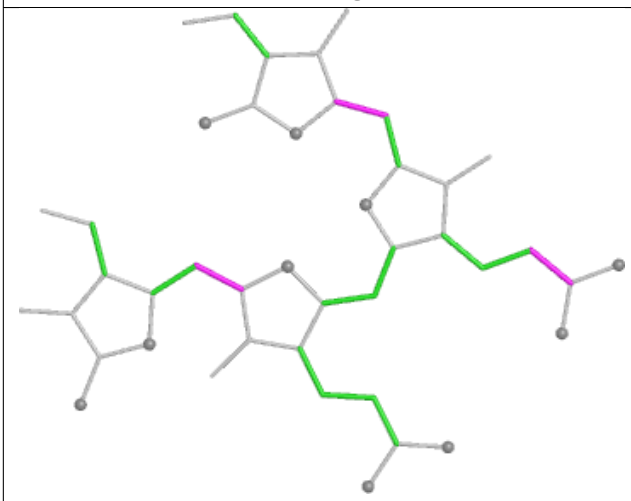
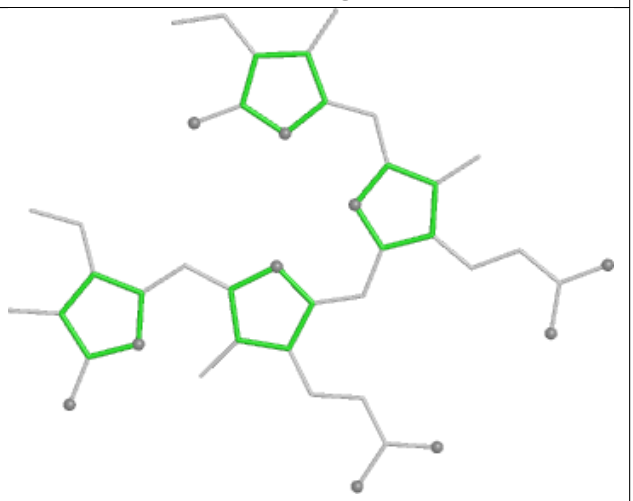


Bond angles

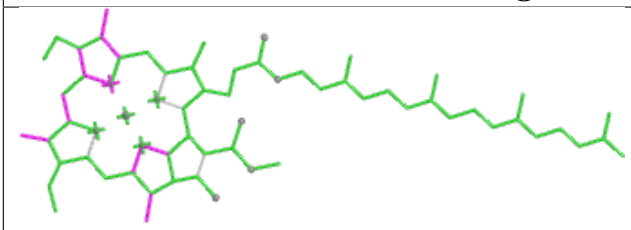


Torsions



Rings

Ligand CLA B6 615



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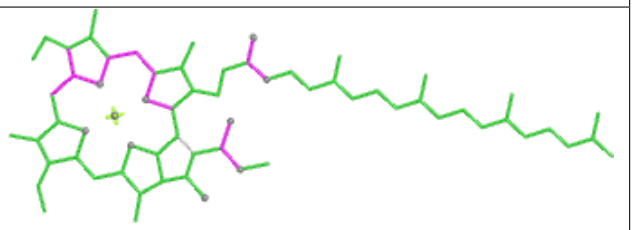

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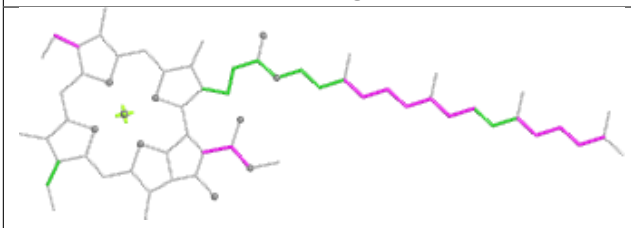

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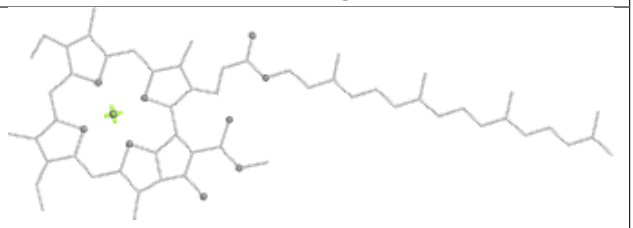
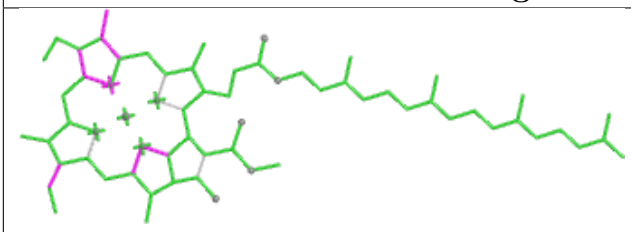


Rings

Ligand CLA LN 203



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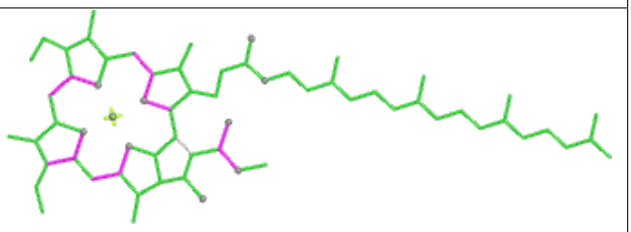

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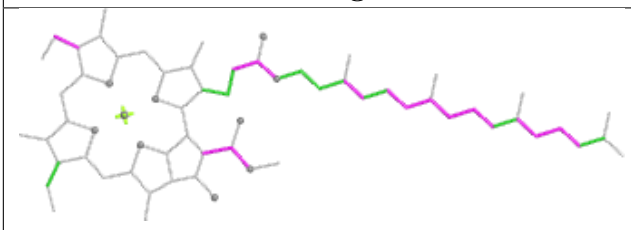

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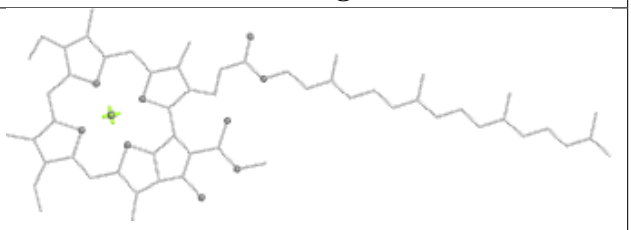
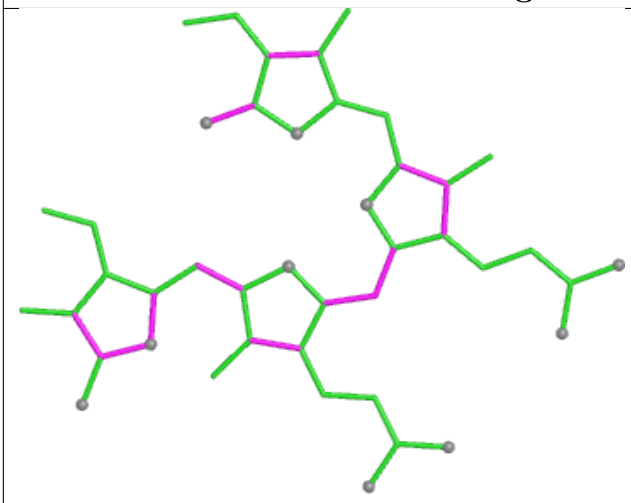


Rings

Ligand PEB bP 502



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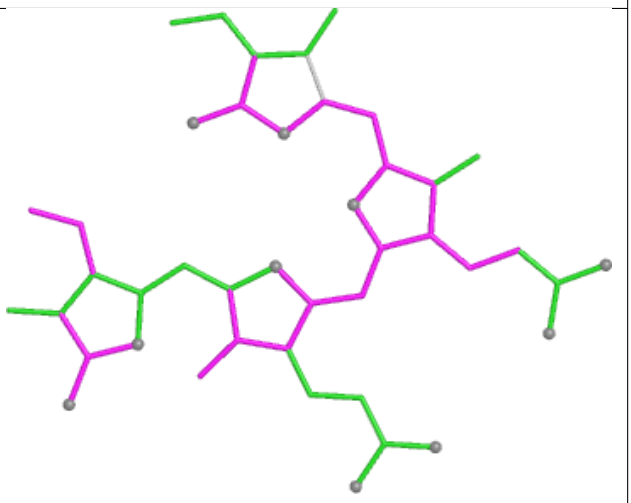

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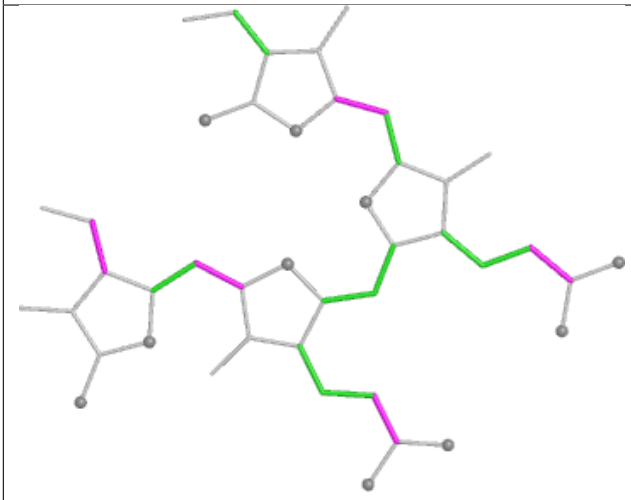

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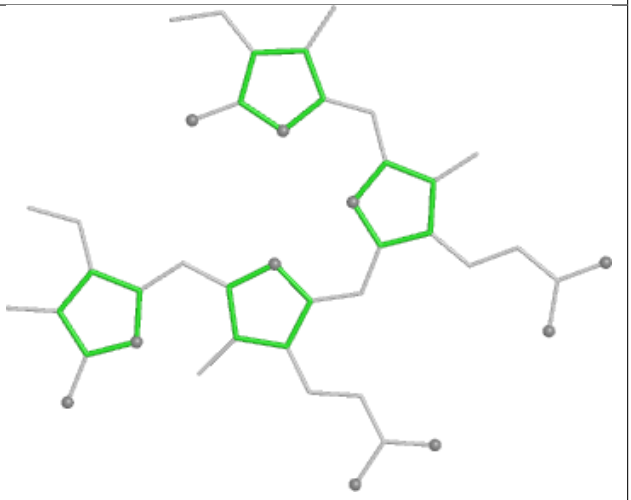
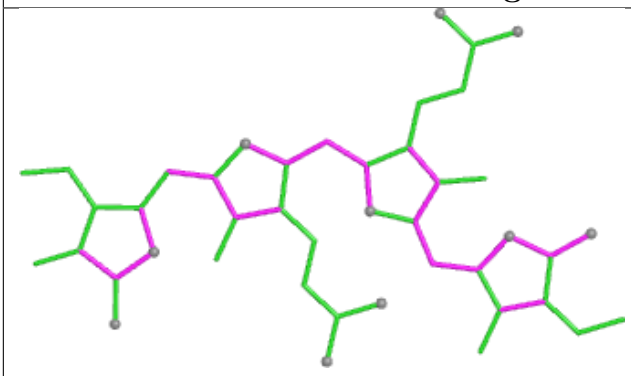


Rings

Ligand CYC LE 1001



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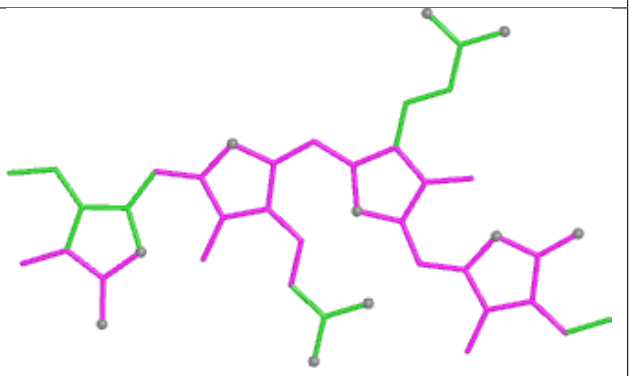

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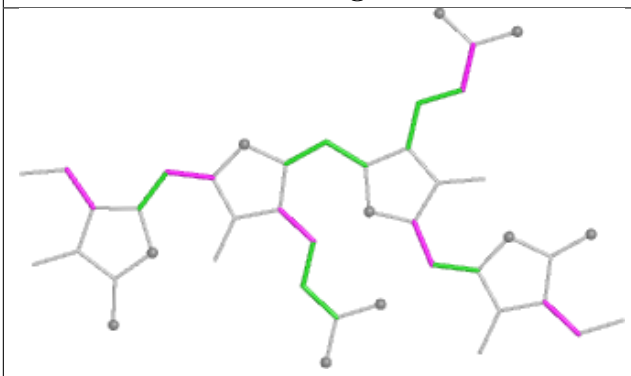

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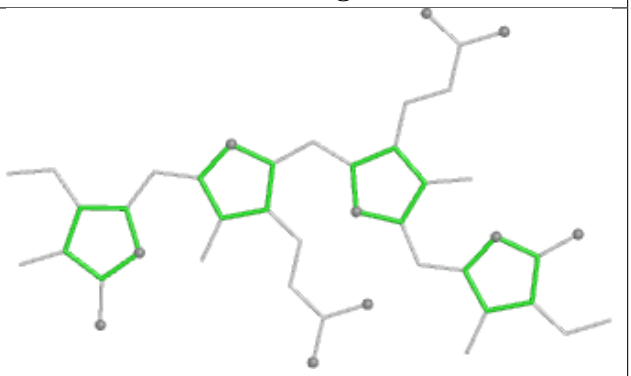
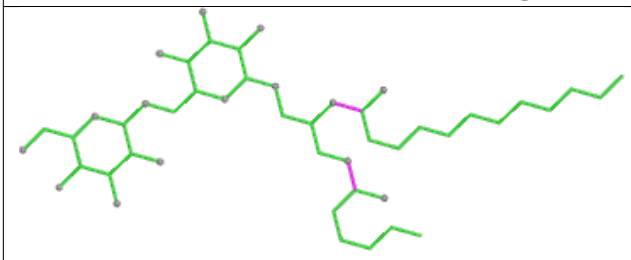


Rings

Ligand DGD c6 620



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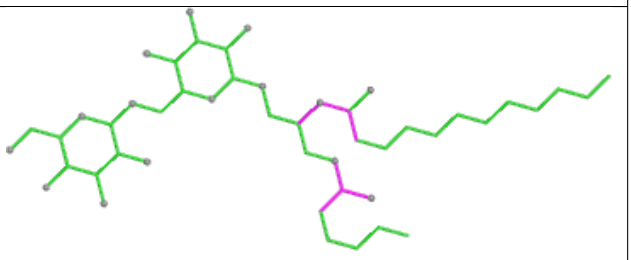
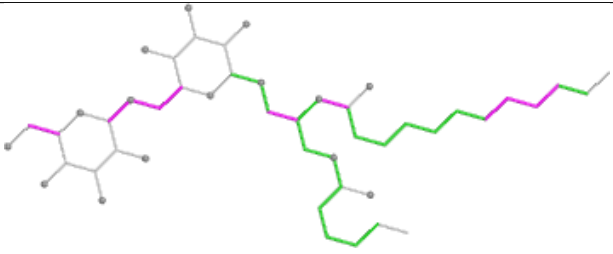


Bond angles



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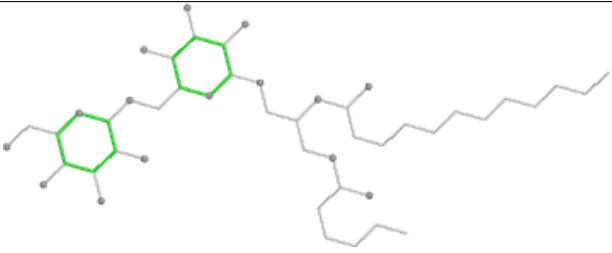
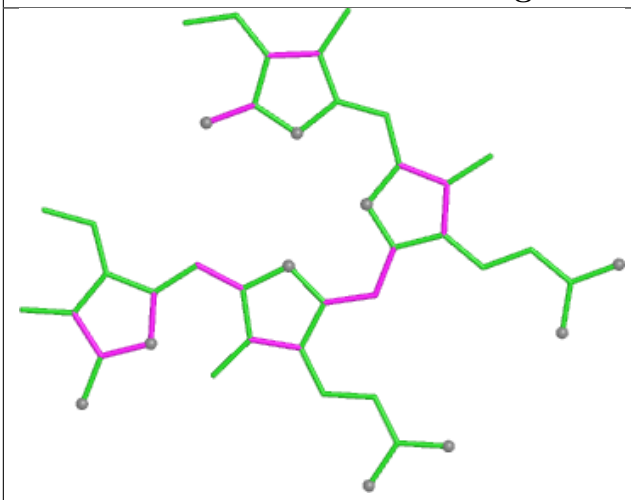


Rings

Ligand PEB UJ 201



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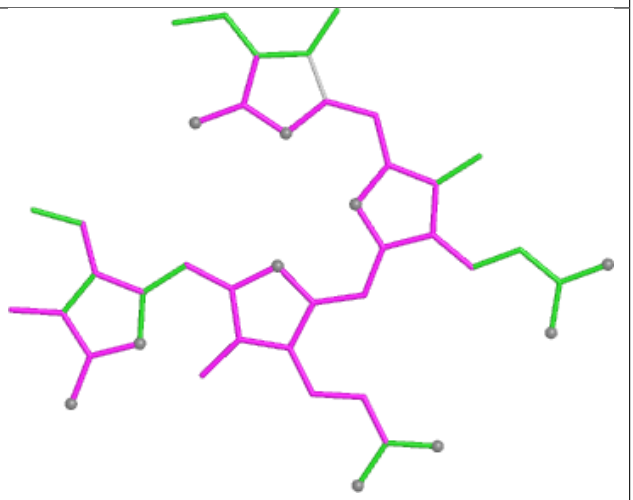
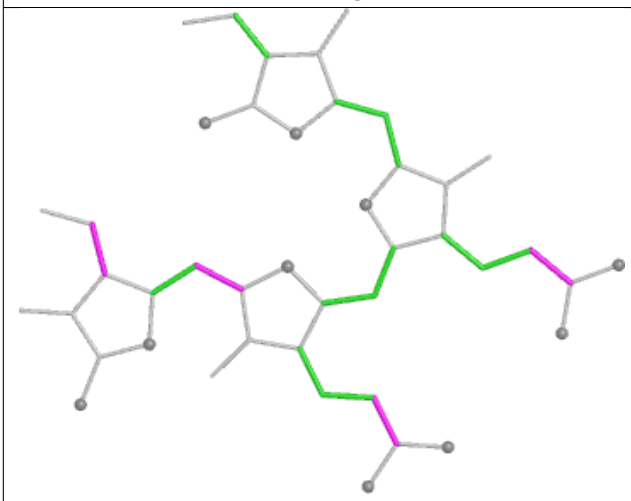


Bond angles



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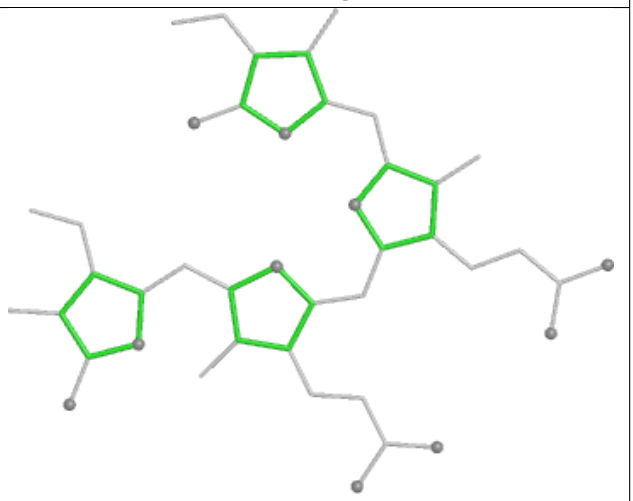
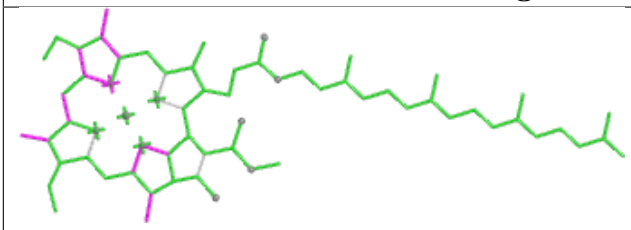


Rings

Ligand CLA B6 603



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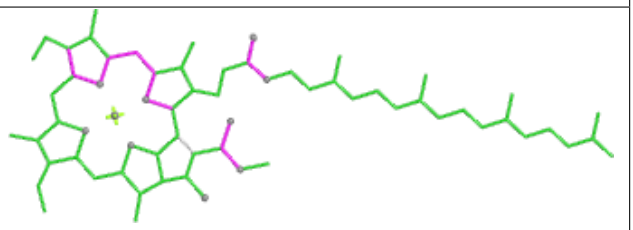

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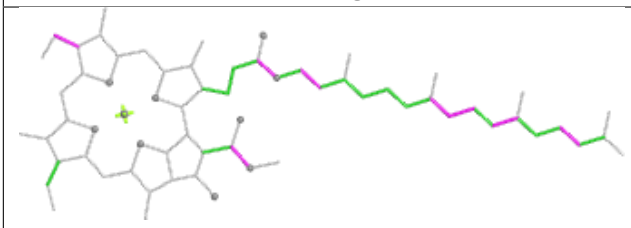

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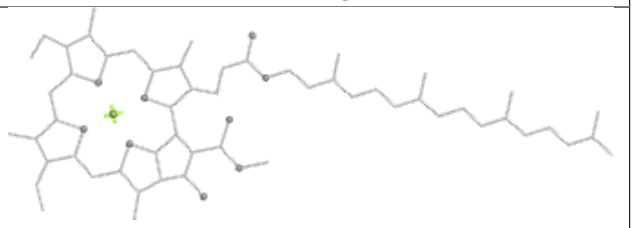
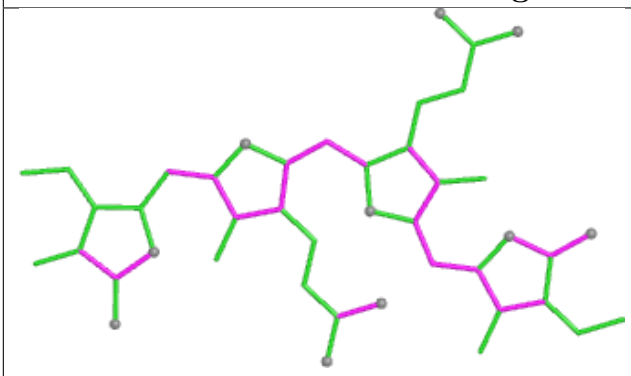


Rings

Ligand CYC f3 1001



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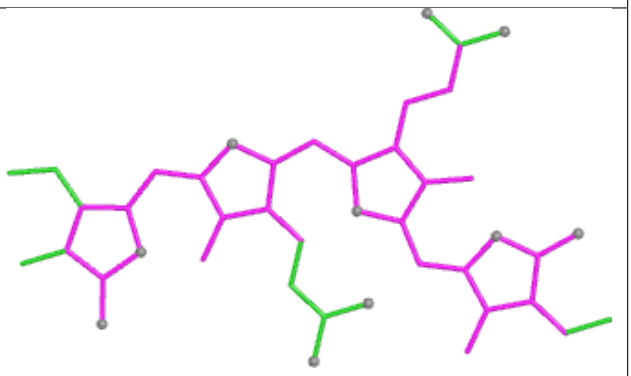
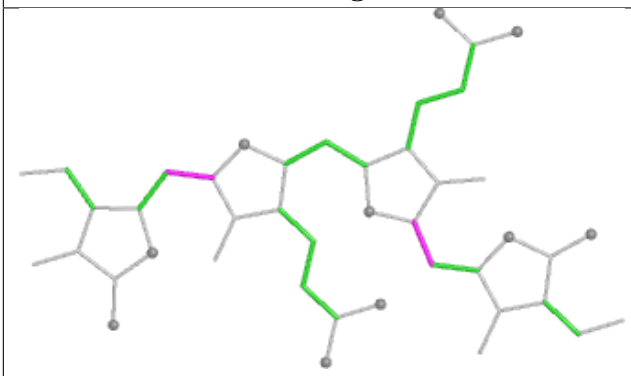


Bond angles



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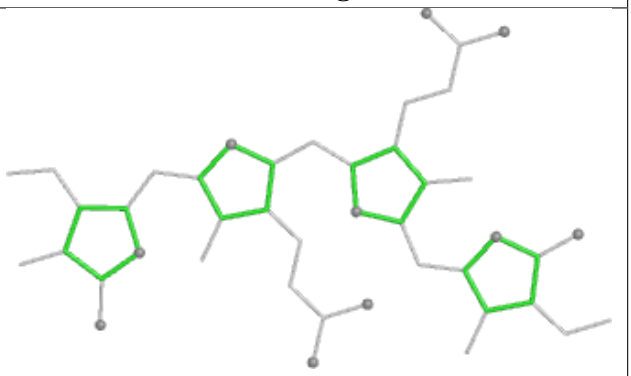
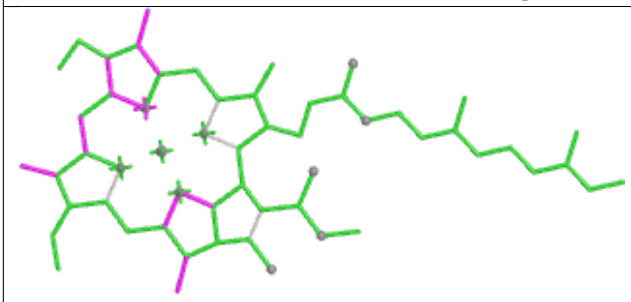


Rings

Ligand CLA bL 620



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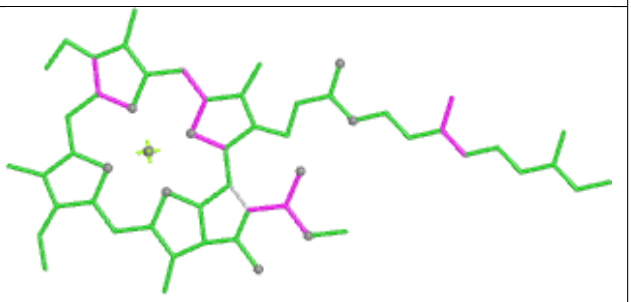
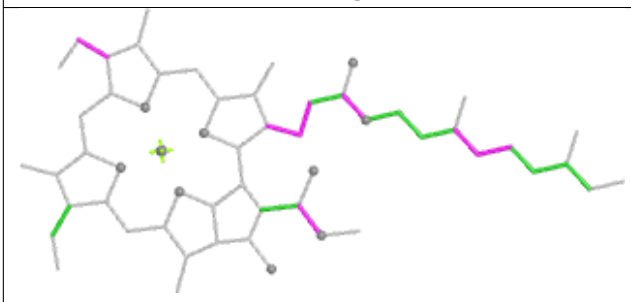


Bond angles



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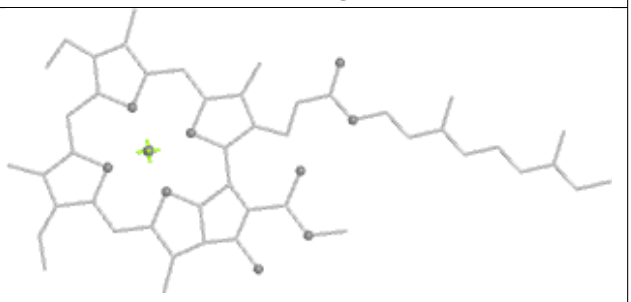
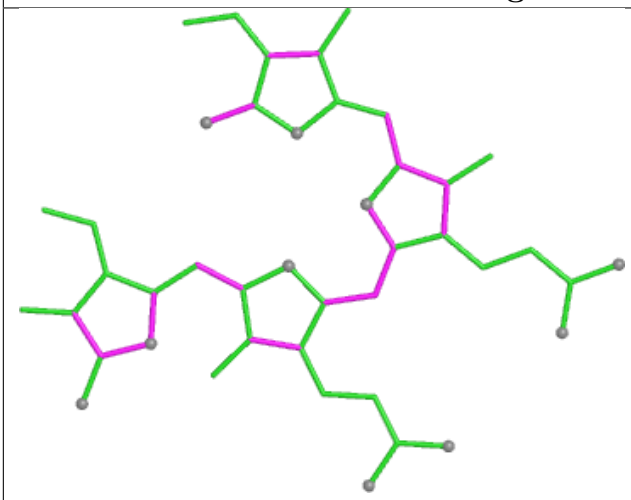


Rings

Ligand PEB VM 201



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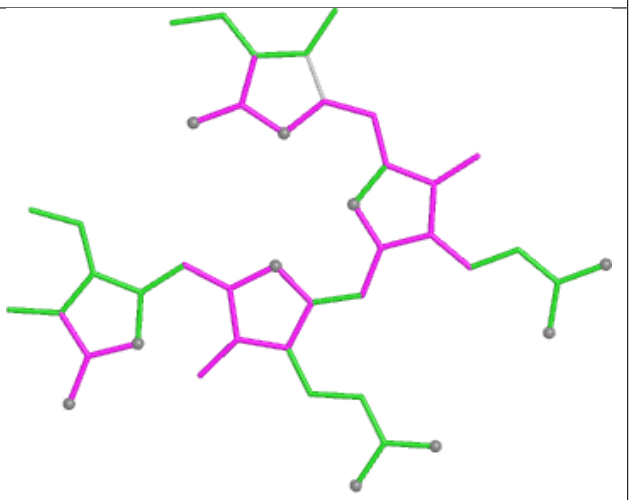
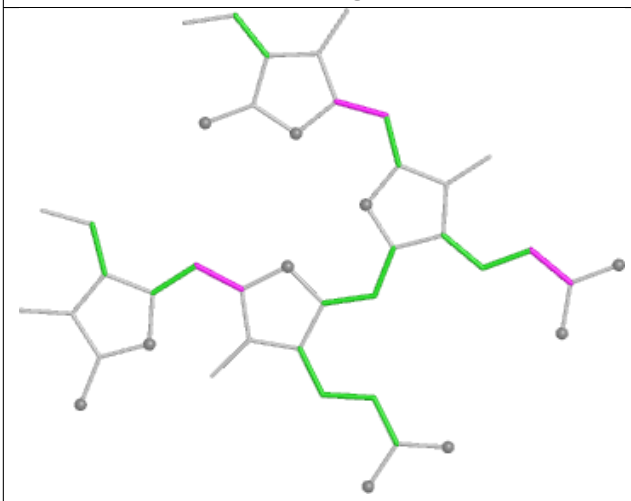


Bond angles



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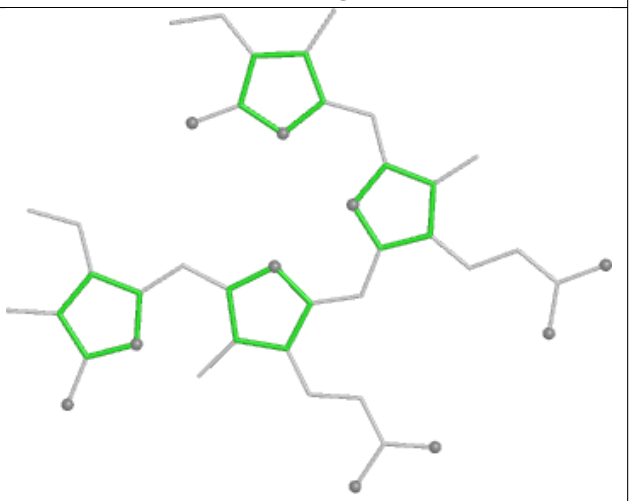
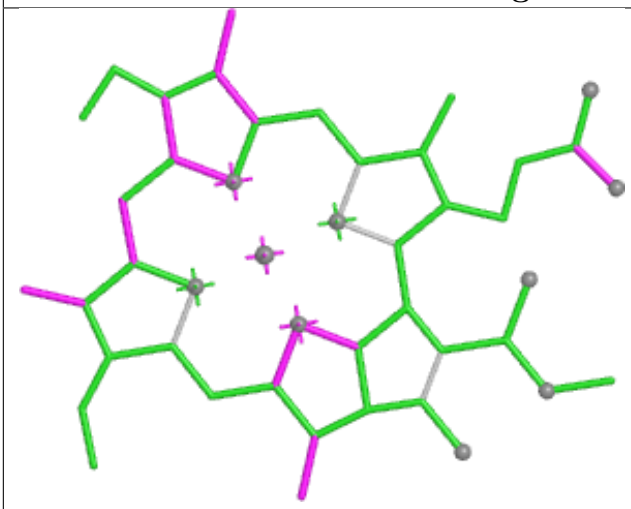


Rings

Ligand CLA FN 203



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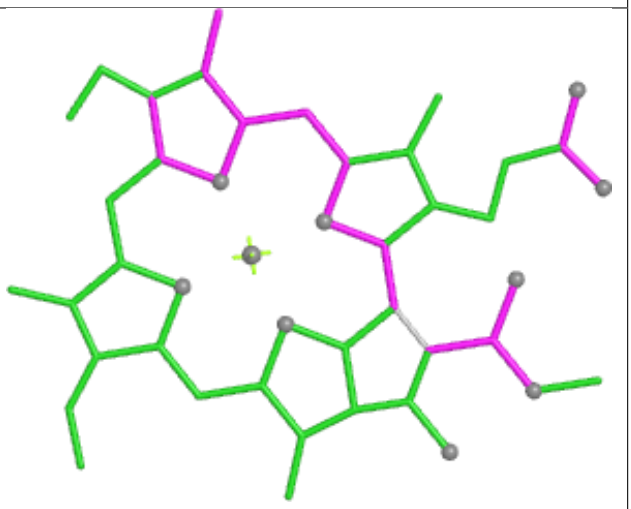

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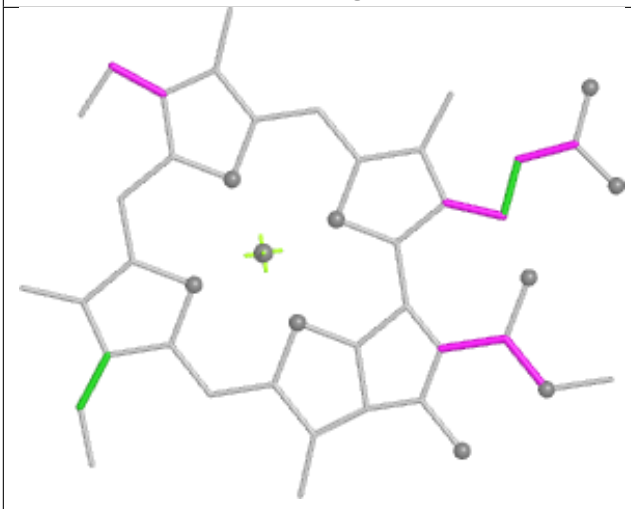
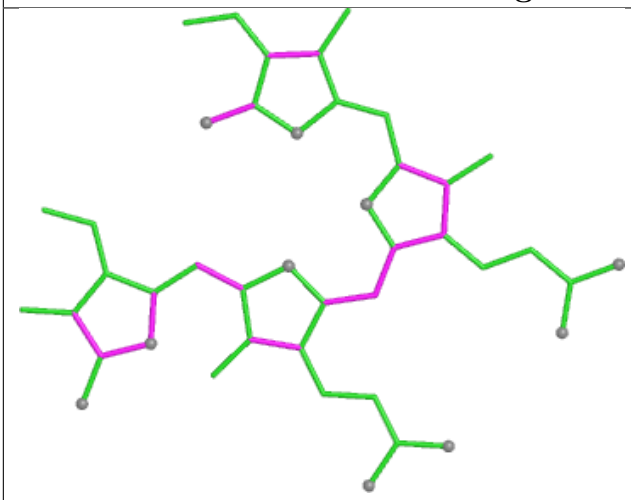


Torsions



Rings

Ligand PEB QJ 202



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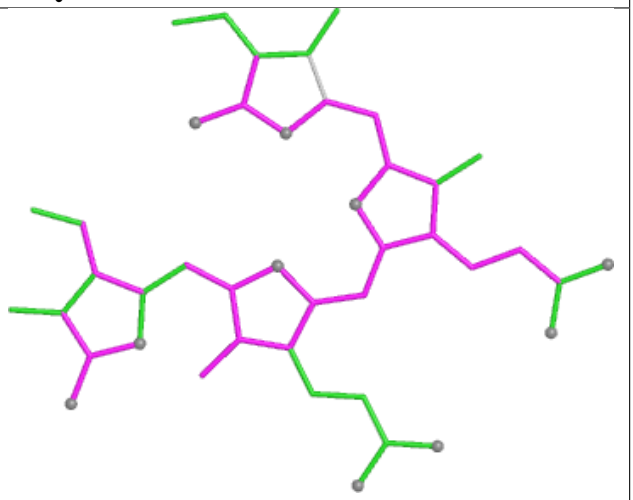
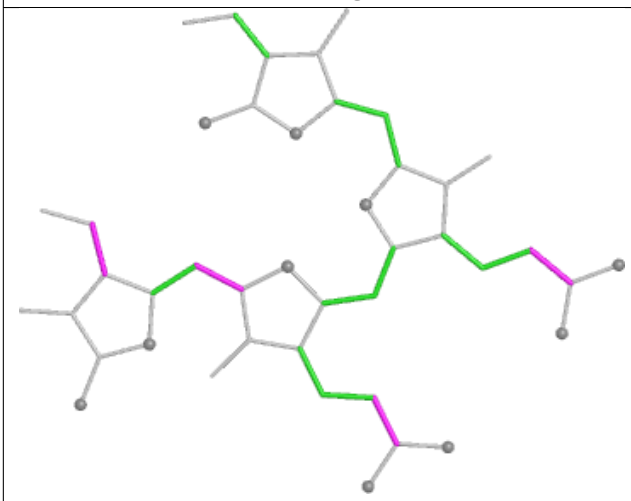


Bond angles



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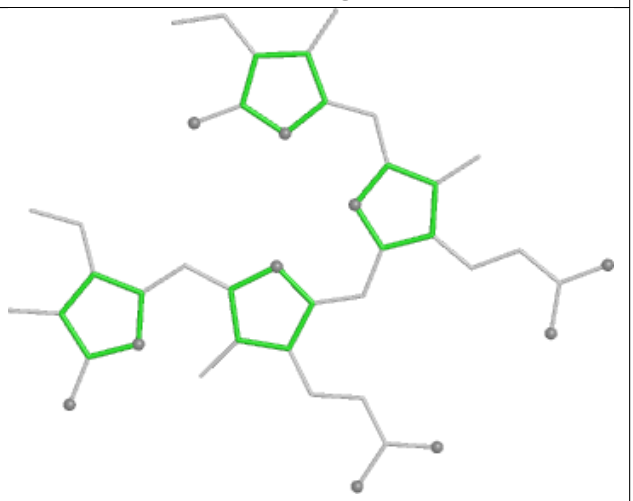
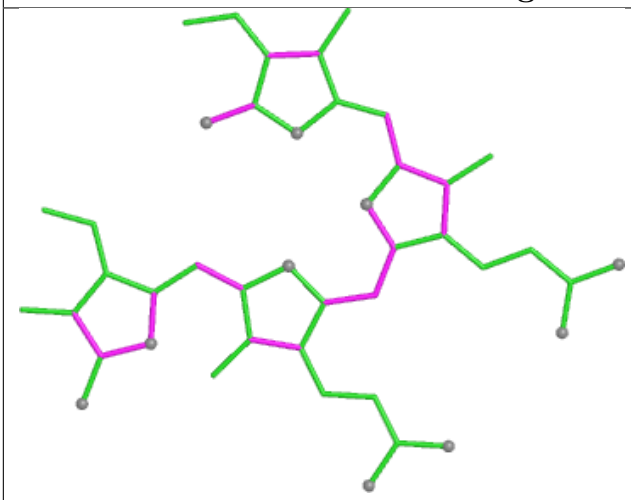


Rings

Ligand PEB F9 201



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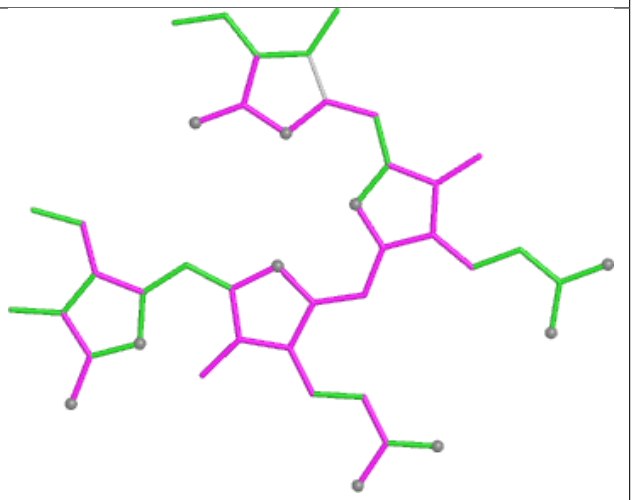
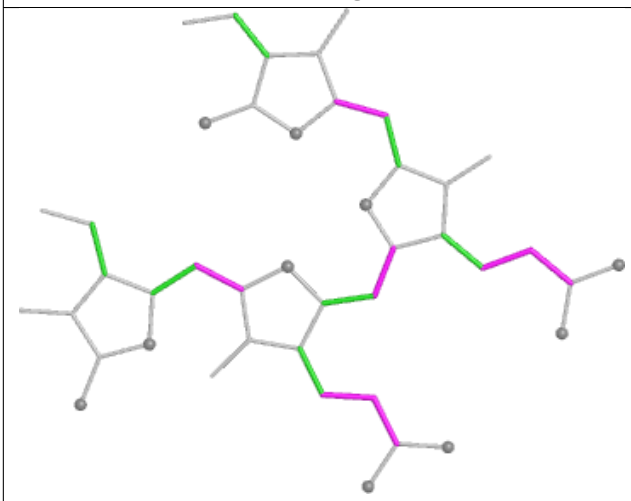


Bond angles



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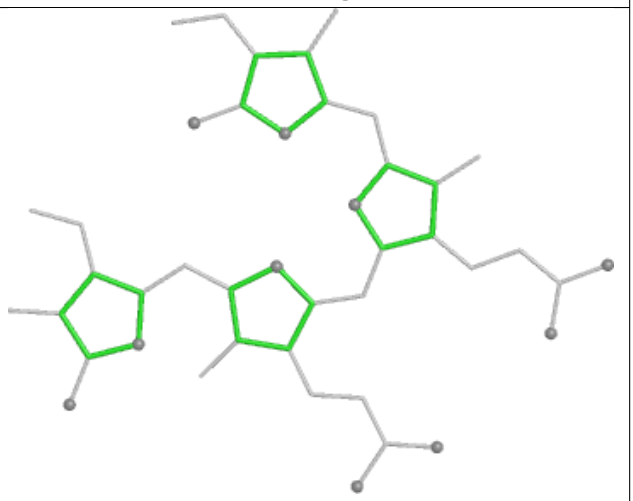
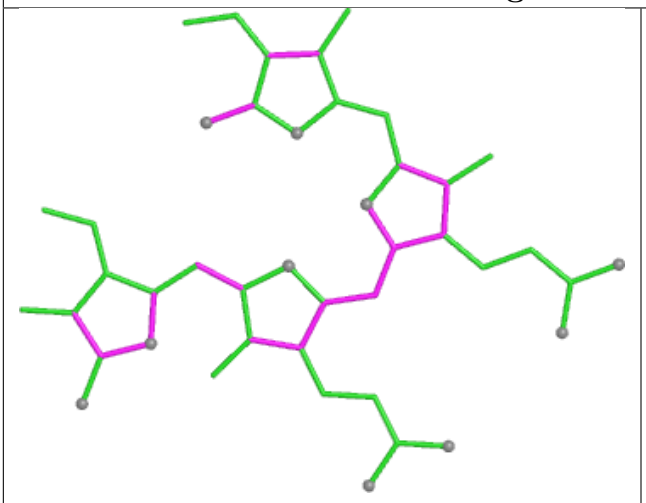


Rings

Ligand PEB GM 202



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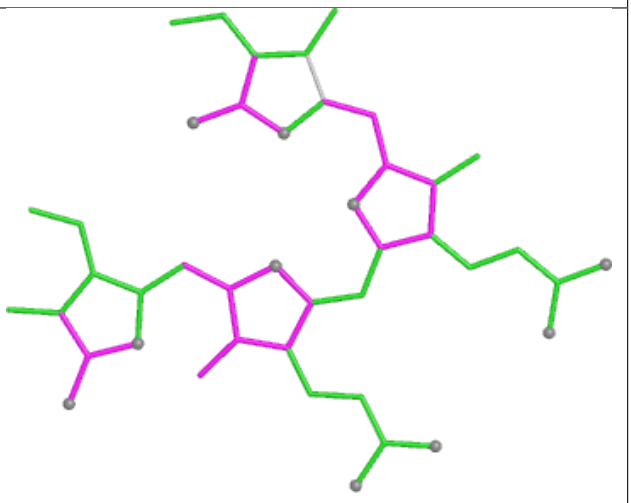
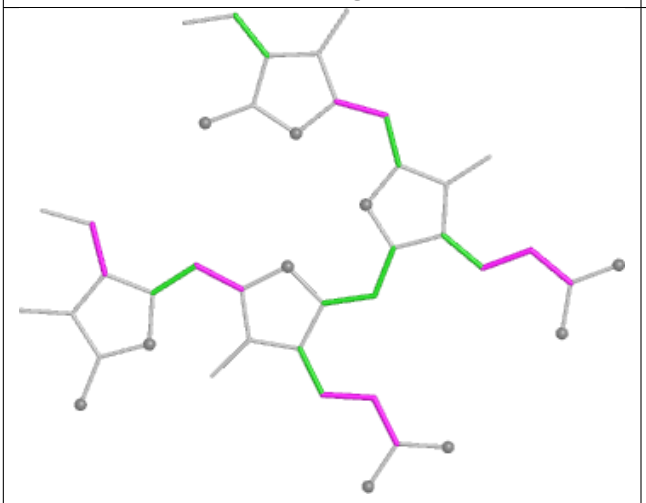


Bond angles



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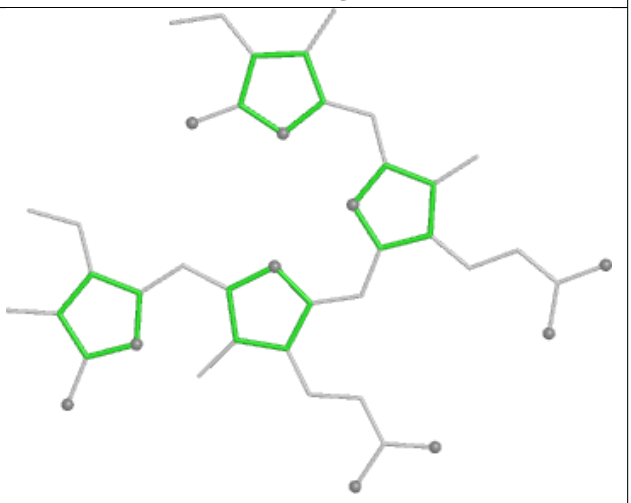
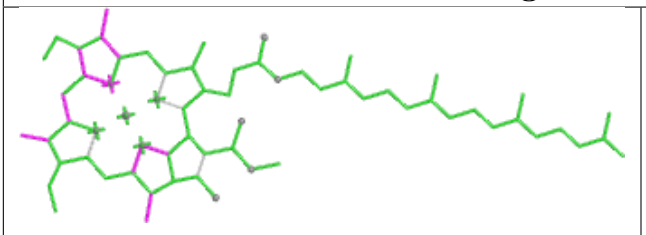


Rings

Ligand CLA c6 609



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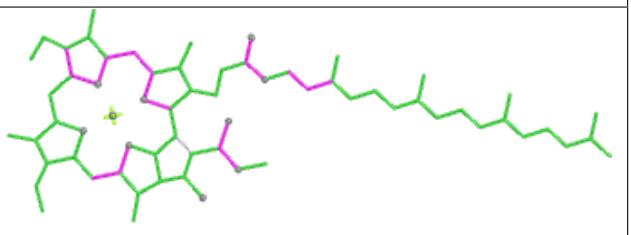

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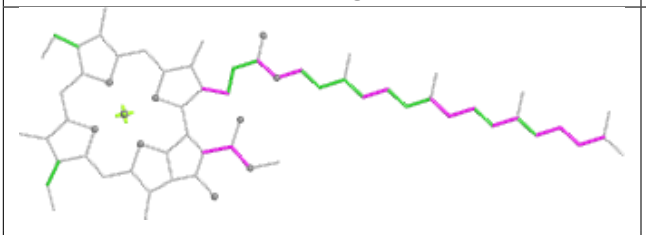
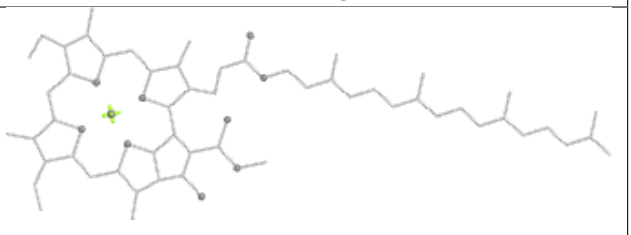
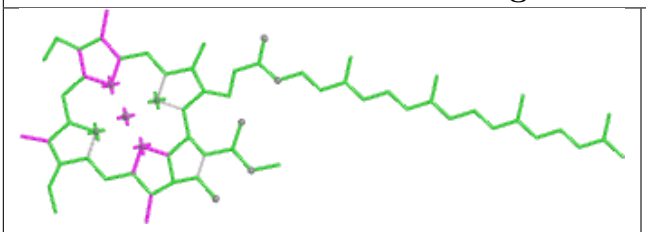


Torsions



Rings

Ligand CLA AN 826



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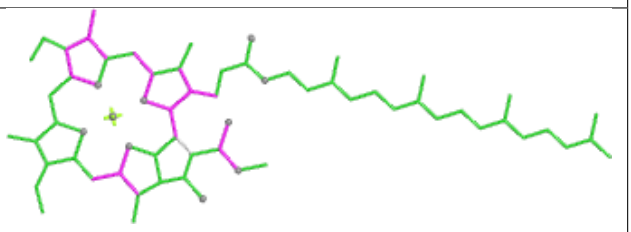

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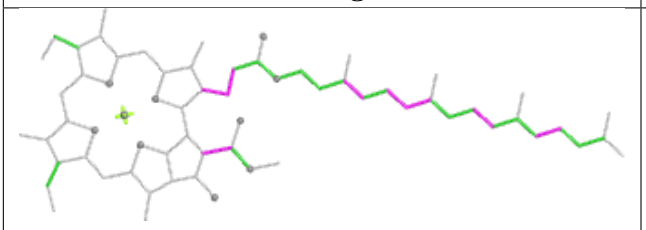

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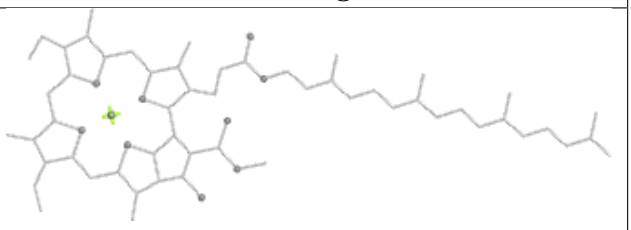
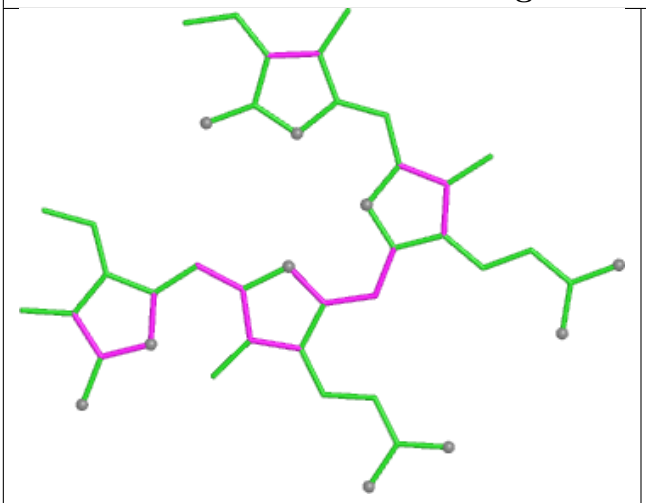


Rings

Ligand PEB Q7 201



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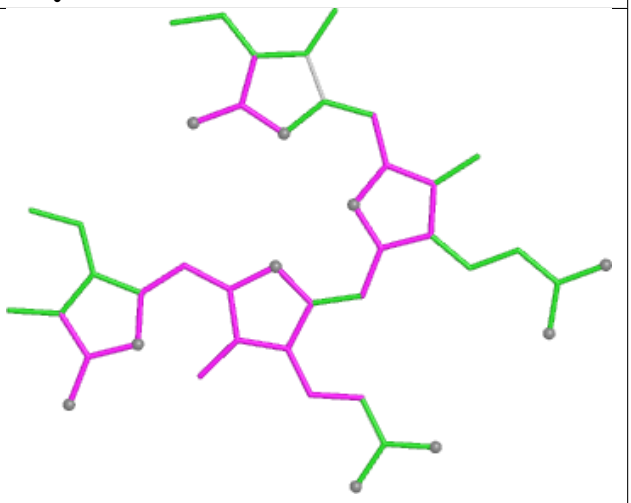

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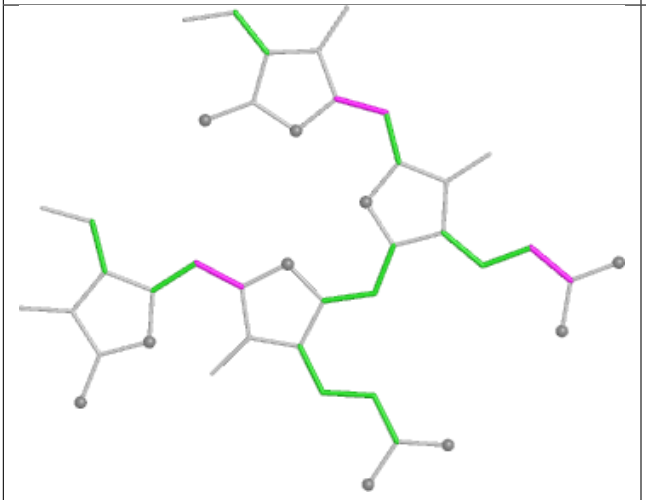

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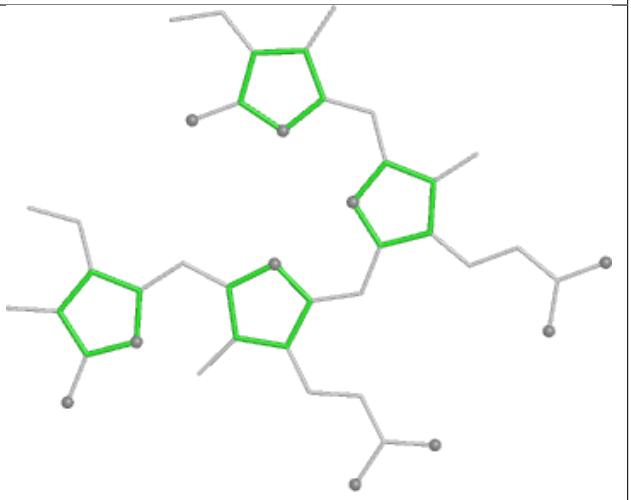
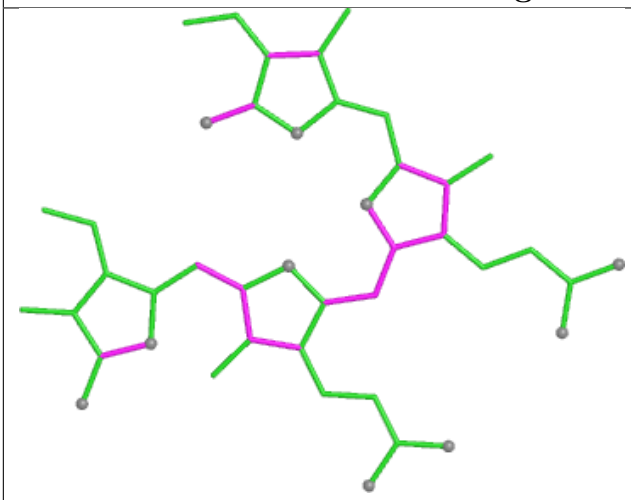


Rings

Ligand PEB oK 202



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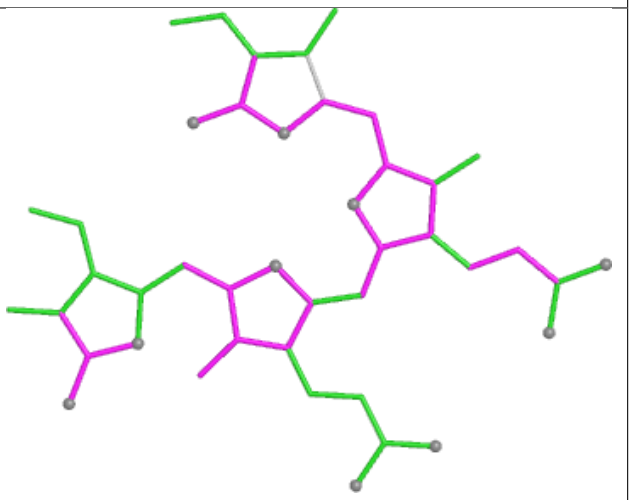

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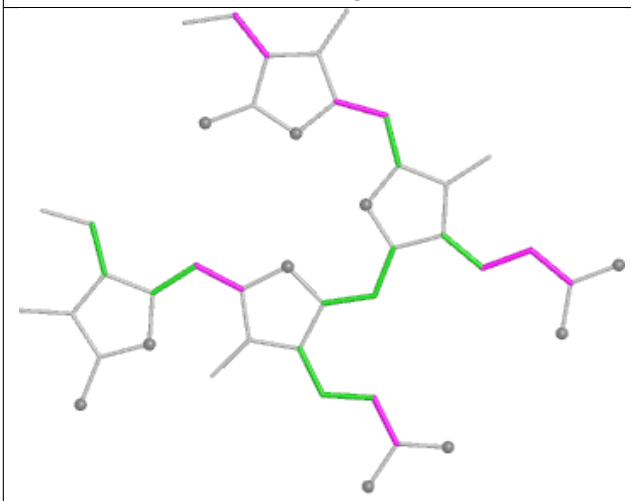

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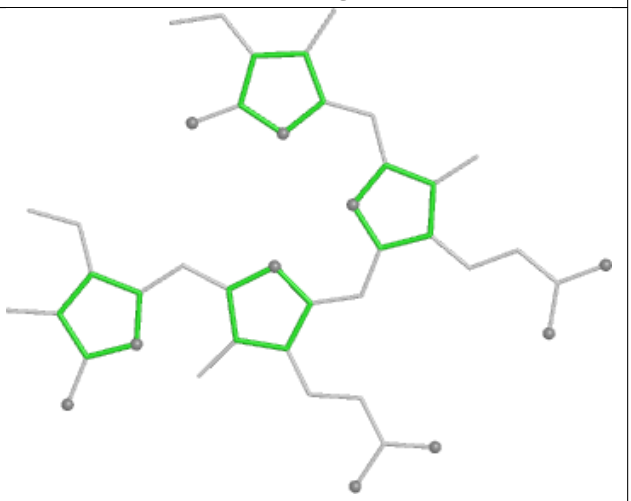
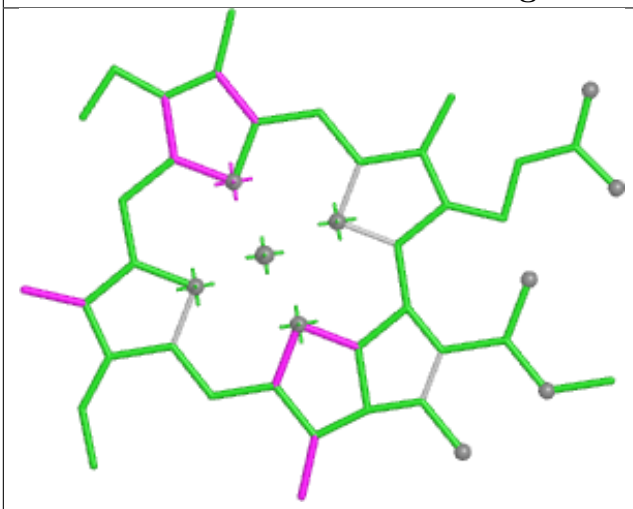


Rings

Ligand CLA 22 608



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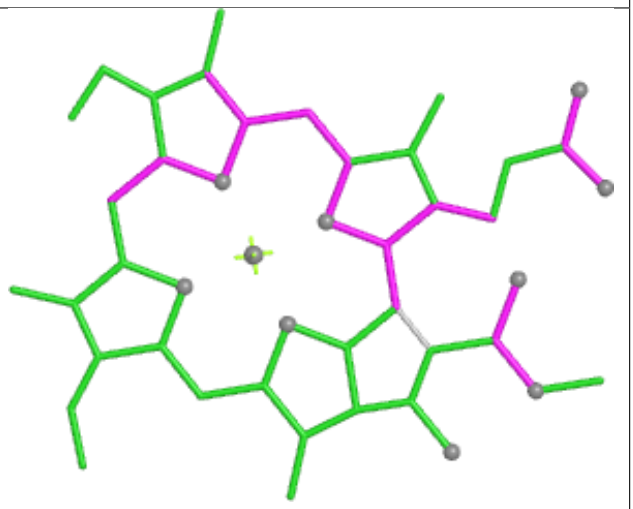

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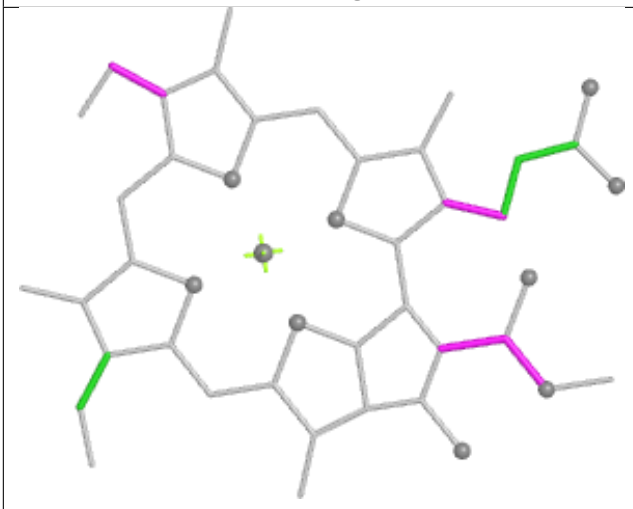
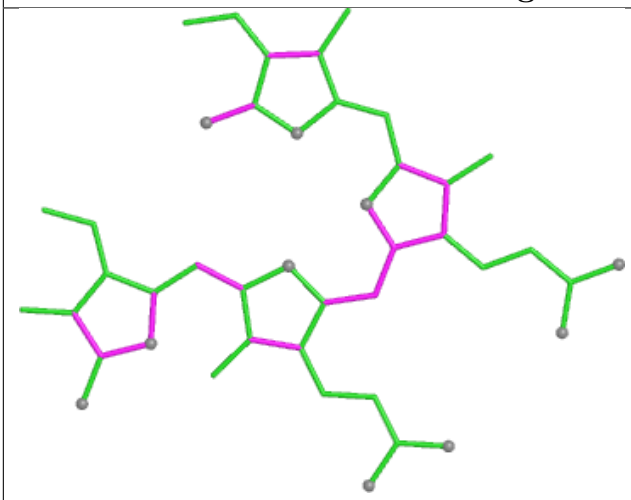


Torsions



Rings

Ligand PEB XI 201



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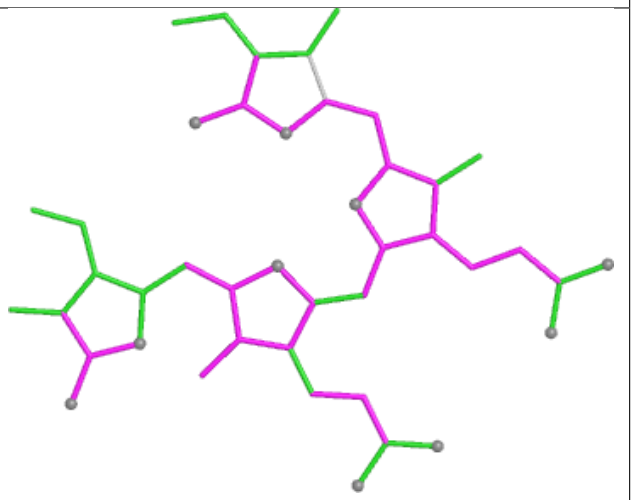

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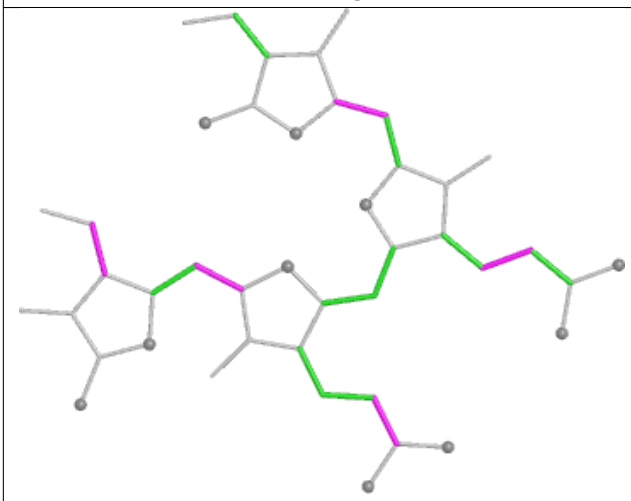

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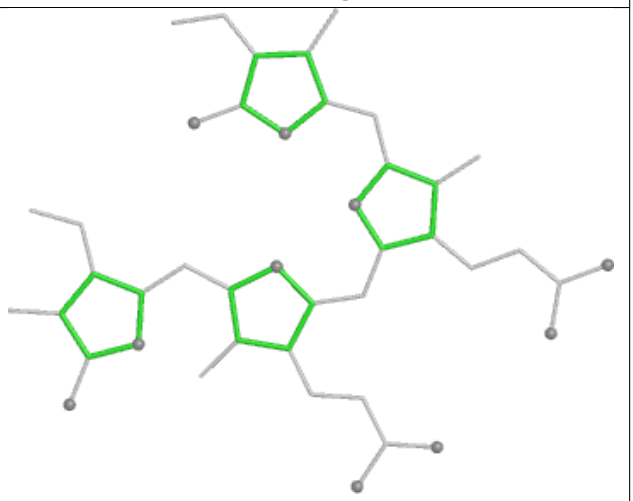

Rings

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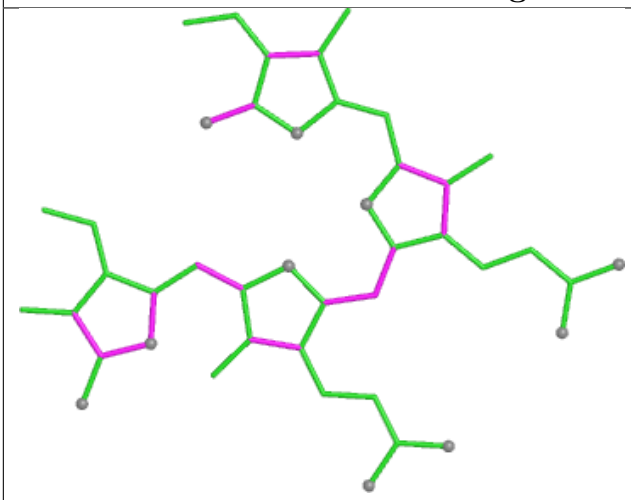

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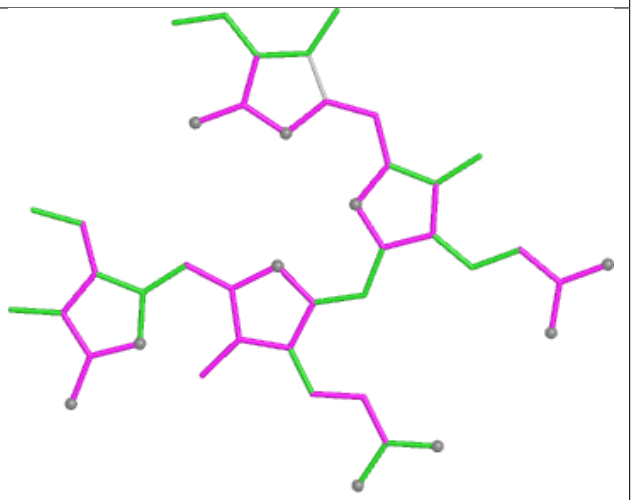

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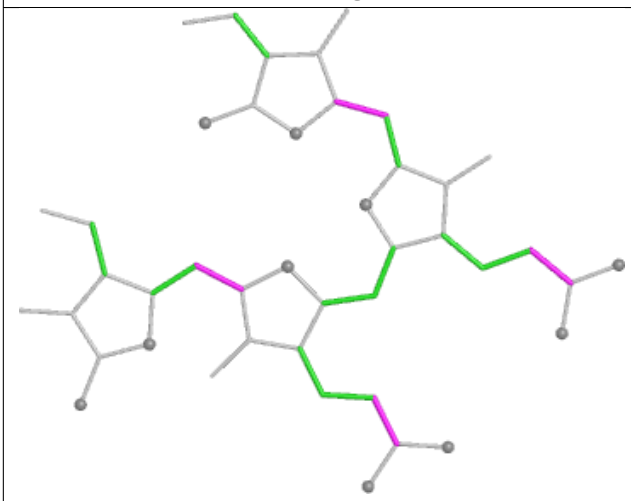

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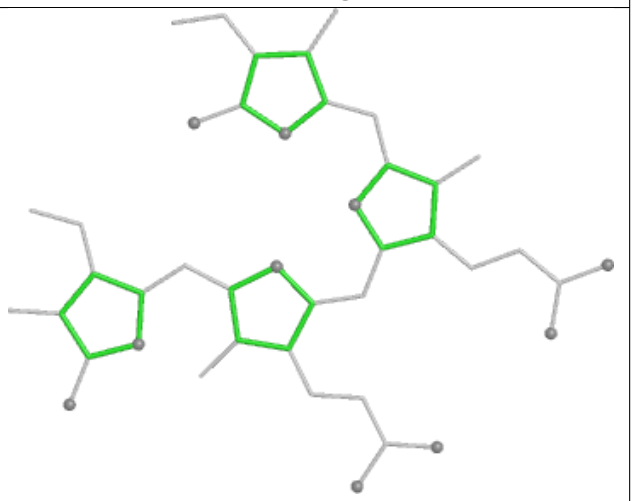

Rings

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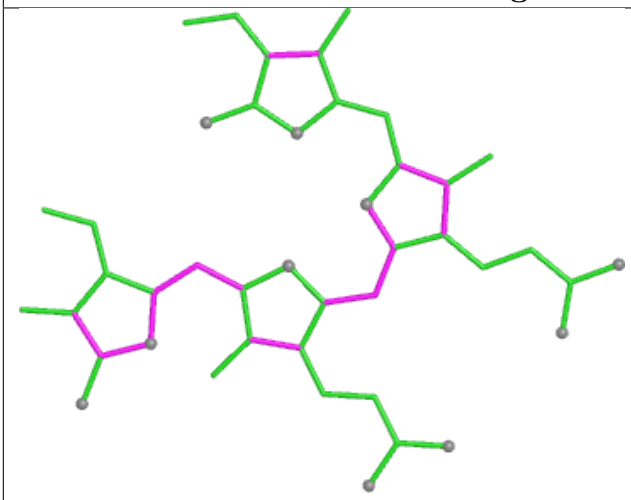

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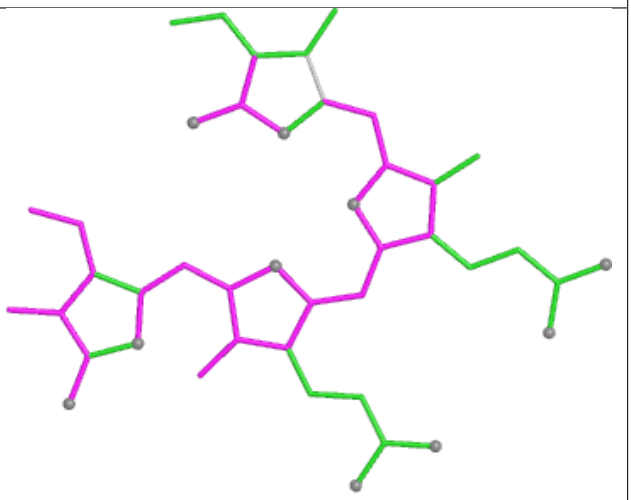

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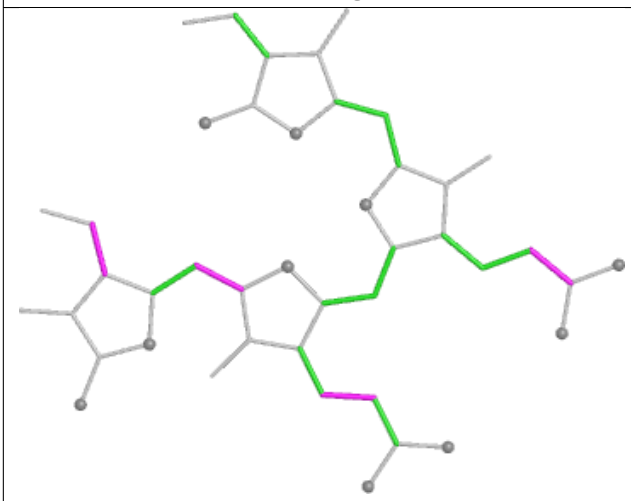

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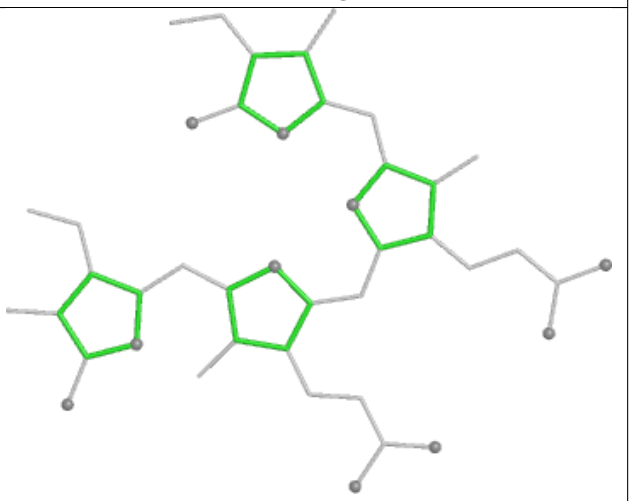
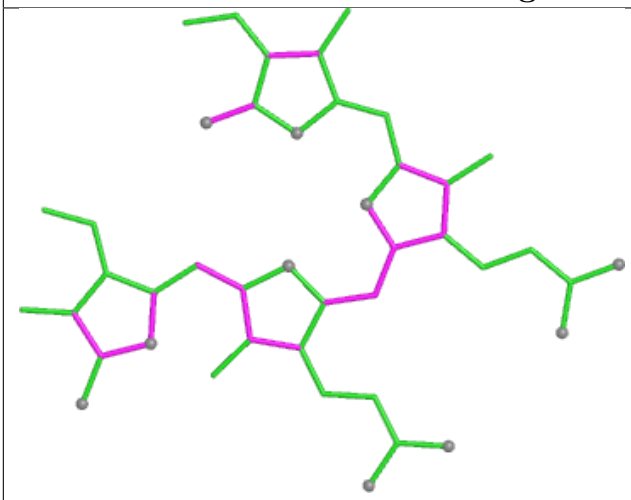


Rings

Ligand PEB S4 201



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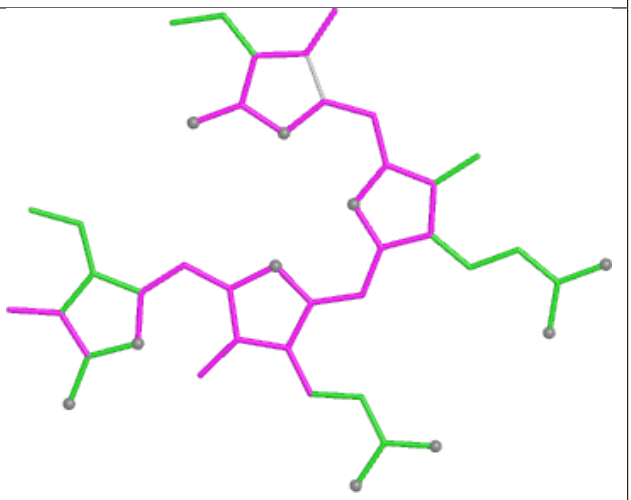

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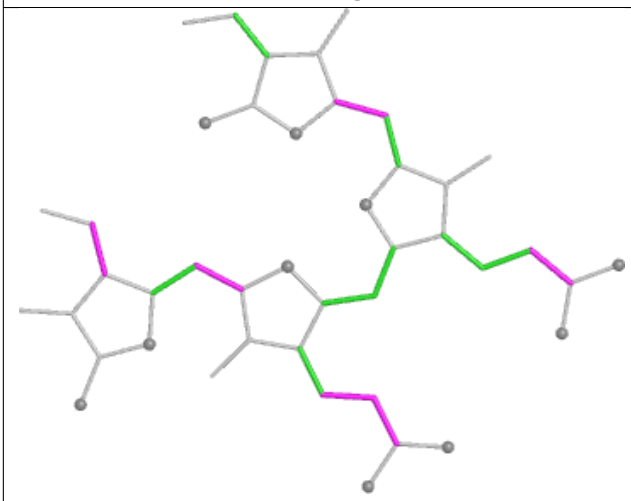

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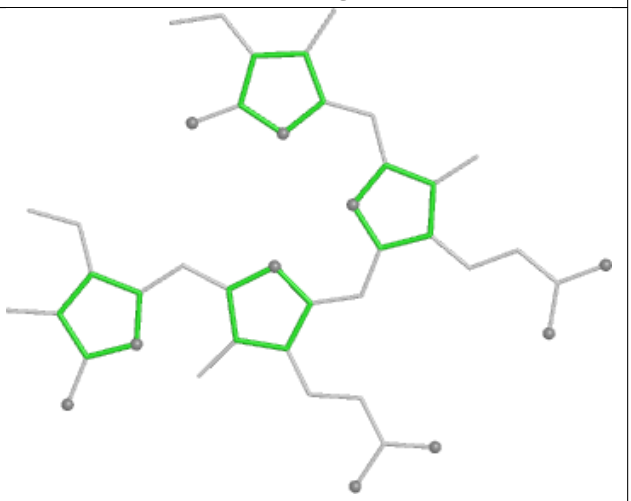
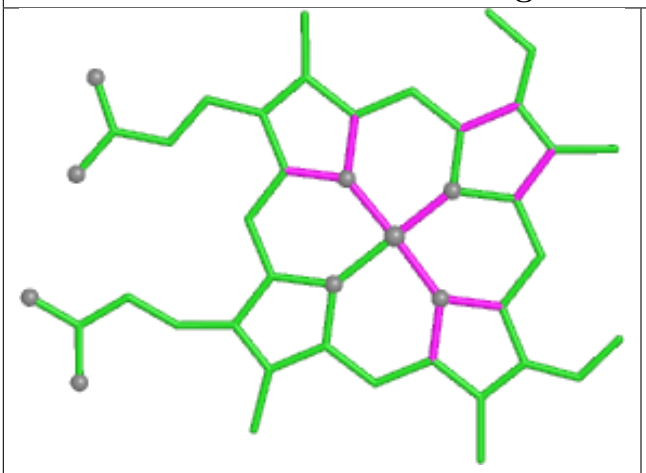


Rings

Ligand HEM fL 102



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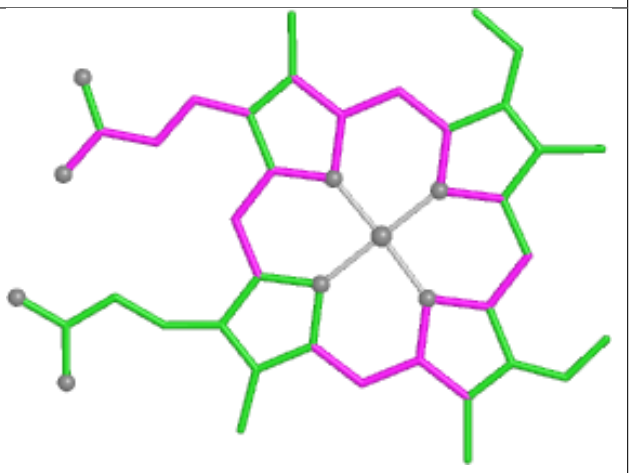

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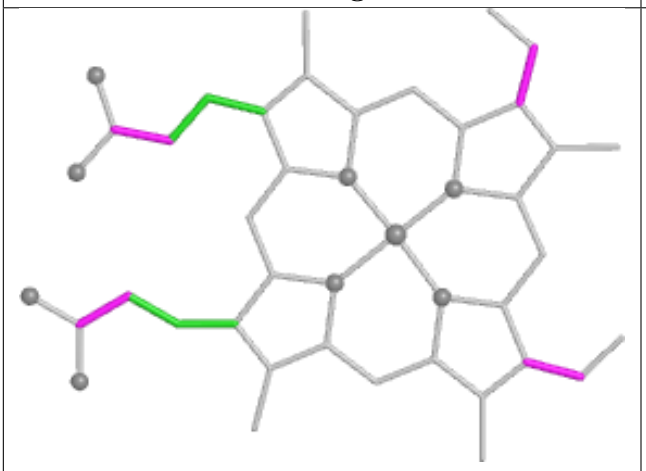

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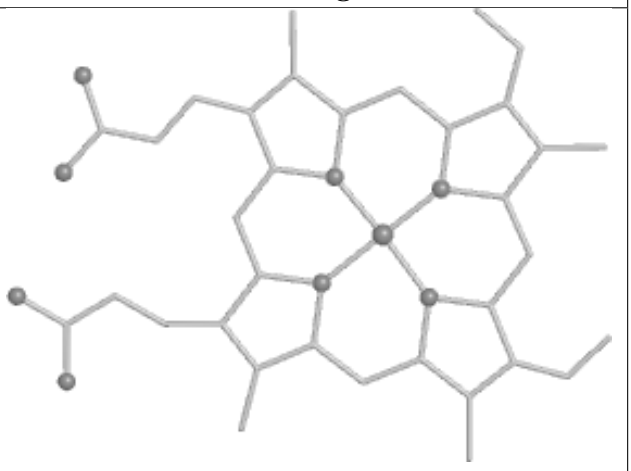
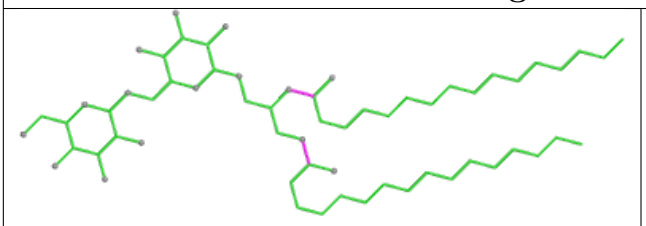


Rings

Ligand DGD CL 517



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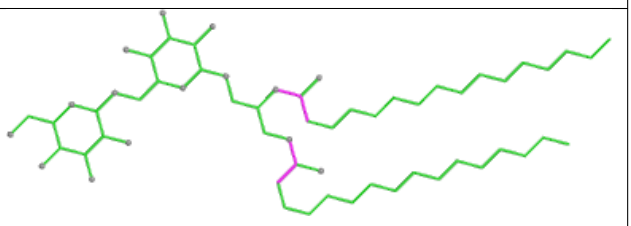

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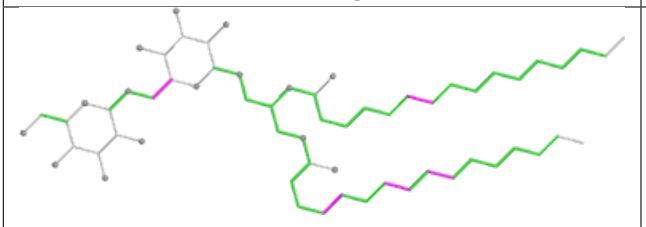

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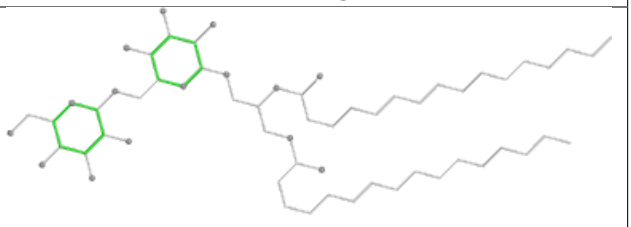
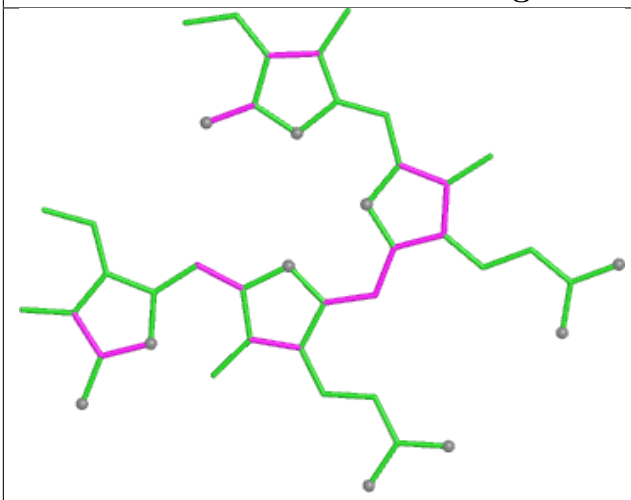


Rings

Ligand PEB VA 202



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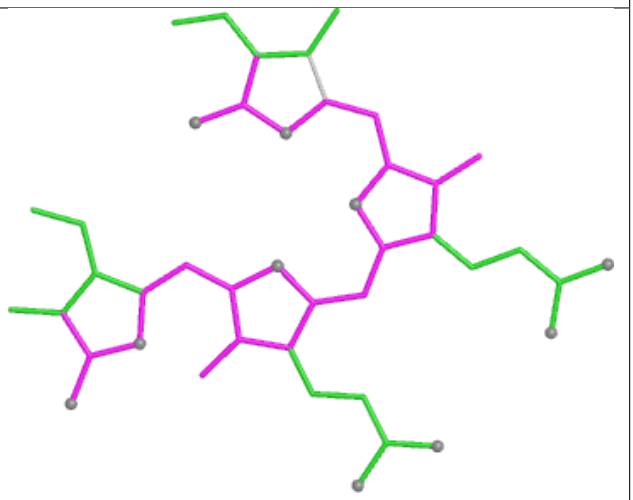

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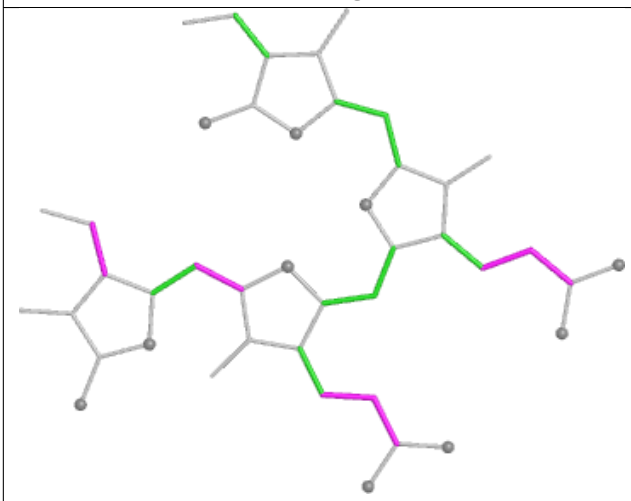

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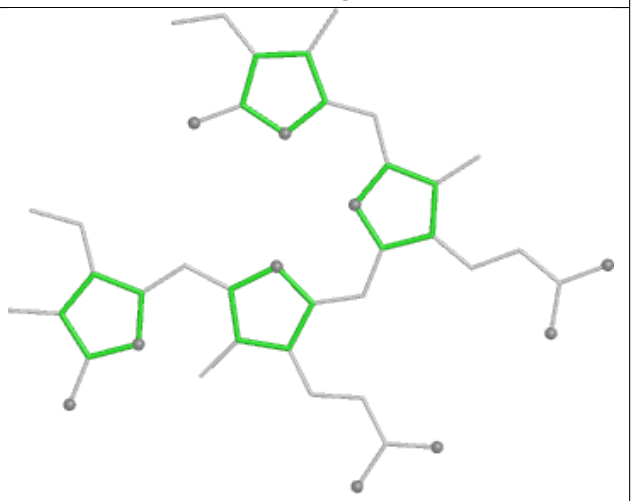
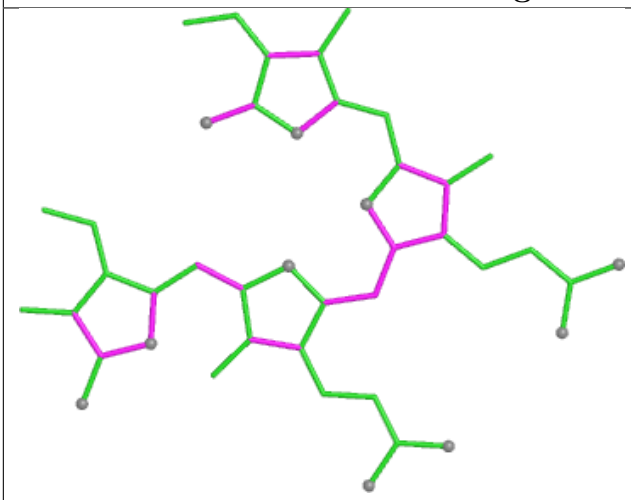


Rings

Ligand PEB hG 202



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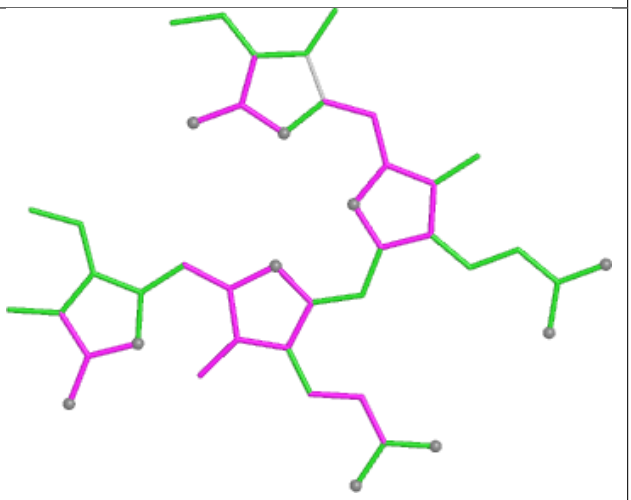

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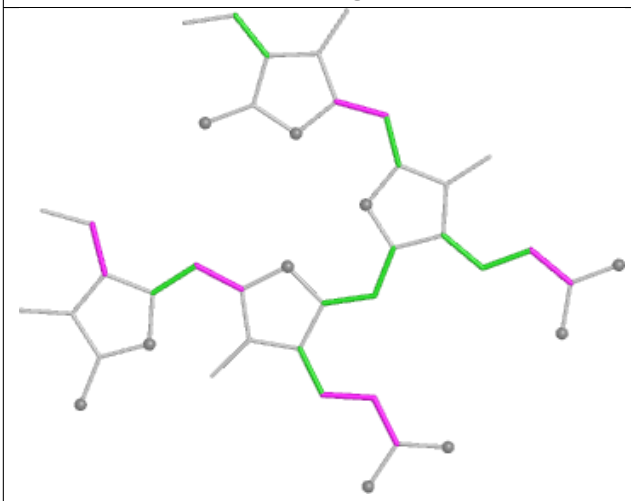

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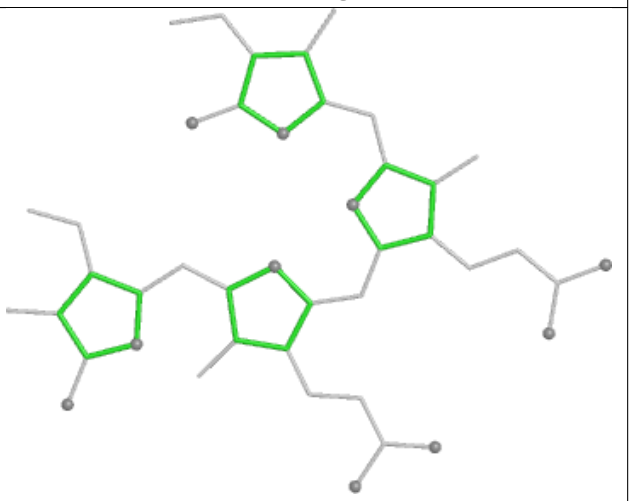
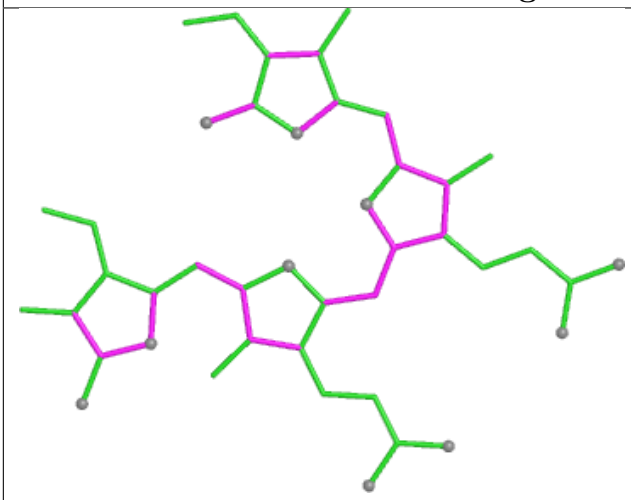


Rings

Ligand PEB rF 202



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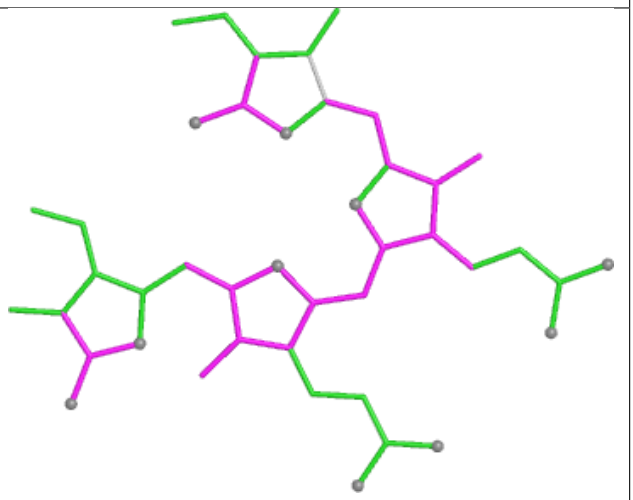
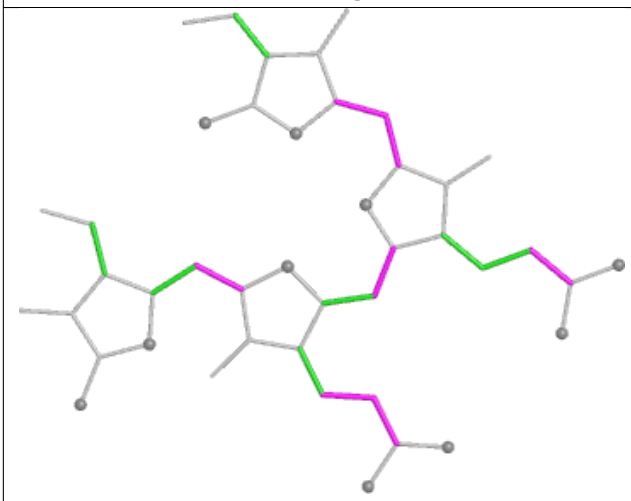


Bond angles



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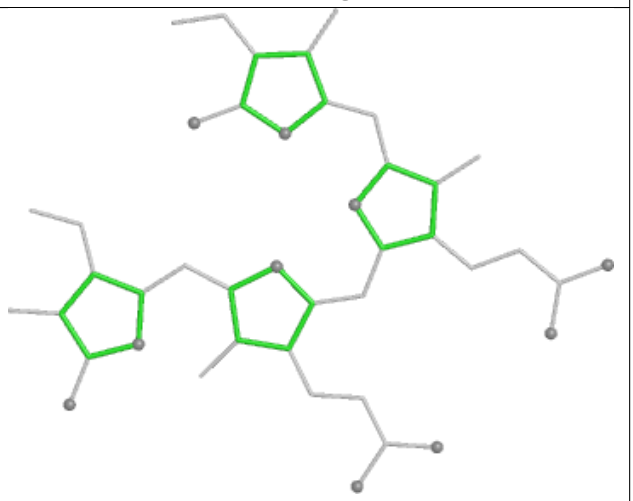
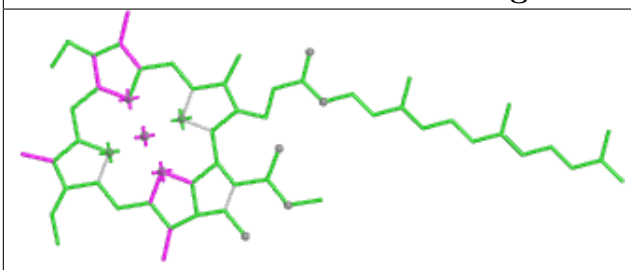


Rings

Ligand CLA BN 831



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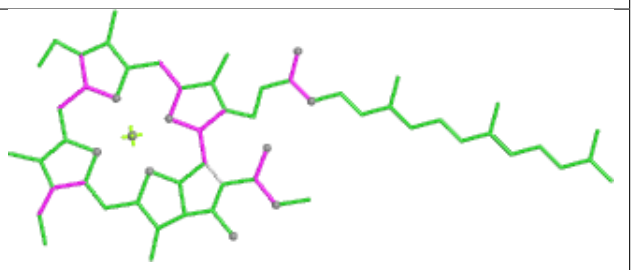
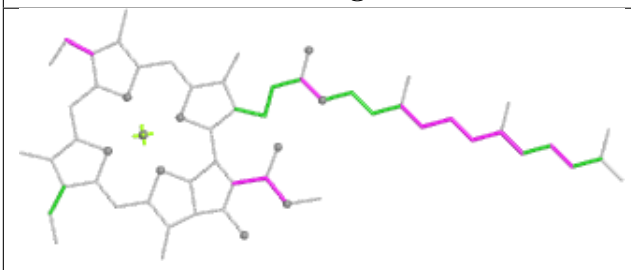


Bond angles



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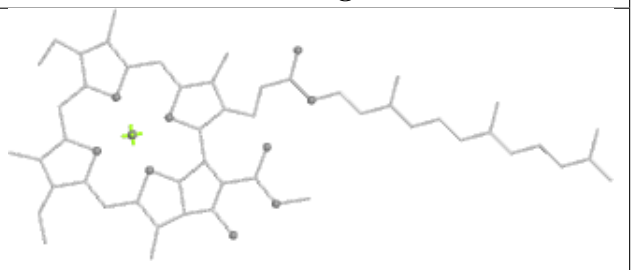
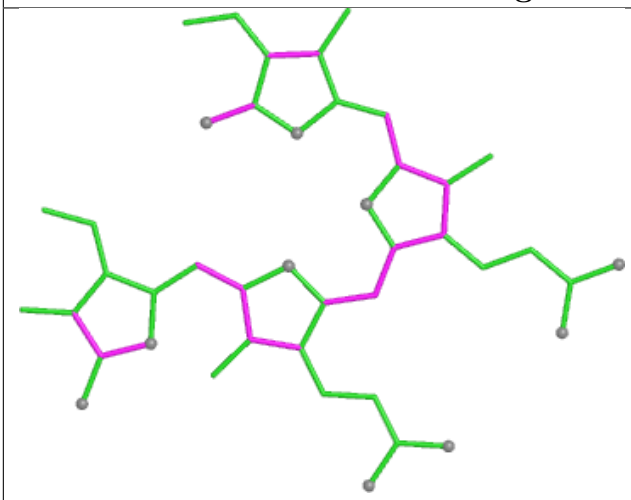


Rings

Ligand PEB aH 202



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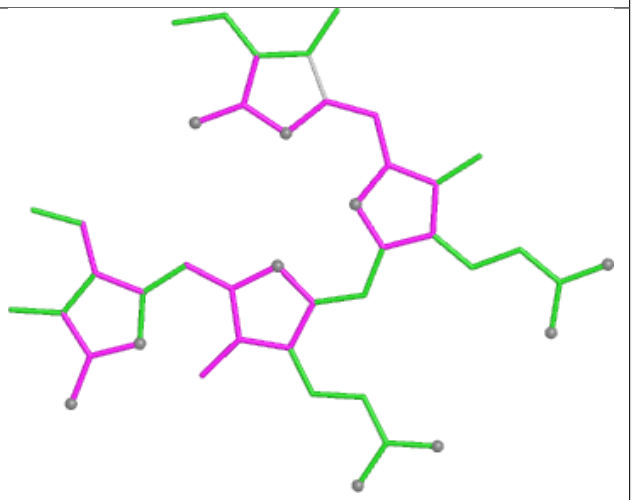

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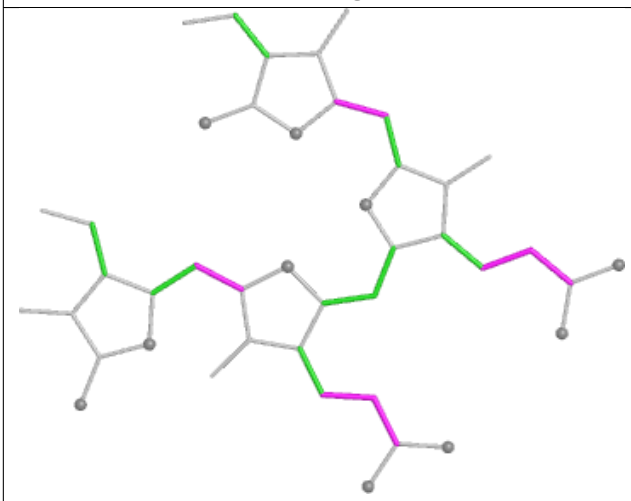

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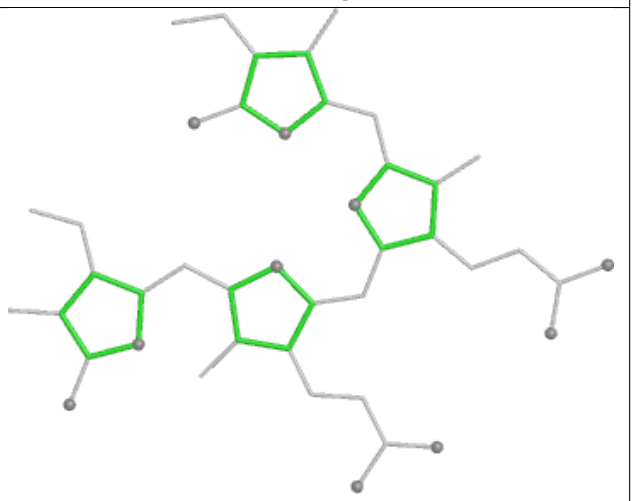
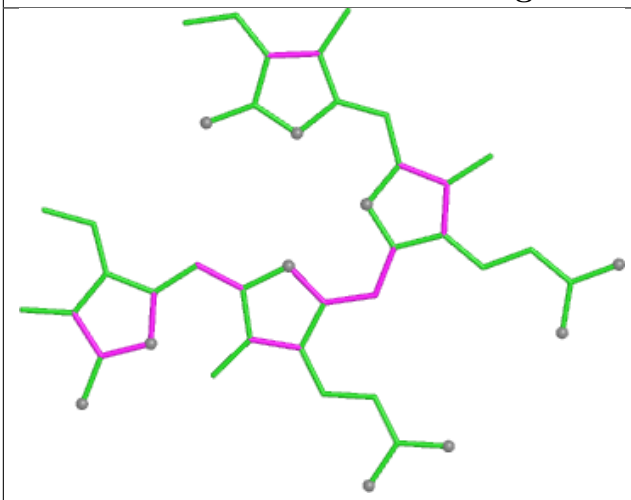


Rings

Ligand PEB O7 201



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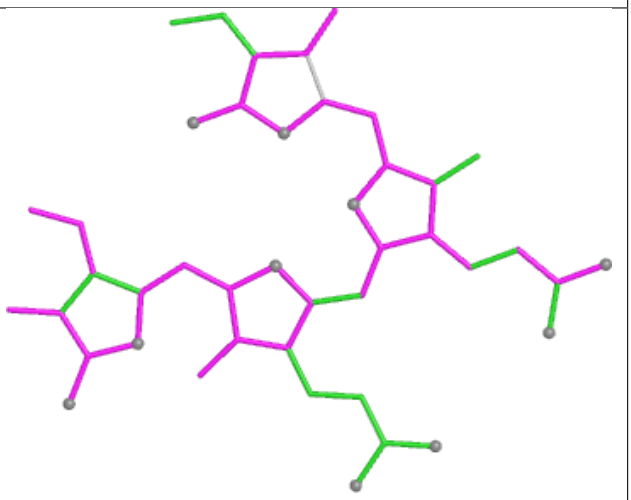

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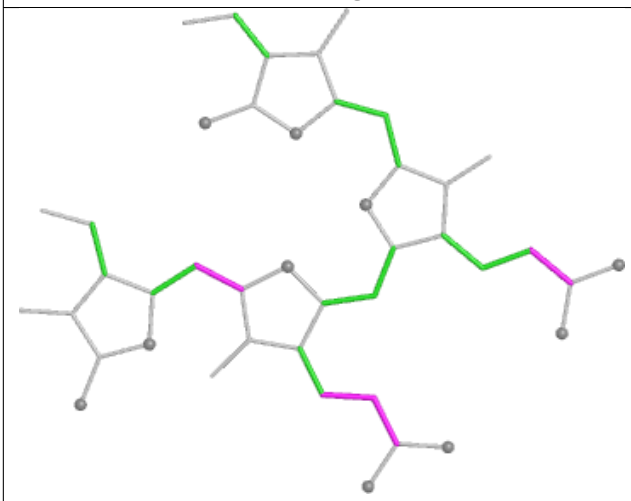

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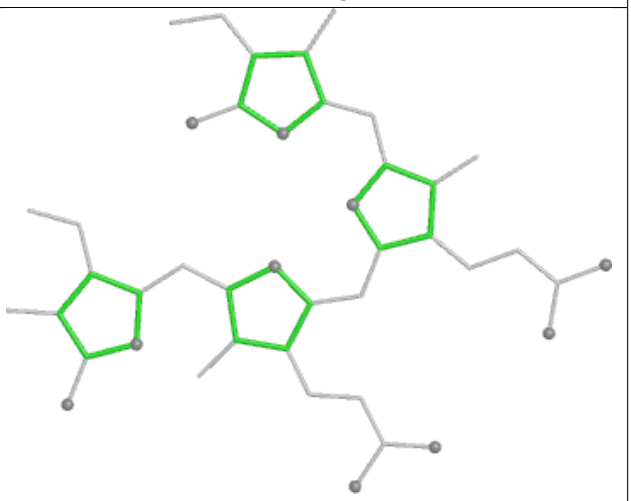
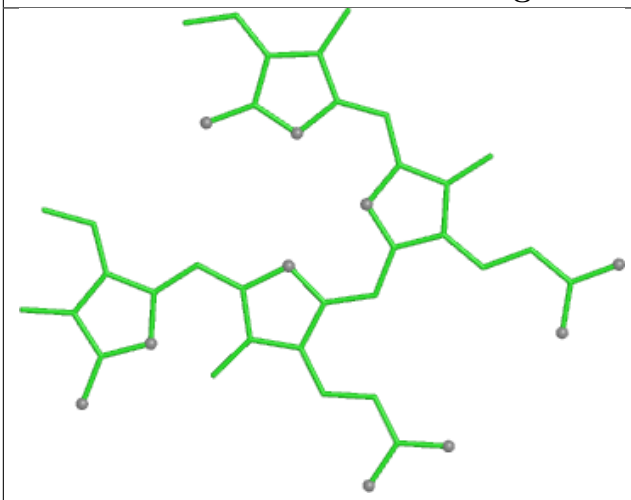


Rings

Ligand PEB SG 202



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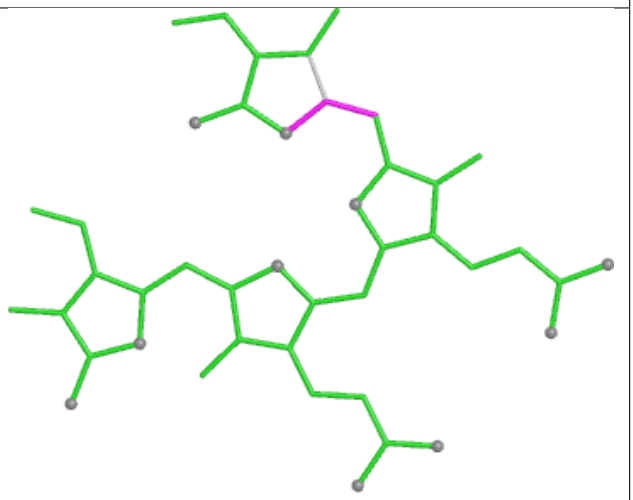

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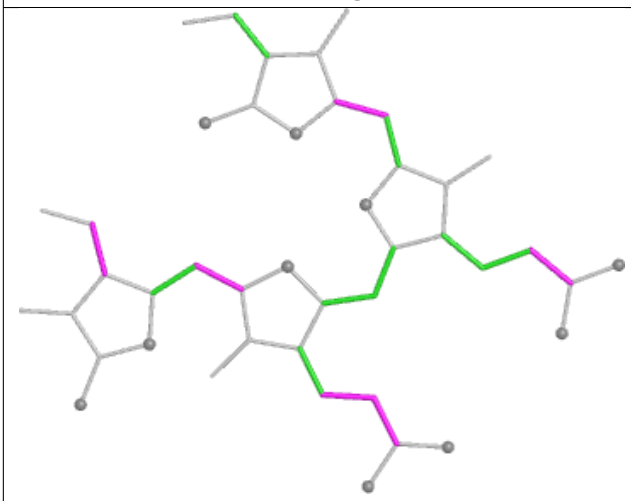

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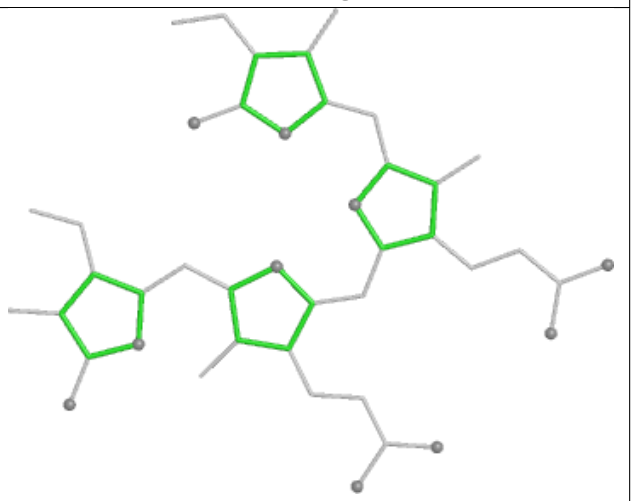
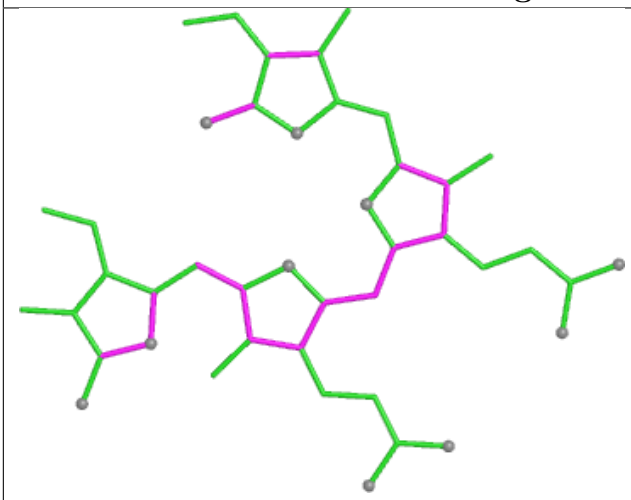


Rings

Ligand PEB qK 202



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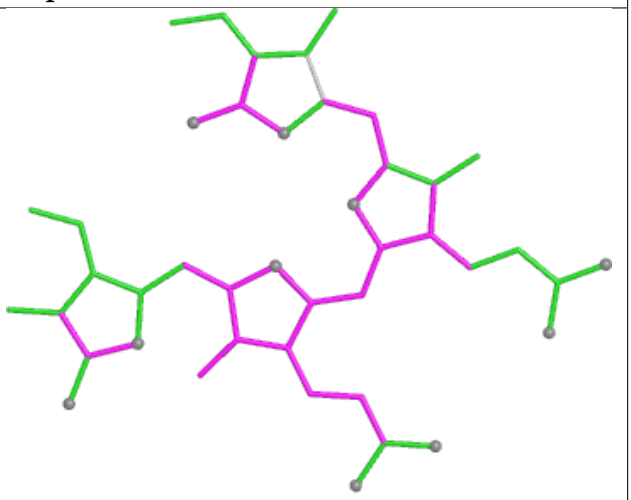

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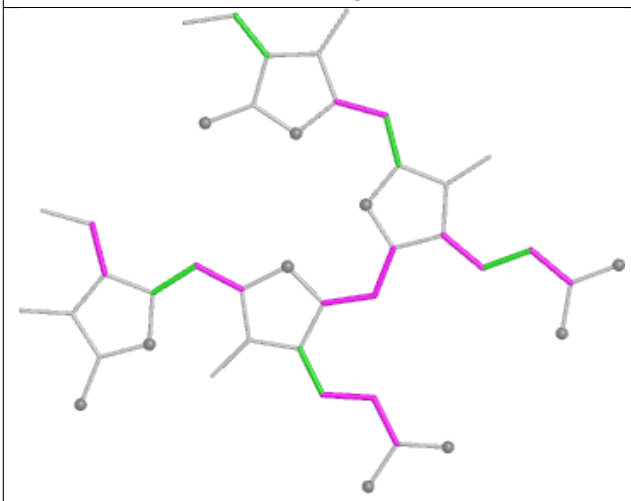

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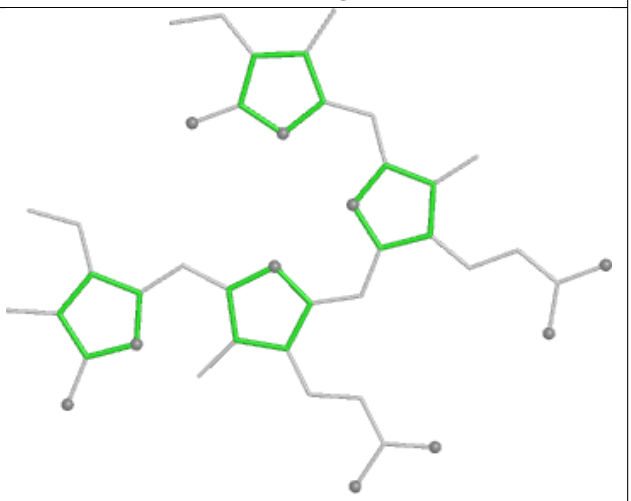
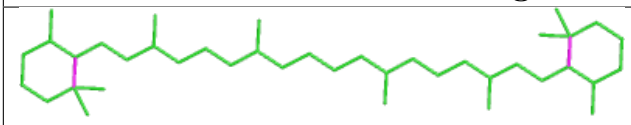


Rings

Ligand BCR H6 101



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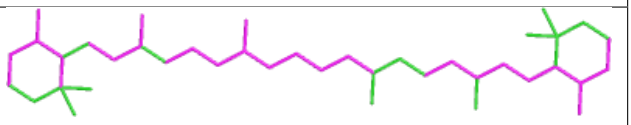

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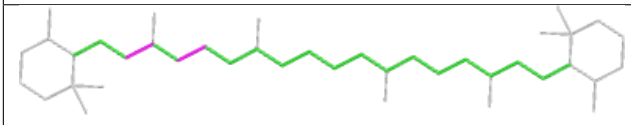

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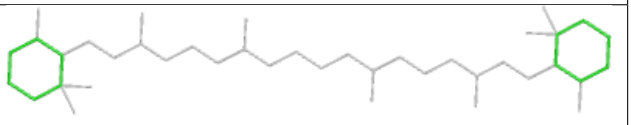
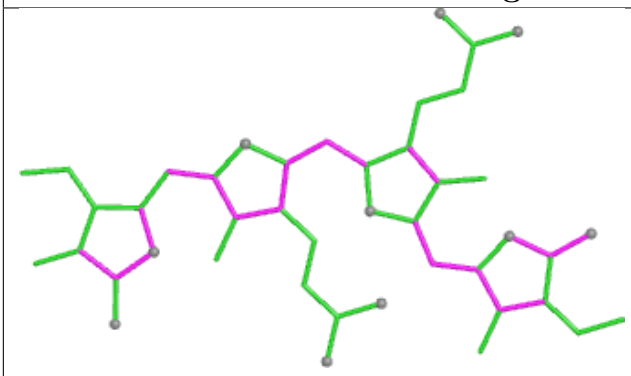


Rings

Ligand CYC K3 1001



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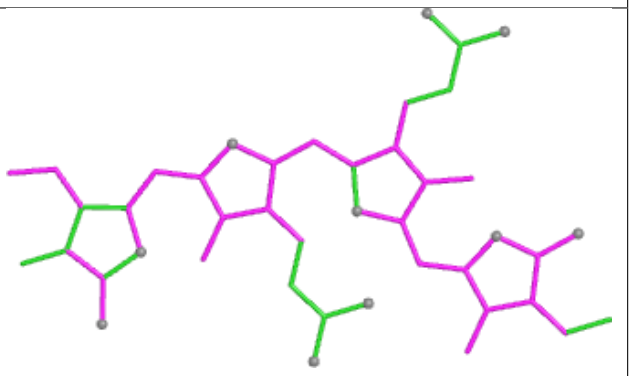

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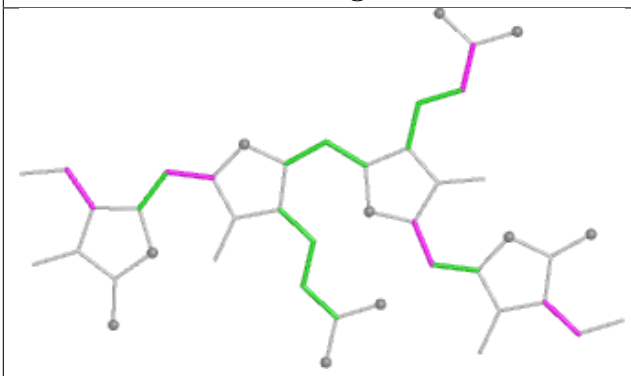

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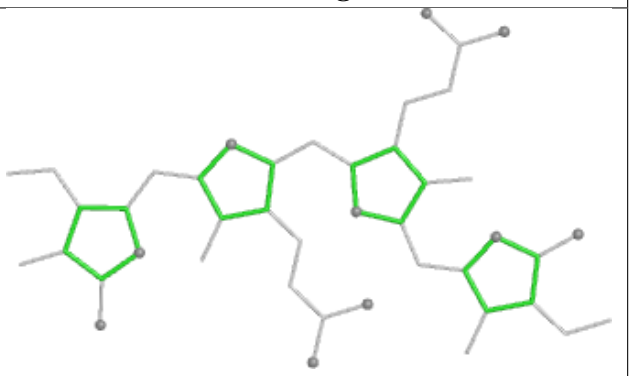
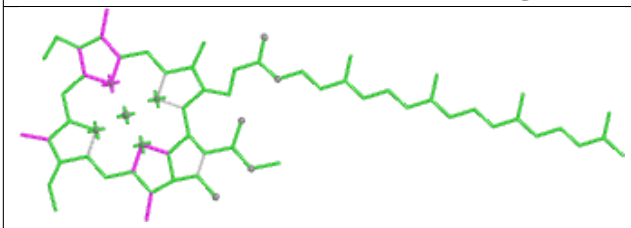


Rings

Ligand CLA nL 101



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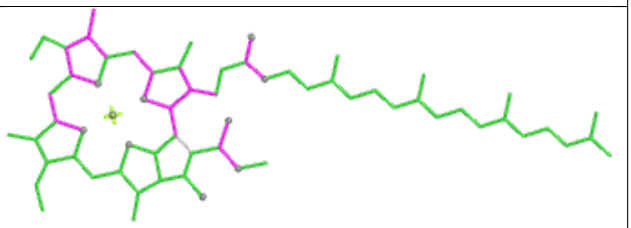

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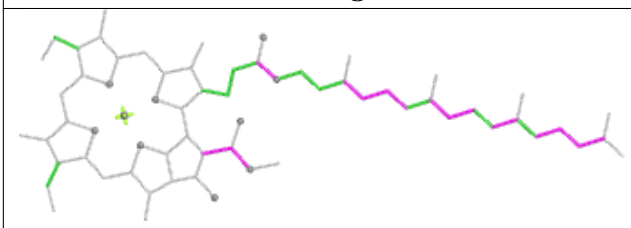

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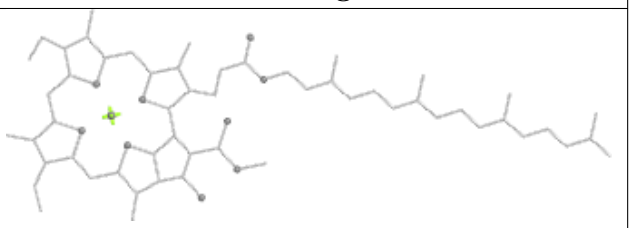
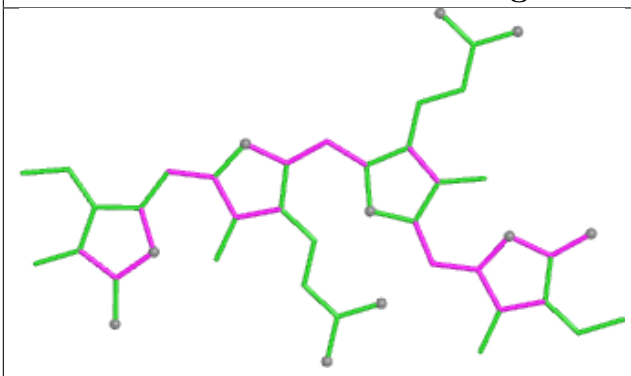


Rings

Ligand CYC I4 1001



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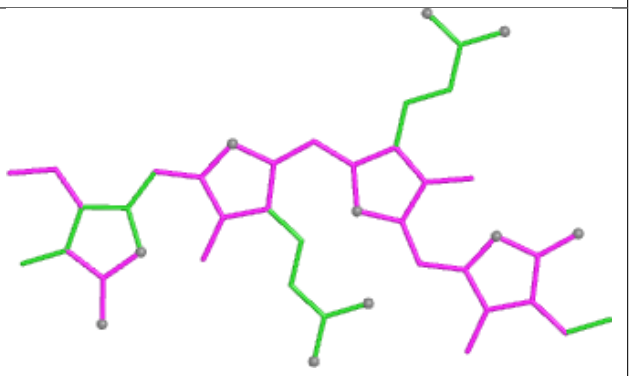

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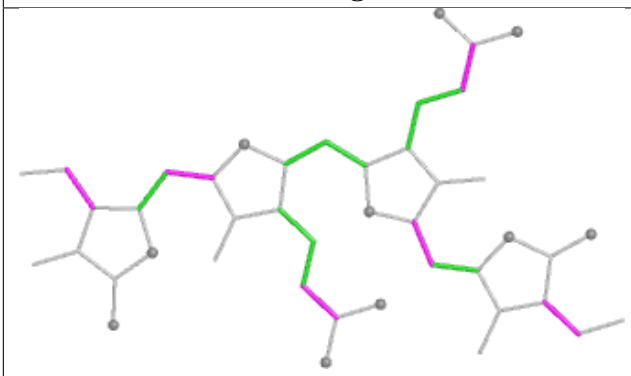

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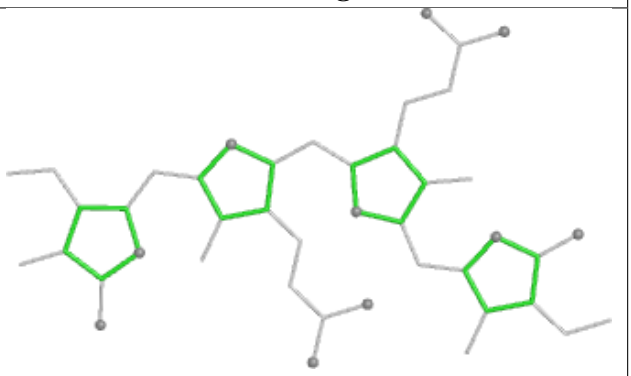
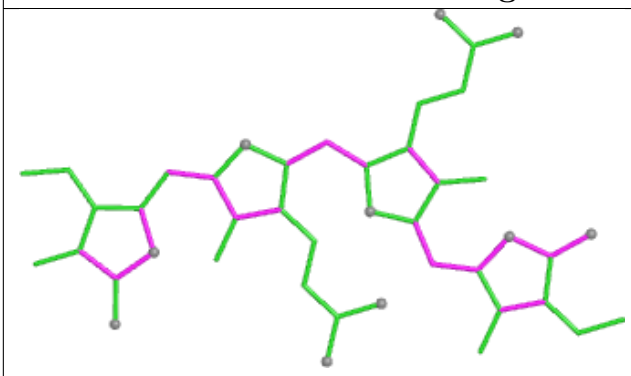


Rings

Ligand CYC GO 1001



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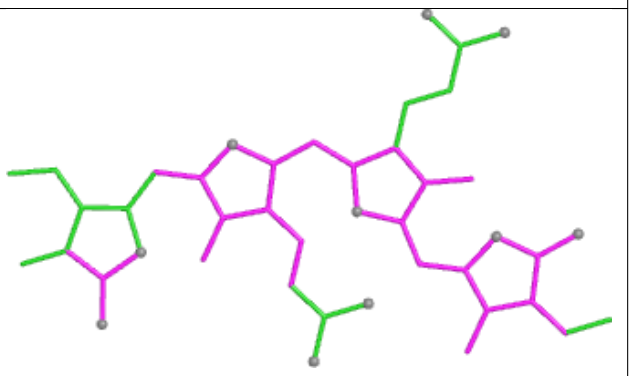

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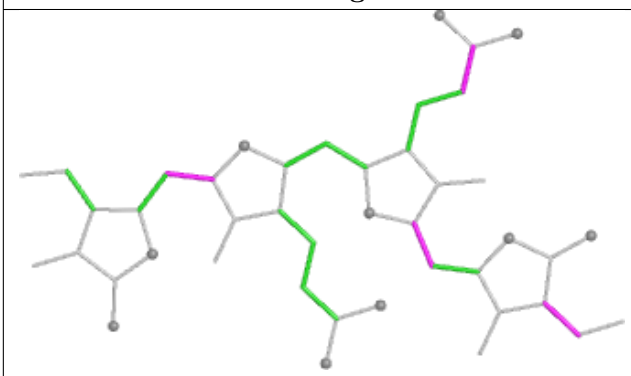

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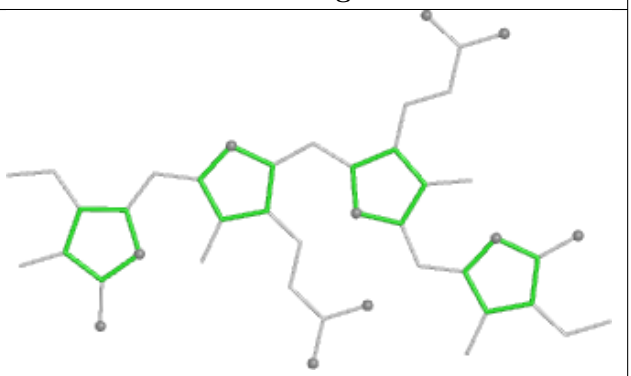
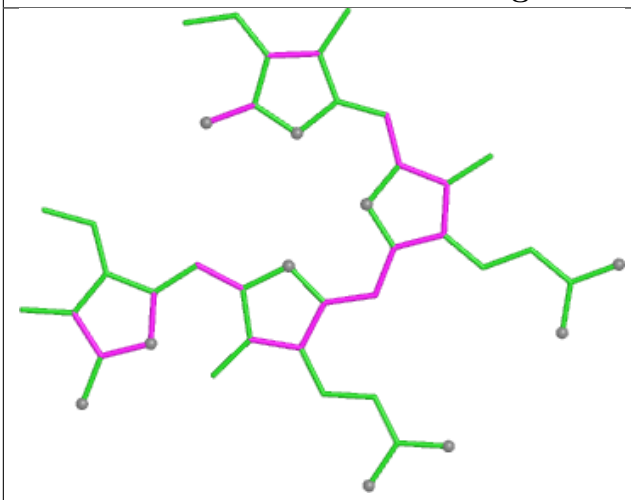


Rings

Ligand PEB wC 204



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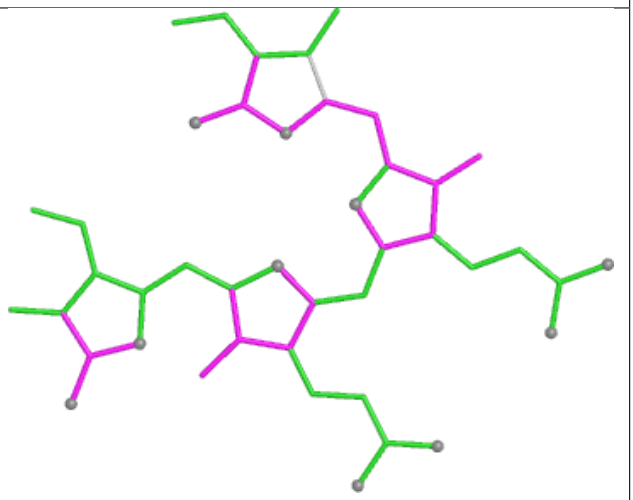

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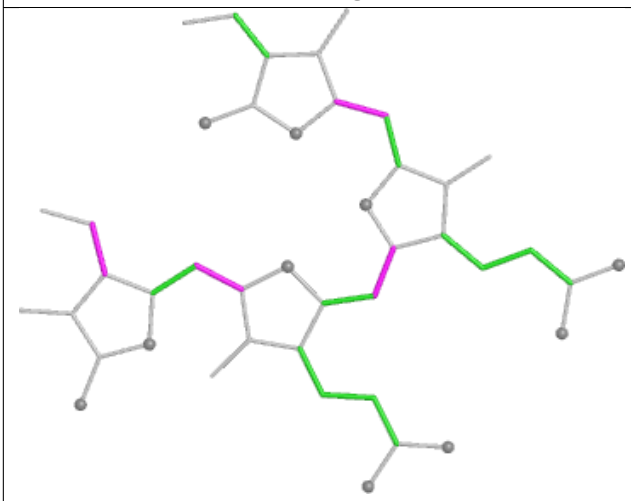

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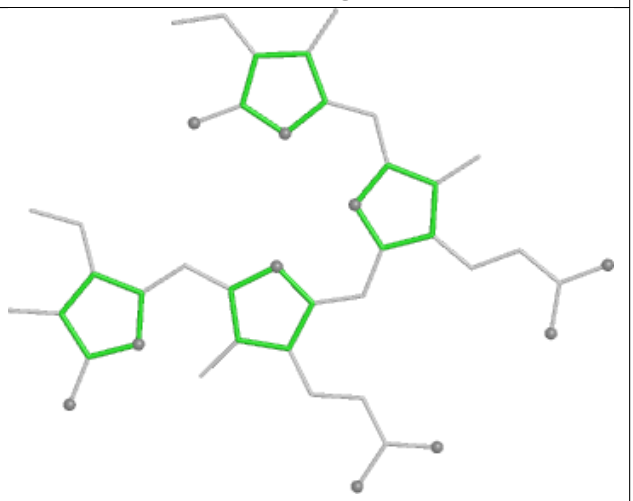

Rings

Ligand BCR b6 601



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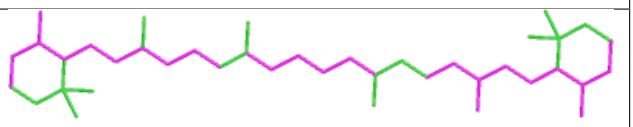

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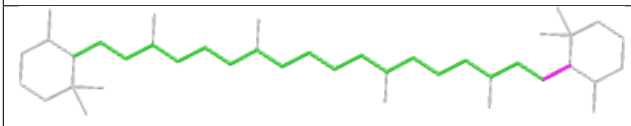

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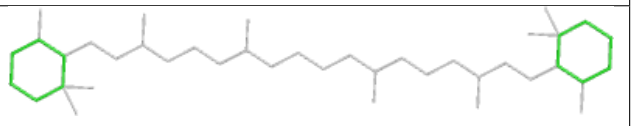
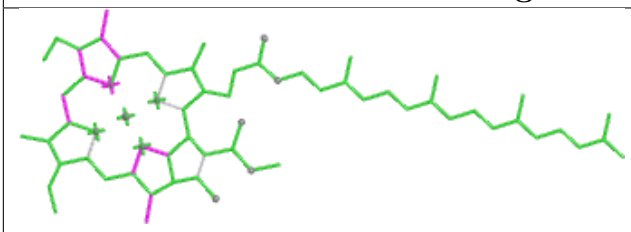


Rings

Ligand CLA B2 830



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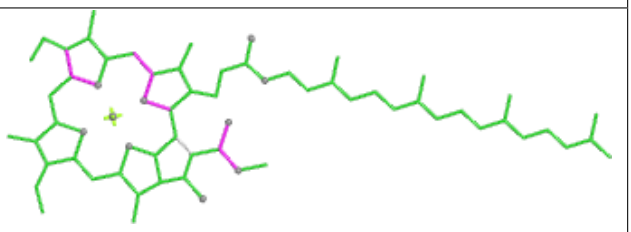

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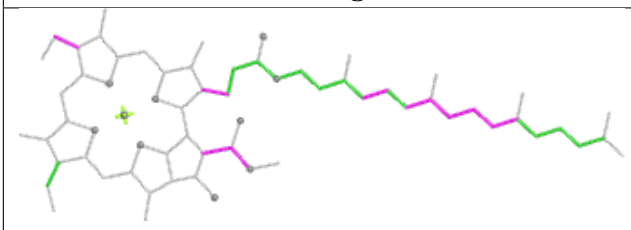

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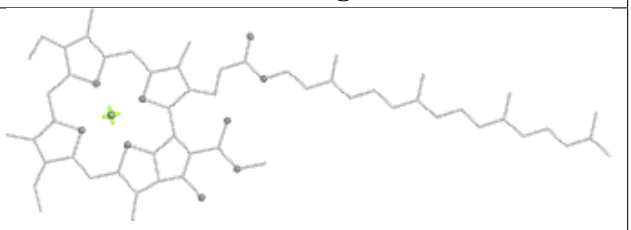
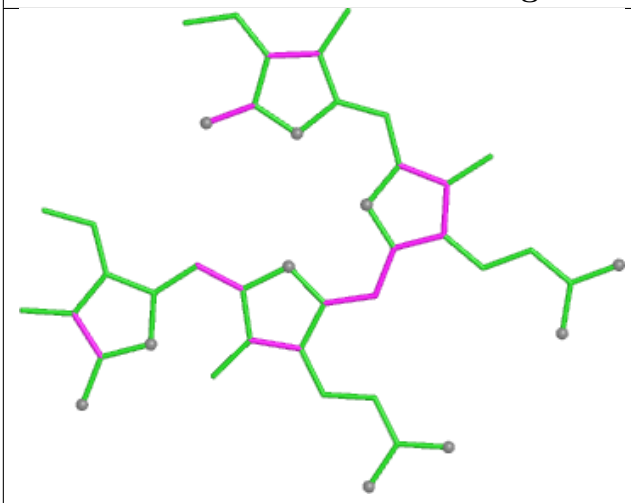


Rings

Ligand PEB fF 201



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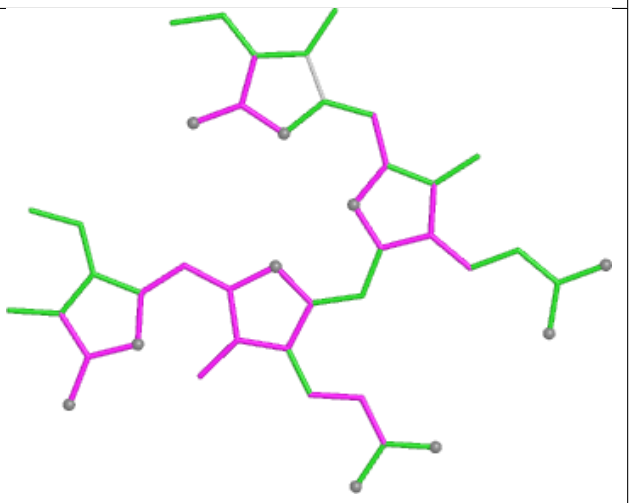
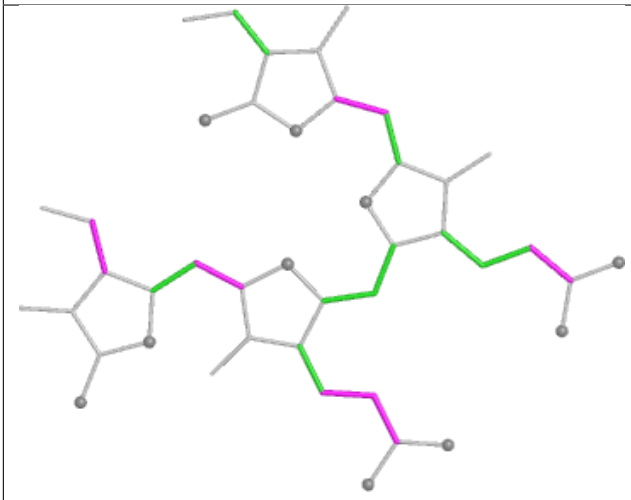


Bond angles



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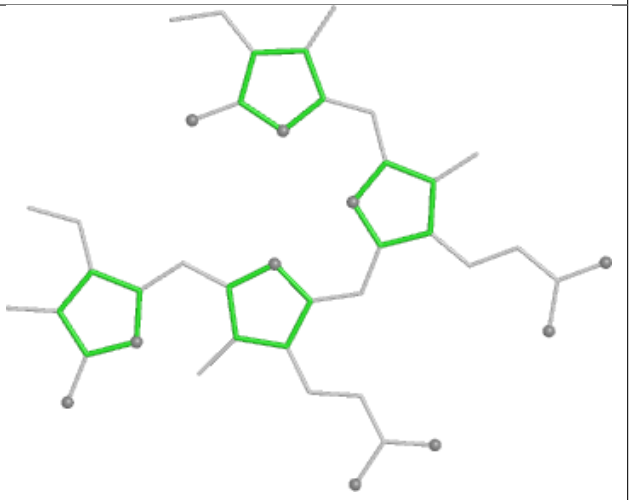
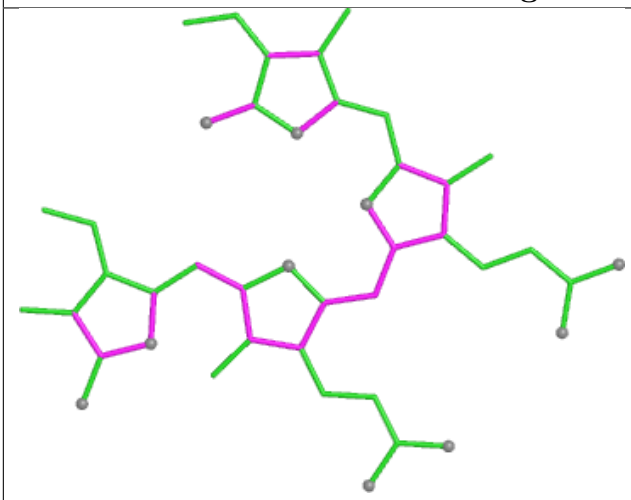


Rings

Ligand PEB fE 202



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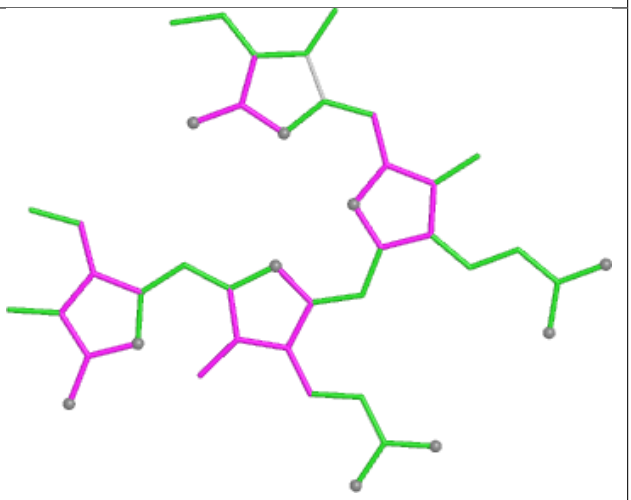

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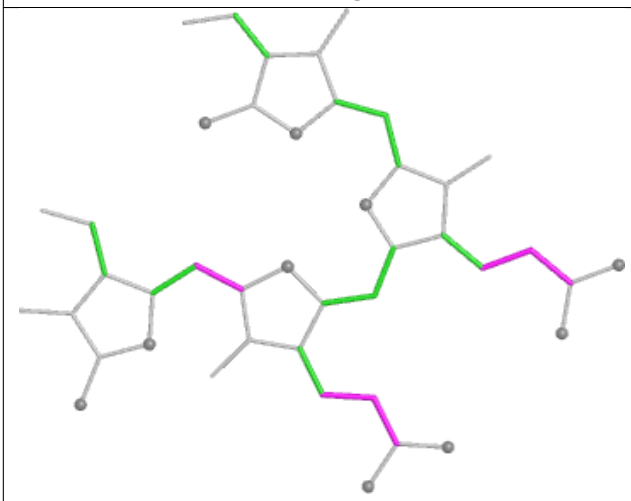

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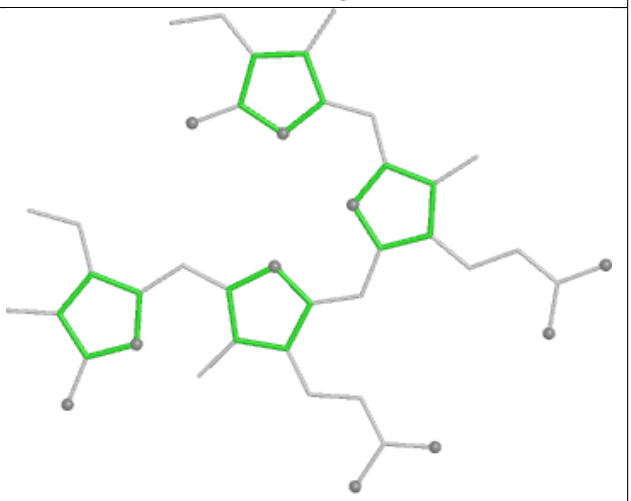

Rings

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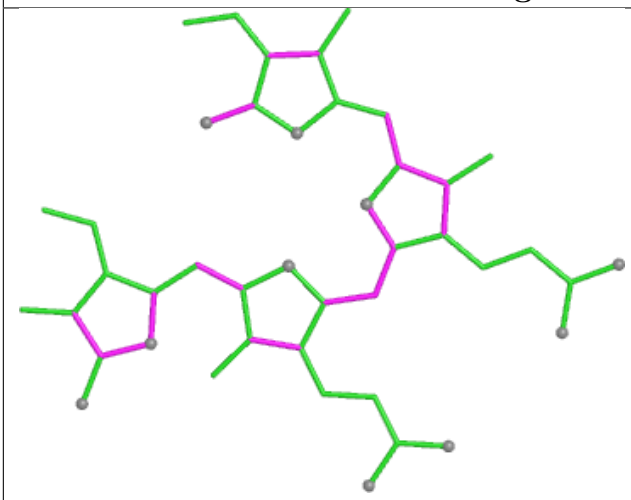

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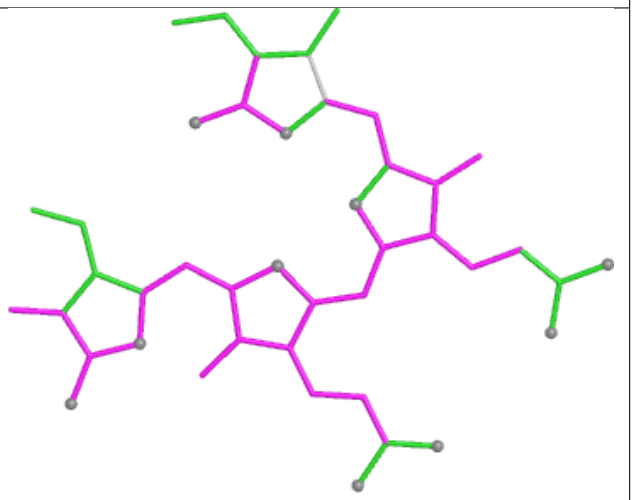
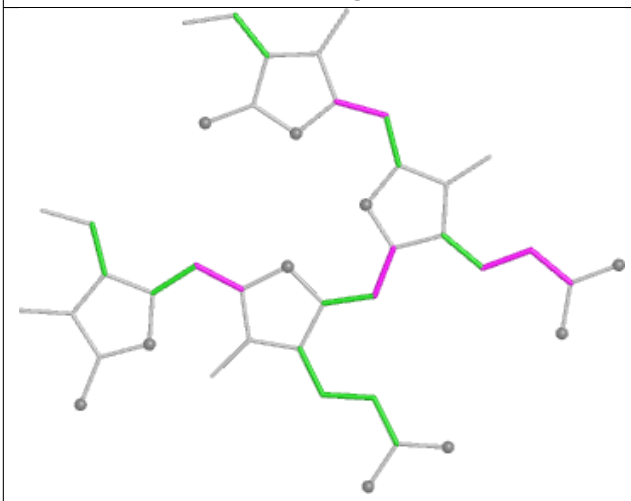


Bond angles



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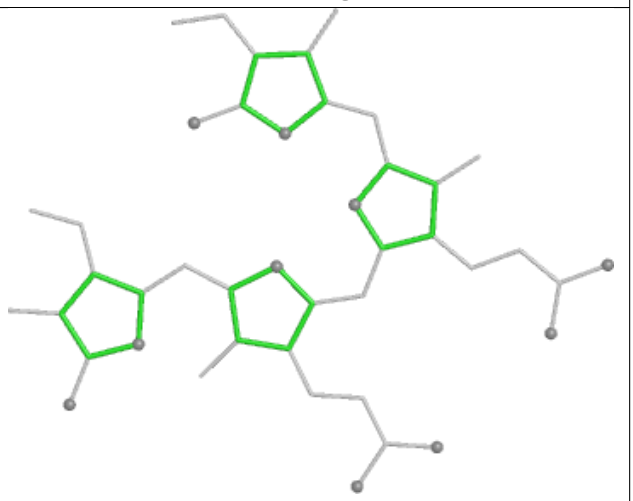
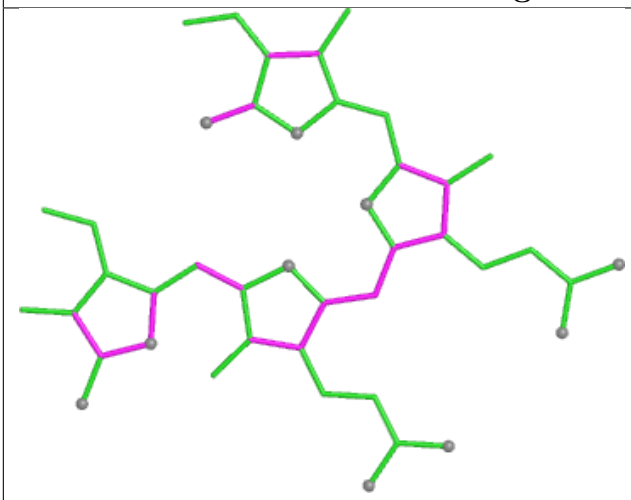


Rings

Ligand PEB m4 203



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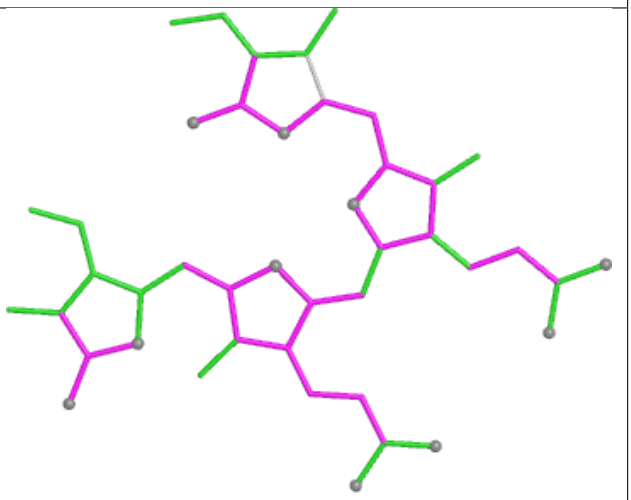

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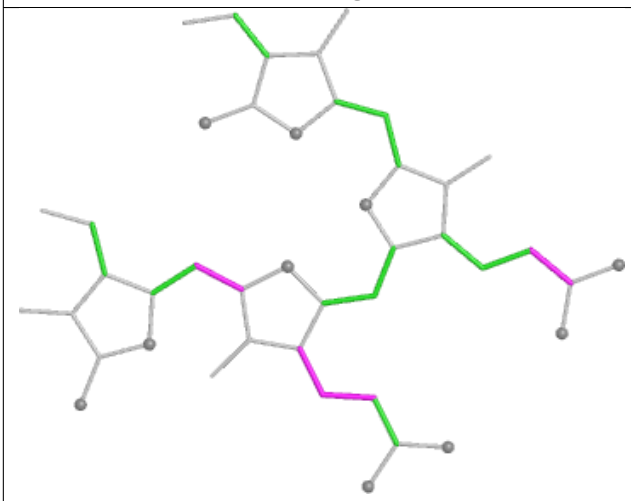
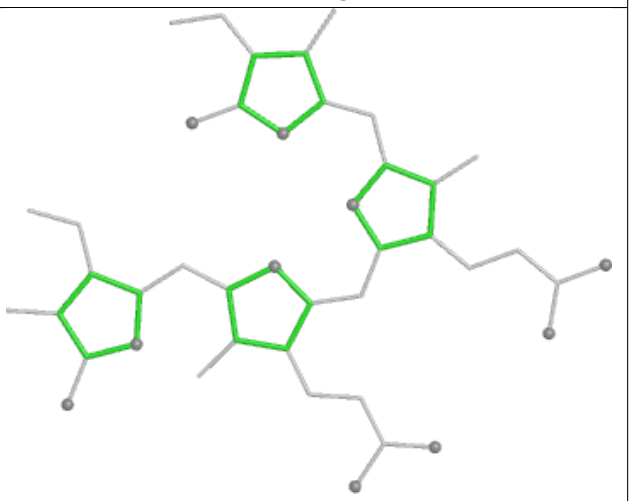
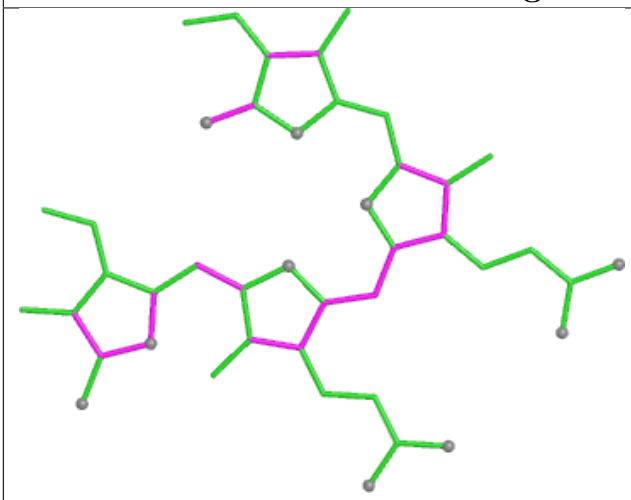


Torsions



Rings

Ligand PEB i4 203



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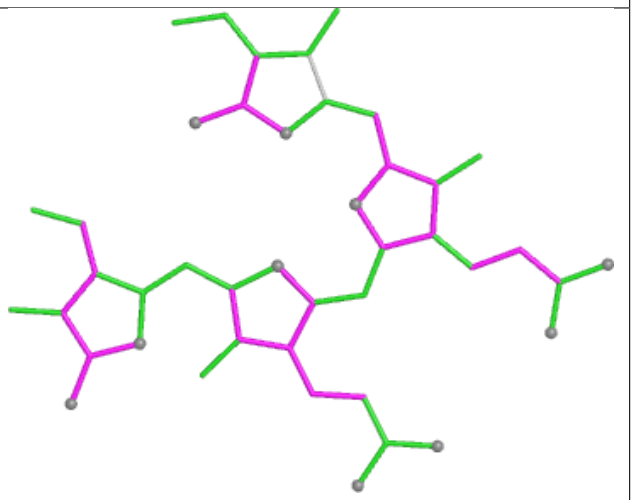

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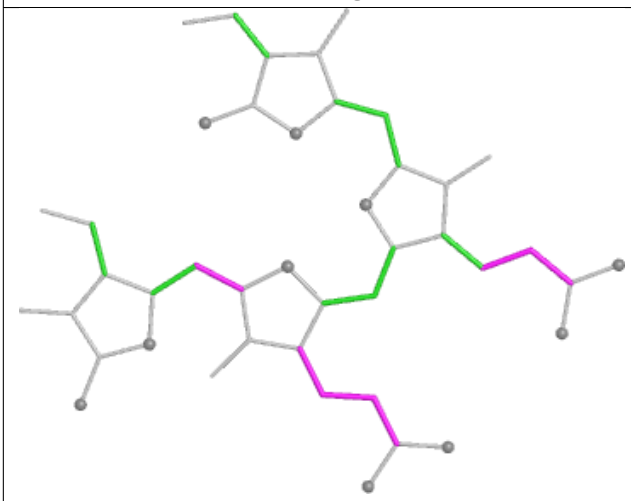

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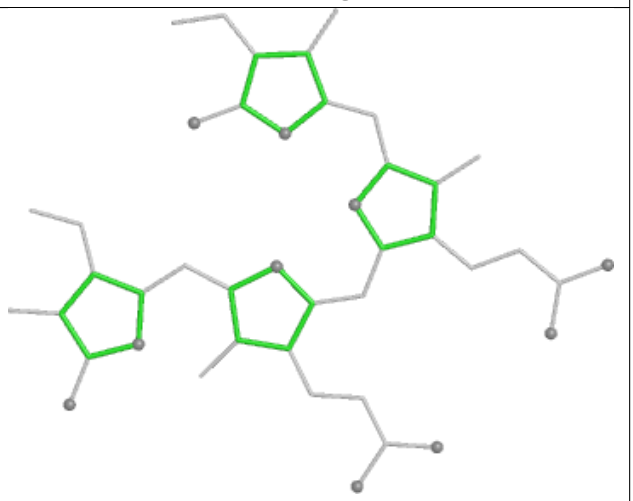
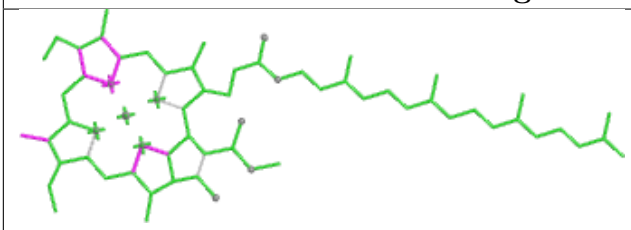


Rings

Ligand CLA BL 606



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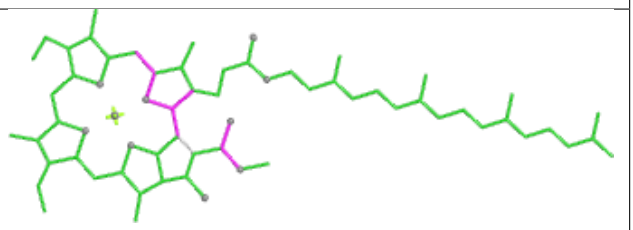

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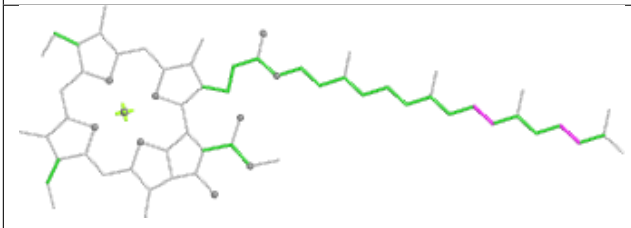

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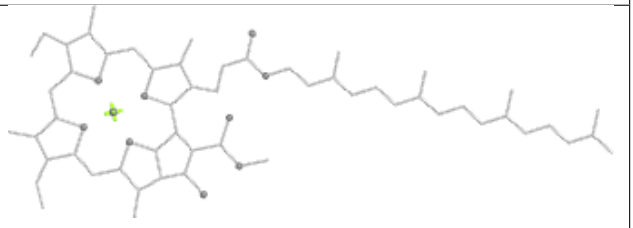
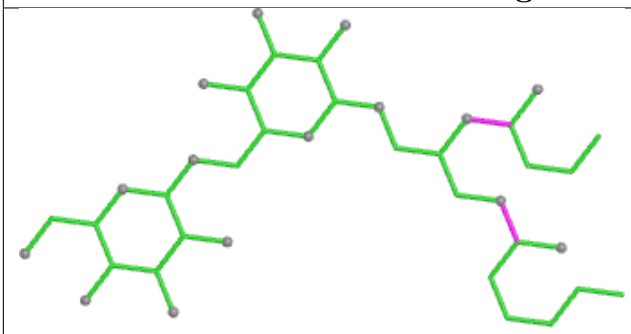


Rings

Ligand DGD a6 603



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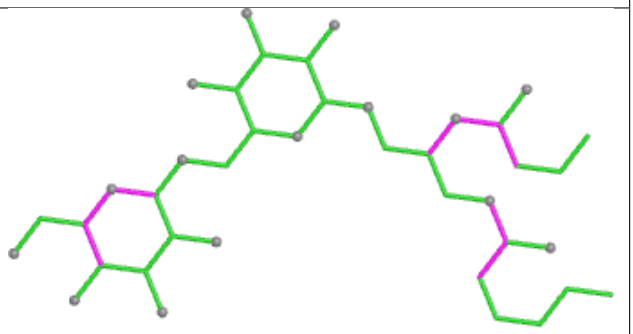

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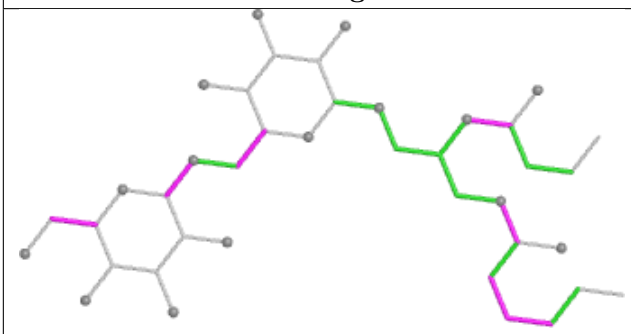

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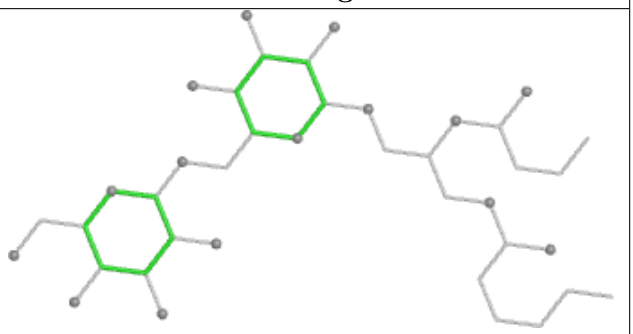
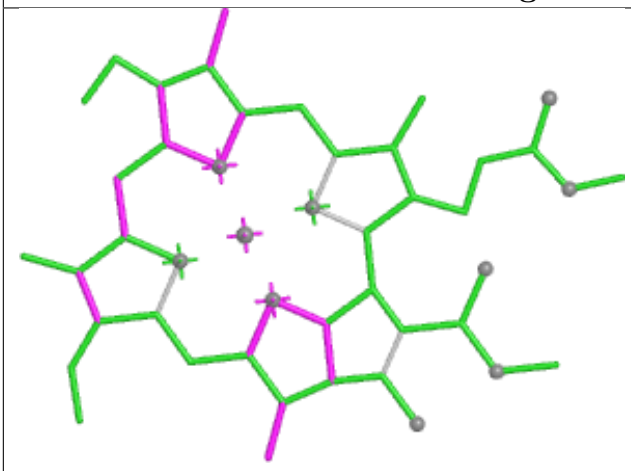


Rings

Ligand CLA 82 306



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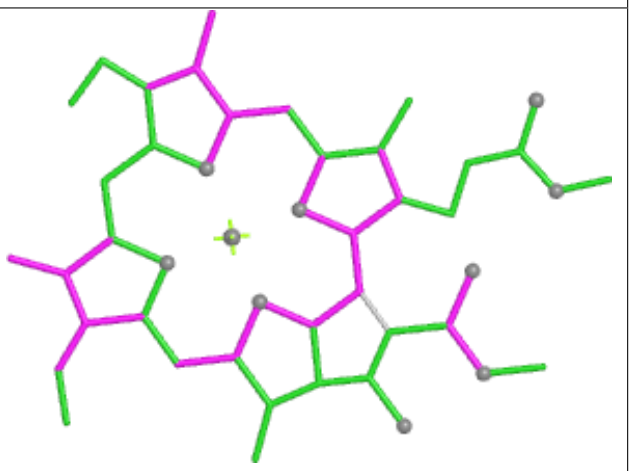

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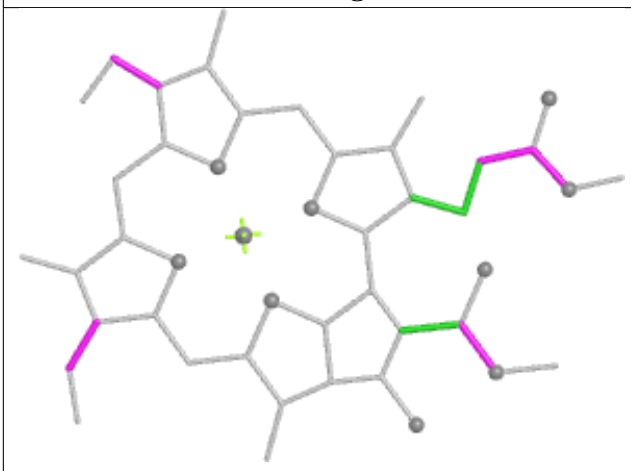

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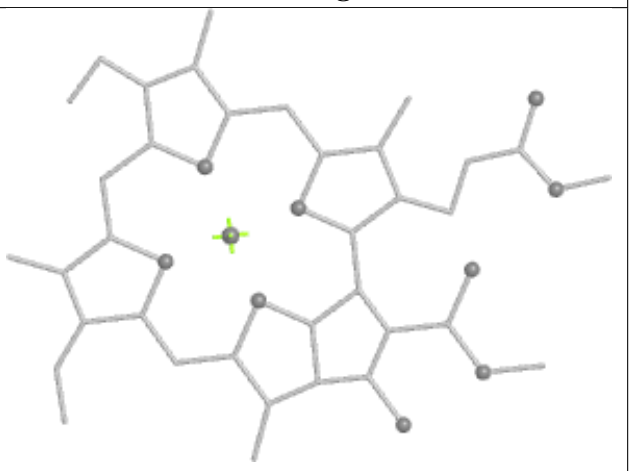
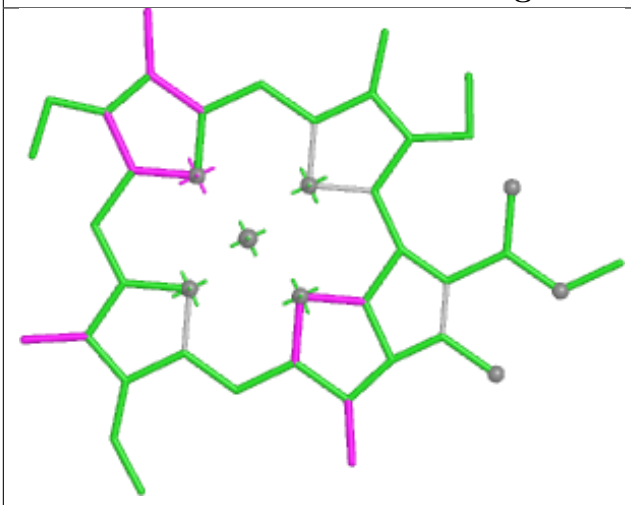


Rings

Ligand CLA 1N 609



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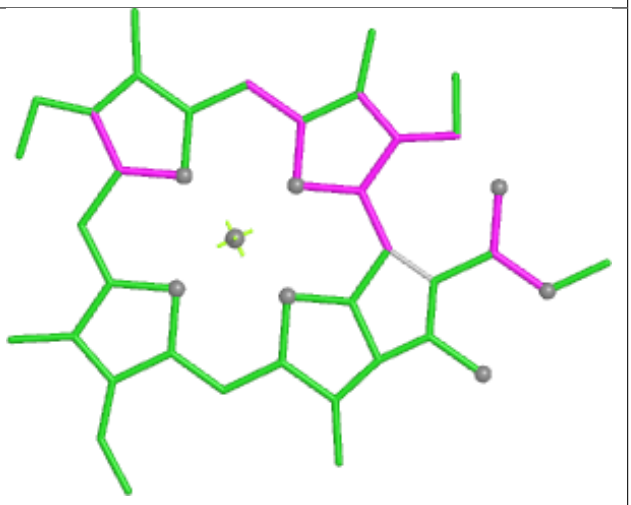

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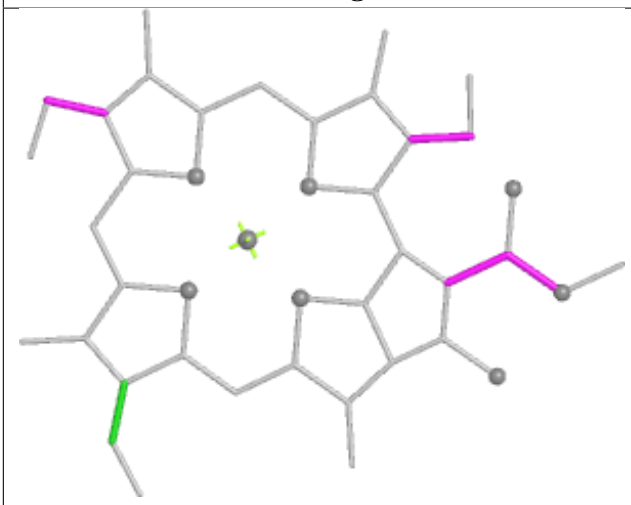
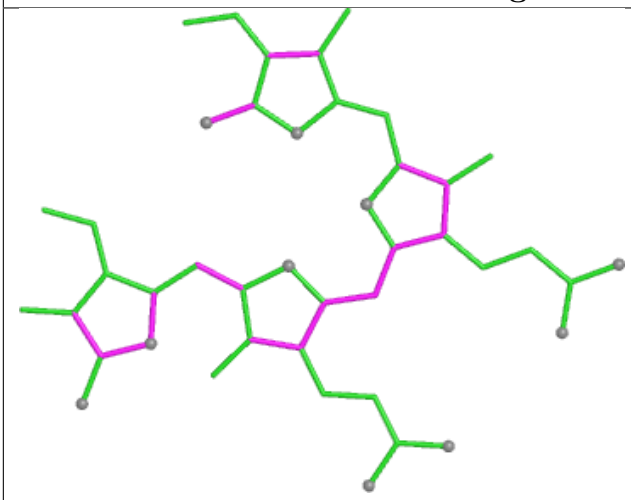


Torsions



Rings

Ligand PEB mO 202



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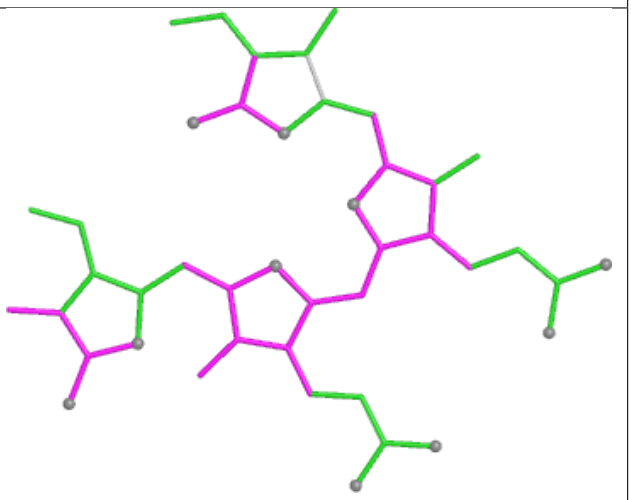

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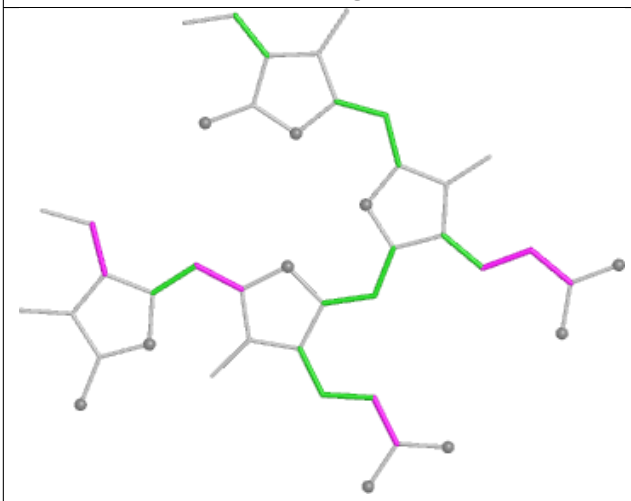

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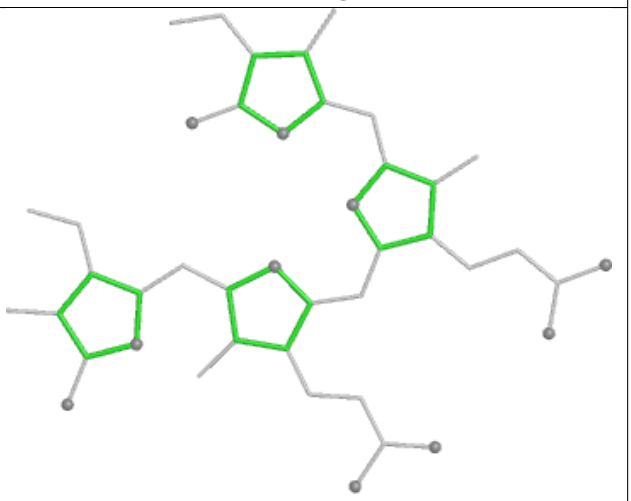
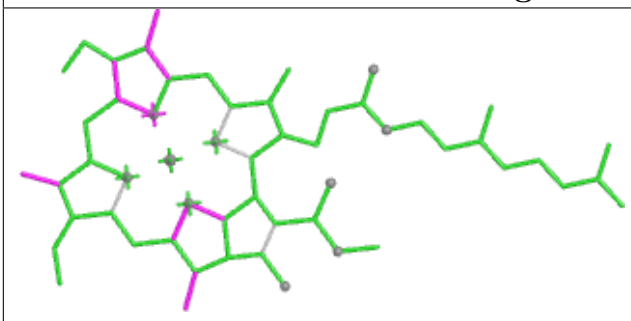


Rings

Ligand CLA A2 812



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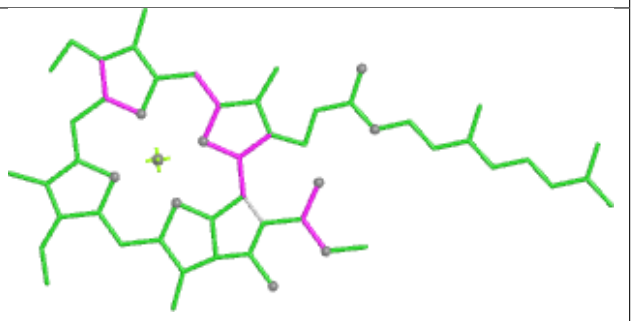

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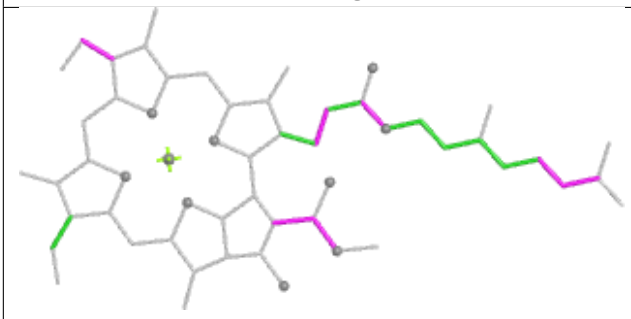

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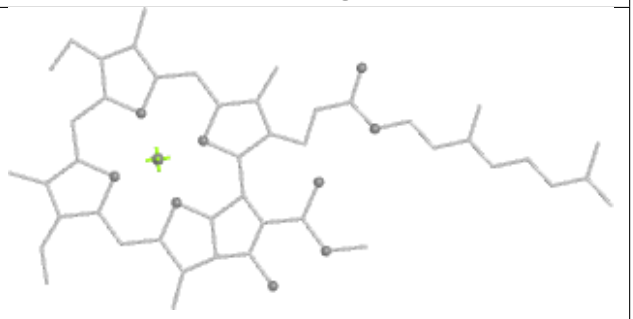
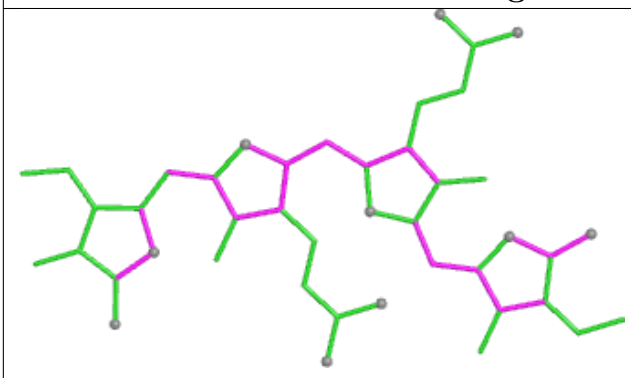


Rings

Ligand CYC y3 1001



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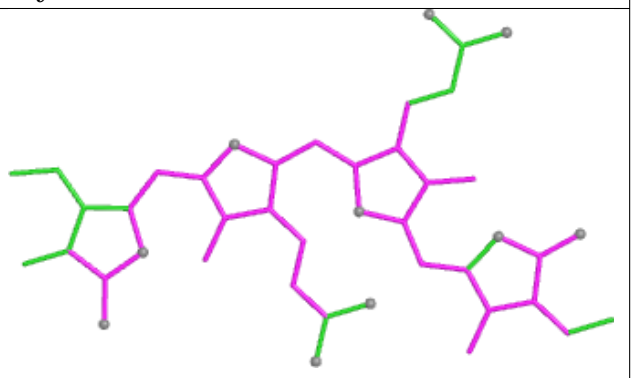

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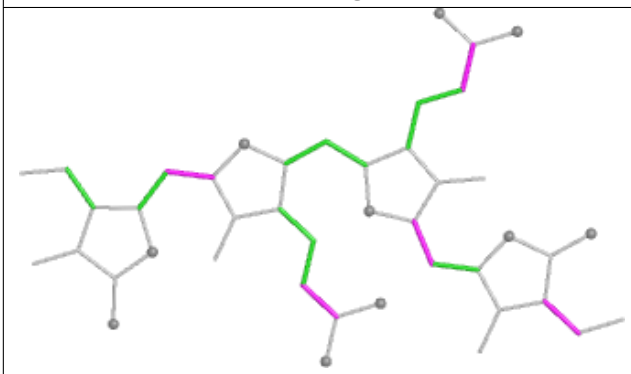

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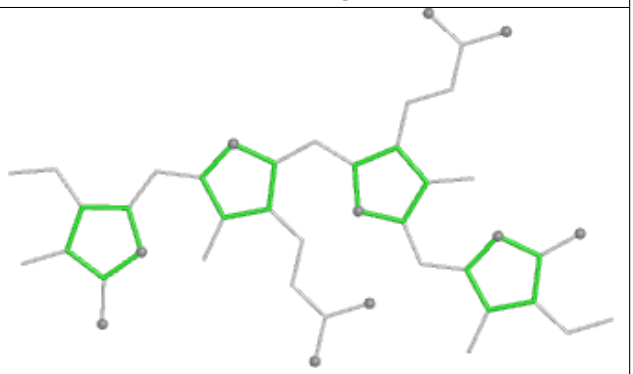
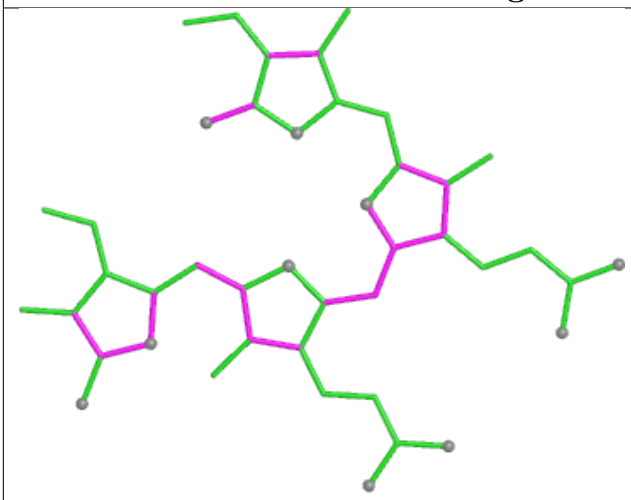


Rings

Ligand PEB WE 201



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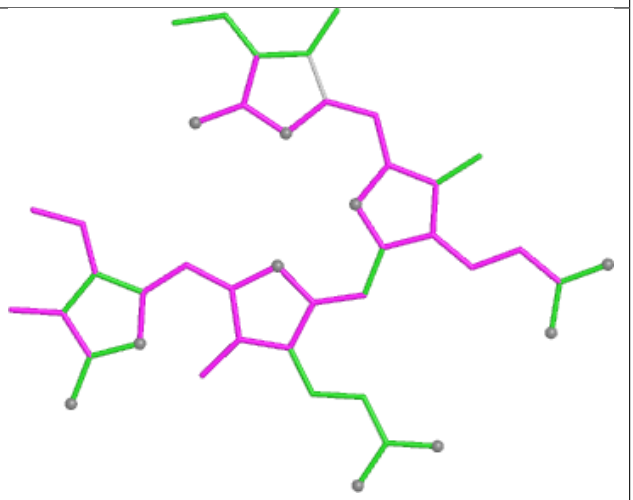

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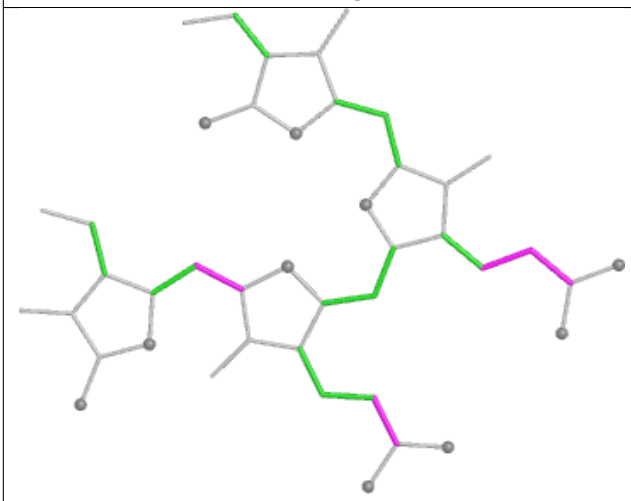

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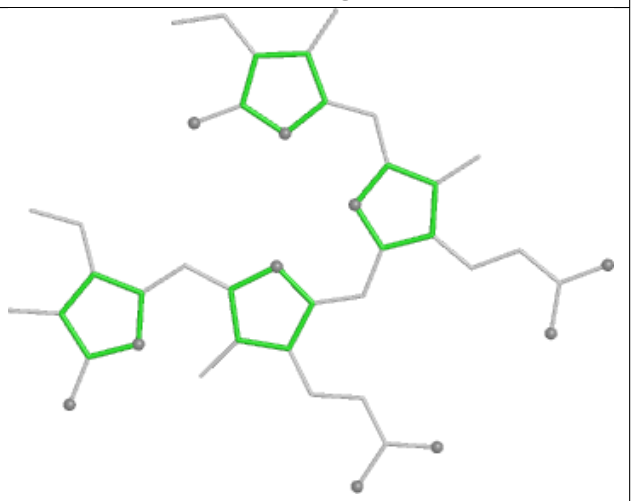
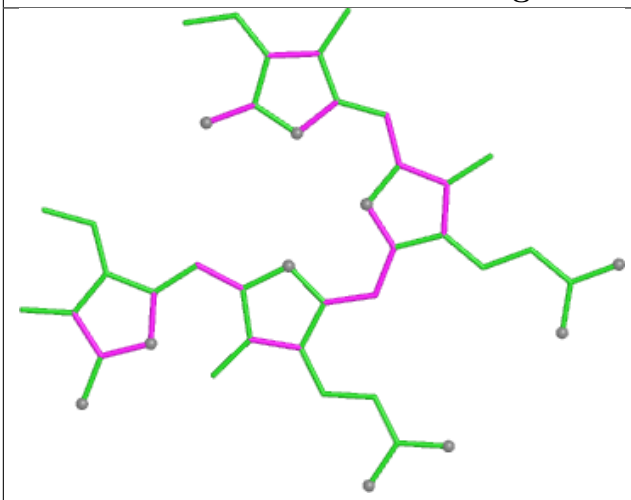


Rings

Ligand PEB cM 201



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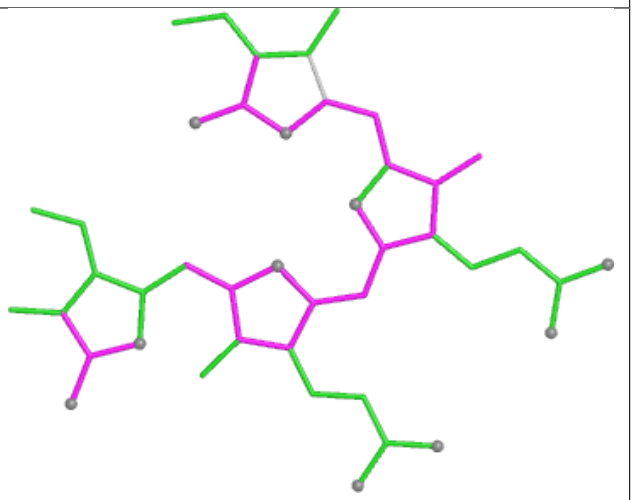

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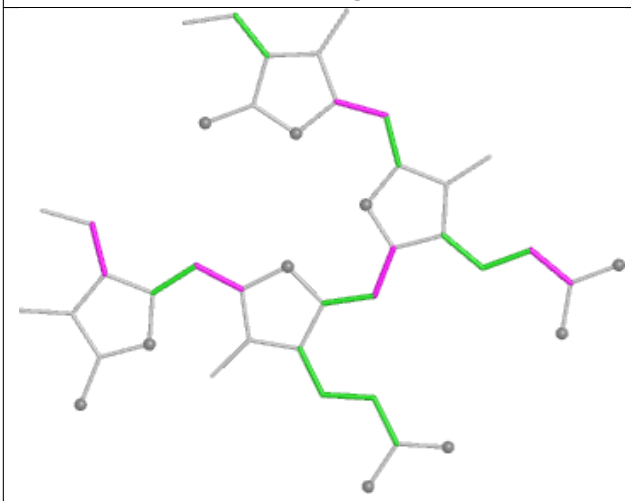

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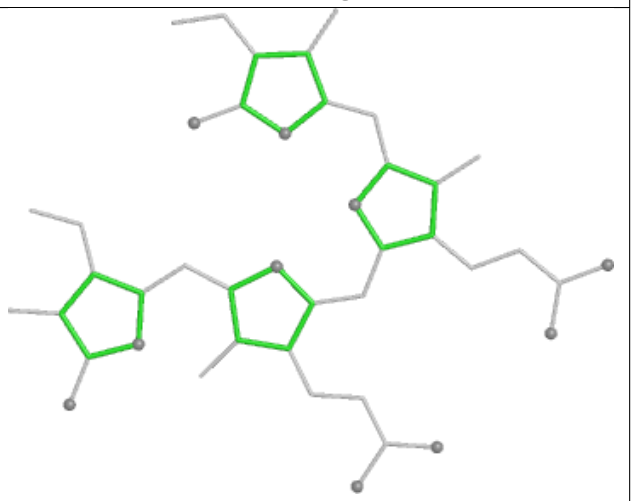
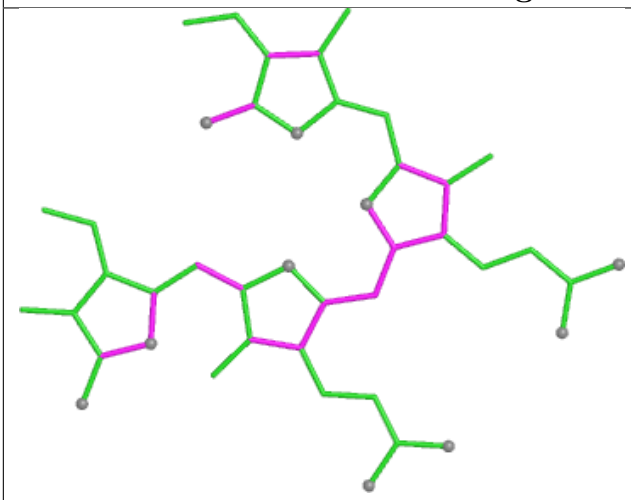


Rings

Ligand PEB Y7 303



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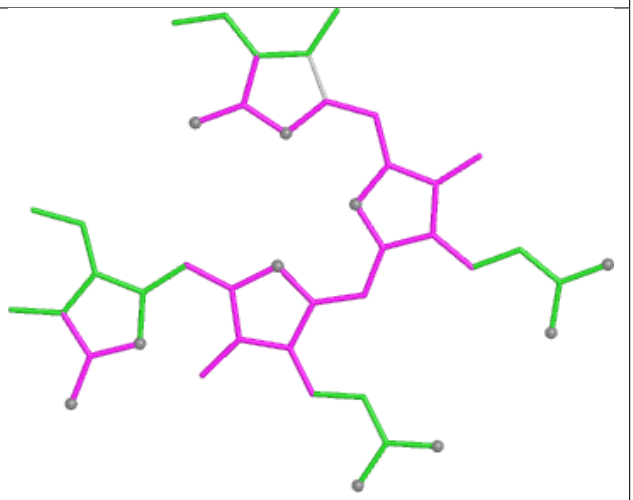

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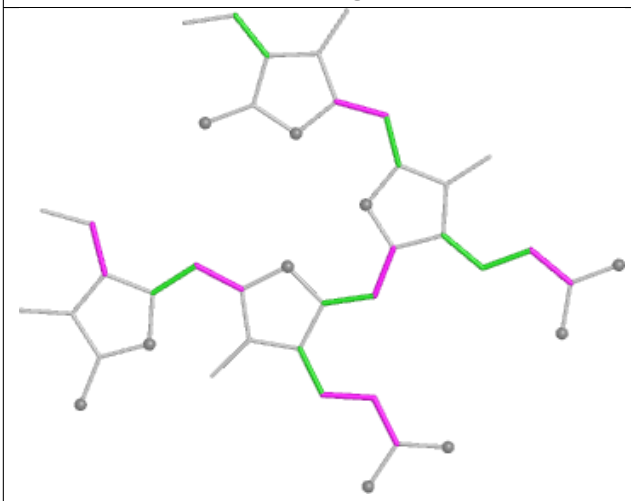

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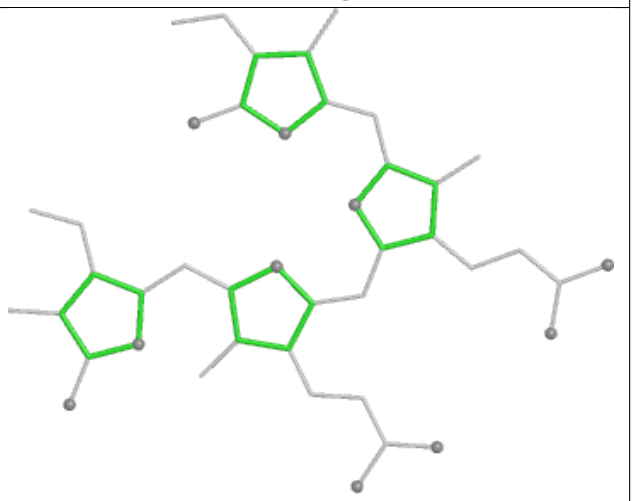
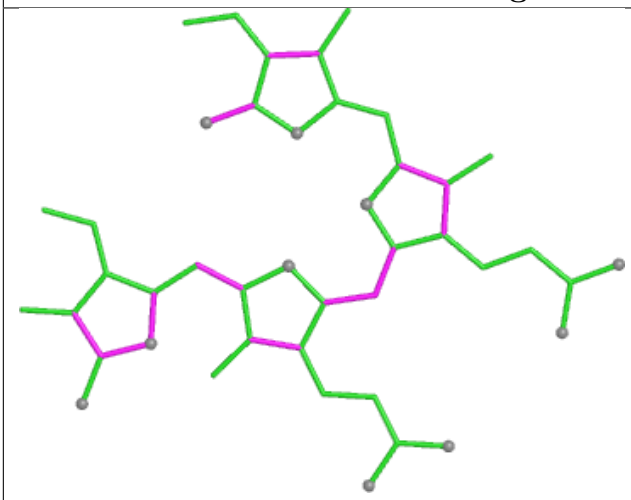


Rings

Ligand PEB KK 201



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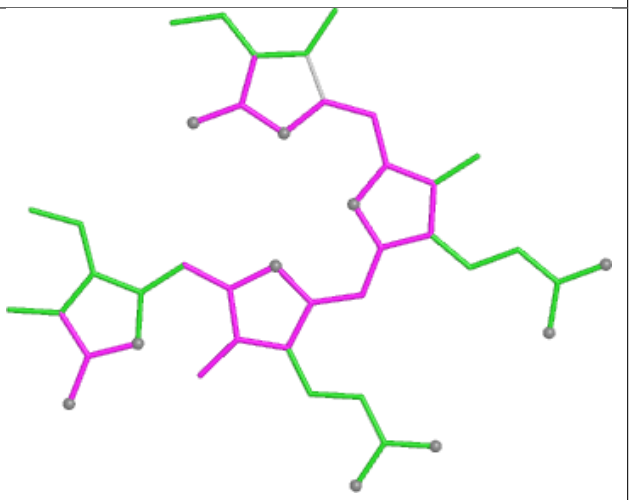
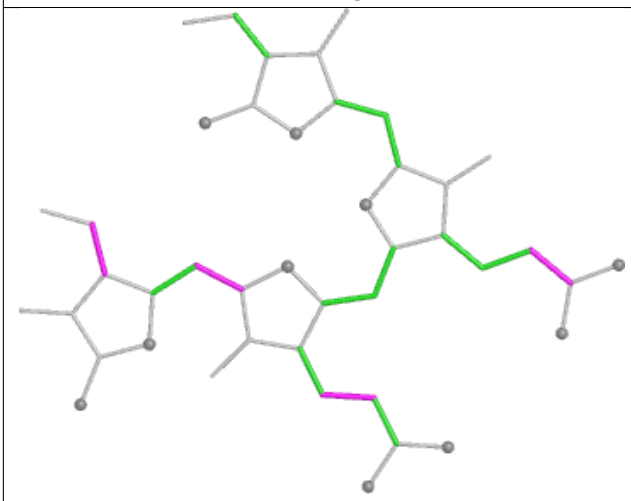


Bond angles



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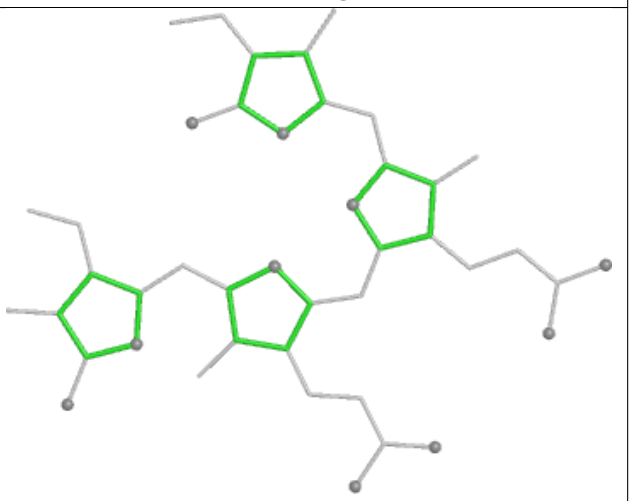
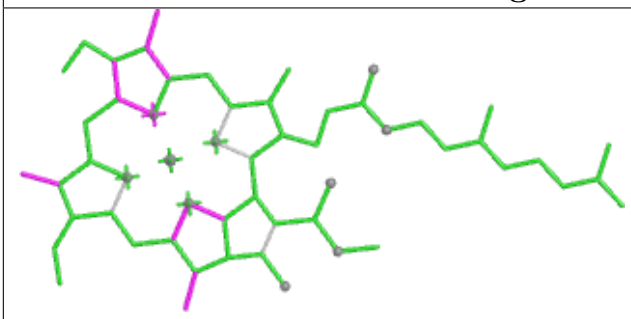


Rings

Ligand CLA AN 812



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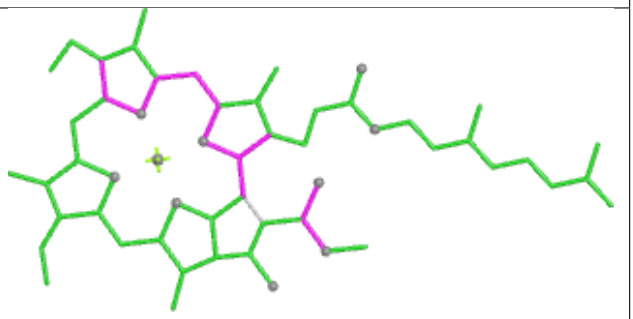

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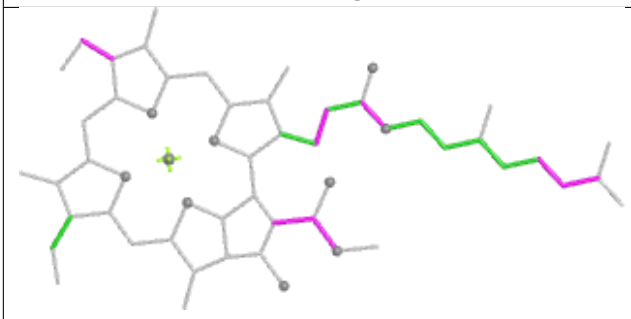

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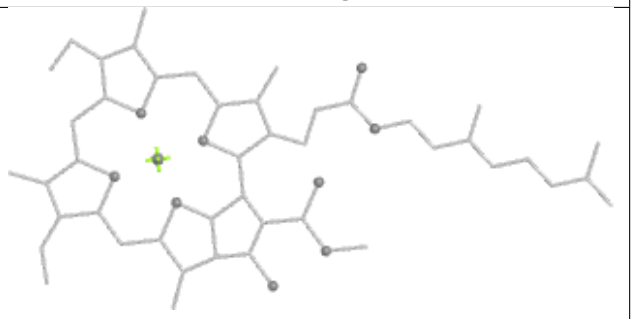
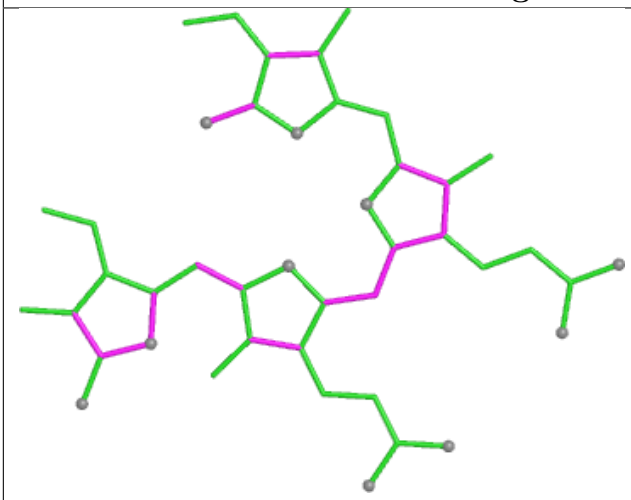


Rings

Ligand PEB aM 202



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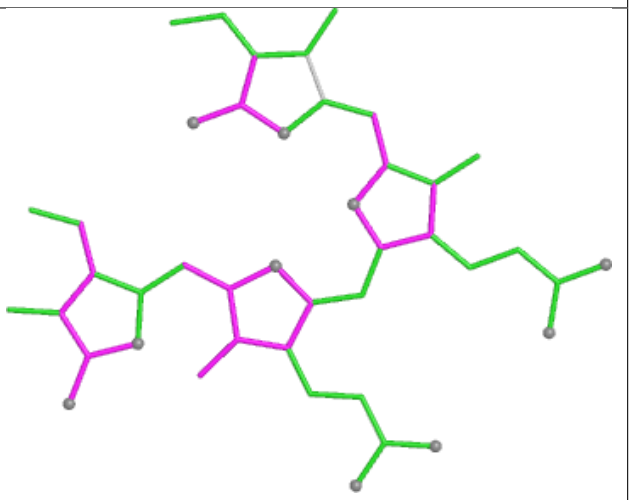
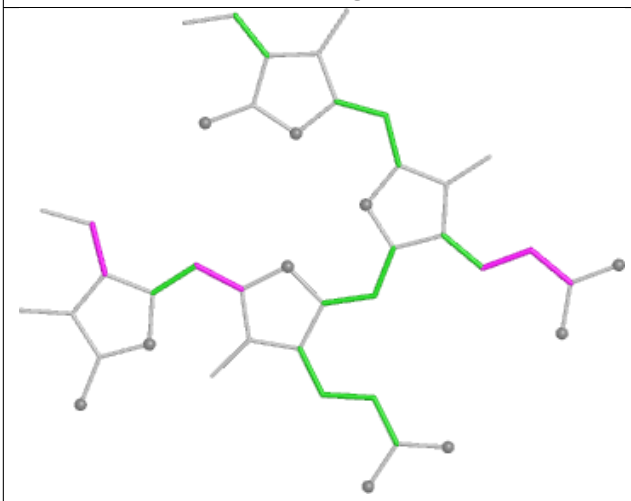


Bond angles



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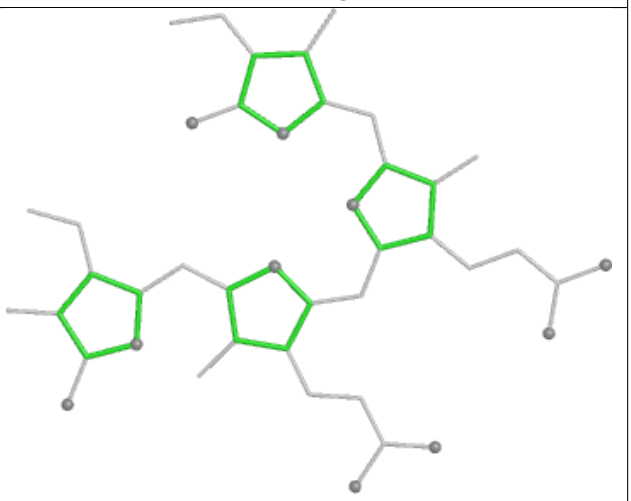
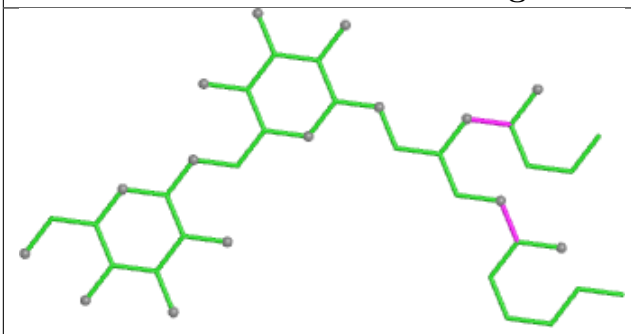


Rings

Ligand DGD AL 415



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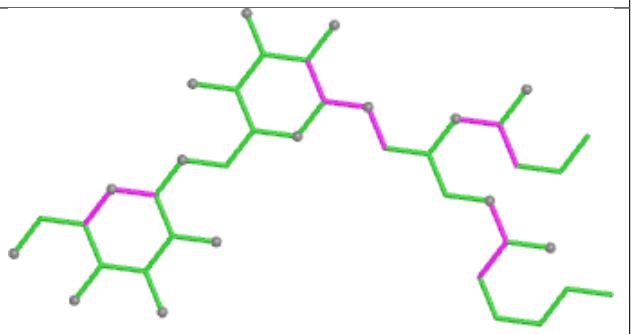

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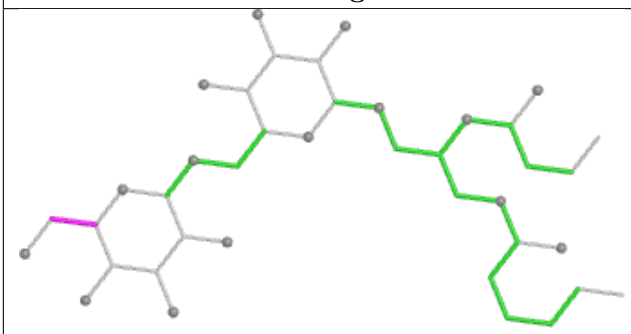
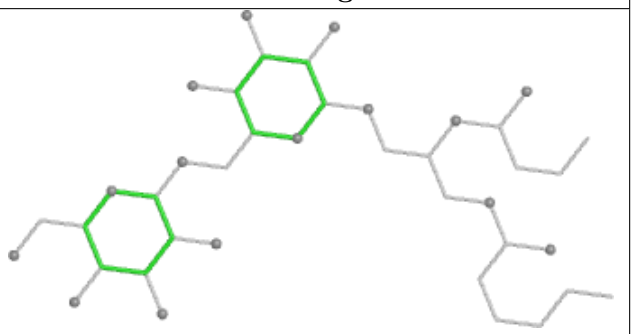
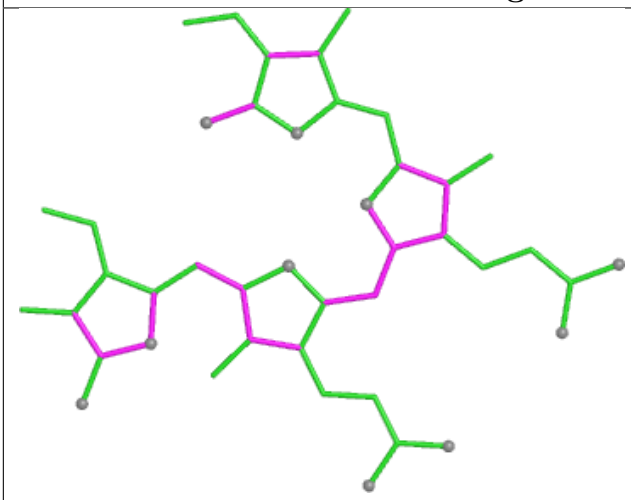


Torsions



Rings

Ligand PEB DM 202



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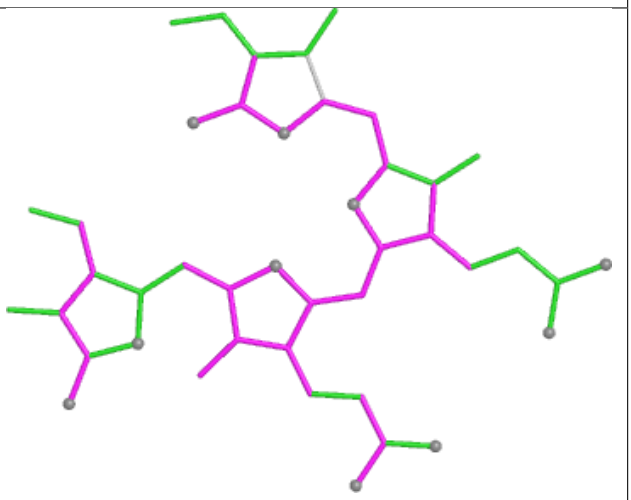

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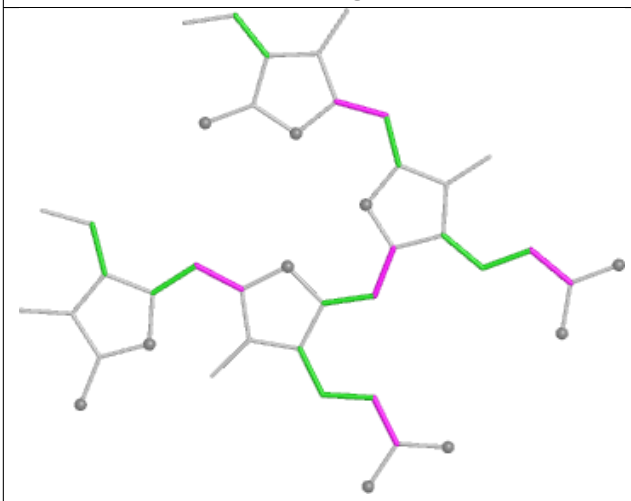

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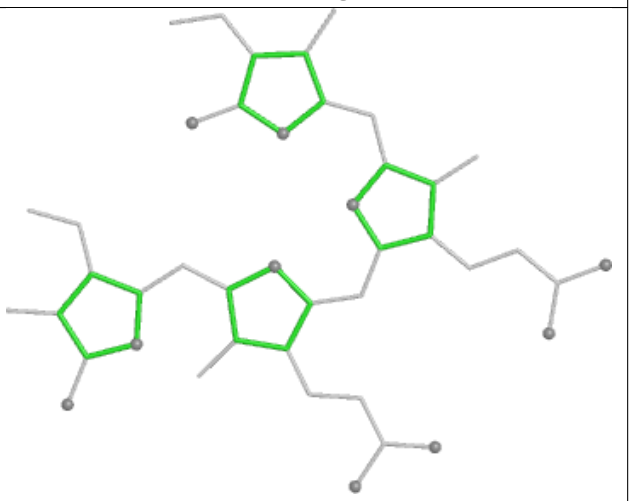
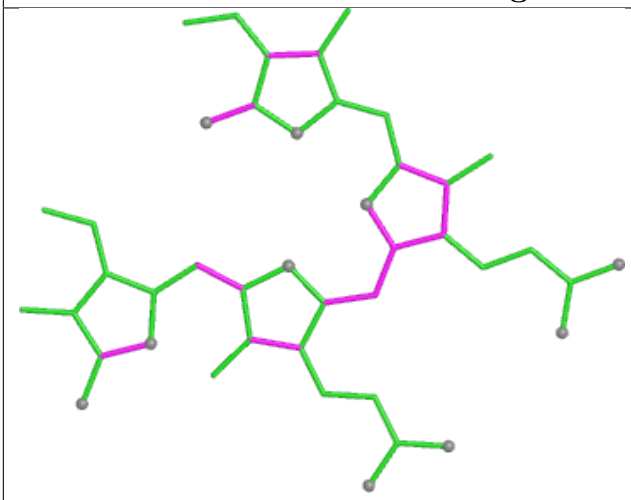


Rings

Ligand PEB GQ 202



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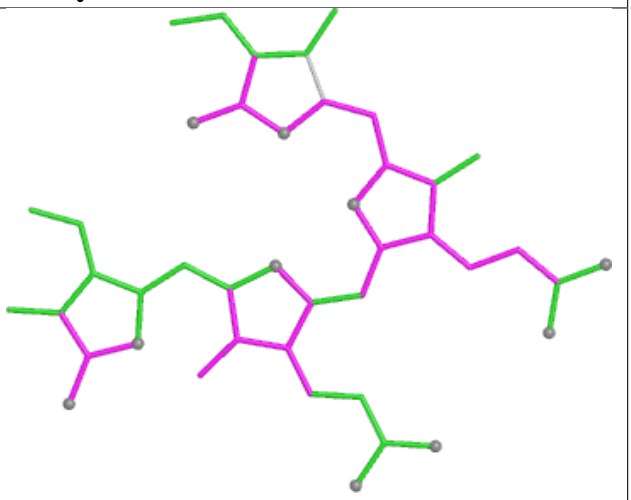

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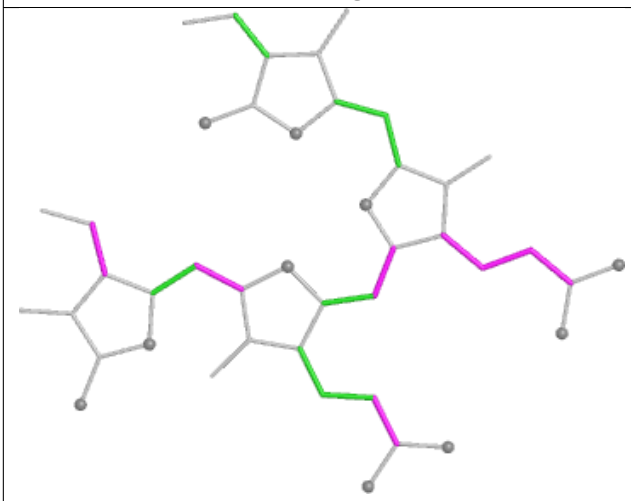

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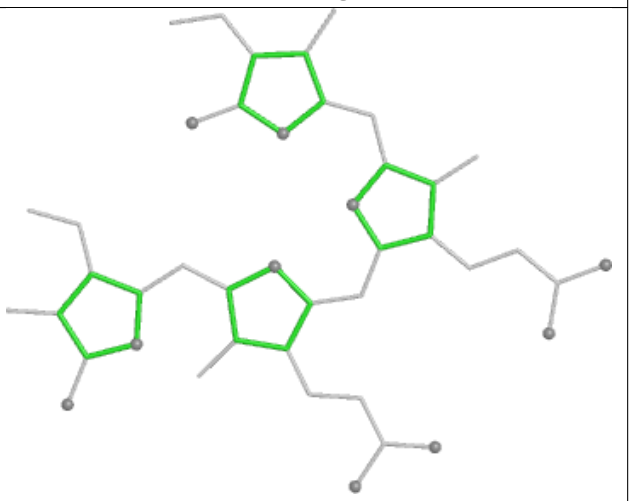
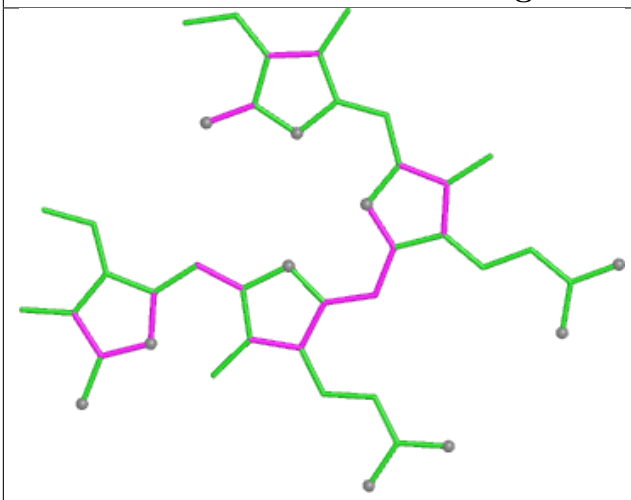


Rings

Ligand PEB SB 202



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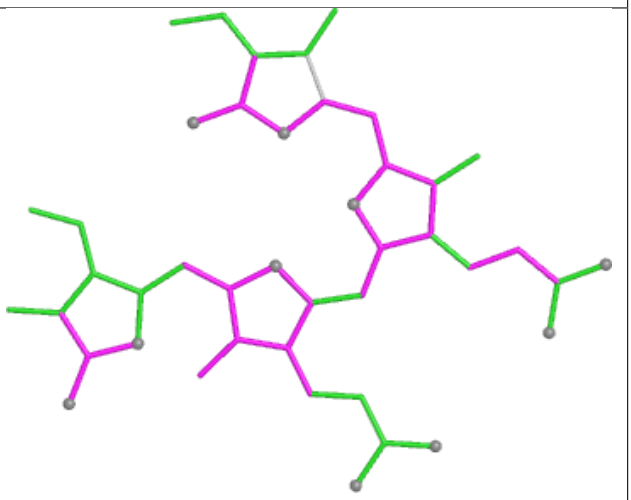

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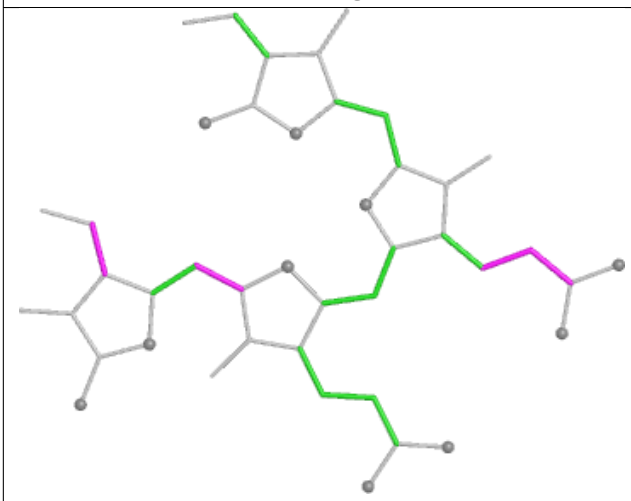

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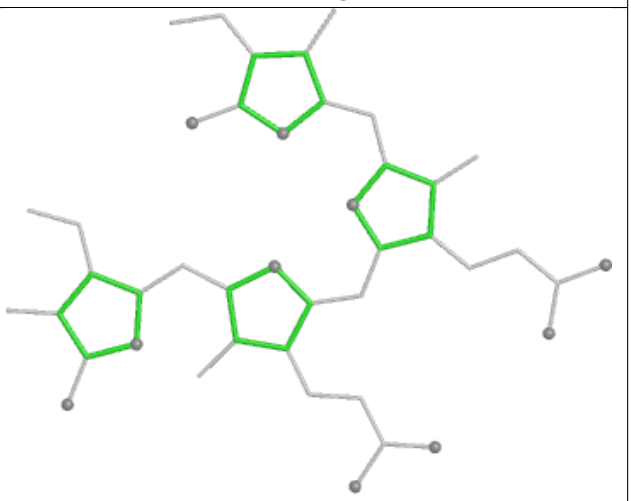
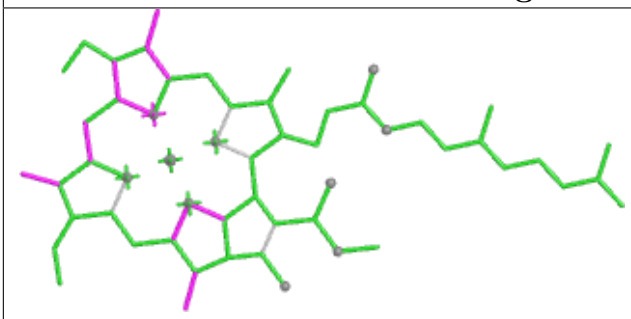


Rings

Ligand CLA C6 519



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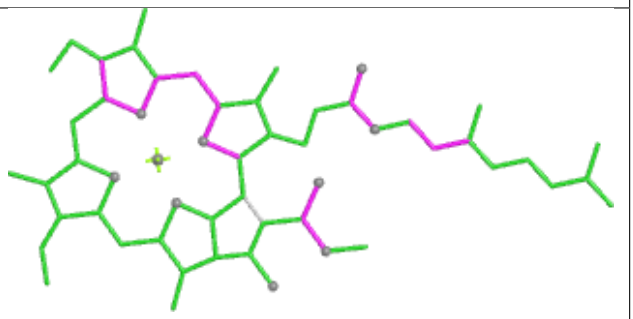

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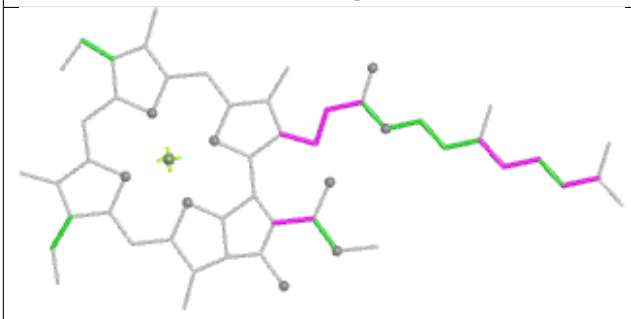

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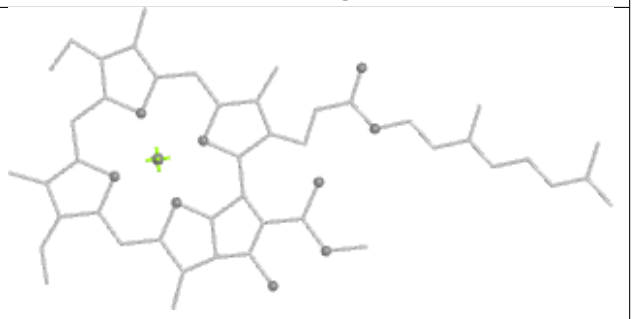
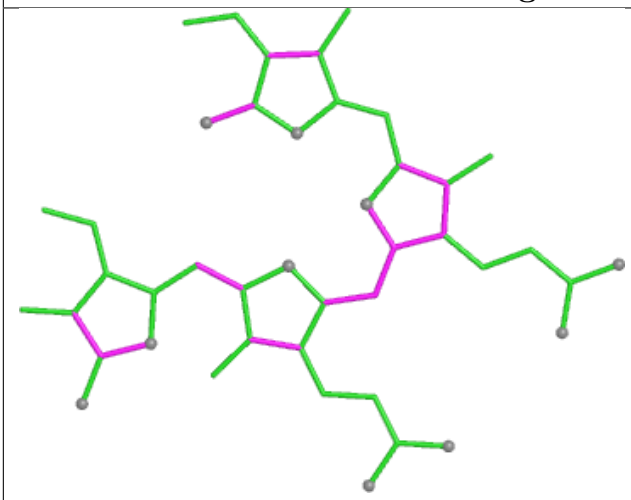


Rings

Ligand PEB p8 201



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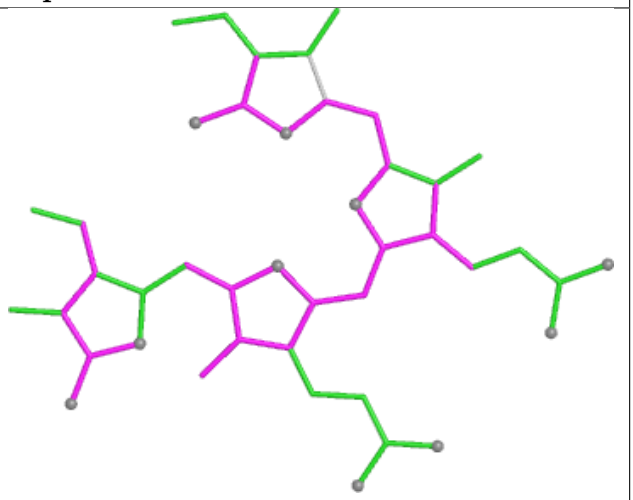

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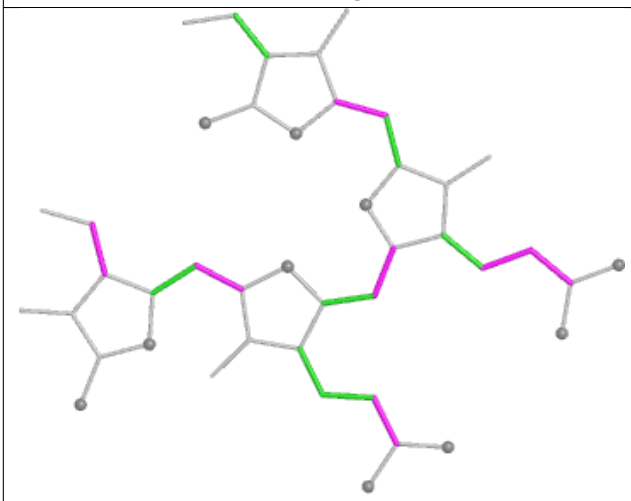

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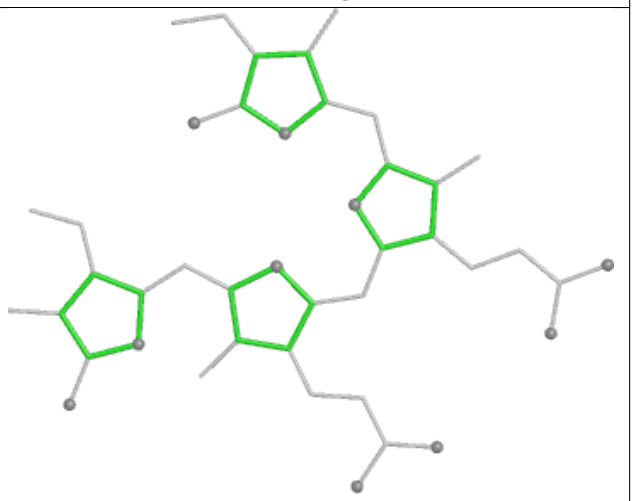
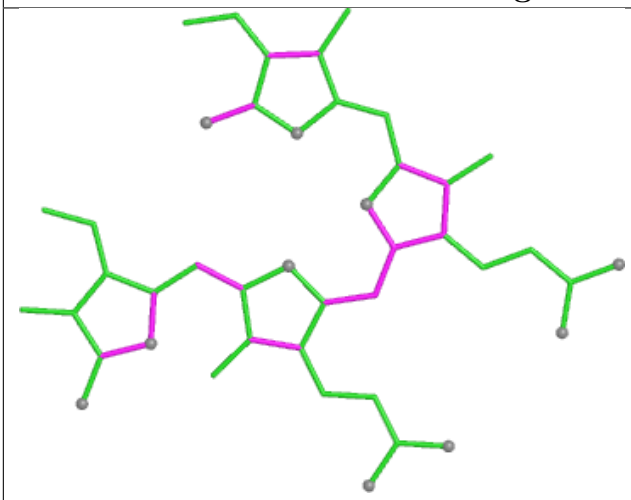


Rings

Ligand PEB IM 203



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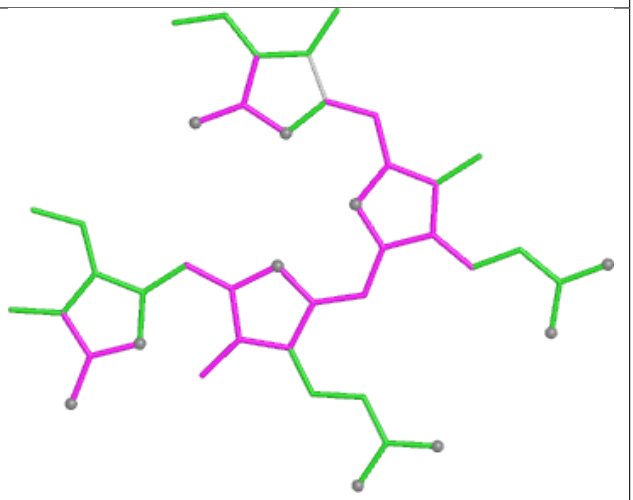

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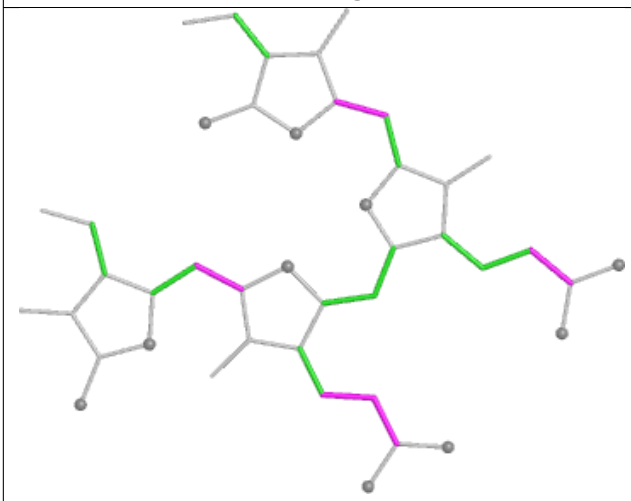

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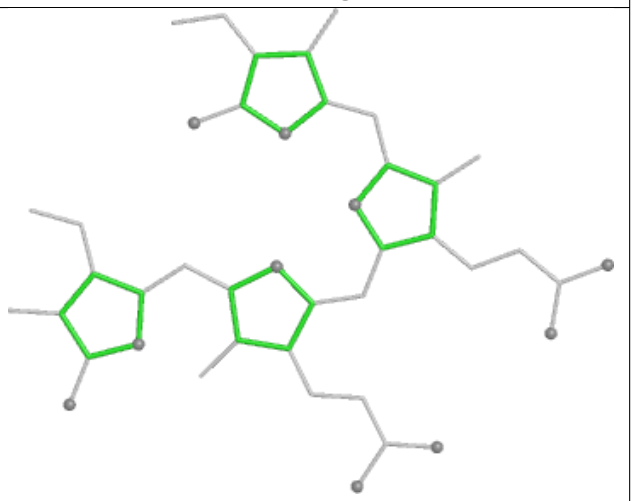
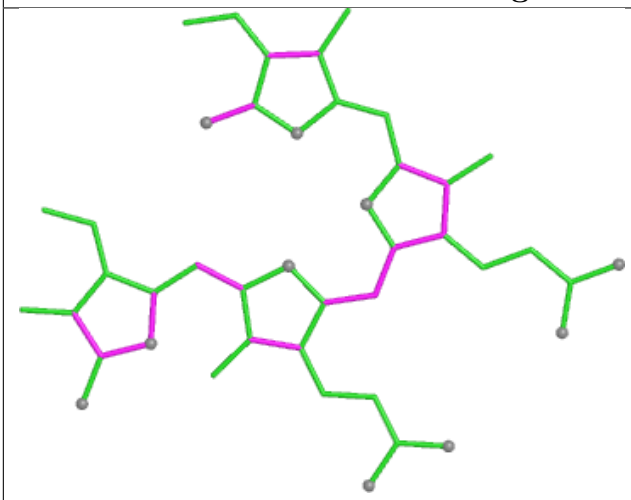


Rings

Ligand PEB JM 202



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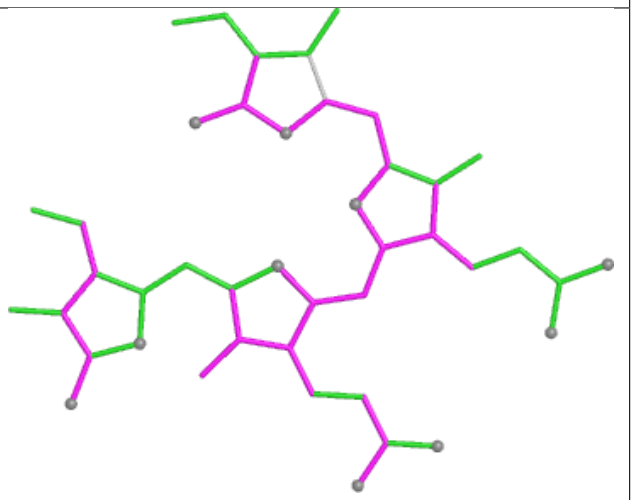

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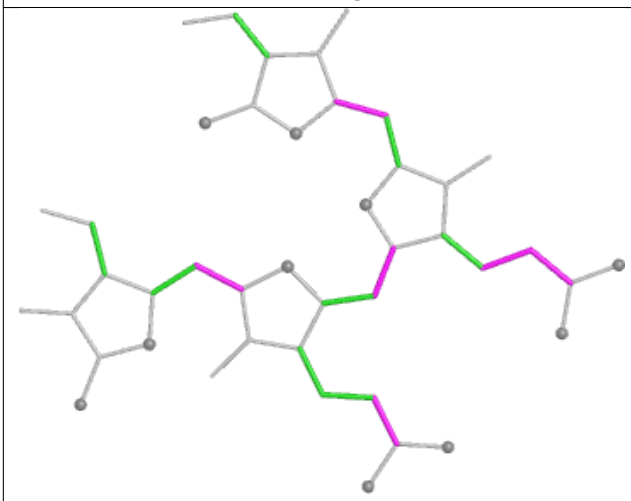

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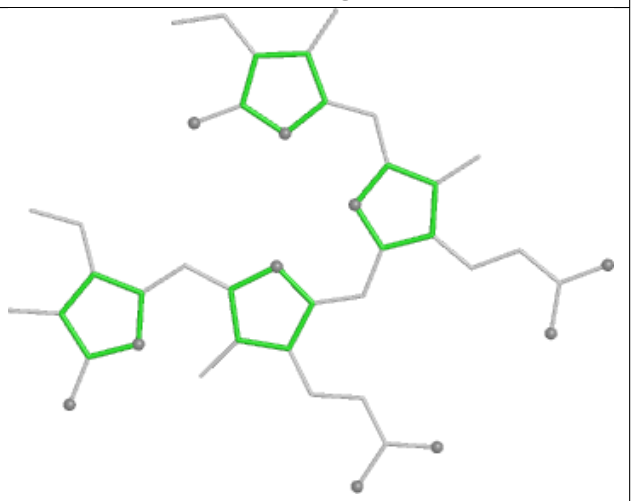
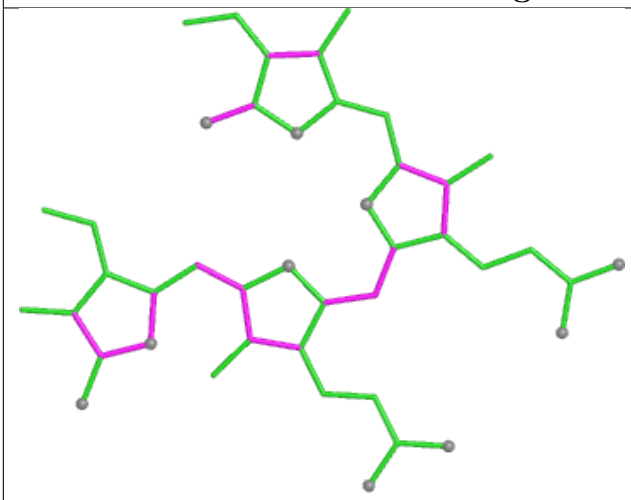


Rings

Ligand PEB LQ 202



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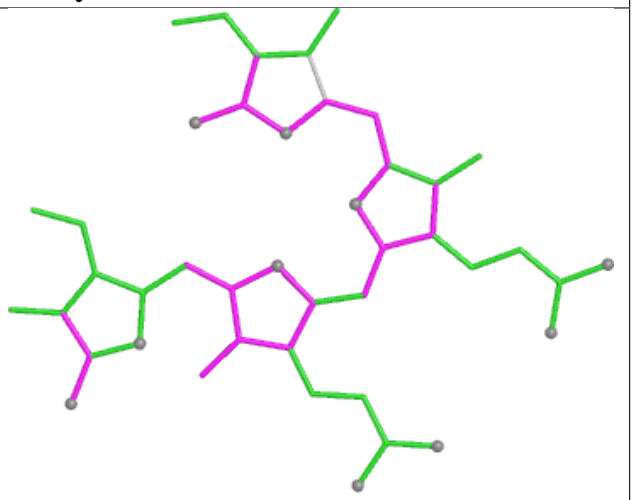

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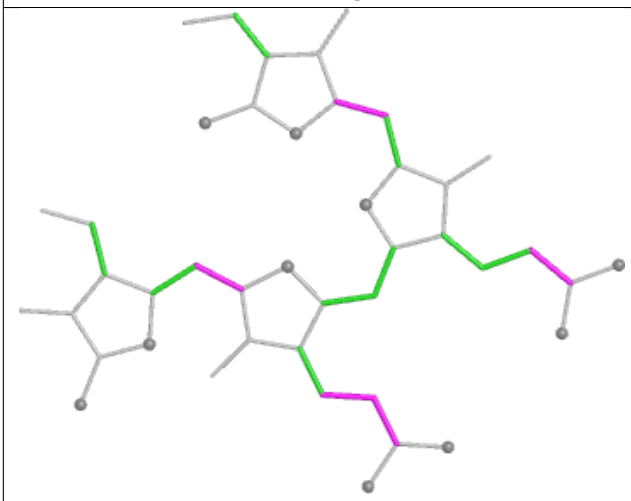

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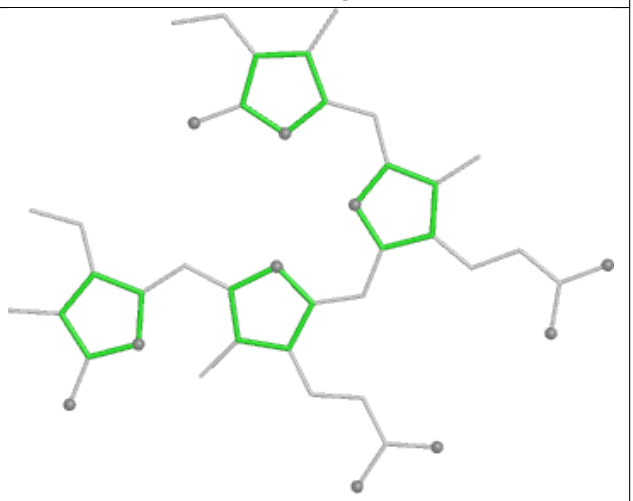
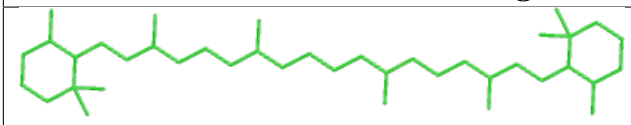


Rings

Ligand BCR bL 603



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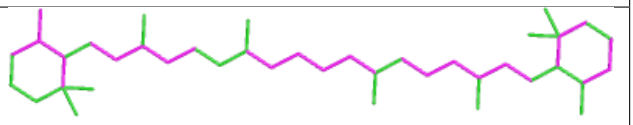

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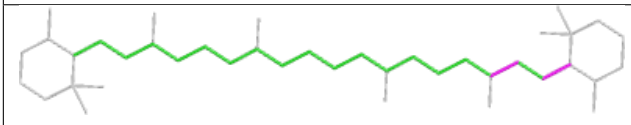

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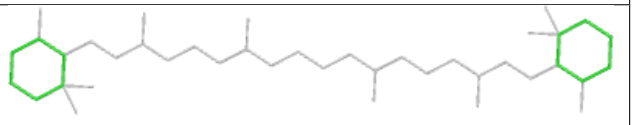
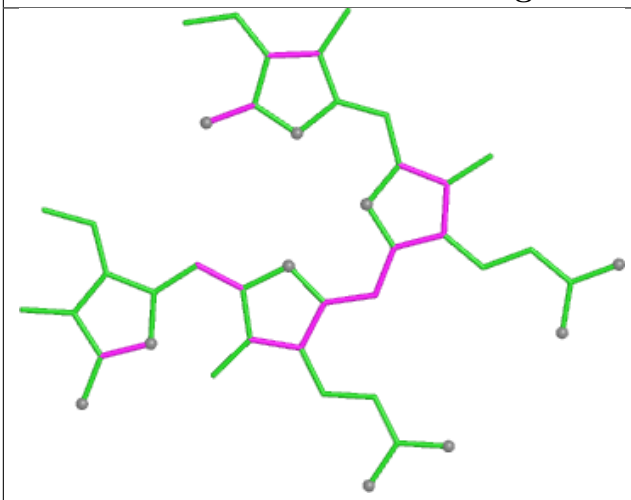


Rings

Ligand PEB U9 202



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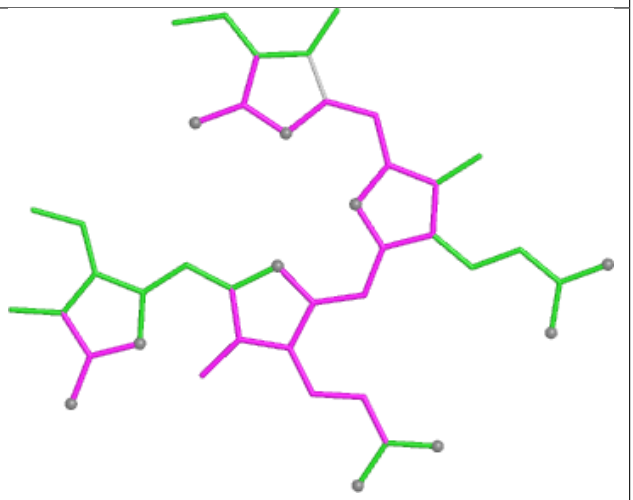

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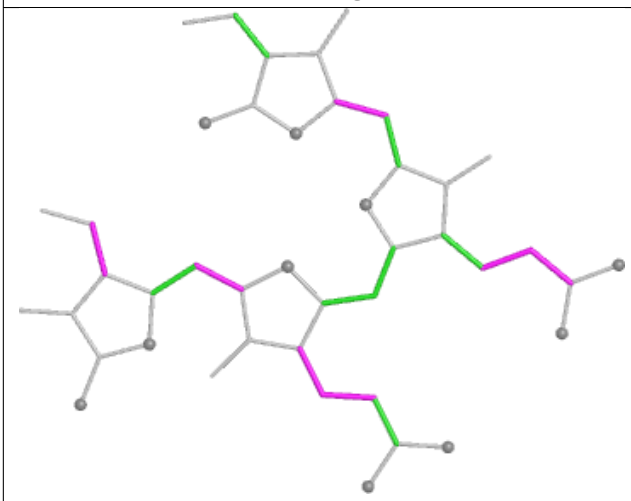

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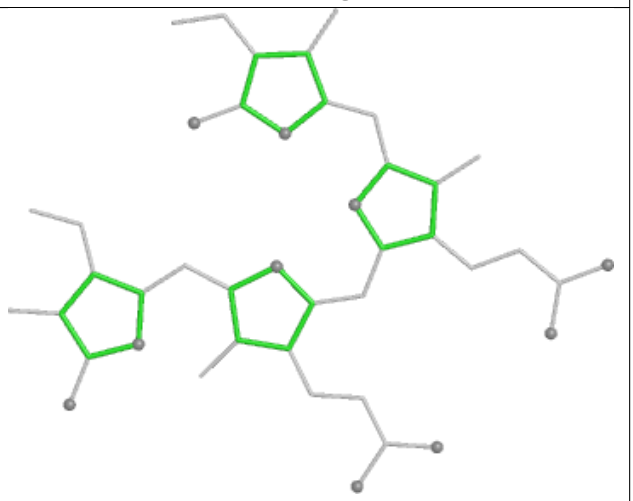
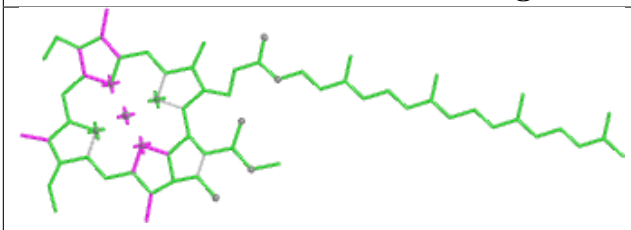


Rings

Ligand CLA A2 807



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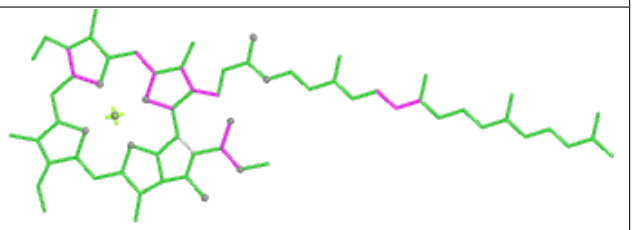

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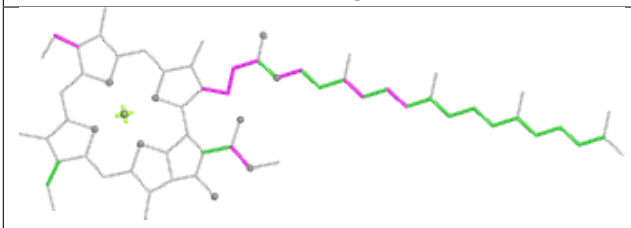

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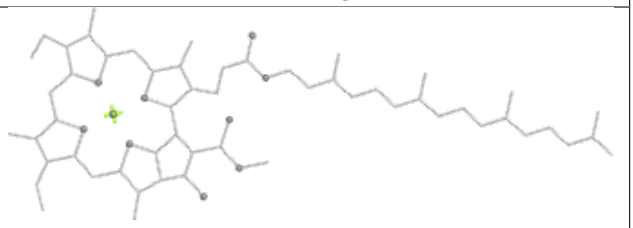
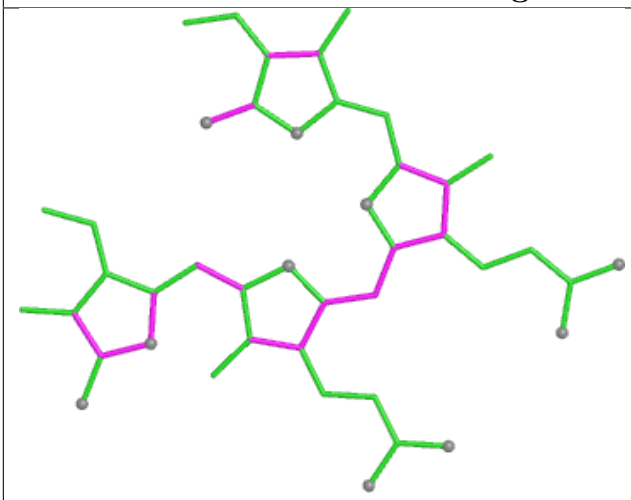


Rings

Ligand PEB RO 202



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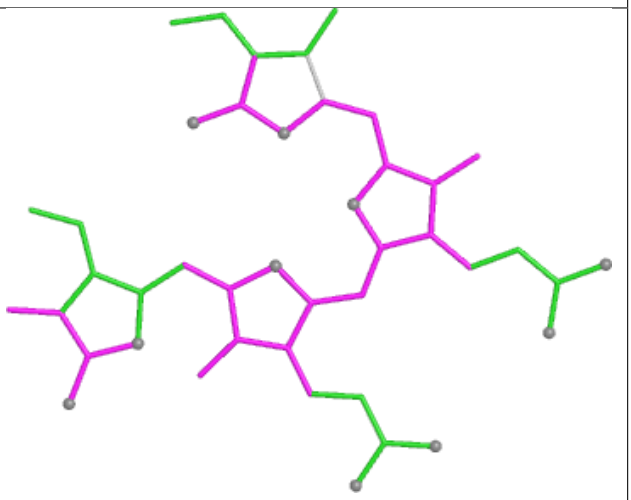
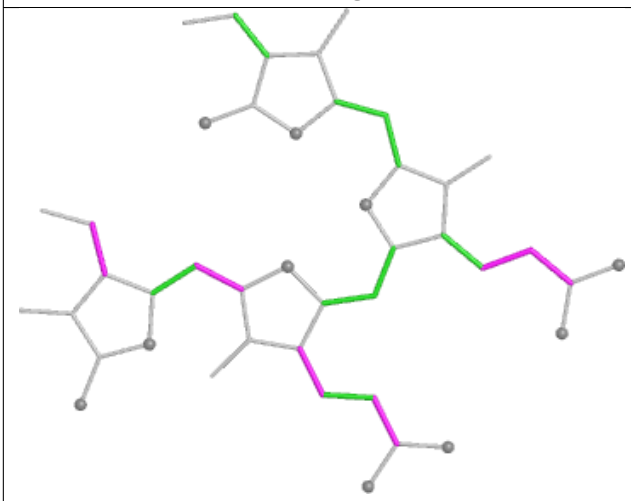


Bond angles



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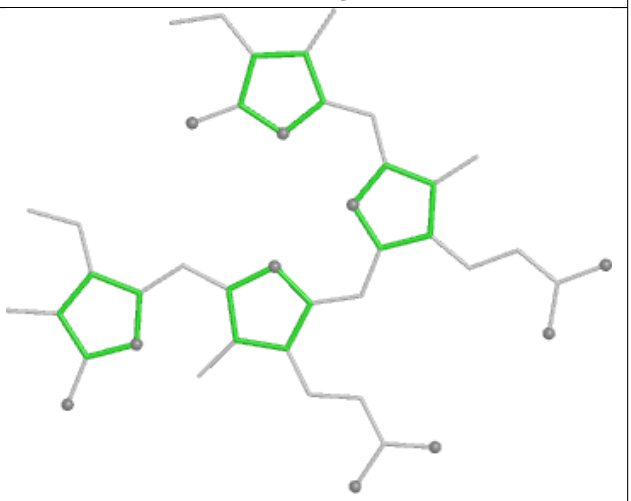
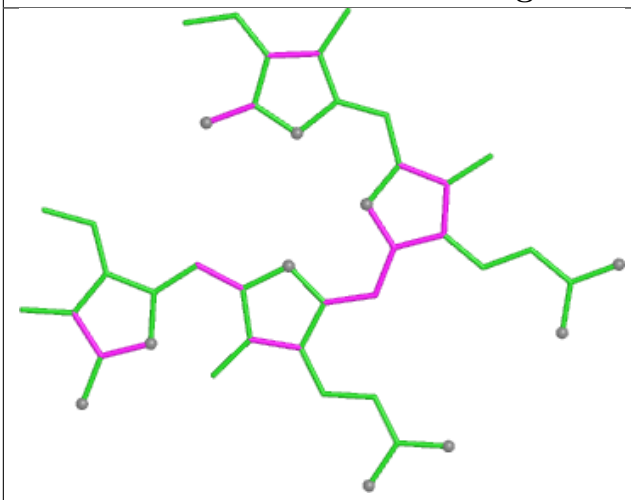


Rings

Ligand PEB B9 203



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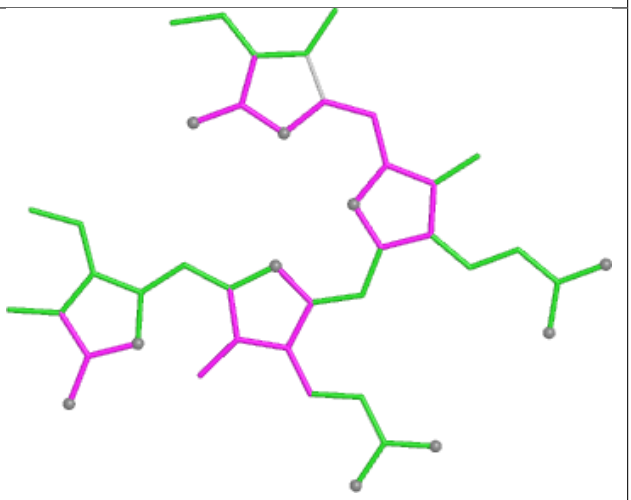
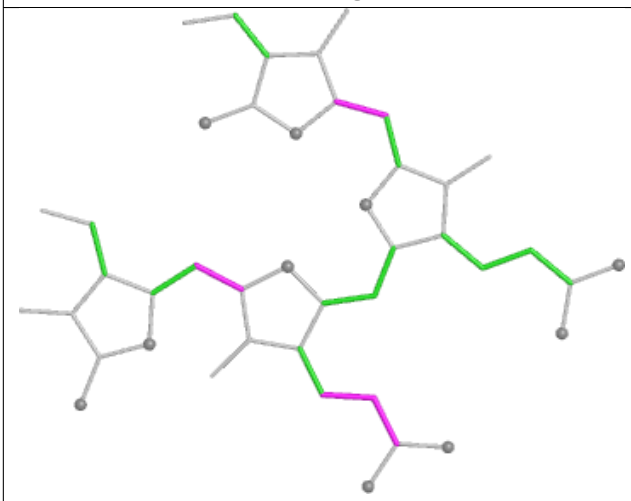


Bond angles



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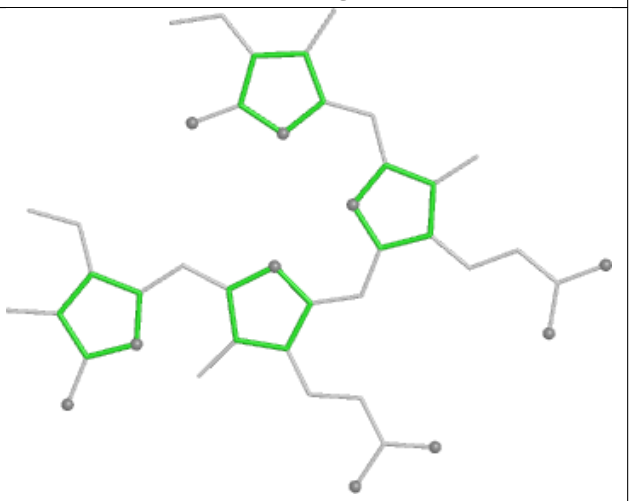
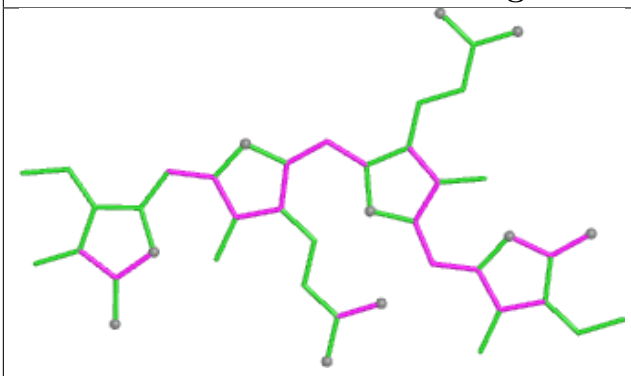


Rings

Ligand CYC u3 1001



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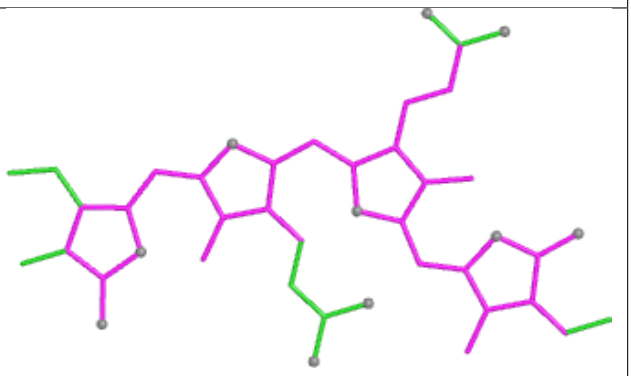
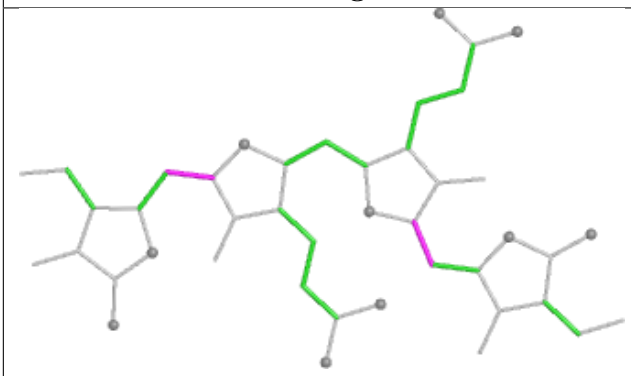
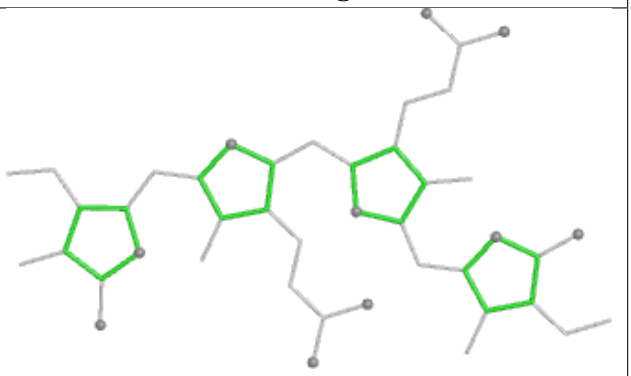


Bond angles

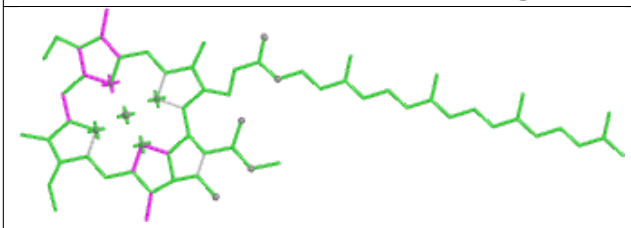


Torsions



Rings

Ligand CLA 6N 602



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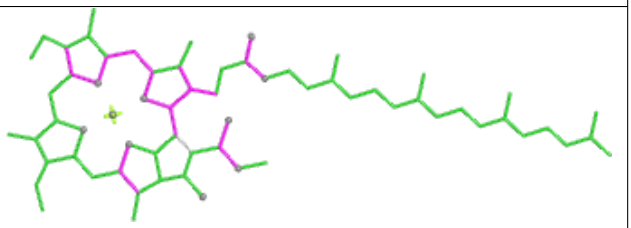
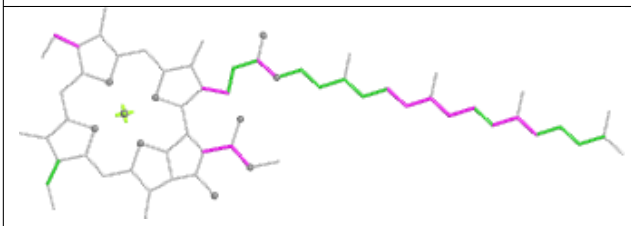


Bond angles



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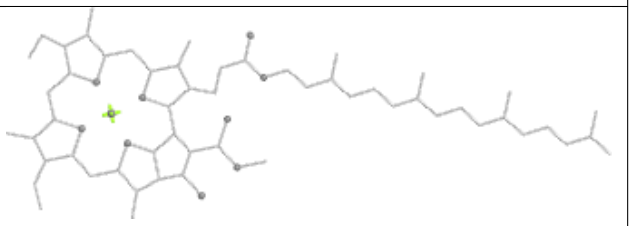
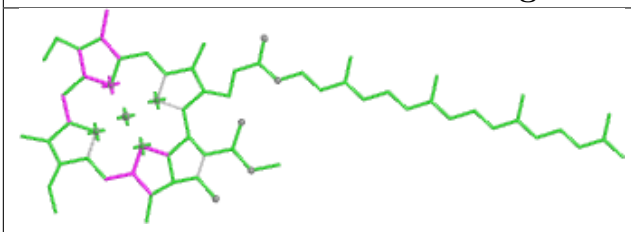


Rings

Ligand CLA 72 602



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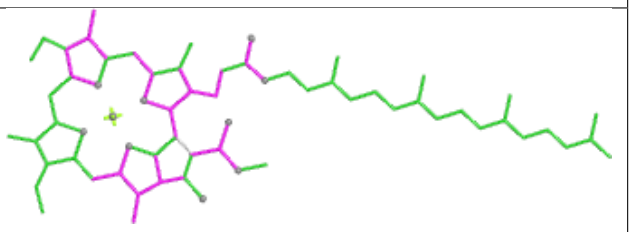

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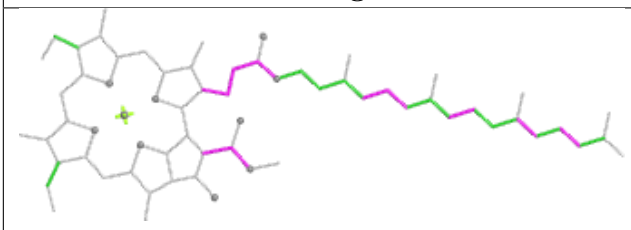

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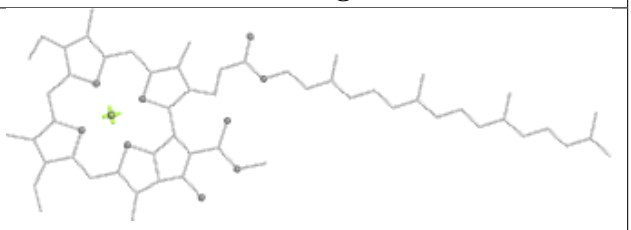
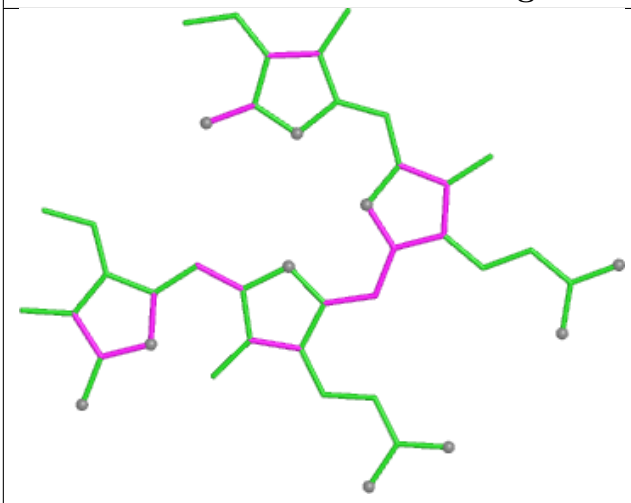


Rings

Ligand PEB FJ 202



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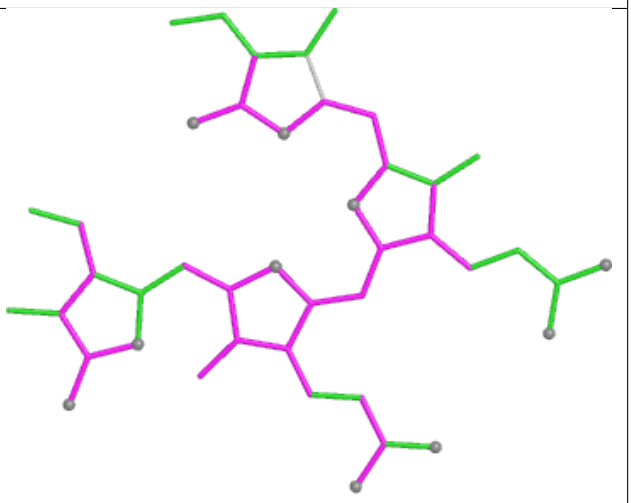
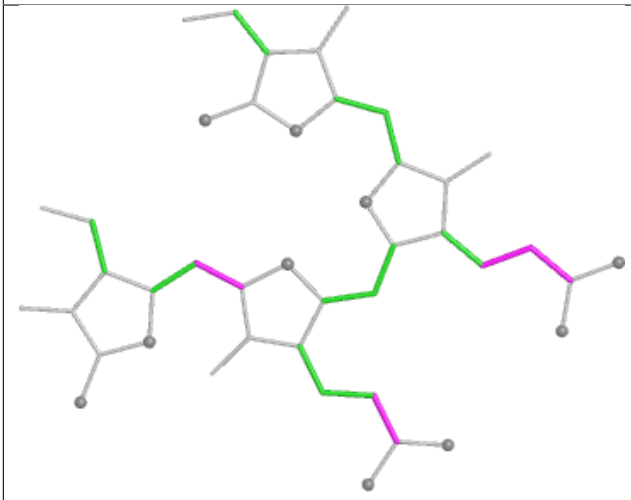


Bond angles



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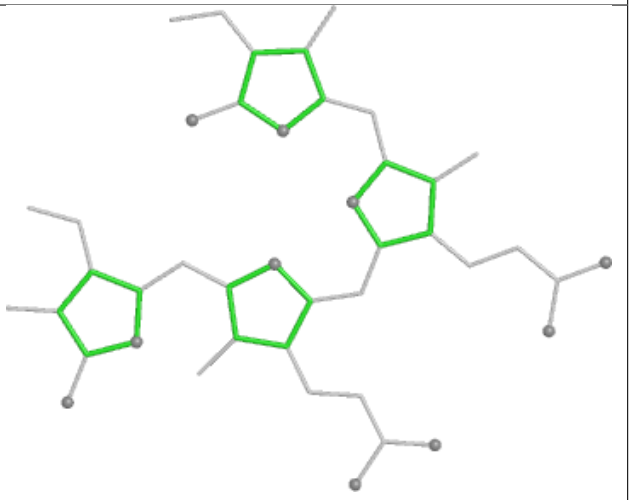
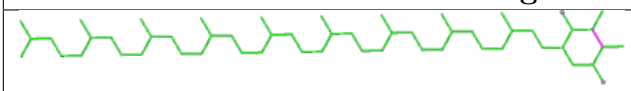


Rings

Ligand PL9 A6 410



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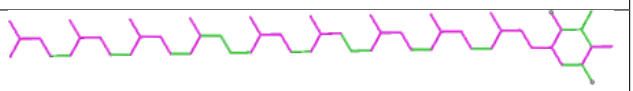

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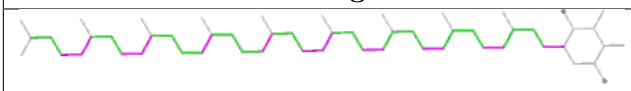

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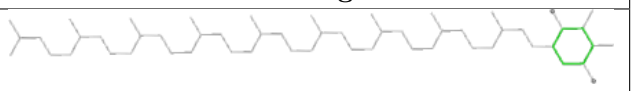
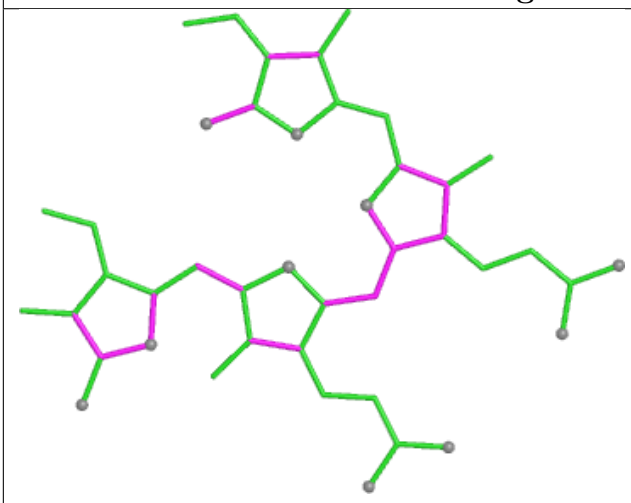


Rings

Ligand PEB eB 201



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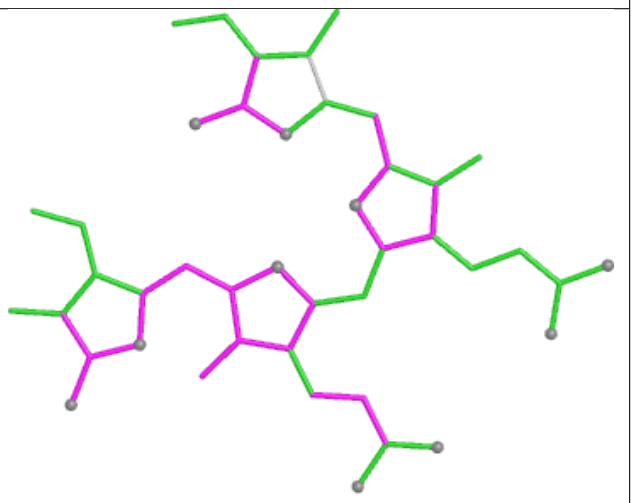

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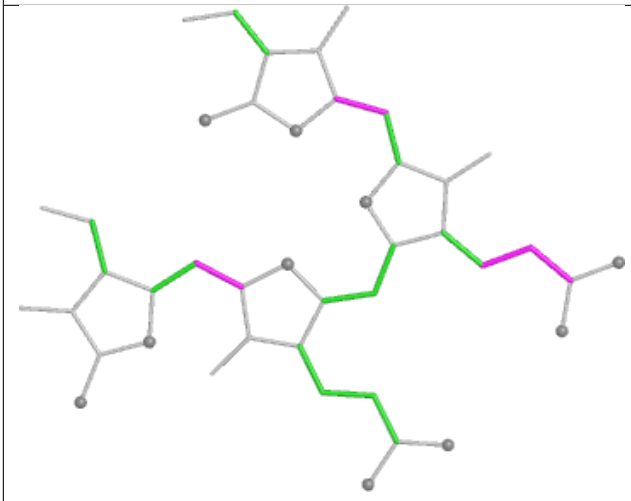

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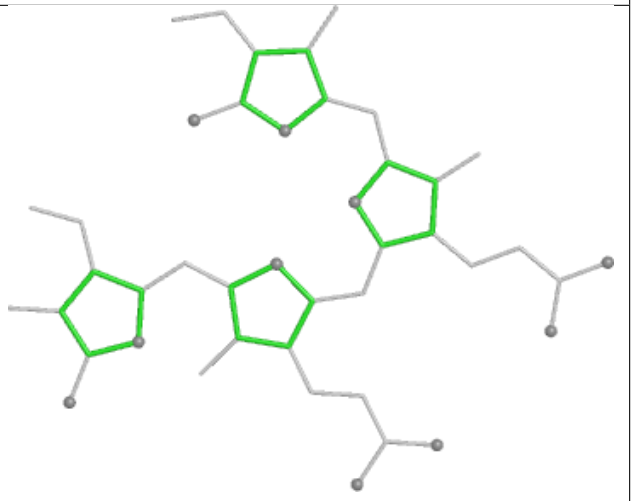
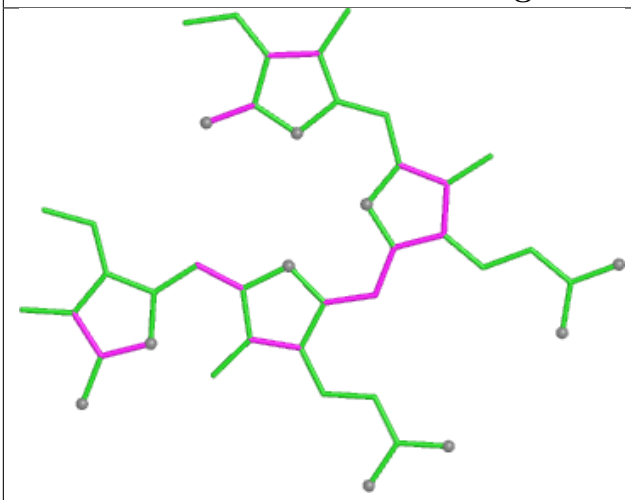


Rings

Ligand PEB PF 201



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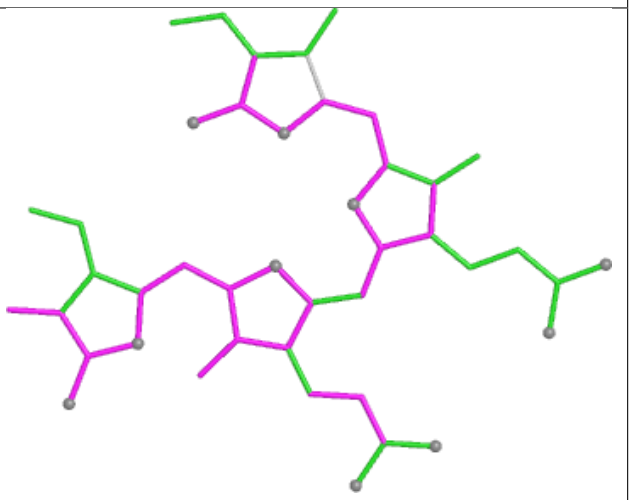

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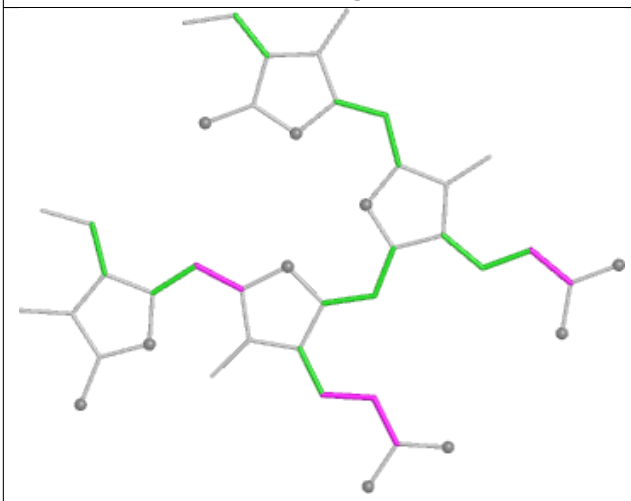

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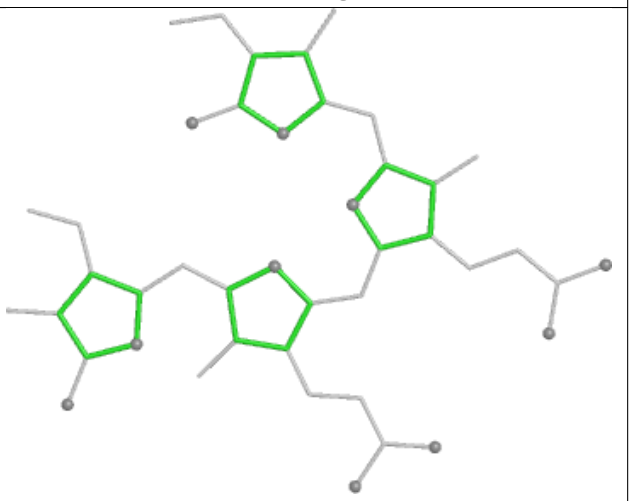
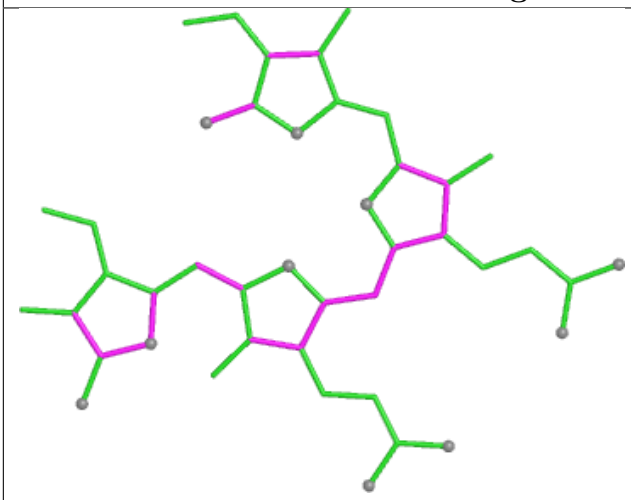


Rings

Ligand PEB OG 203



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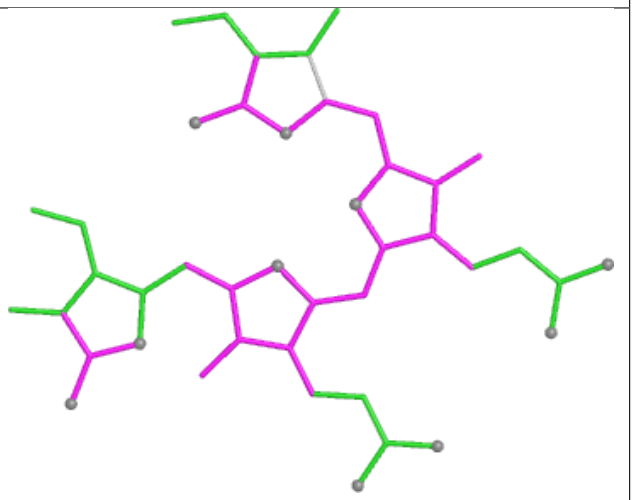

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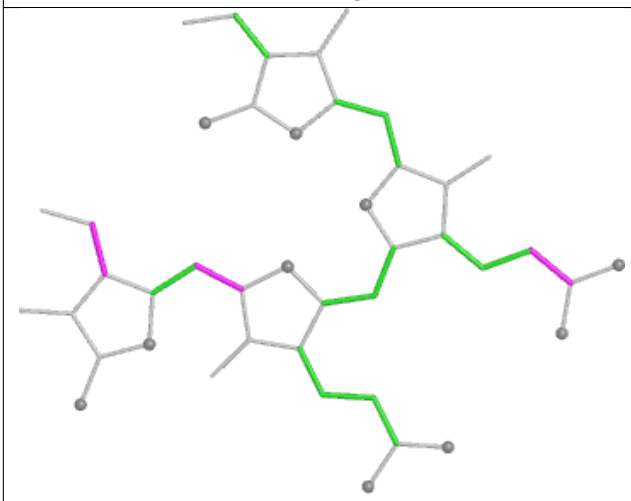

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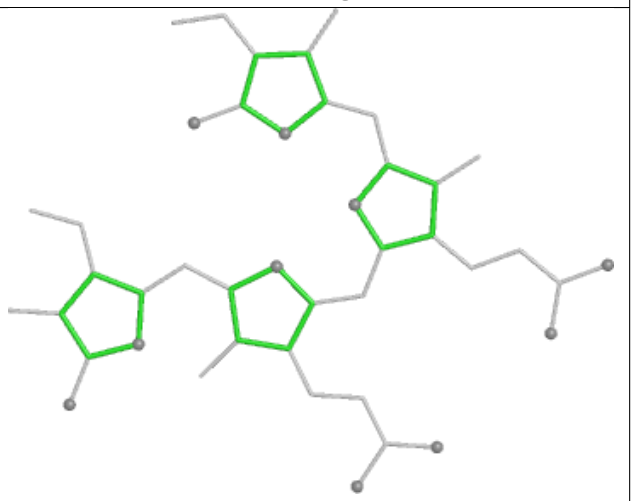
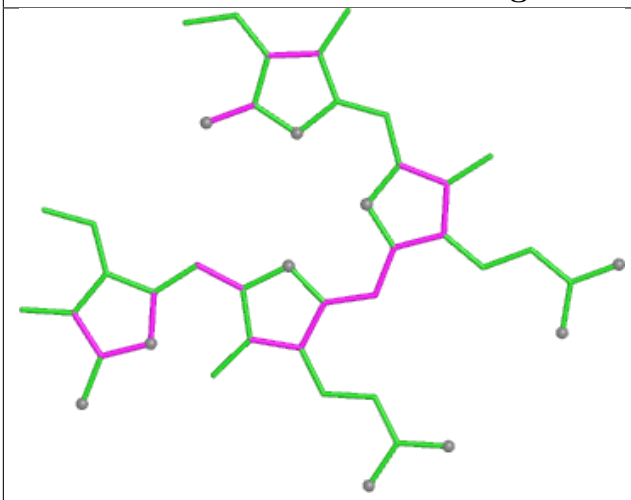


Rings

Ligand PEB QG 201



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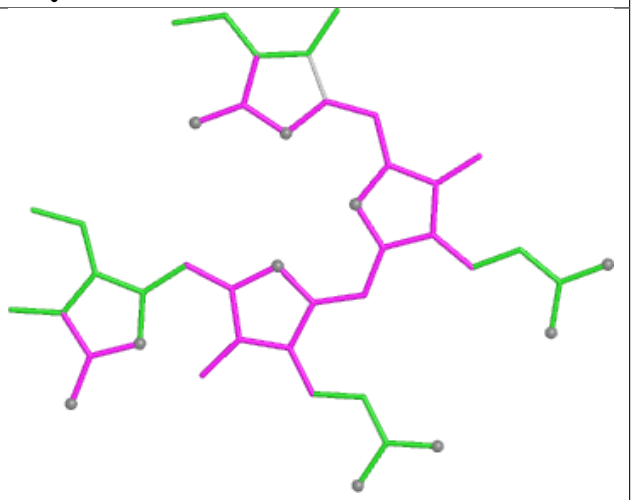

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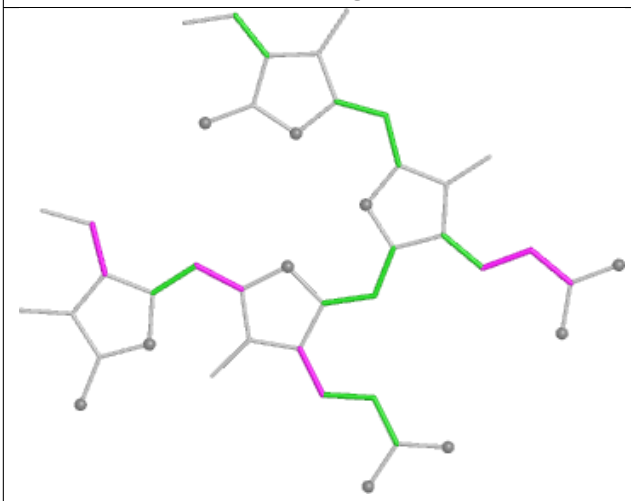

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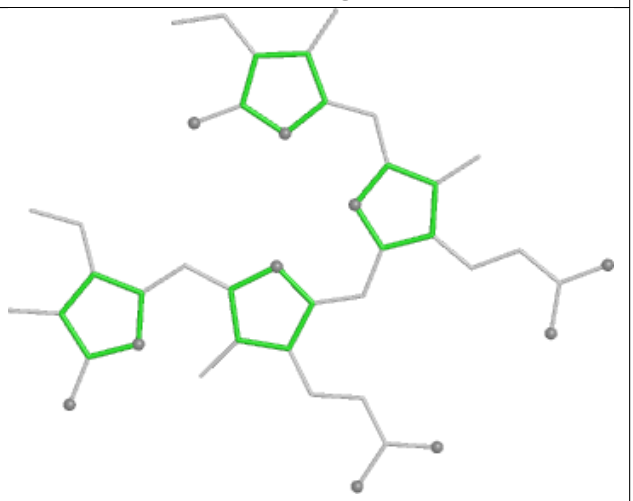
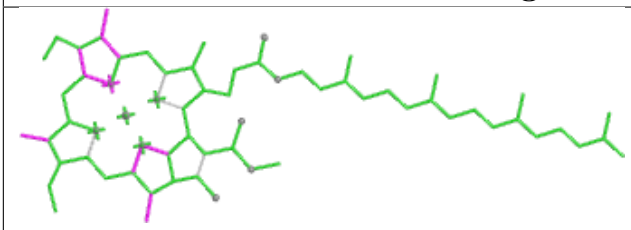


Rings

Ligand CLA c6 610



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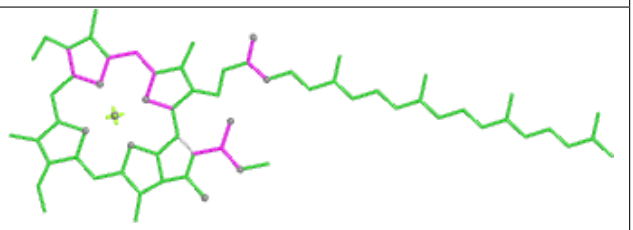
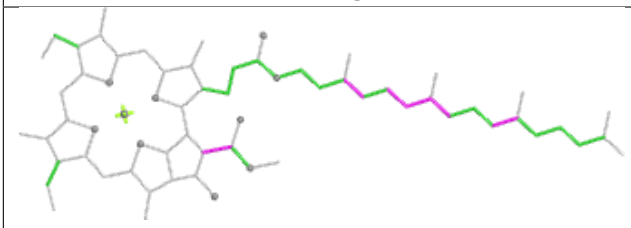


Bond angles



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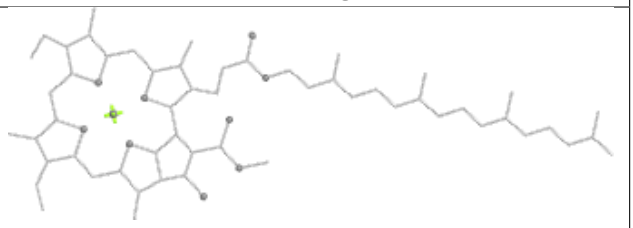
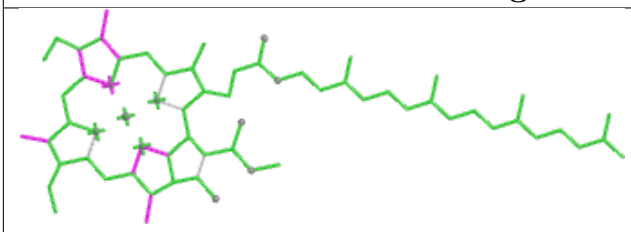


Rings

Ligand CLA AN 833



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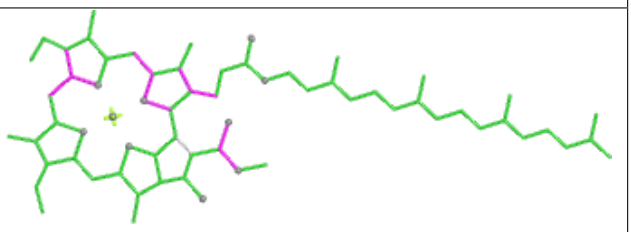
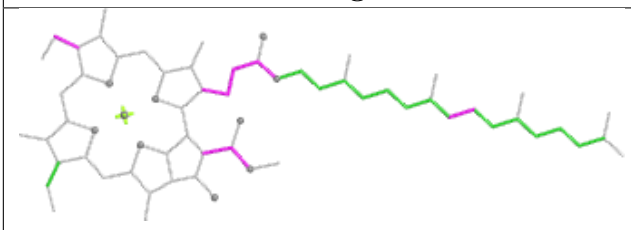


Bond angles



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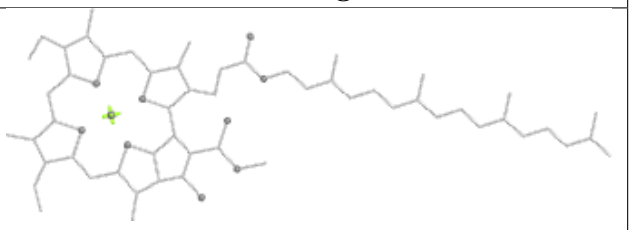
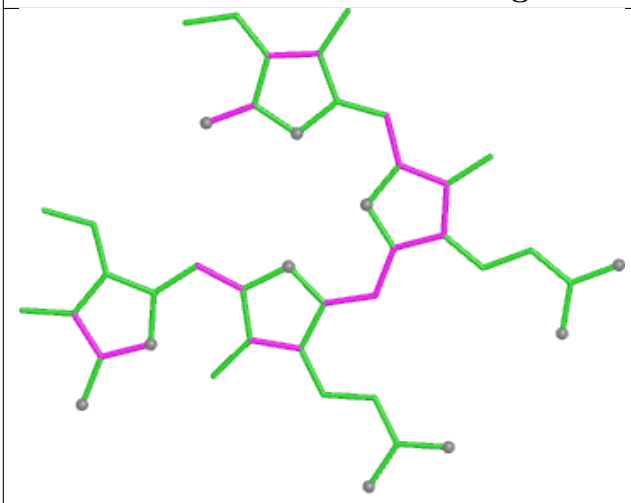


Rings

Ligand PEB TD 202



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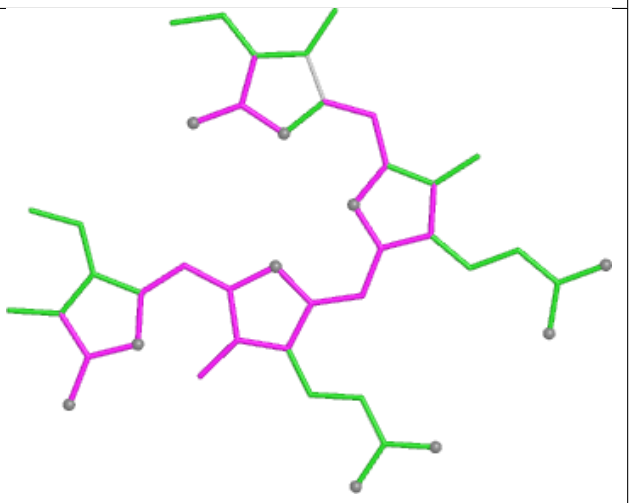

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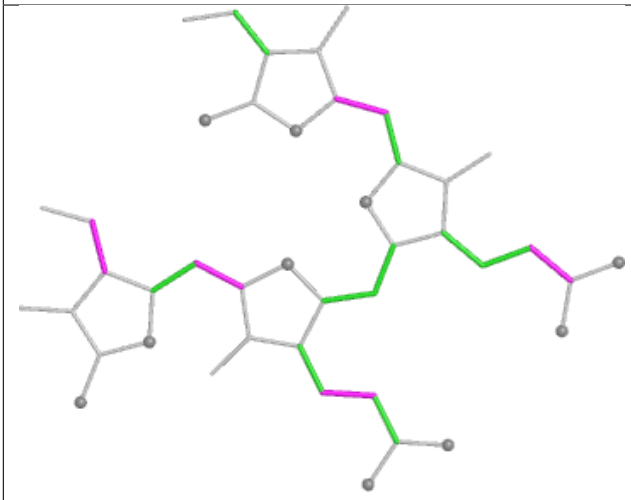

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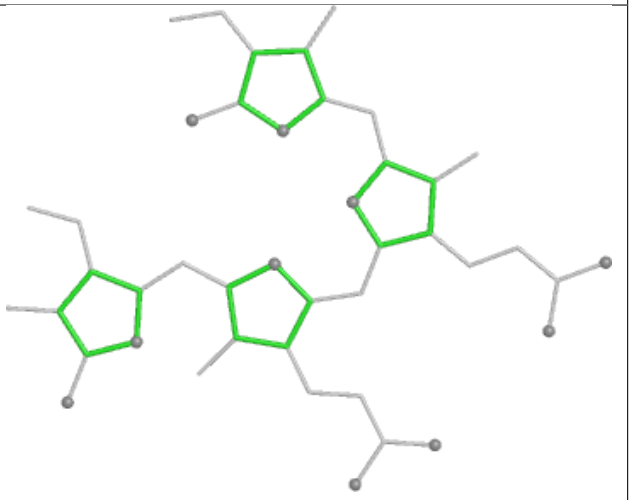
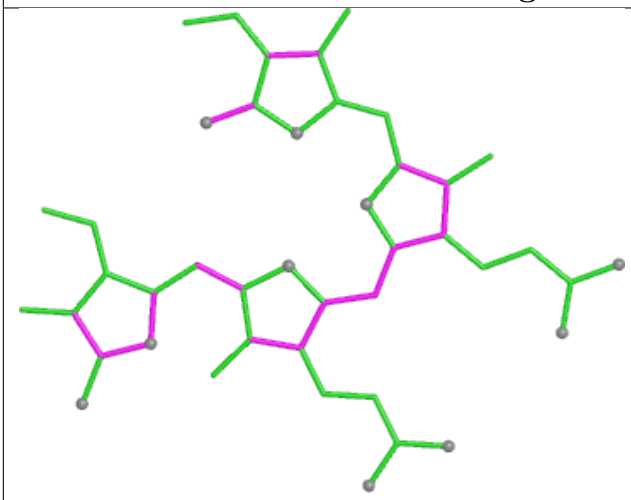


Rings

Ligand PEB S9 202



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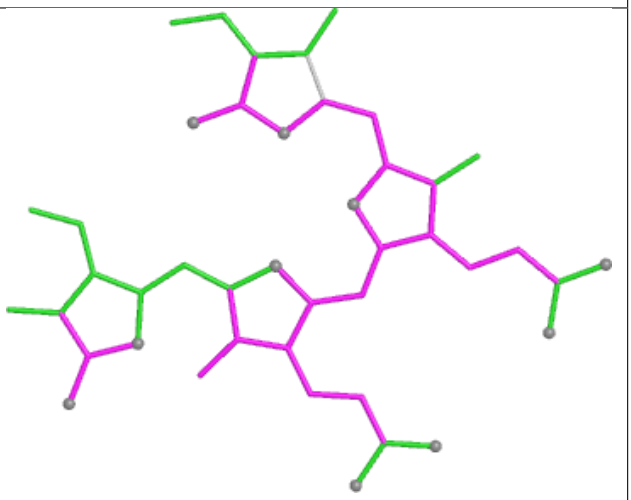

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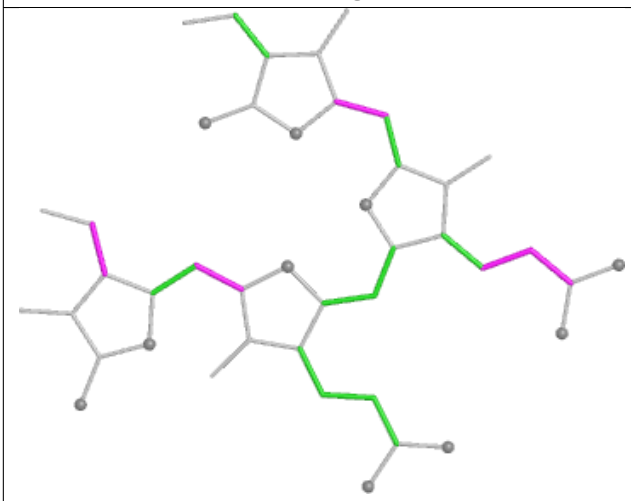

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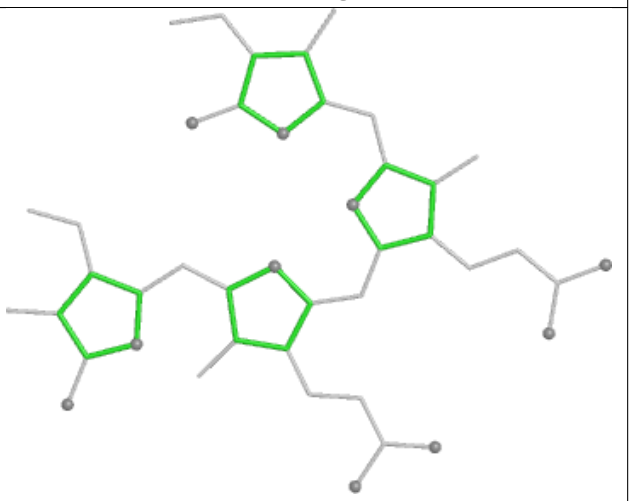
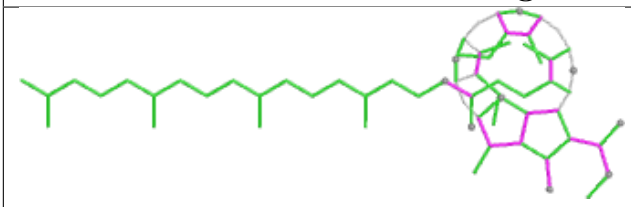


Rings

Ligand PHO a6 613



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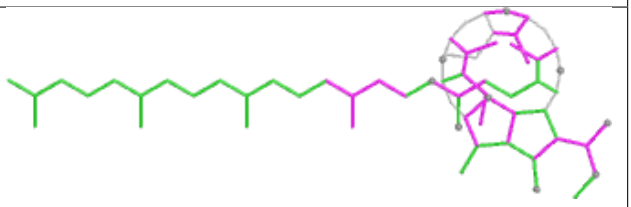
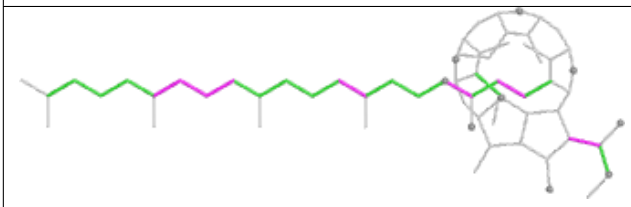


Bond angles



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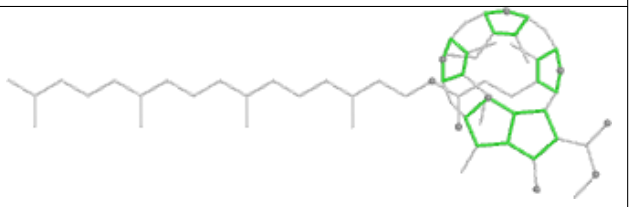
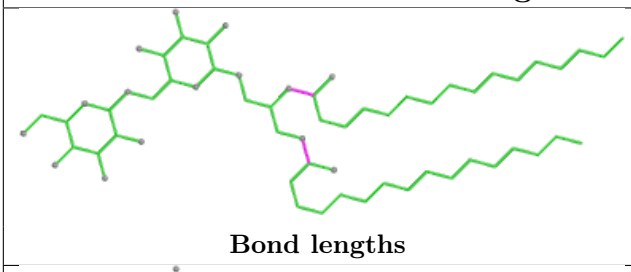


Rings

Ligand DGD cL 502



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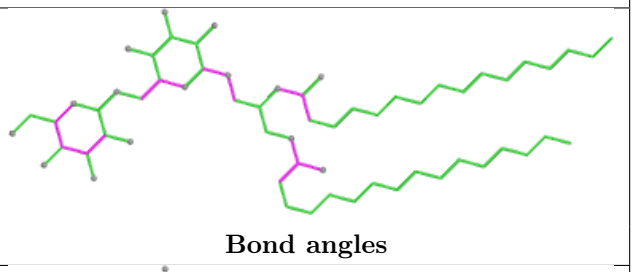
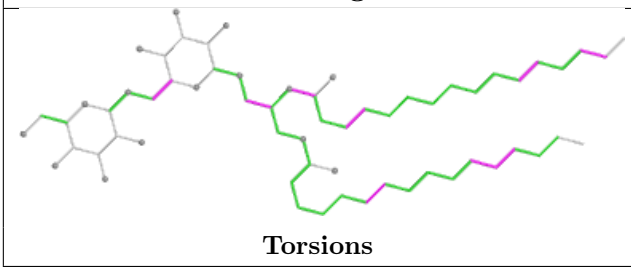


Bond angles



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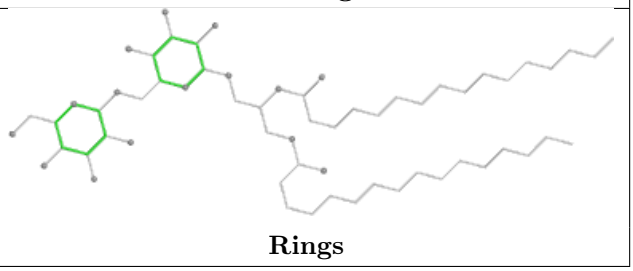
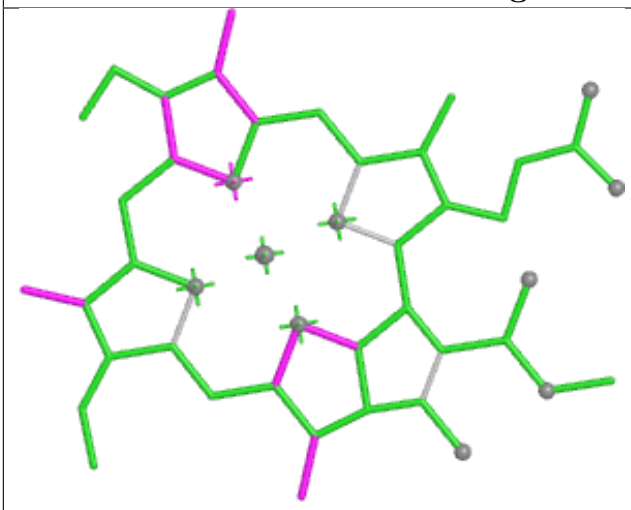
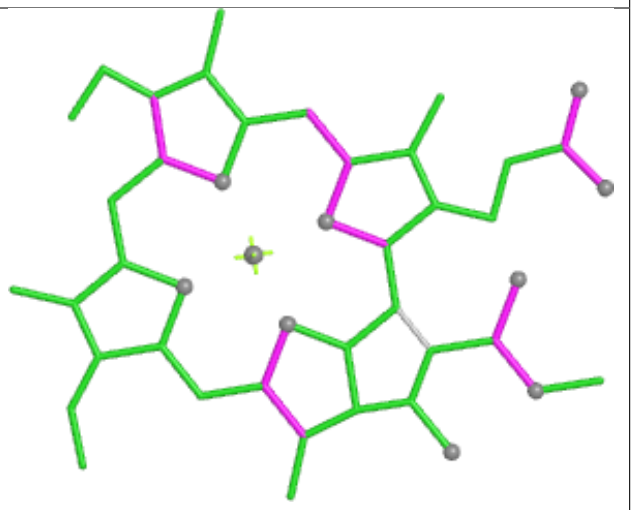


Rings

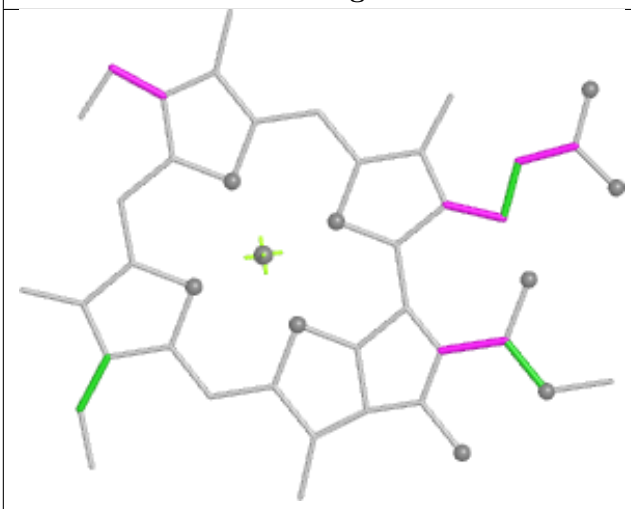
Ligand CLA AN 816



Bond lengths



Bond angles

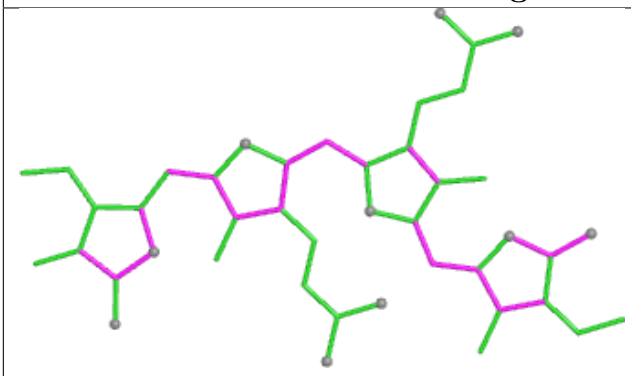


Torsions



Rings

Ligand CYC t3 1001



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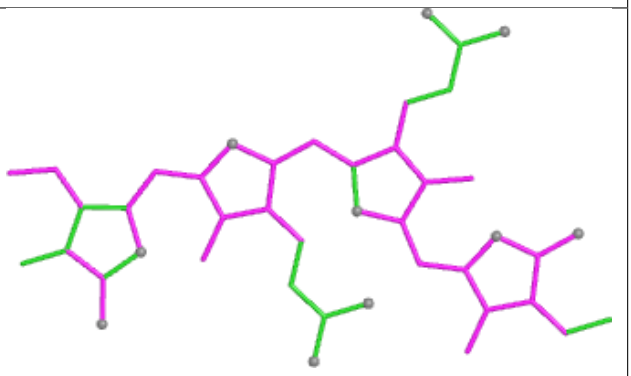

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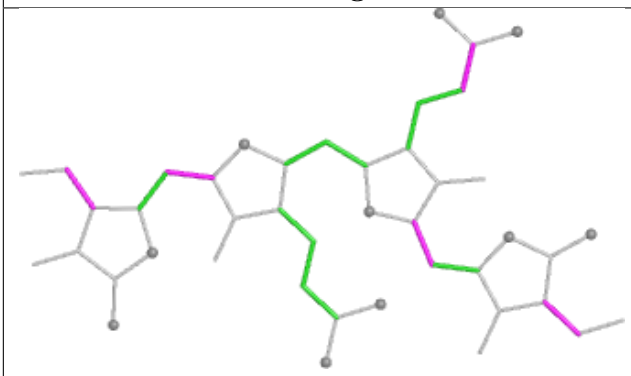

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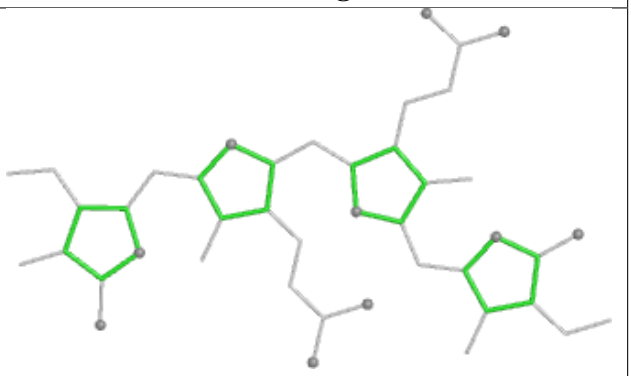

Rings

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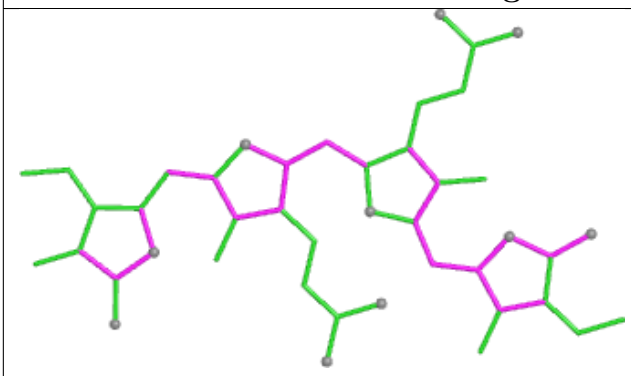

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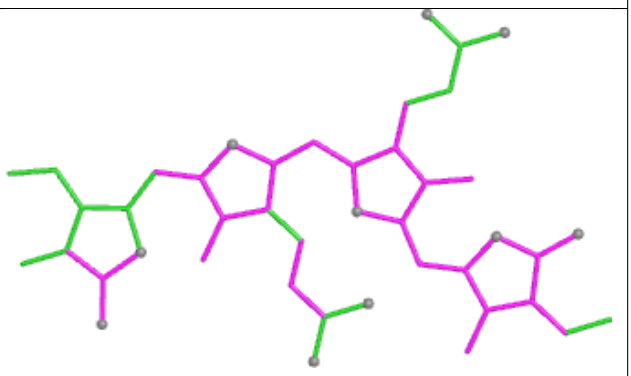

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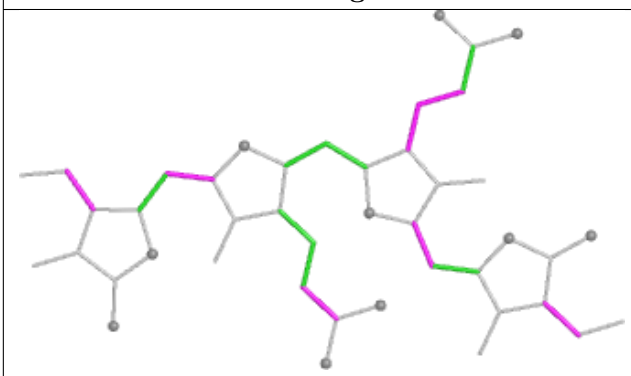

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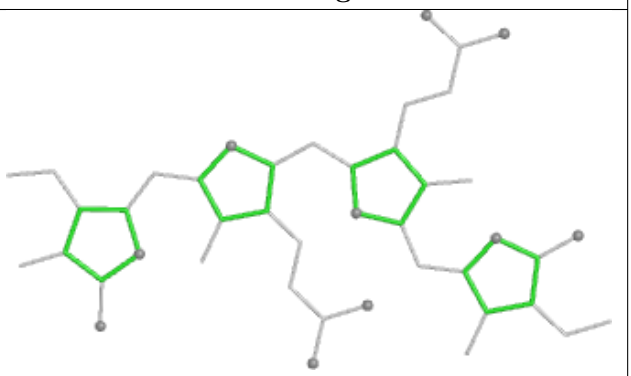
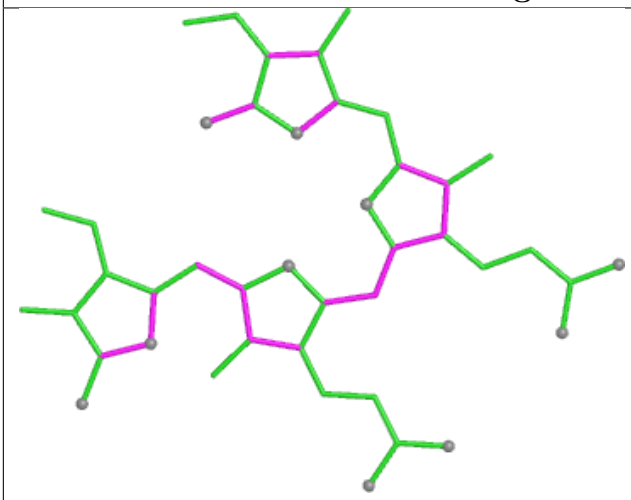


Rings

Ligand PEB uK 201



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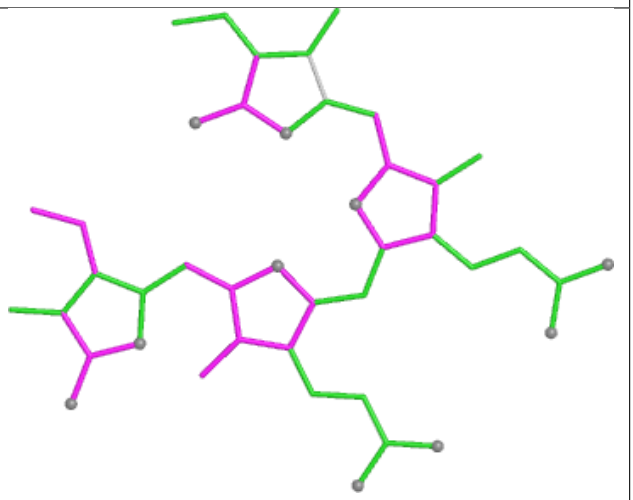

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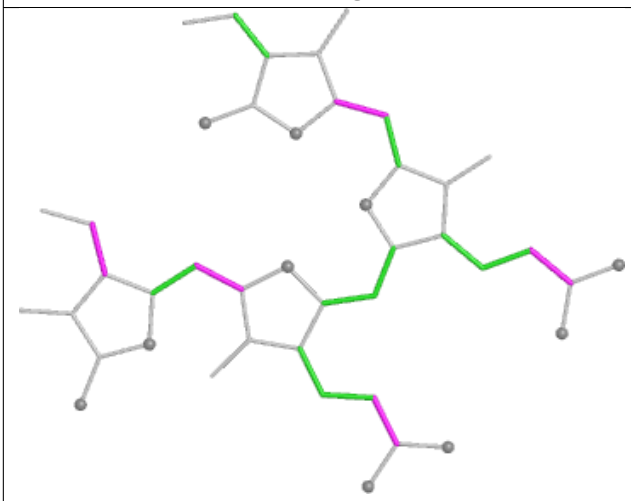

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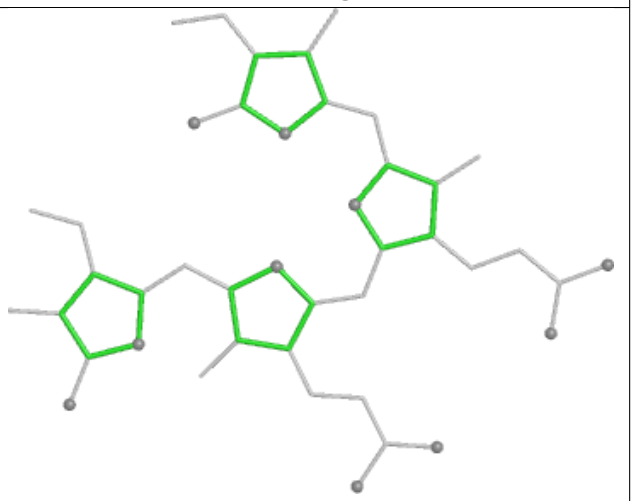
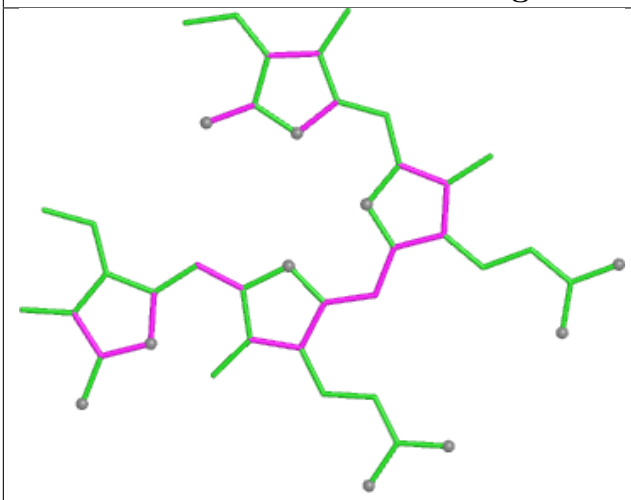


Rings

Ligand PEB PD 201



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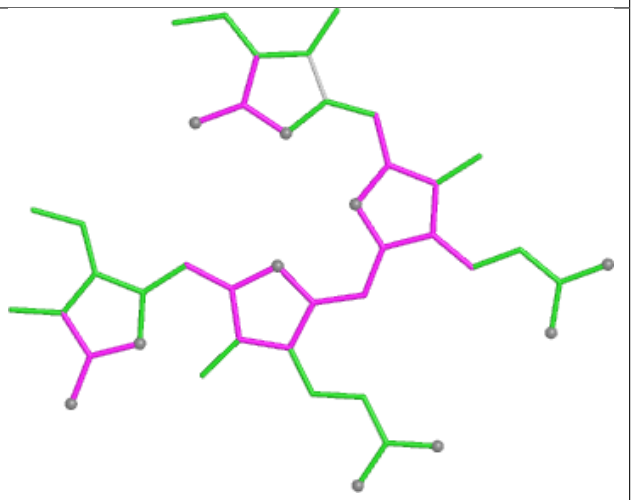

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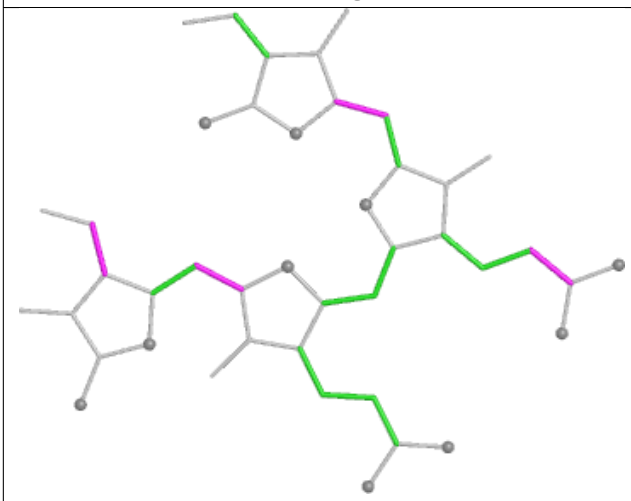

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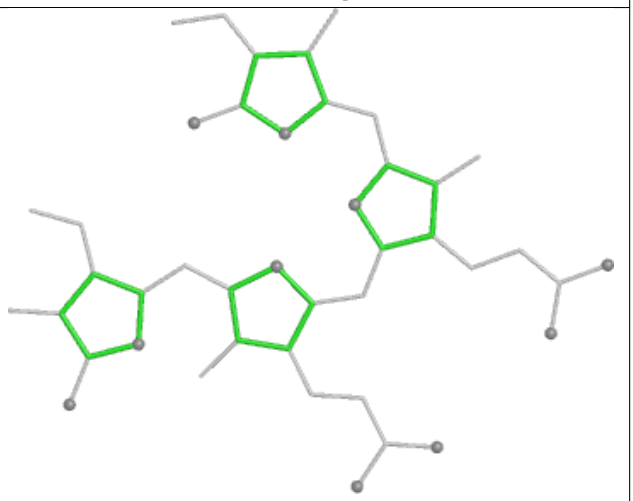
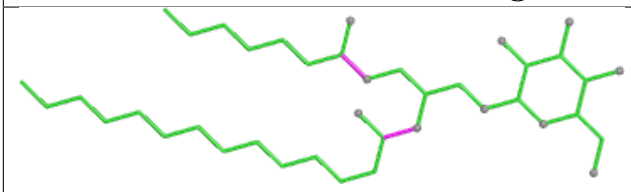


Rings

Ligand LMG BL 611



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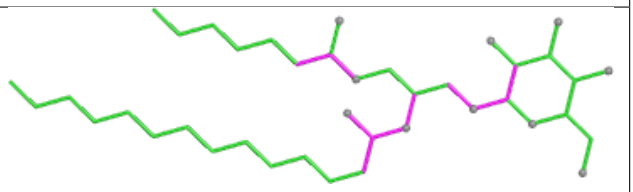

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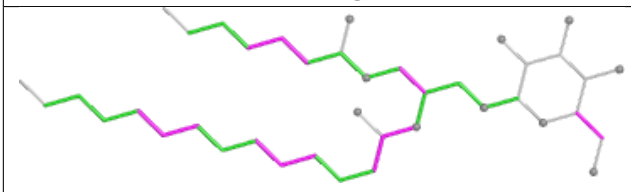

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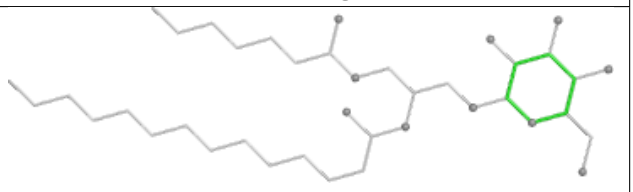
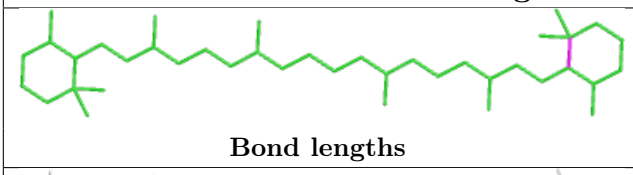


Rings

Ligand BCR C6 508



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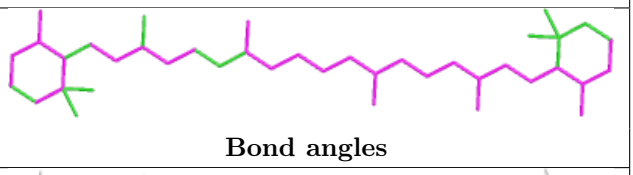

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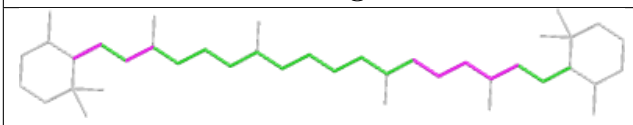

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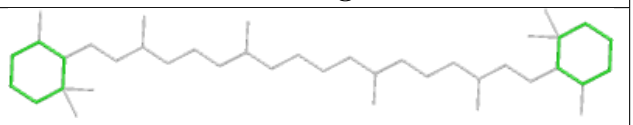
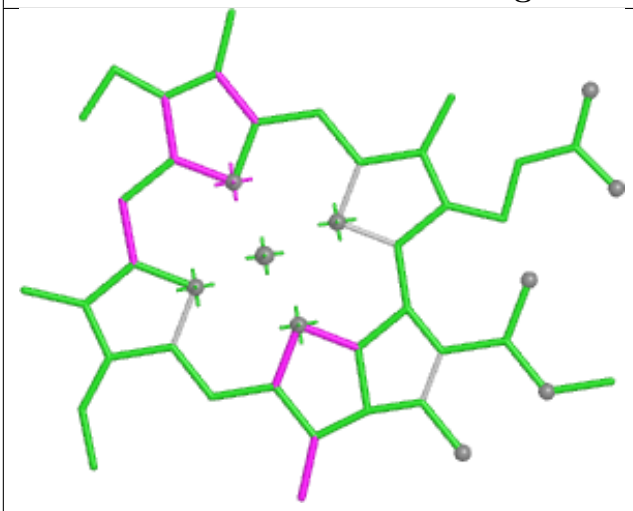


Rings

Ligand CLA 6N 605



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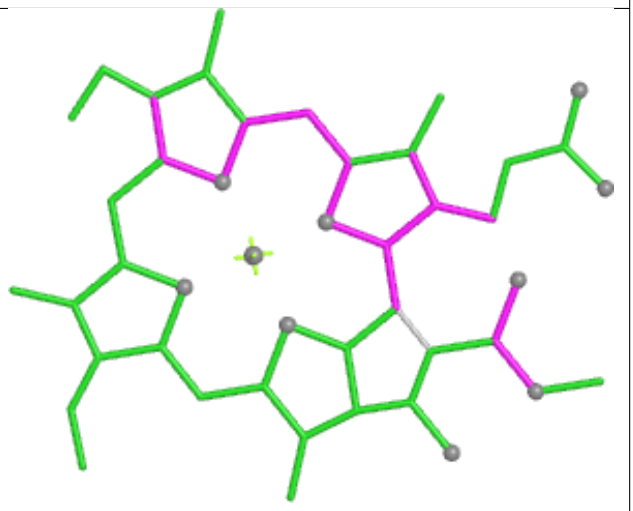

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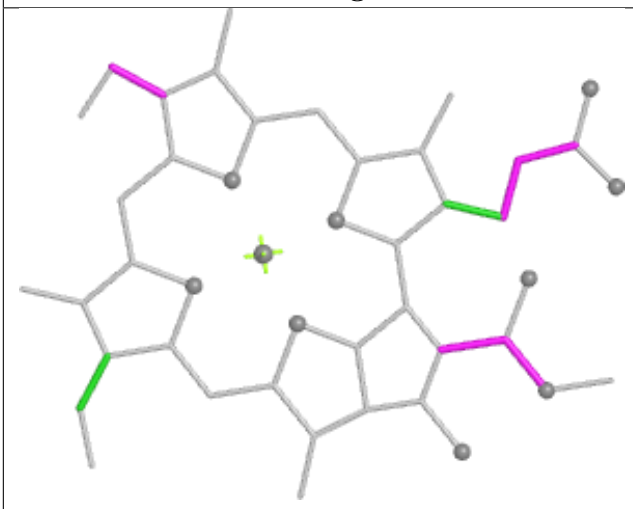

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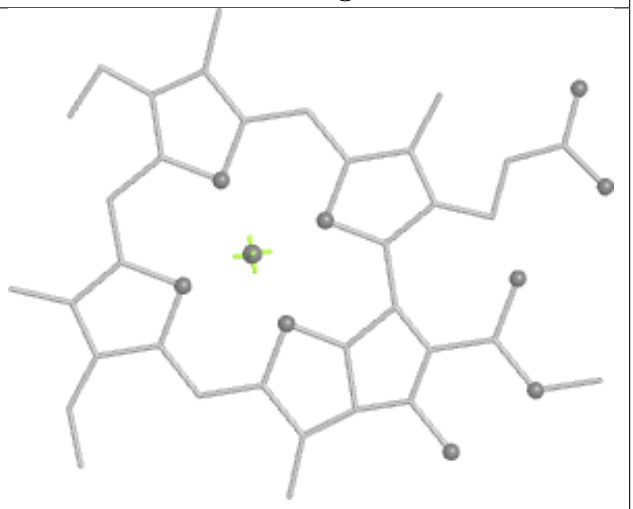
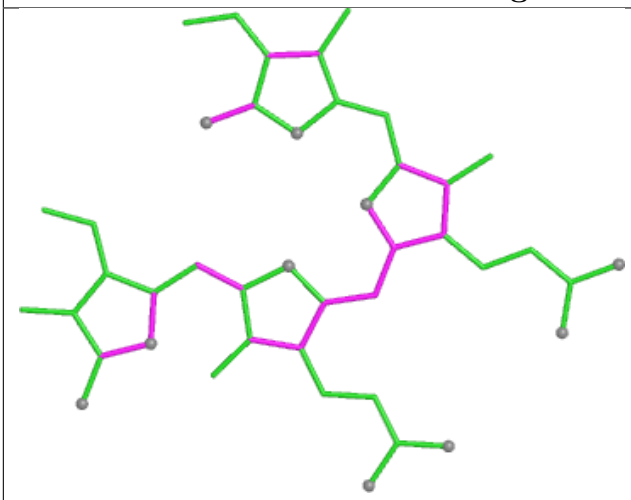


Rings

Ligand PEB HQ 203



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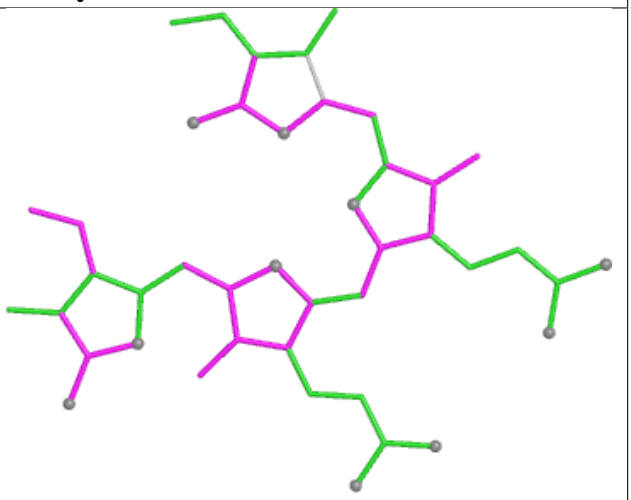

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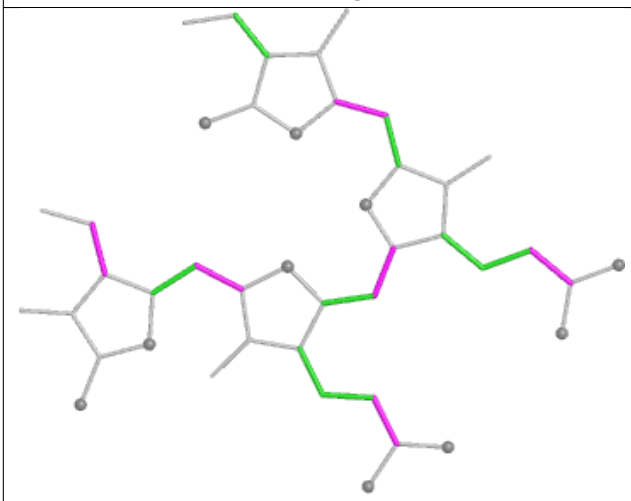

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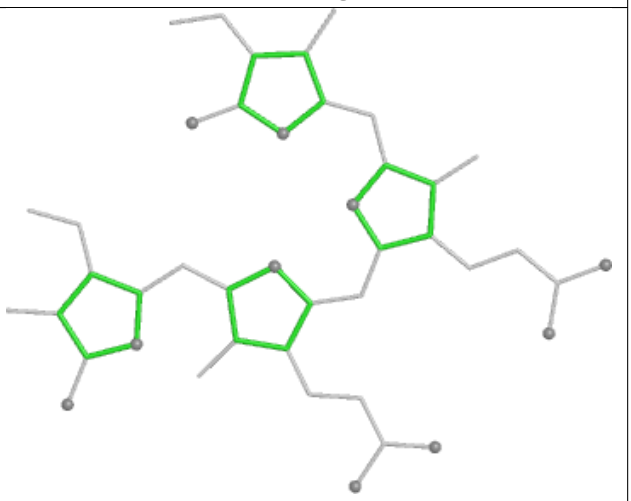
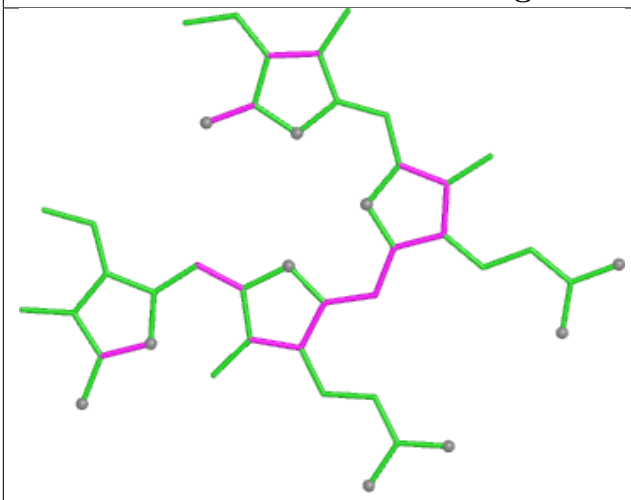


Rings

Ligand PEB xK 304



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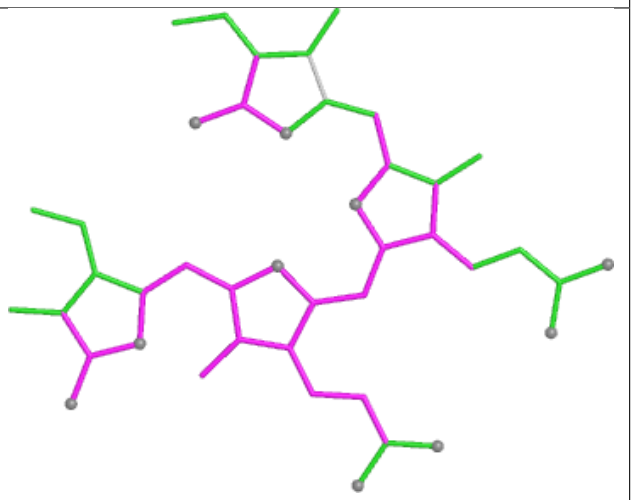

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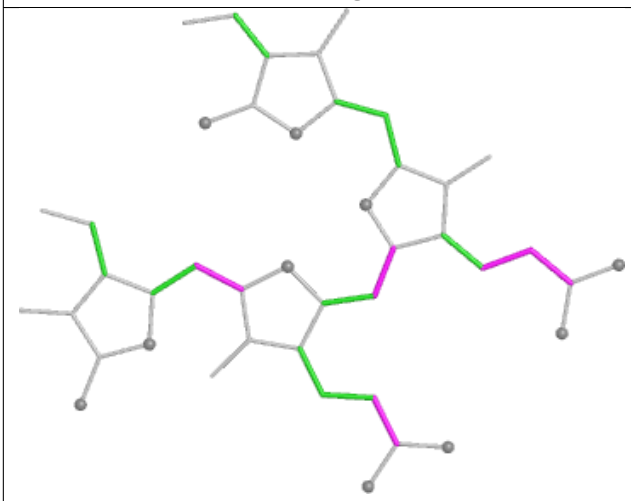

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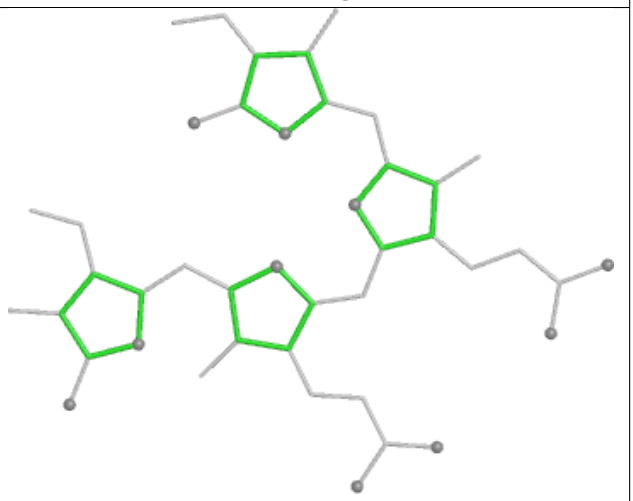
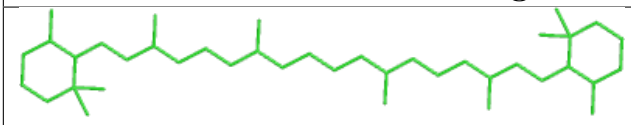


Rings

Ligand BCR KL 100



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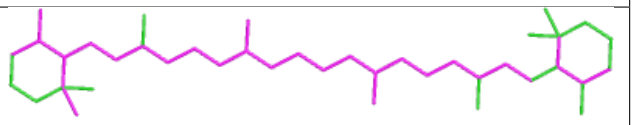

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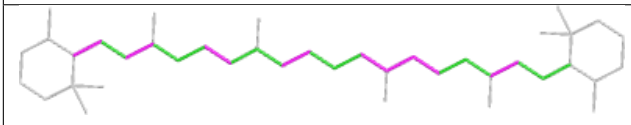

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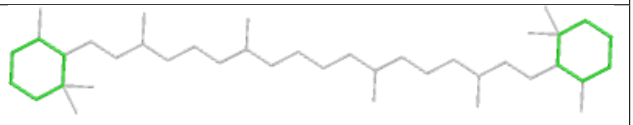
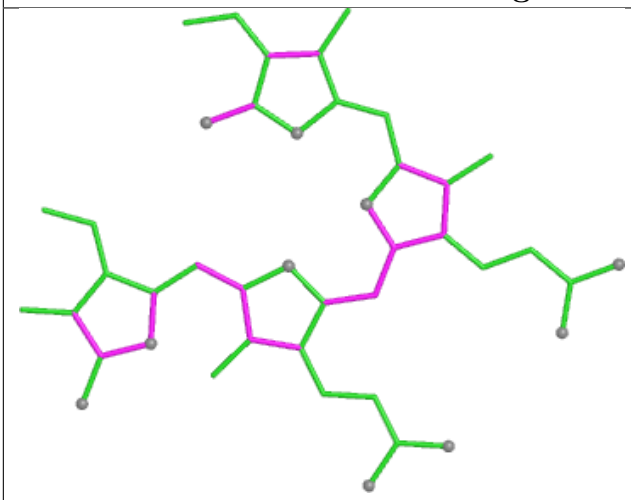


Rings

Ligand PEB CP 202



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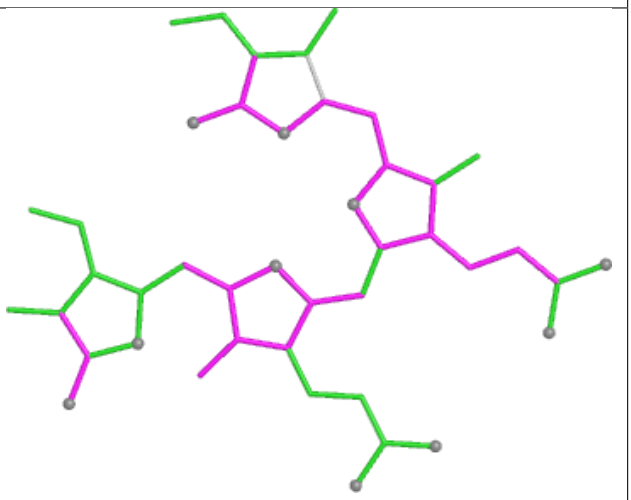

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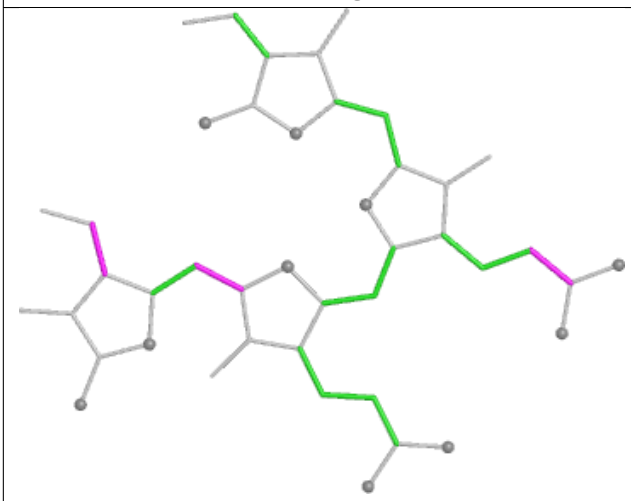

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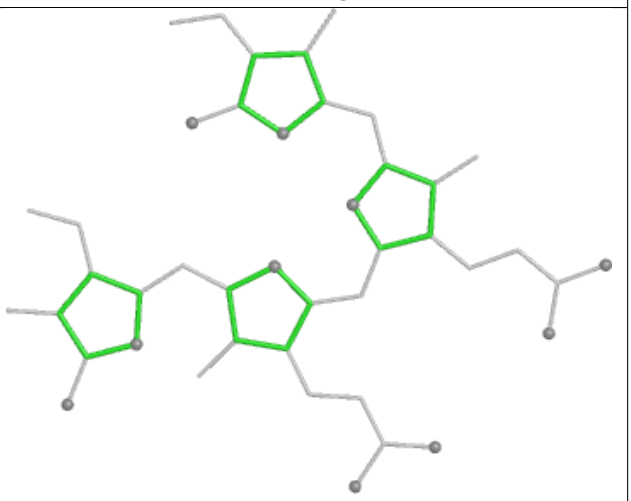
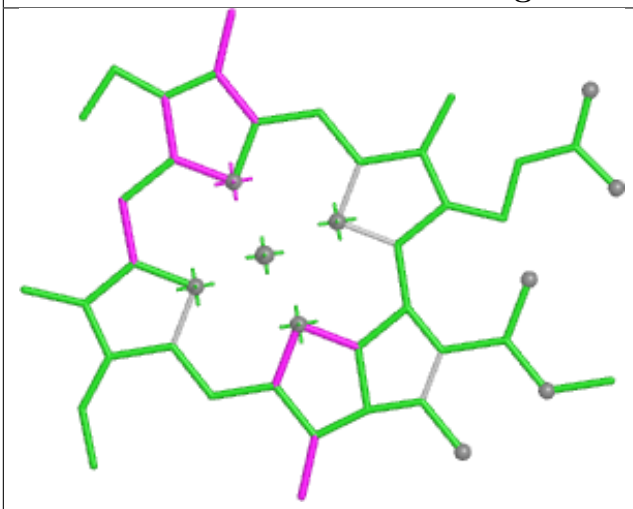


Rings

Ligand CLA 6N 606



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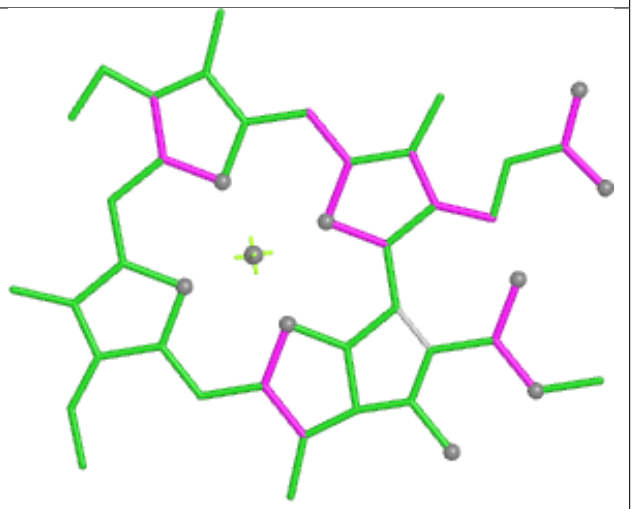
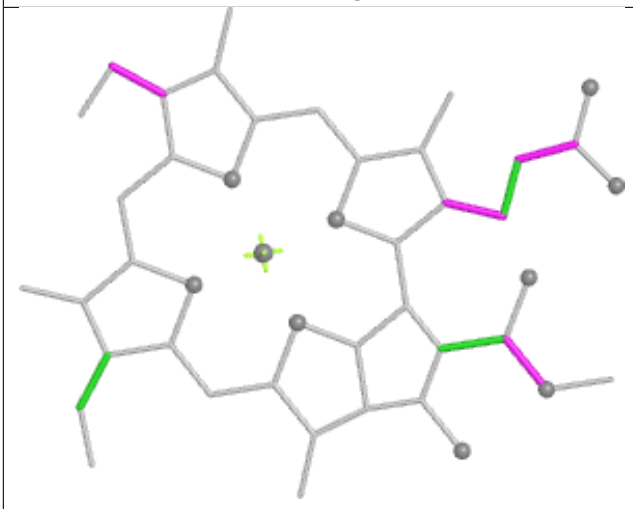


Bond angles

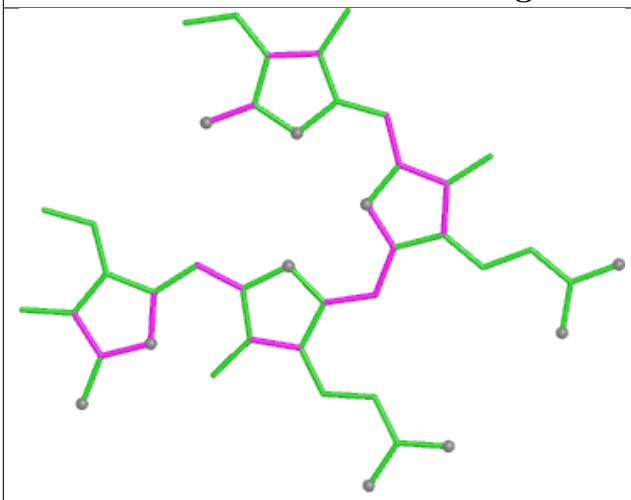


Torsions



Rings

Ligand PEB VJ 201



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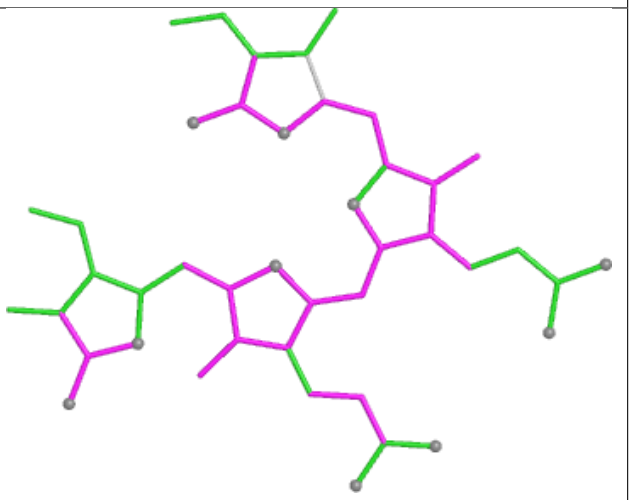
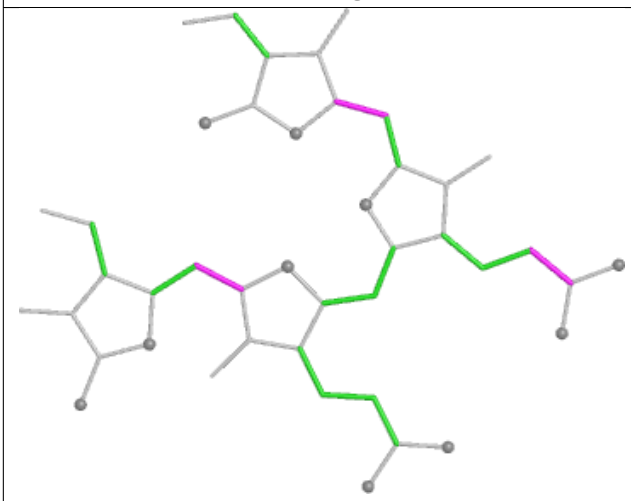


Bond angles



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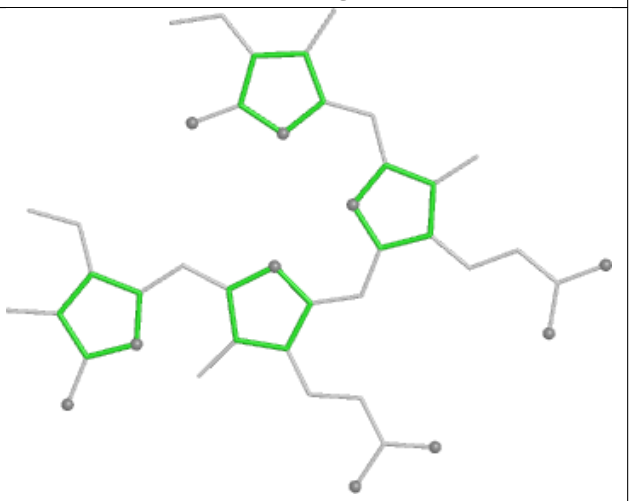
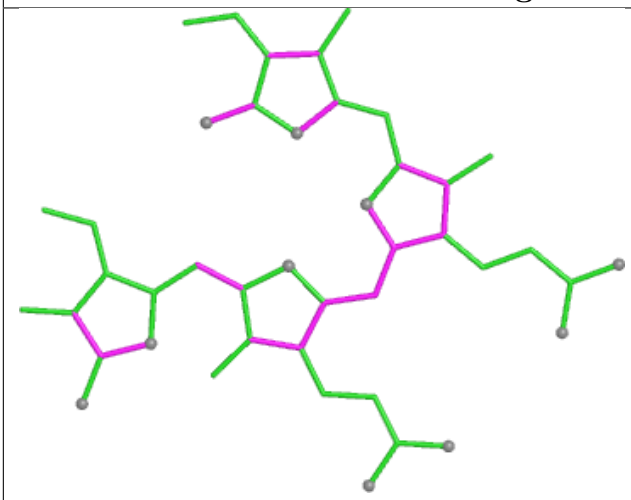


Rings

Ligand PEB R9 202



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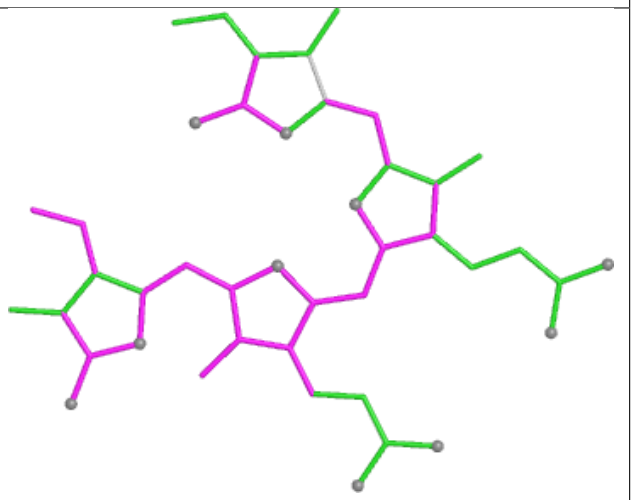
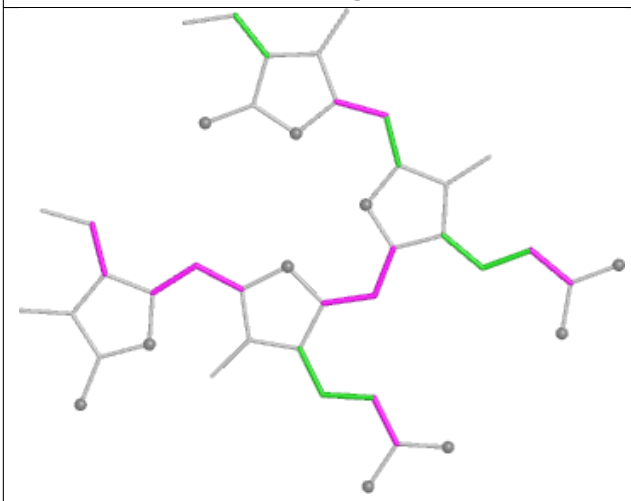


Bond angles



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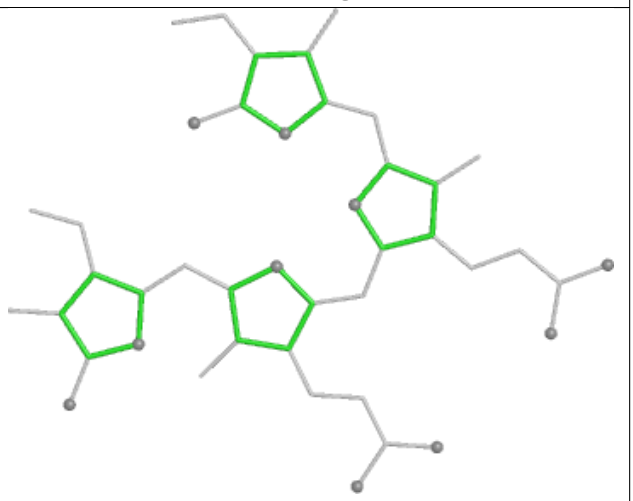
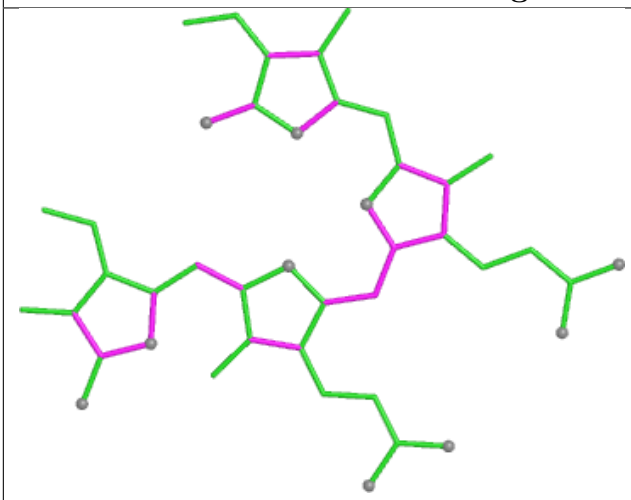
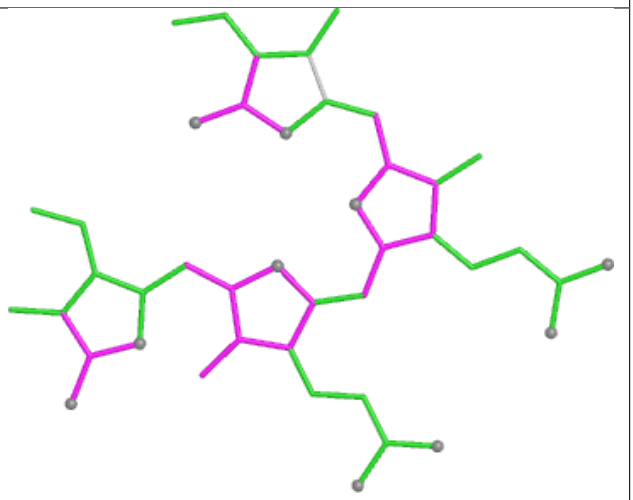


Rings

Ligand PEB AA 202



Bond lengths



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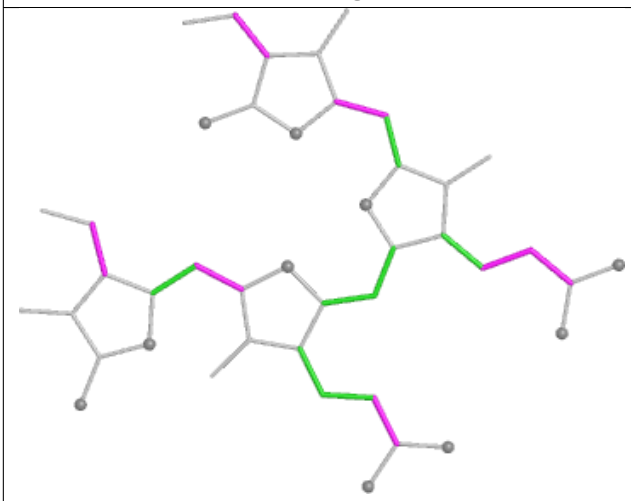

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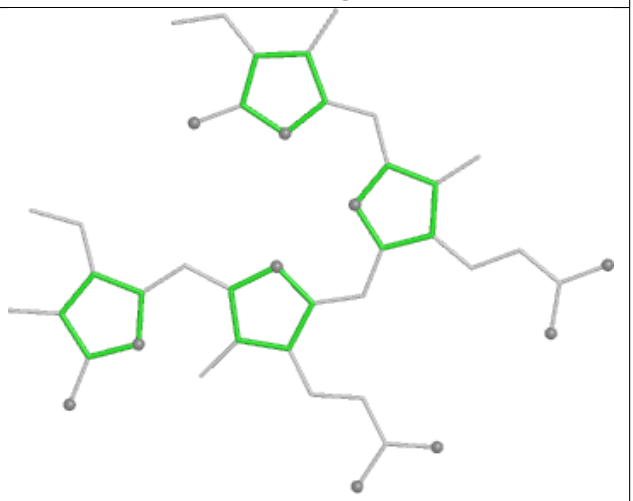
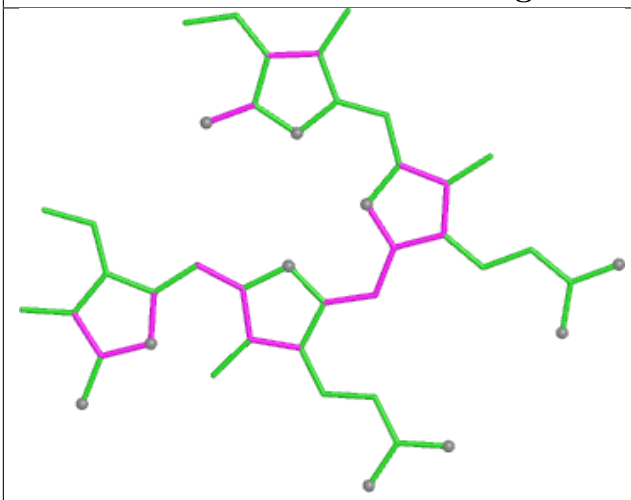


Rings

Ligand PEB ZE 202



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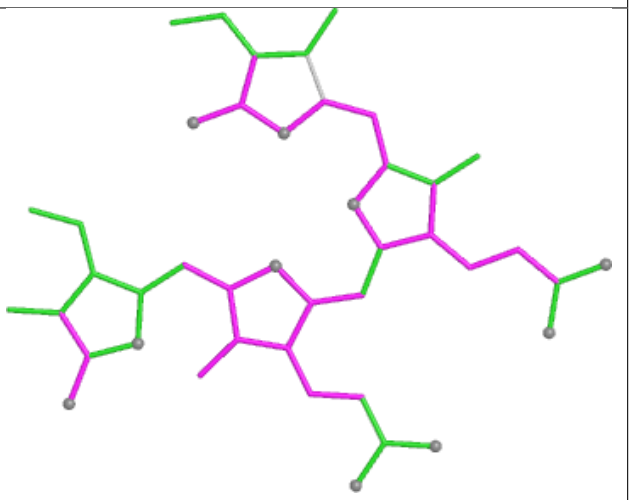

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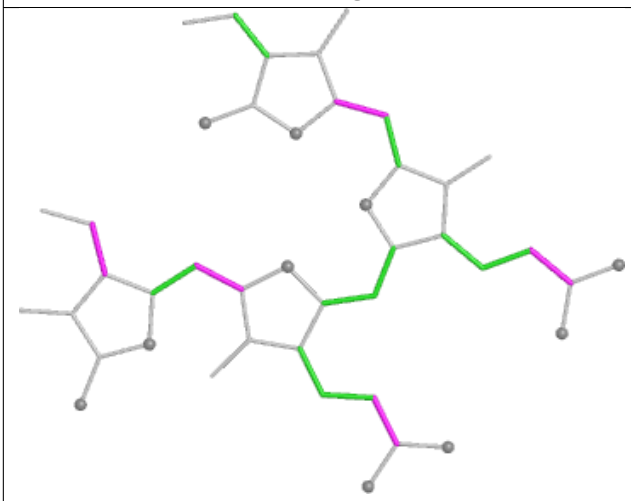

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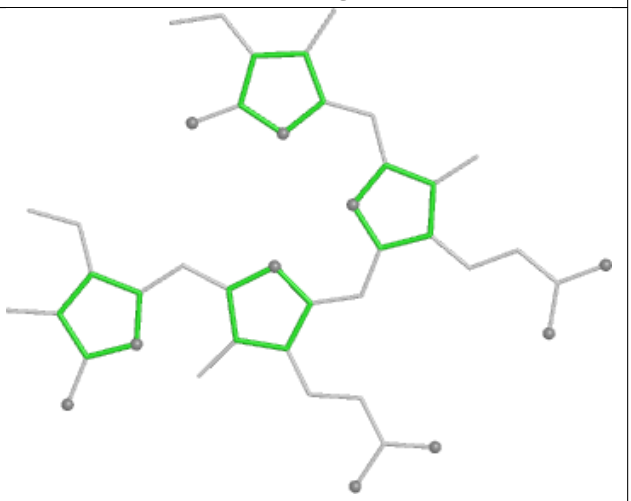
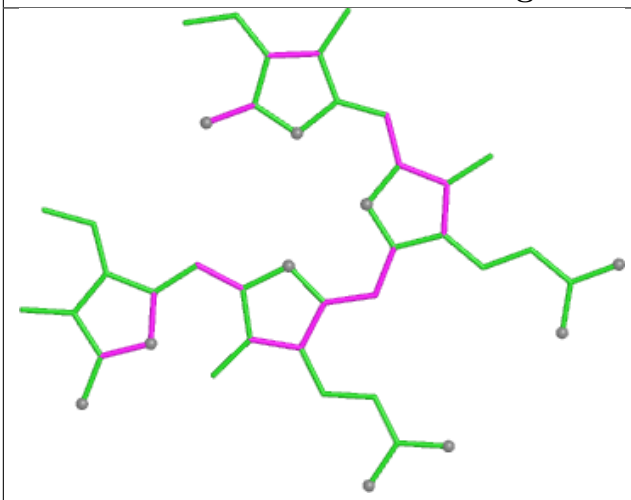


Rings

Ligand PEB hF 202



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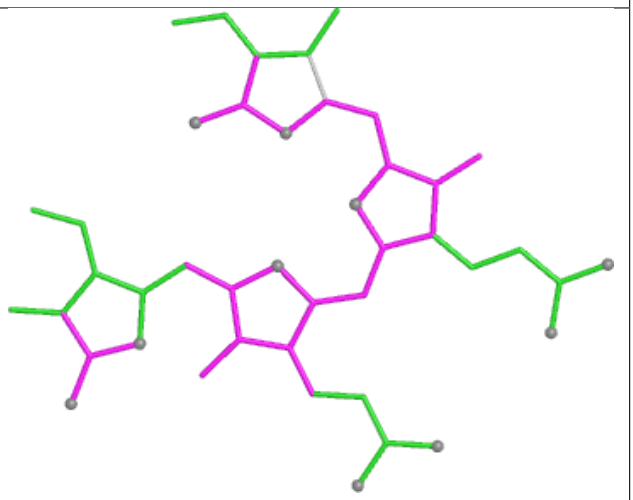

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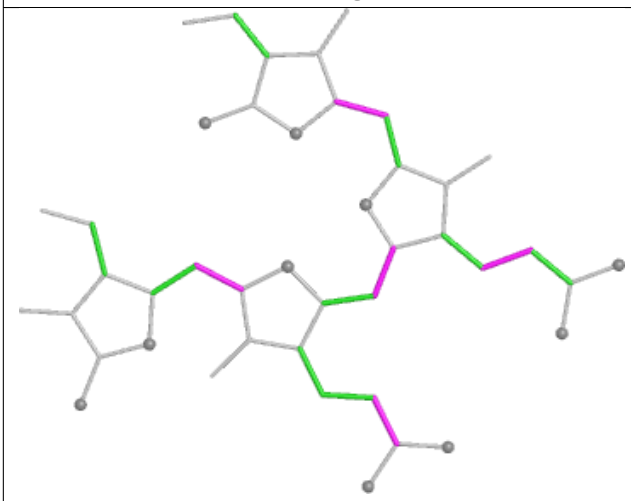

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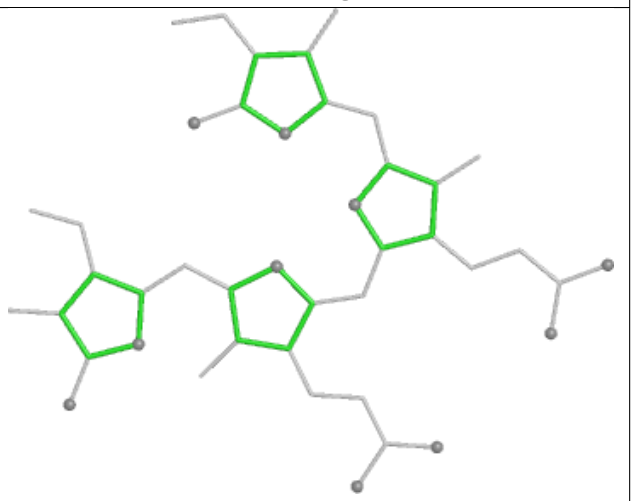
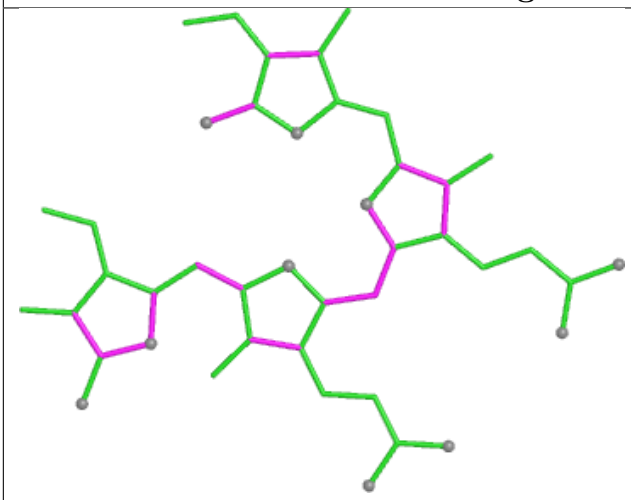


Rings

Ligand PEB F5 201



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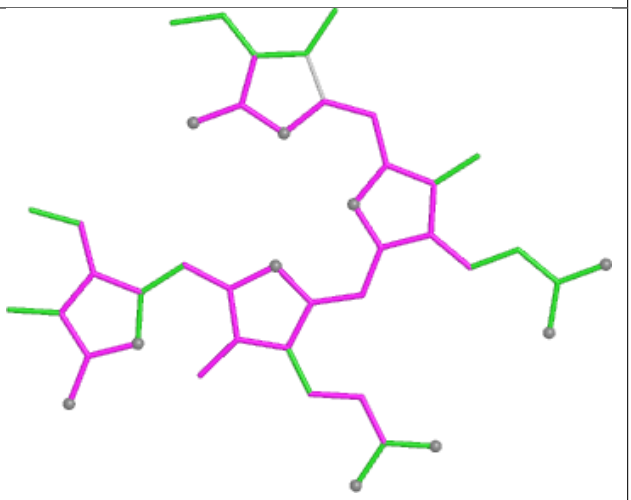

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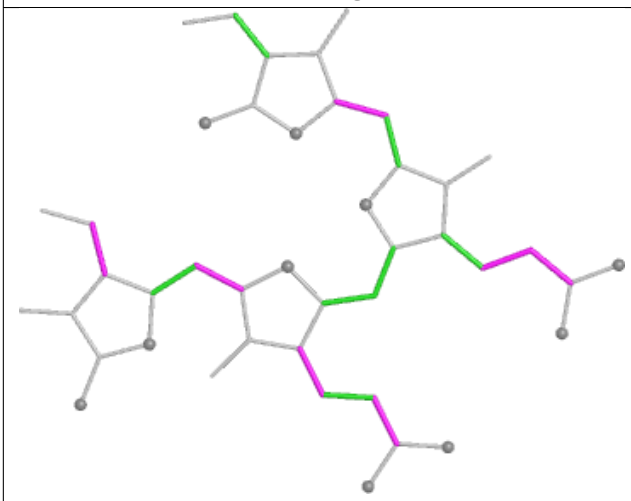

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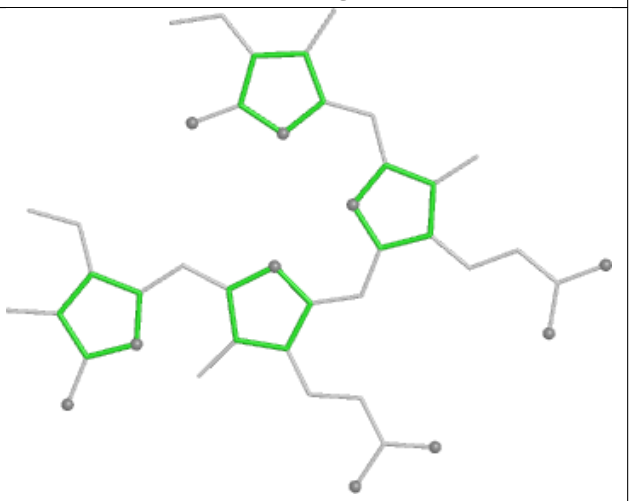
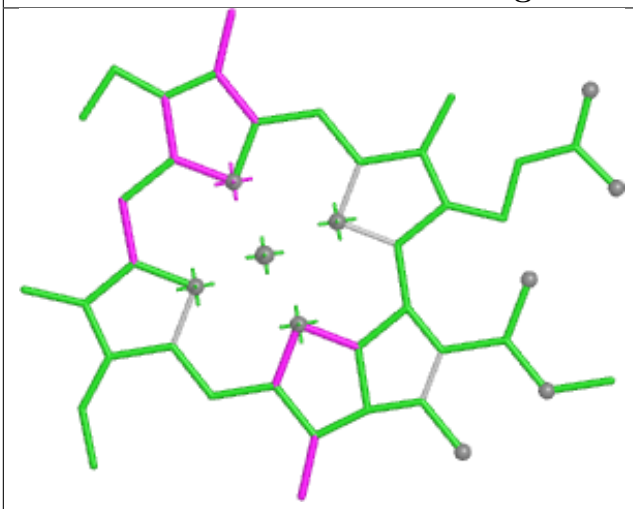


Rings

Ligand CLA 5N 605



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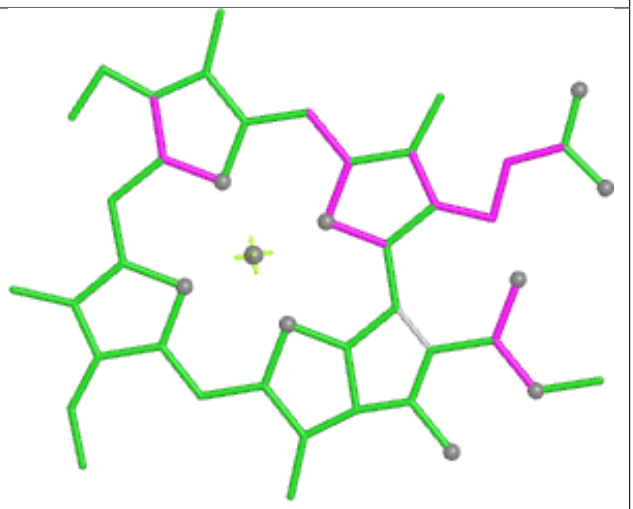

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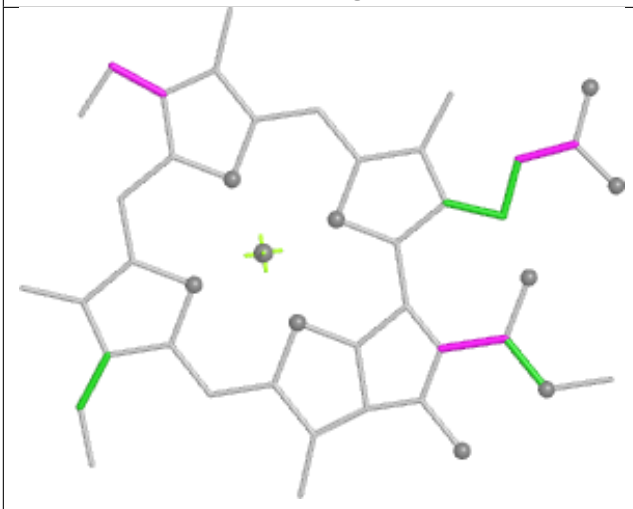
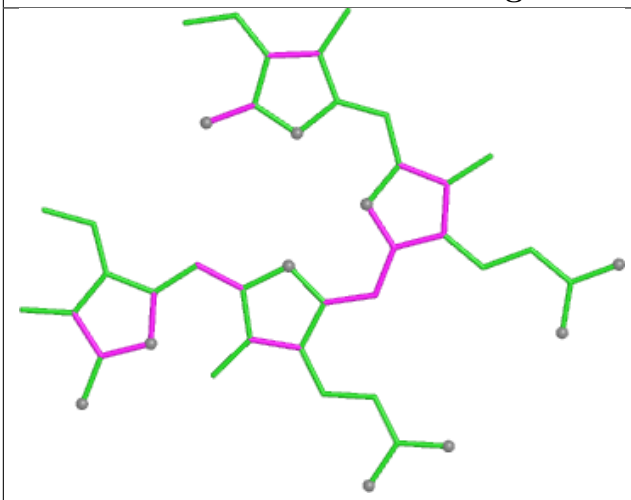


Torsions



Rings

Ligand PEB JH 1002



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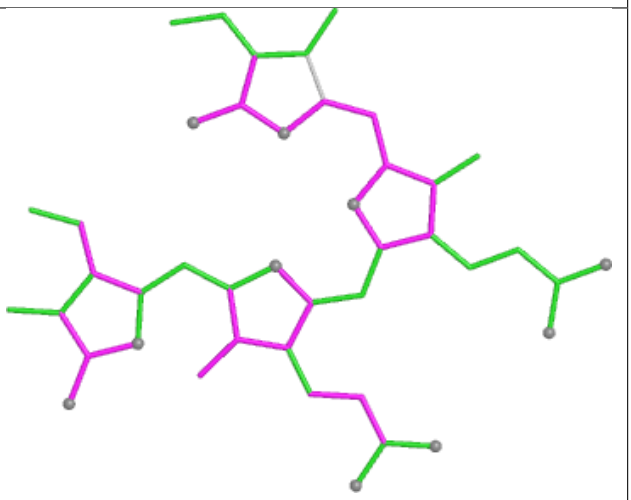

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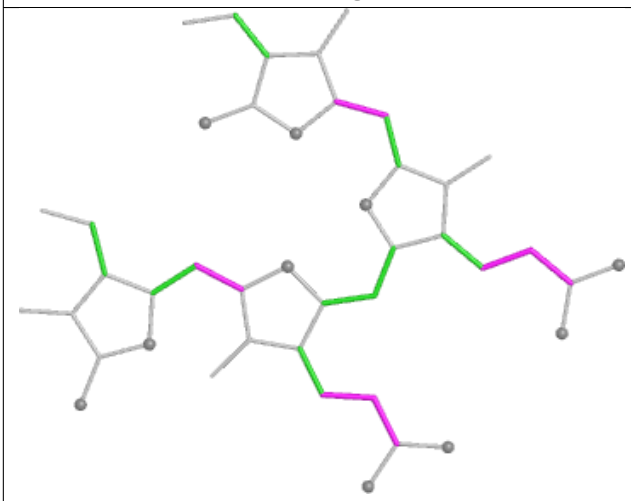

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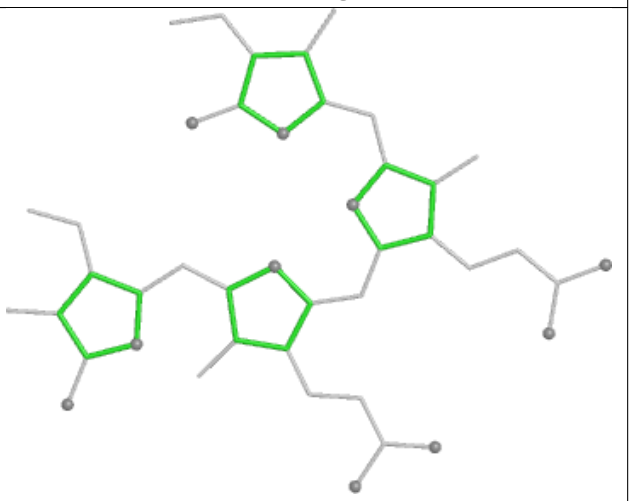
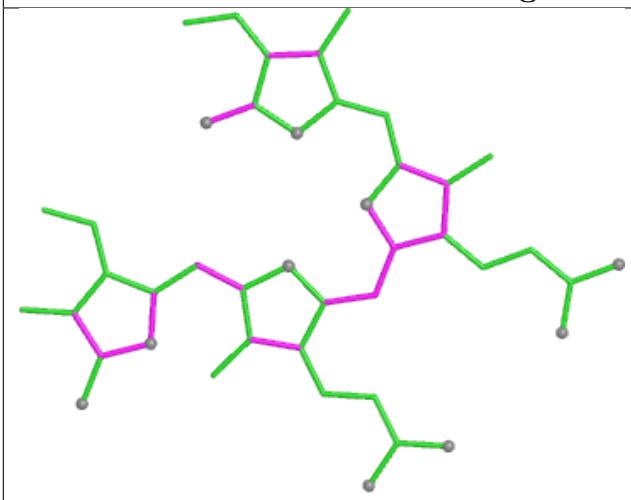


Rings

Ligand PEB J5 203



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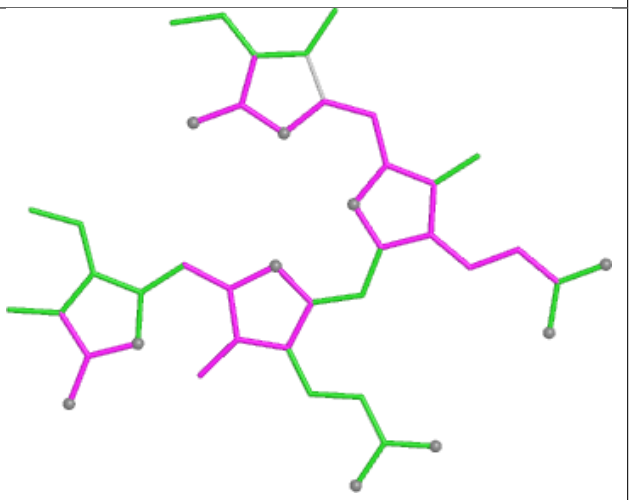

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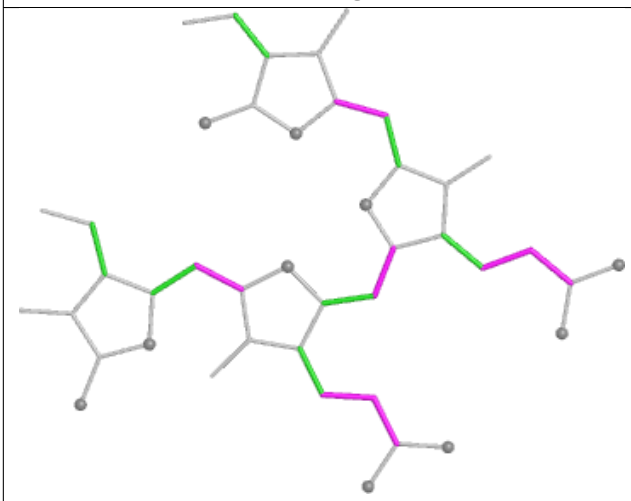

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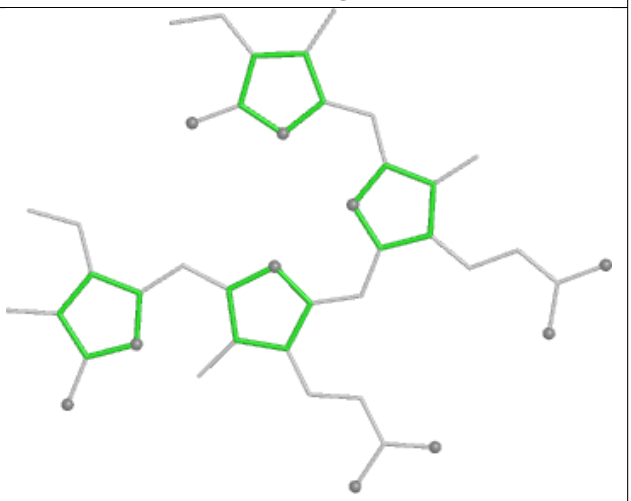
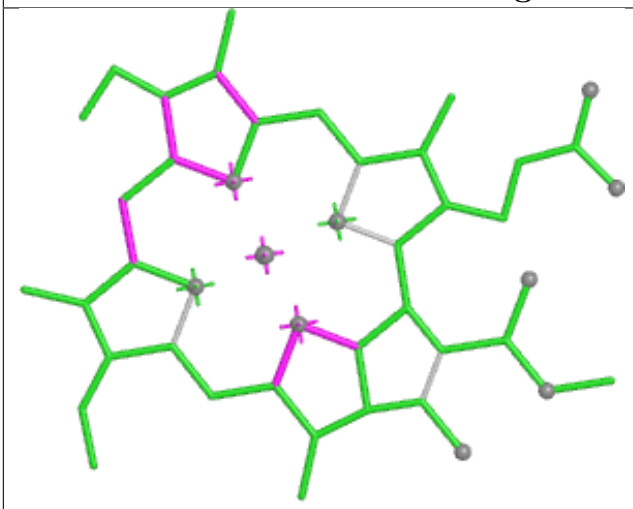


Rings

Ligand CLA 1N 610



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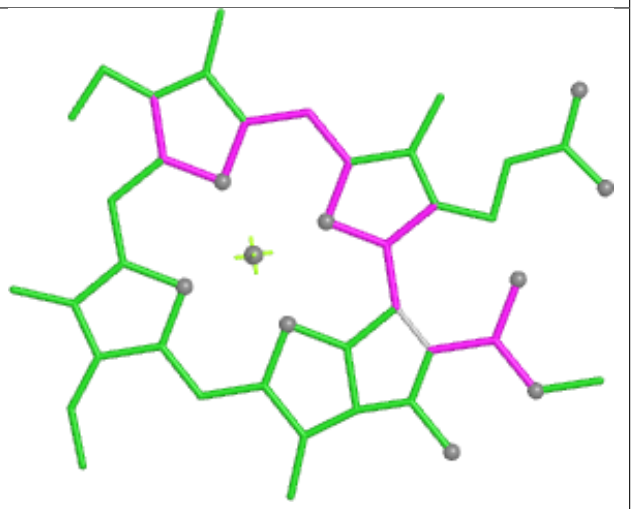
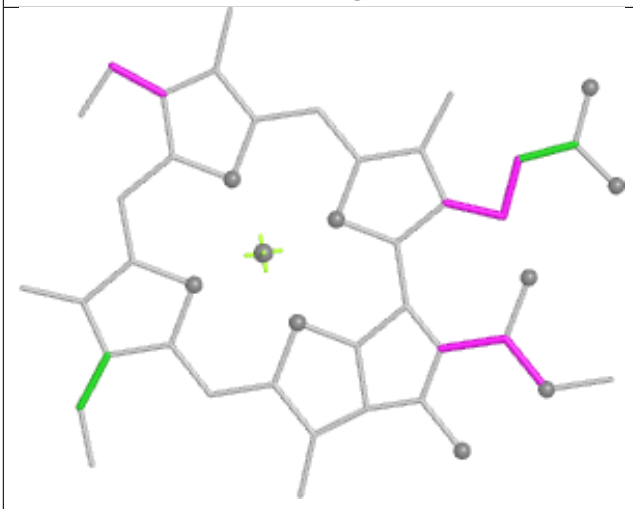


Bond angles

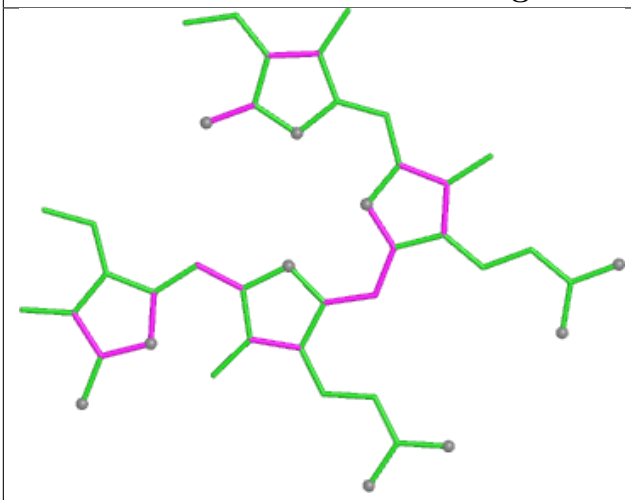


Torsions



Rings

Ligand PEB M5 301



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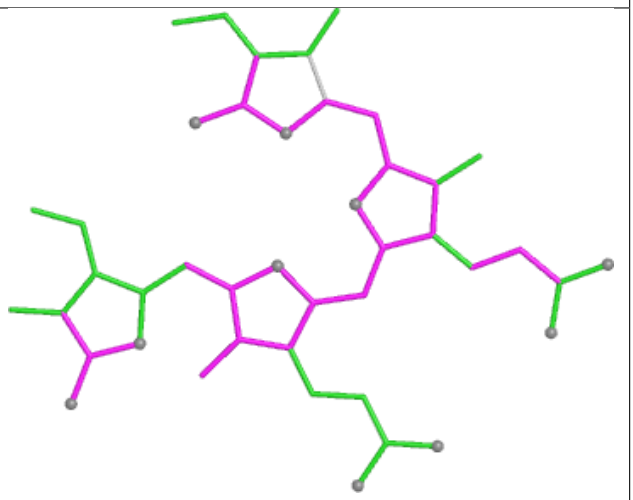

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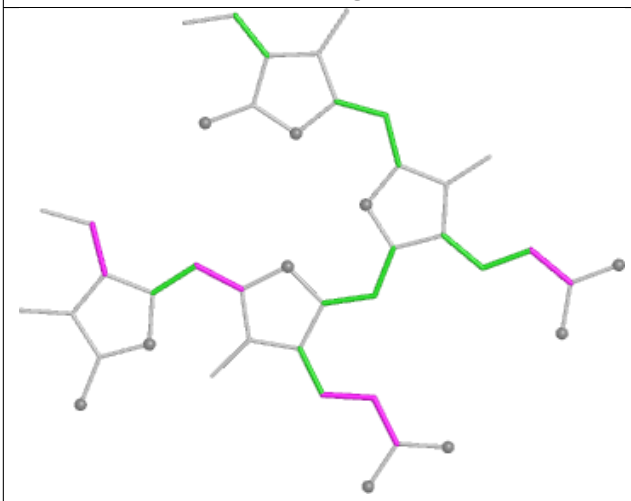

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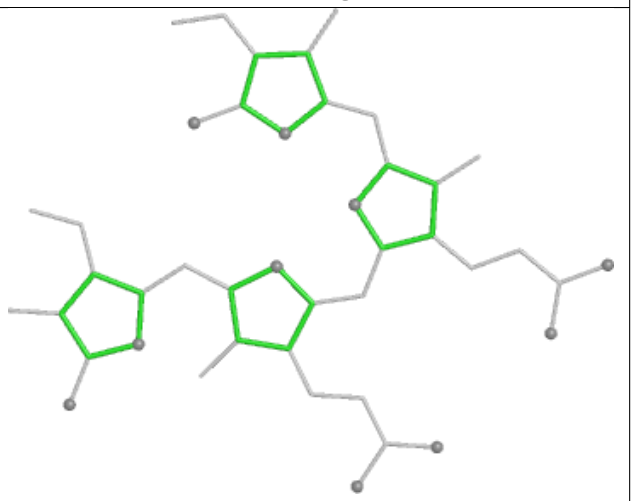
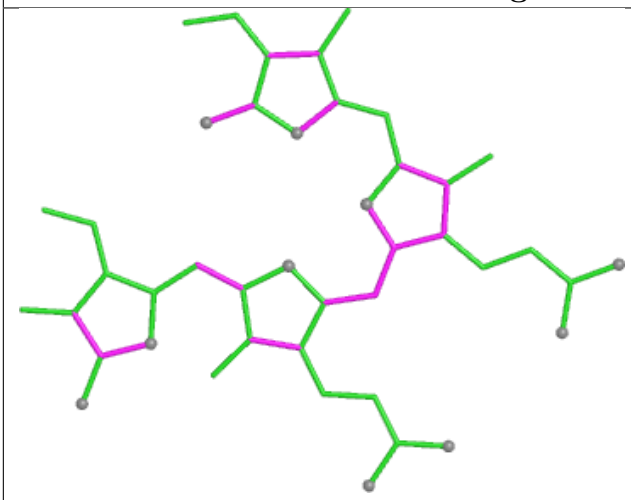


Rings

Ligand PEB KA 202



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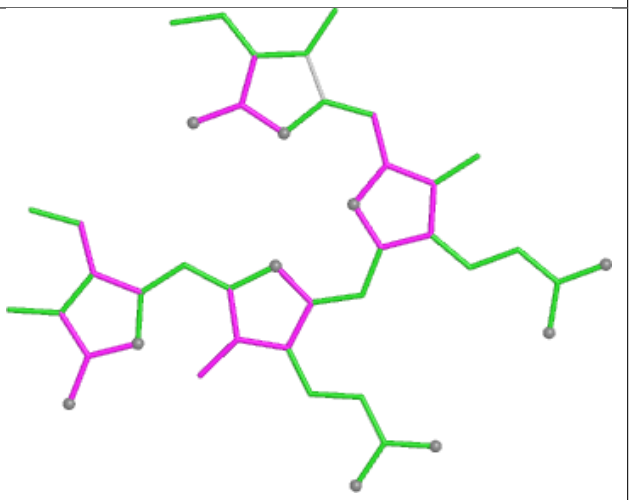

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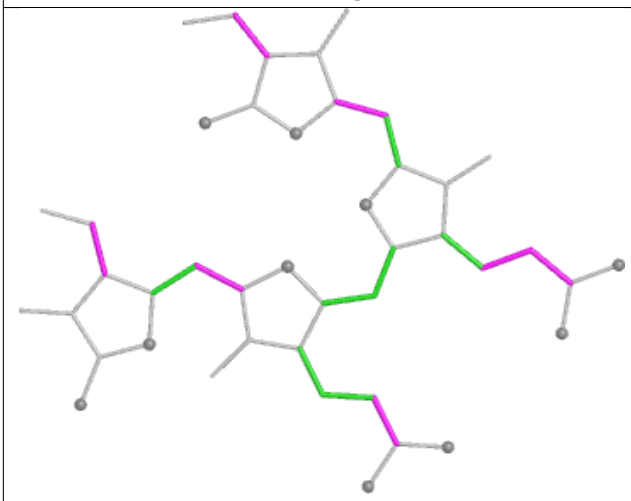

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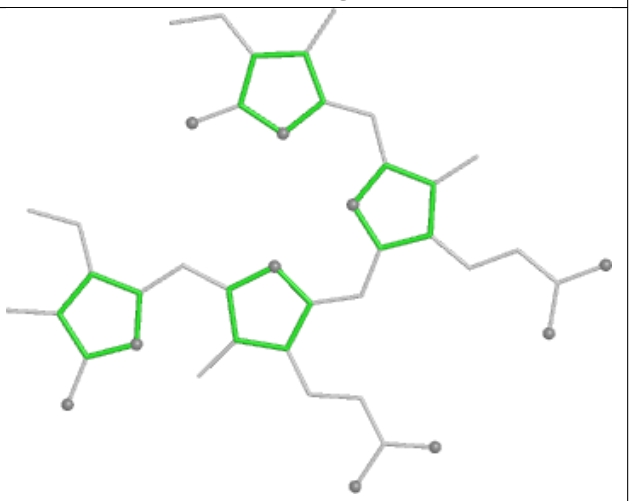
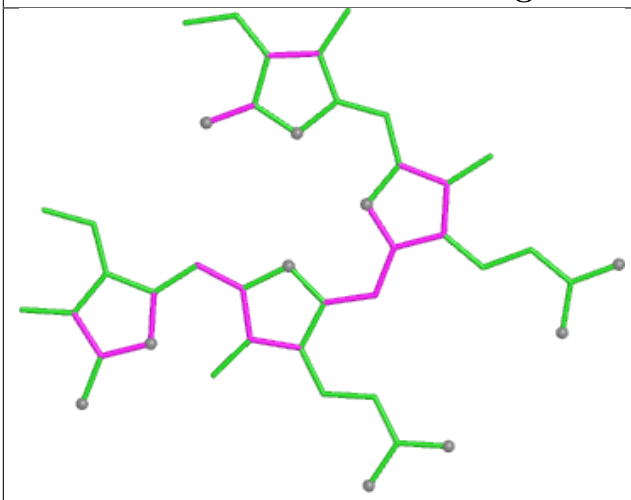


Rings

Ligand PEB V1 201



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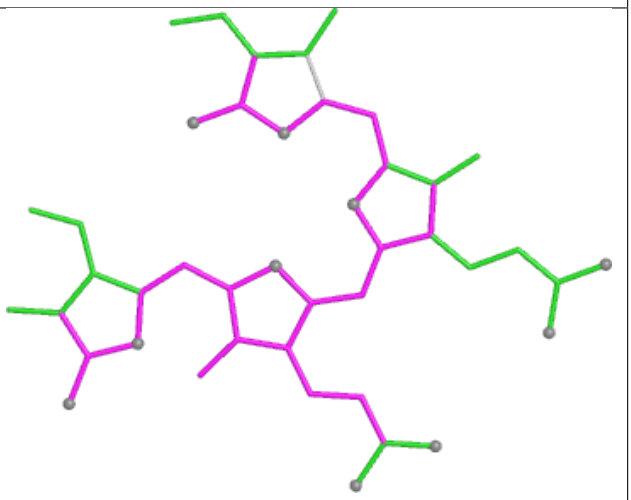

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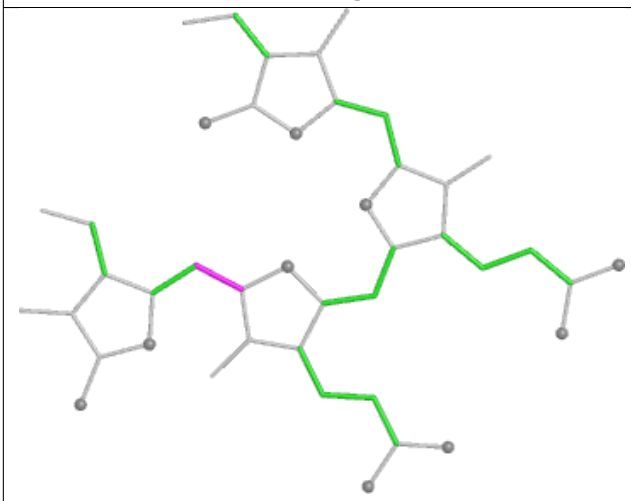

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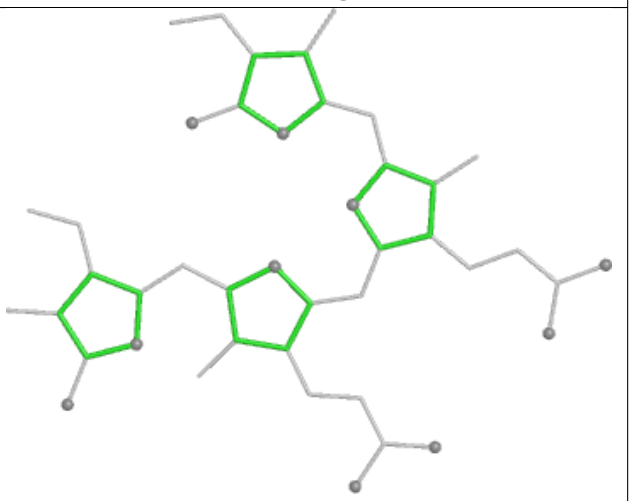
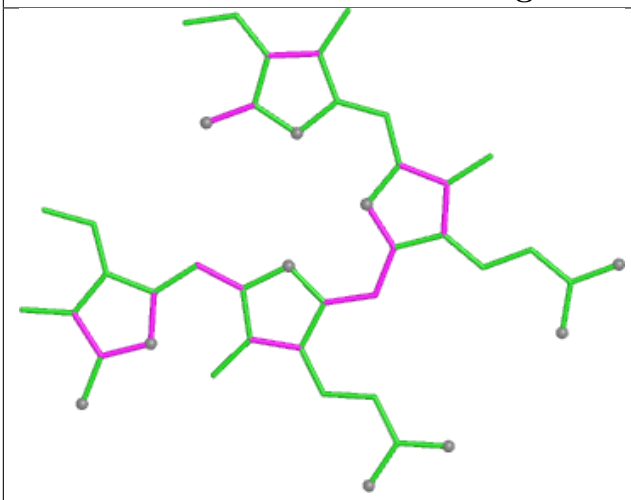


Rings

Ligand PEB aO 201



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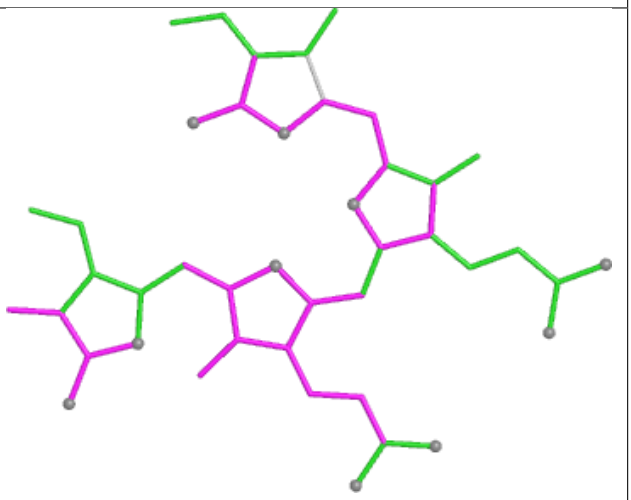
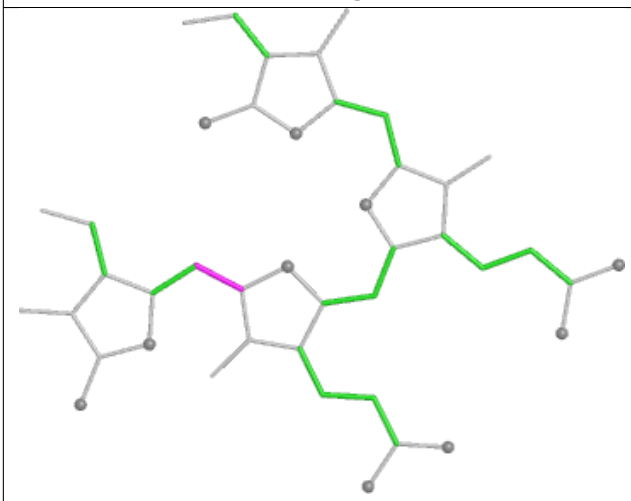


Bond angles



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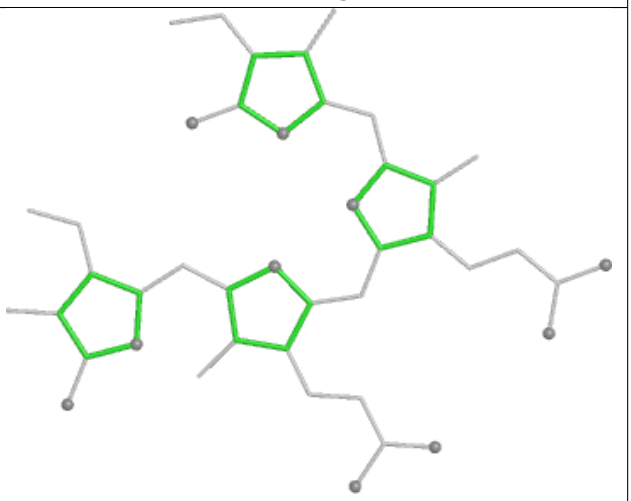
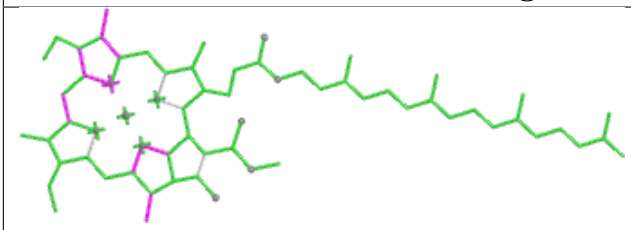


Rings

Ligand CLA cL 507



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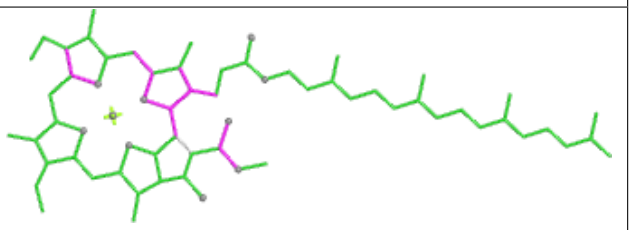
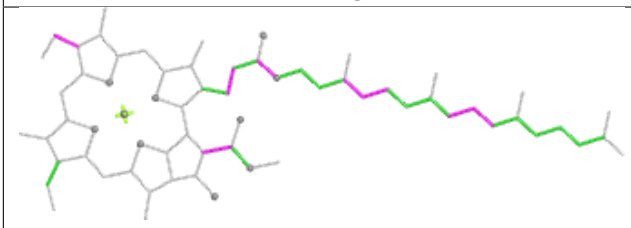


Bond angles



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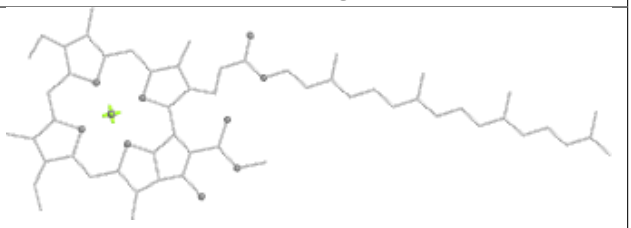
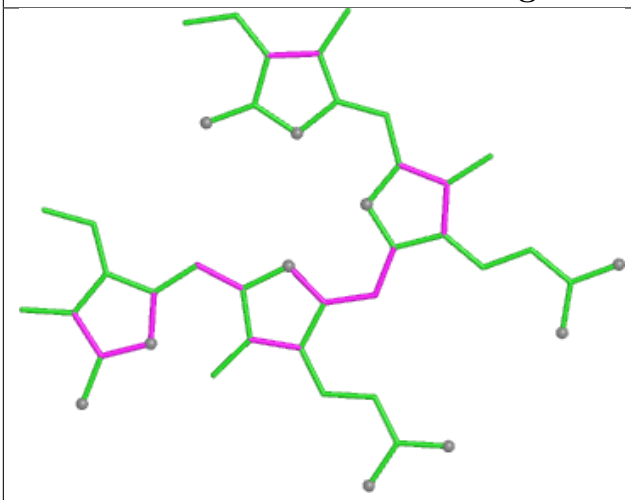


Rings

Ligand PEB S7 201



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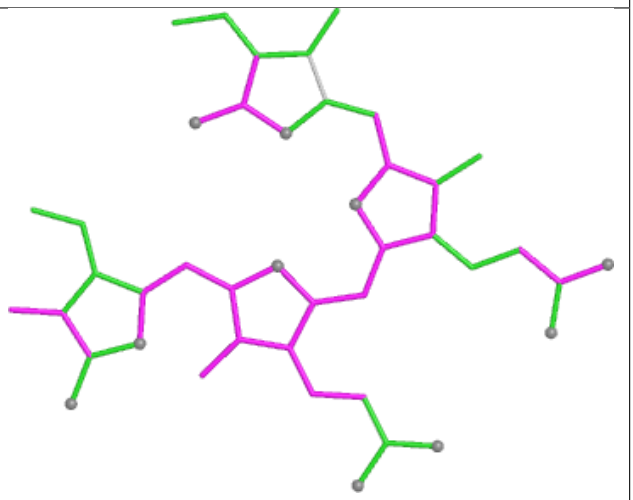
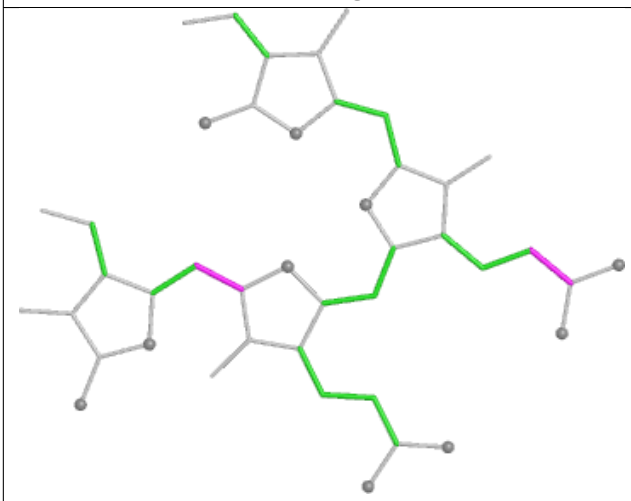


Bond angles



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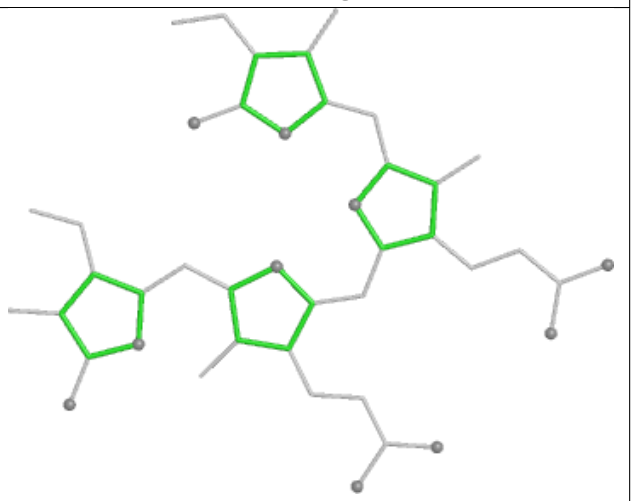
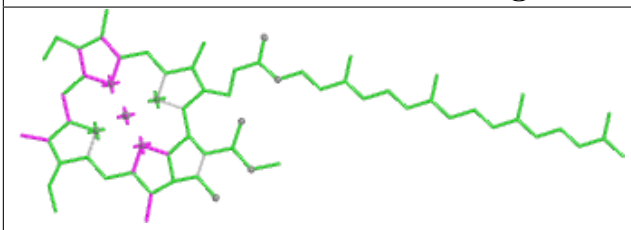


Rings

Ligand CLA BN 824



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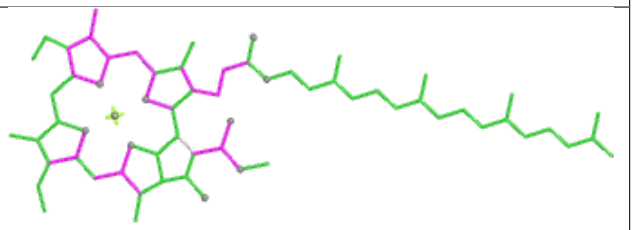
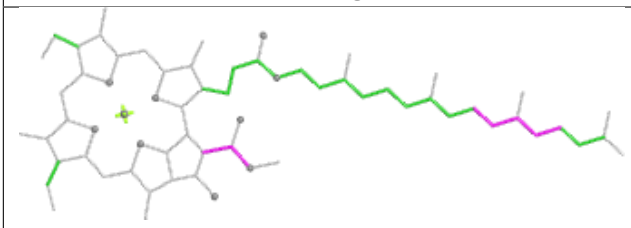


Bond angles



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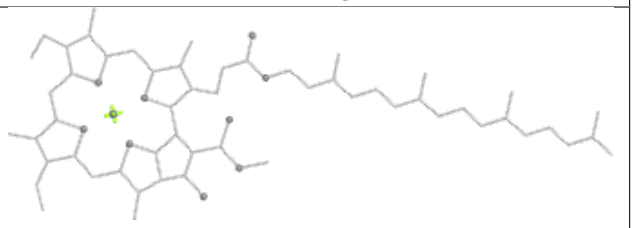
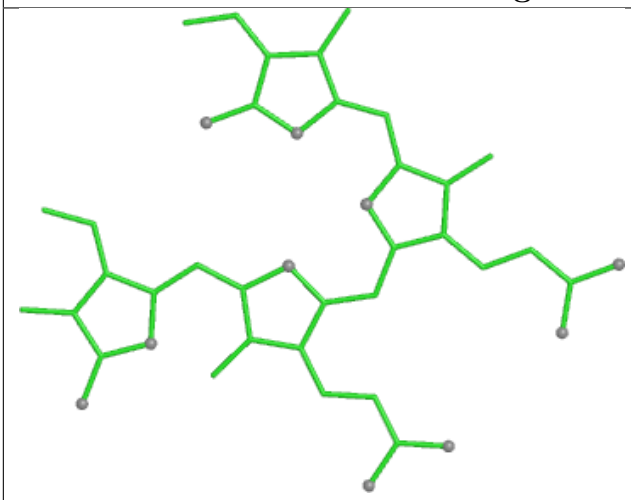
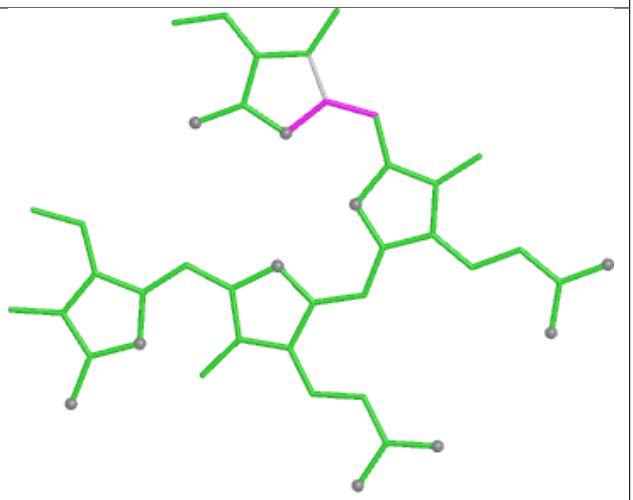


Rings

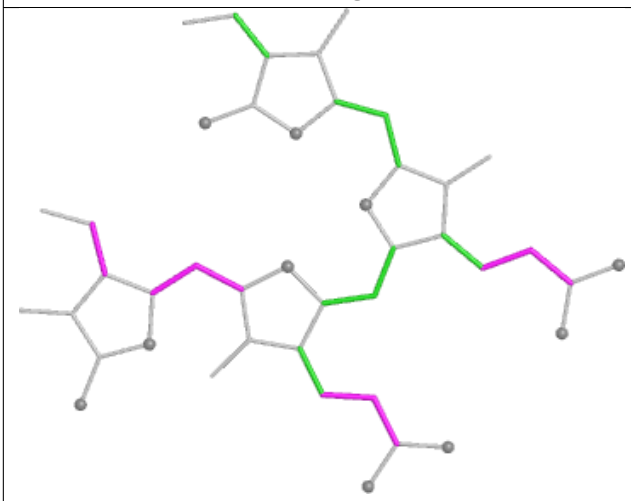
Ligand PEB hH 202



Bond lengths



Bond angles



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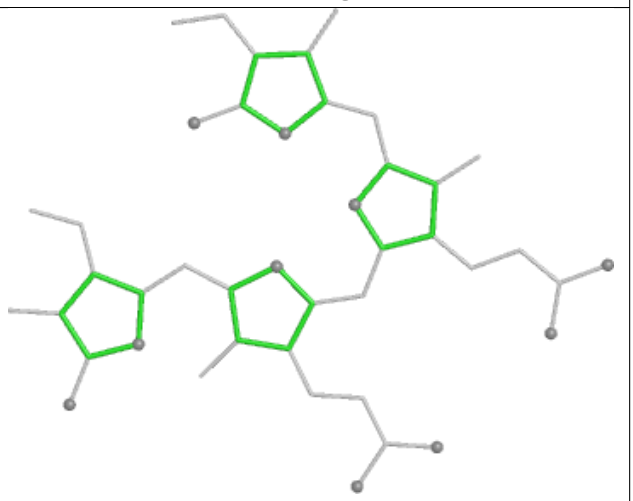
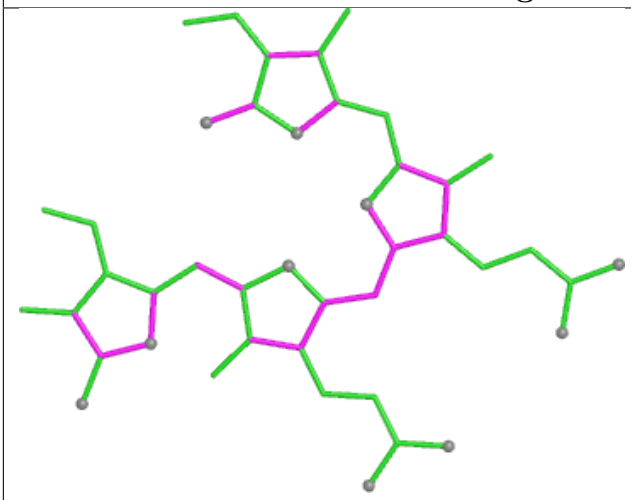


Rings

Ligand PEB T1 201



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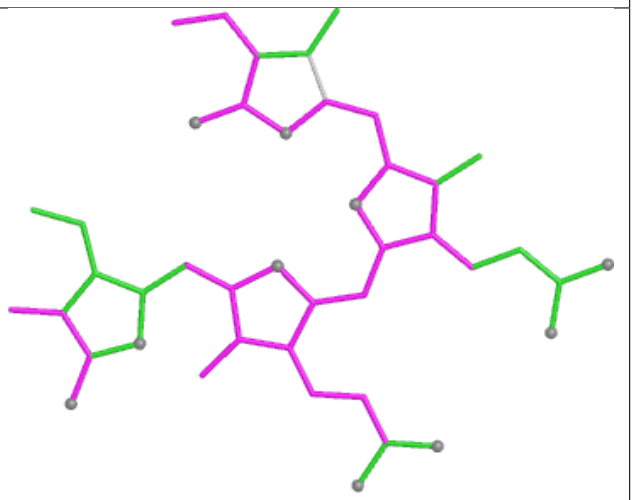

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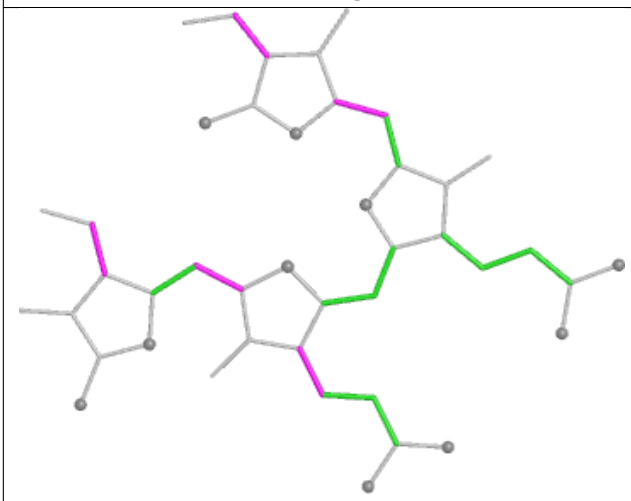

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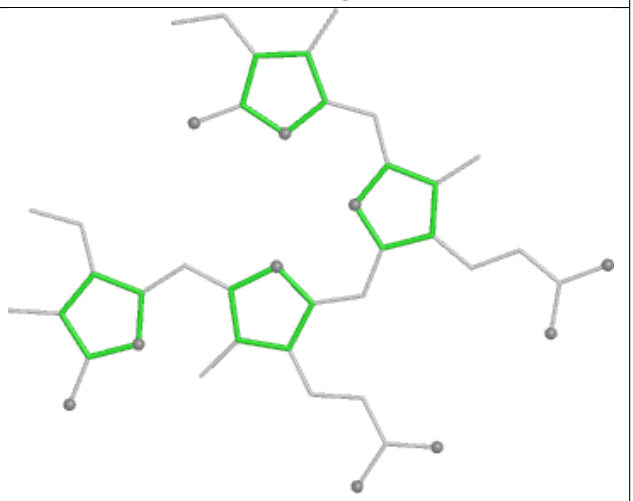
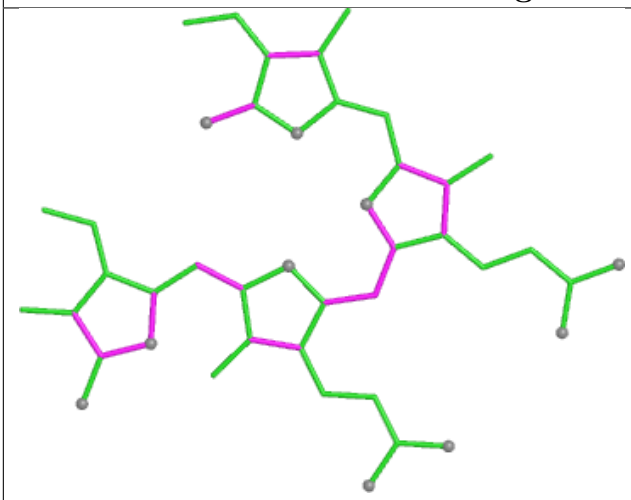


Rings

Ligand PEB OJ 201



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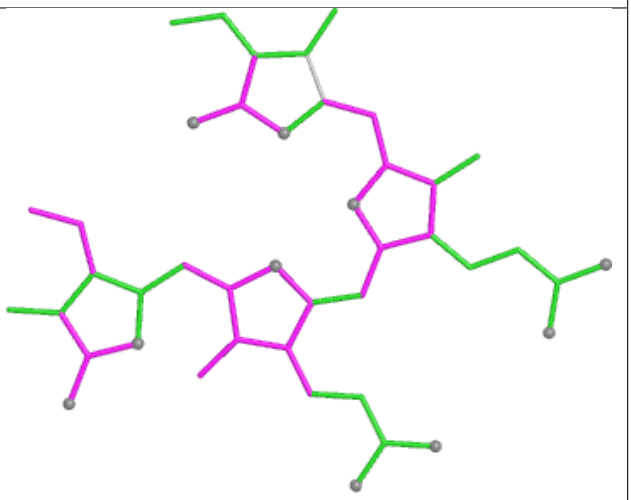

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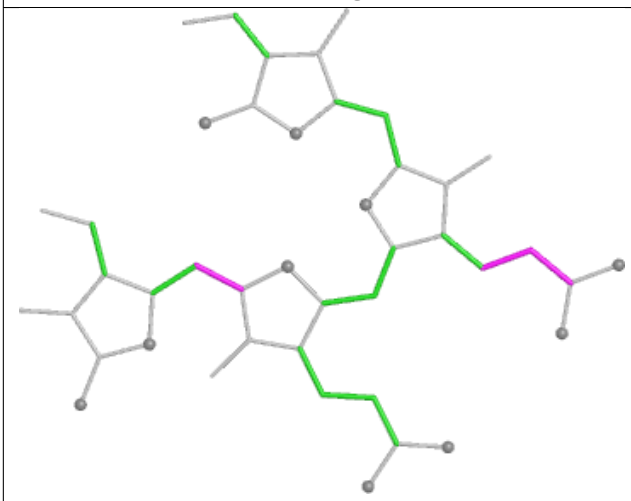

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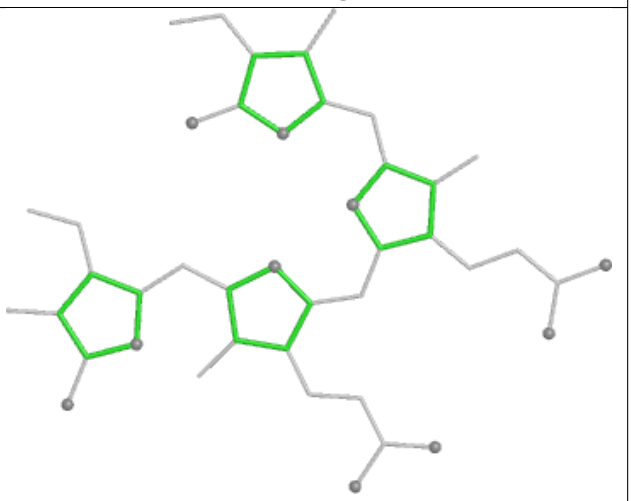
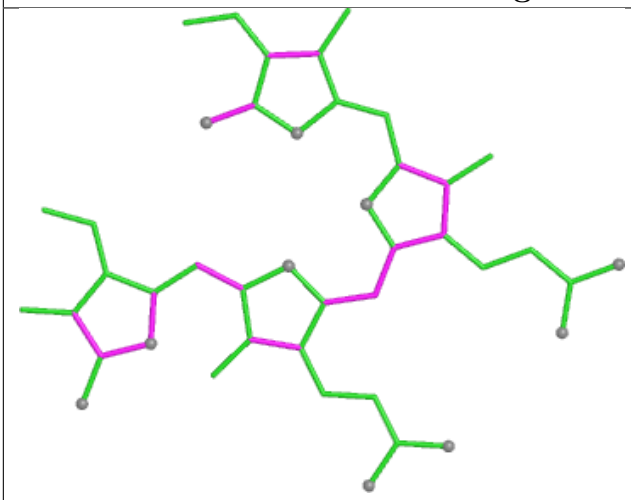


Rings

Ligand PEB FB 201



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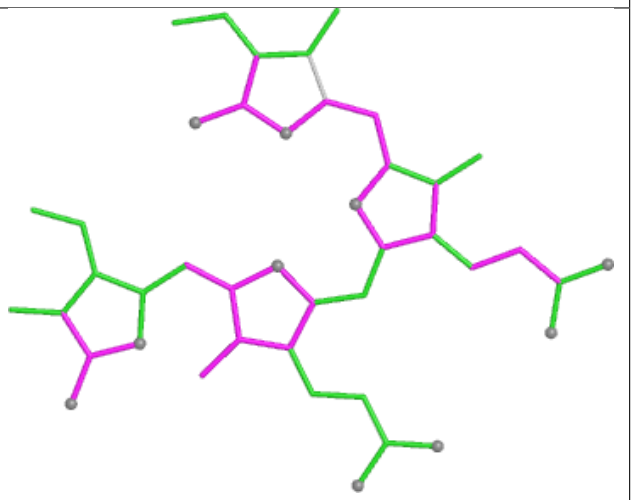

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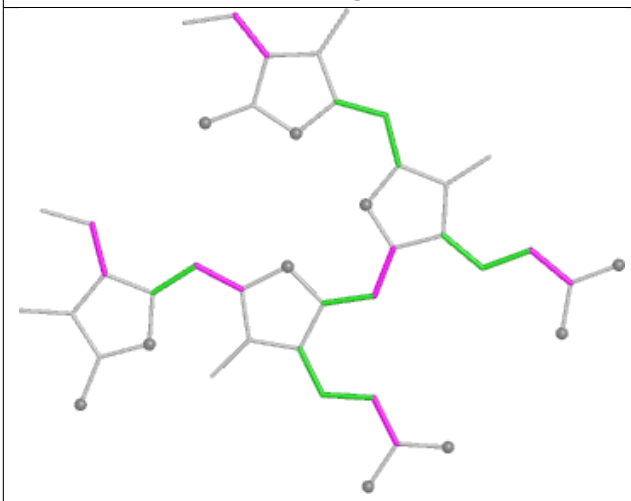

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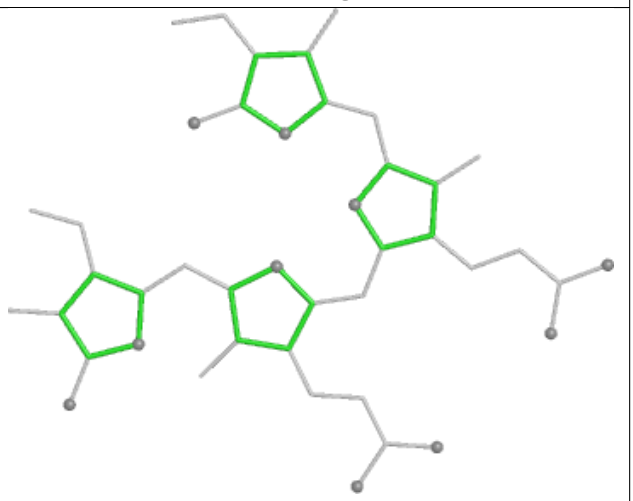
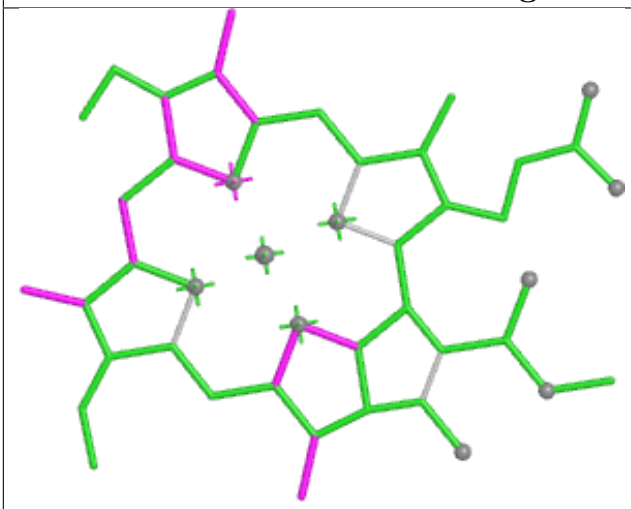


Rings

Ligand CLA 42 607



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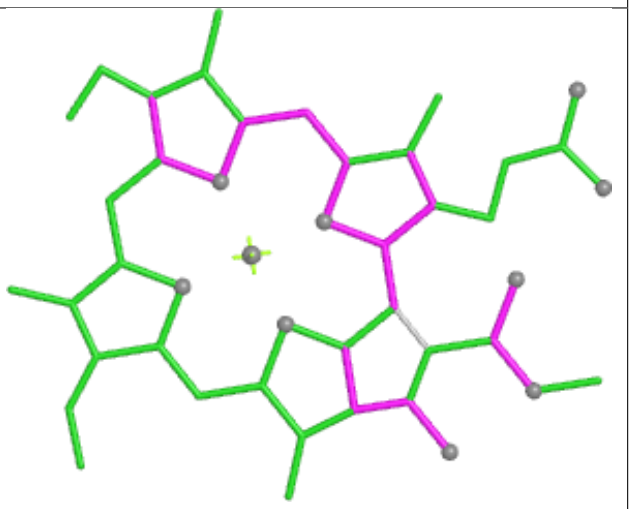

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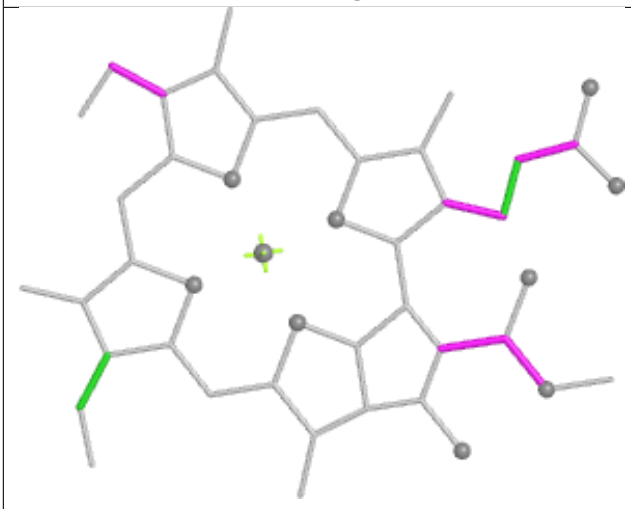
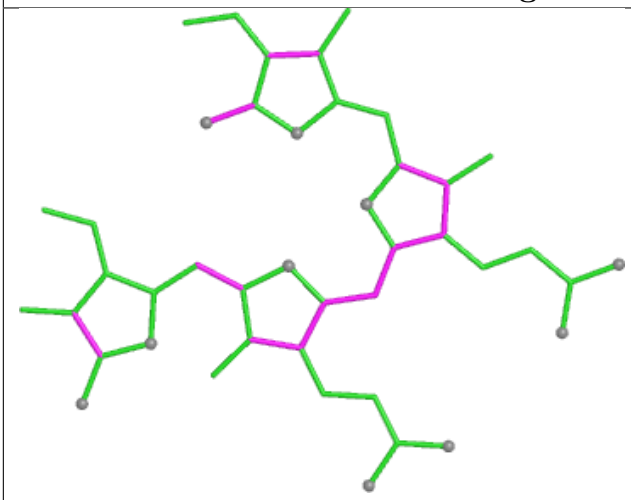


Torsions



Rings

Ligand PEB tF 201



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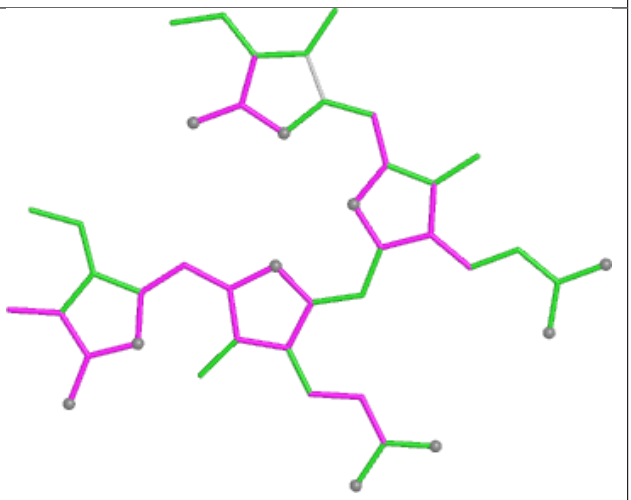

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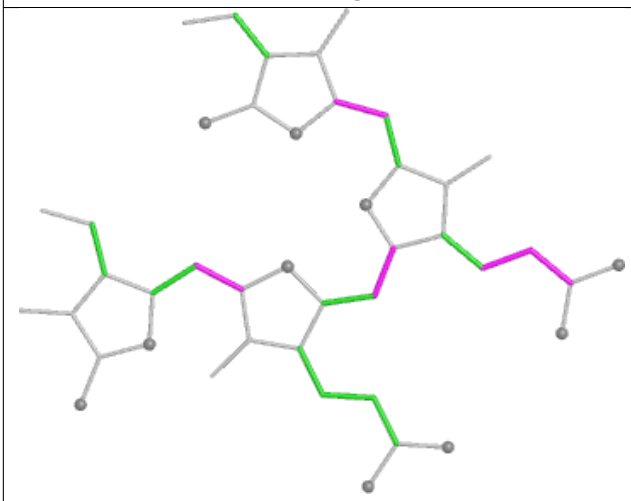

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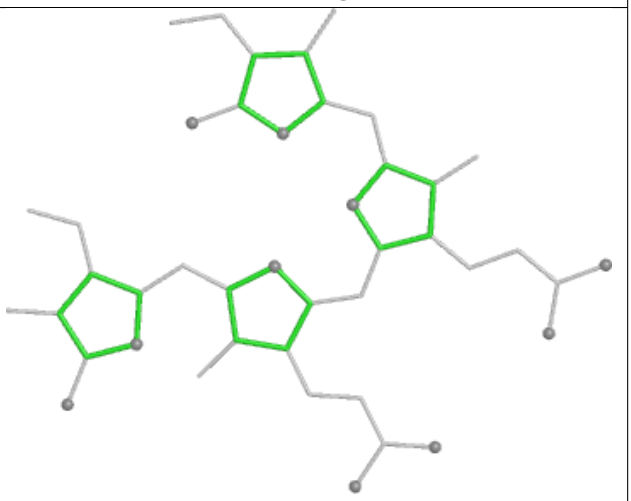

Rings

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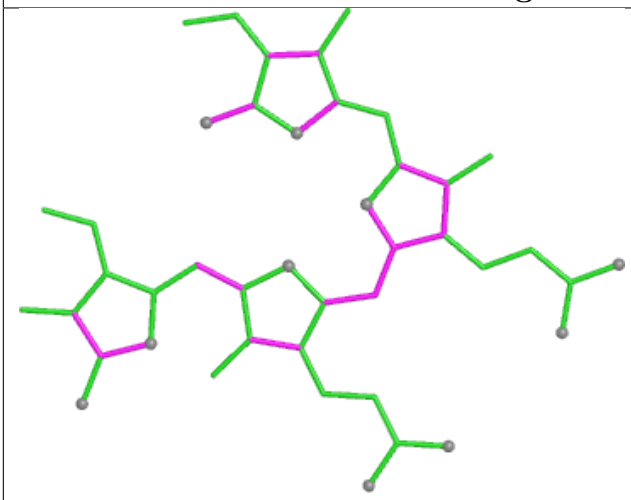

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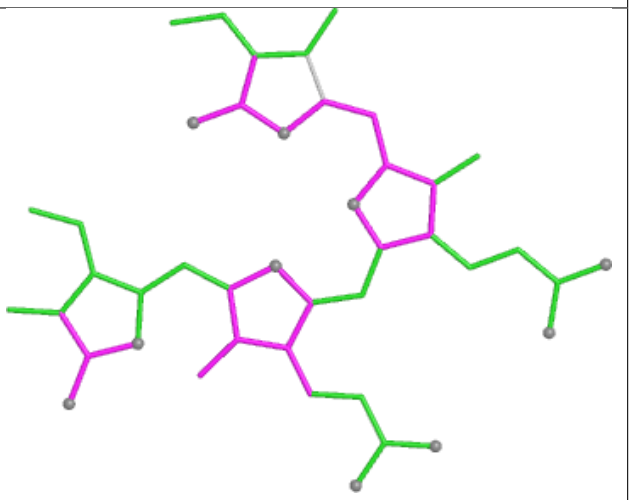

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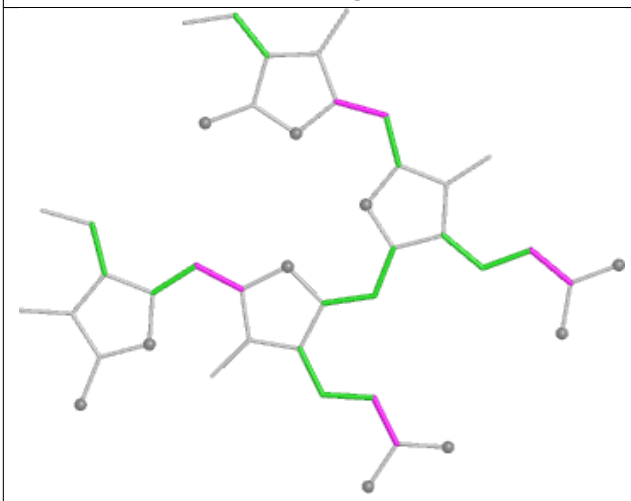

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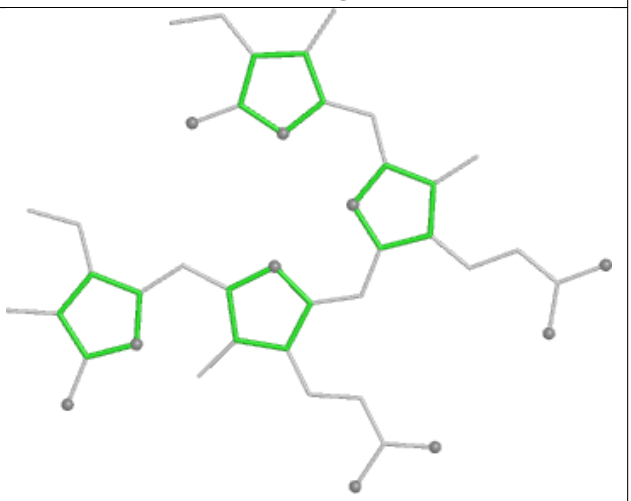

Rings

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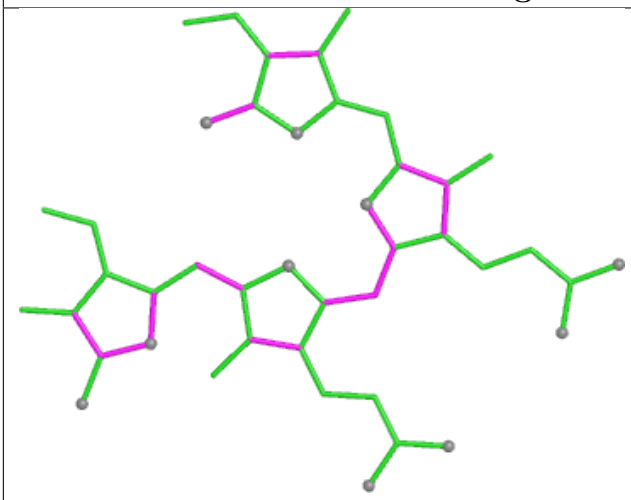

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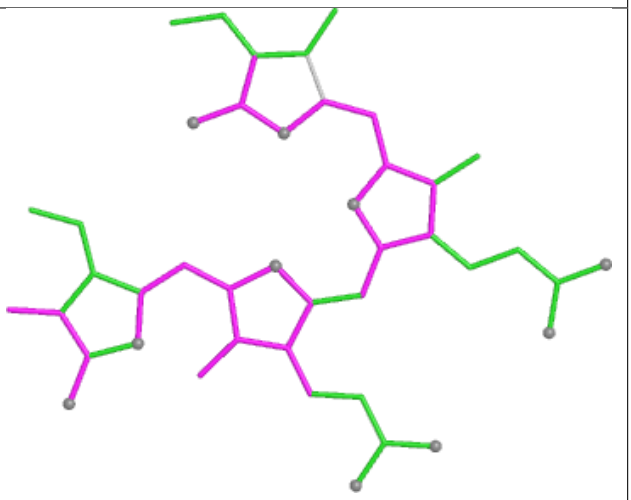

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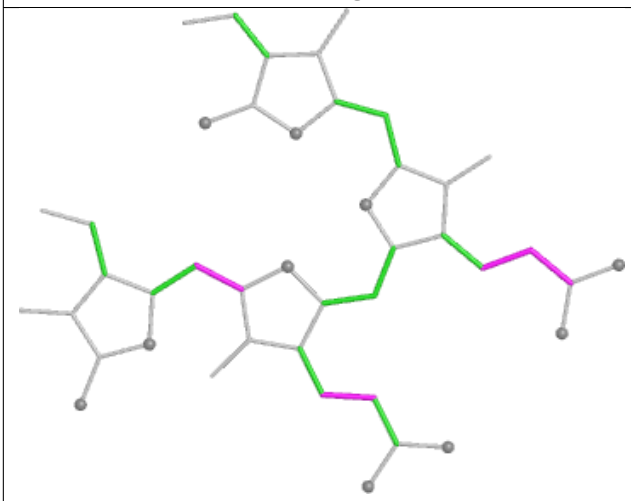

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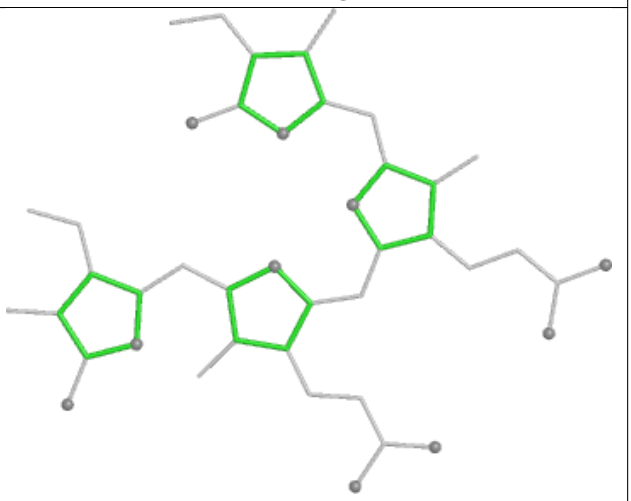
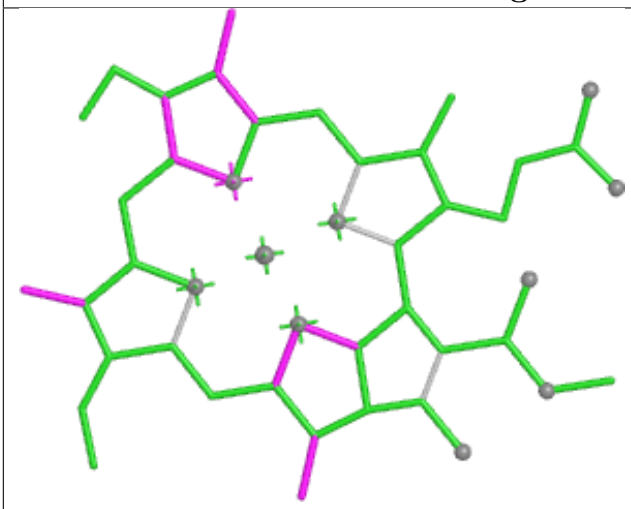


Rings

Ligand CLA BN 814



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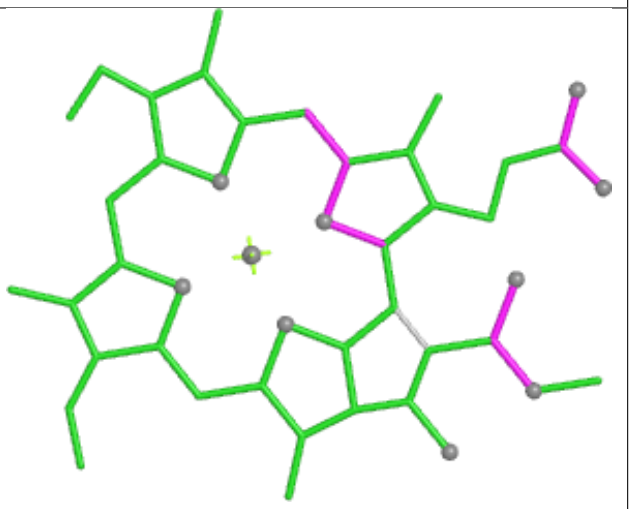

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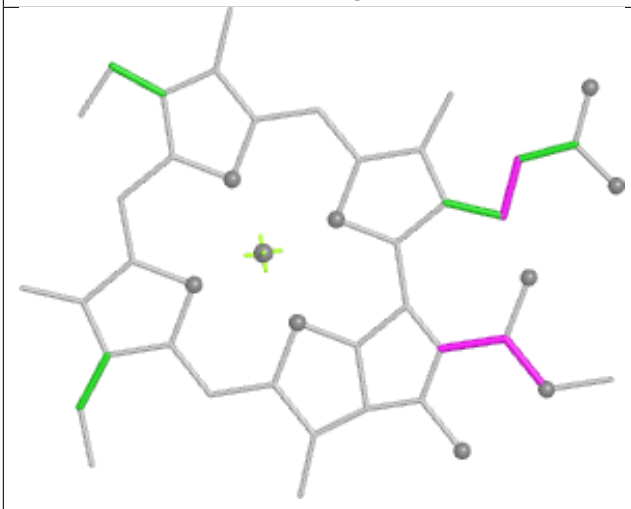
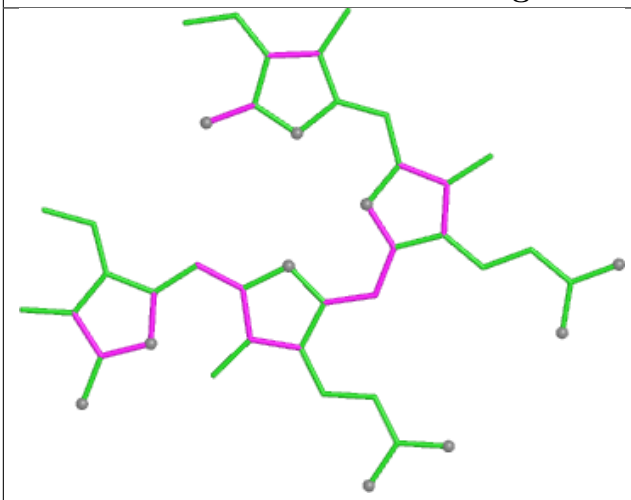


Torsions



Rings

Ligand PEB TB 201



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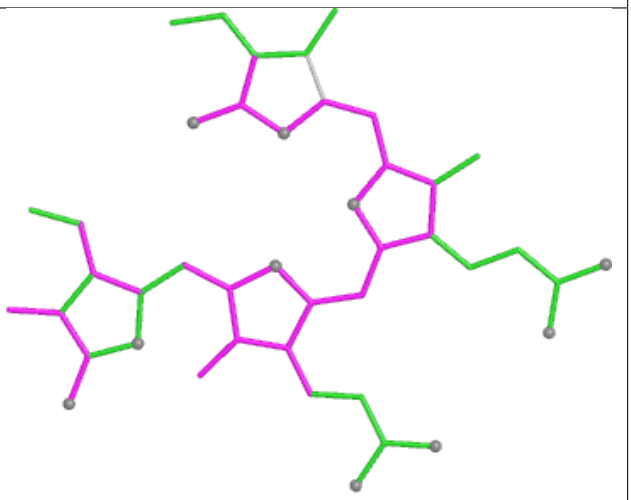

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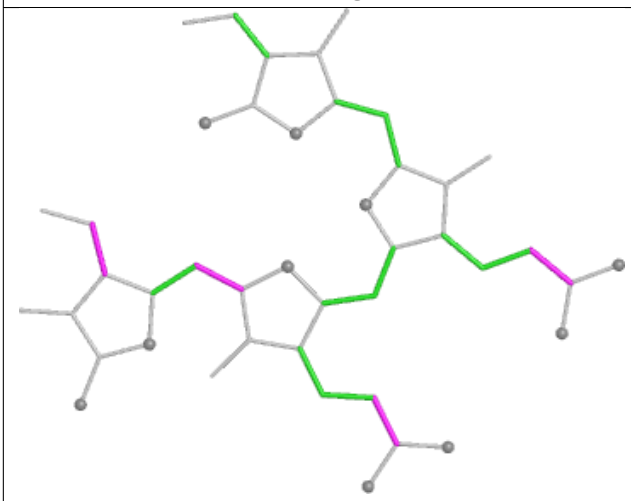

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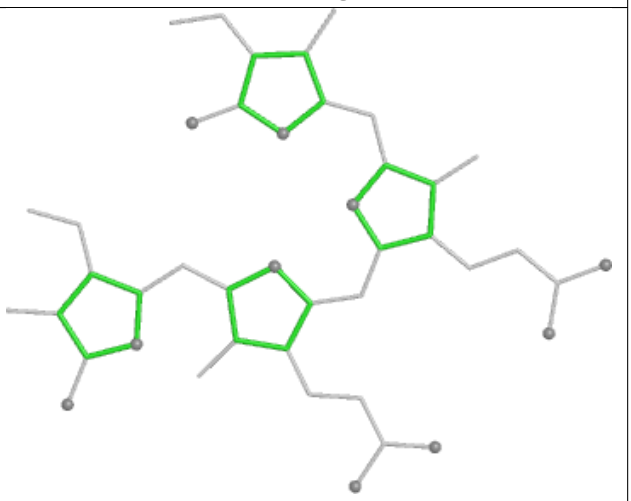

Rings

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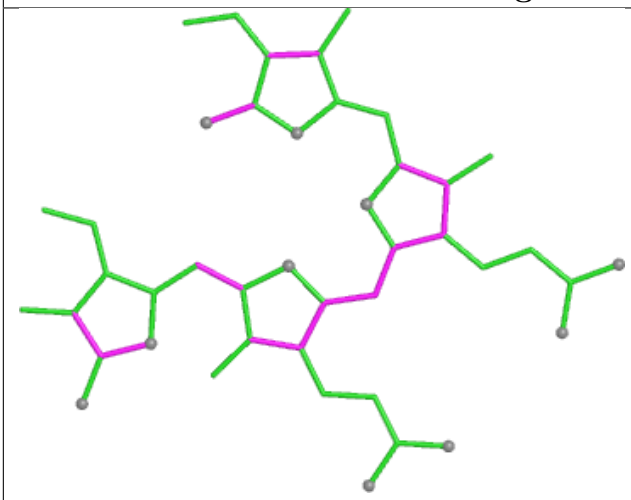

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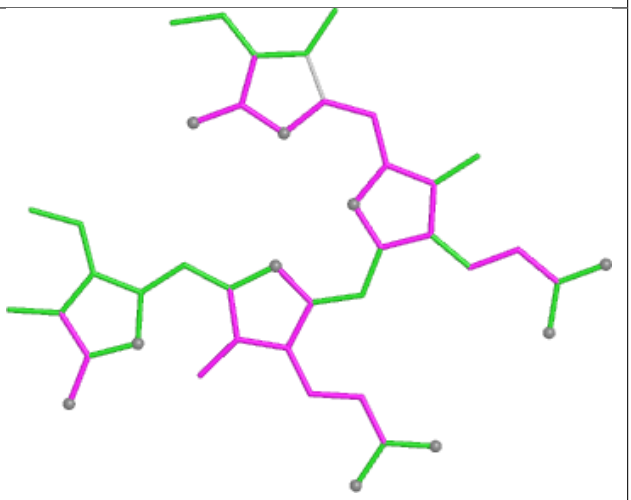

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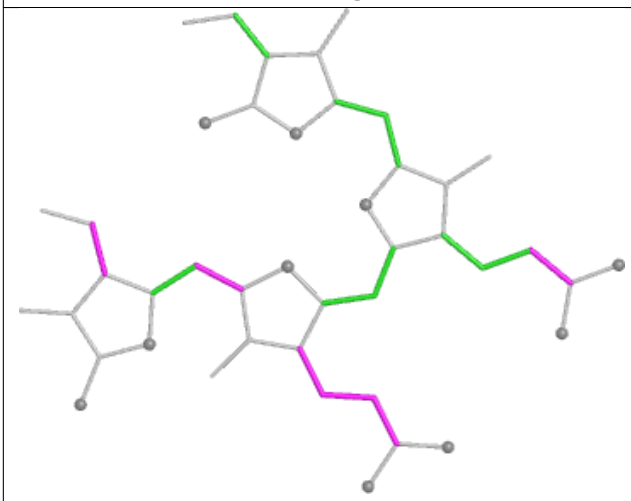

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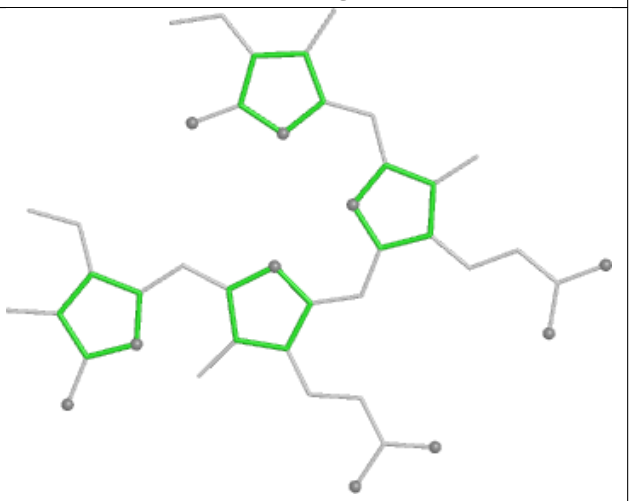
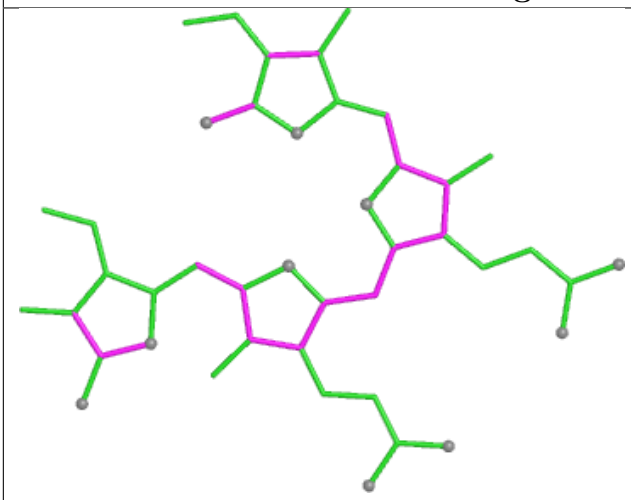


Rings

Ligand PEB pK 202



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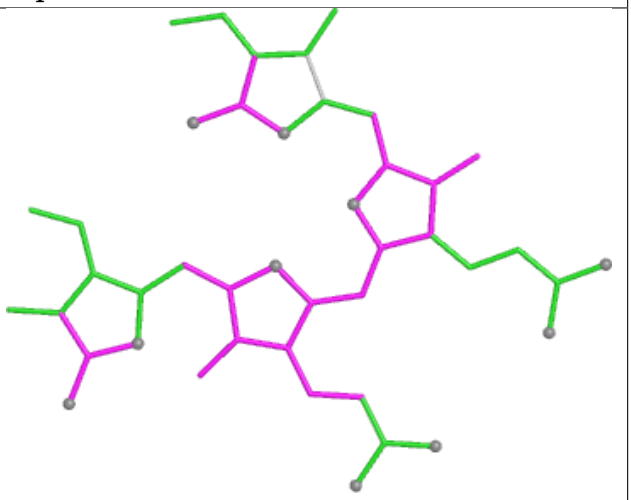

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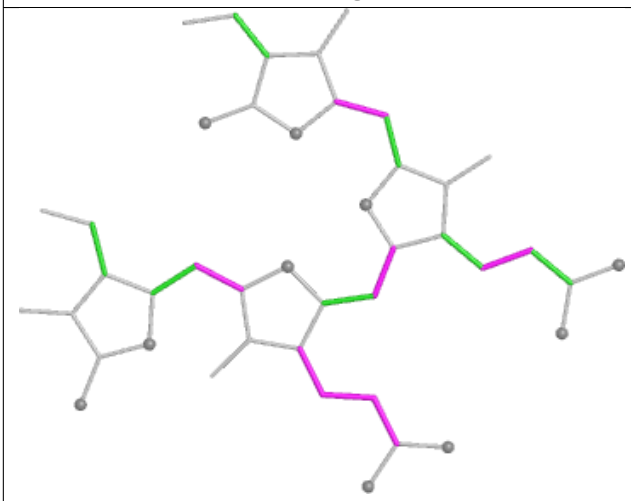

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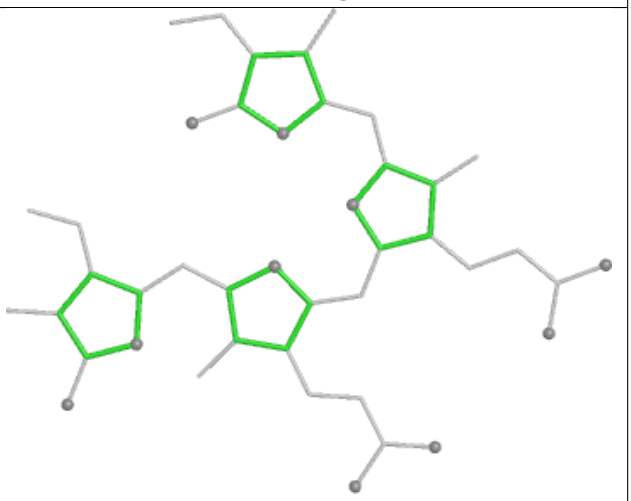
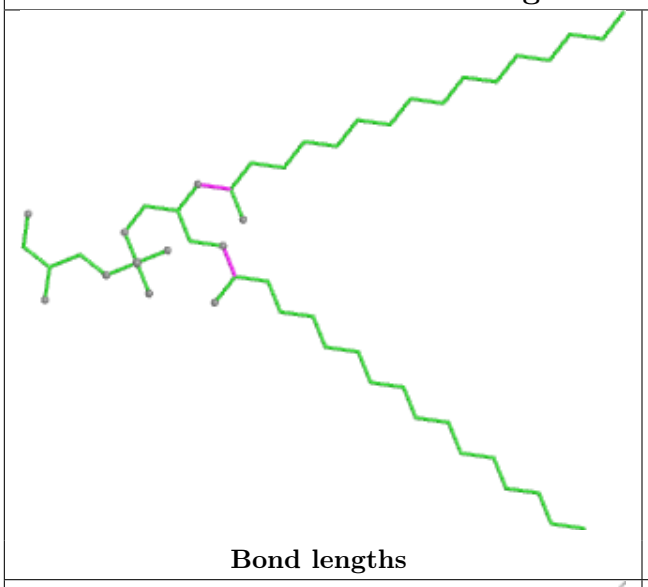


Rings

Ligand LHG l6 101



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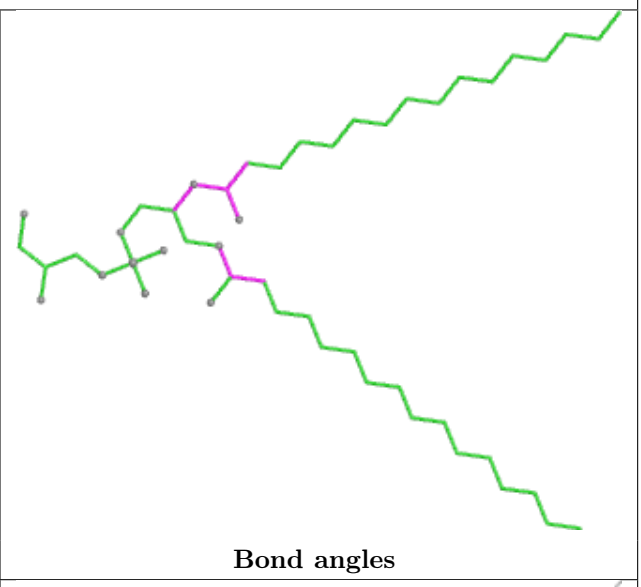
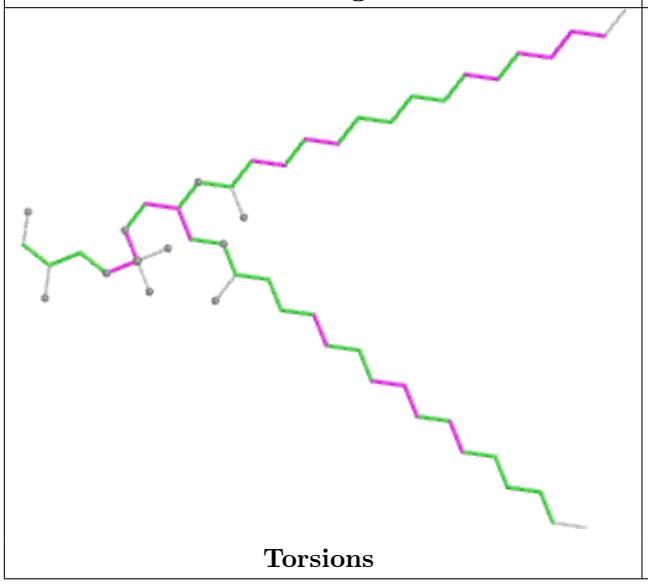


Bond angles



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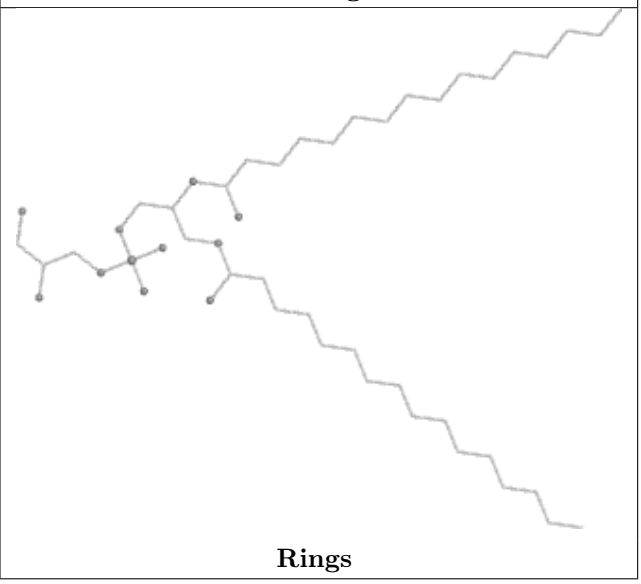
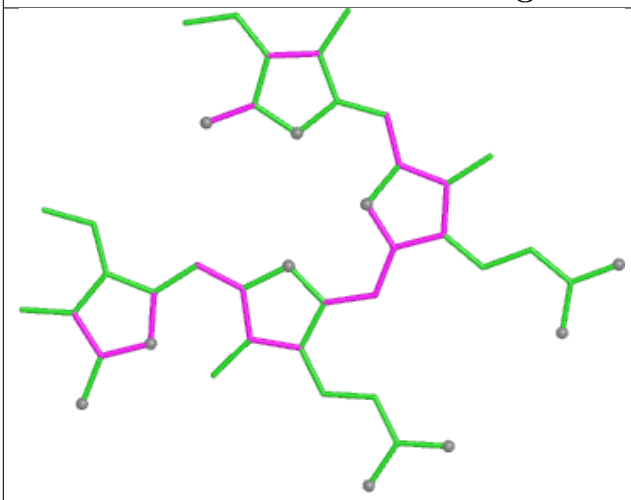


Rings

Ligand PEB dF 202



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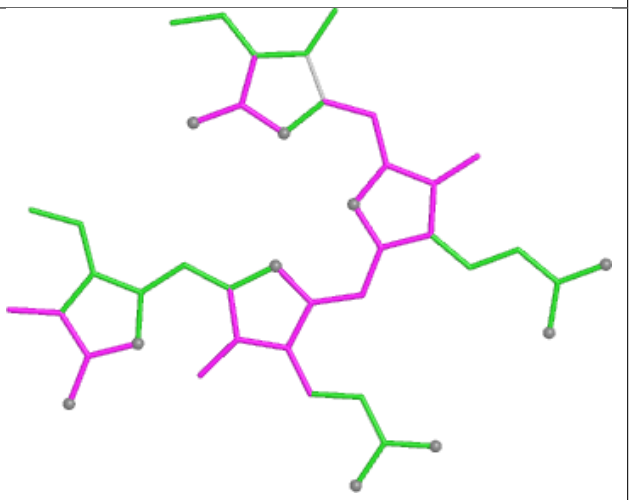
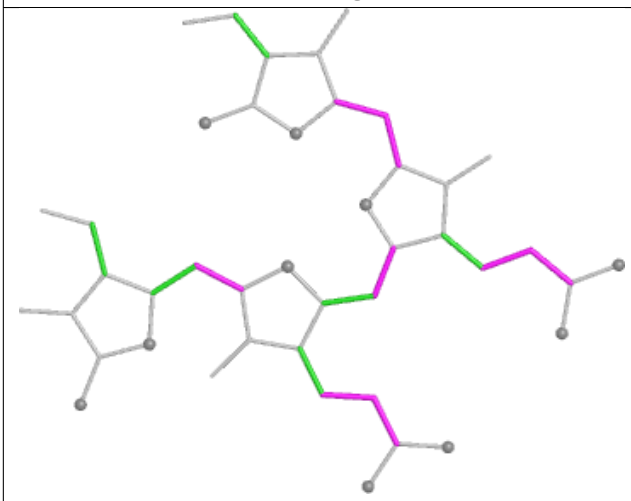


Bond angles



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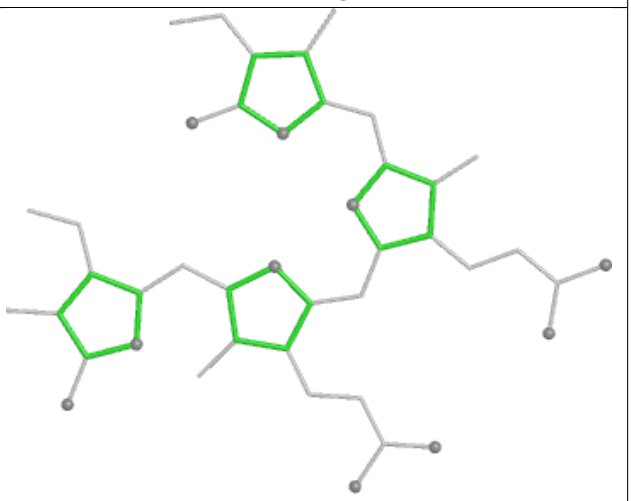
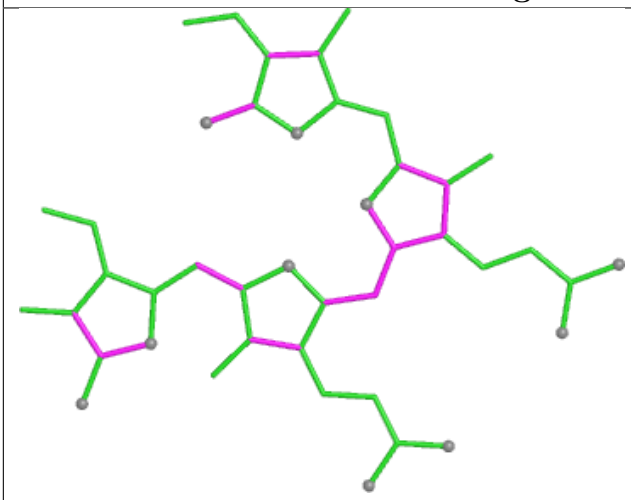


Rings

Ligand PEB CF 201



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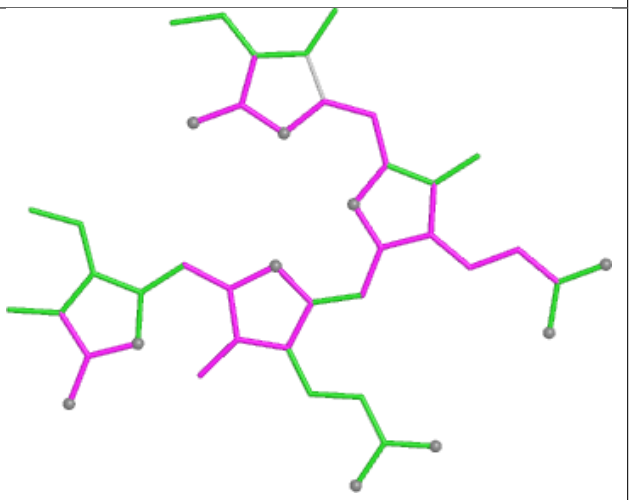
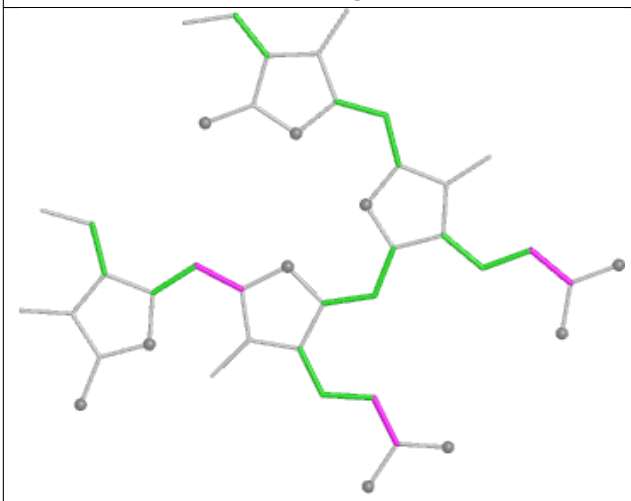


Bond angles



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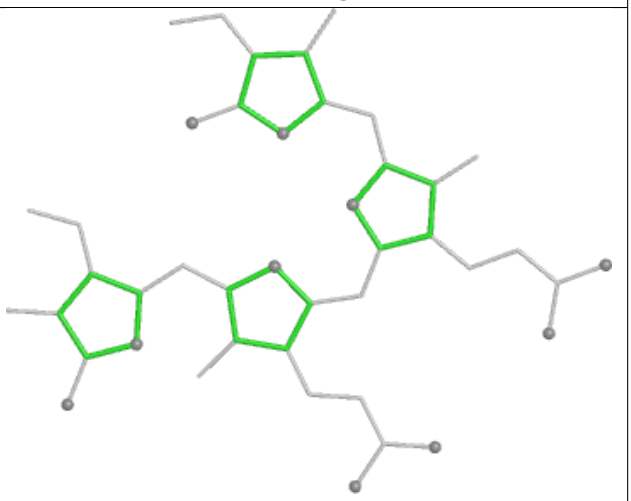
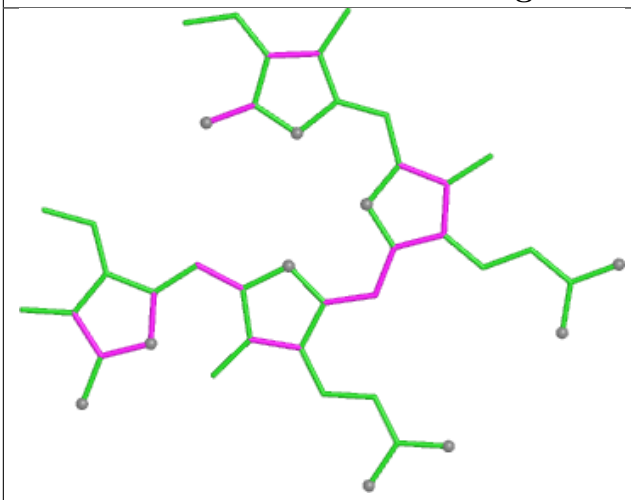
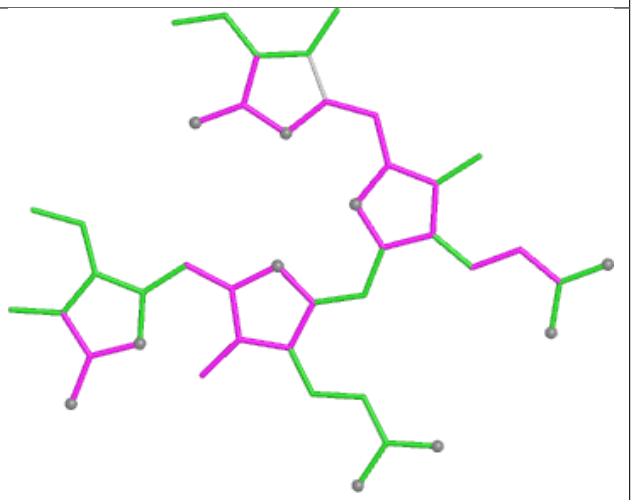


Rings

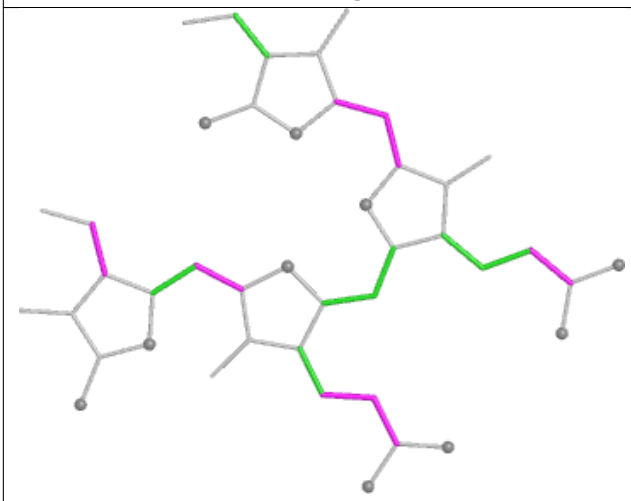
Ligand PEB A4 305



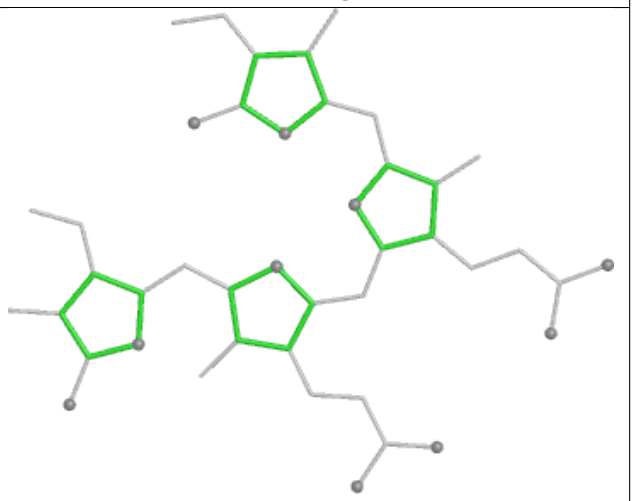
Bond lengths



Bond angles

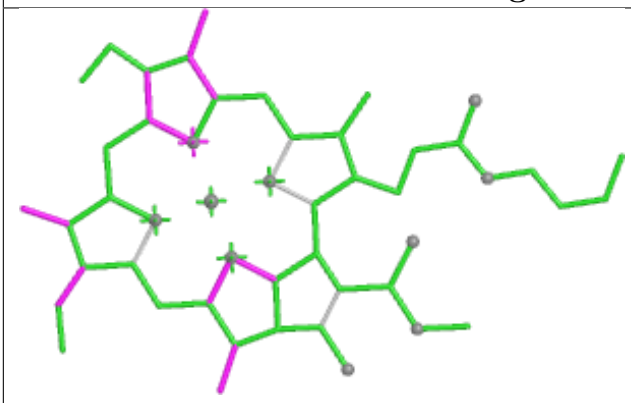


Torsions



Rings

Ligand CLA KN 105



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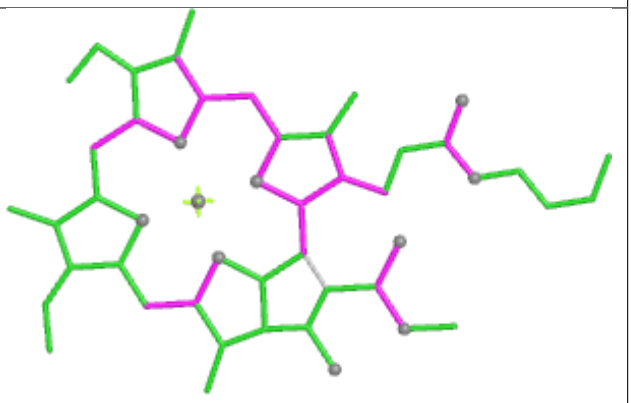

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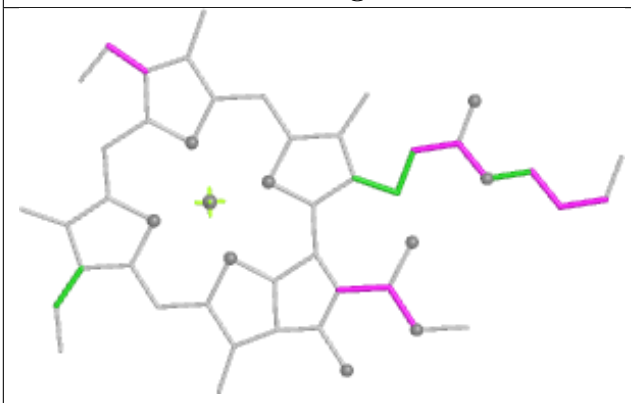

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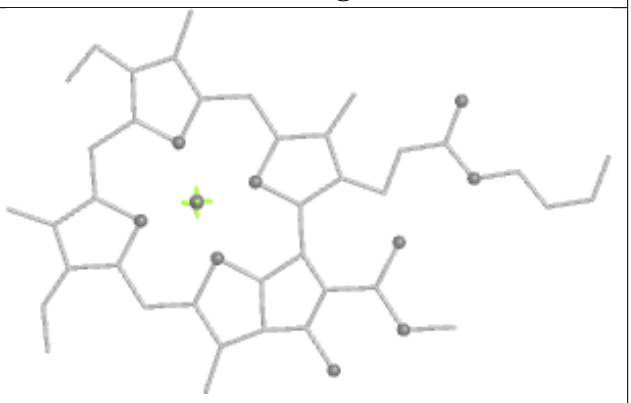
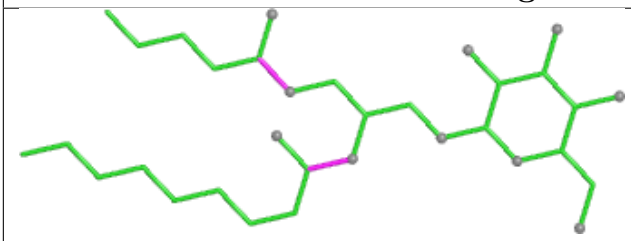


Rings

Ligand LMG j6 102



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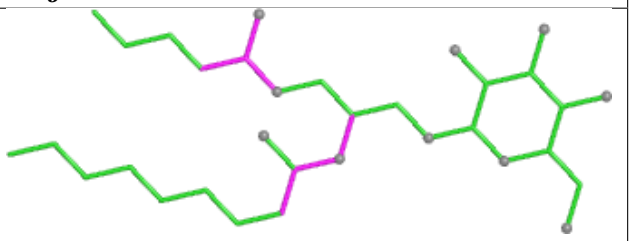

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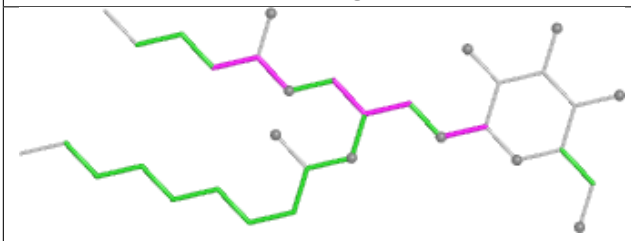

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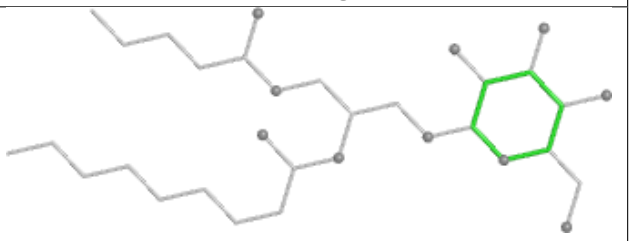
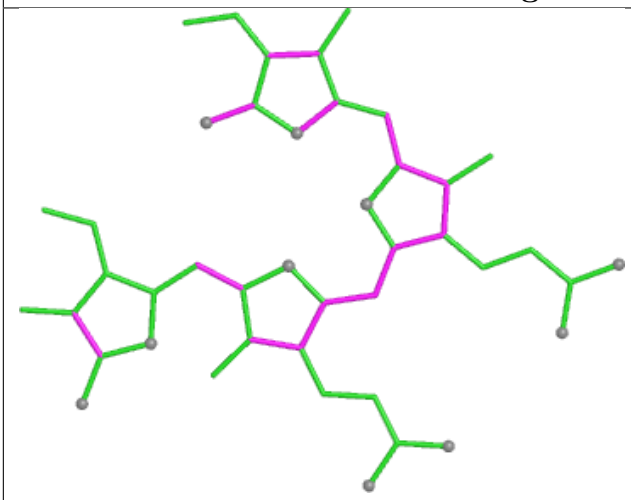


Rings

Ligand PEB lF 201



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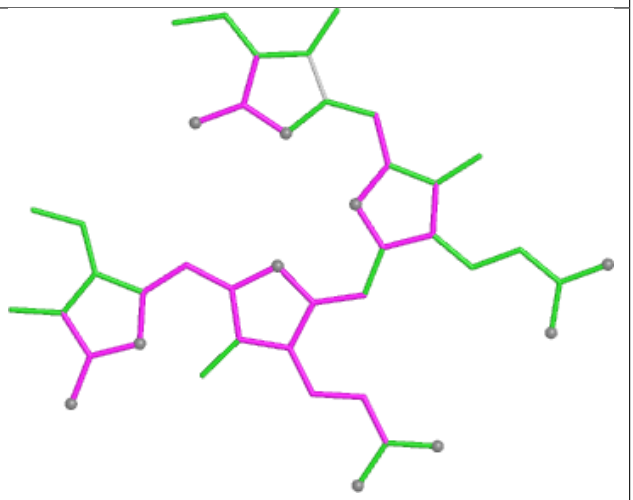

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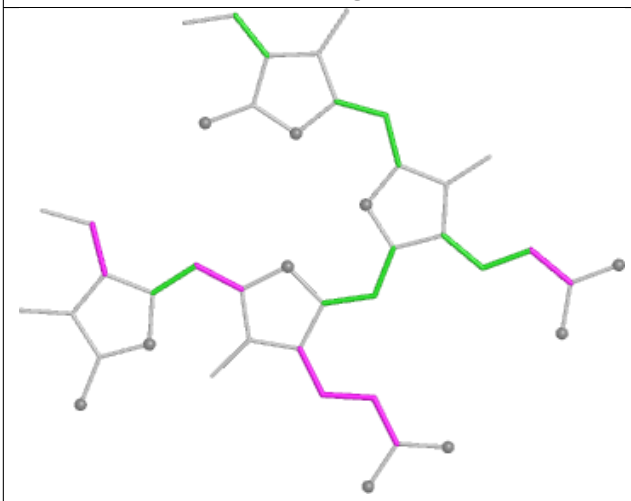

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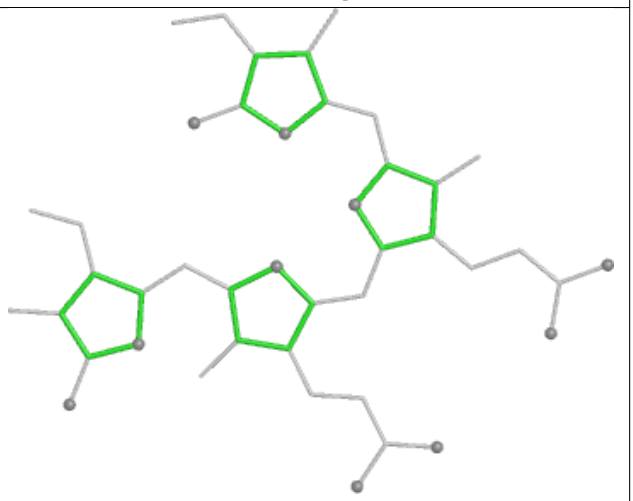
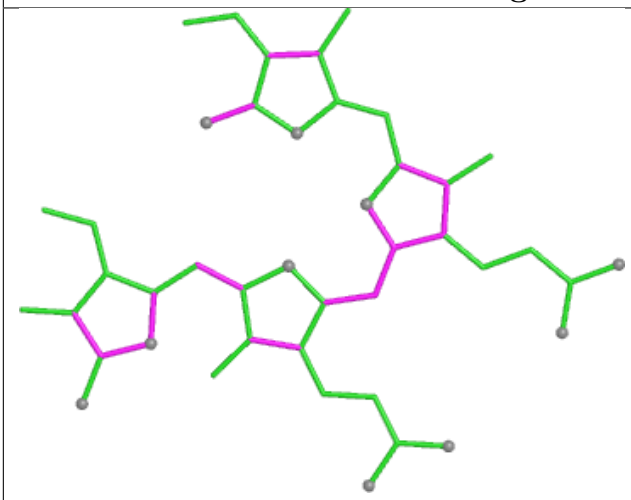


Rings

Ligand PEB YG 202



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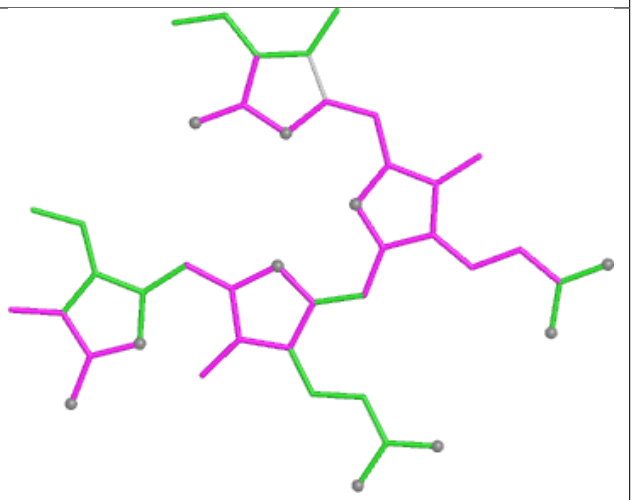

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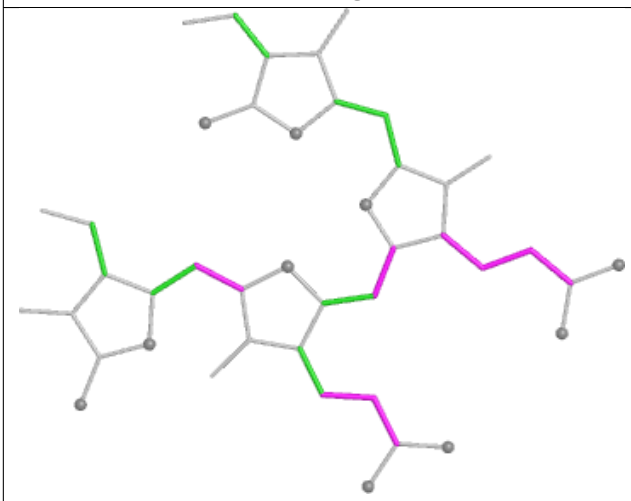

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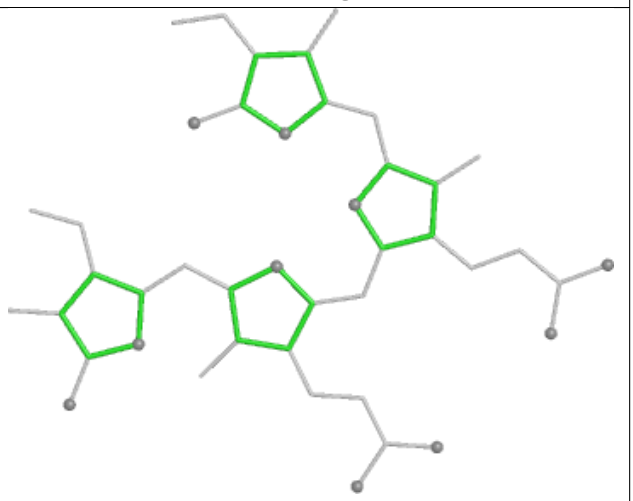
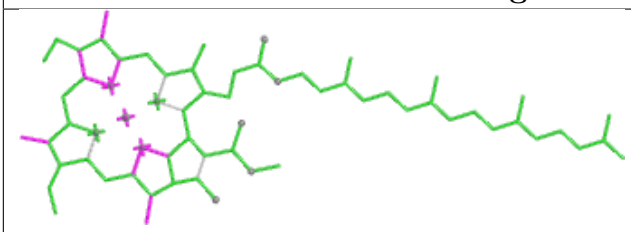


Rings

Ligand CLA AN 820



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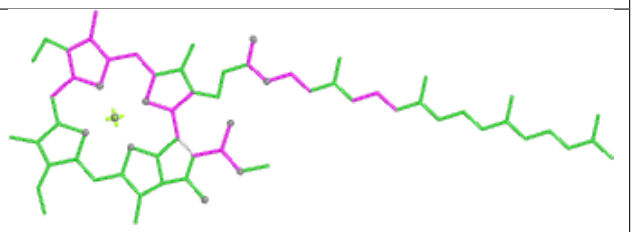
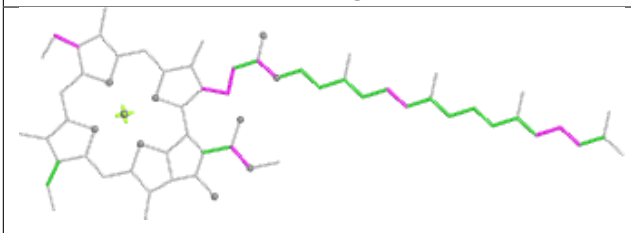


Bond angles



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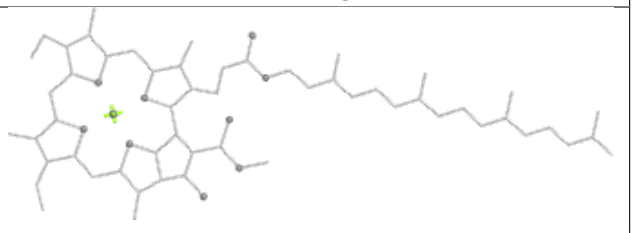
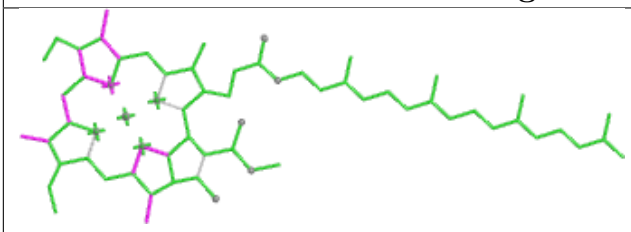


Rings

Ligand CLA b6 611



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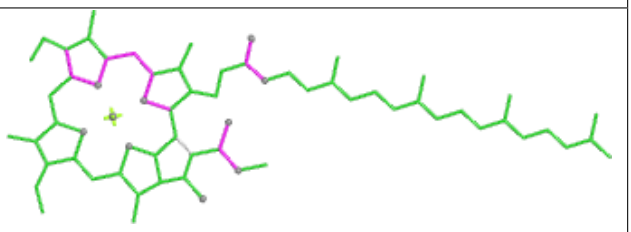
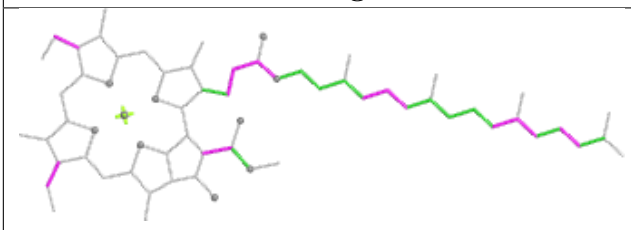


Bond angles



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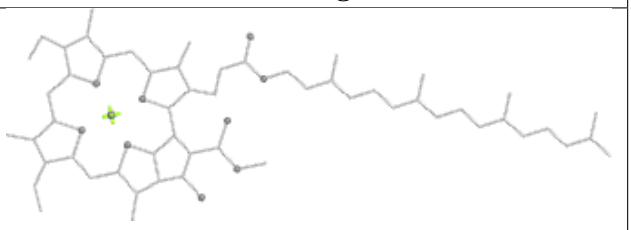
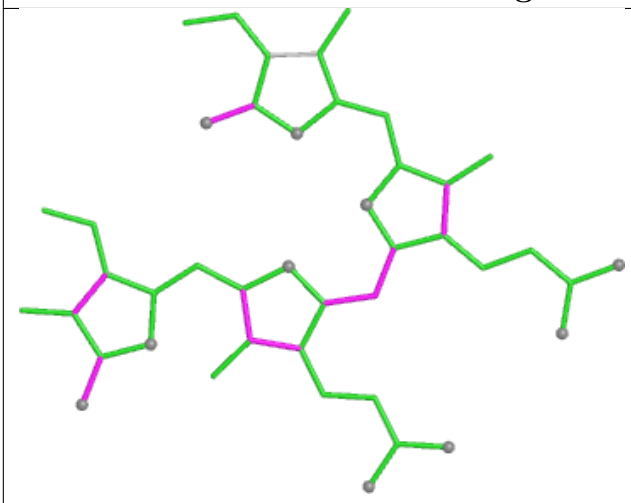


Rings

Ligand PUB yF 302



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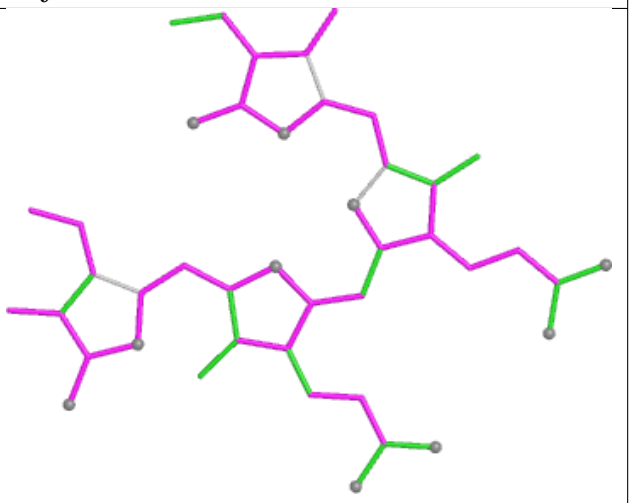

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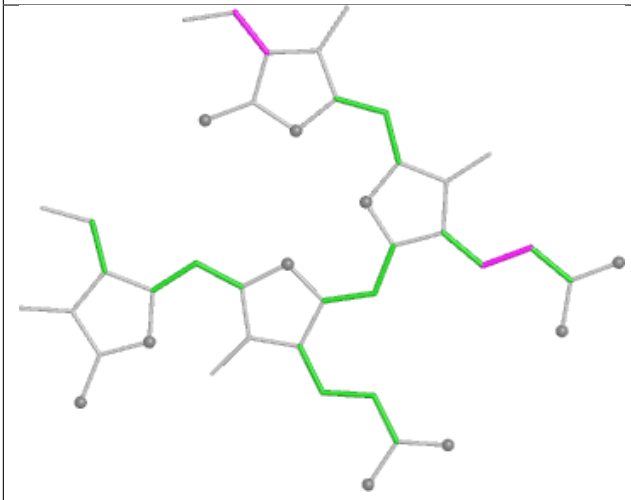

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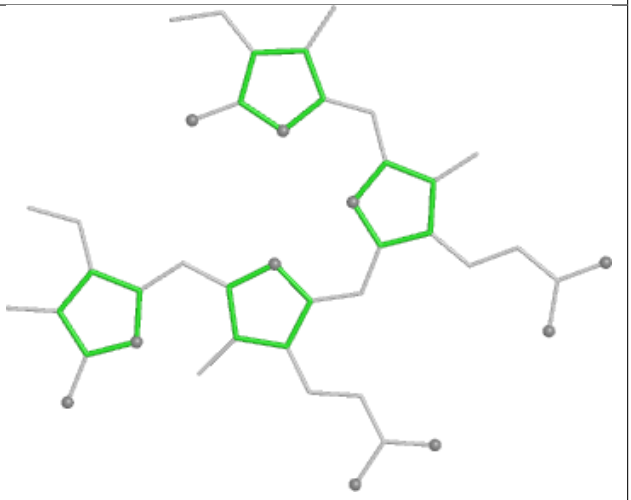
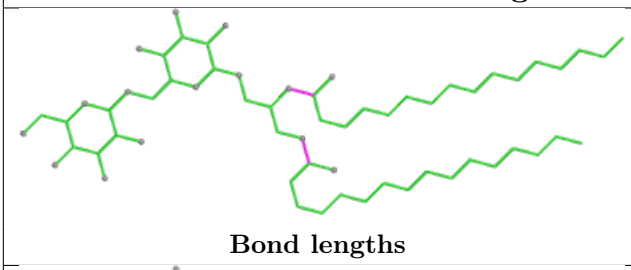


Rings

Ligand DGD C6 521



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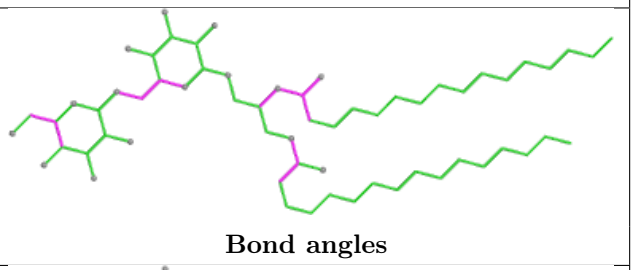

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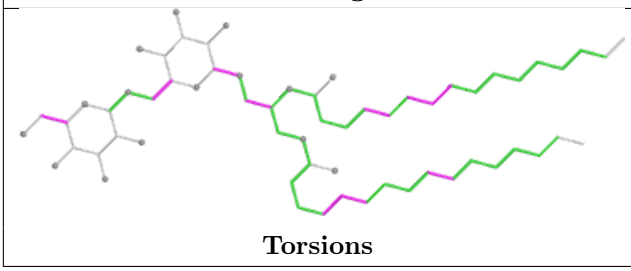

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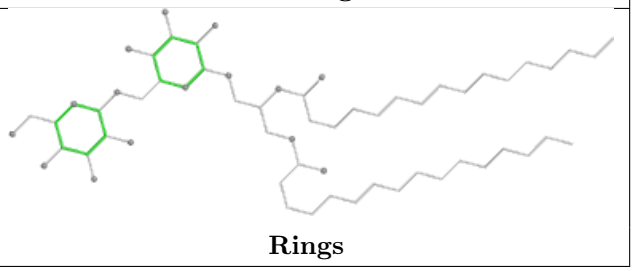
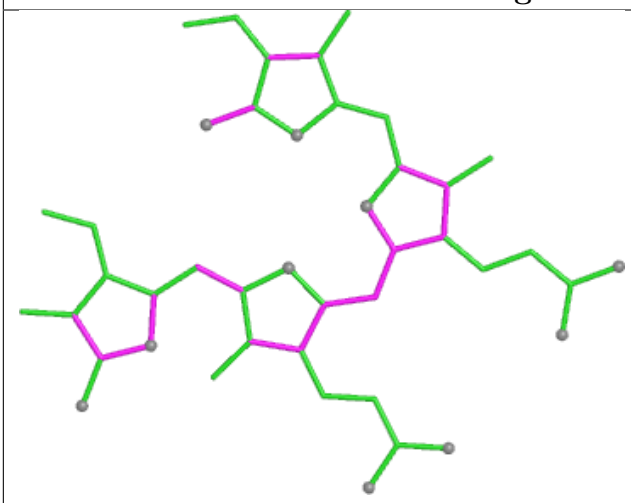


Rings

Ligand PEB vK 202



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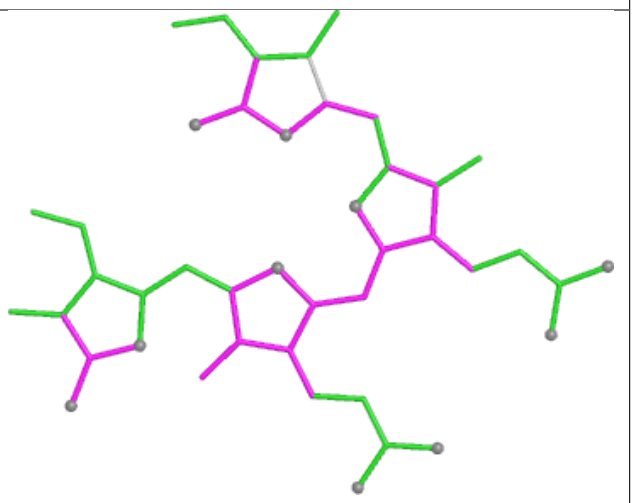
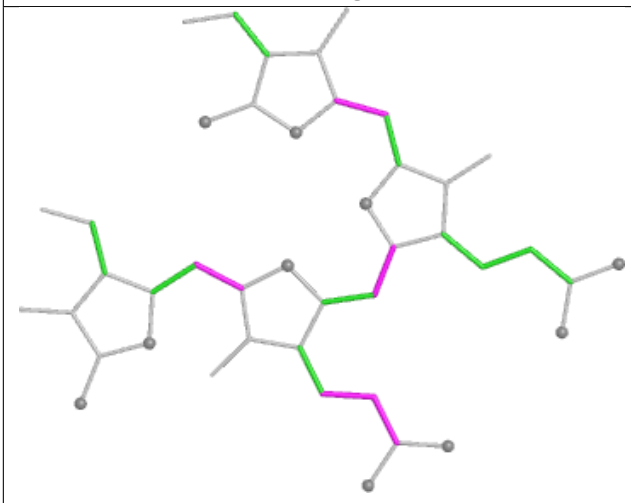


Bond angles



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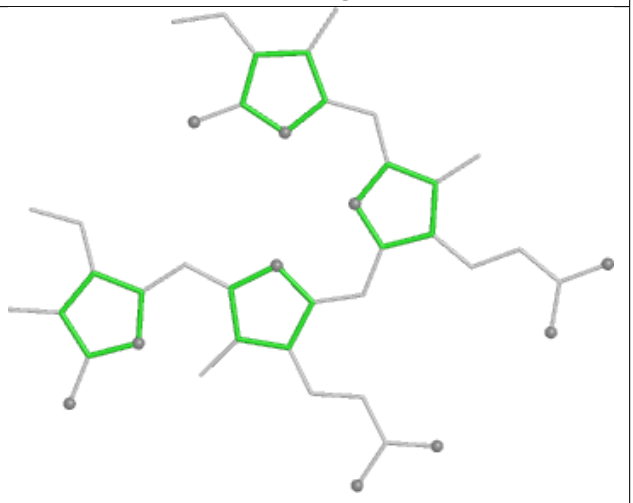
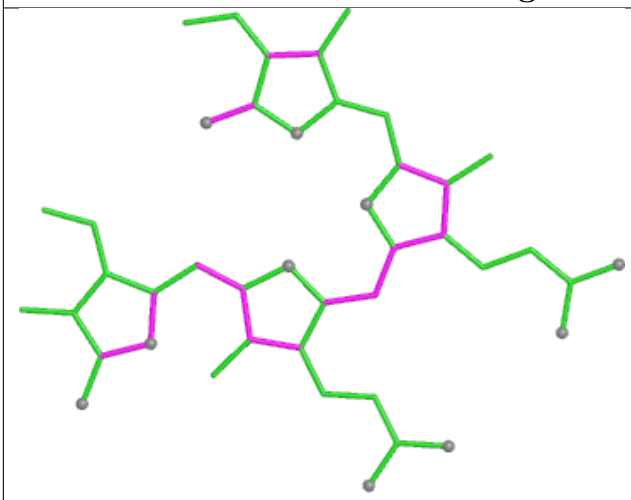


Rings

Ligand PEB jH 201



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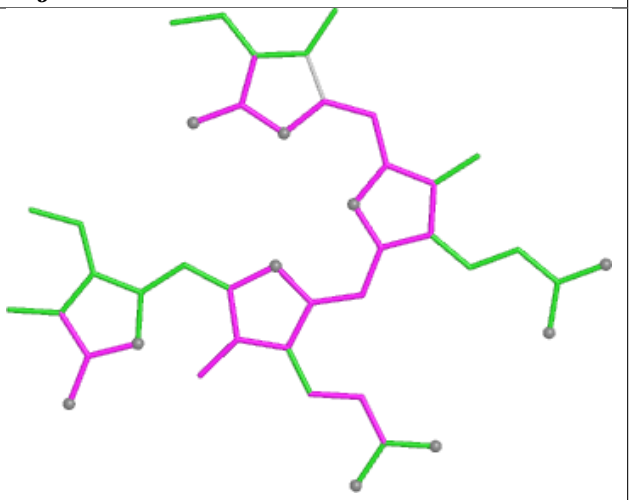

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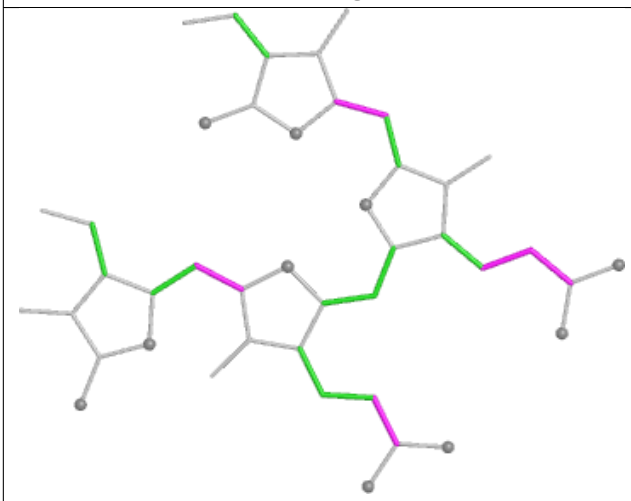

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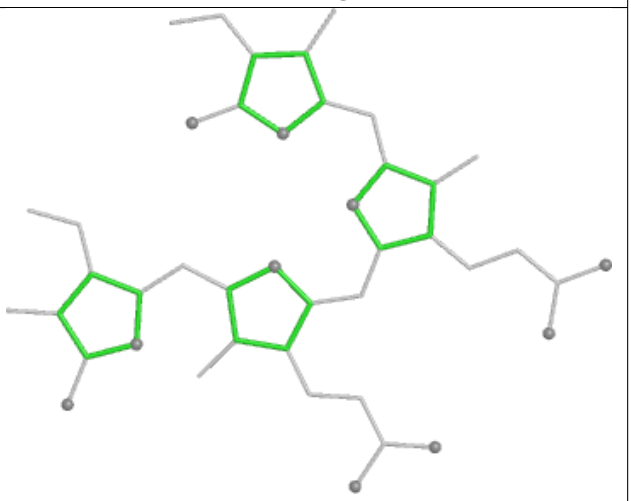
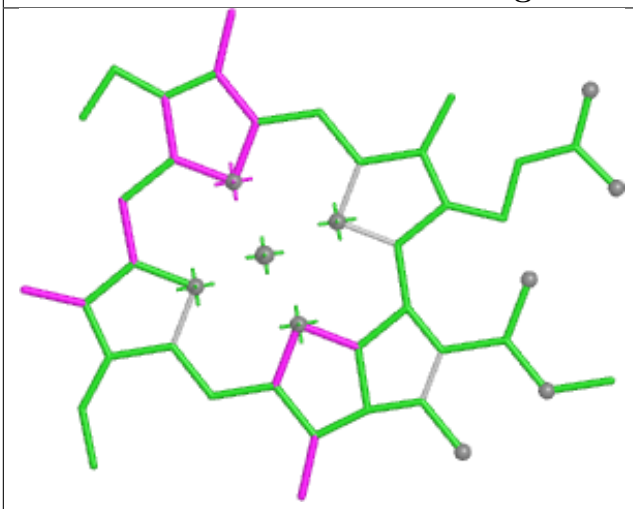


Rings

Ligand CLA 4N 603



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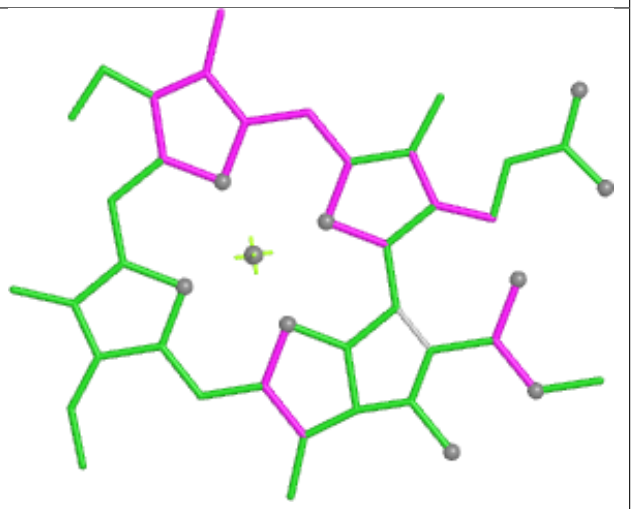
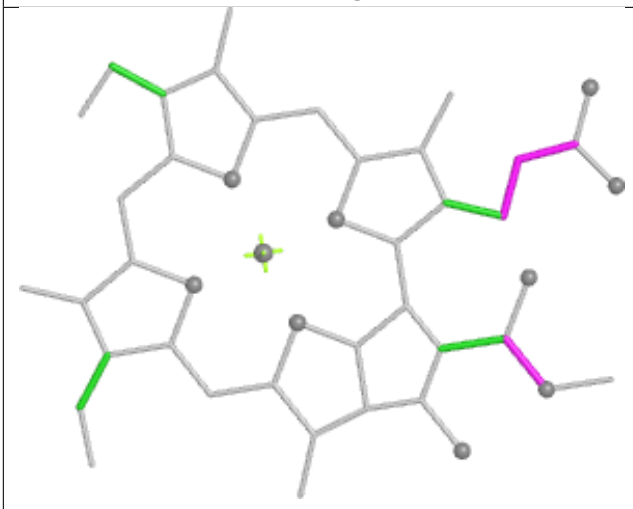


Bond angles

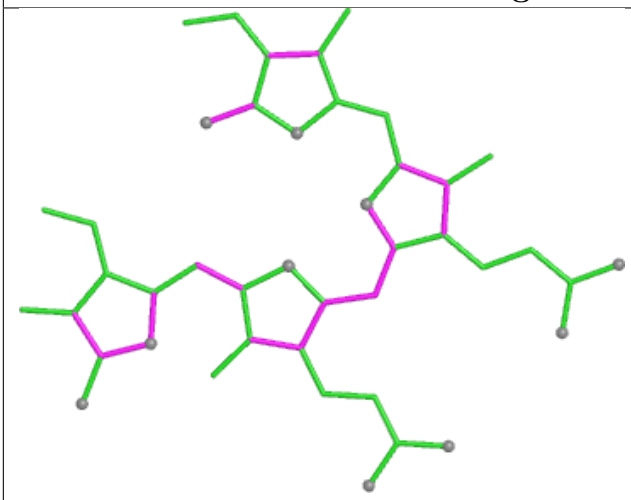


Torsions



Rings

Ligand PEB GF 203



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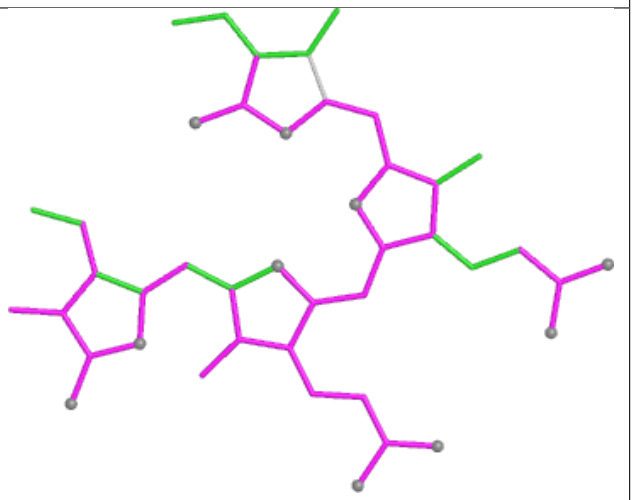
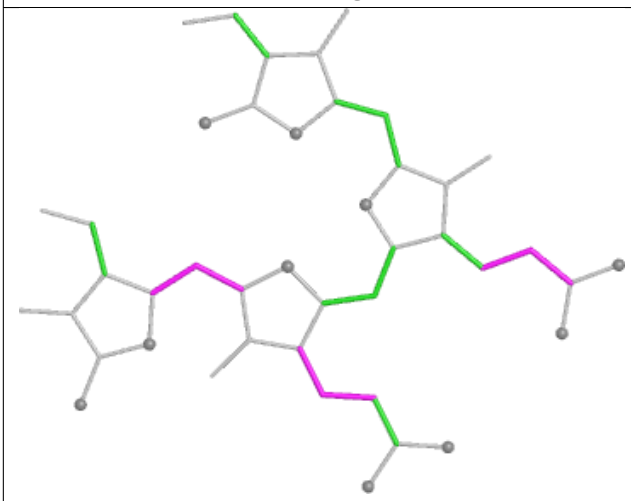


Bond angles



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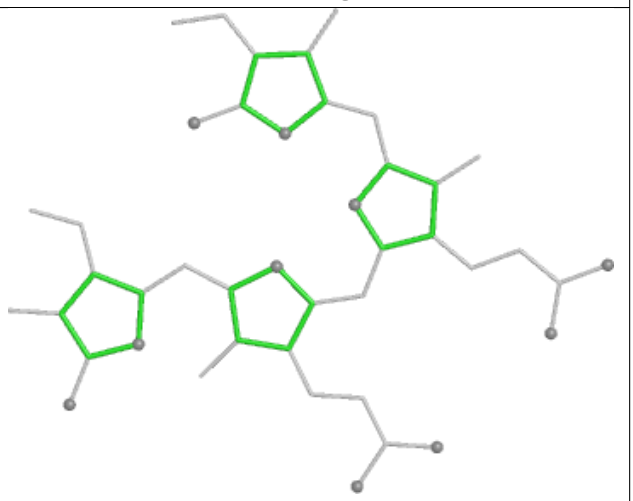
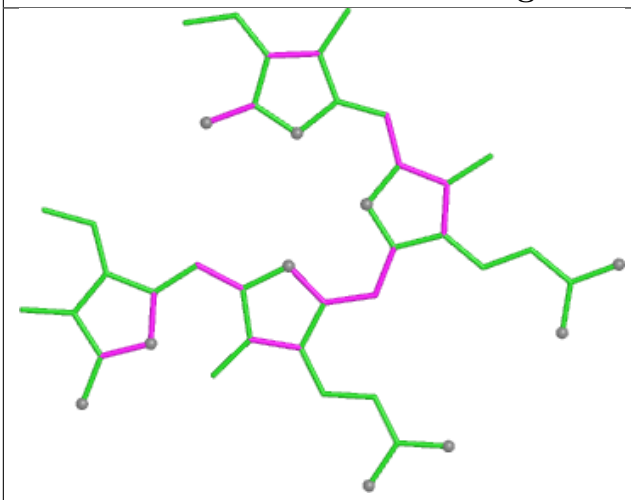


Rings

Ligand PEB gF 203



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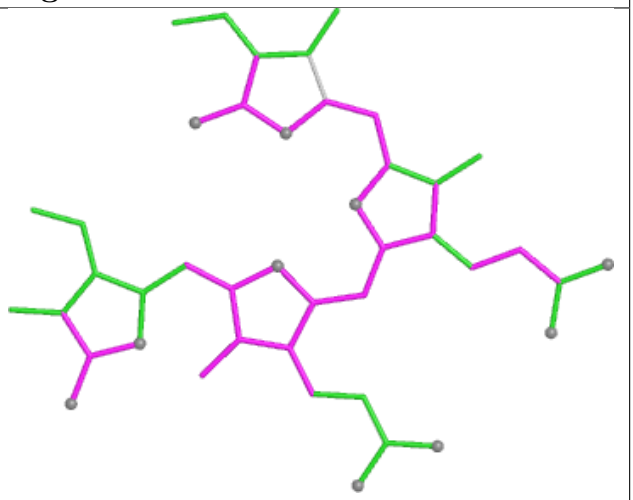
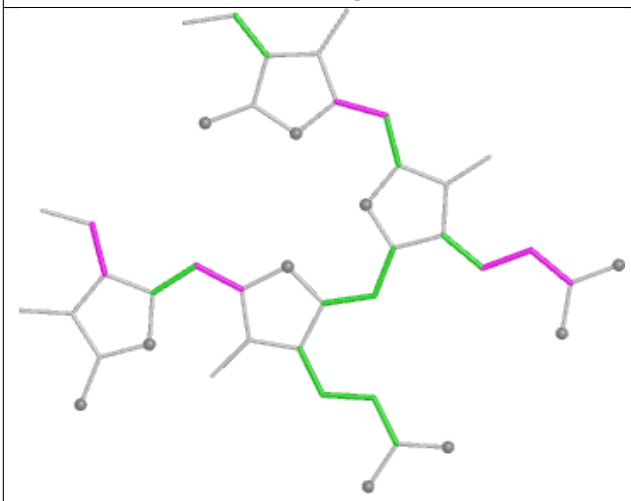


Bond angles



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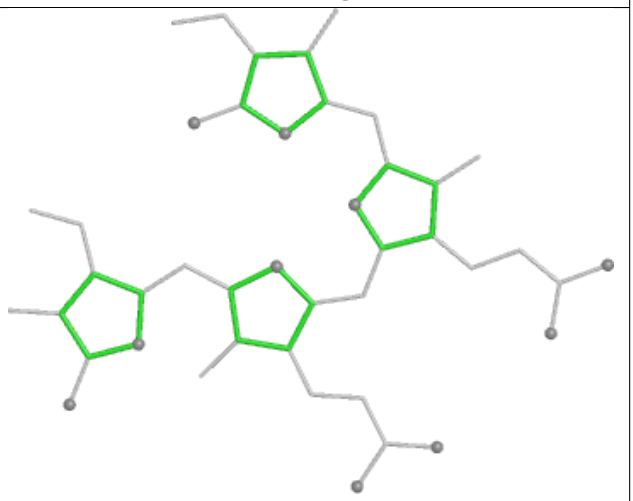
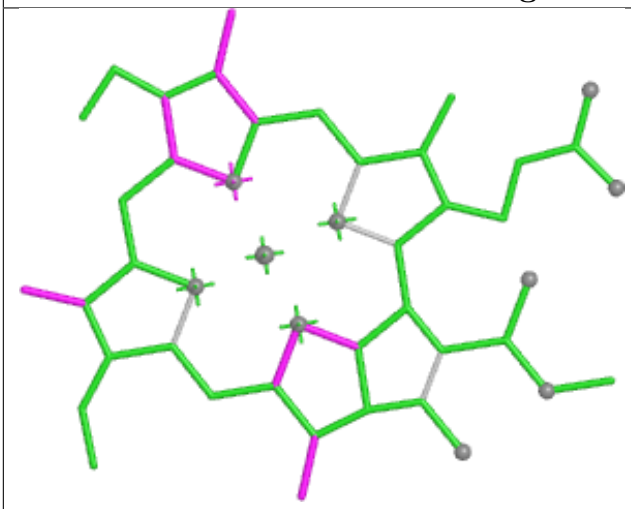


Rings

Ligand CLA 42 601



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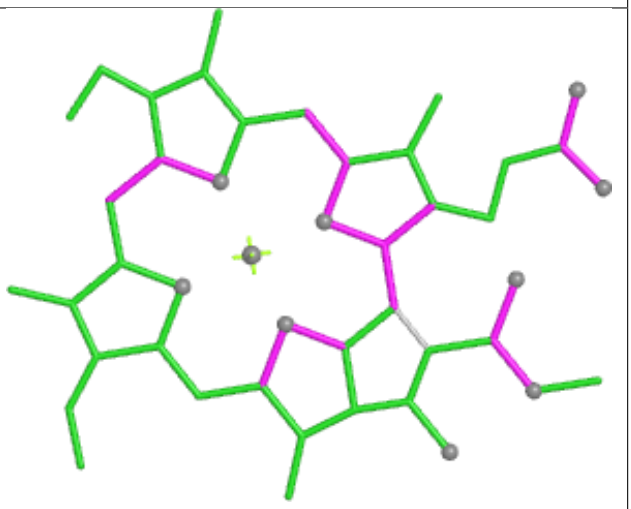
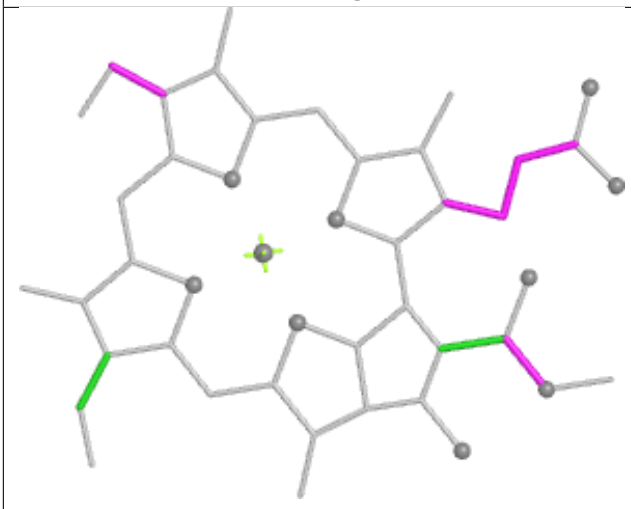


Bond angles

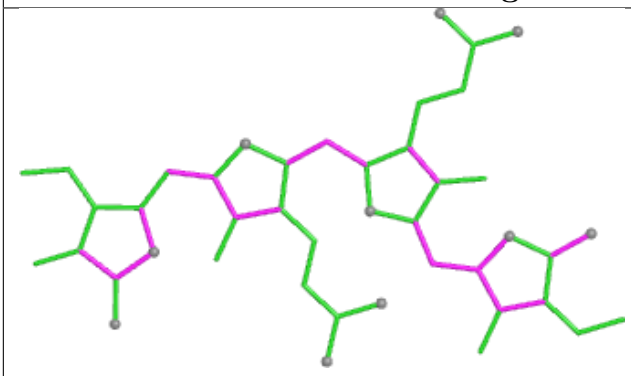


Torsions

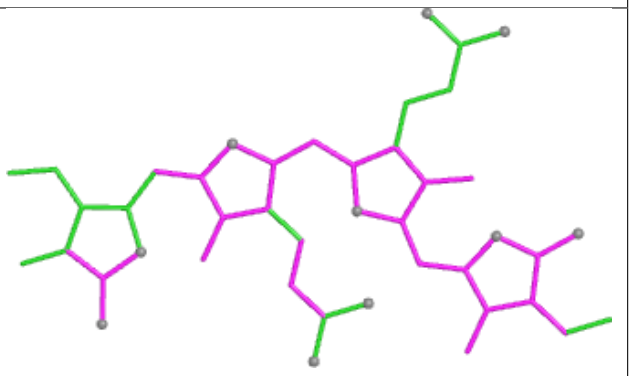


Rings

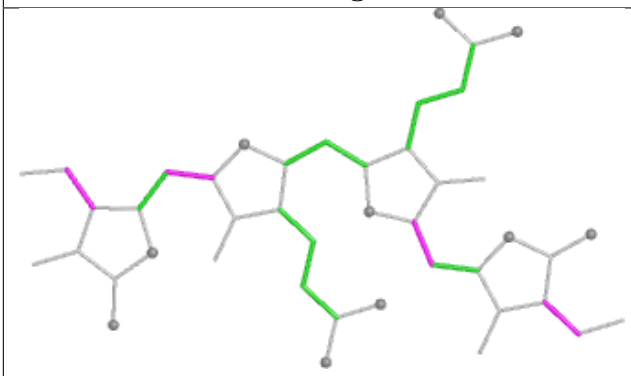
Ligand CYC FG 1001



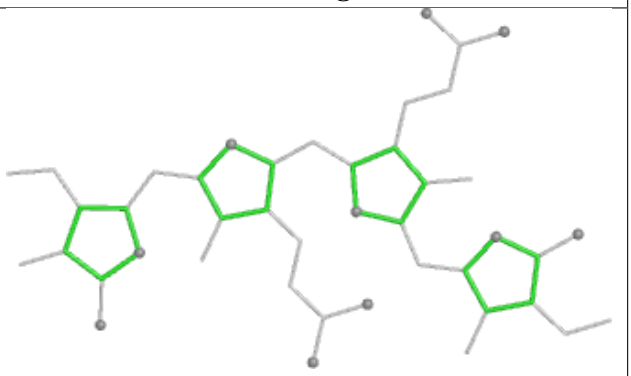
Bond lengths



Bond angles

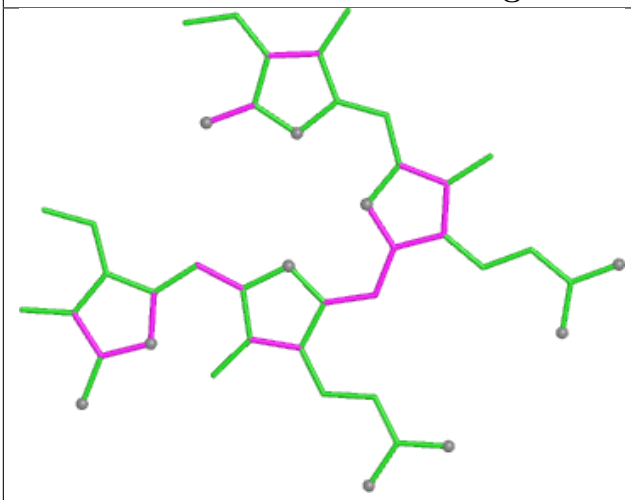


Torsions



Rings

Ligand PEB FH 1002



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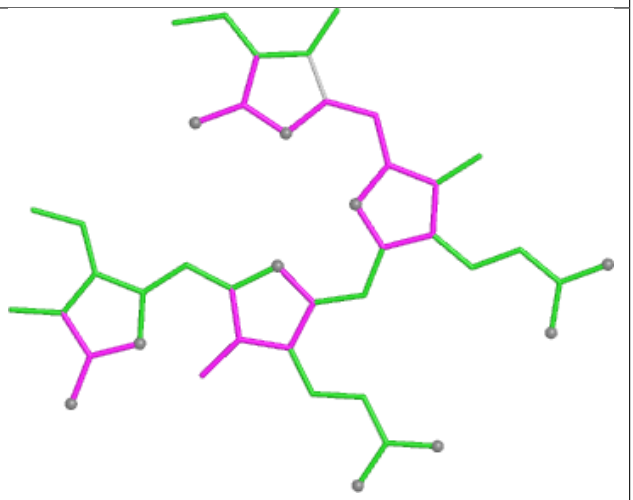

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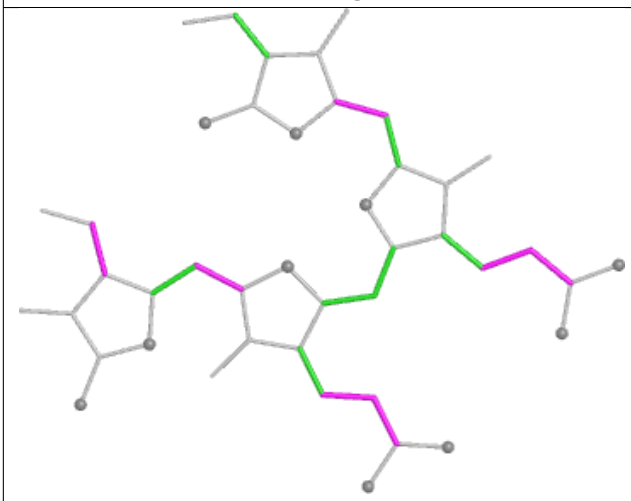

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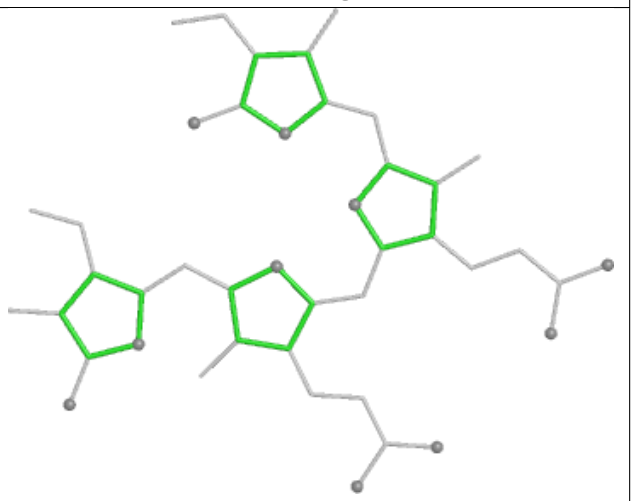
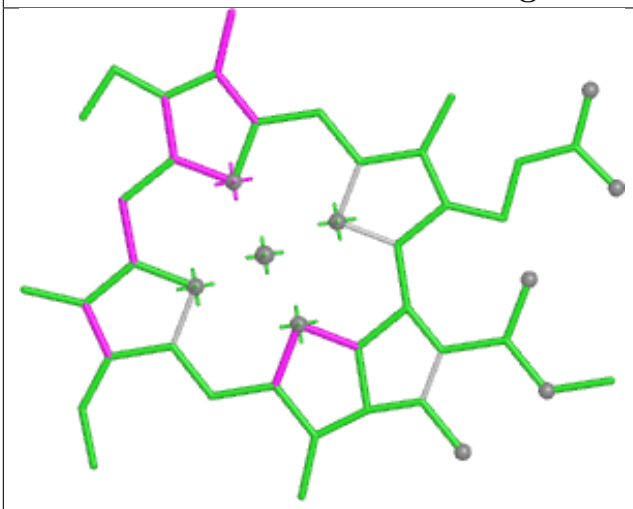


Rings

Ligand CLA 22 612



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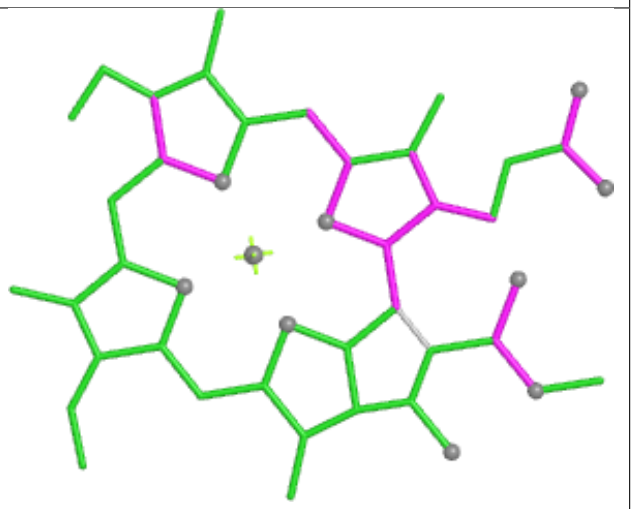

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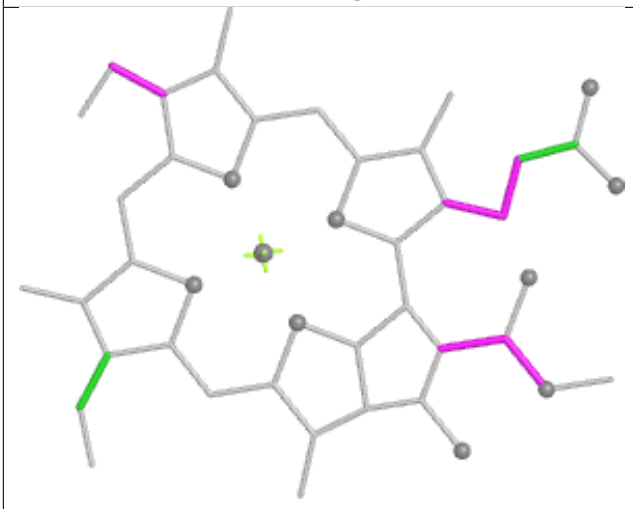
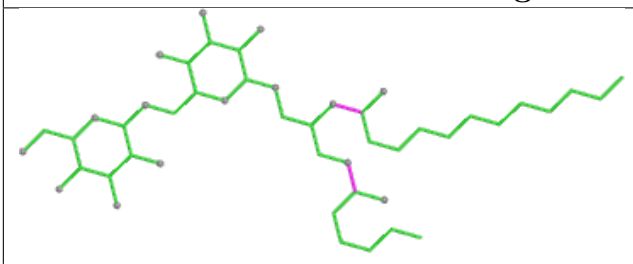


Torsions



Rings

Ligand DGD cL 520



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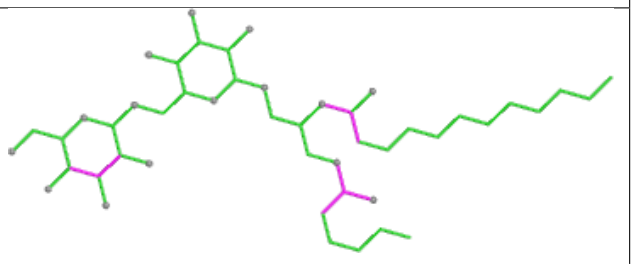

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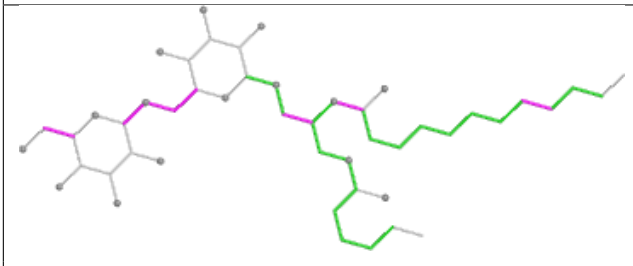

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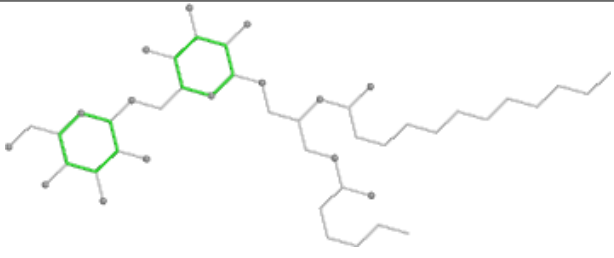
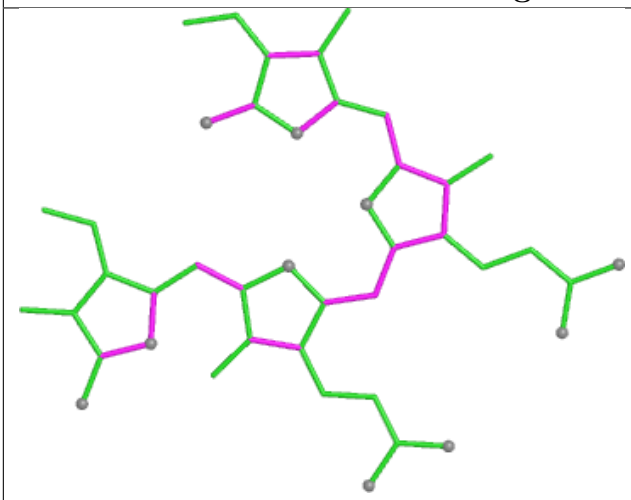


Rings

Ligand PEB hH 201



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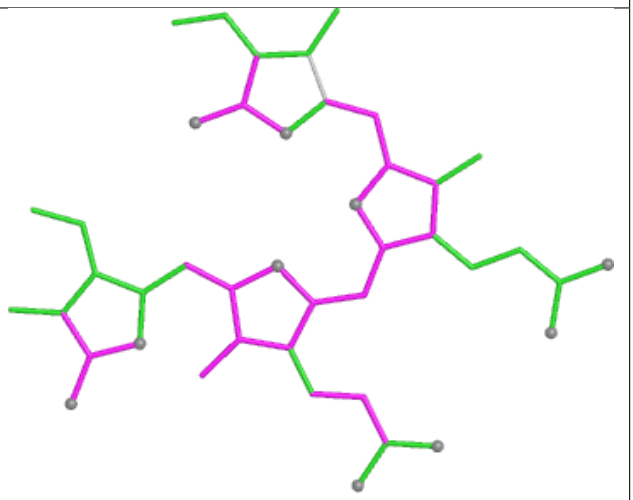
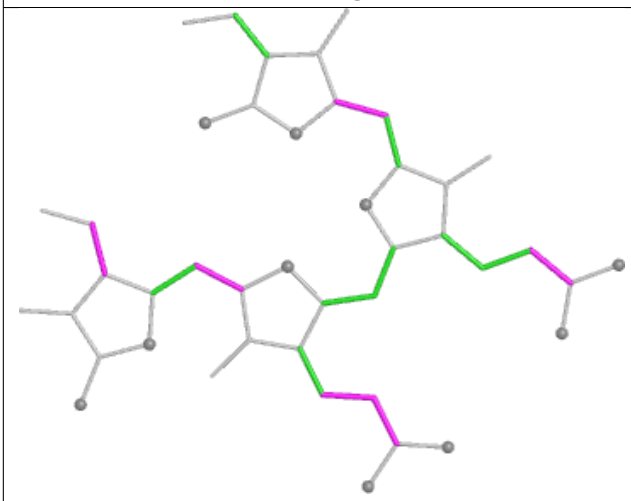


Bond angles



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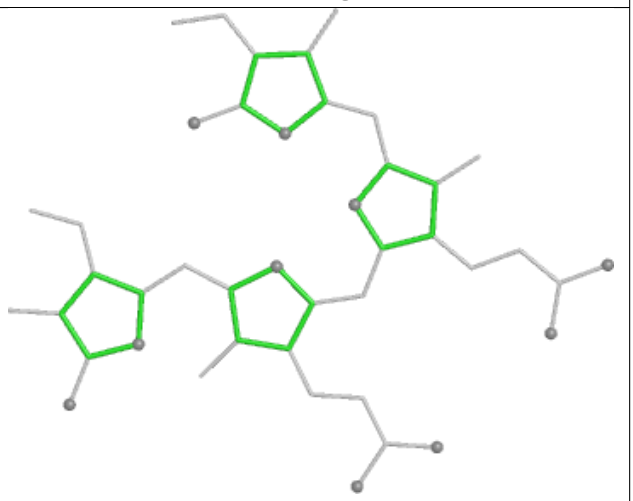
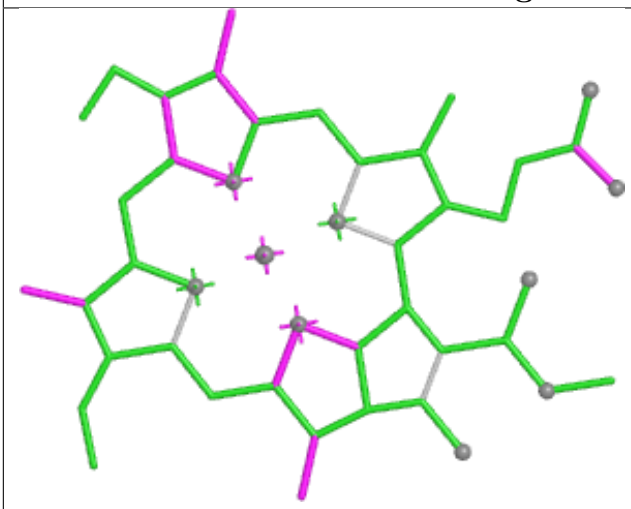


Rings

Ligand CLA B2 819



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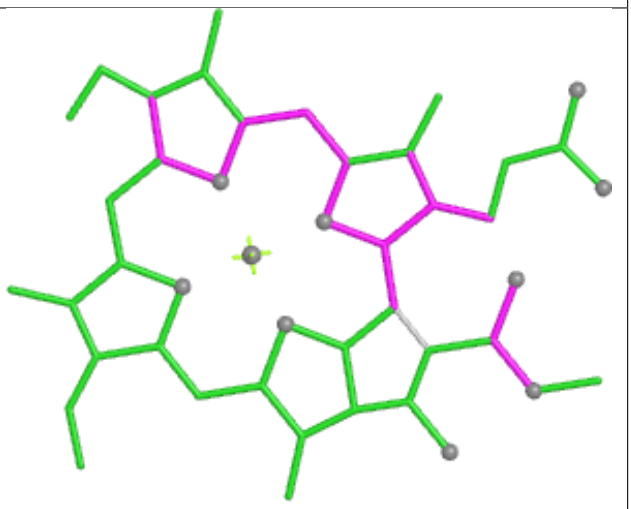

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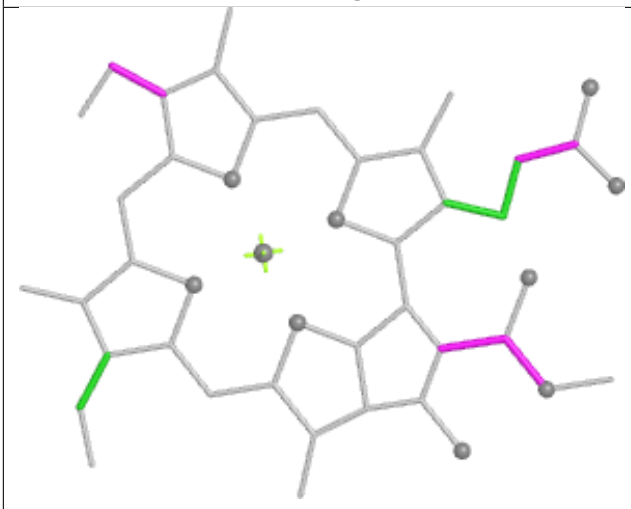
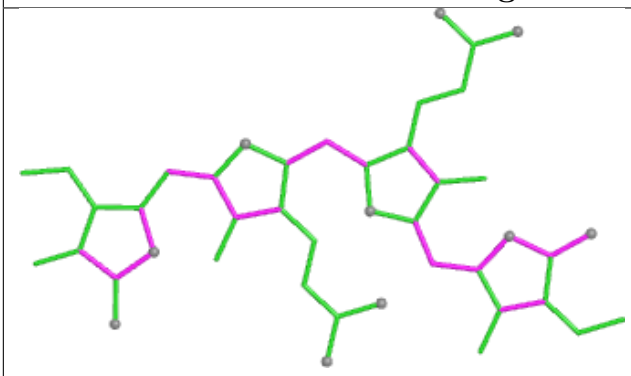


Torsions



Rings

Ligand CYC GG 1001



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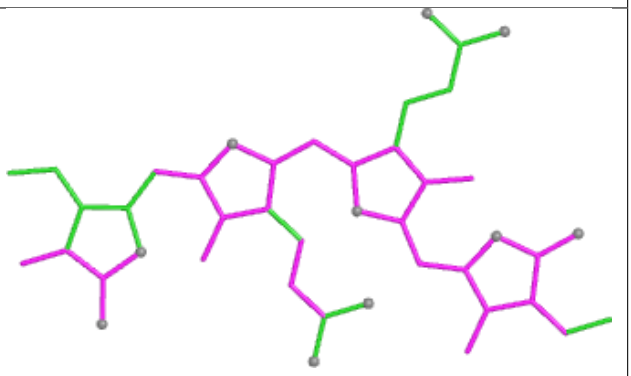

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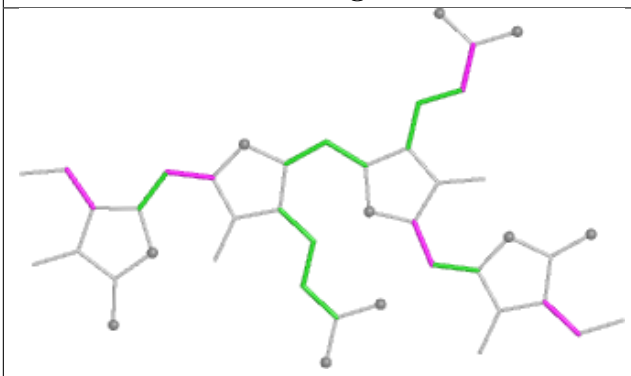

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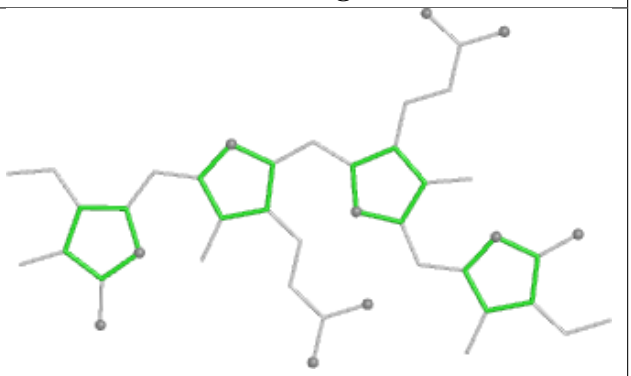
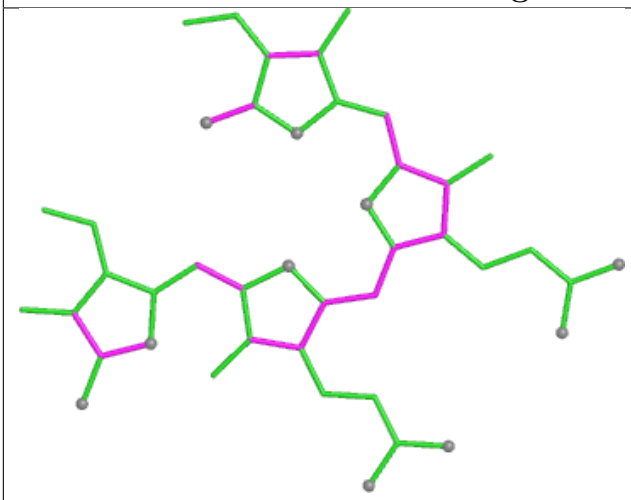


Rings

Ligand PEB BA 202



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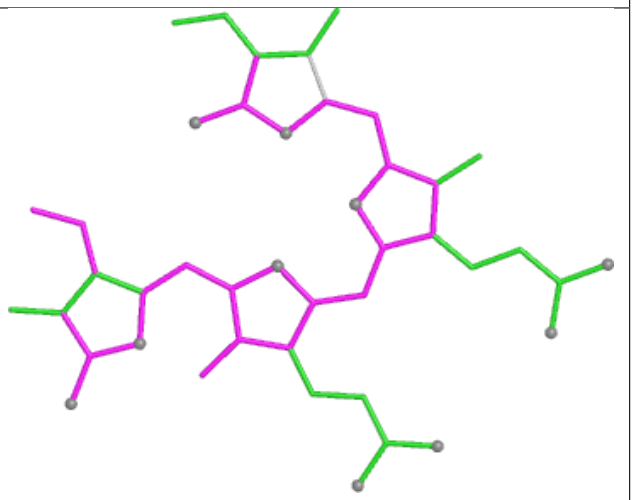

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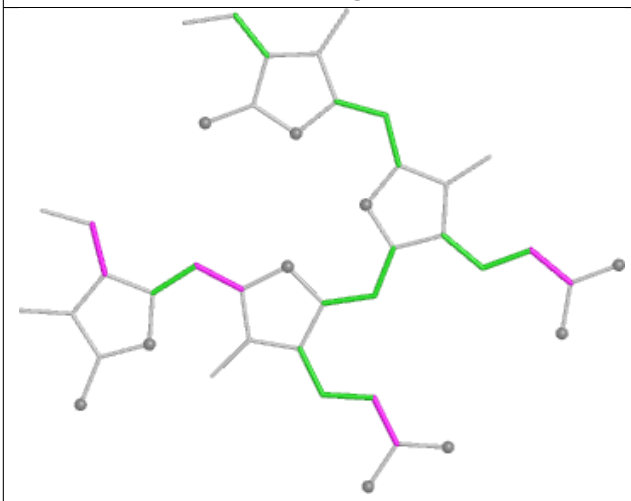

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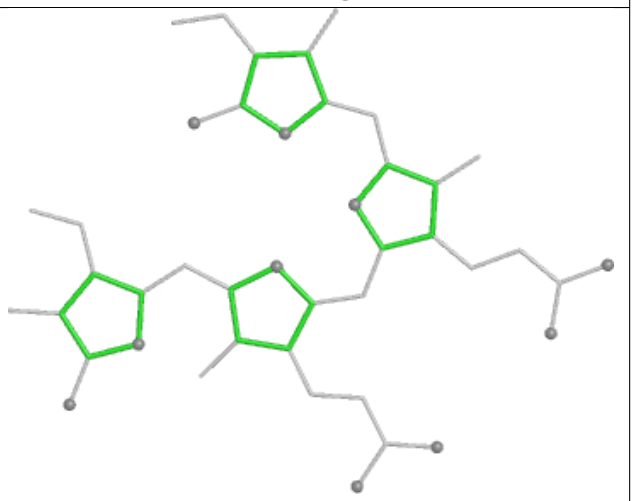
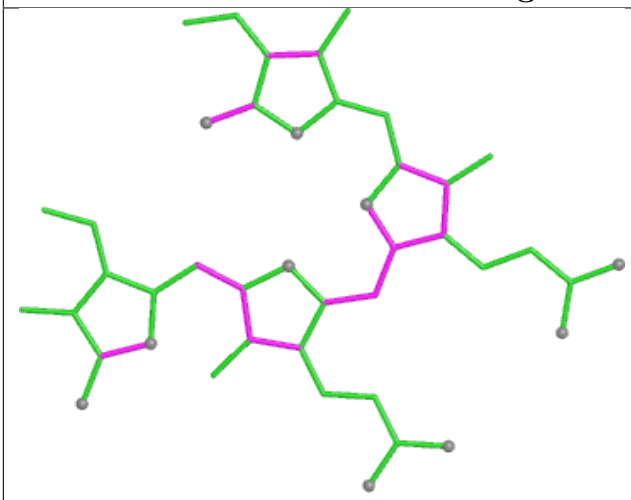


Rings

Ligand PEB oF 202



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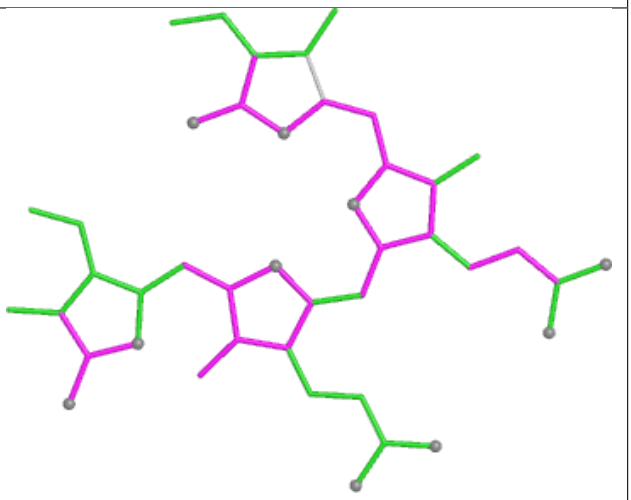

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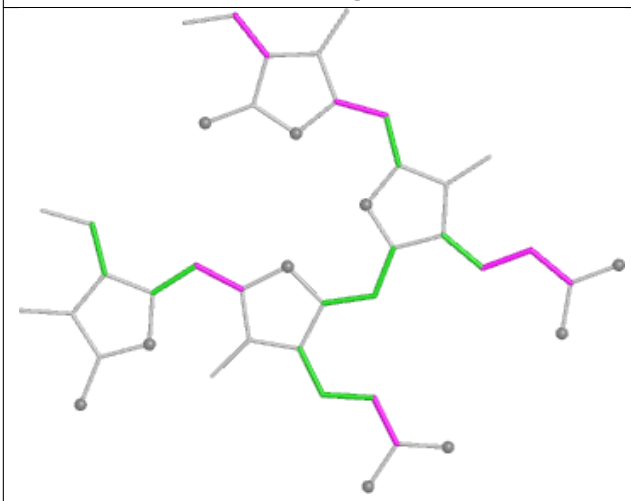

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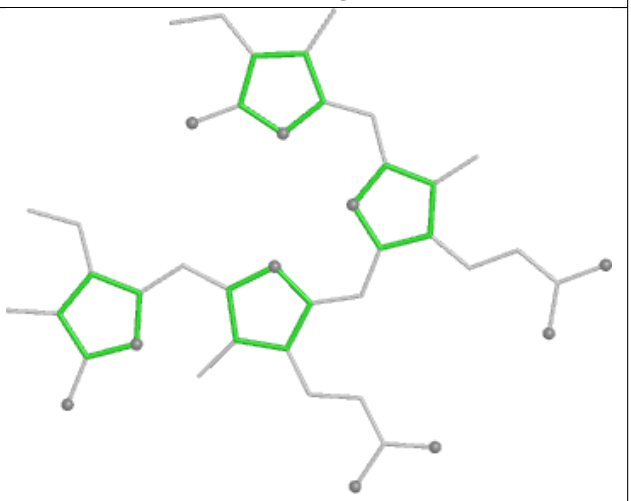
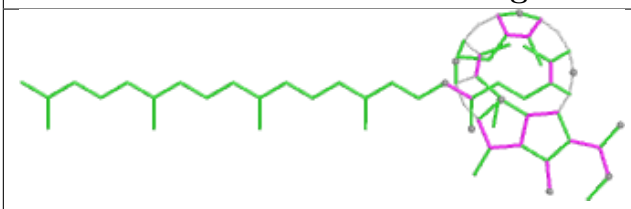


Rings

Ligand PHO AL 410



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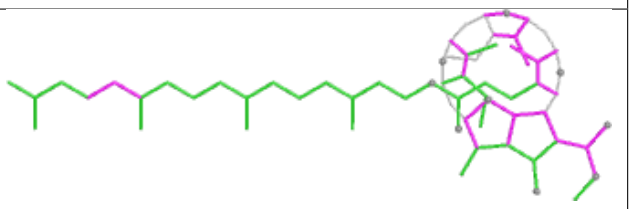

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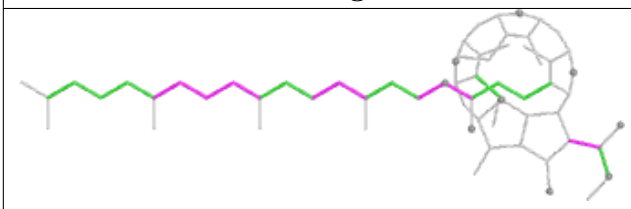

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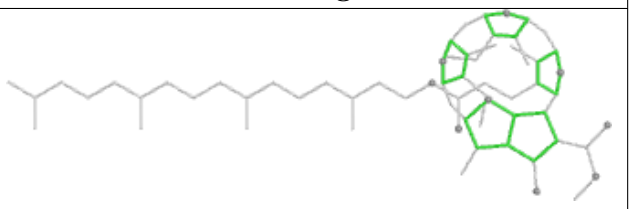
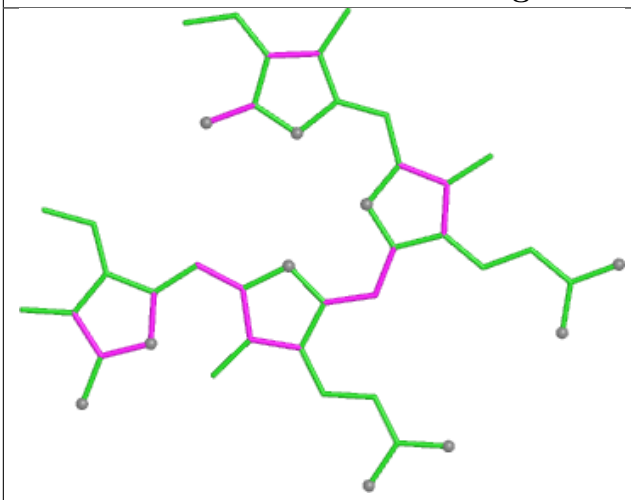


Rings

Ligand PEB KF 202



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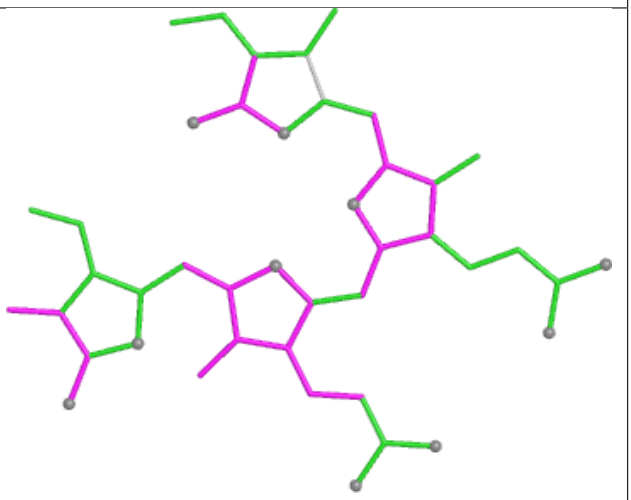
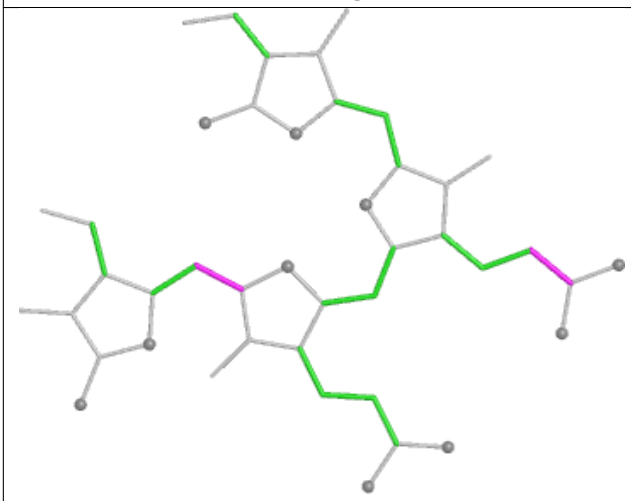


Bond angles



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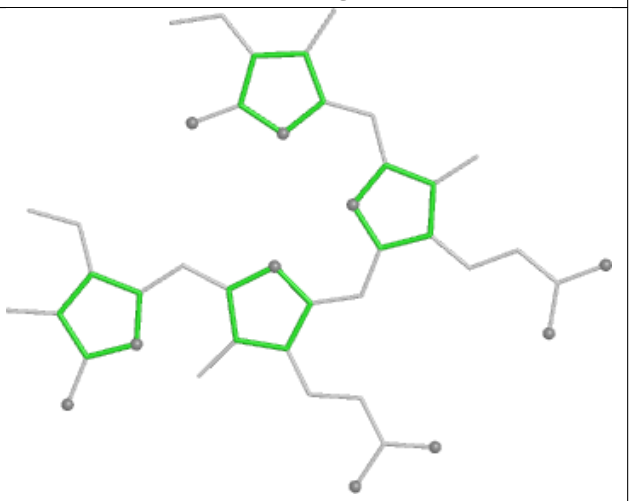
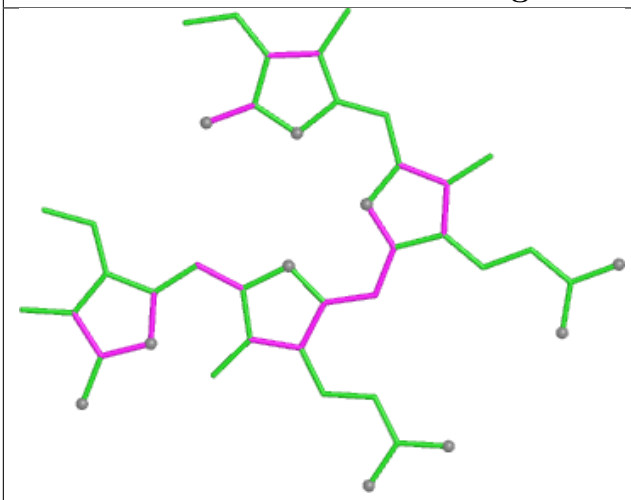


Rings

Ligand PEB NP 201



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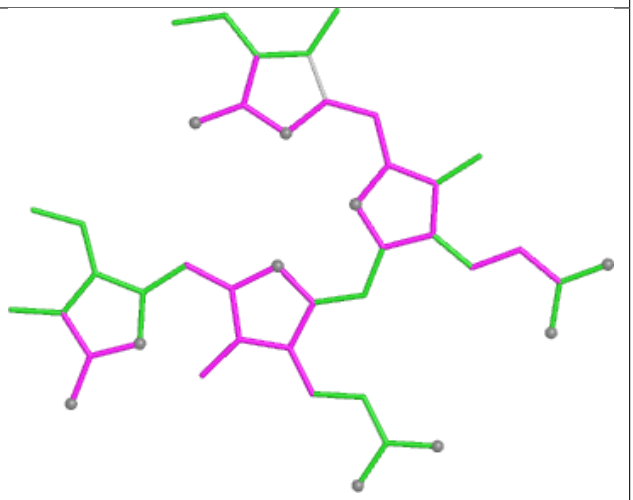

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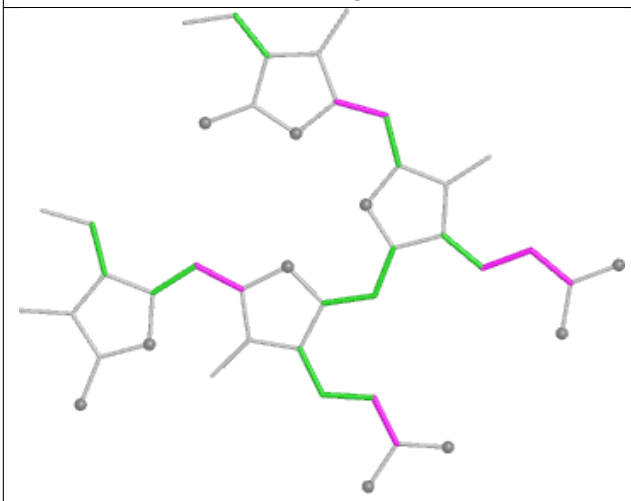

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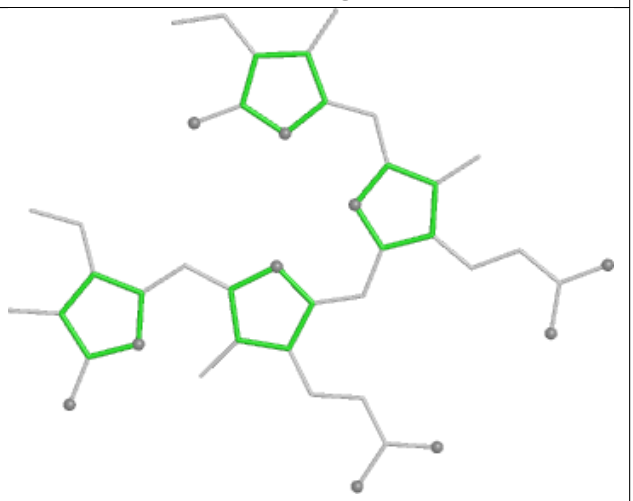
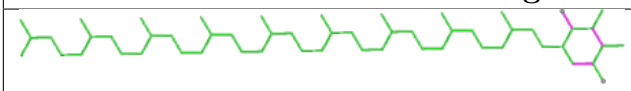


Rings

Ligand PL9 aL 601



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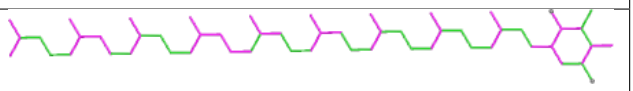

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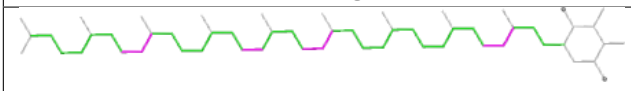

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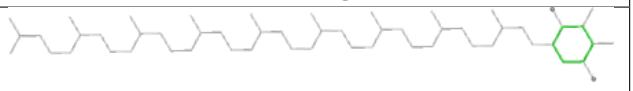
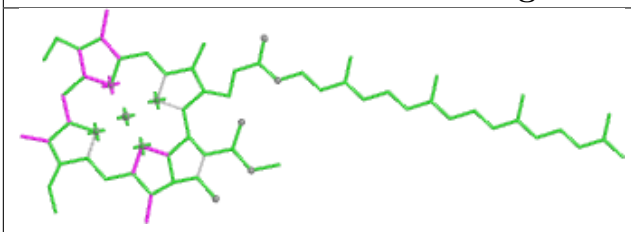


Rings

Ligand CLA b6 618



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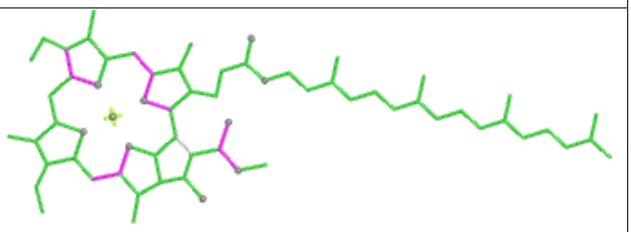
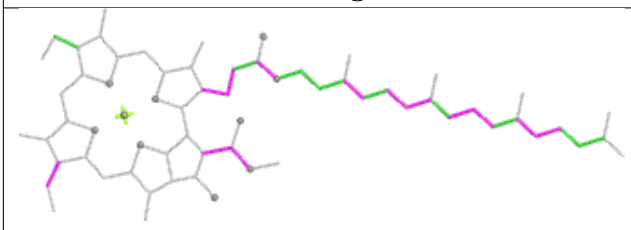


Bond angles



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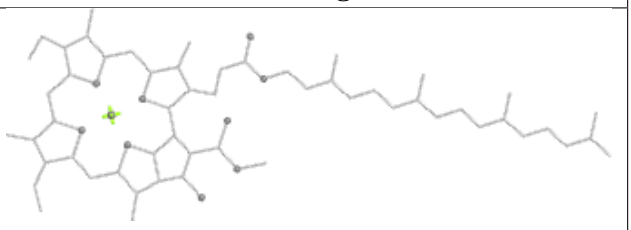
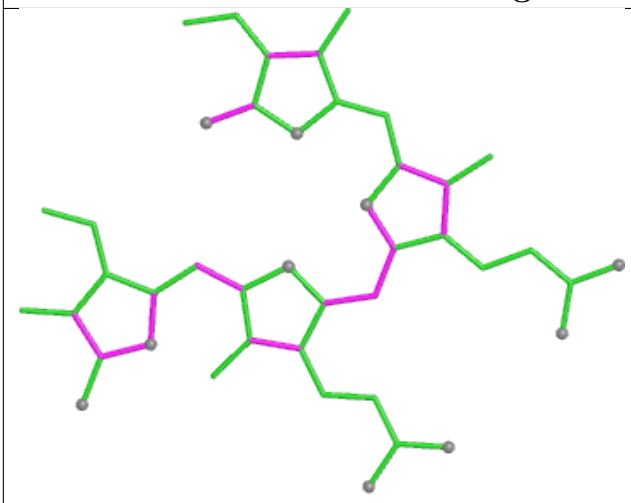


Rings

Ligand PEB TE 201



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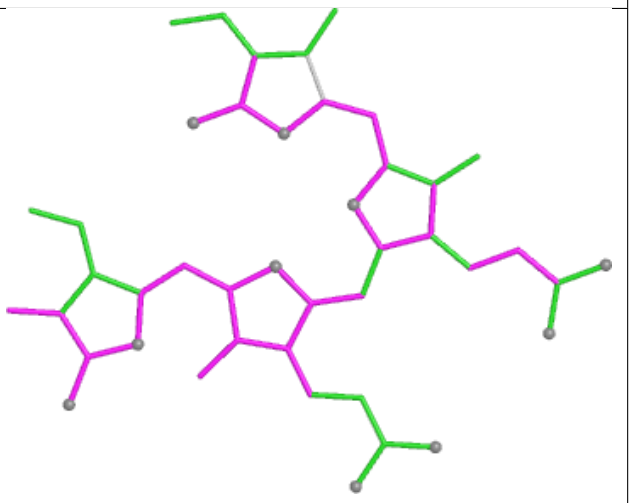
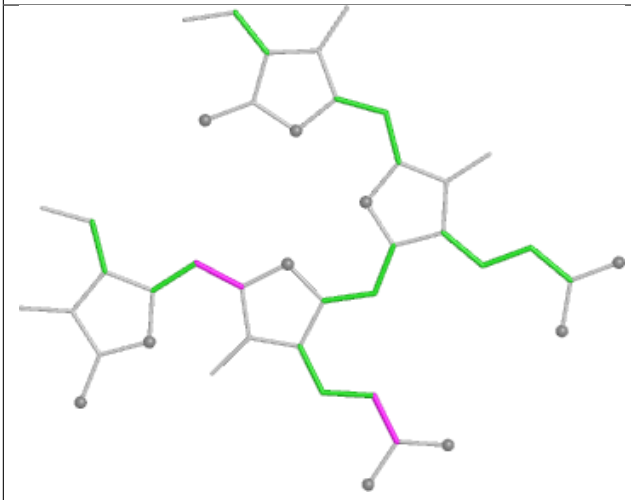


Bond angles



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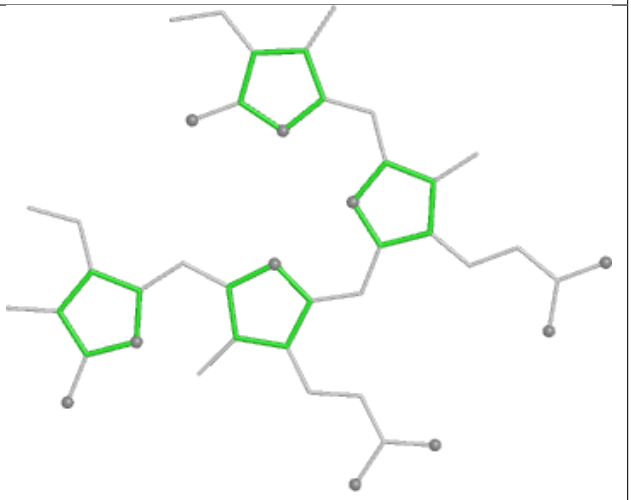
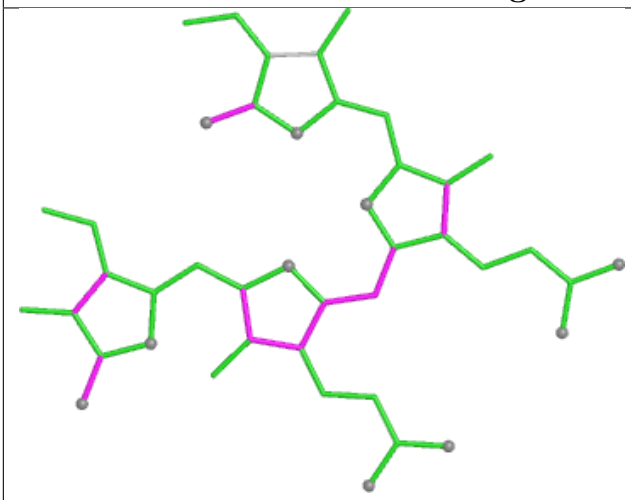
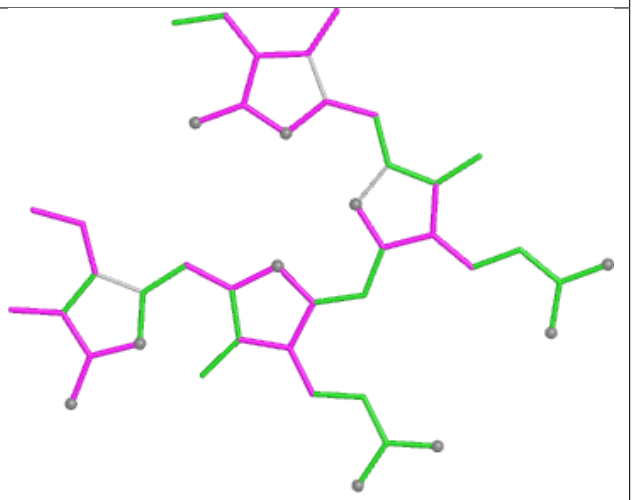


Rings

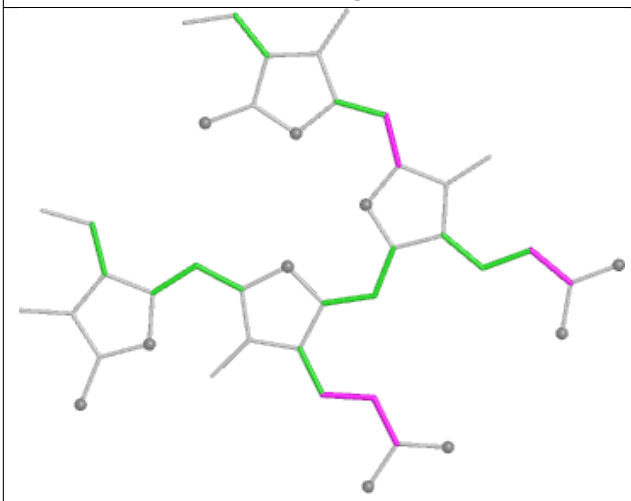
Ligand PUB AO 303



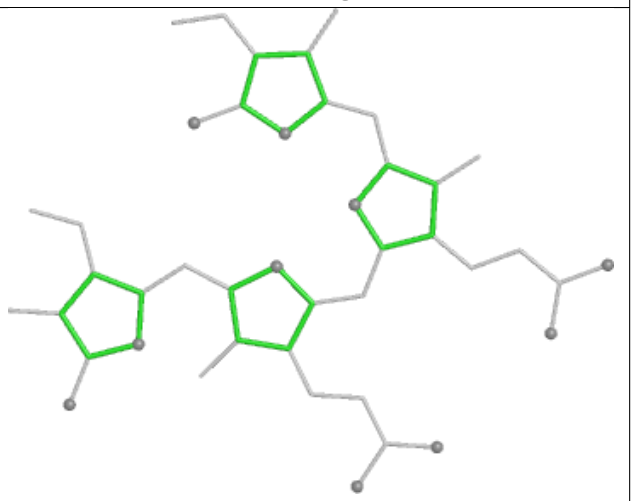
Bond lengths



Bond angles

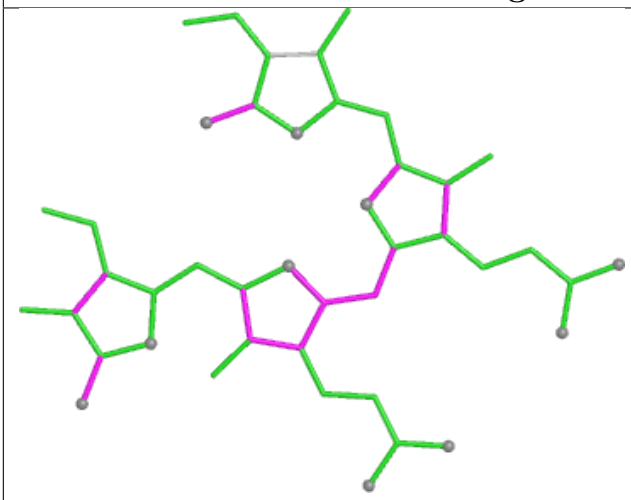


Torsions



Rings

Ligand PUB NQ 201



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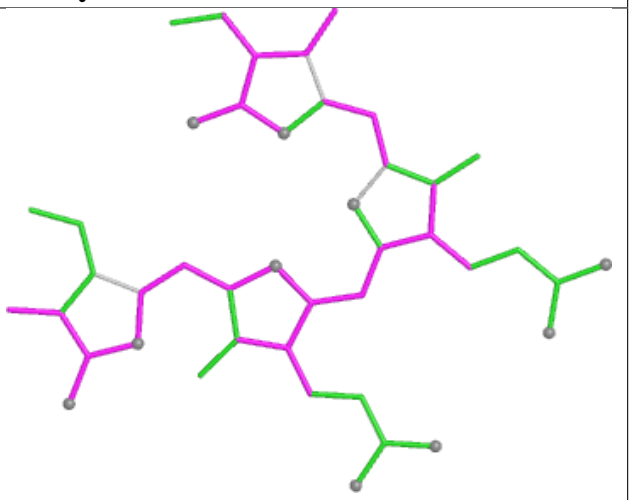

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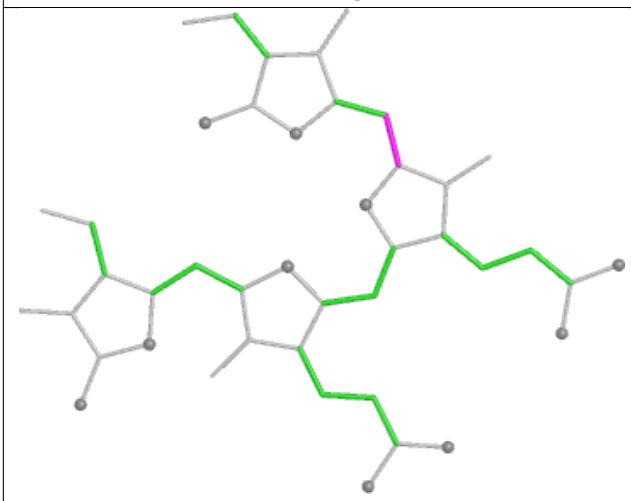

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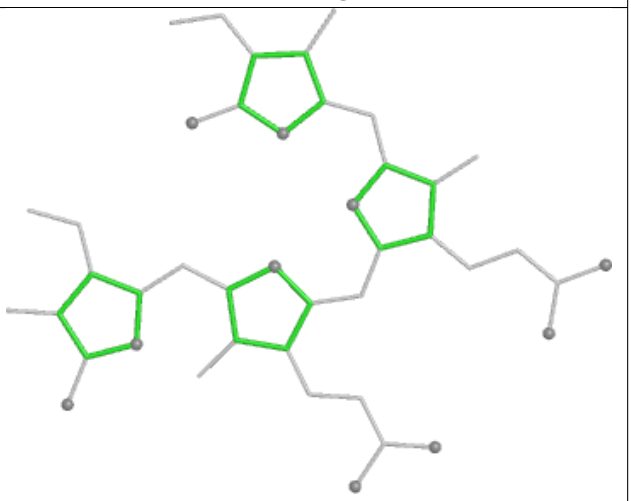
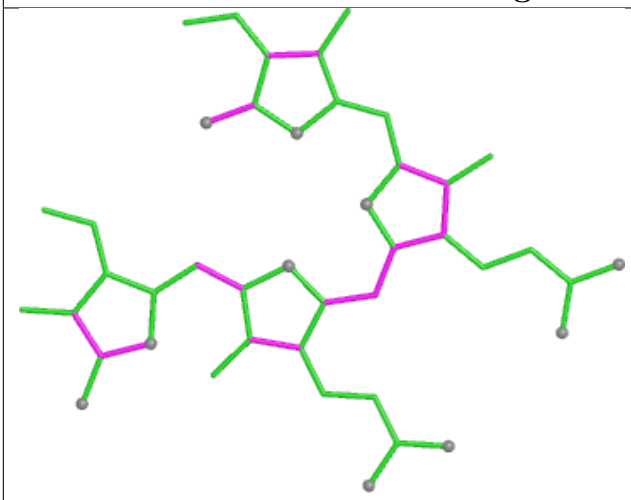


Rings

Ligand PEB SH 202



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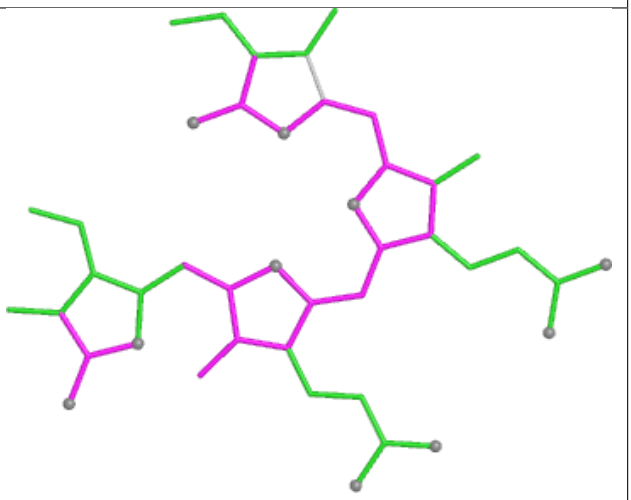

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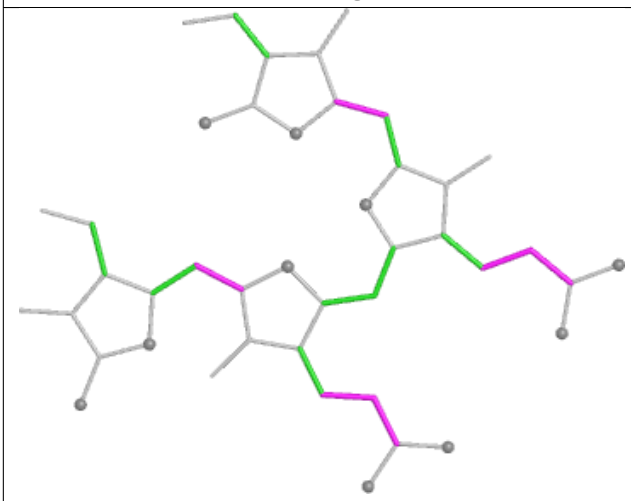

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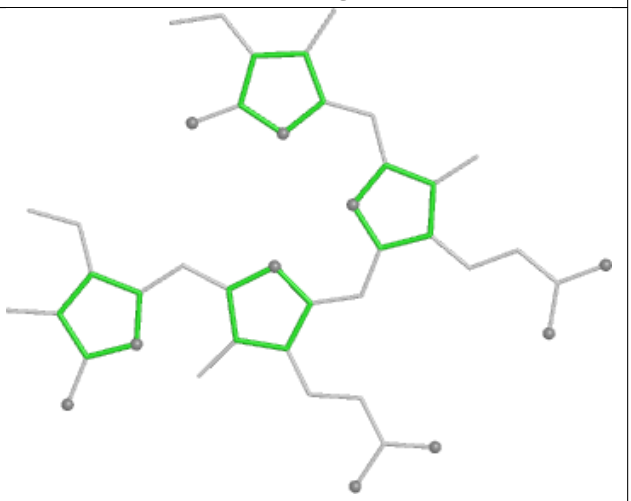
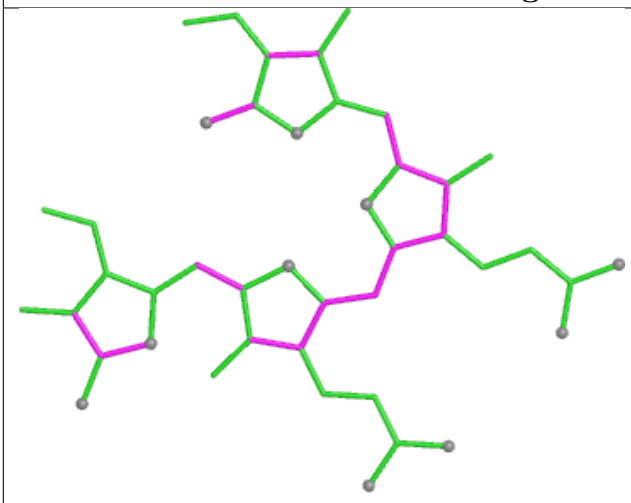


Rings

Ligand PEB s8 202



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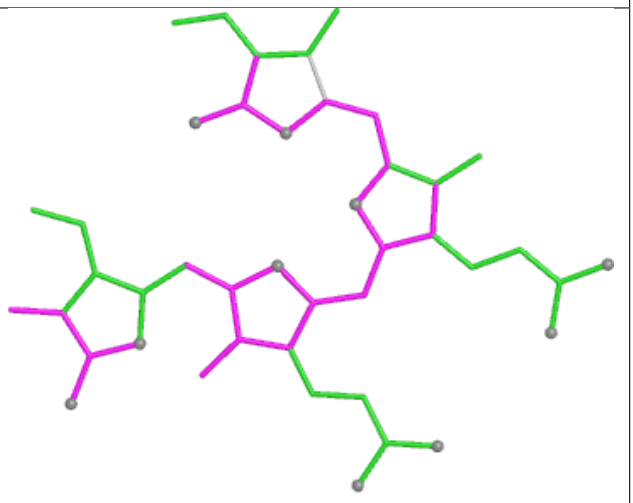

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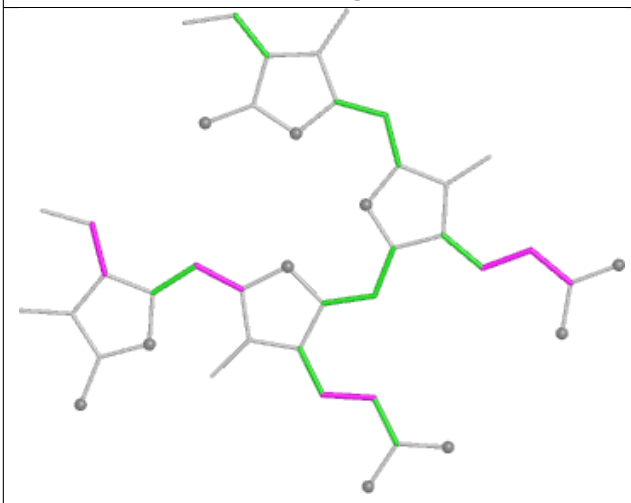

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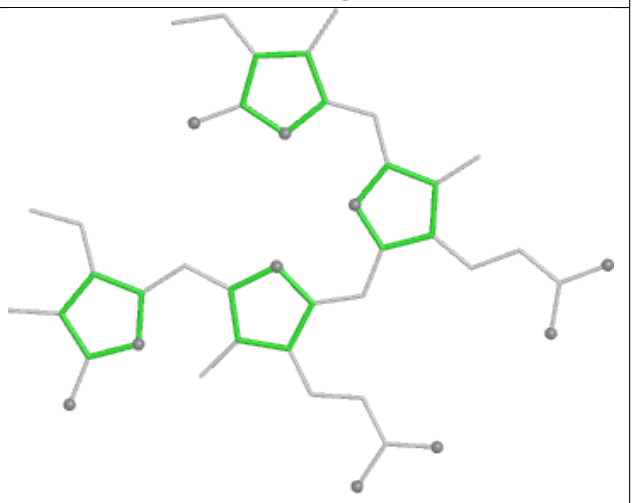
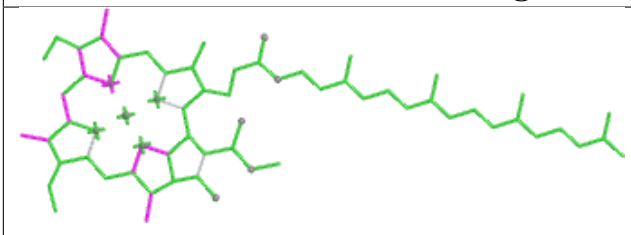


Rings

Ligand CLA DL 406



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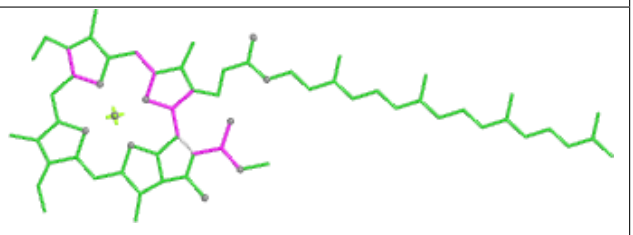

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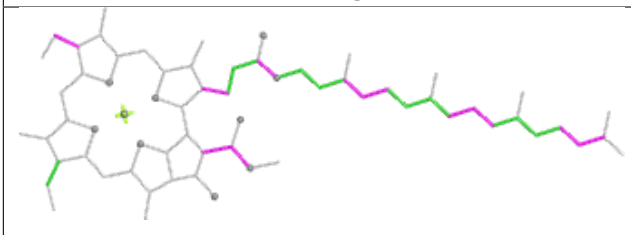

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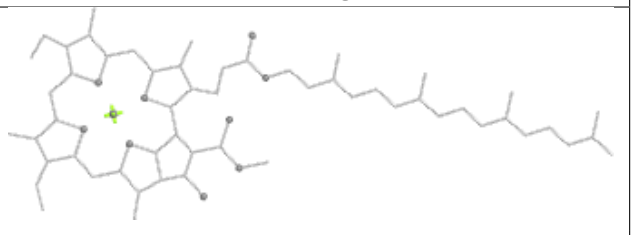
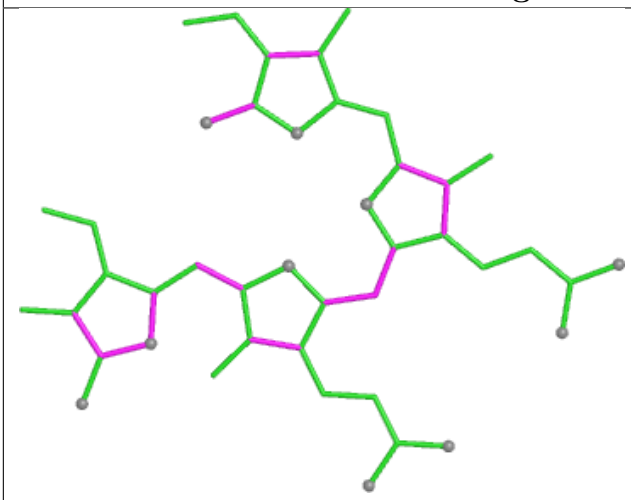


Rings

Ligand PEB ZG 201



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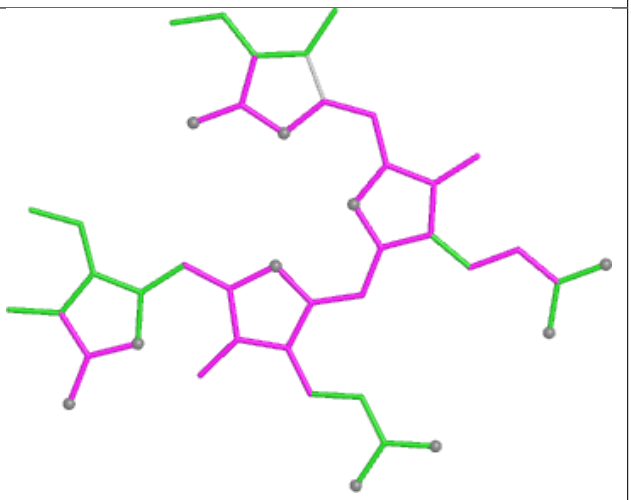

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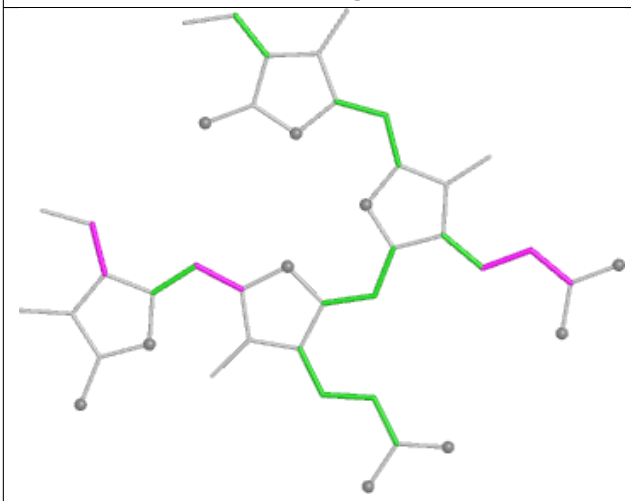

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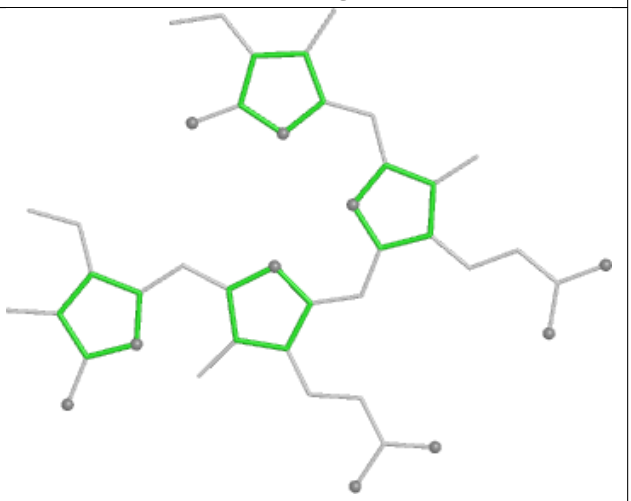
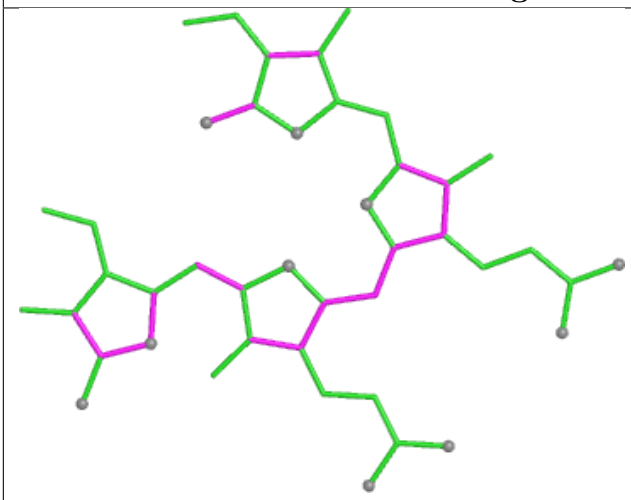


Rings

Ligand PEB SM 202



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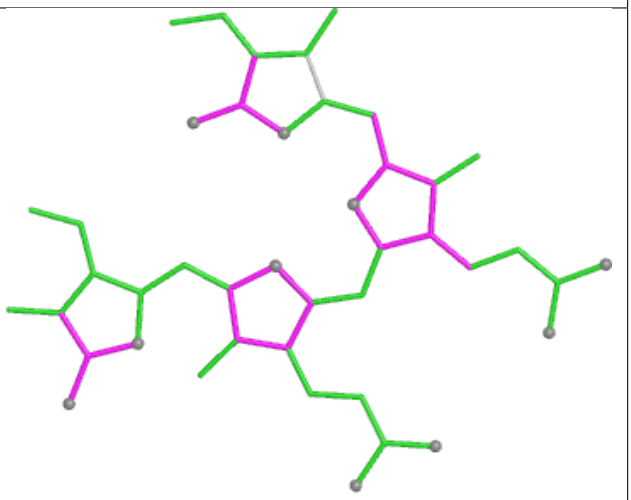

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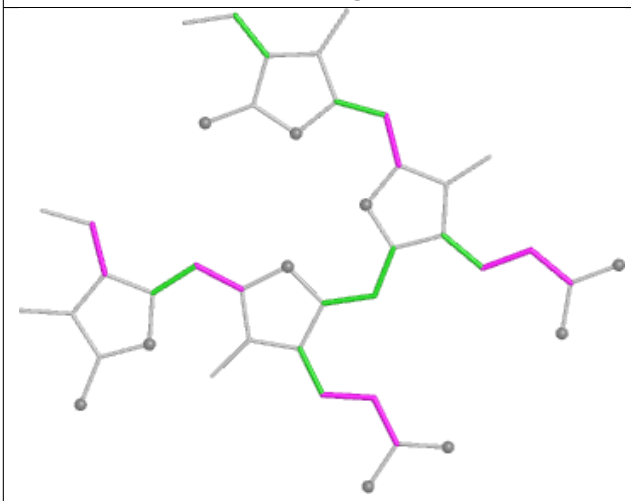

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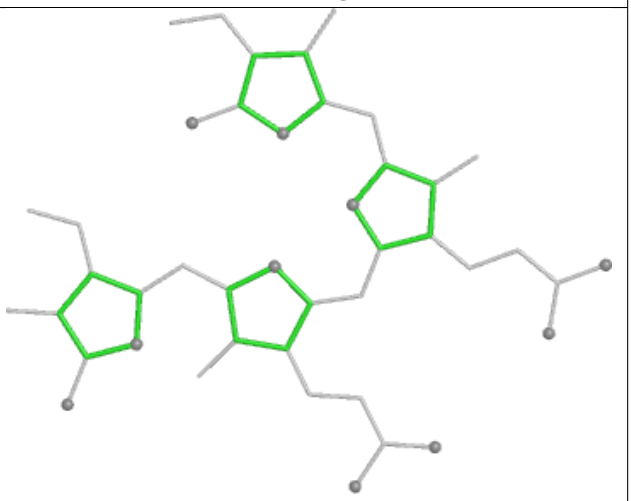
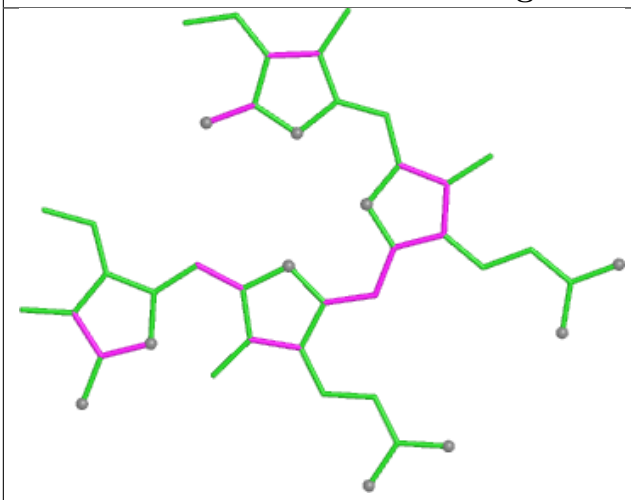


Rings

Ligand PEB dF 201



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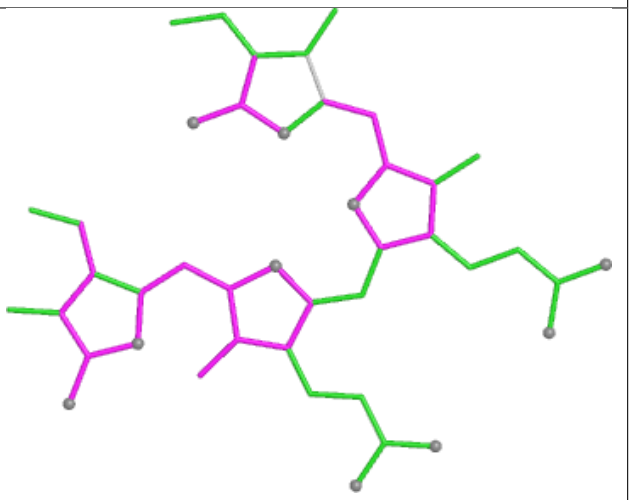

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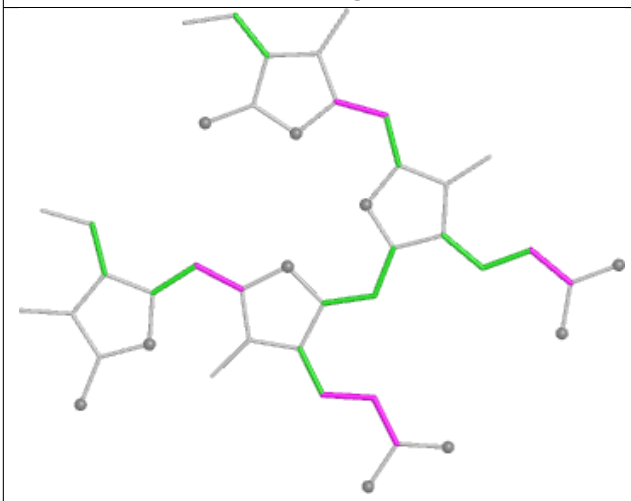

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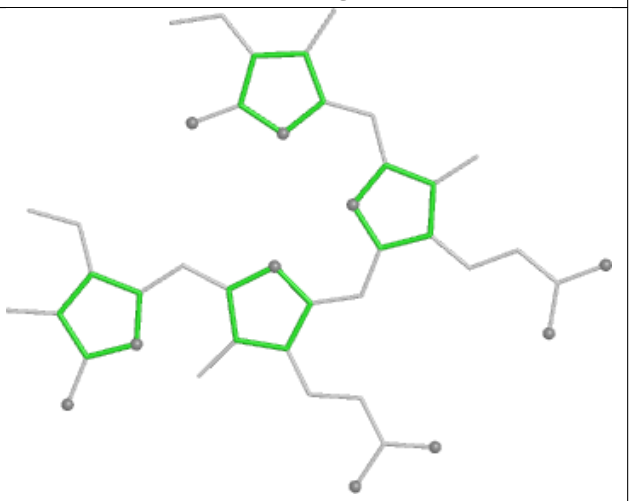
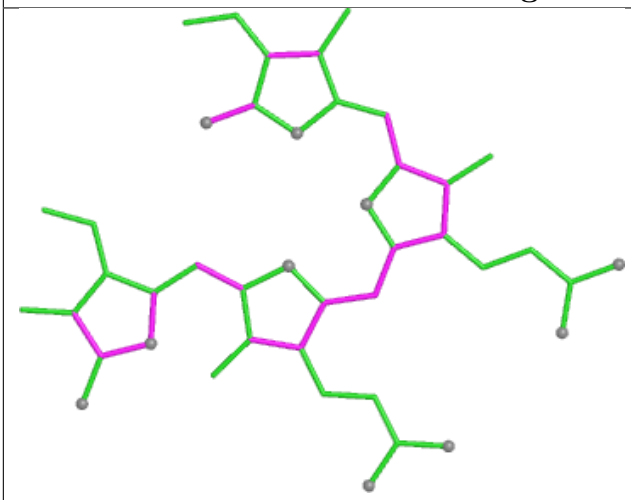


Rings

Ligand PEB c4 202



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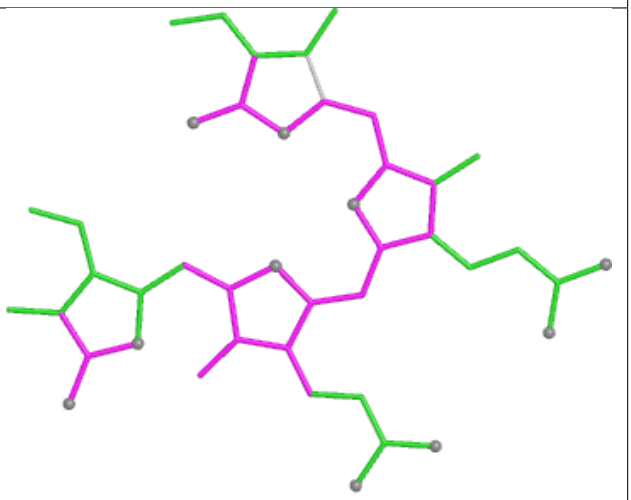
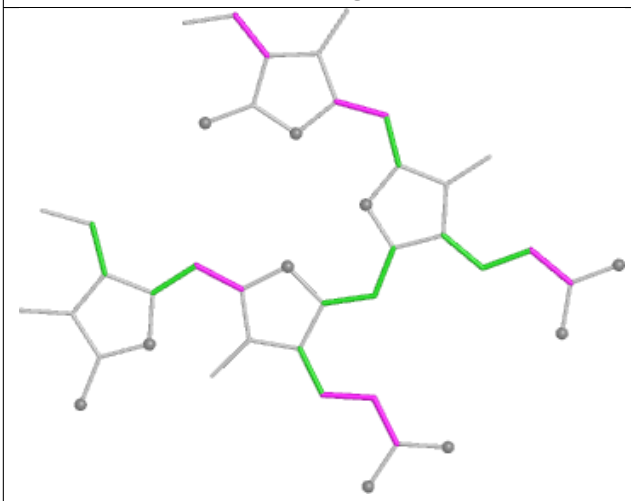


Bond angles



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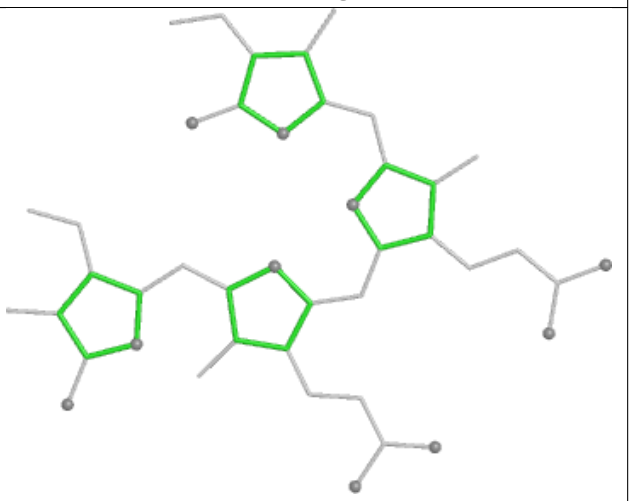
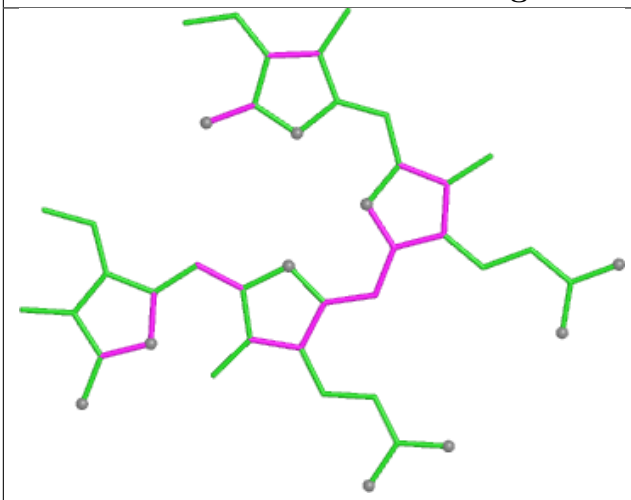


Rings

Ligand PEB YD 202



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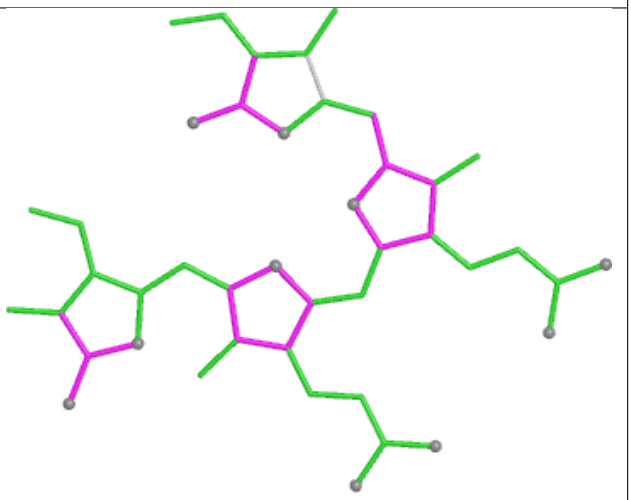
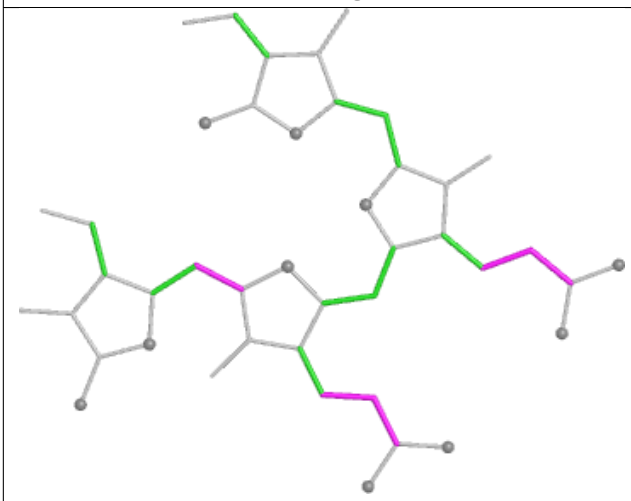


Bond angles



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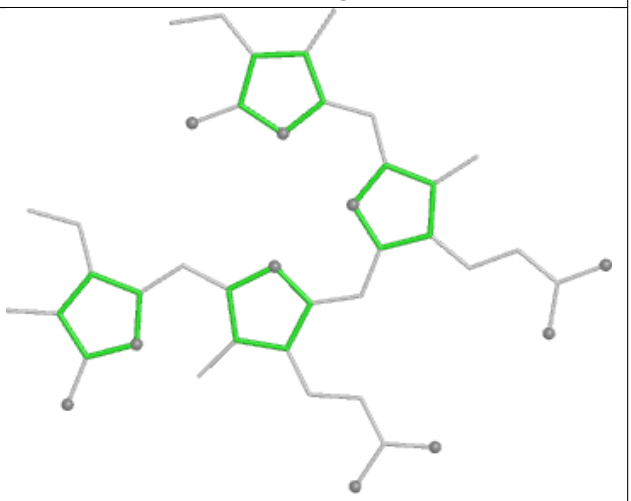
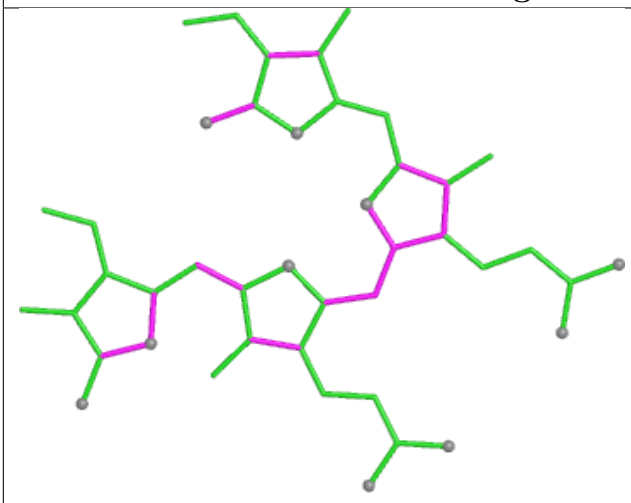


Rings

Ligand PEB LA 203



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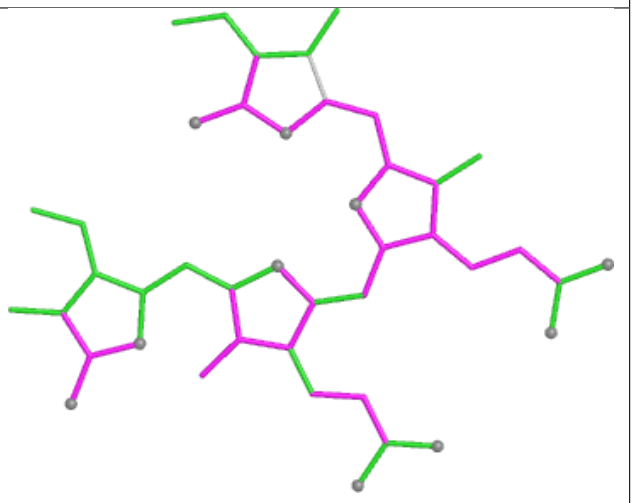
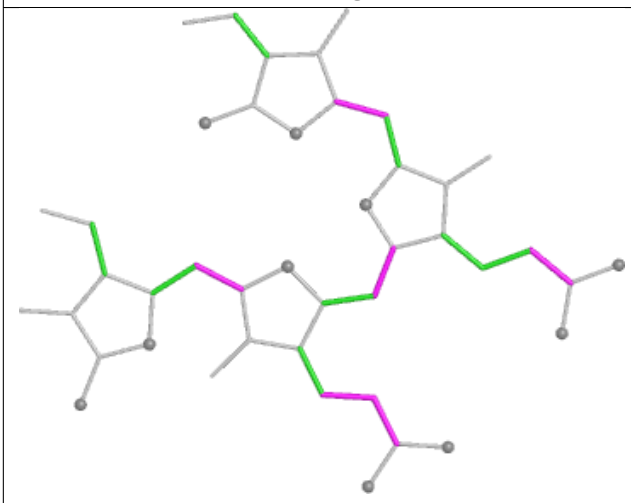


Bond angles



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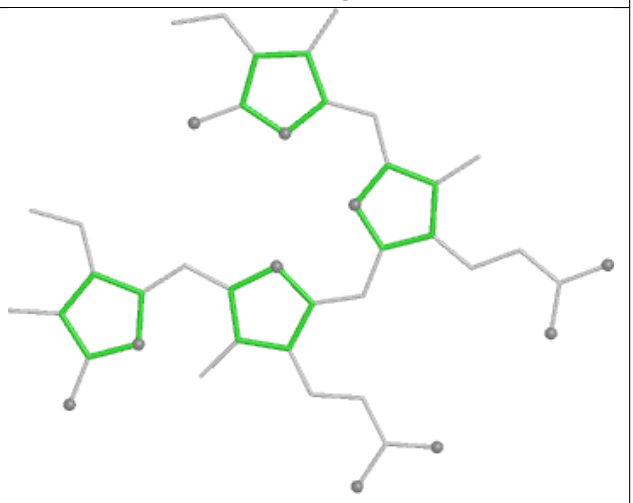
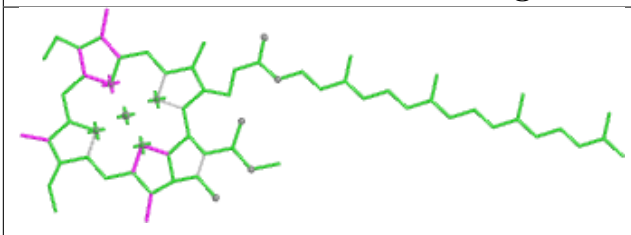


Rings

Ligand CLA BL 622



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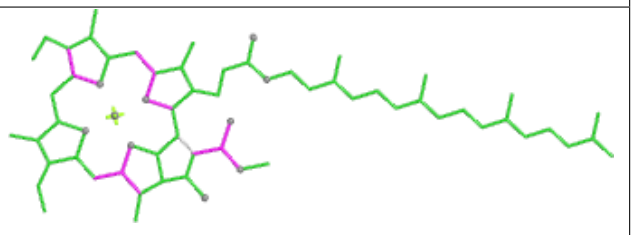
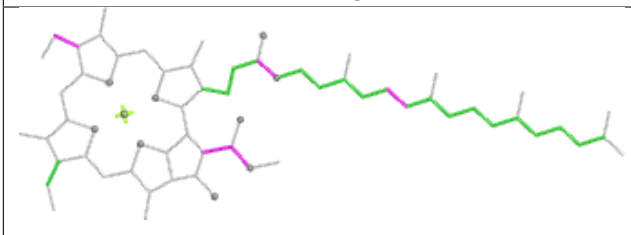


Bond angles



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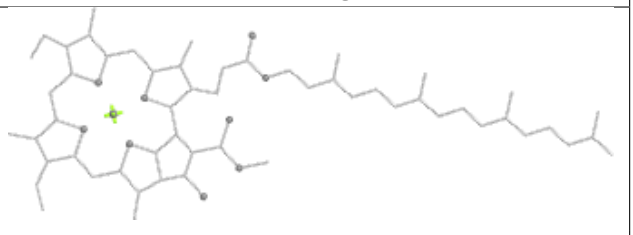
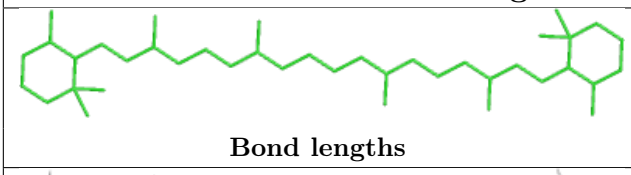


Rings

Ligand BCR FN 204



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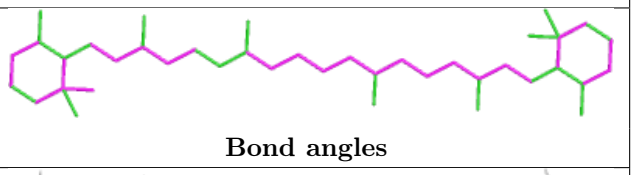

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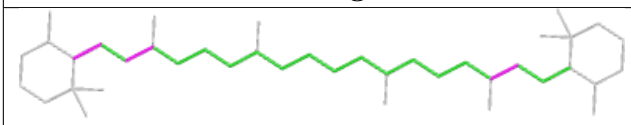

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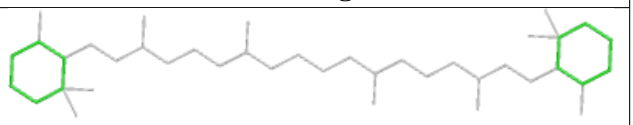
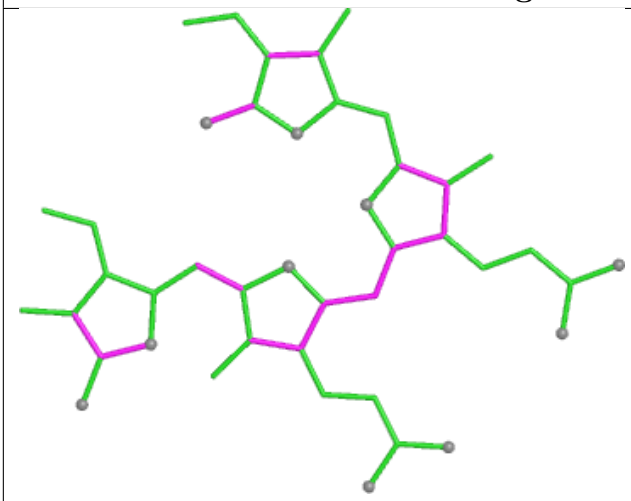
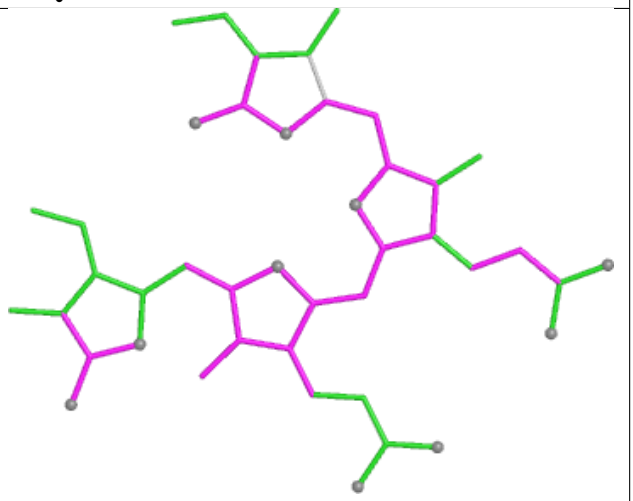


Rings

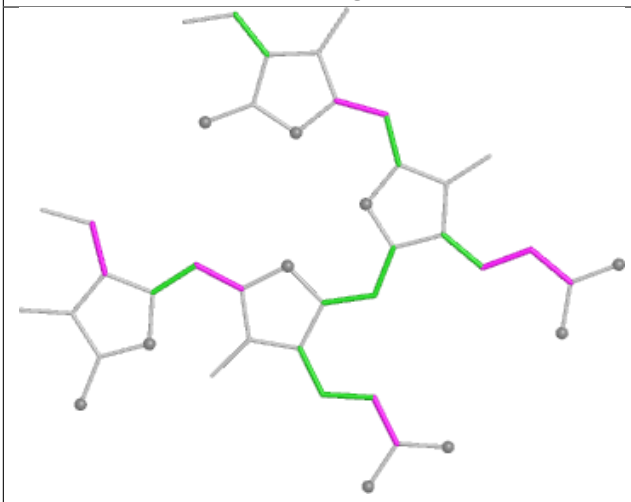
Ligand PEB Q1 201



Bond lengths



Bond angles



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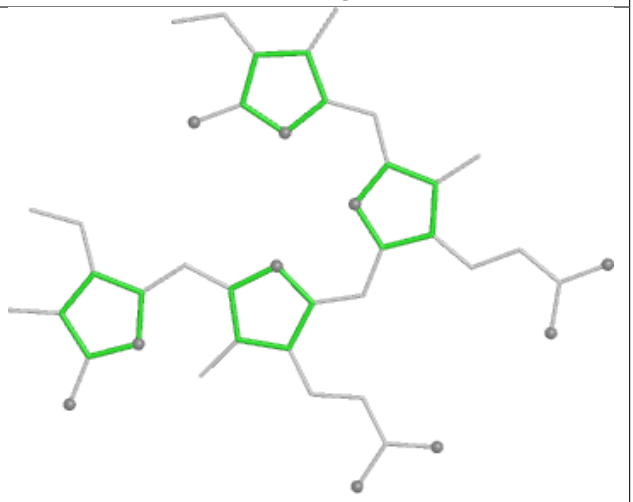
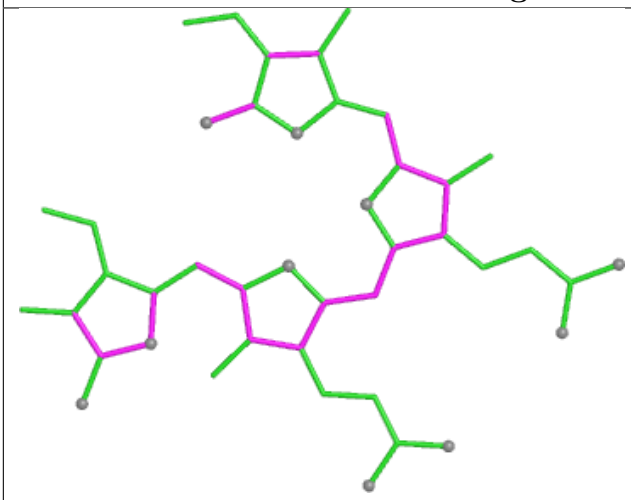
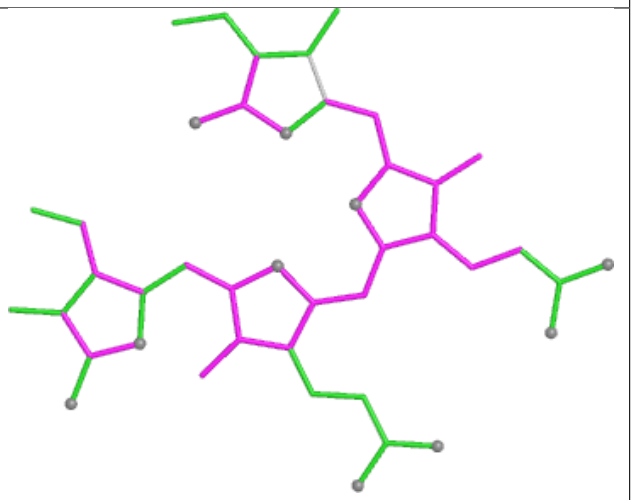


Rings

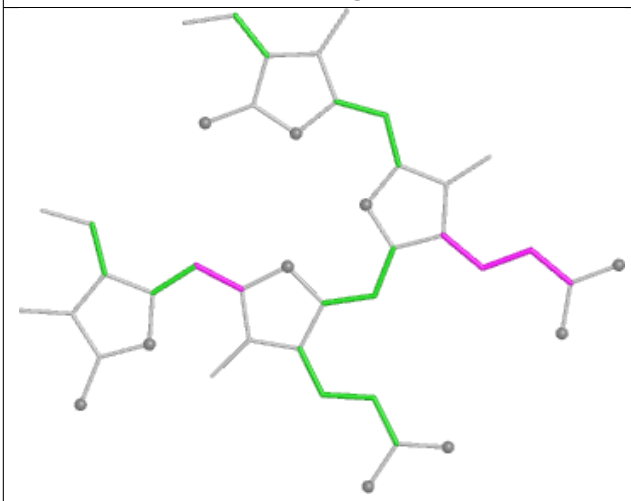
Ligand PEB KA 201



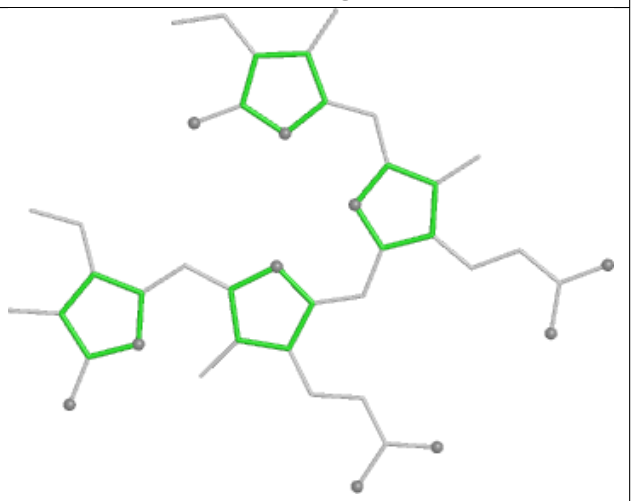
Bond lengths



Bond angles

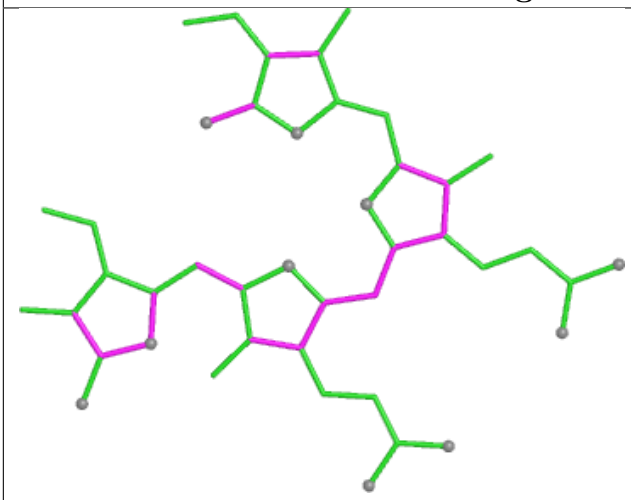


Torsions



Rings

Ligand PEB R4 202



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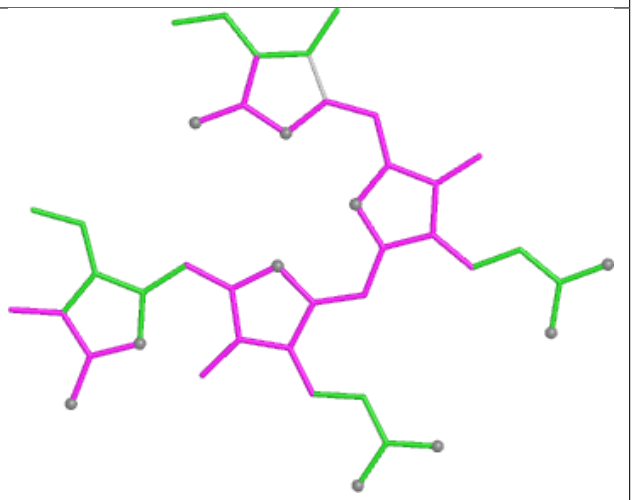
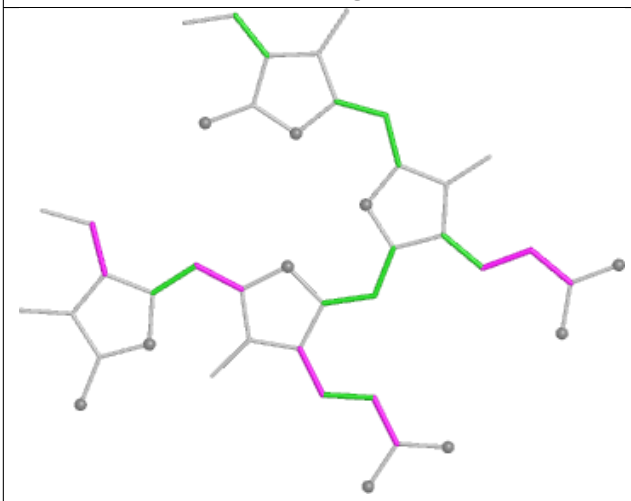


Bond angles



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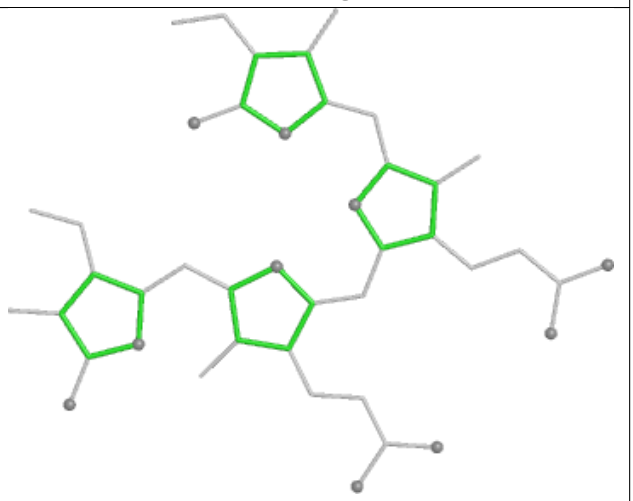
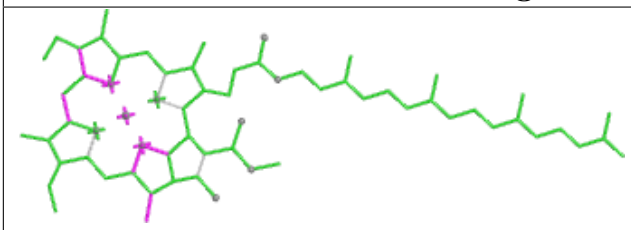


Rings

Ligand CLA B2 805



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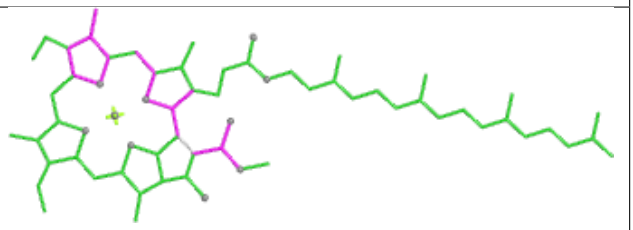

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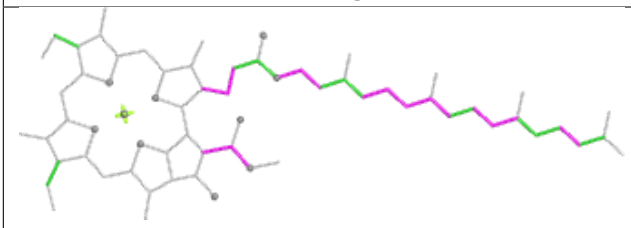

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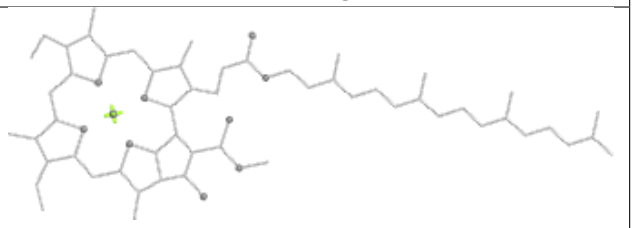
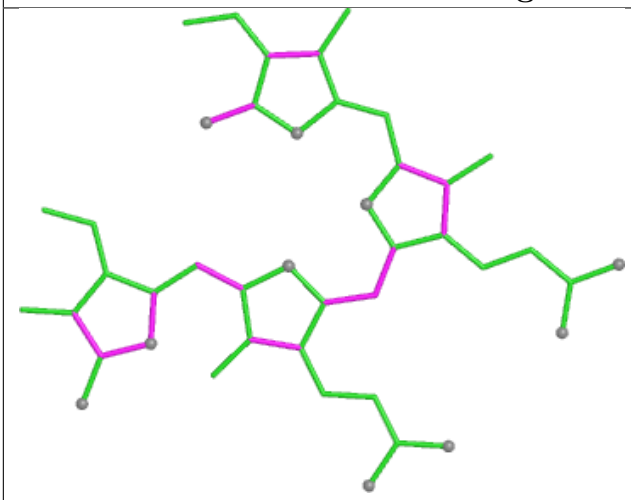


Rings

Ligand PEB EJ 202



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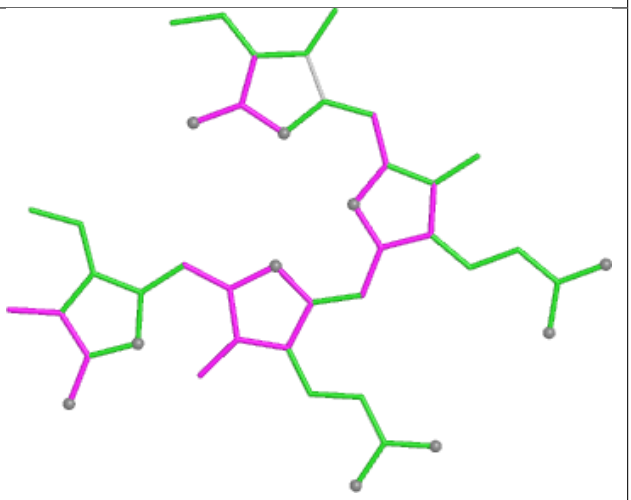

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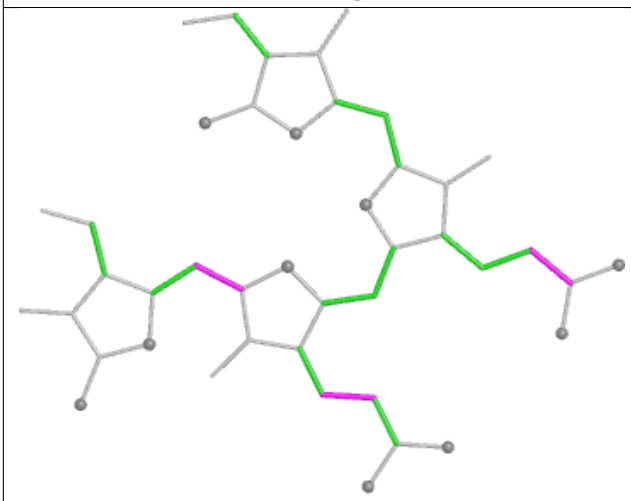

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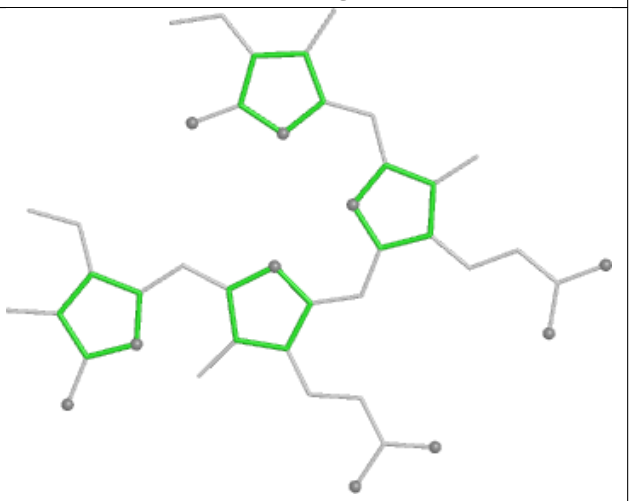
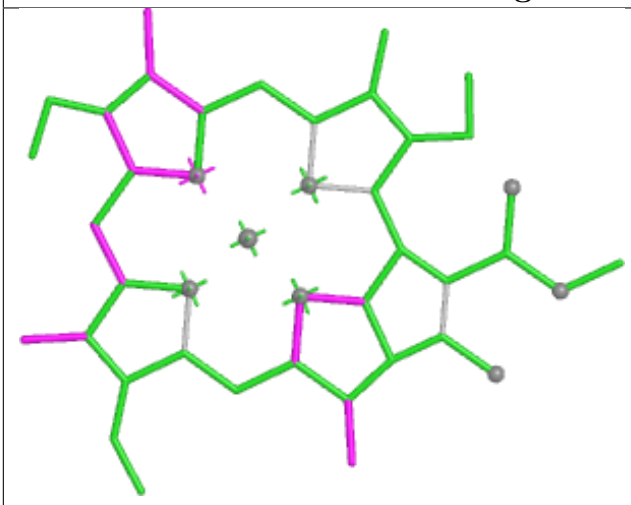


Rings

Ligand CLA 5N 604



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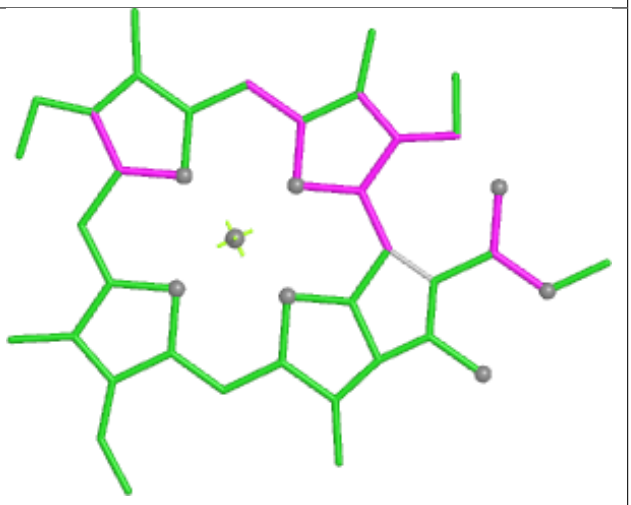

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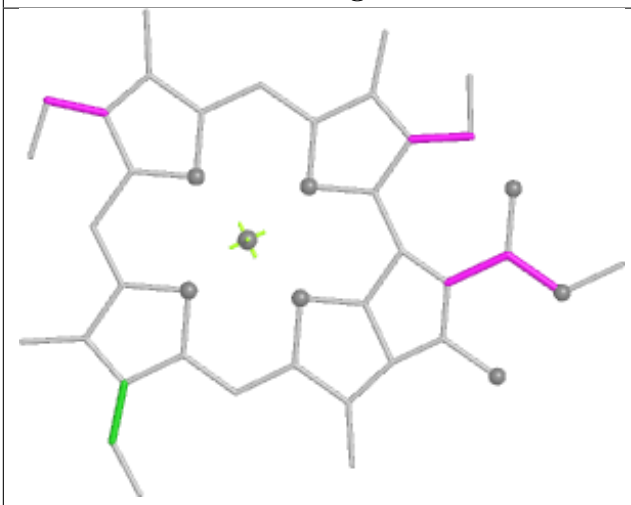
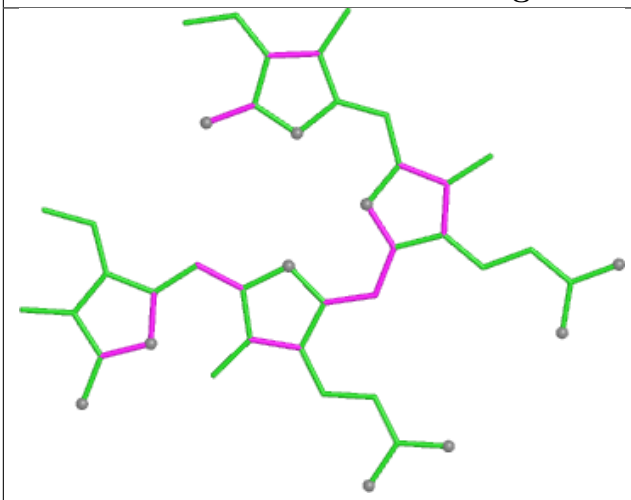


Torsions



Rings

Ligand PEB UF 202



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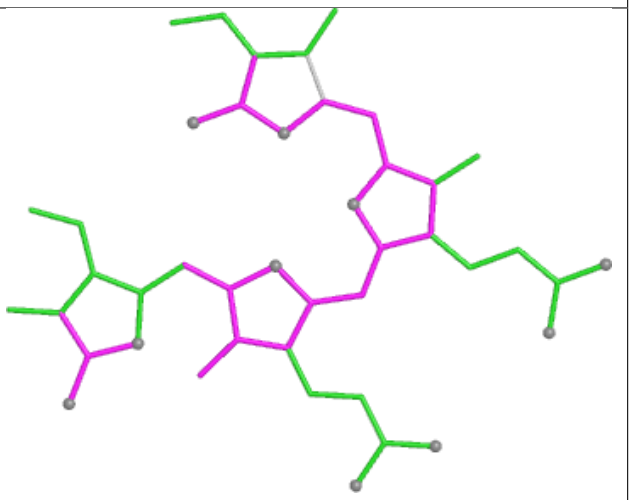

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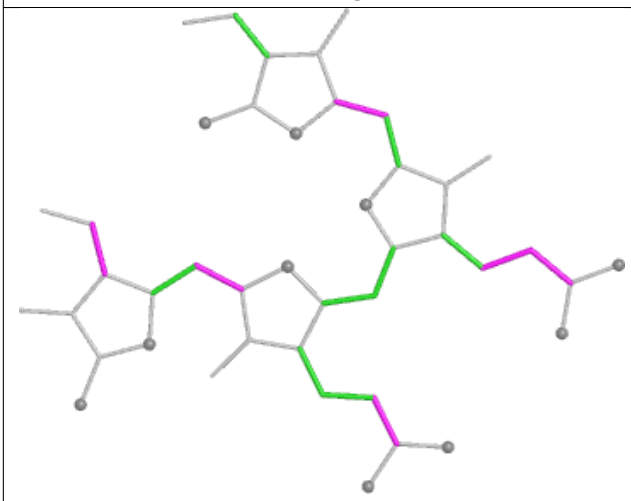

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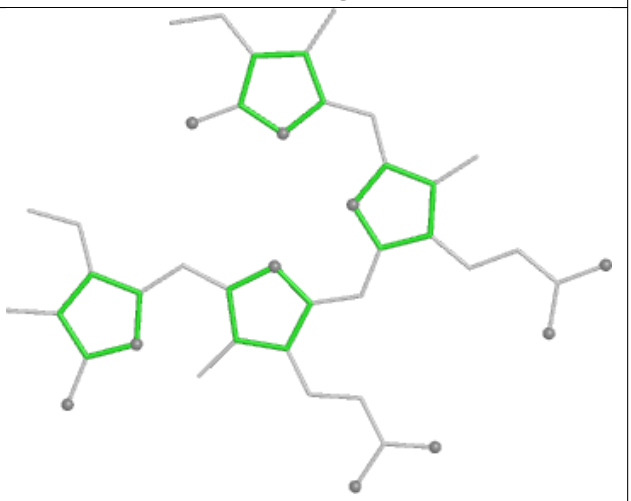

Rings

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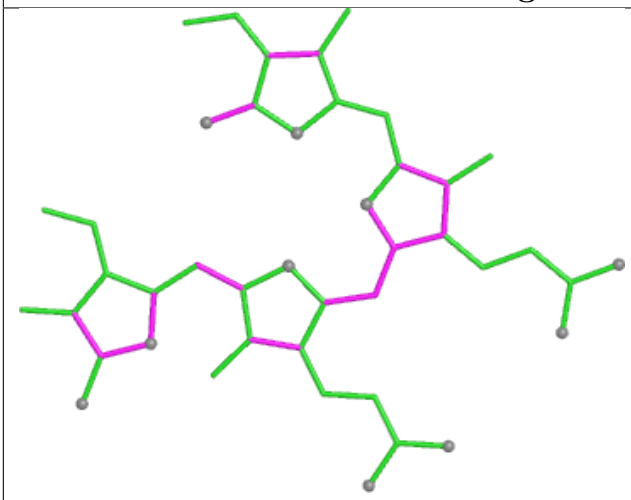

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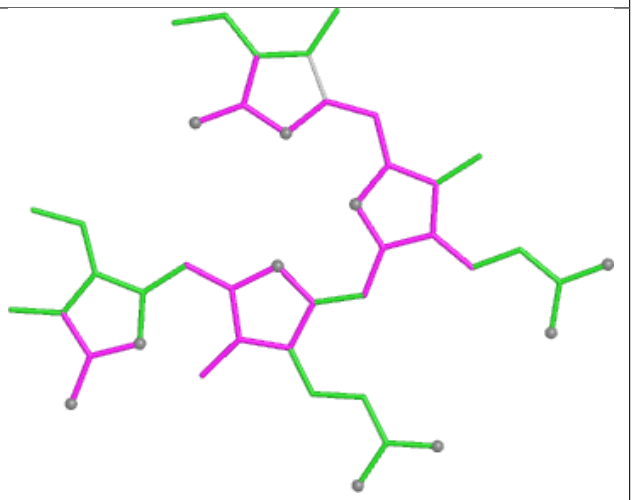

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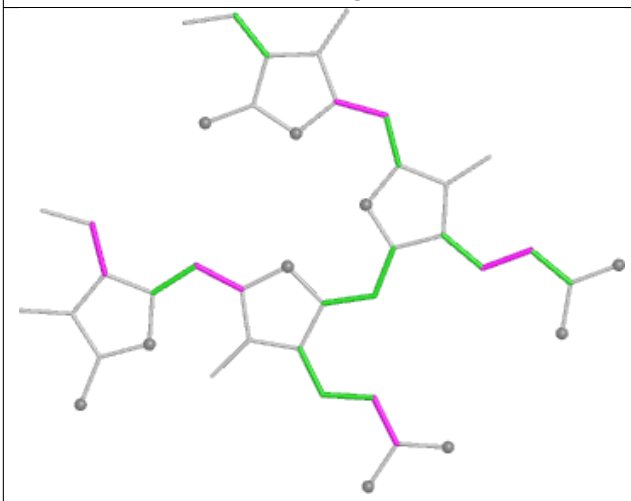

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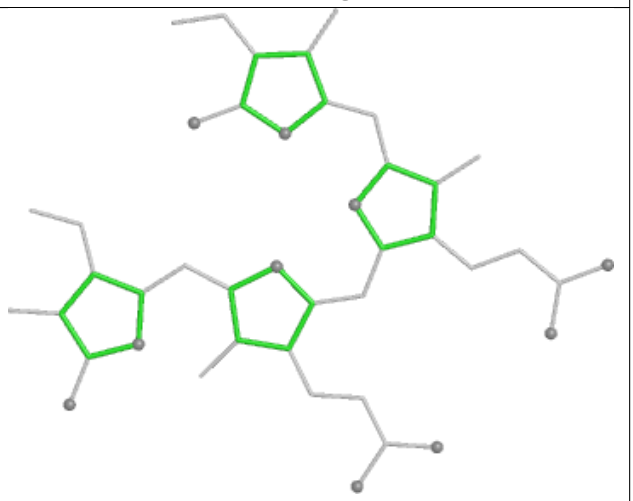
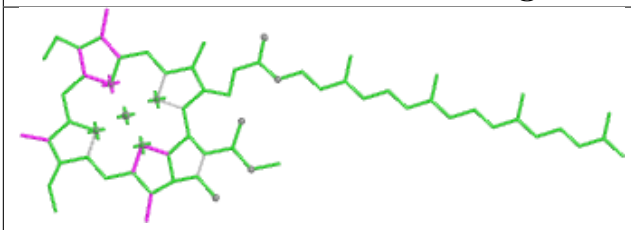


Rings

Ligand CLA cL 510



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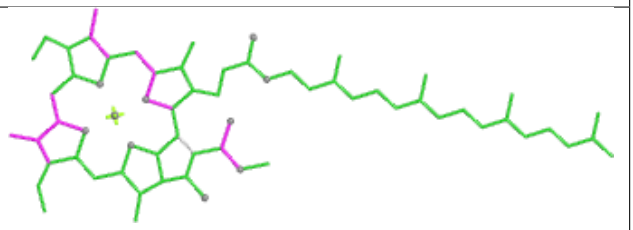
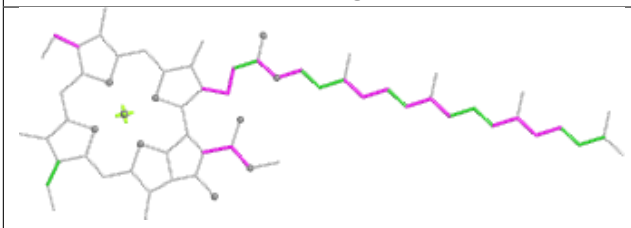


Bond angles



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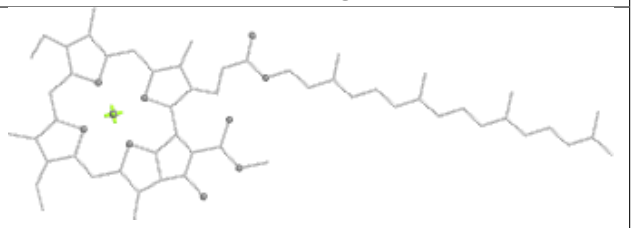
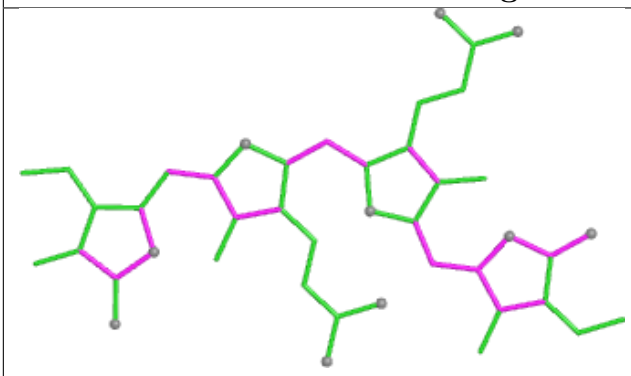


Rings

Ligand CYC HE 1001



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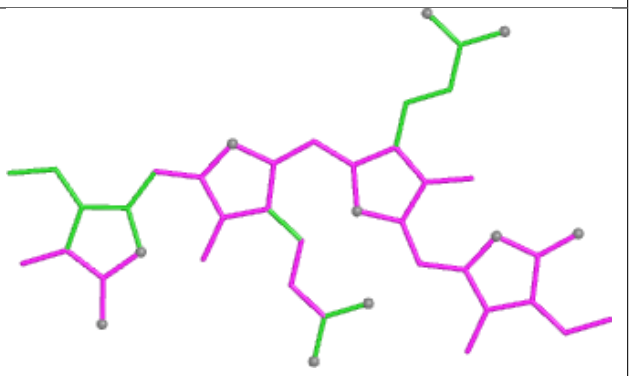

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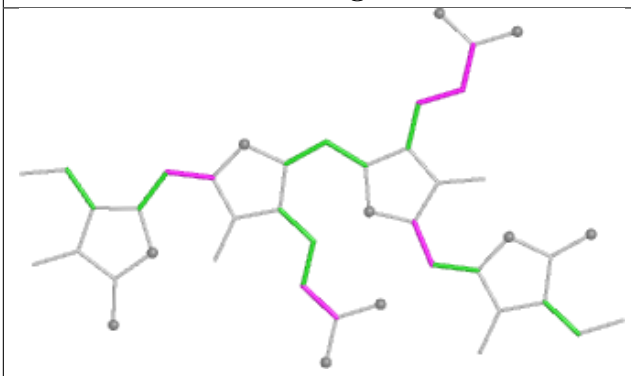

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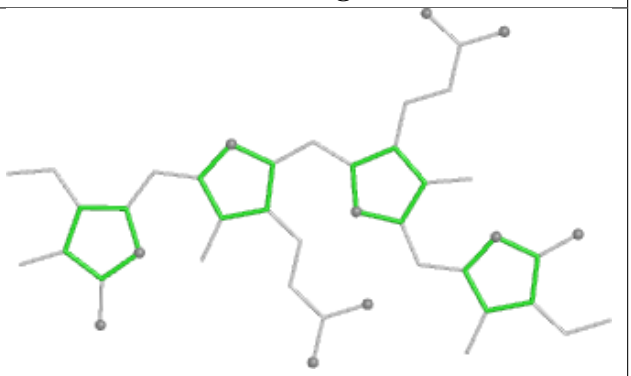
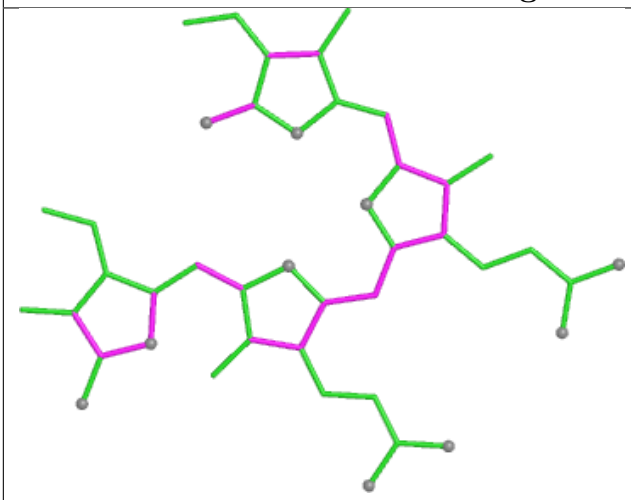


Rings

Ligand PEB 18 202



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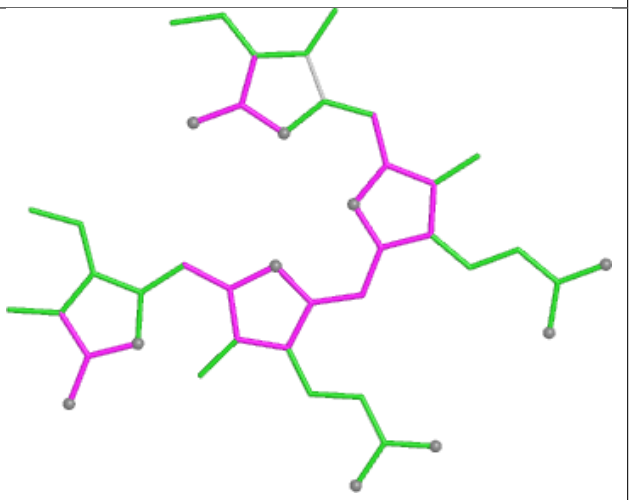

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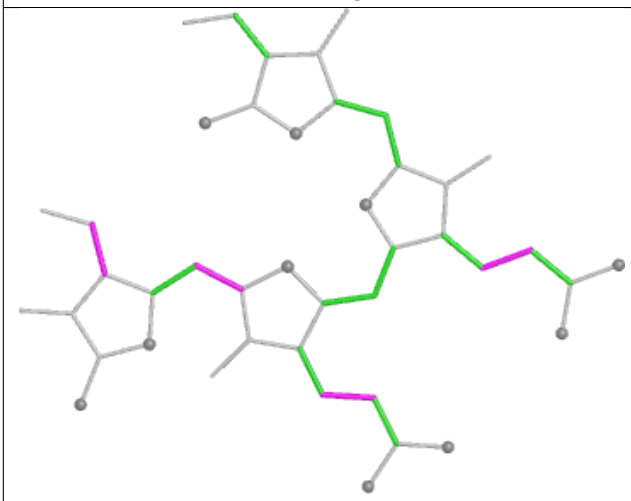

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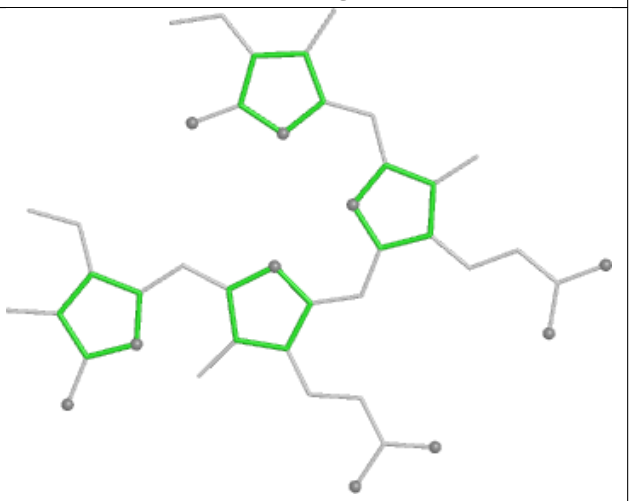
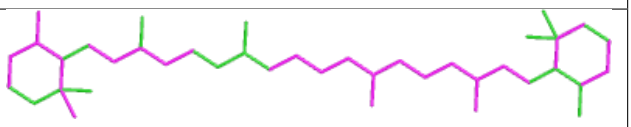


Rings

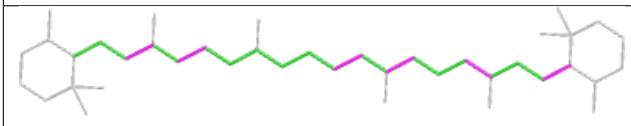
Ligand BCR A2 846



Bond lengths



Bond angles



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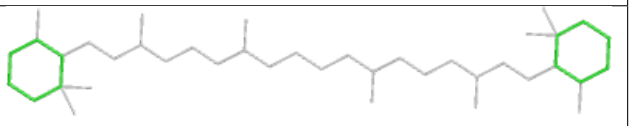
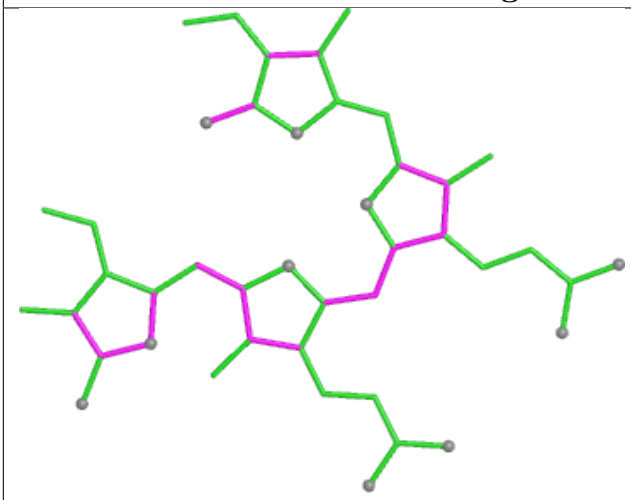


Rings

Ligand PEB DH 1002



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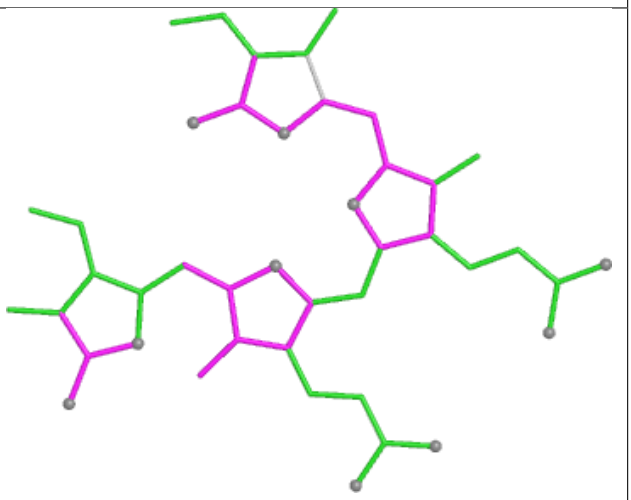
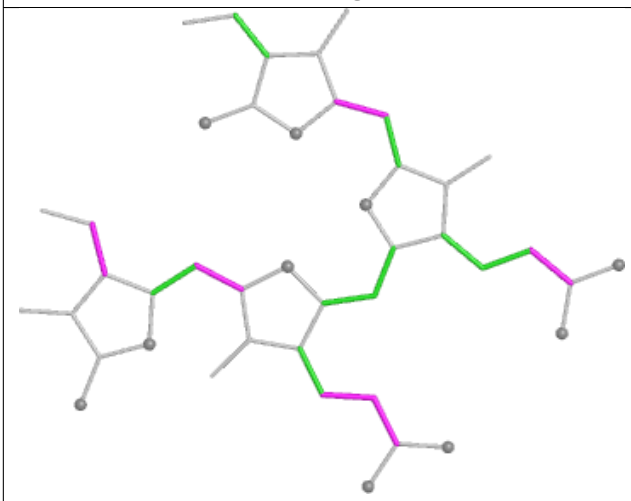


Bond angles



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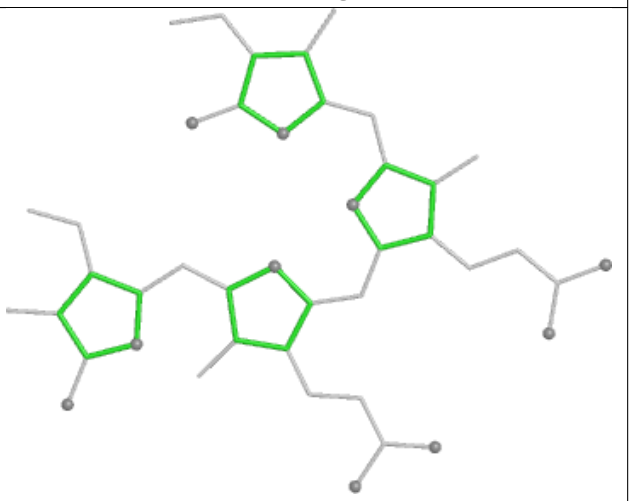
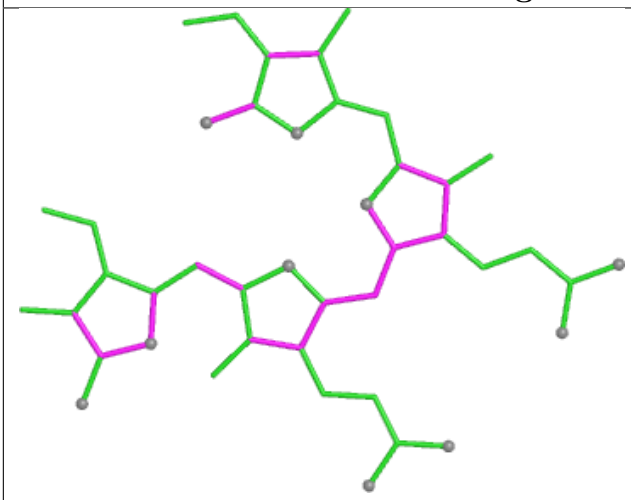


Rings

Ligand PEB vC 201



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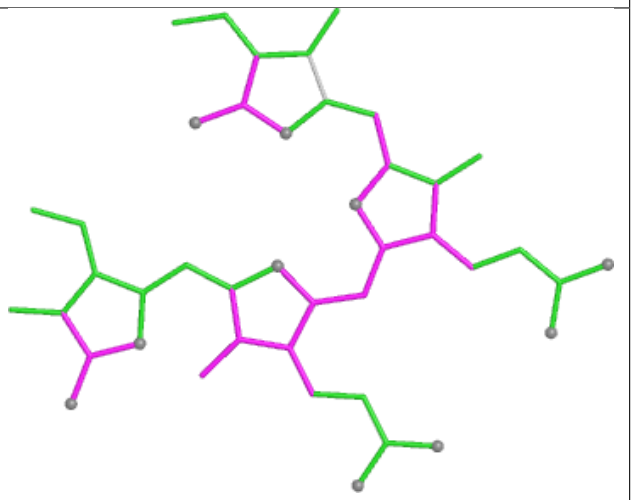

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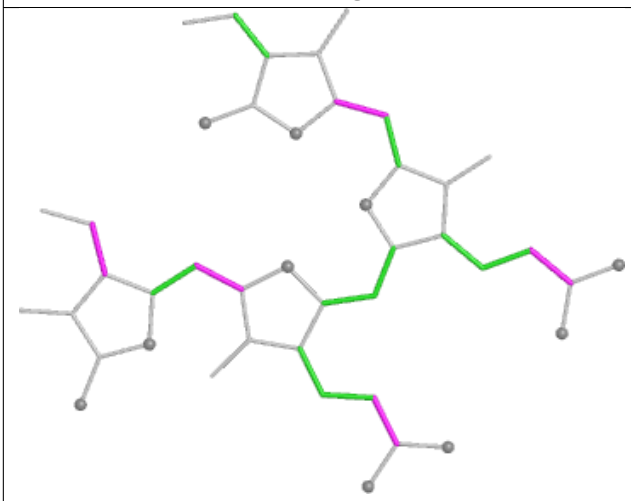

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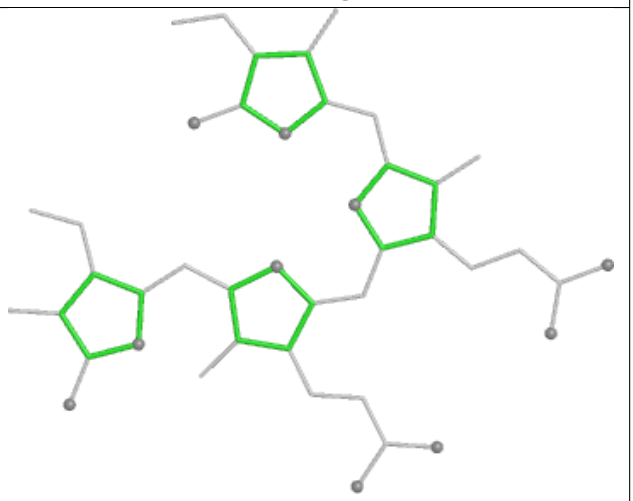
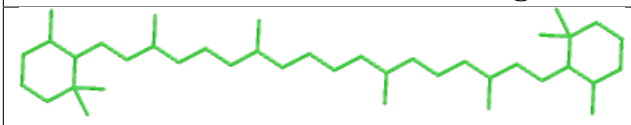


Rings

Ligand BCR K2 105



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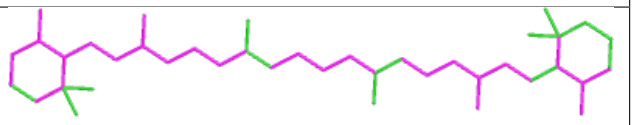
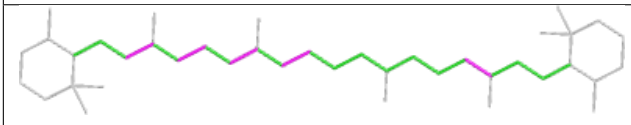


Bond angles



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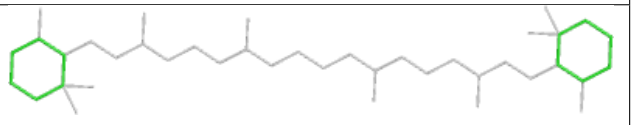
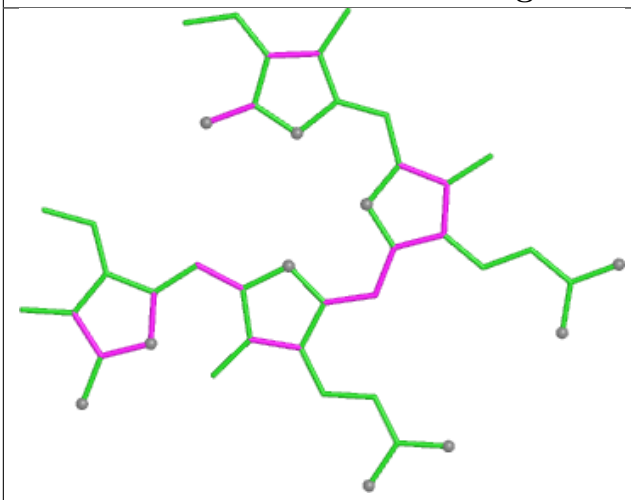


Rings

Ligand PEB dE 202



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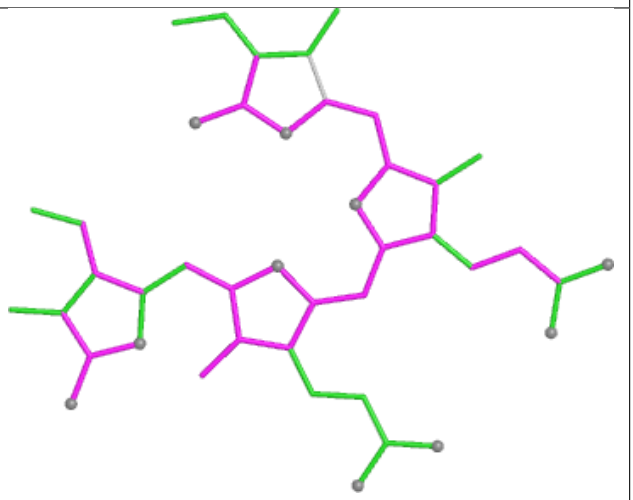
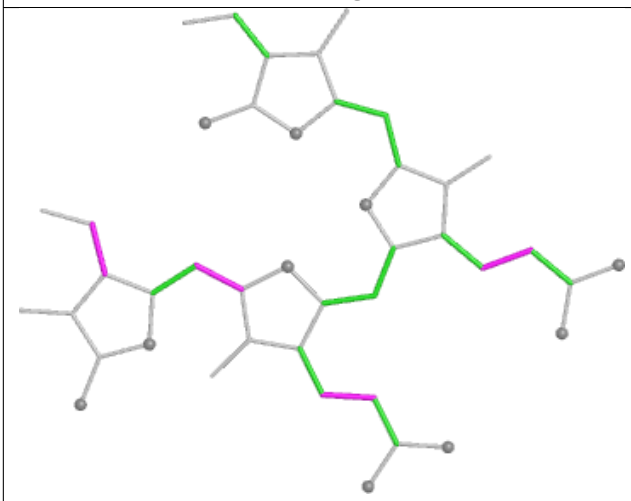


Bond angles



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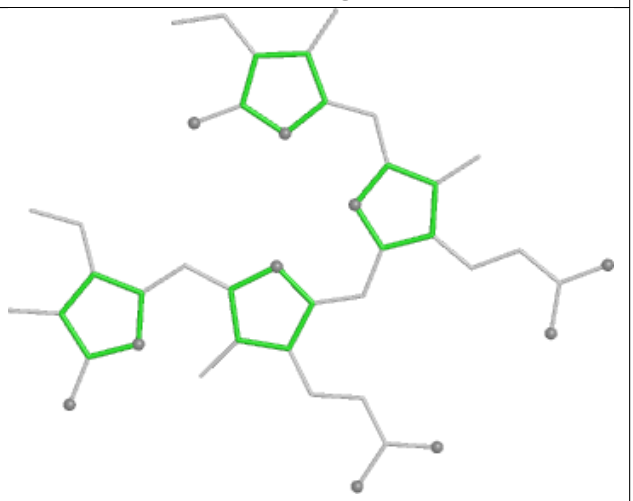
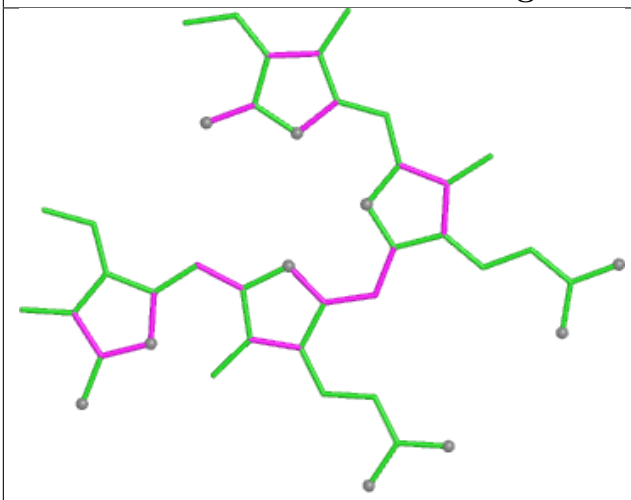


Rings

Ligand PEB GI 201



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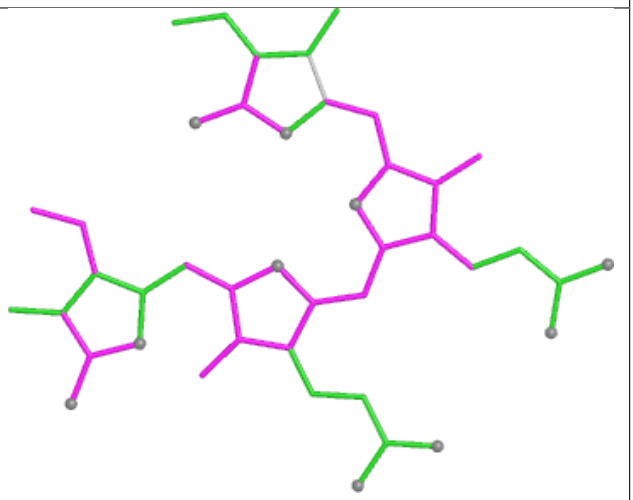
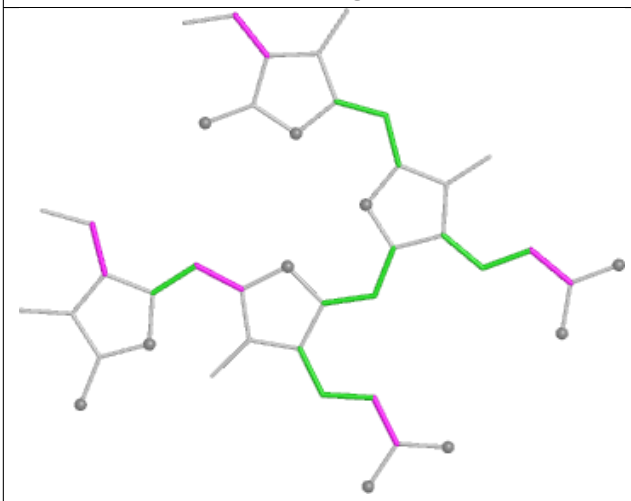
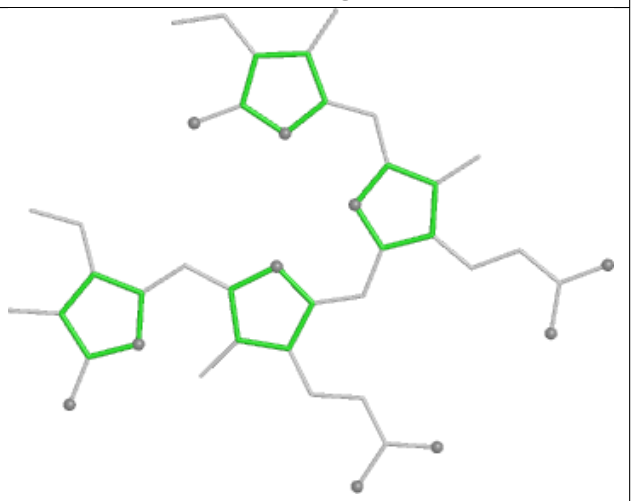


Bond angles

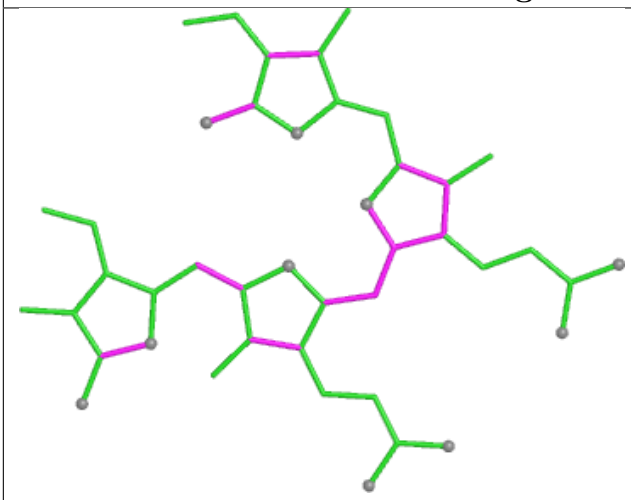


Torsions



Rings

Ligand PEB A1 301



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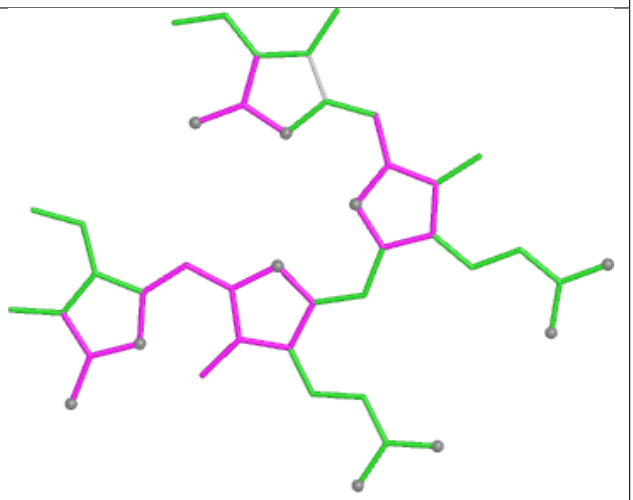
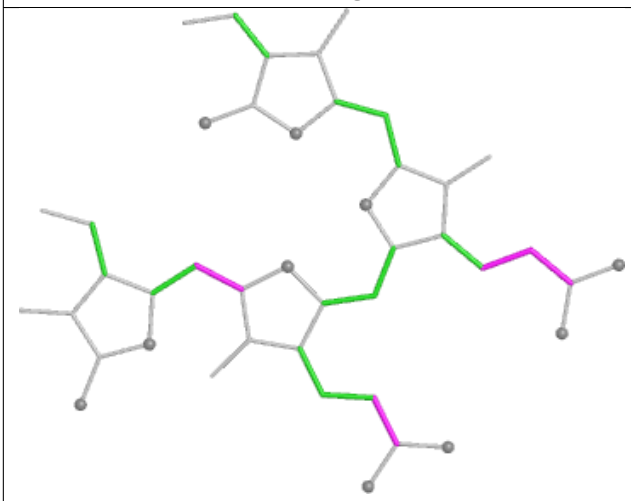


Bond angles



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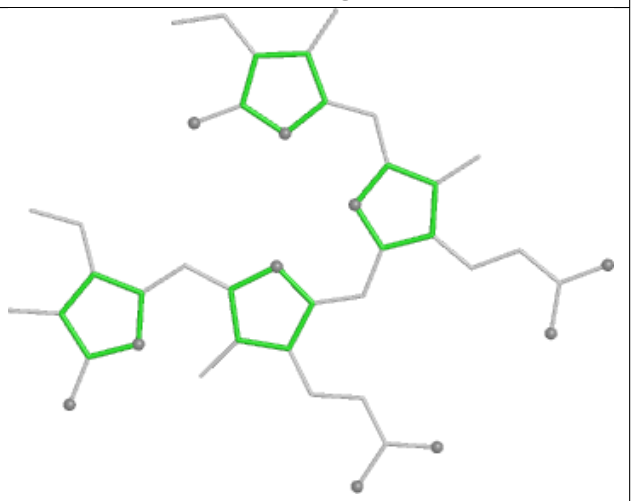
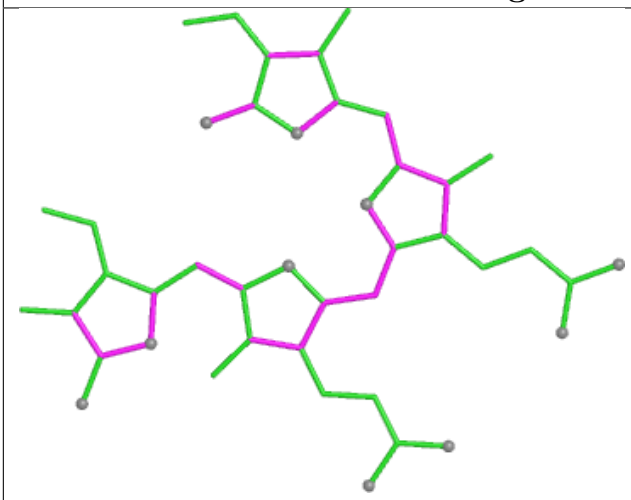


Rings

Ligand PEB PM 201



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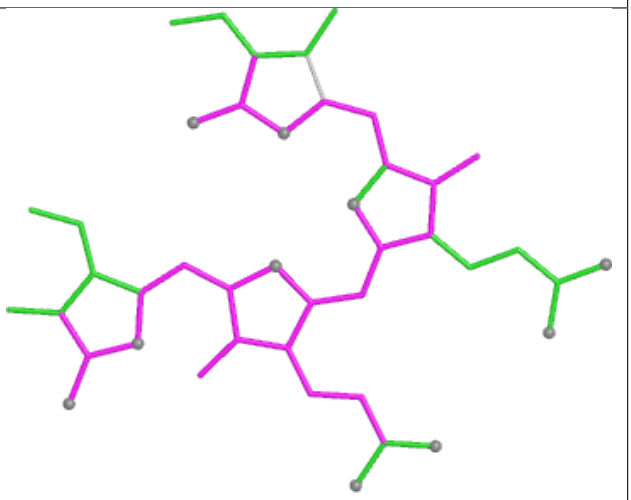

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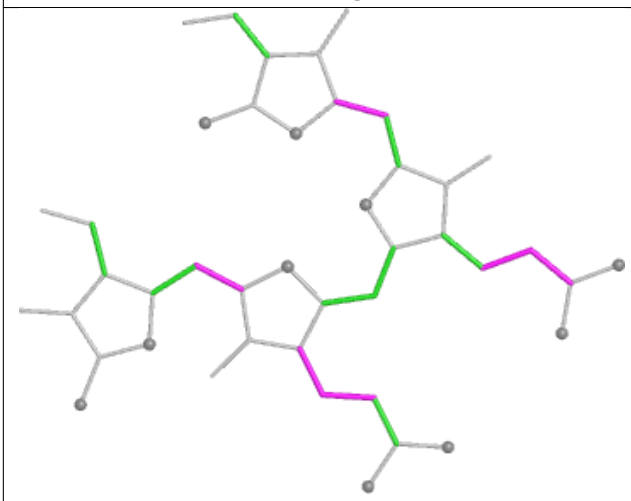

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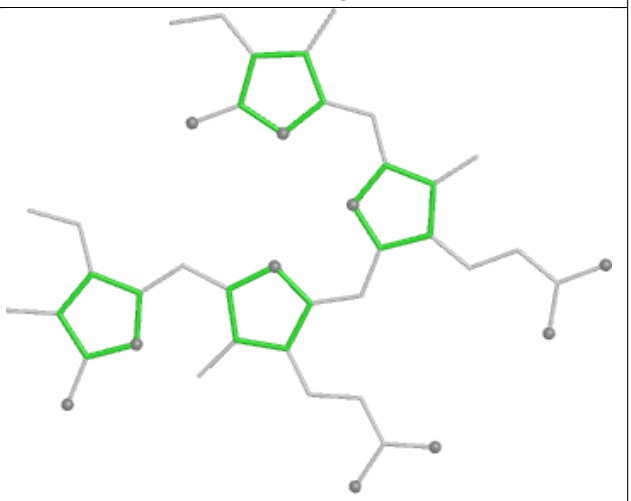
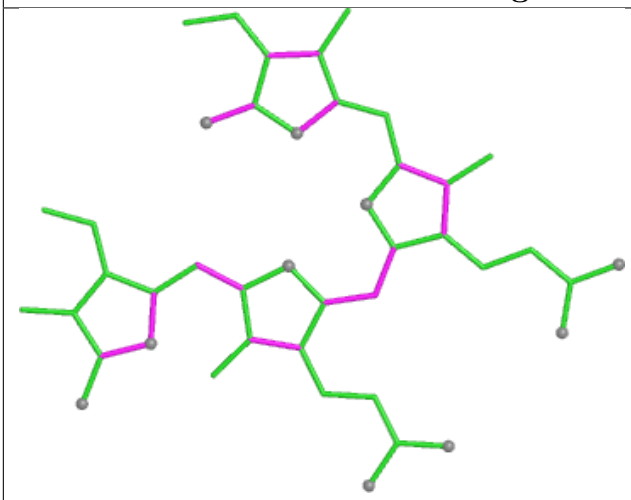


Rings

Ligand PEB VQ 201



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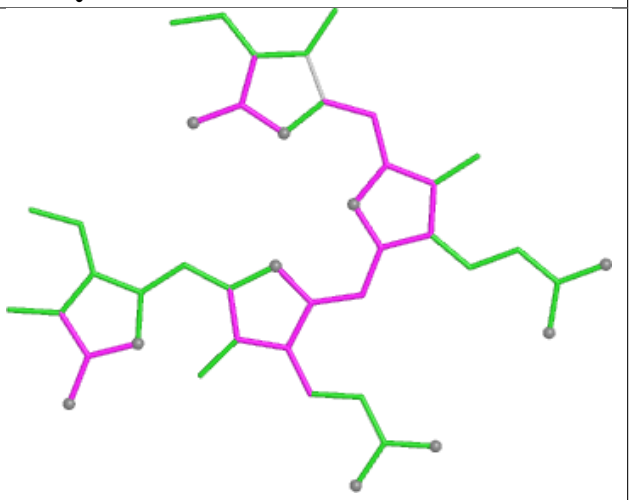

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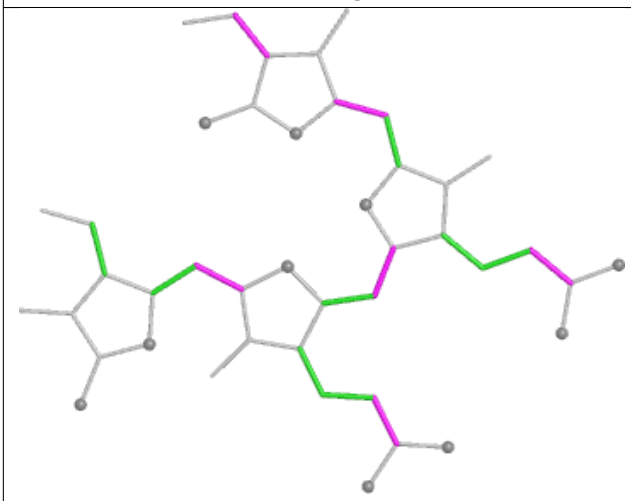

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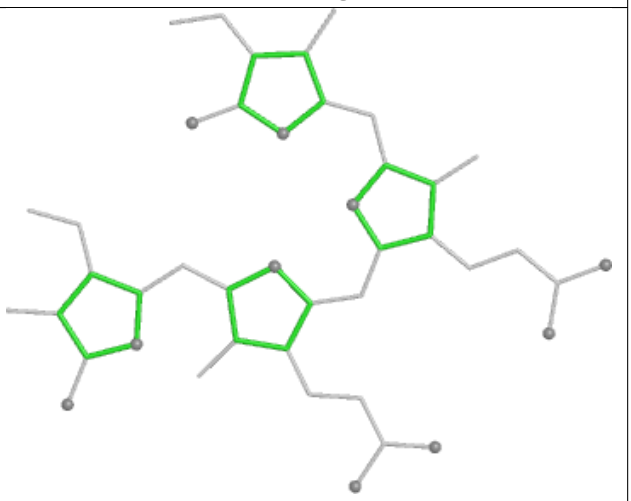
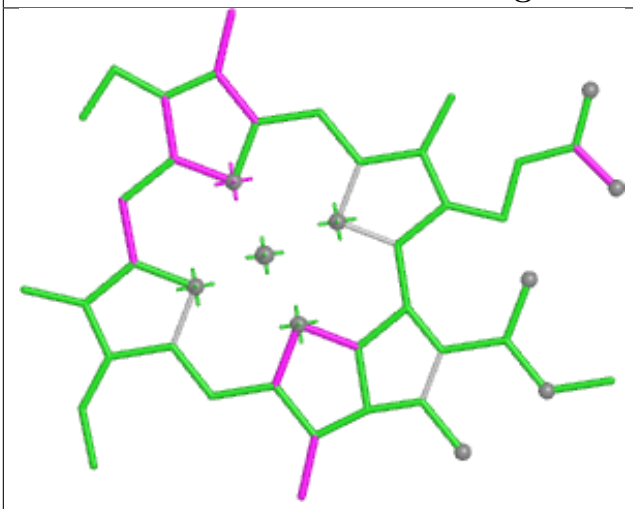


Rings

Ligand CLA 6N 613



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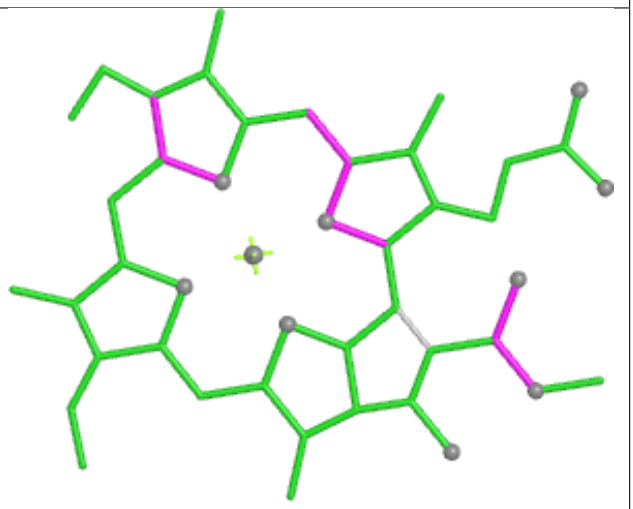

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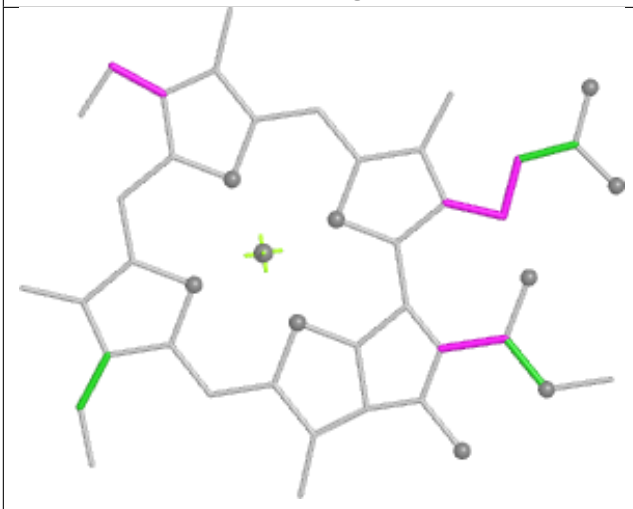
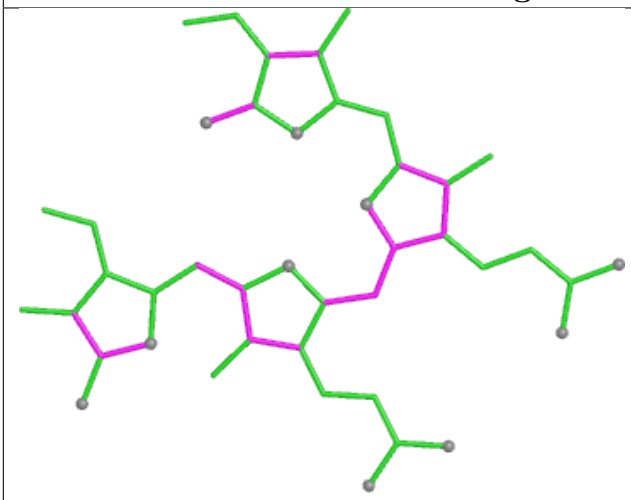


Torsions



Rings

Ligand PEB hK 201



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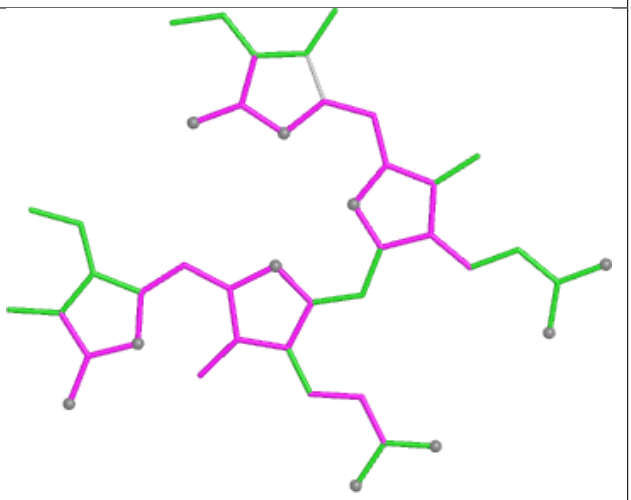

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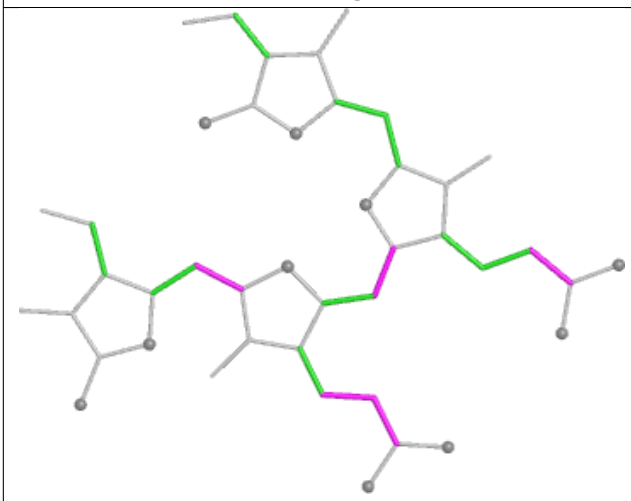

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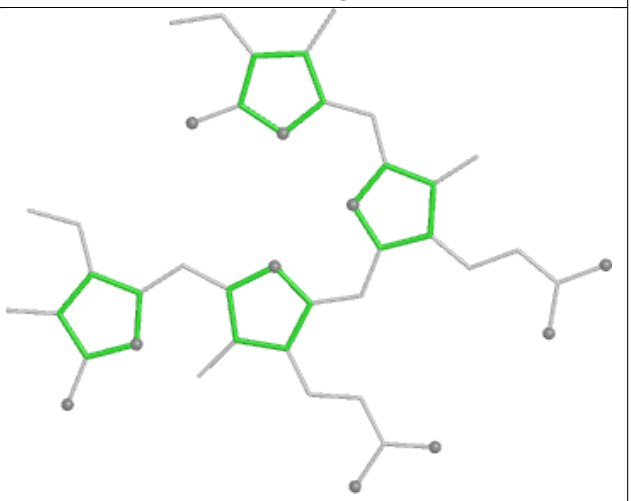

Rings

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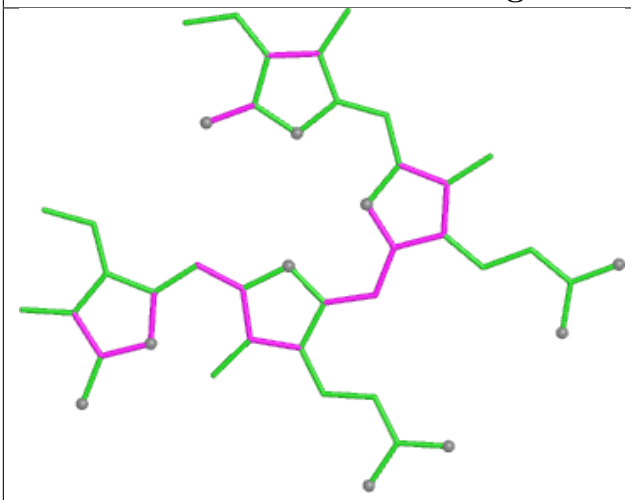

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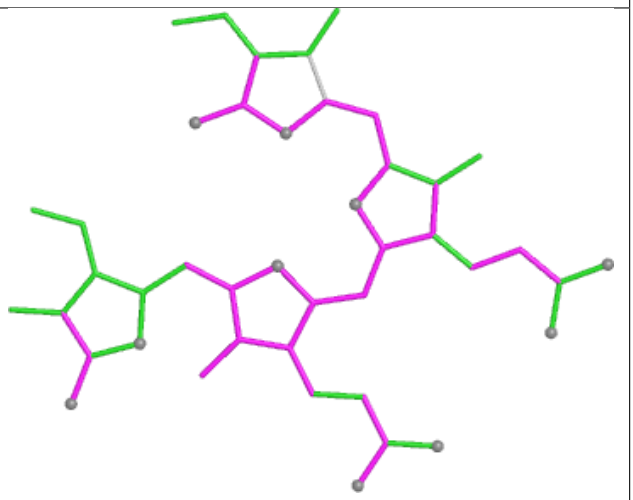

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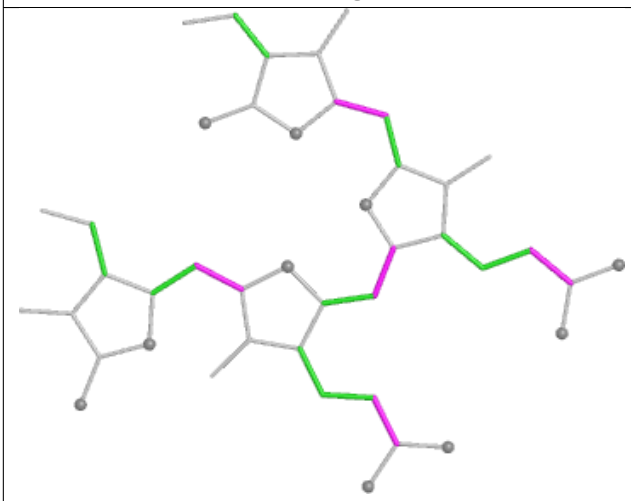

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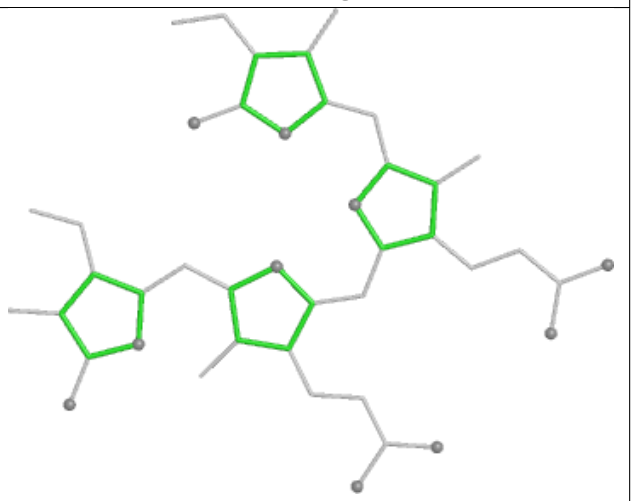
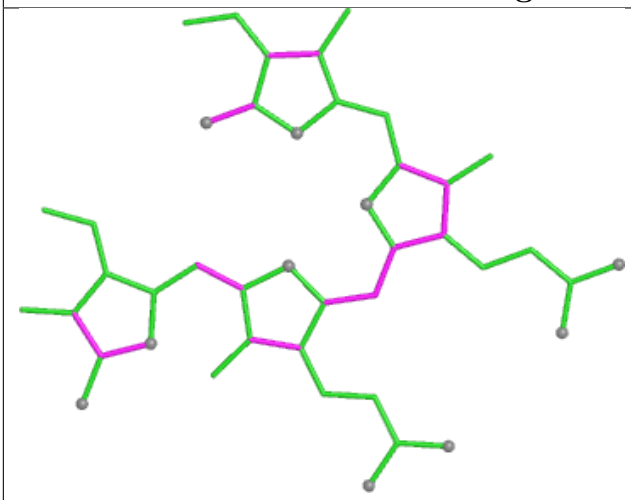


Rings

Ligand PEB jM 202



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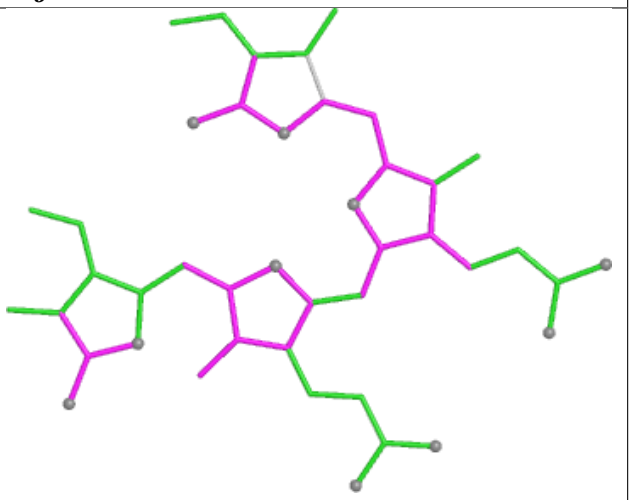

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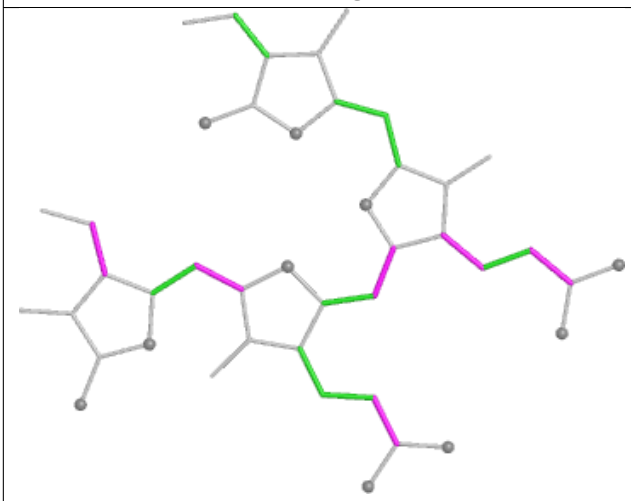

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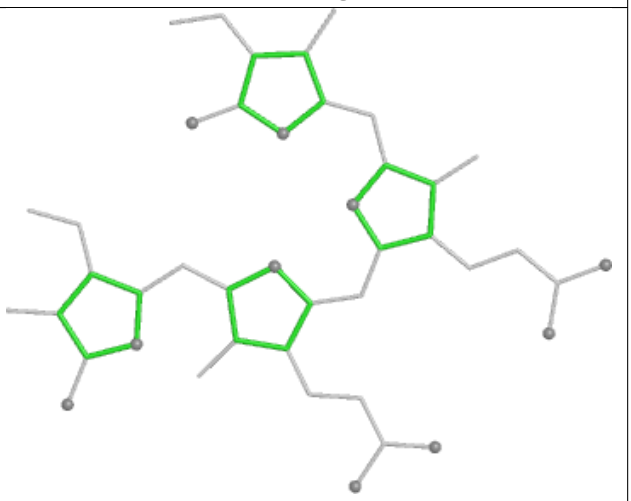
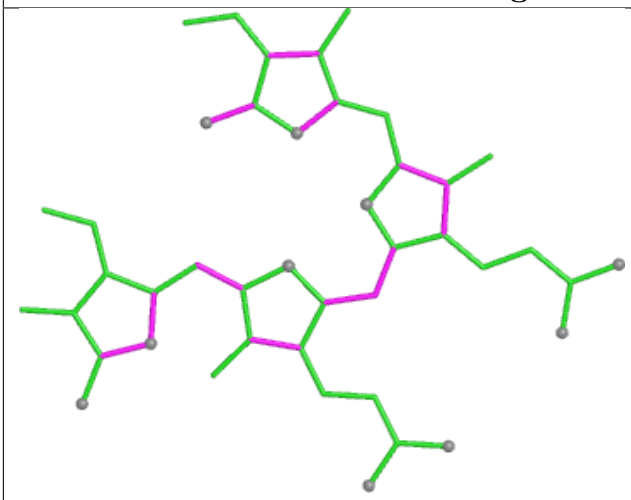


Rings

Ligand PEB VD 201



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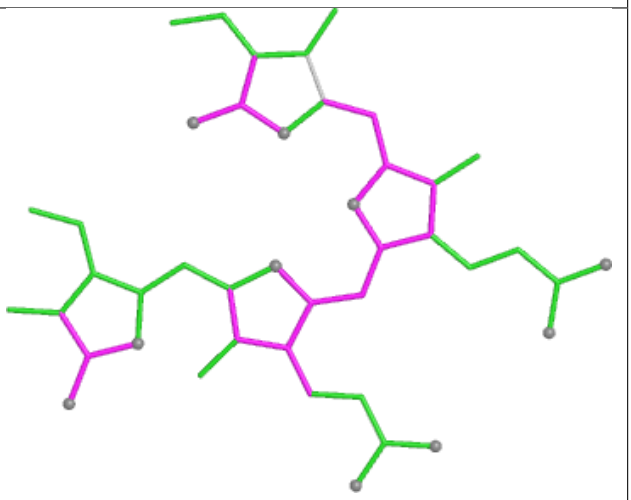

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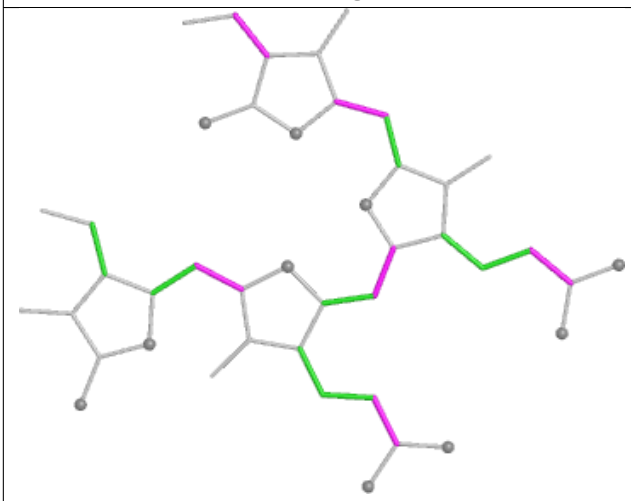

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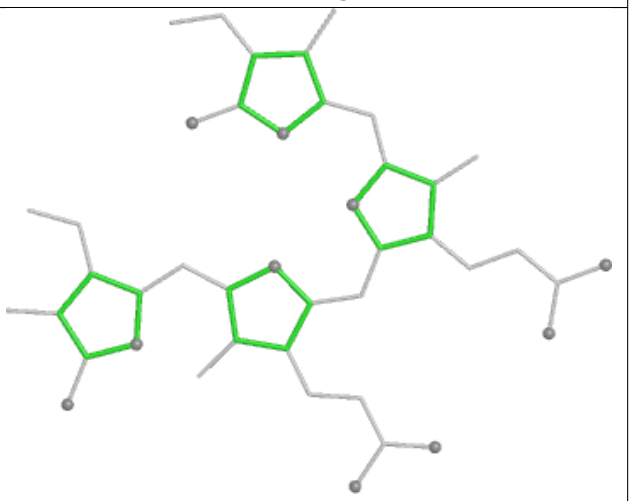
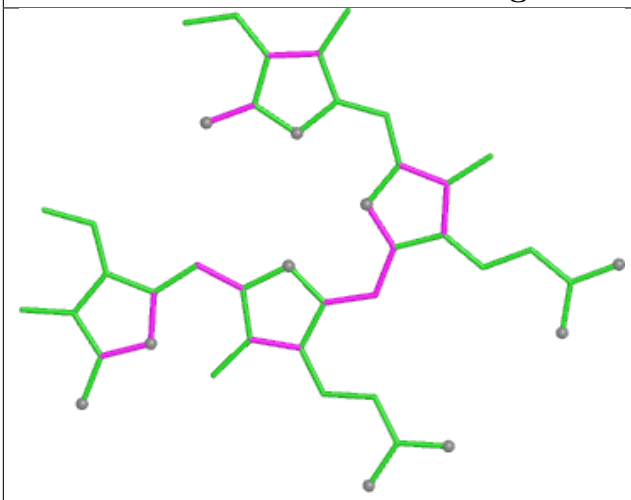


Rings

Ligand PEB KK 203



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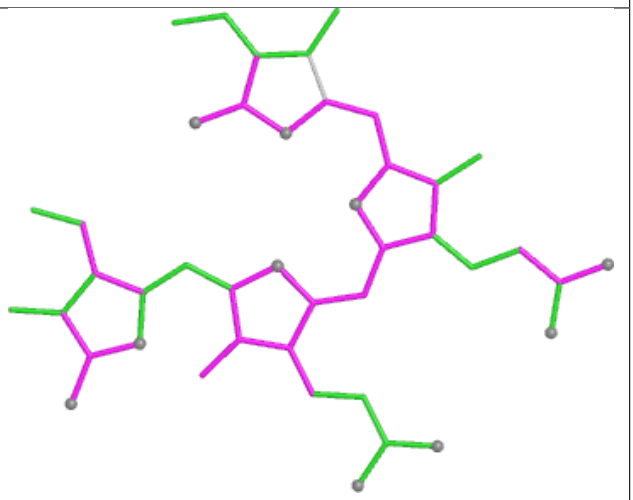
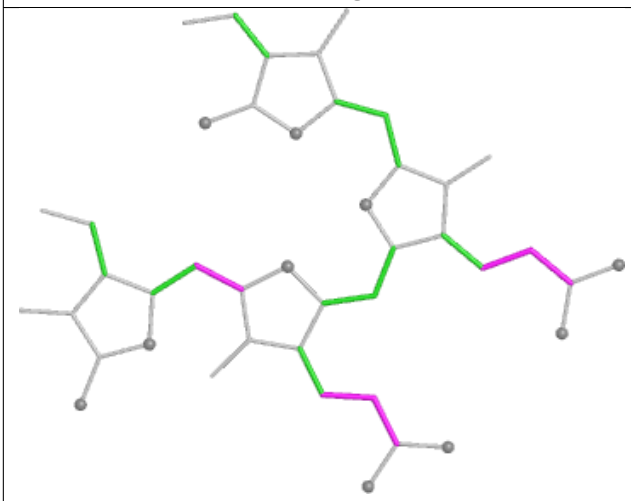


Bond angles



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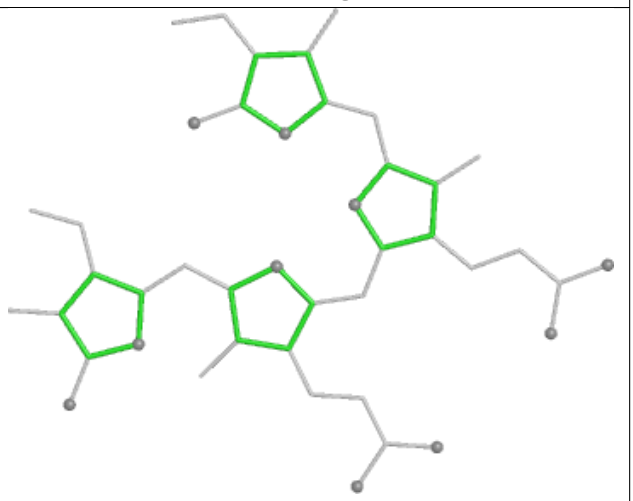
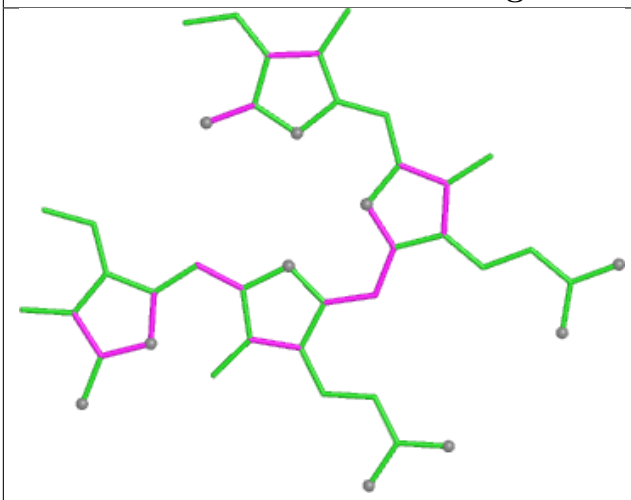


Rings

Ligand PEB WB 402



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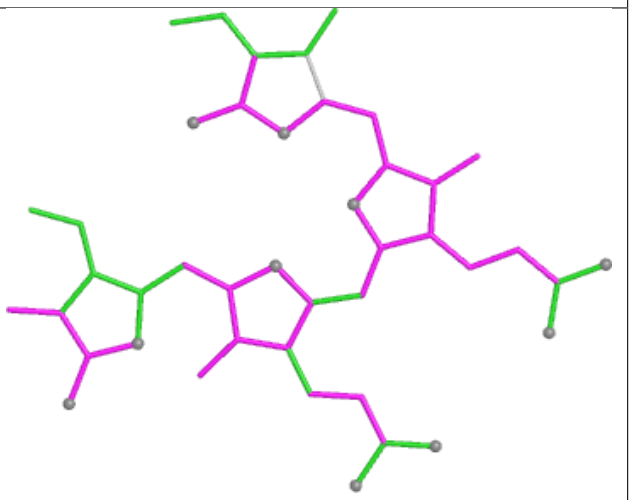
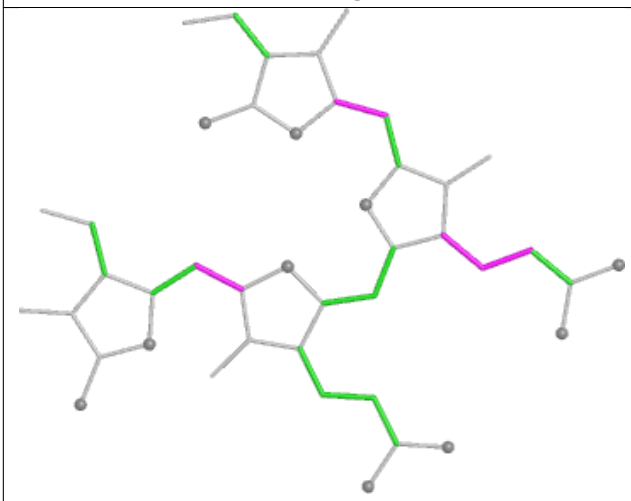


Bond angles



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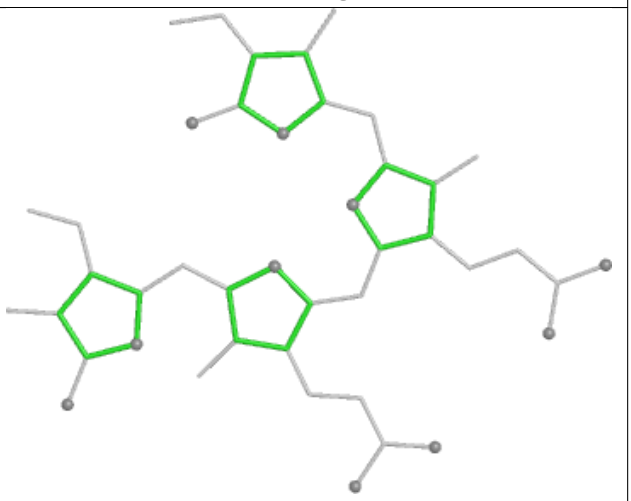
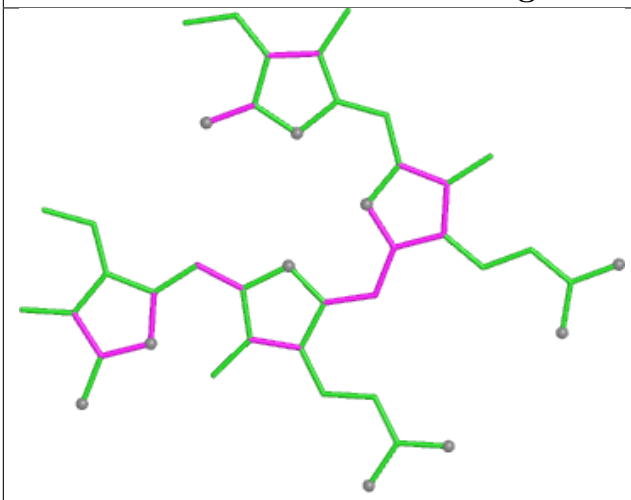


Rings

Ligand PEB L5 201



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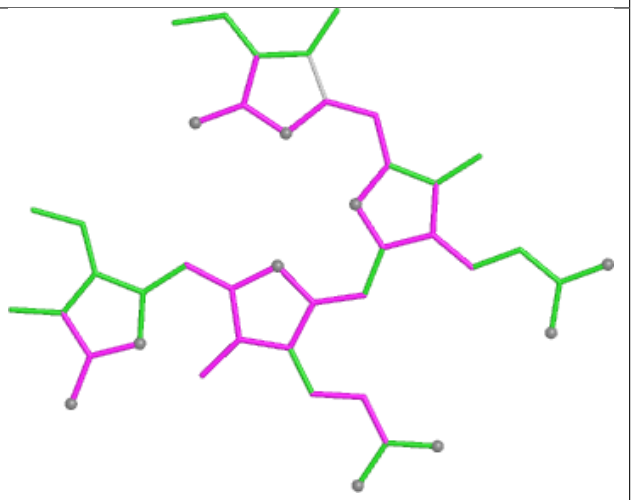

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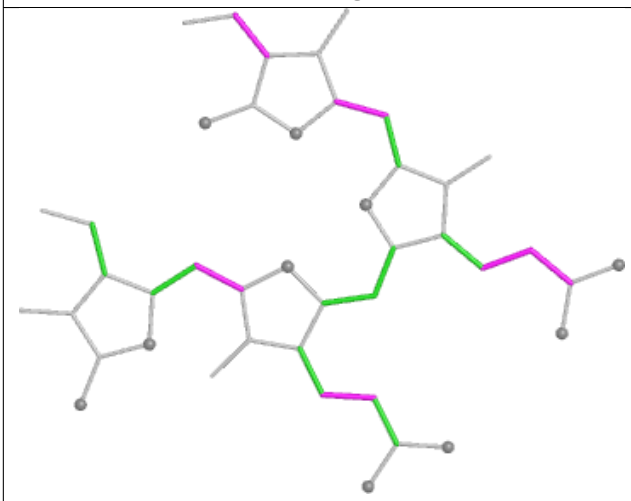

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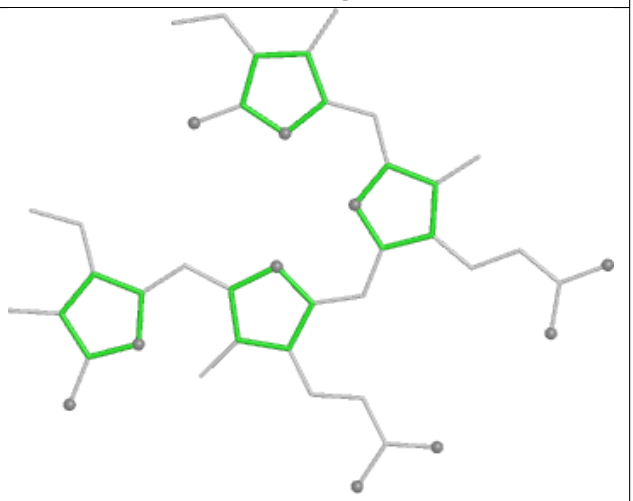
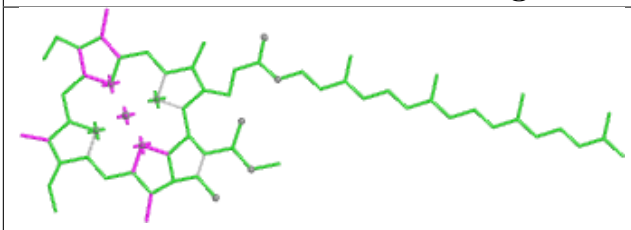


Rings

Ligand CLA BN 808



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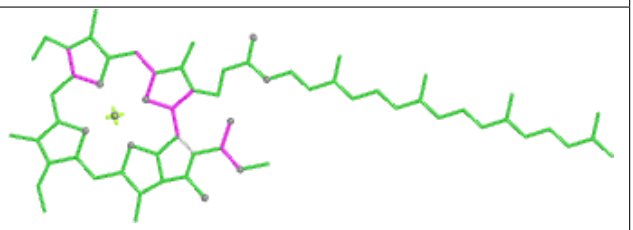
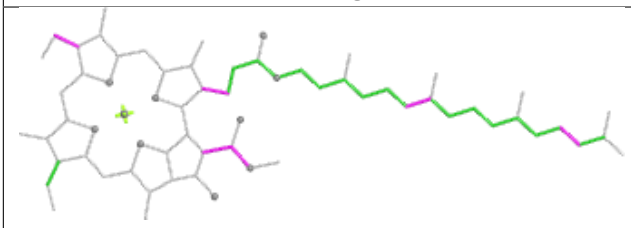


Bond angles



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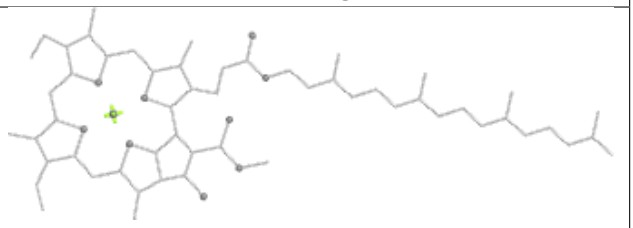
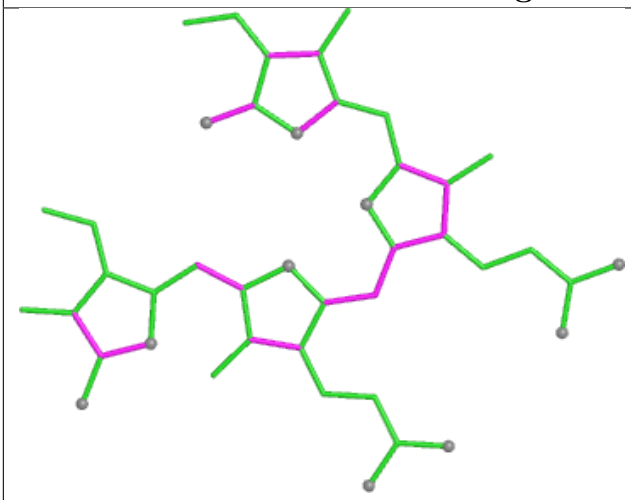


Rings

Ligand PEB JQ 201



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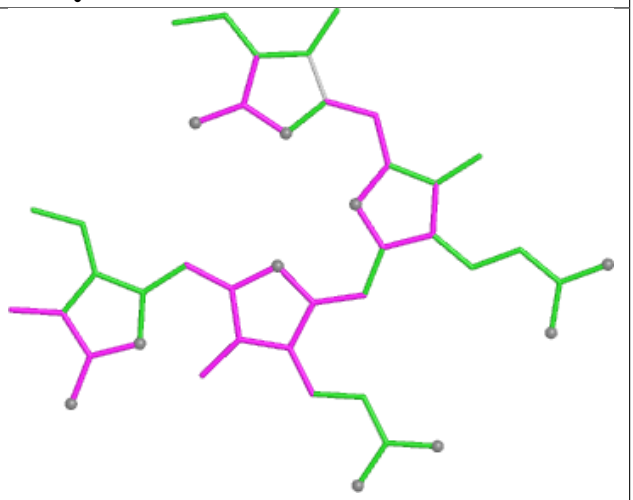
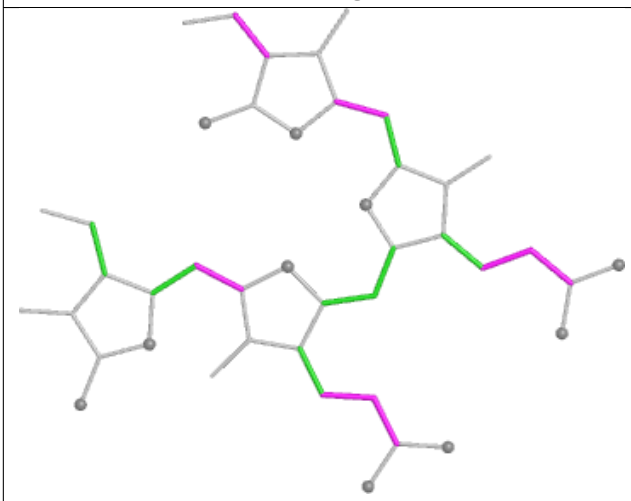


Bond angles



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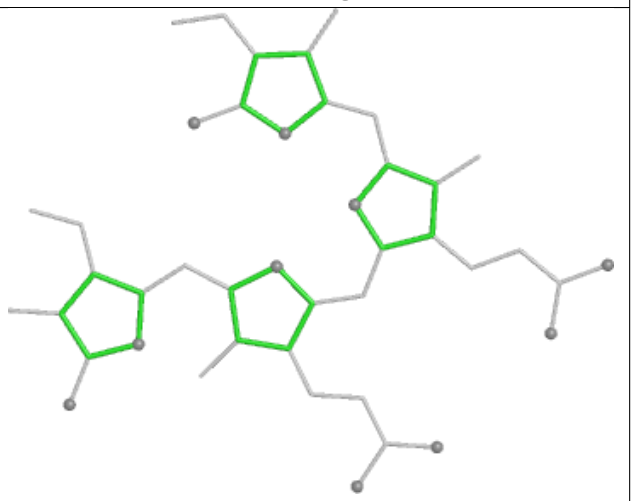
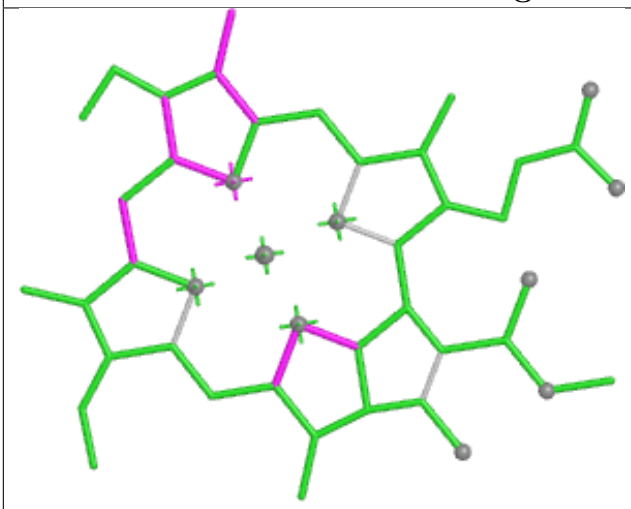


Rings

Ligand CLA 6N 601



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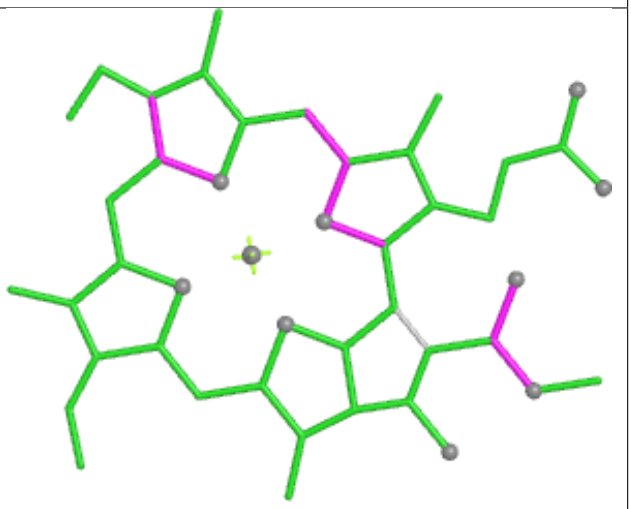
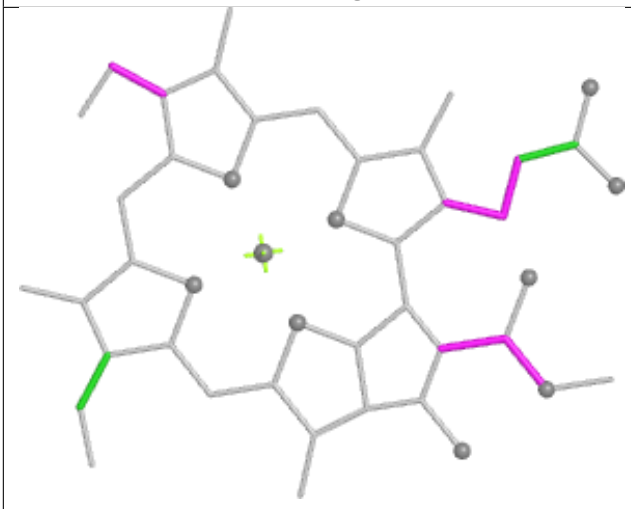


Bond angles

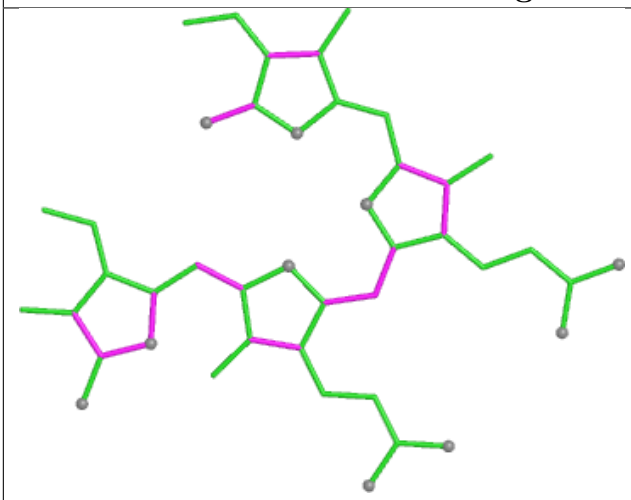


Torsions



Rings

Ligand PEB CJ 201



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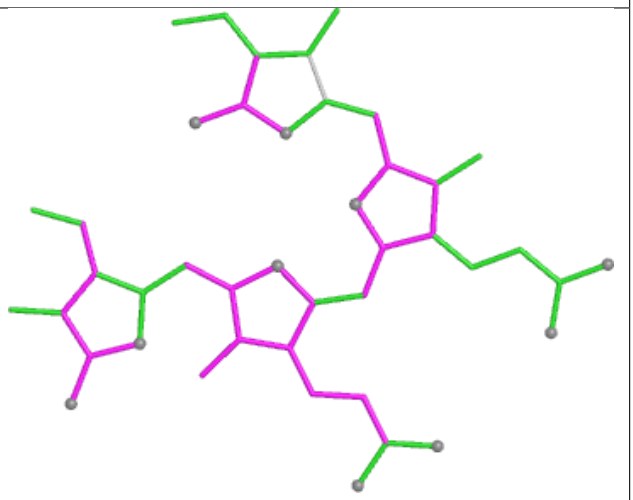
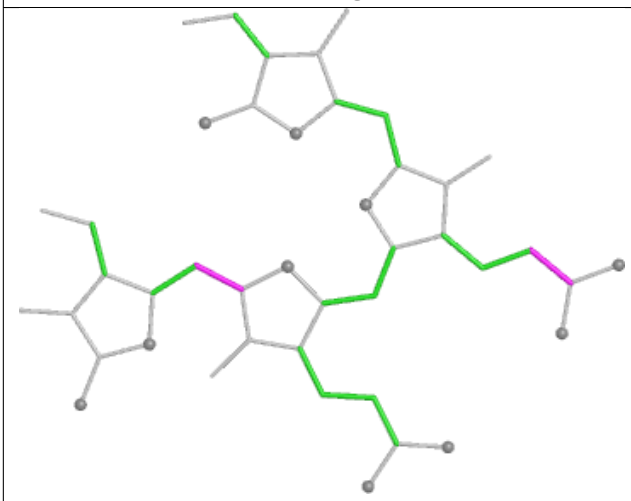
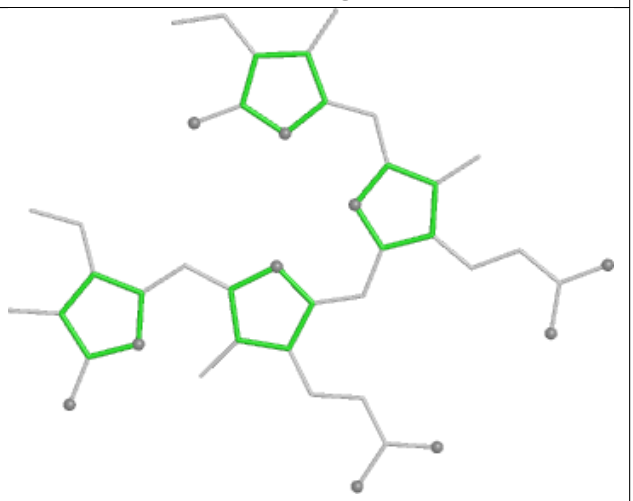


Bond angles

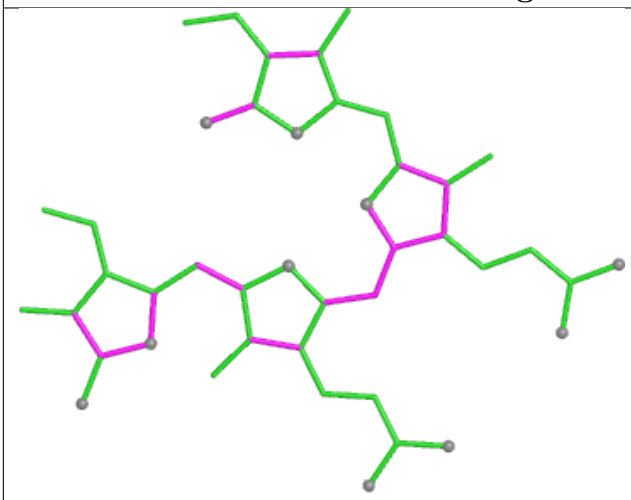


Torsions



Rings

Ligand PEB P1 201



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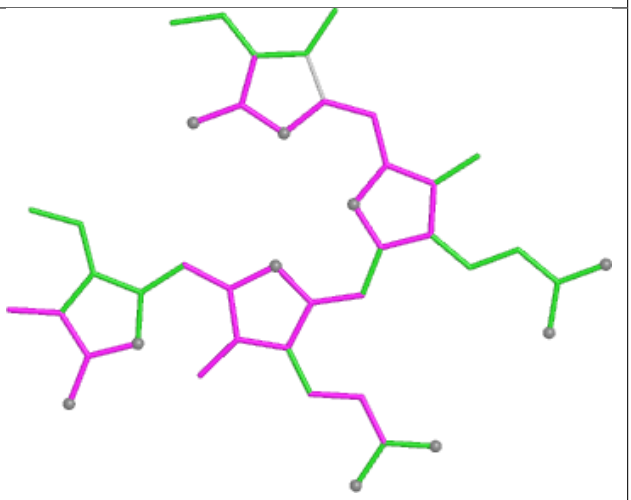

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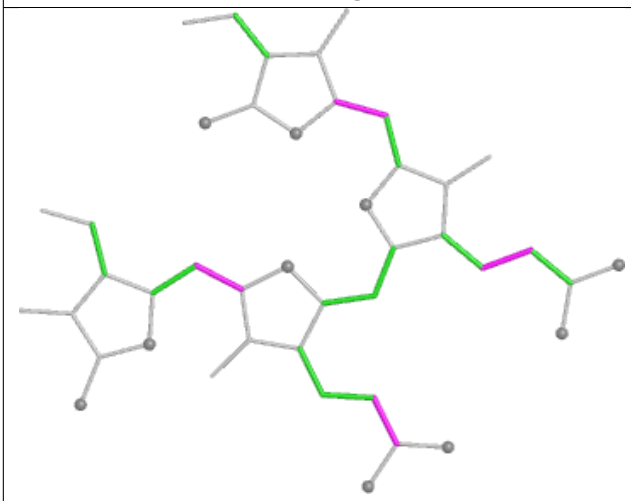

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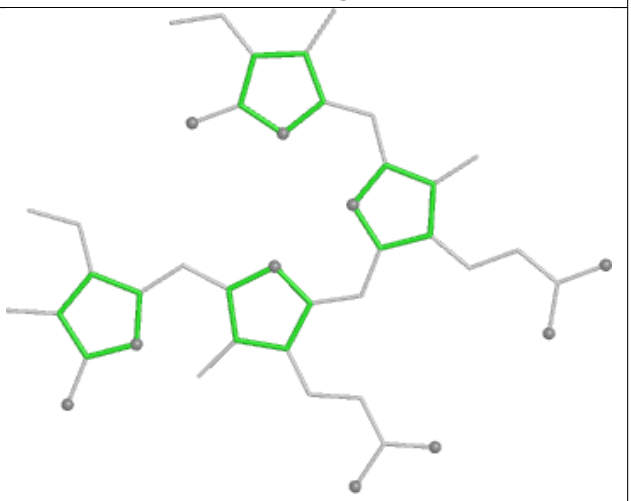
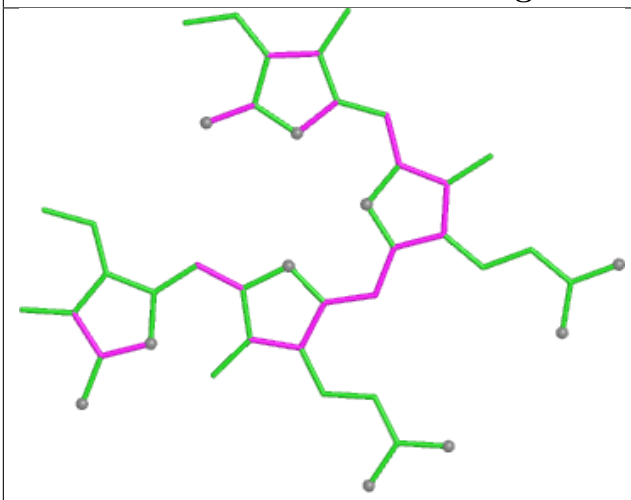


Rings

Ligand PEB D9 202



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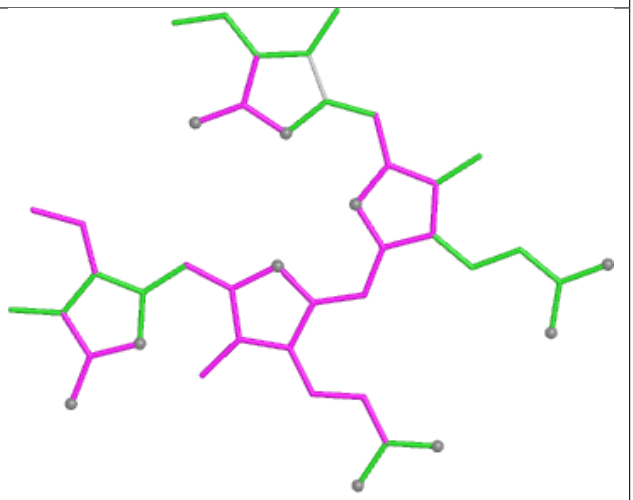

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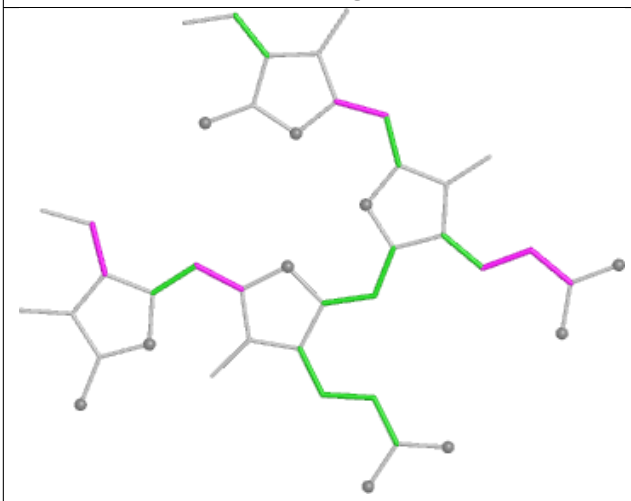

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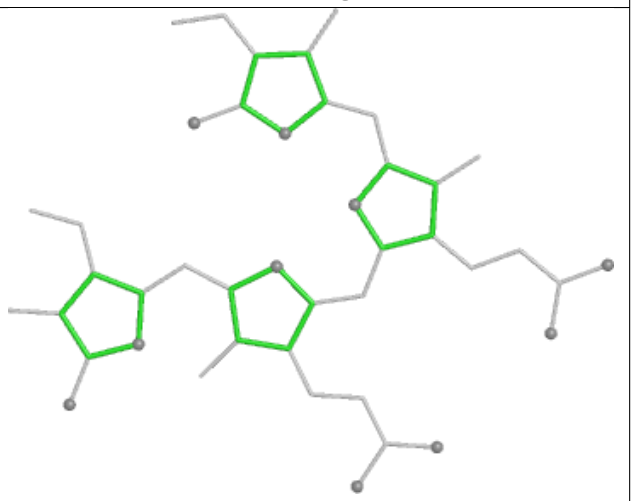
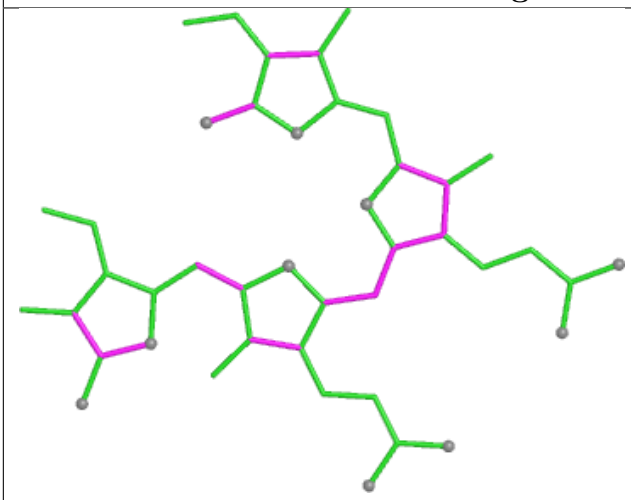


Rings

Ligand PEB AO 301



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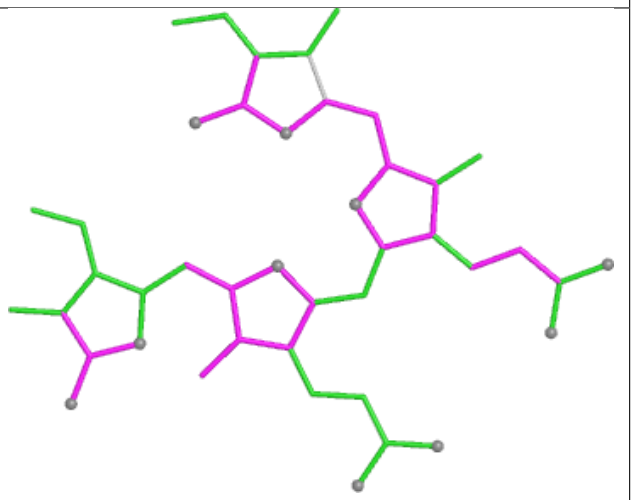

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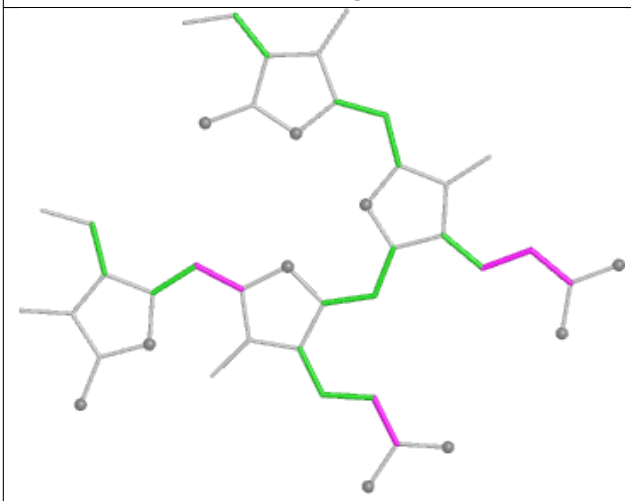

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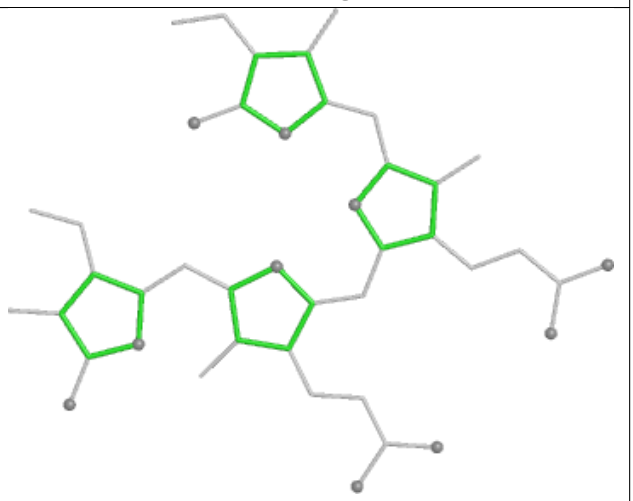
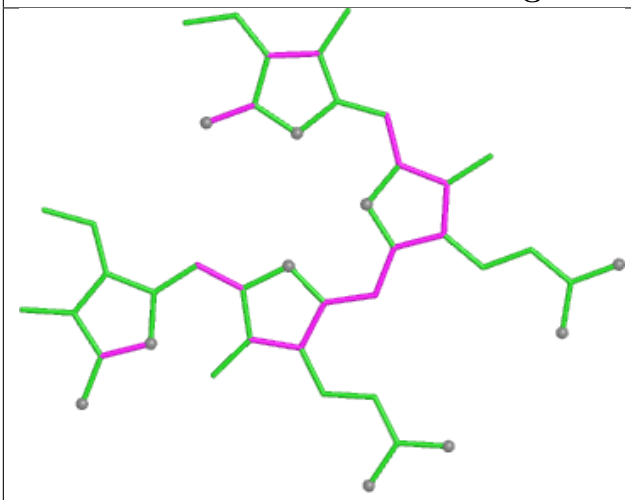


Rings

Ligand PEB l1 201



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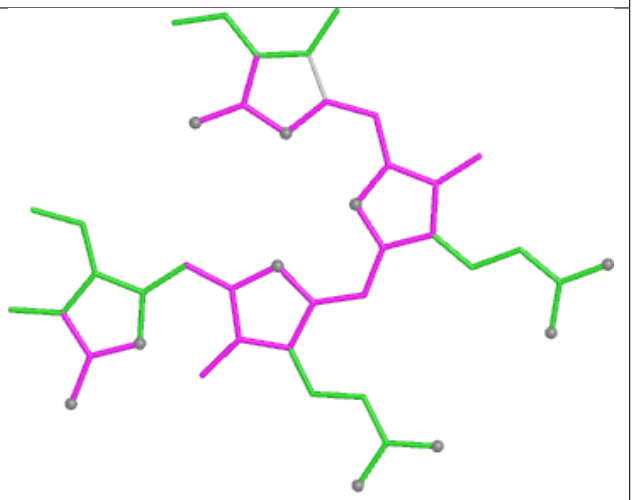

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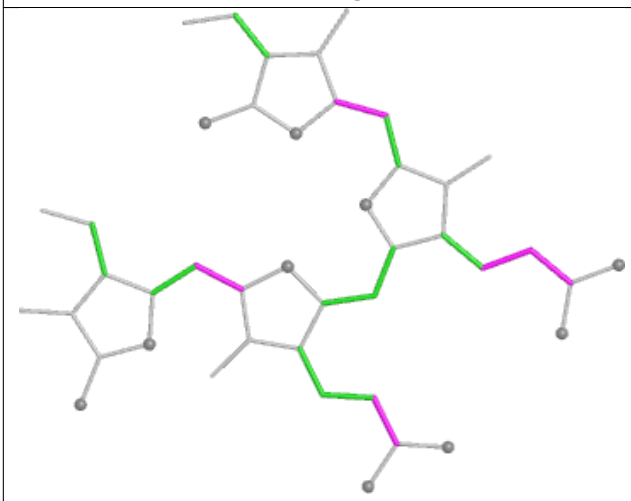

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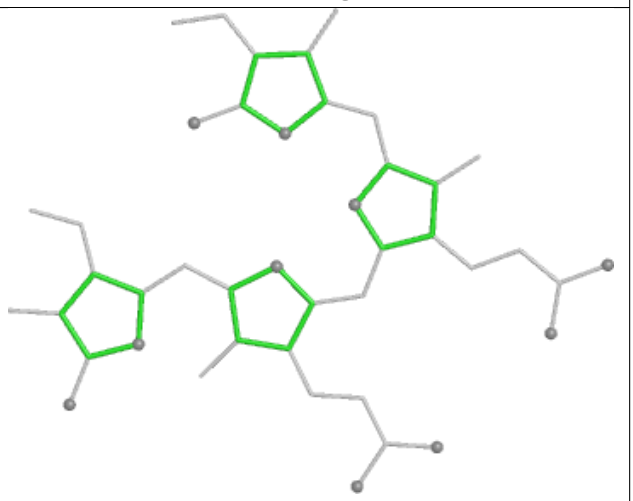
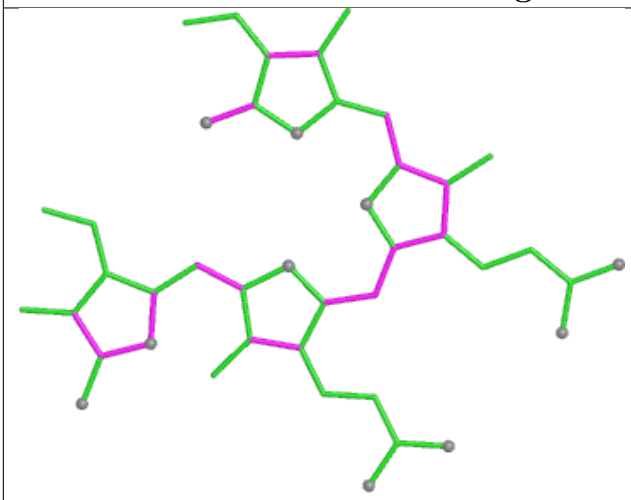


Rings

Ligand PEB H7 201



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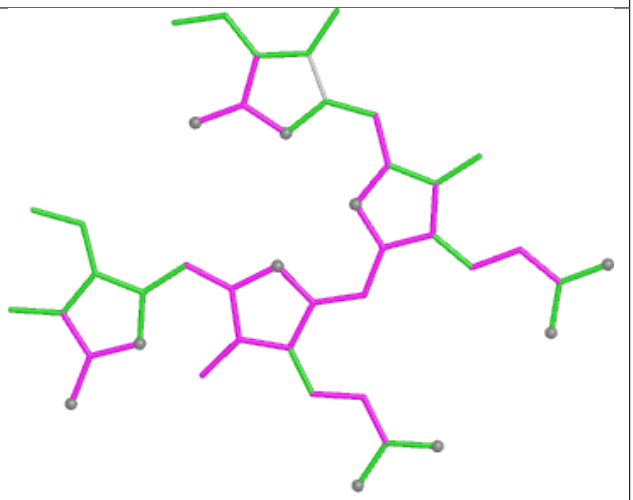

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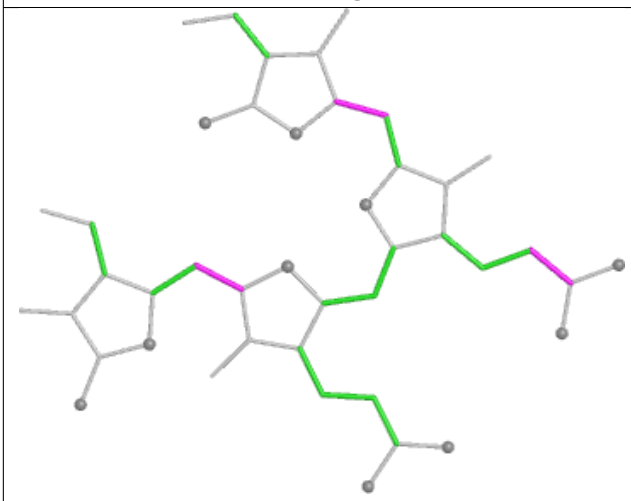

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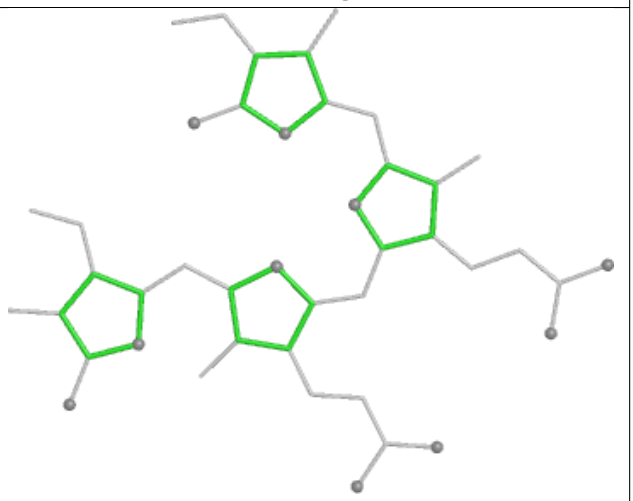
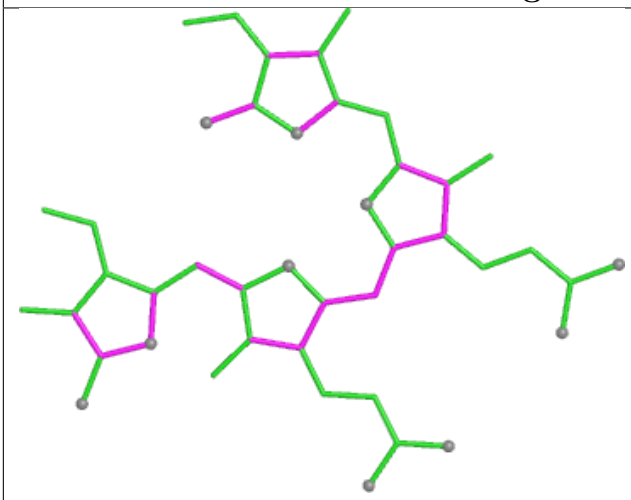


Rings

Ligand PEB f1 201



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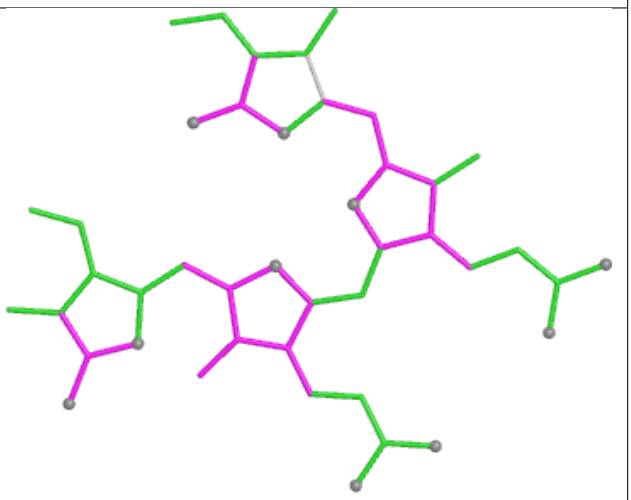

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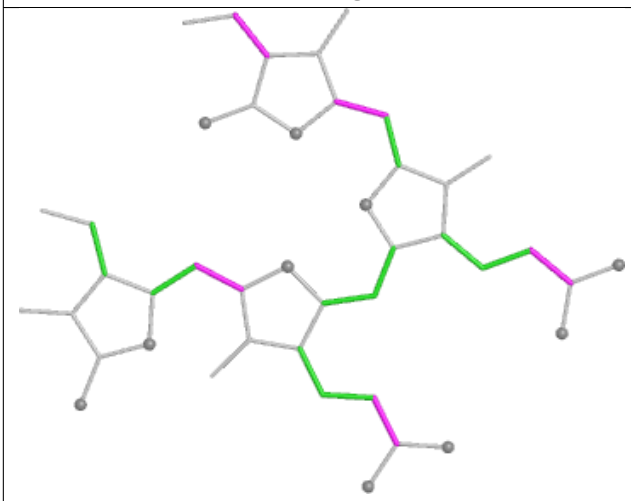

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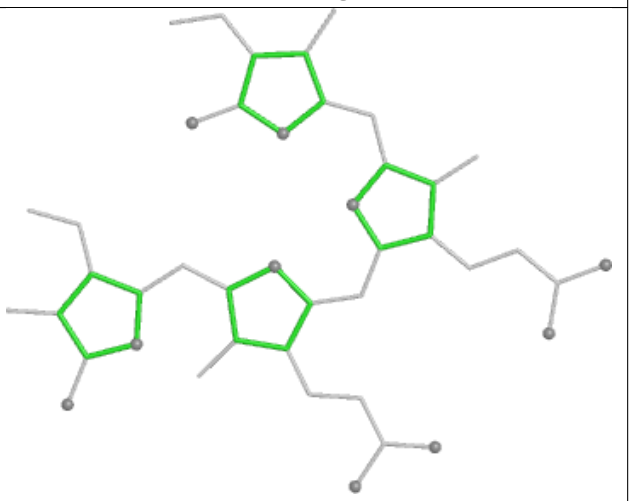
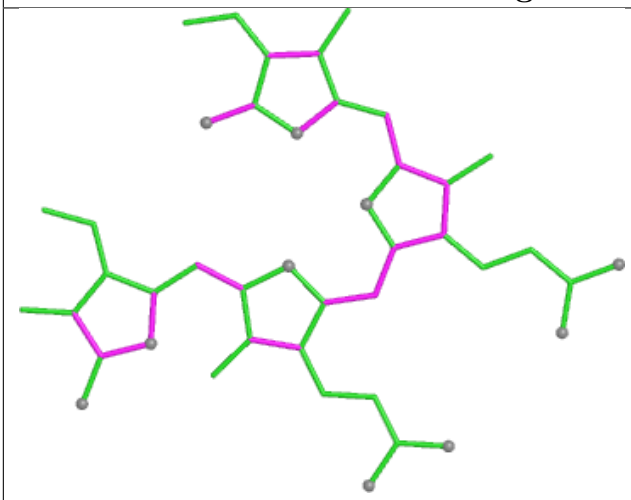


Rings

Ligand PEB eH 203



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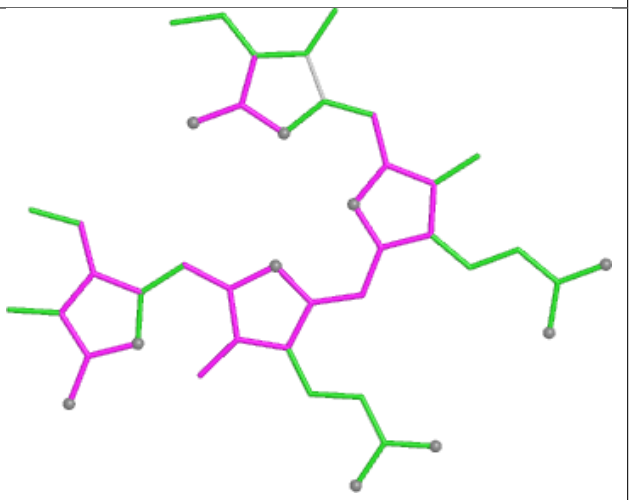

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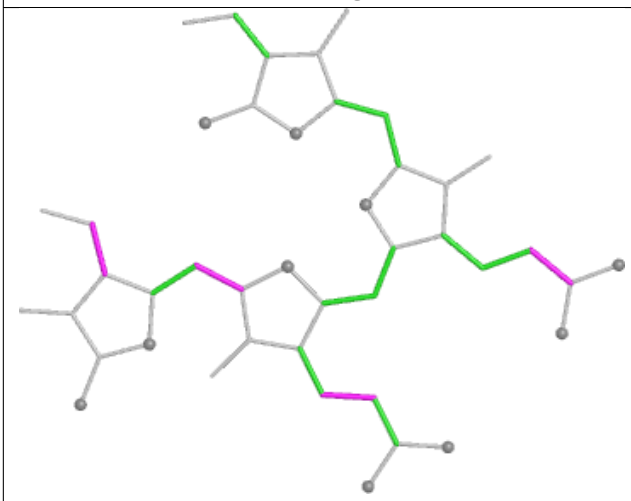

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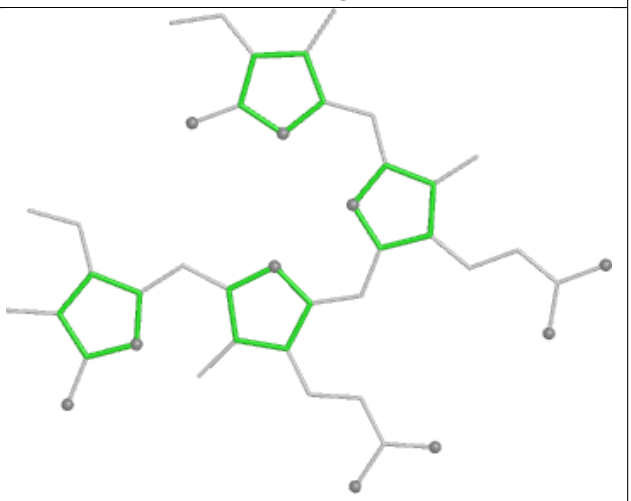
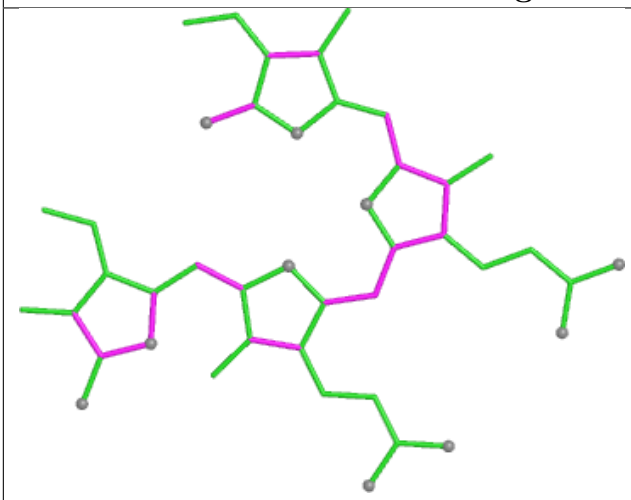


Rings

Ligand PEB U1 201



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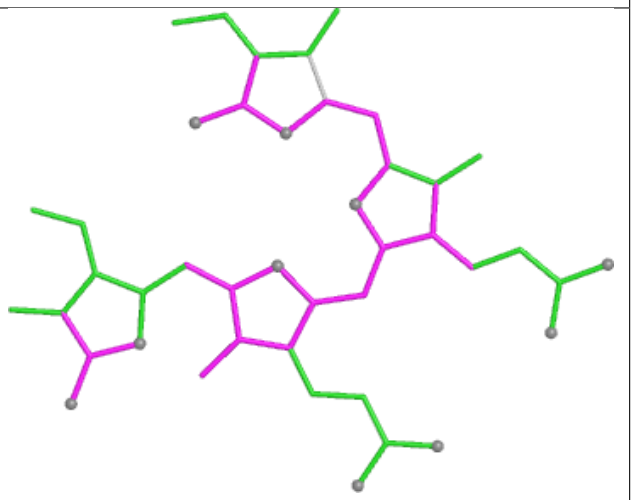

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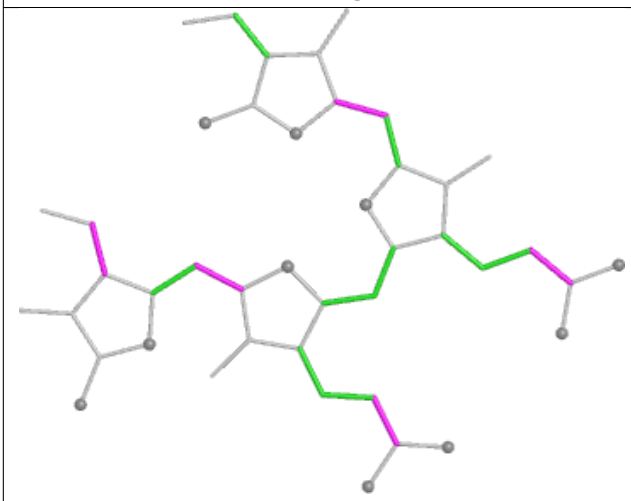

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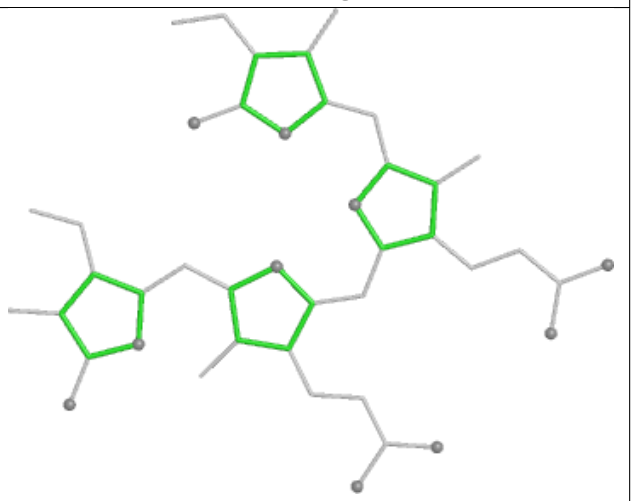
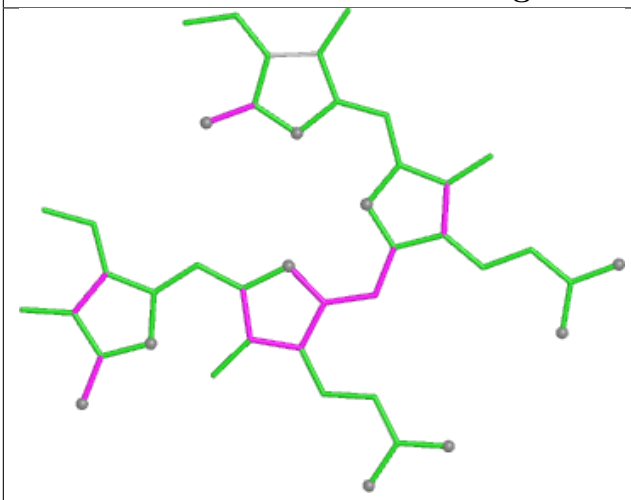


Rings

Ligand PUB QJ 201



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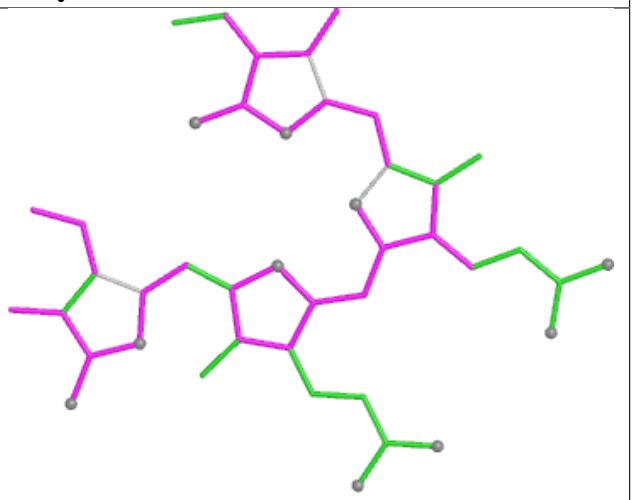

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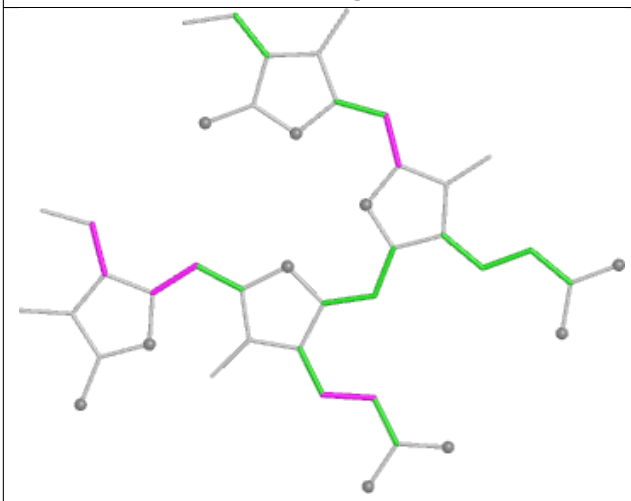

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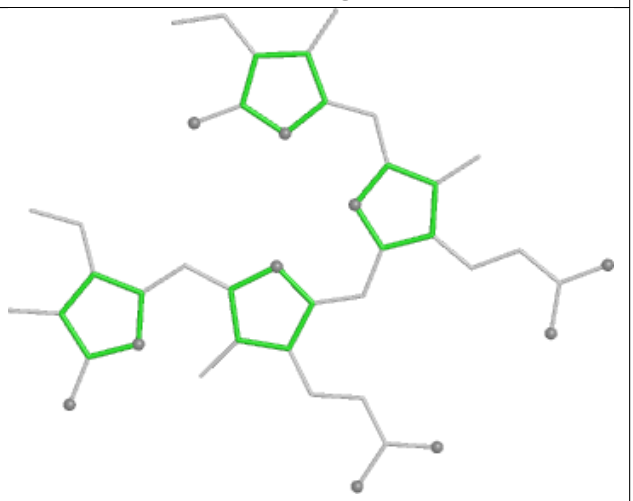
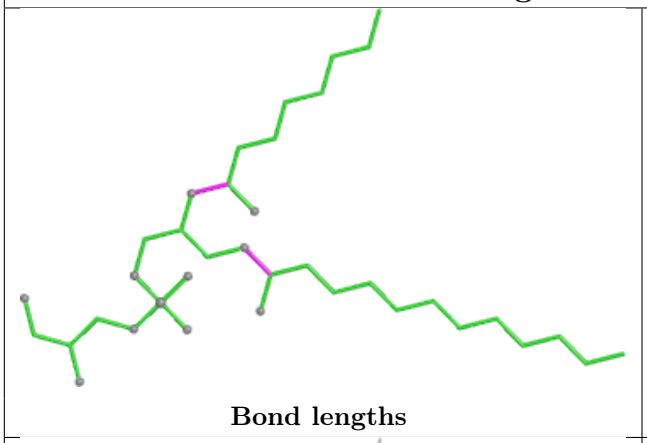


Rings

Ligand LHG C6 505



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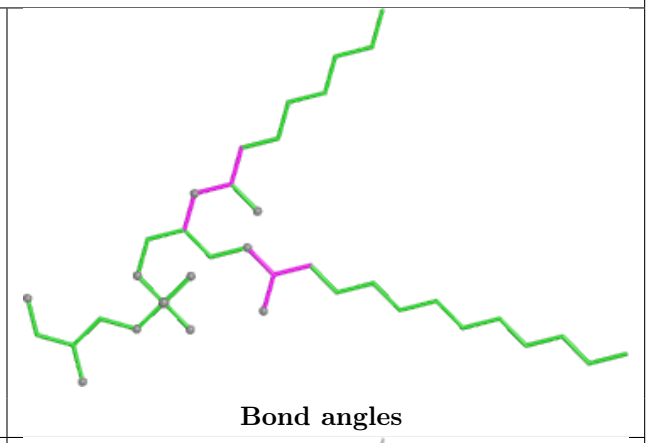

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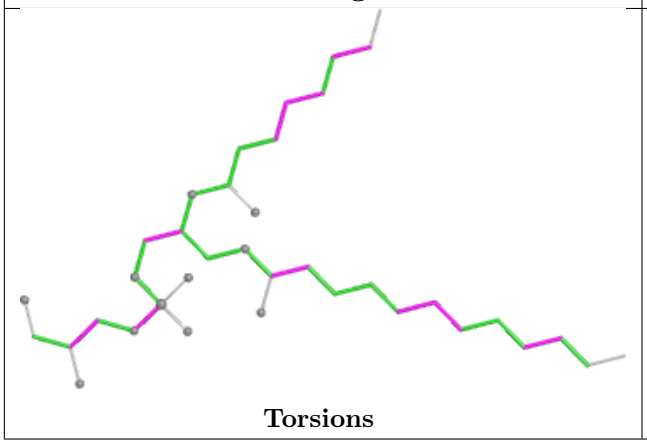

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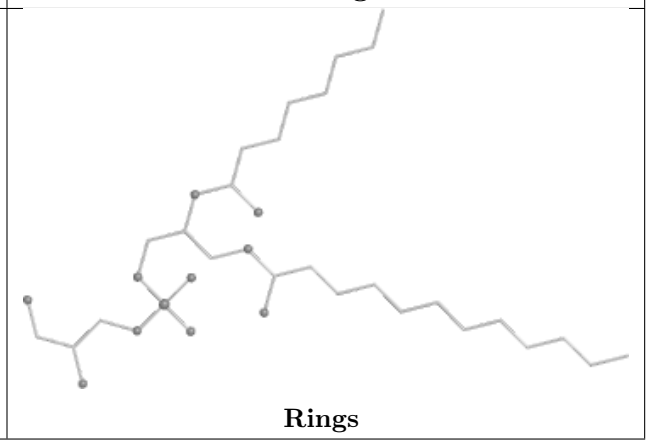
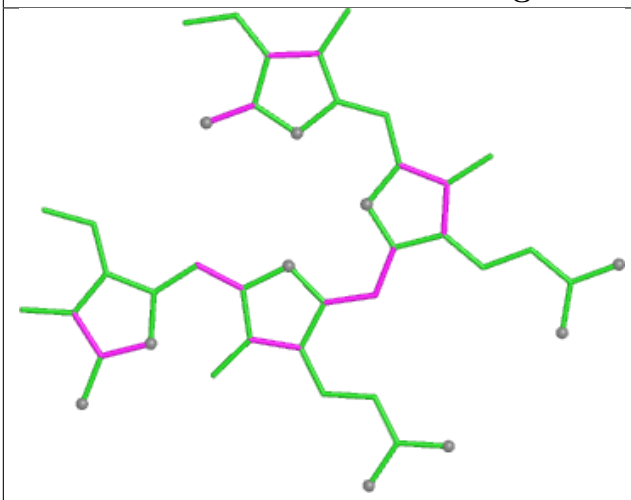


Rings

Ligand PEB LQ 203



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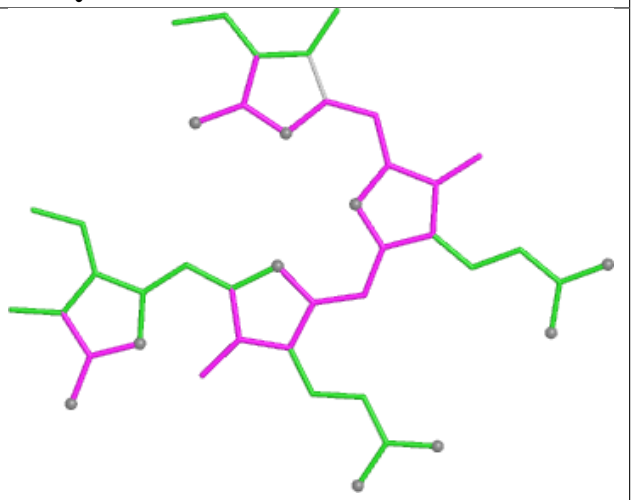

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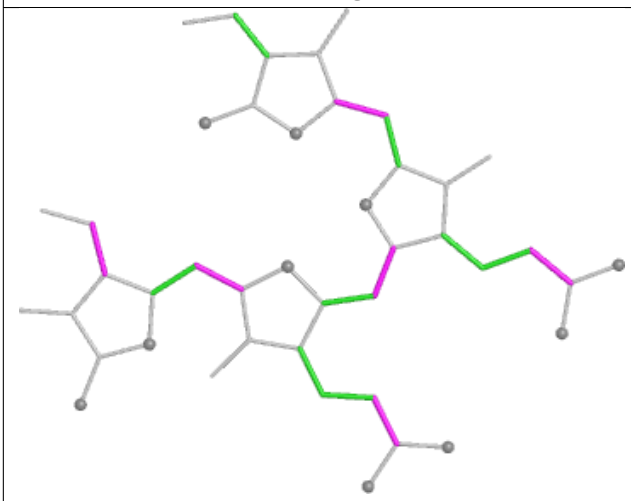

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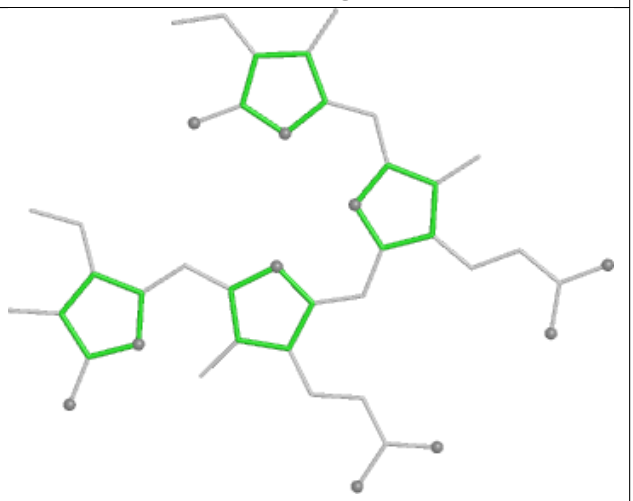
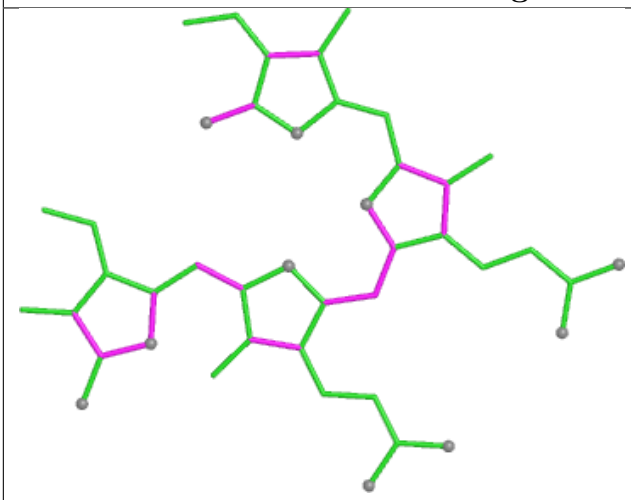


Rings

Ligand PEB NB 201



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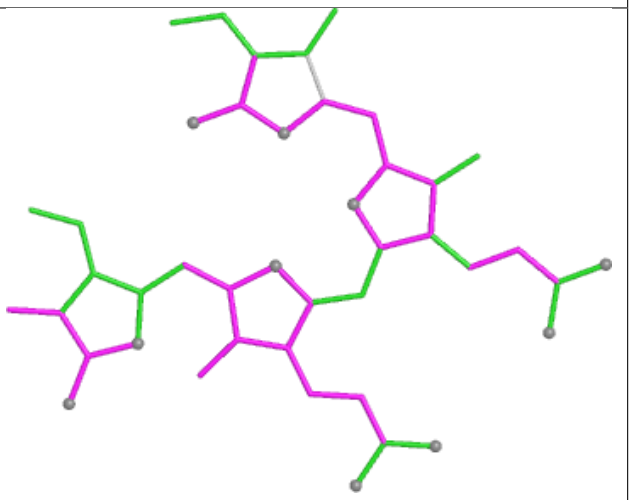
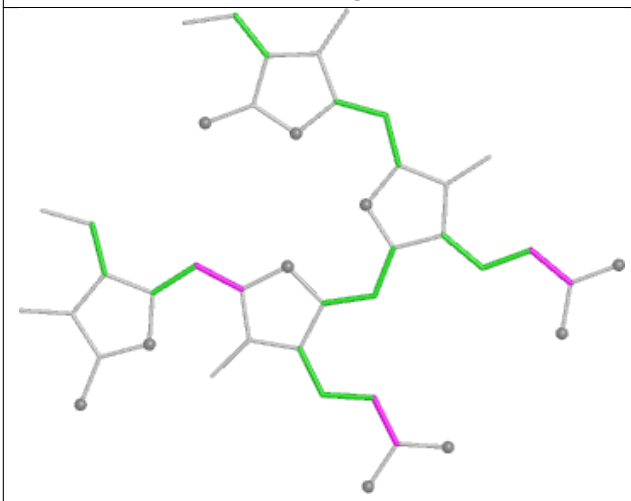


Bond angles



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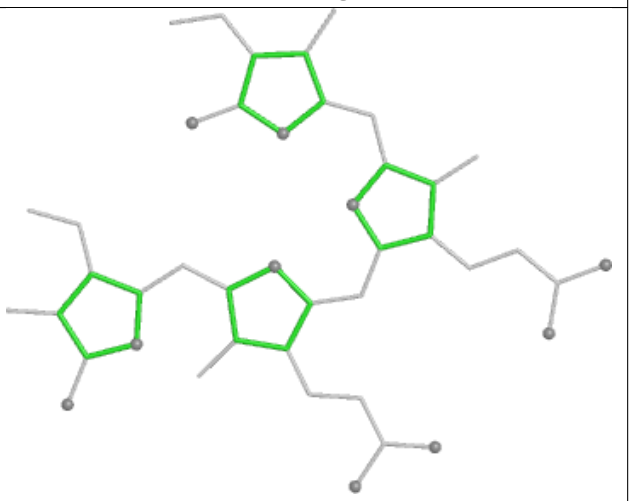
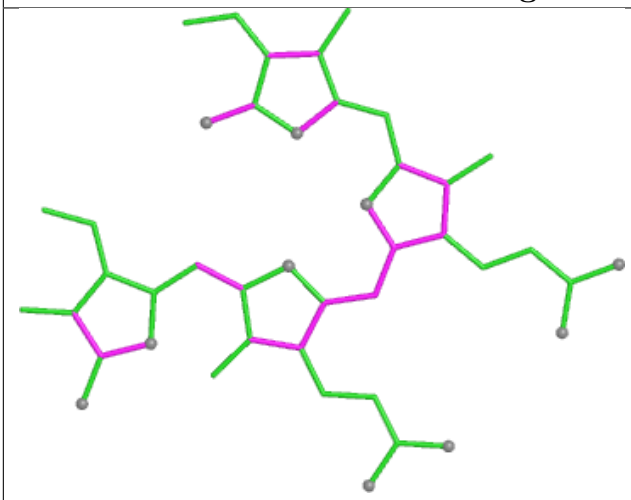


Rings

Ligand PEB v8 202



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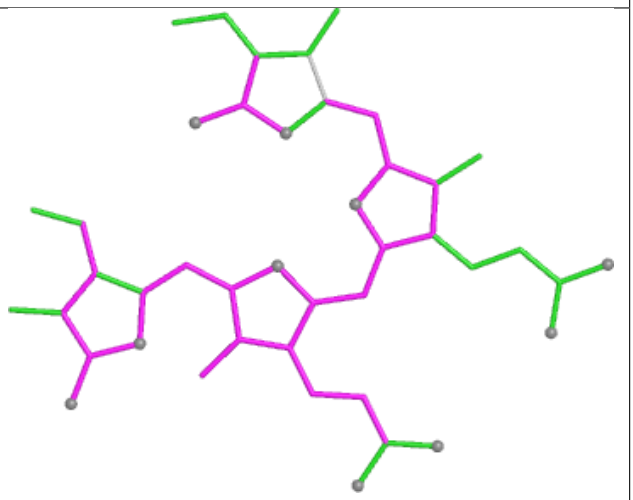
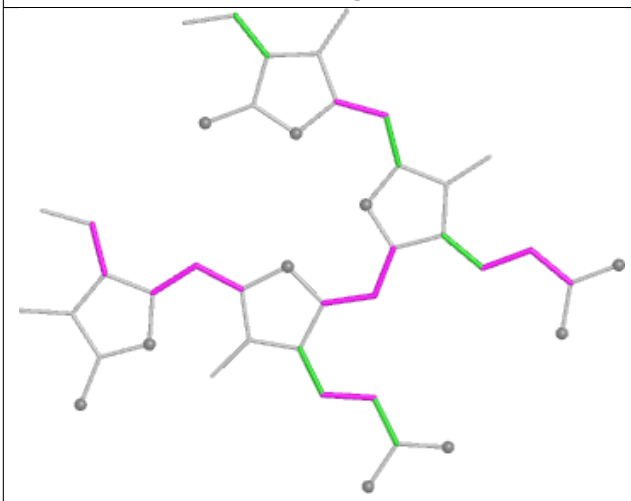


Bond angles



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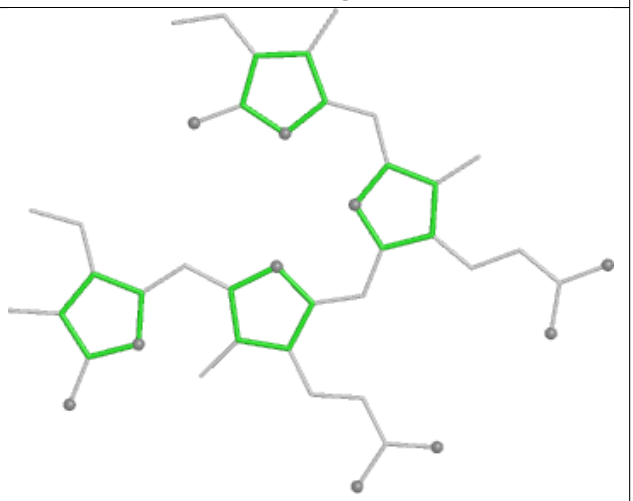
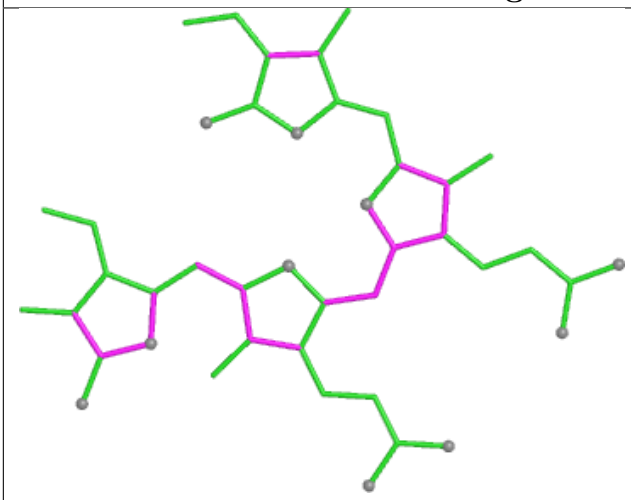


Rings

Ligand PEB WG 201



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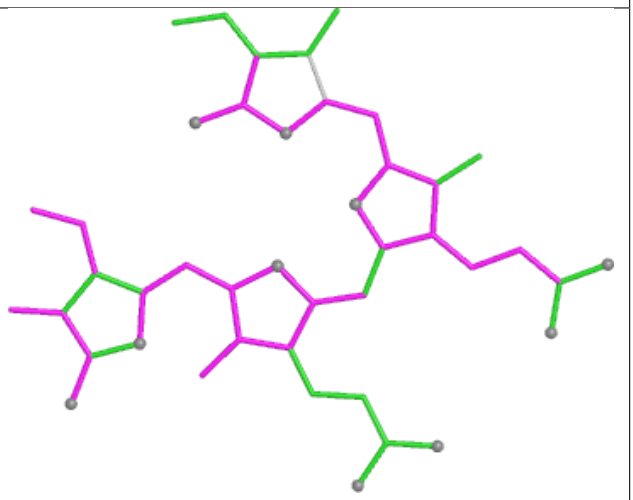
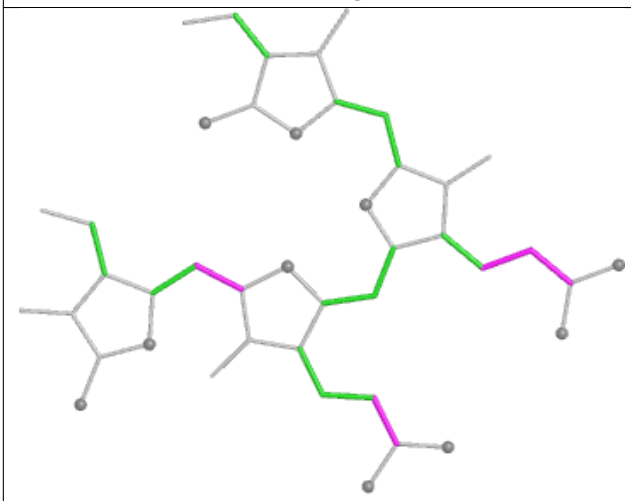


Bond angles



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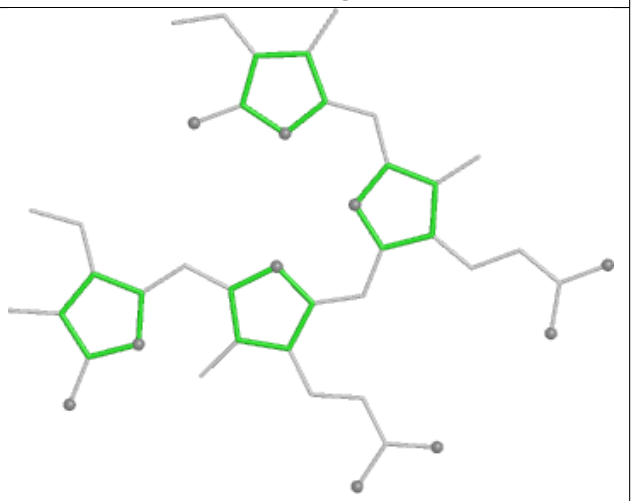
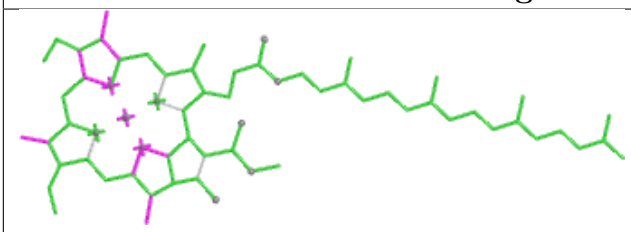
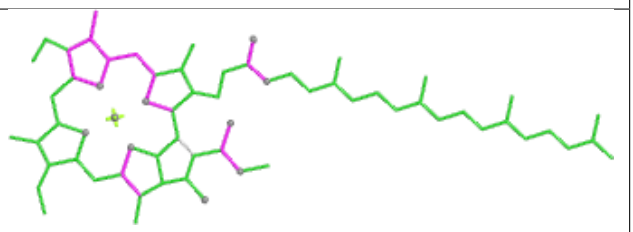


Rings

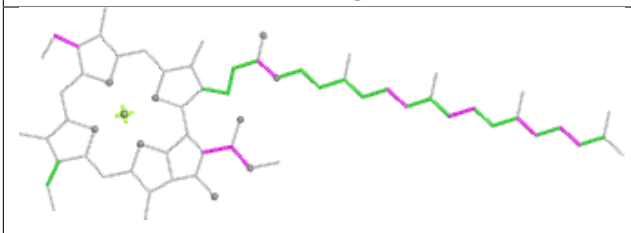
Ligand CLA B2 832



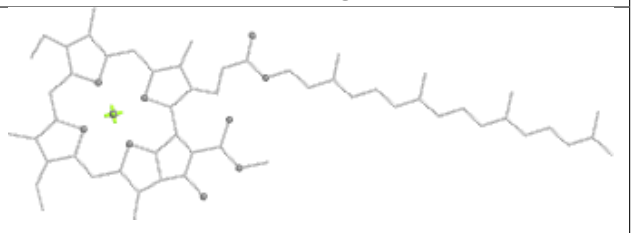
Bond lengths



Bond angles

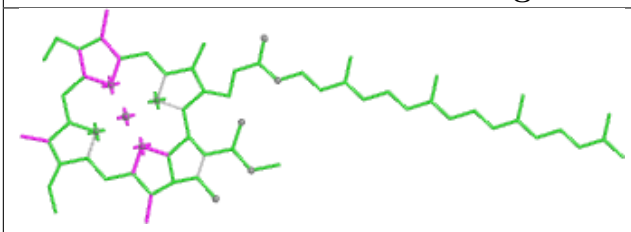


Torsions



Rings

Ligand CLA BL 621



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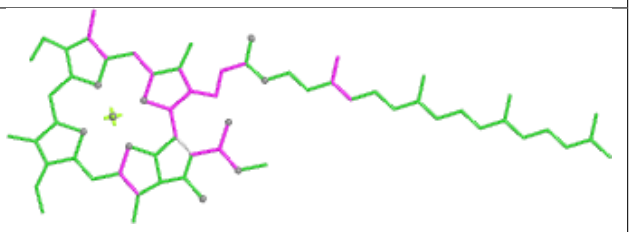

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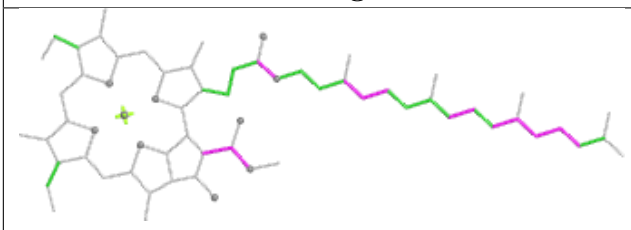

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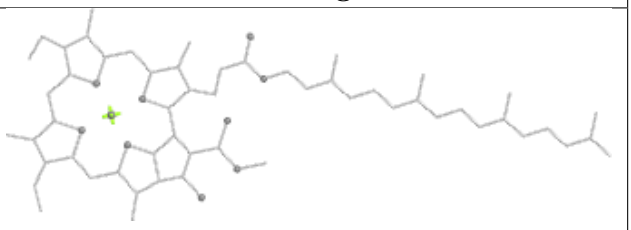
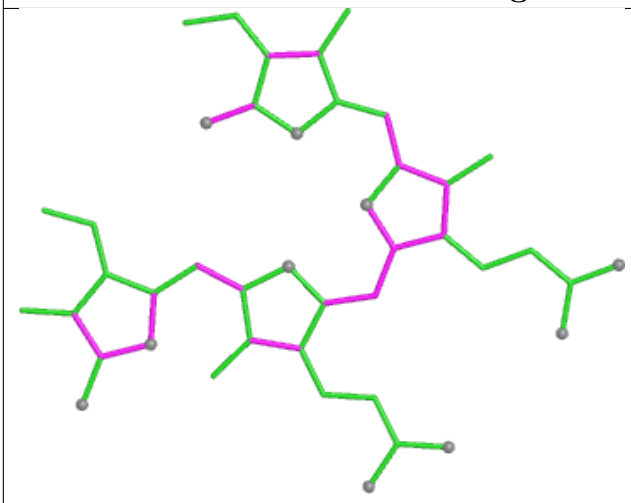


Rings

Ligand PEB DK 203



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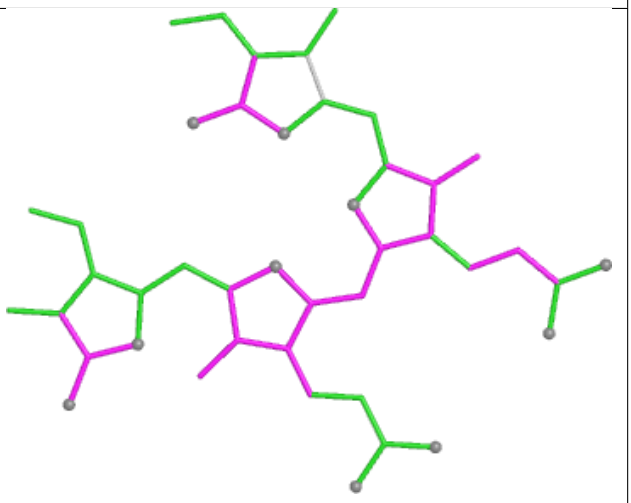

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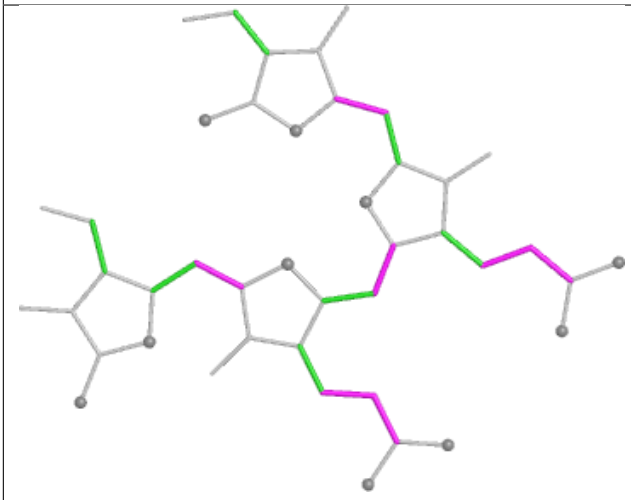

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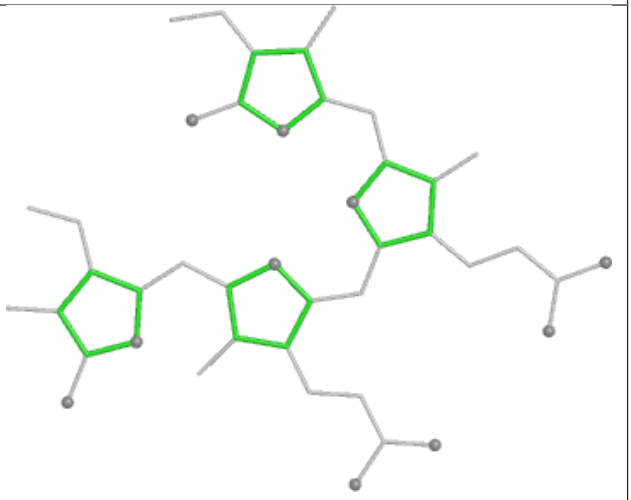
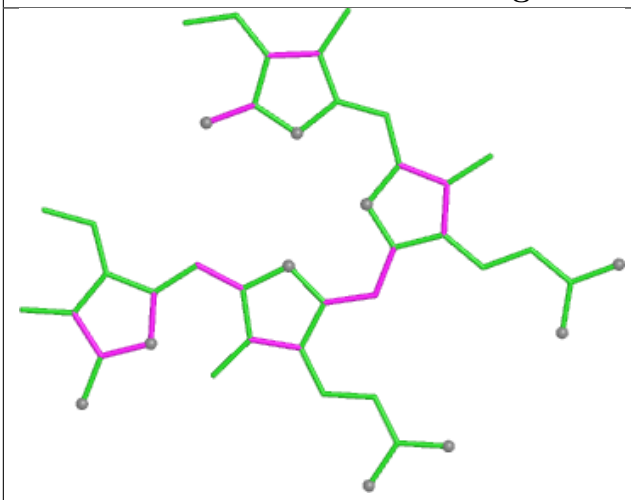


Rings

Ligand PEB BP 202



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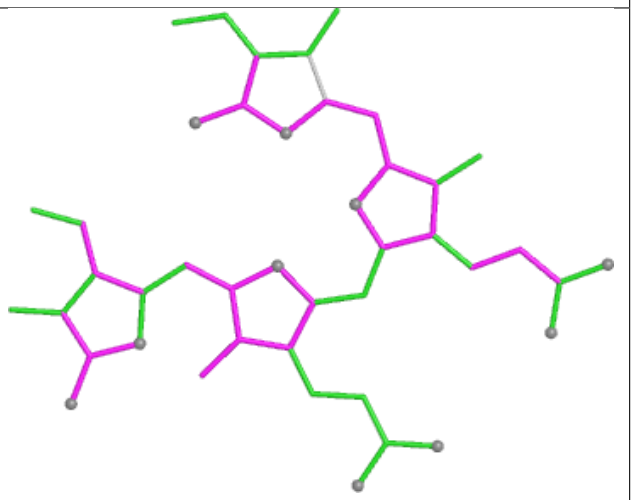
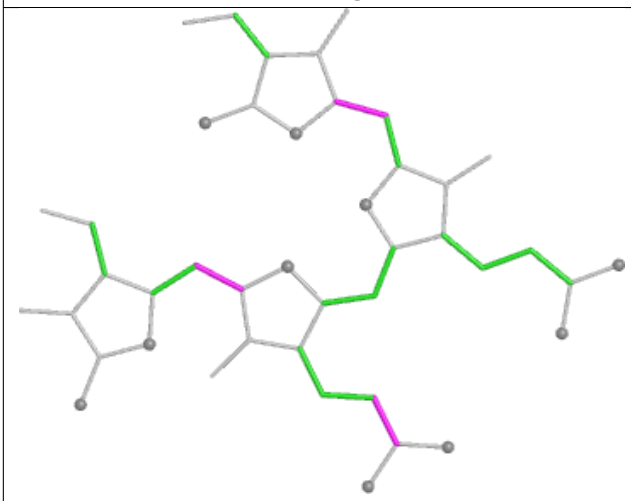


Bond angles



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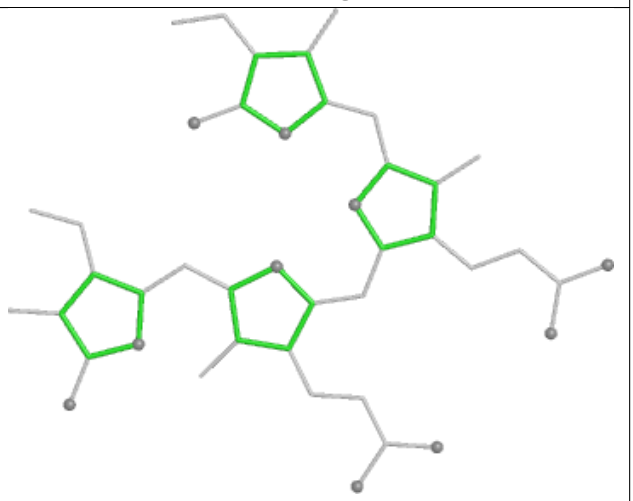
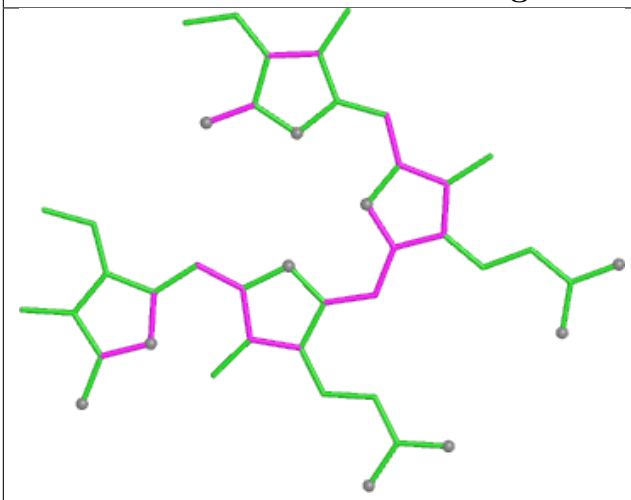


Rings

Ligand PEB wK 303



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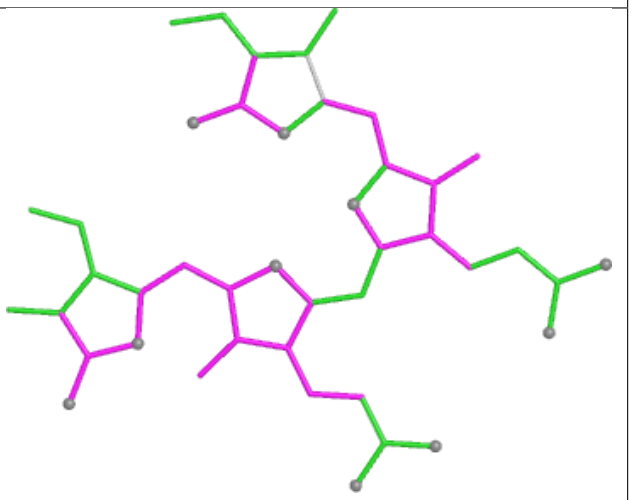

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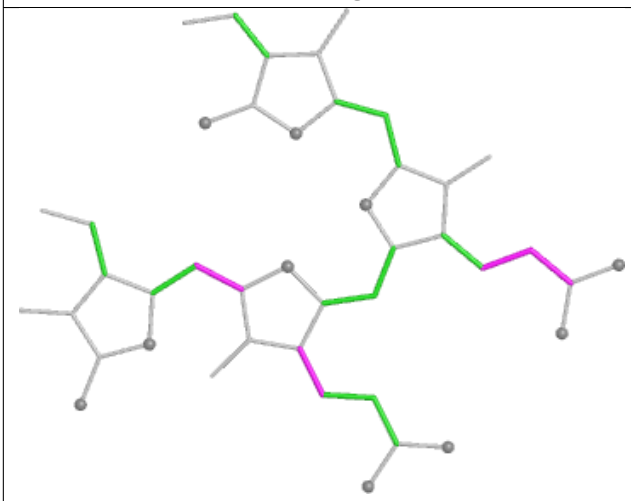

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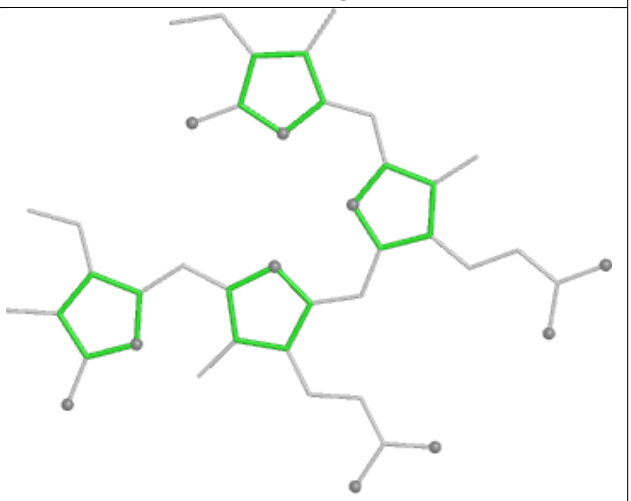
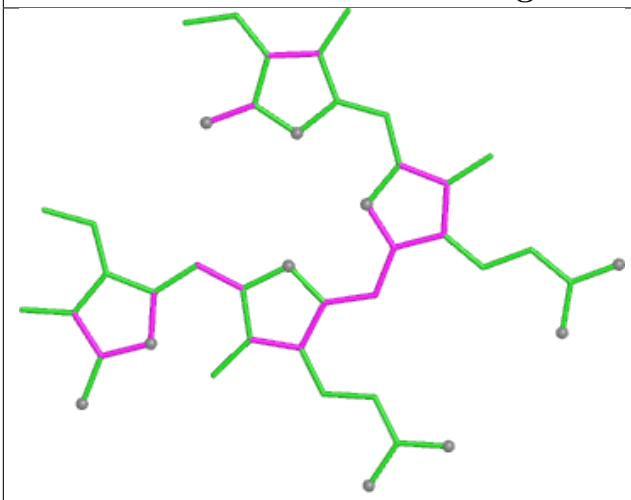


Rings

Ligand PEB JP 201



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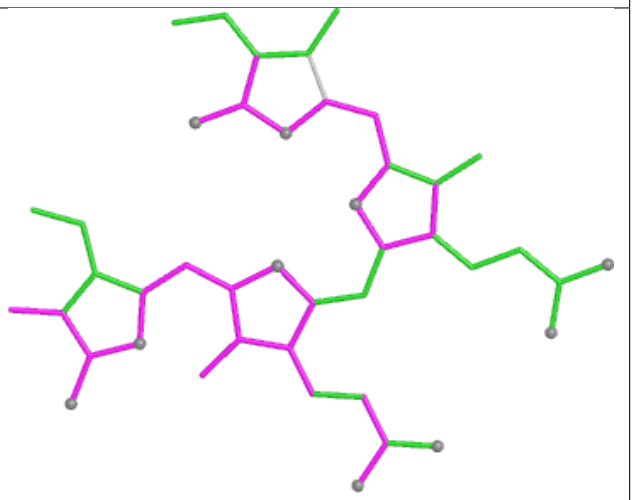

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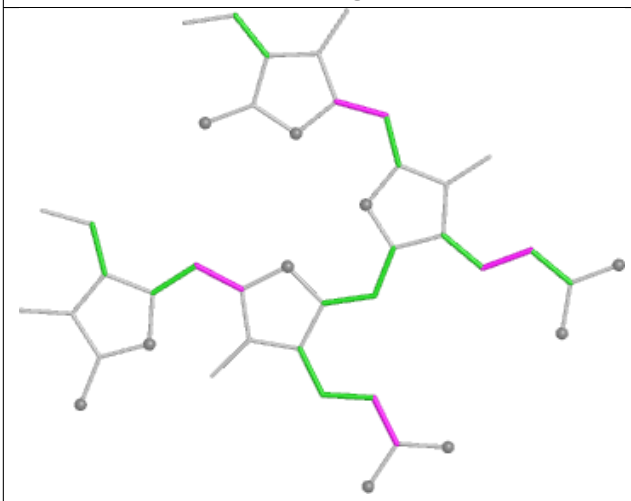

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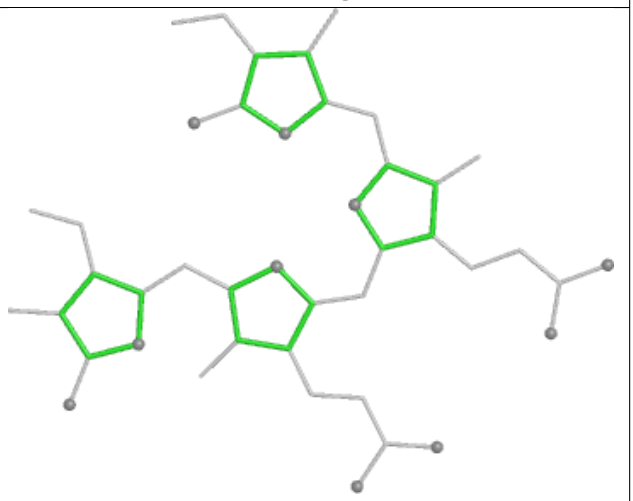
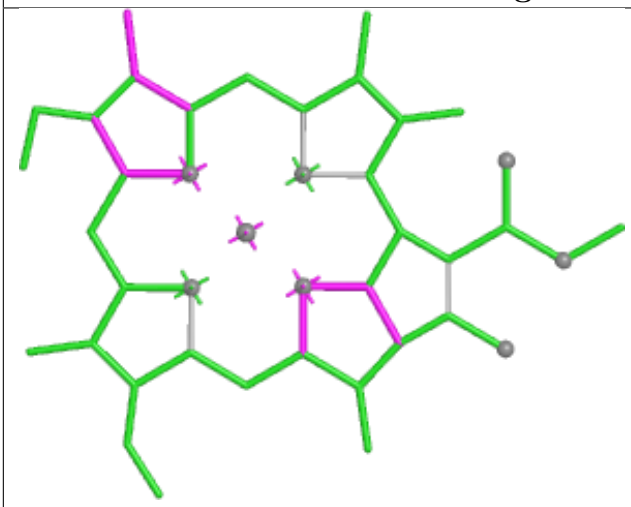


Rings

Ligand CLA 2N 310



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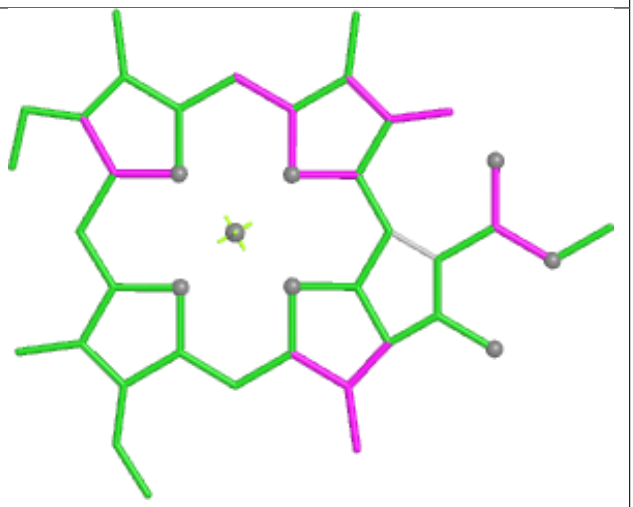
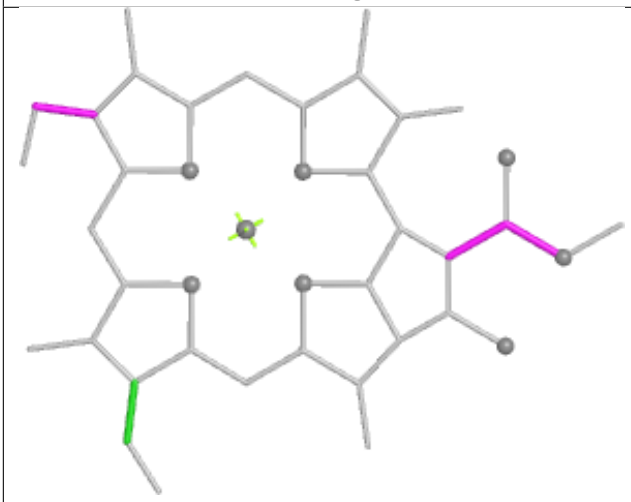


Bond angles



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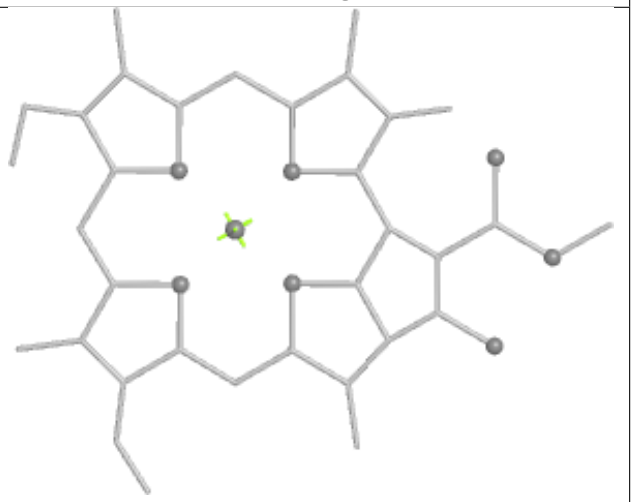
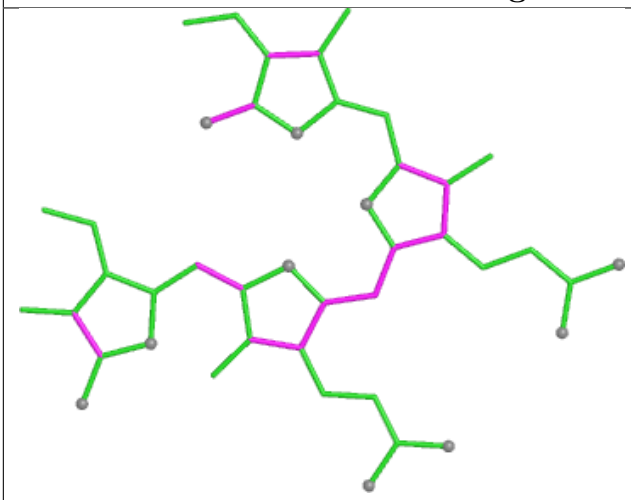


Rings

Ligand PEB mH 202



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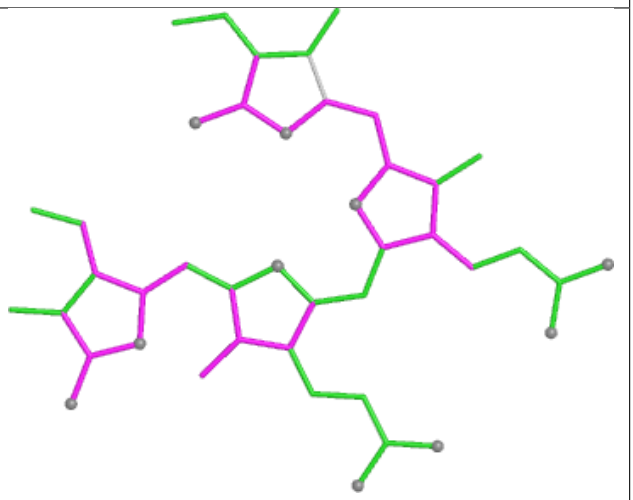

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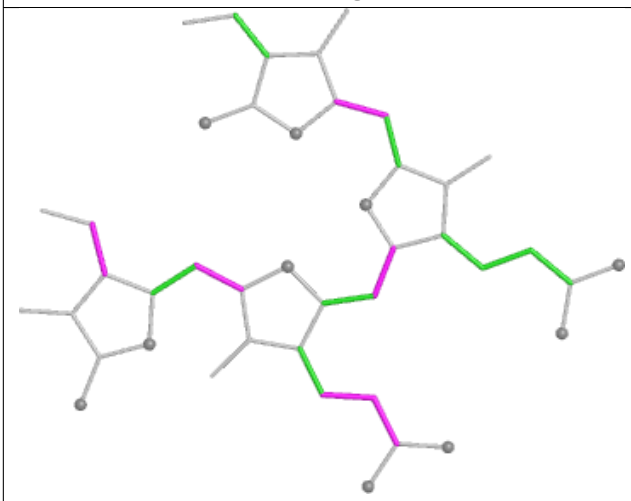

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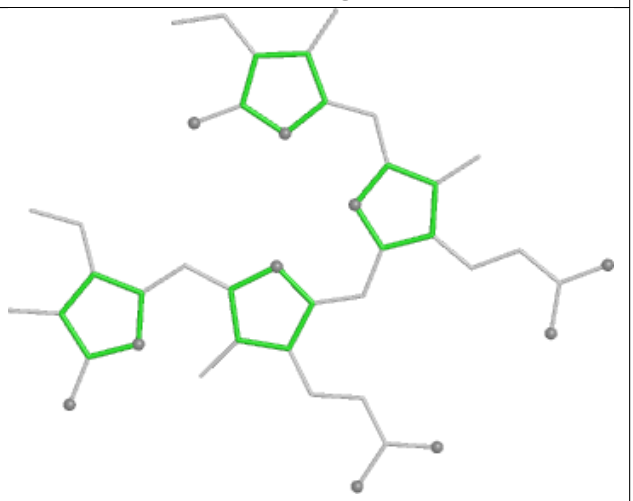
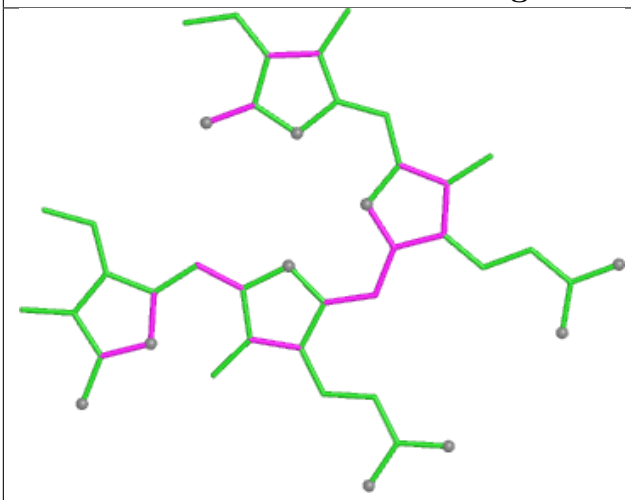


Rings

Ligand PEB wK 302



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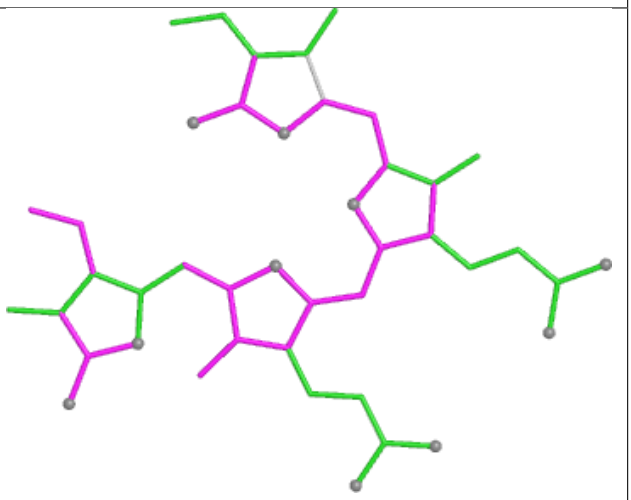
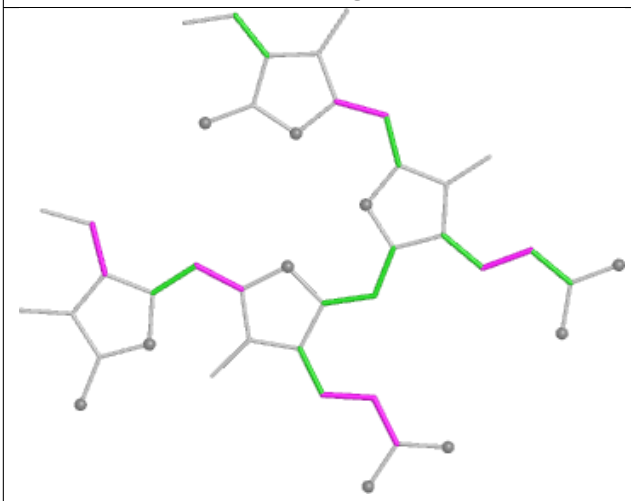


Bond angles



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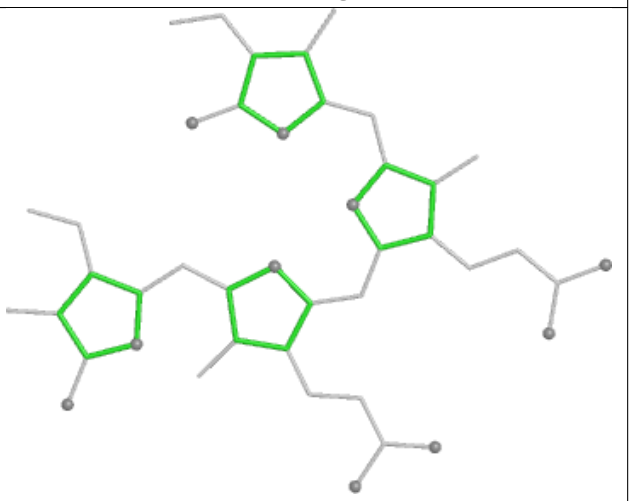
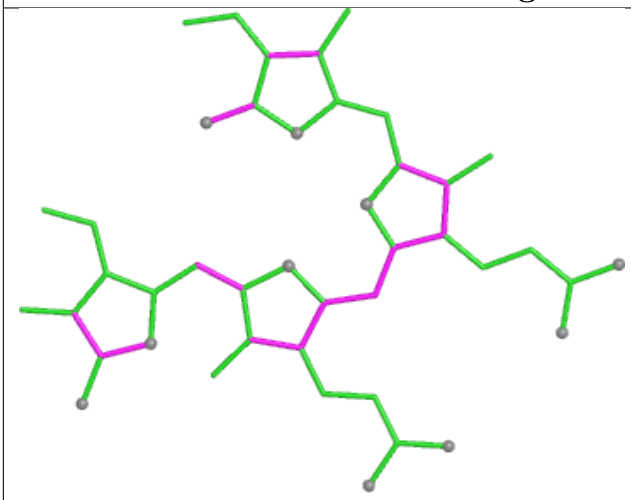


Rings

Ligand PEB hJ 203



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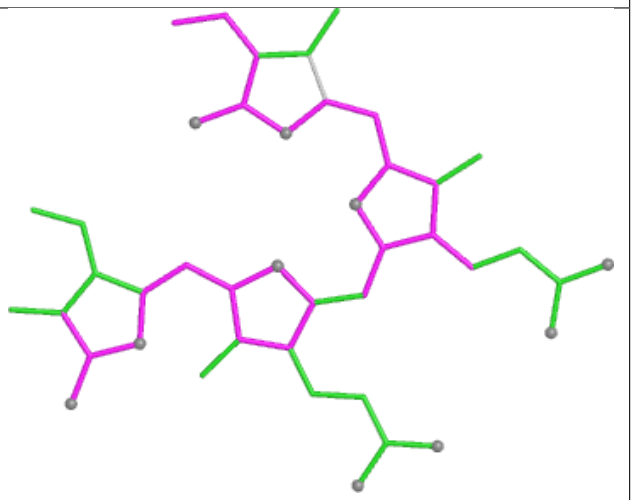
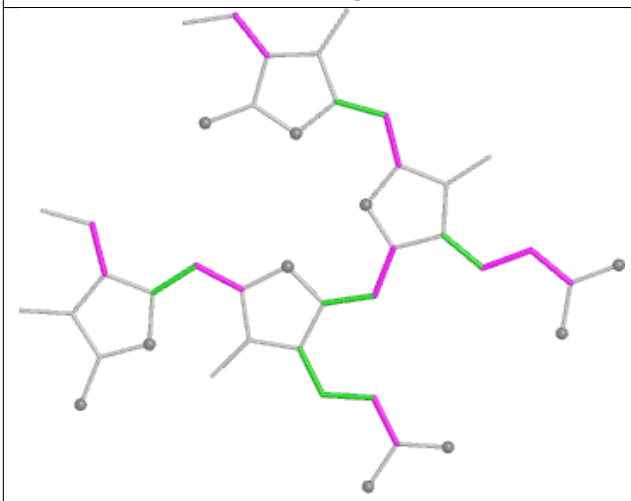


Bond angles



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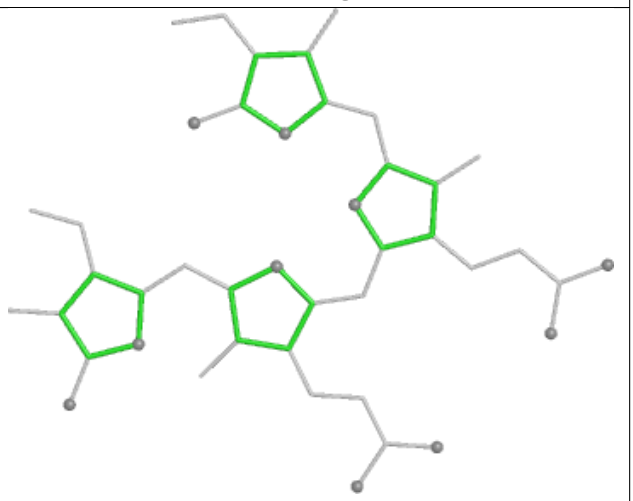
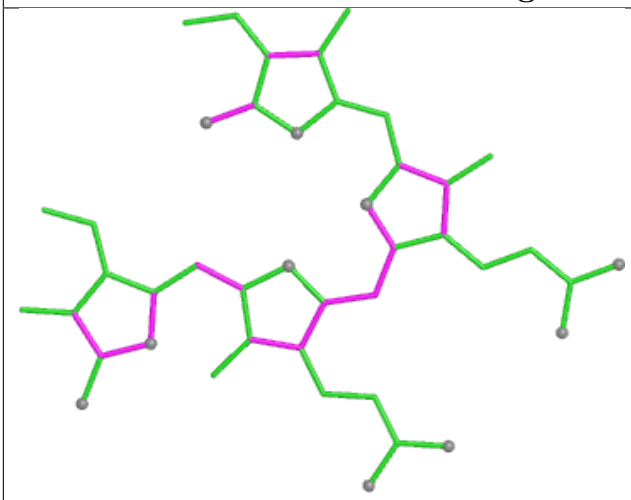


Rings

Ligand PEB IQ 202



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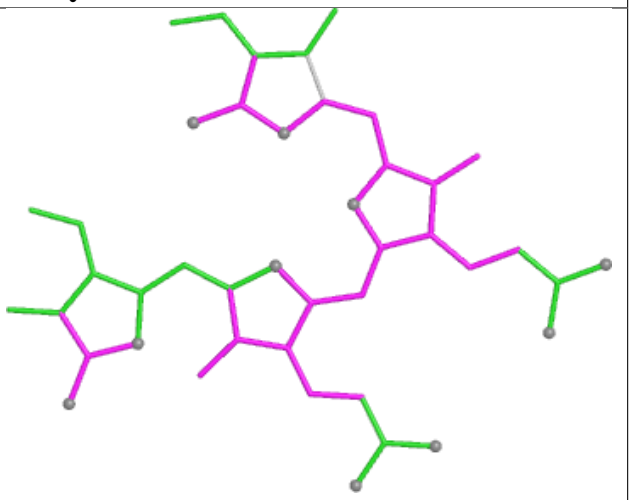

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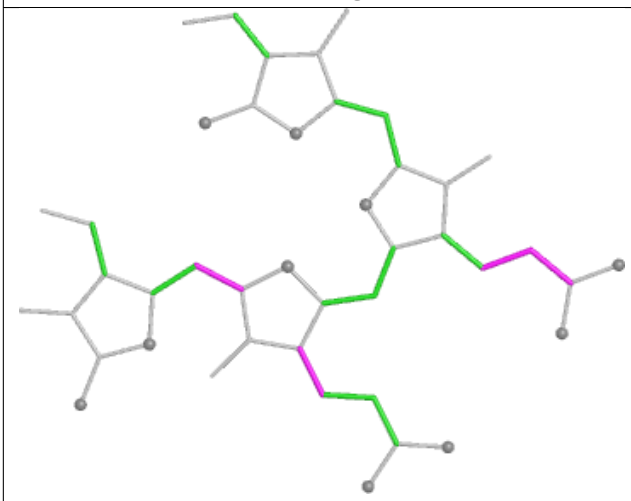

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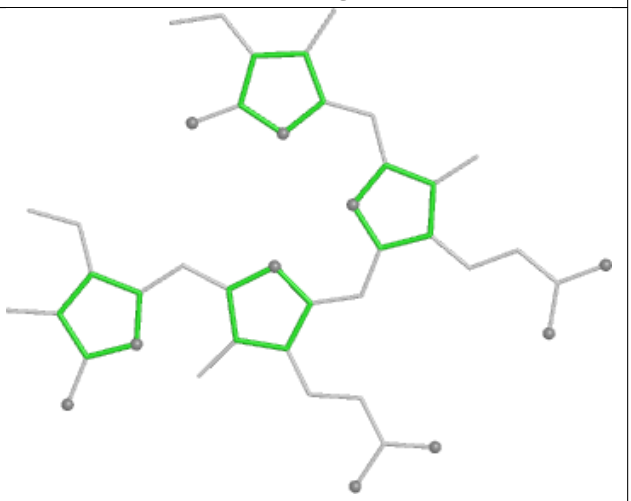
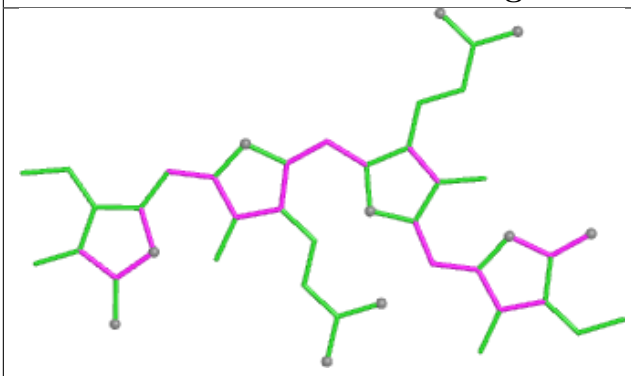


Rings

Ligand CYC P3 1001



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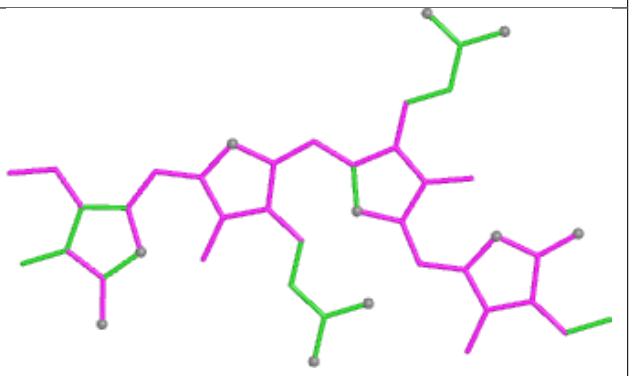
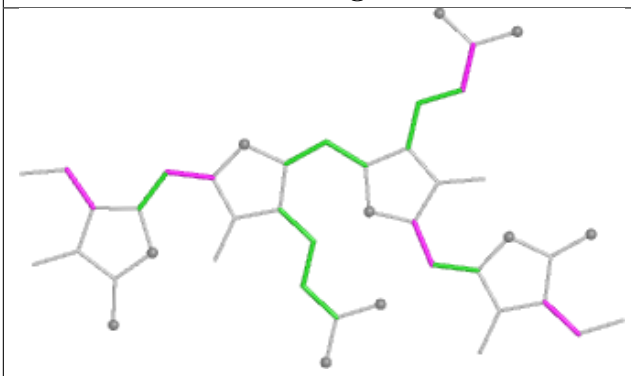


Bond angles



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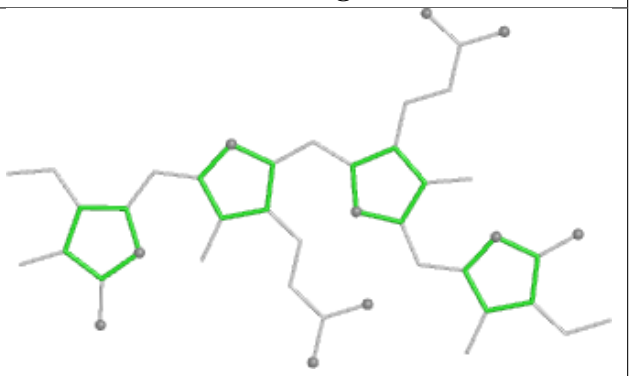
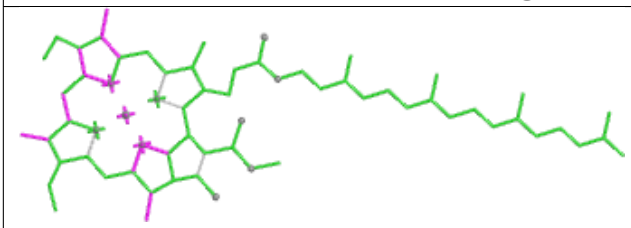


Rings

Ligand CLA cL 511



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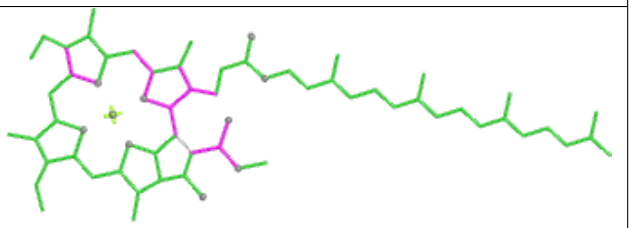
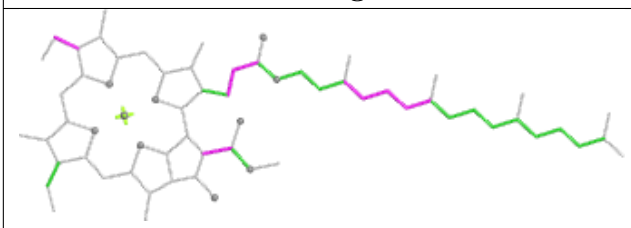


Bond angles



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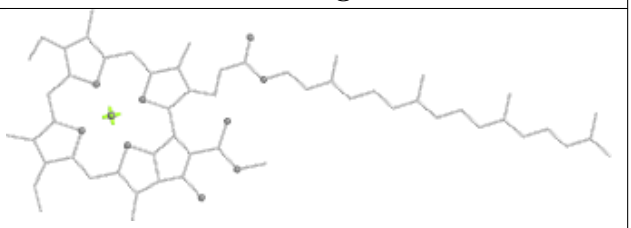
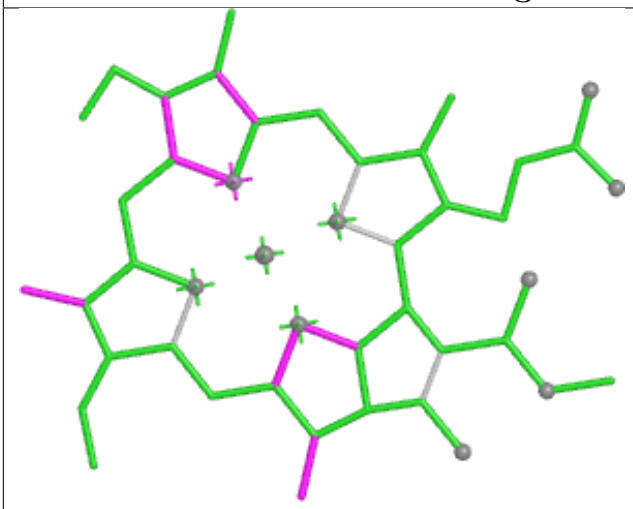


Rings

Ligand CLA 3N 306



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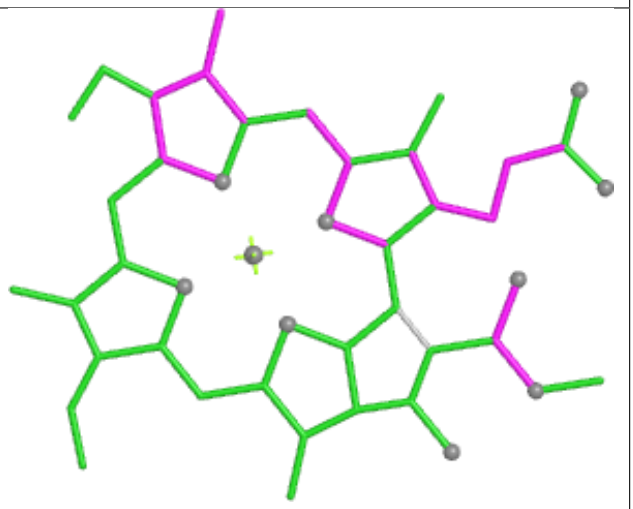
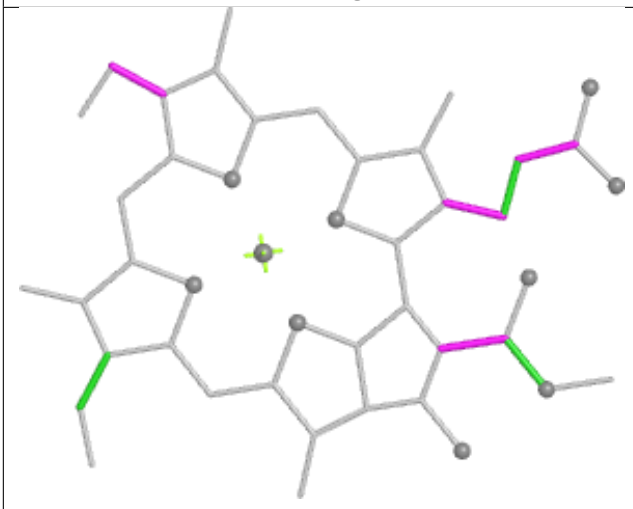


Bond angles

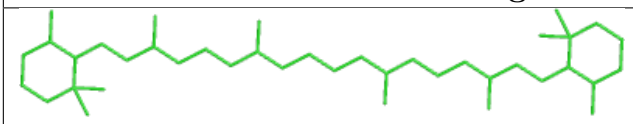


Torsions



Rings

Ligand BCR BN 840



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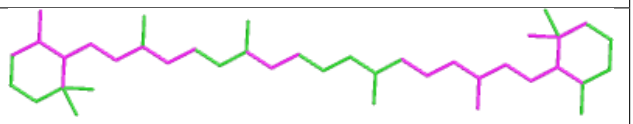
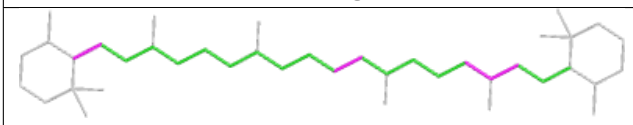


Bond angles



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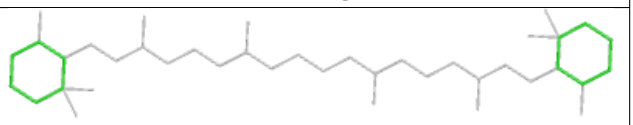
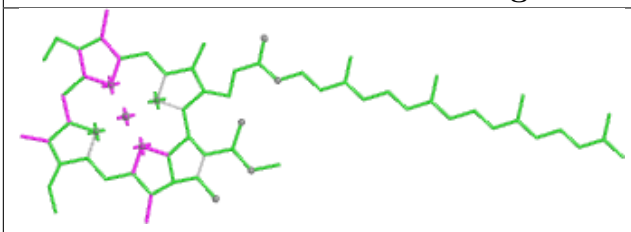
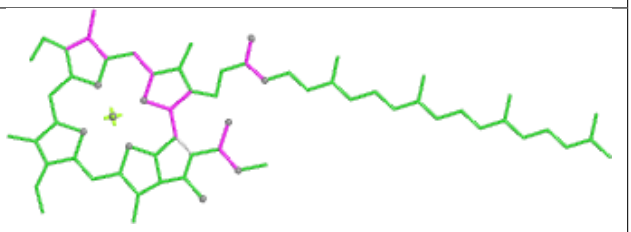


Rings

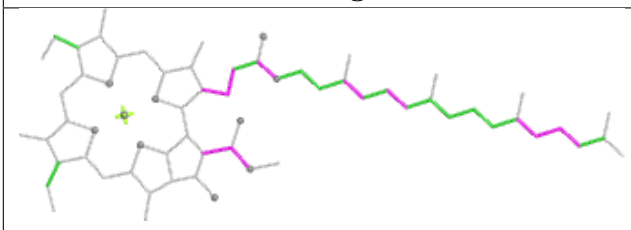
Ligand CLA BN 801



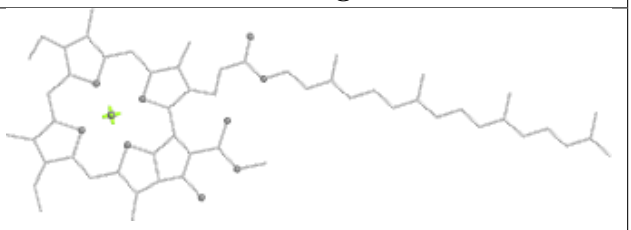
Bond lengths



Bond angles

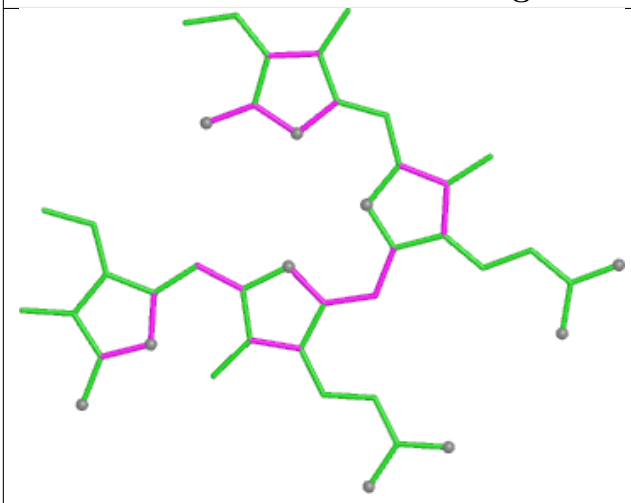


Torsions



Rings

Ligand PEB WI 202



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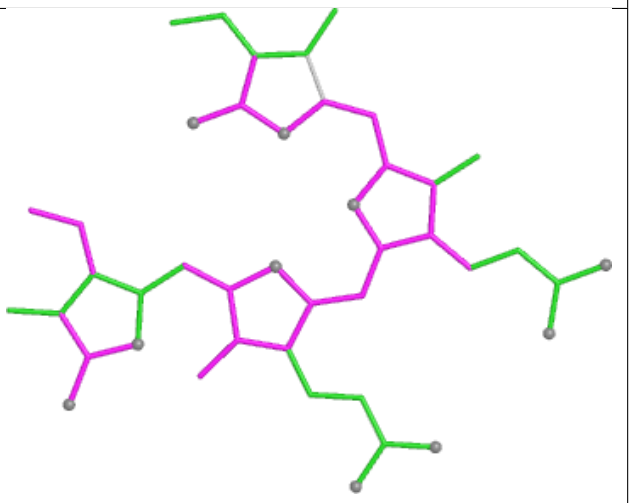

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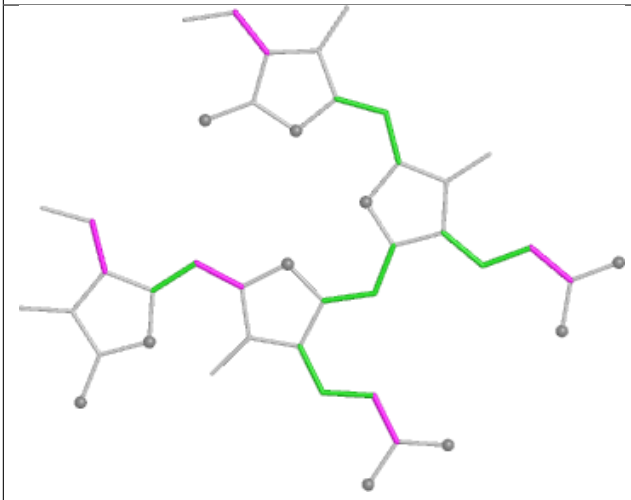

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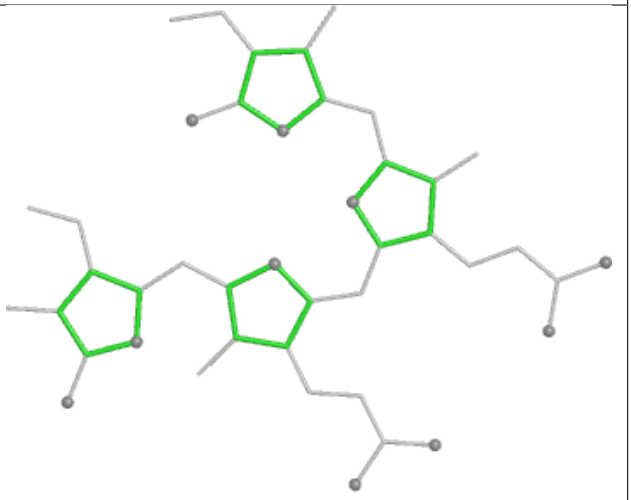
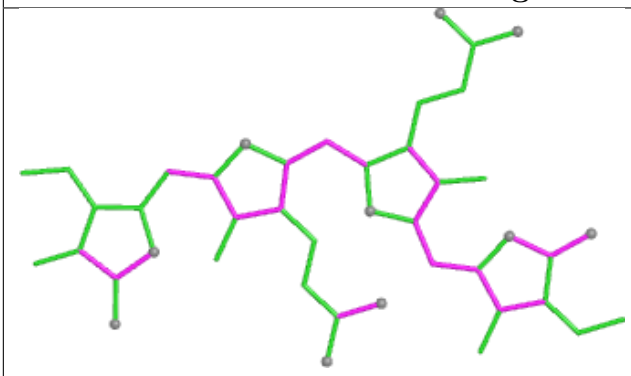


Rings

Ligand CYC j3 1001



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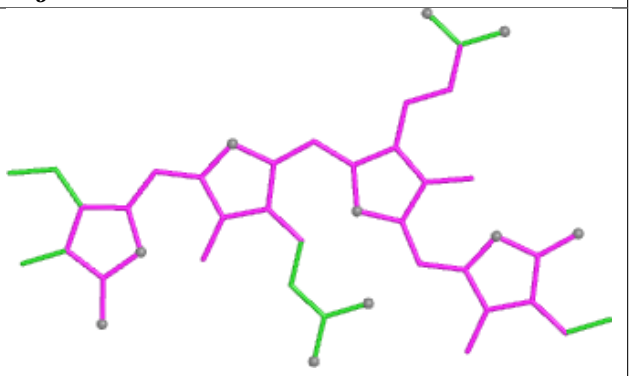

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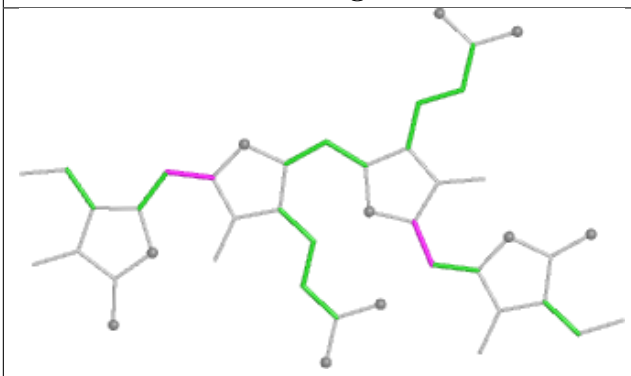

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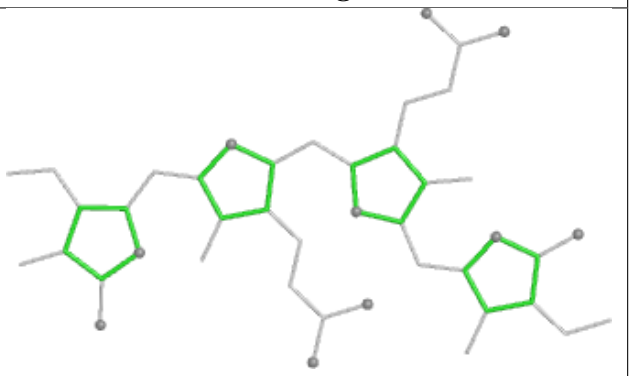
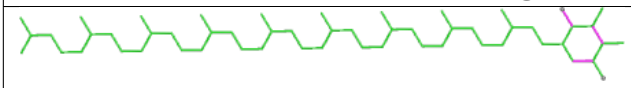


Rings

Ligand PL9 DL 401



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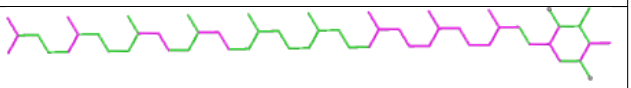

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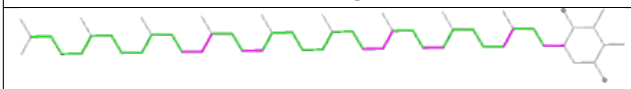

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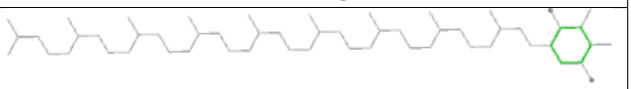
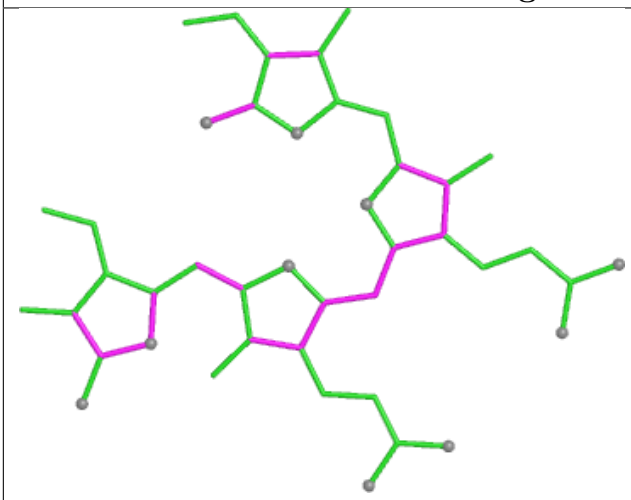


Rings

Ligand PEB u8 203



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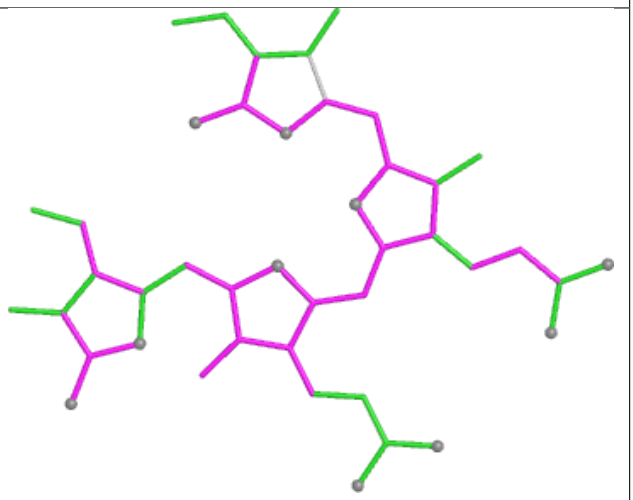

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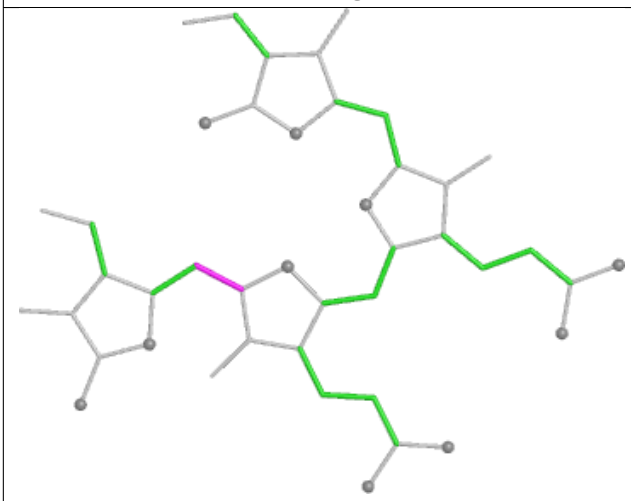

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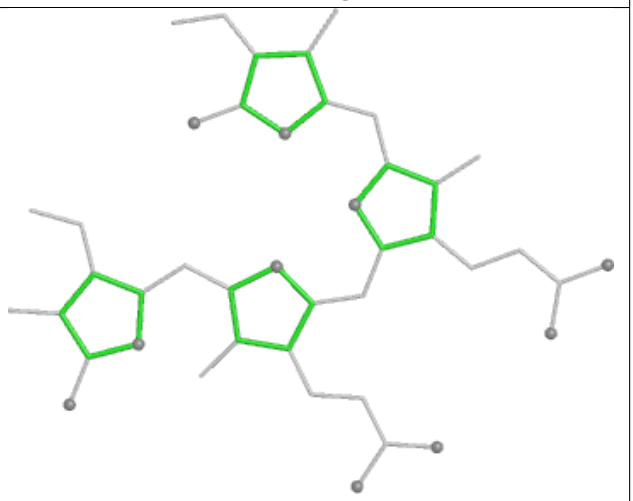
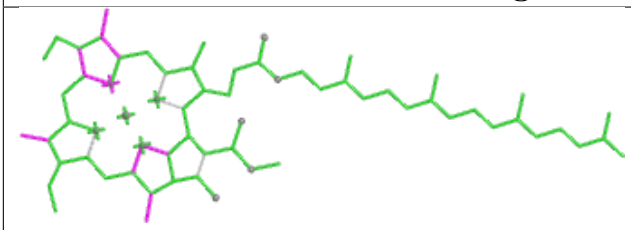


Rings

Ligand CLA HL 102



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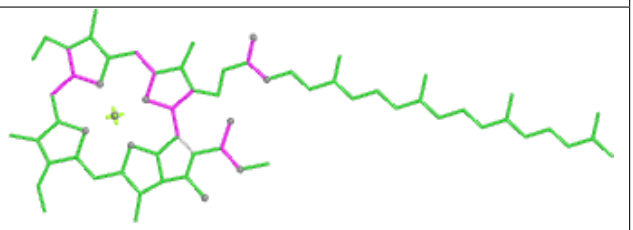

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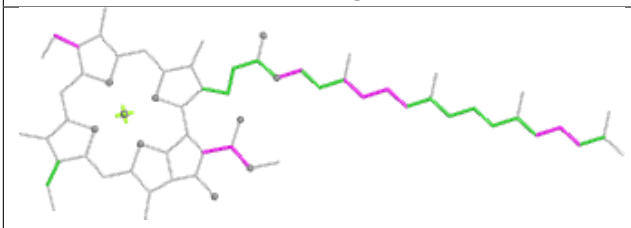

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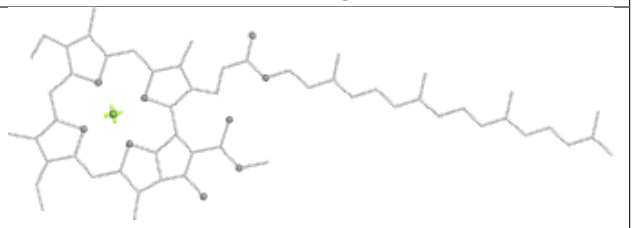
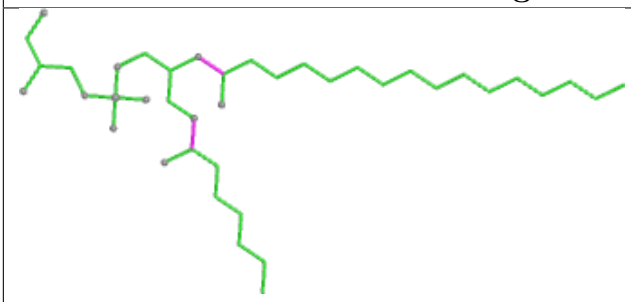


Rings

Ligand LHG A2 844



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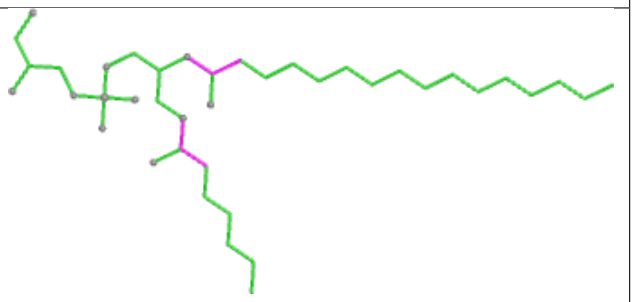
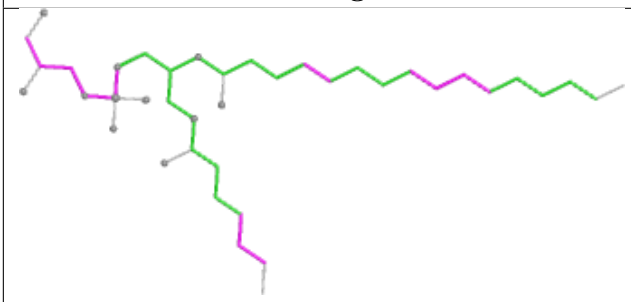


Bond angles



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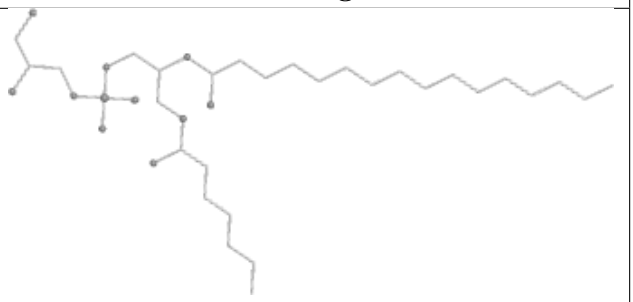
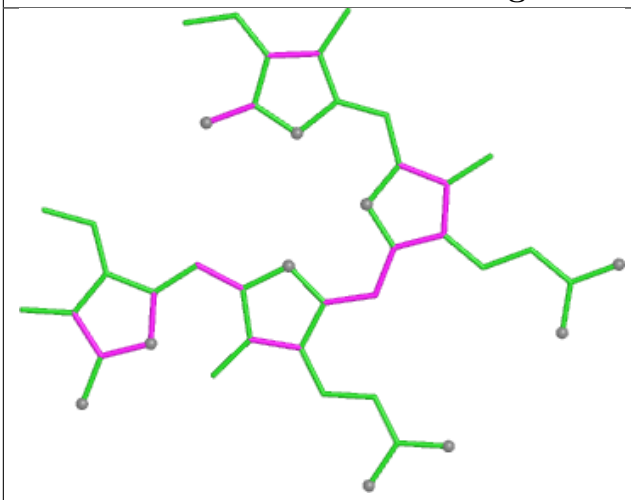


Rings

Ligand PEB MP 202



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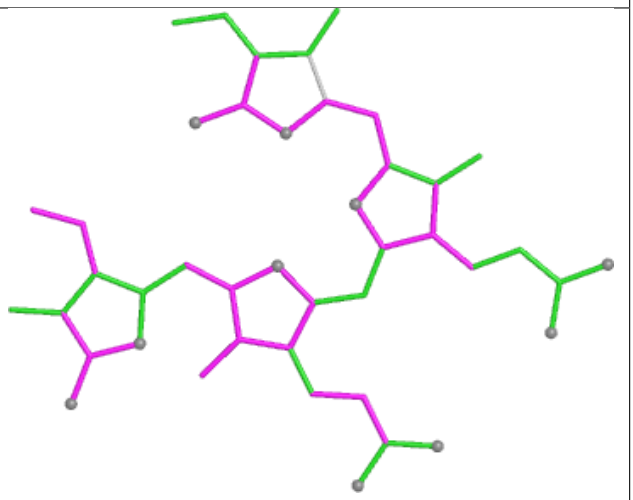

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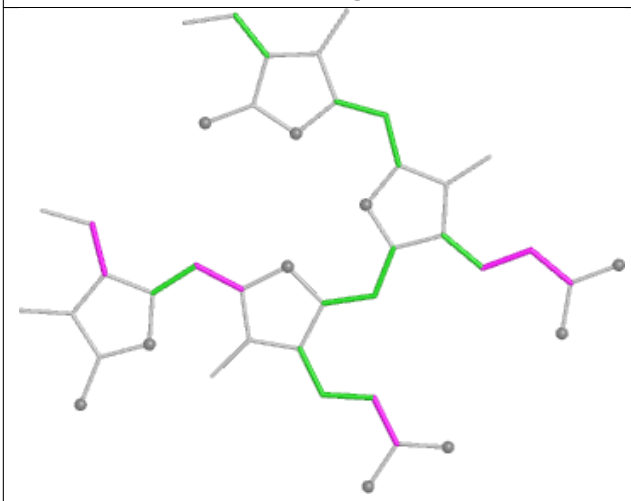

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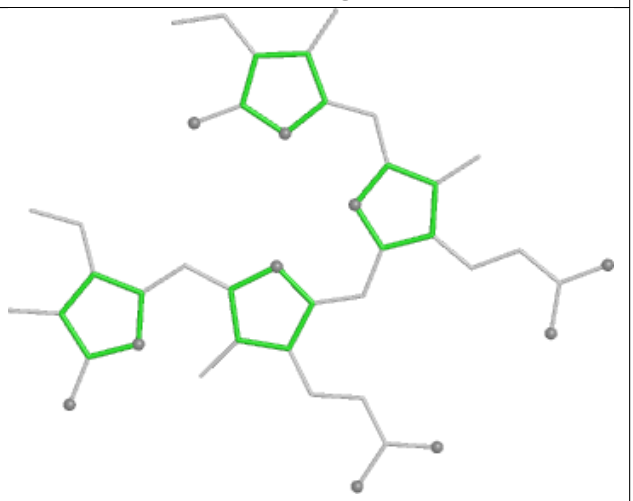
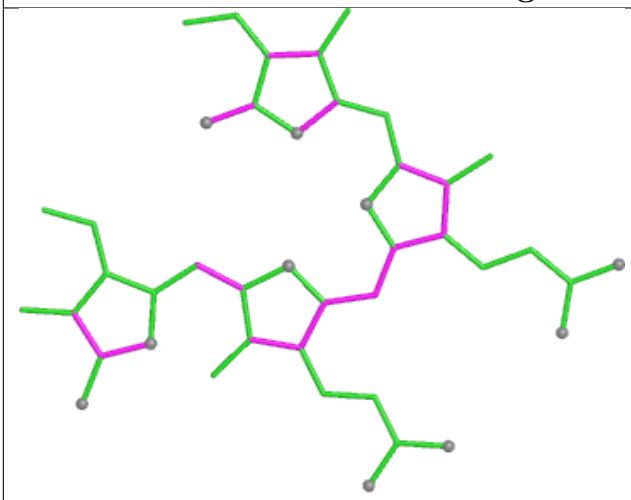


Rings

Ligand PEB oF 203



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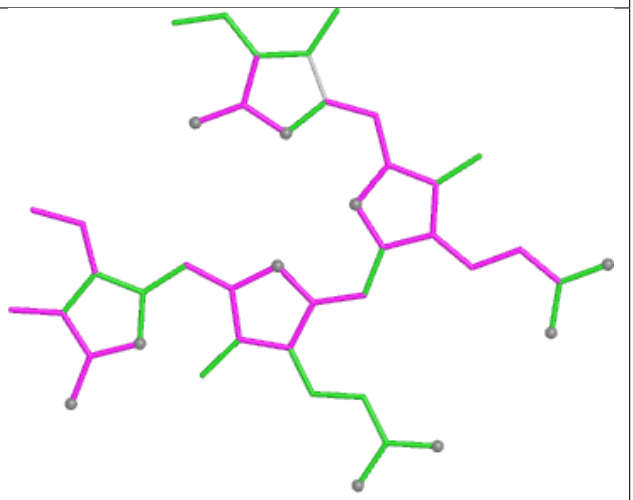

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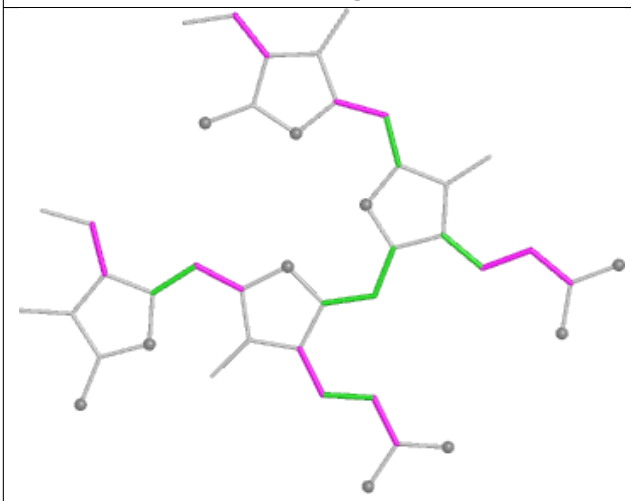

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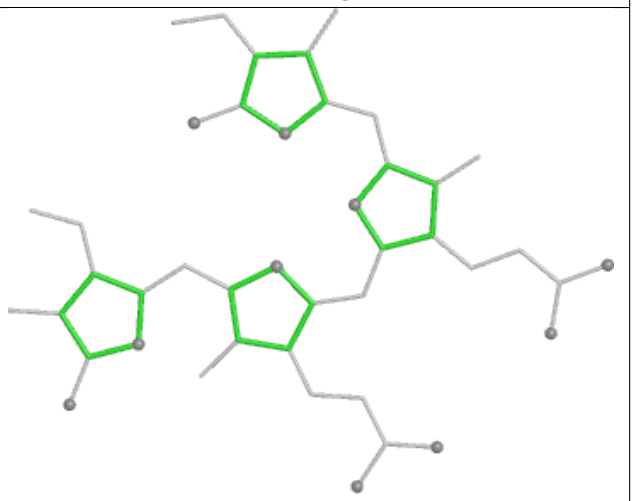
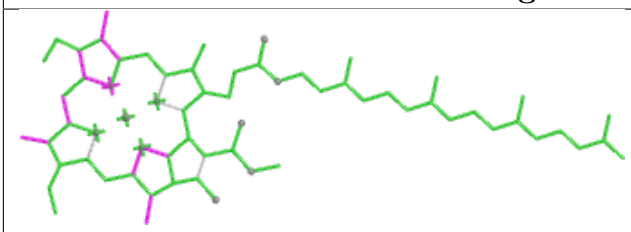


Rings

Ligand CLA d6 401



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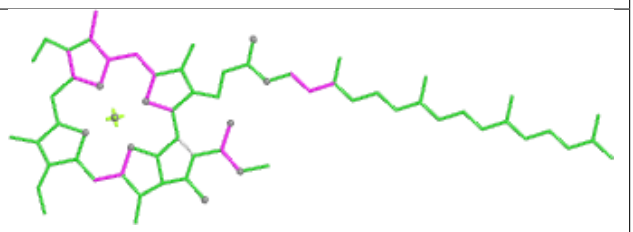
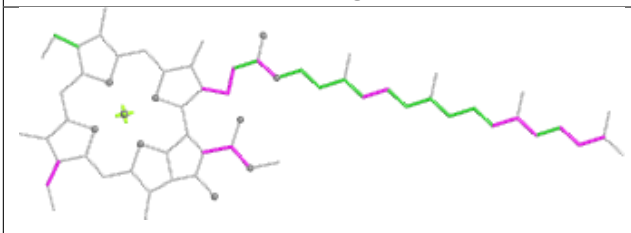


Bond angles



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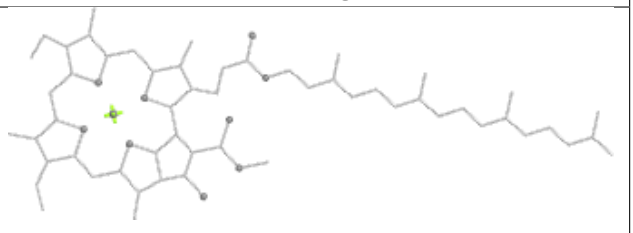
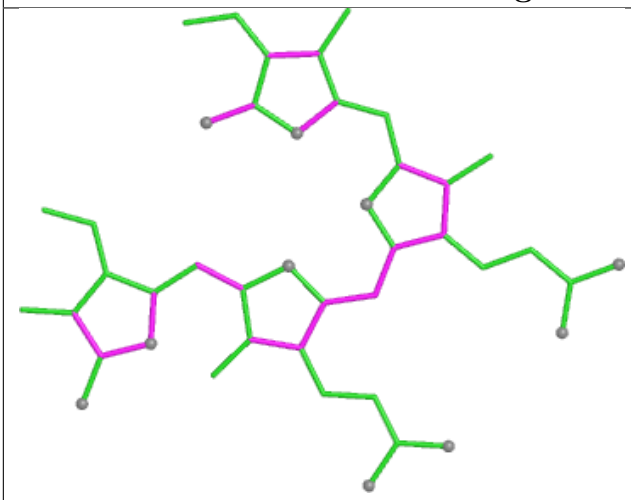


Rings

Ligand PEB JD 201



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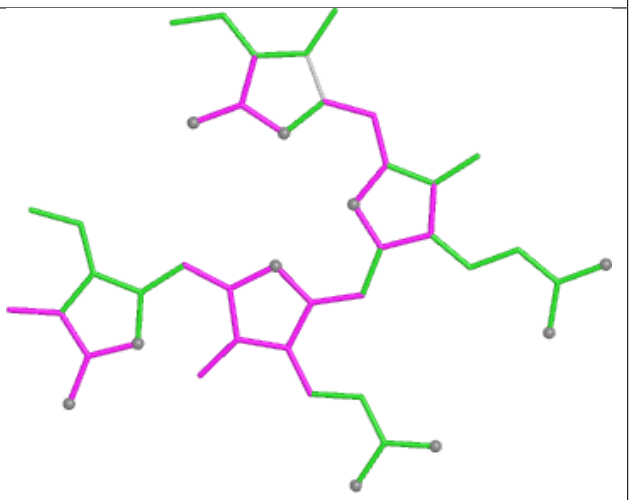
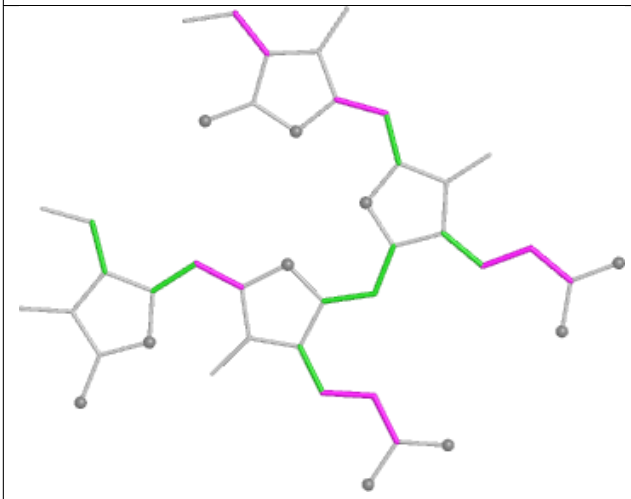


Bond angles



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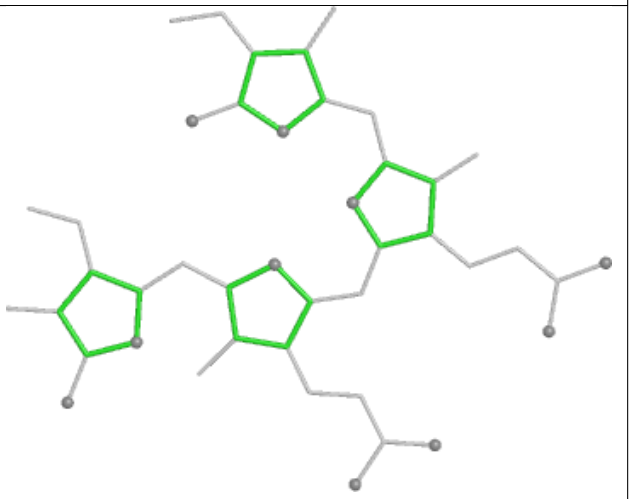
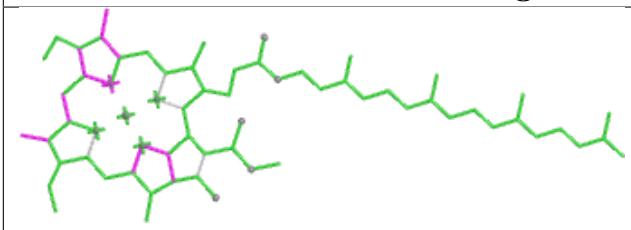


Rings

Ligand CLA A2 810



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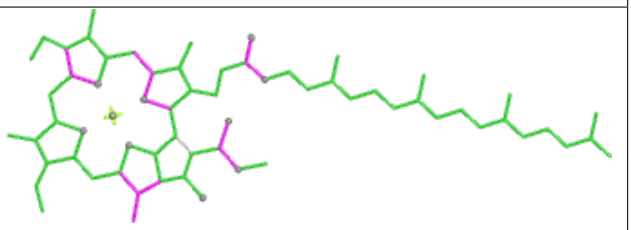
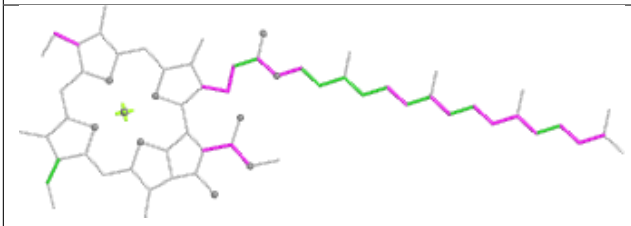


Bond angles



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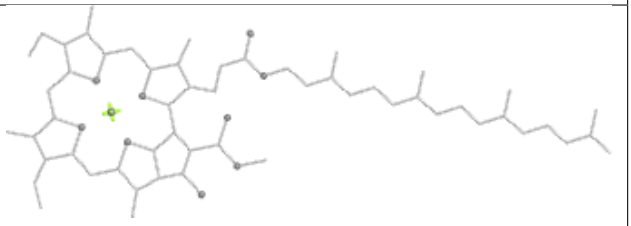
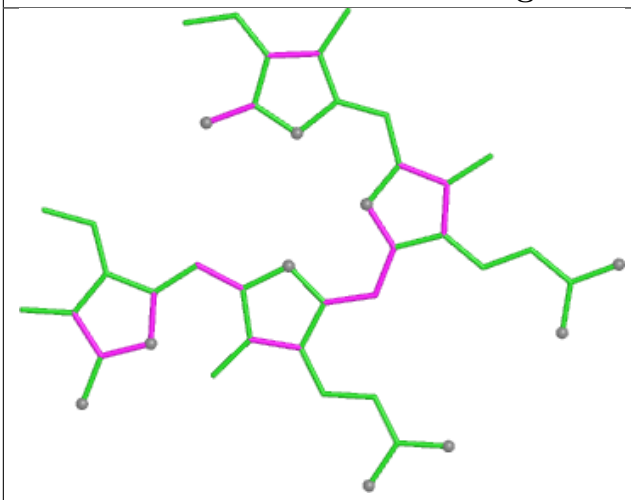


Rings

Ligand PEB eB 202



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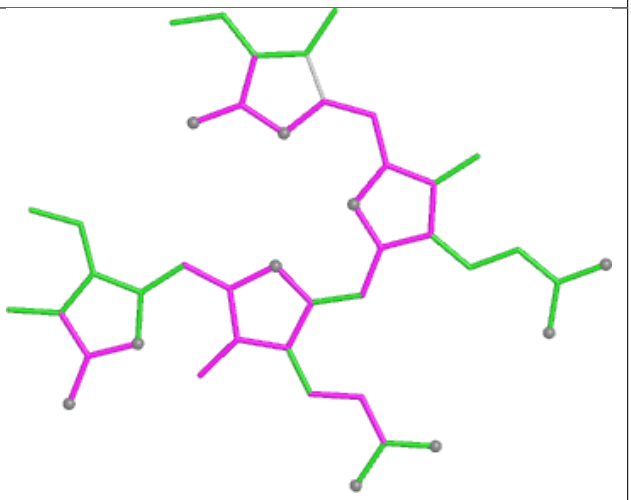
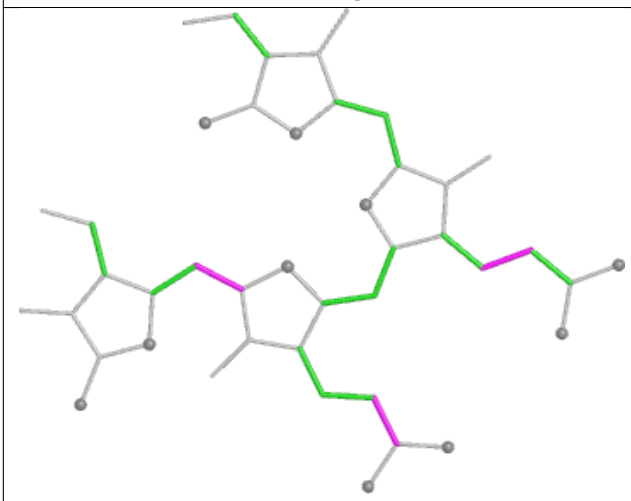


Bond angles



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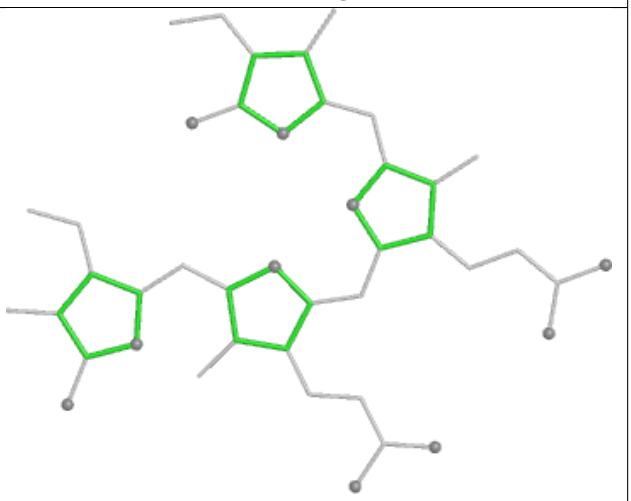
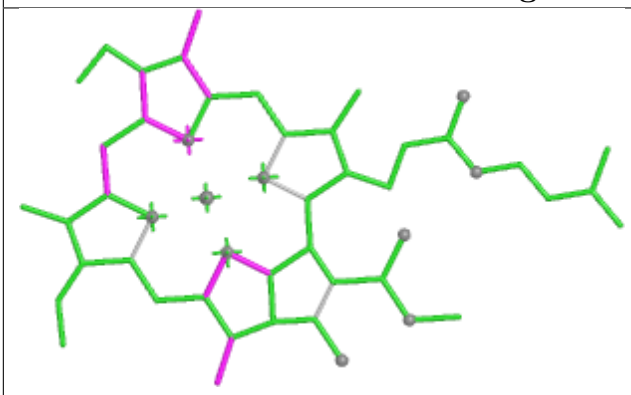


Rings

Ligand CLA 72 607



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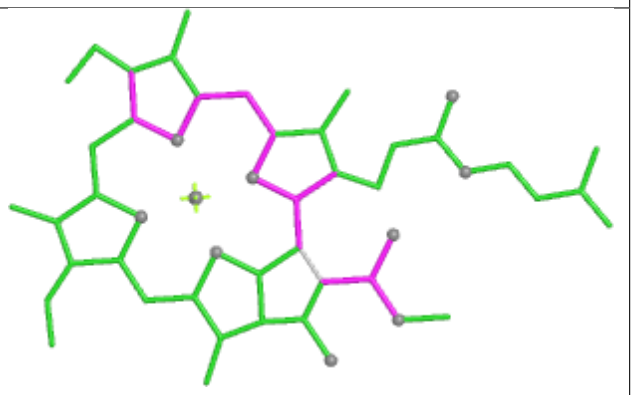
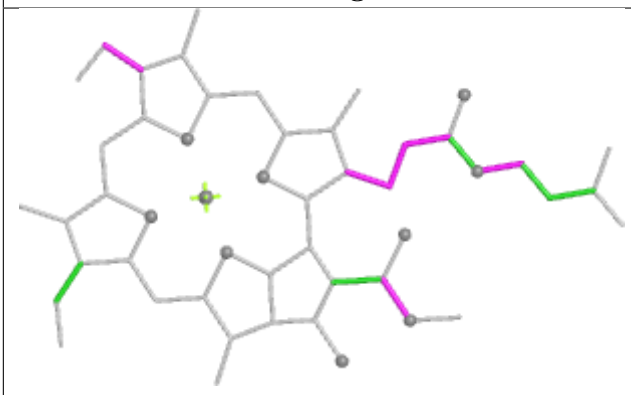


Bond angles



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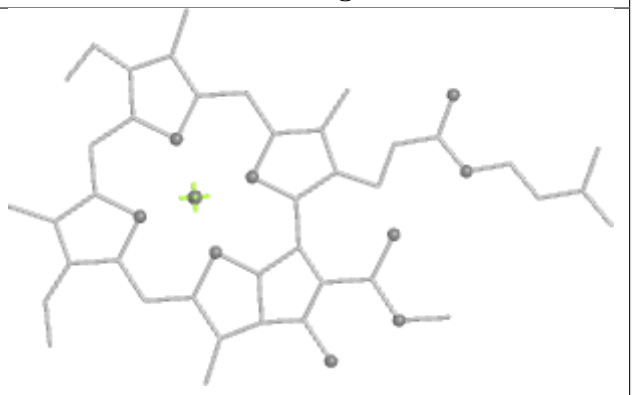
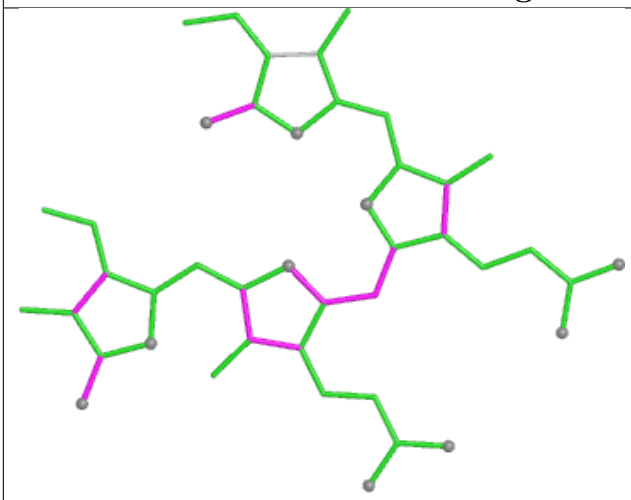
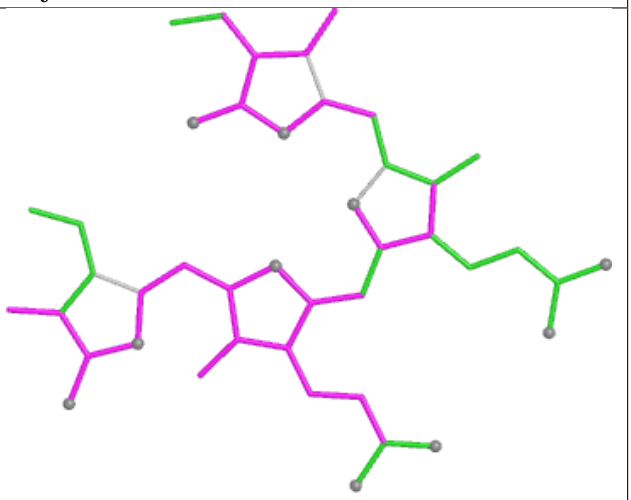


Rings

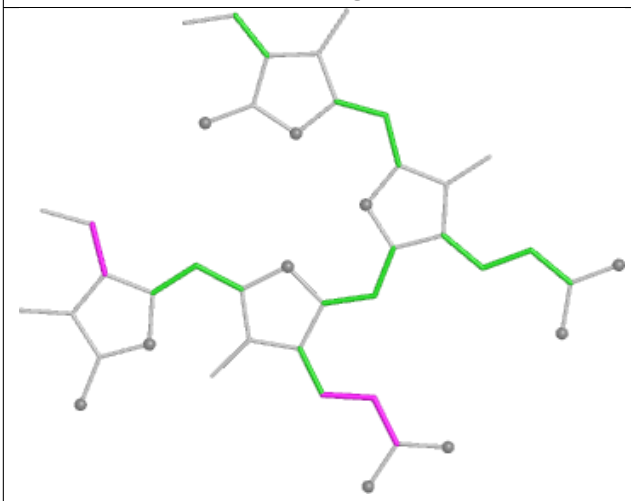
Ligand PUB yF 303



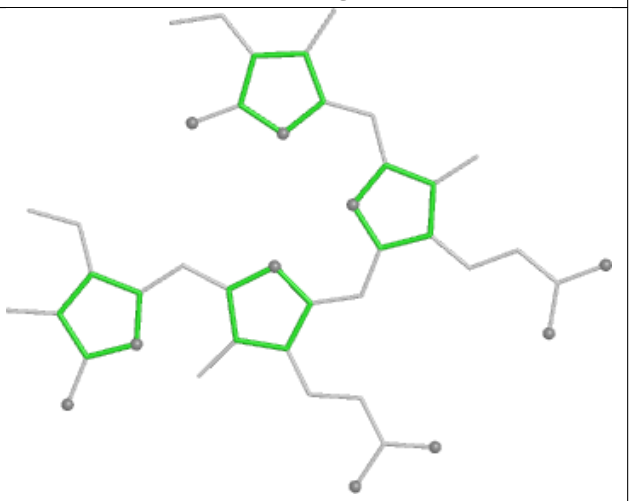
Bond lengths



Bond angles



Torsions



Rings

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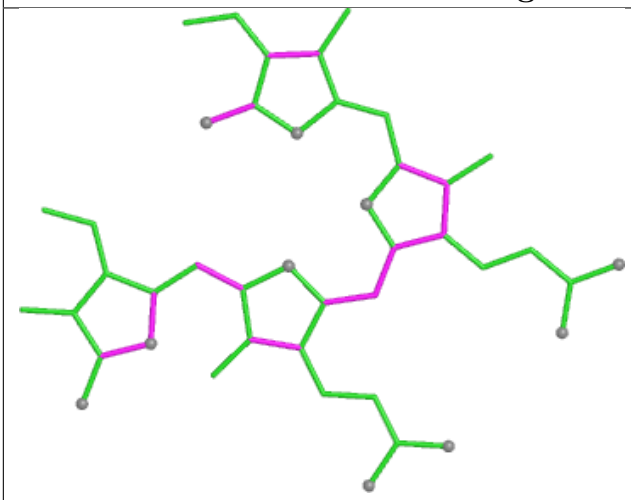

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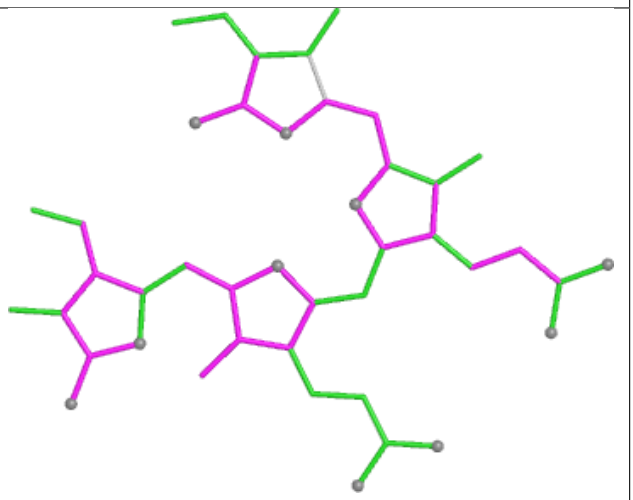

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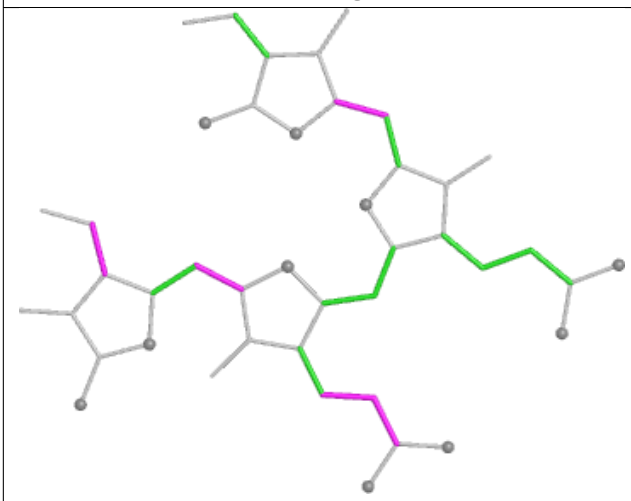

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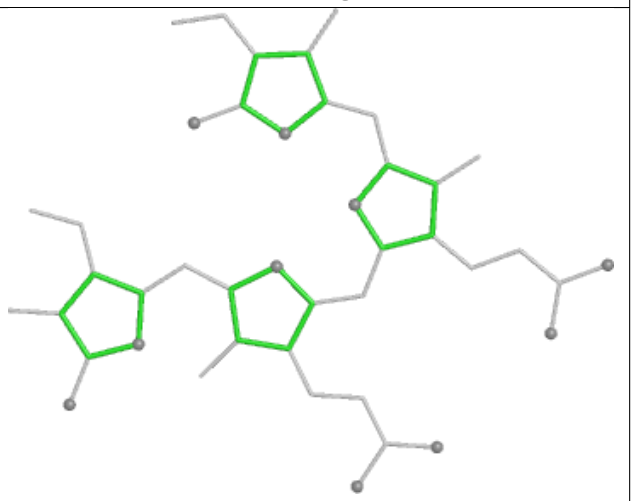

Rings

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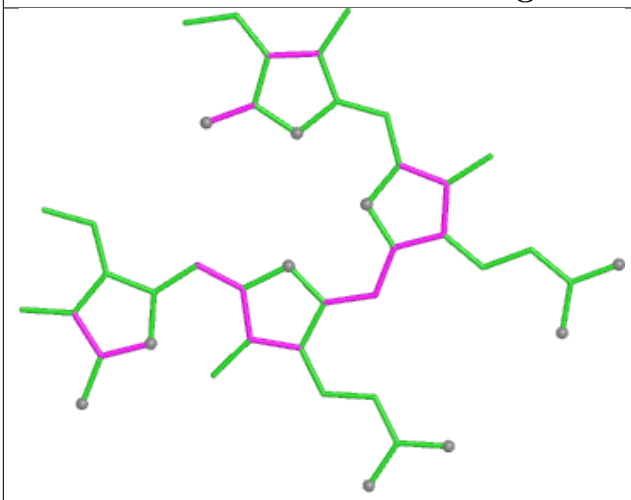

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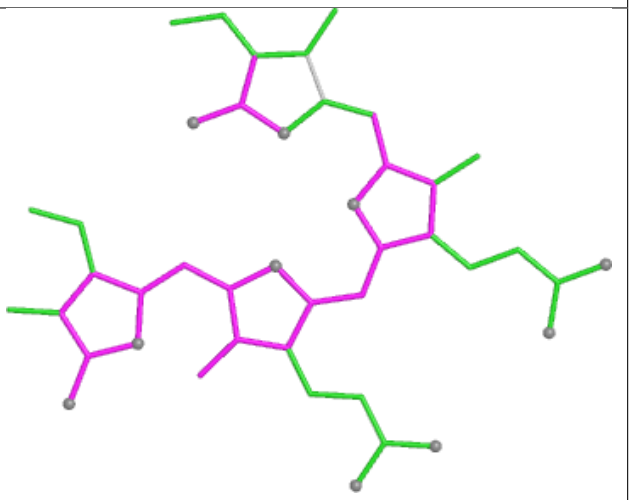

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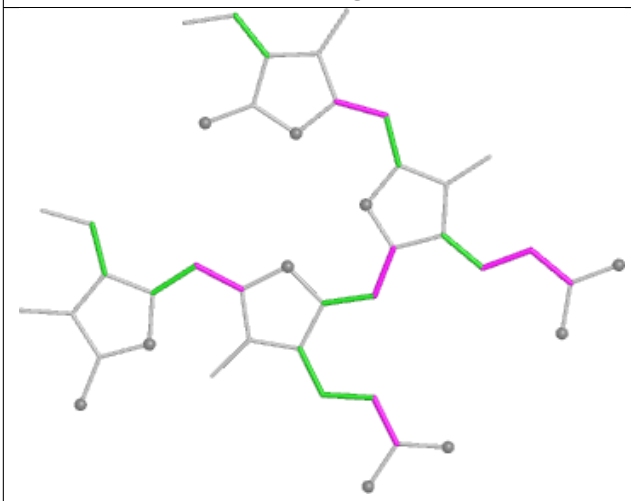

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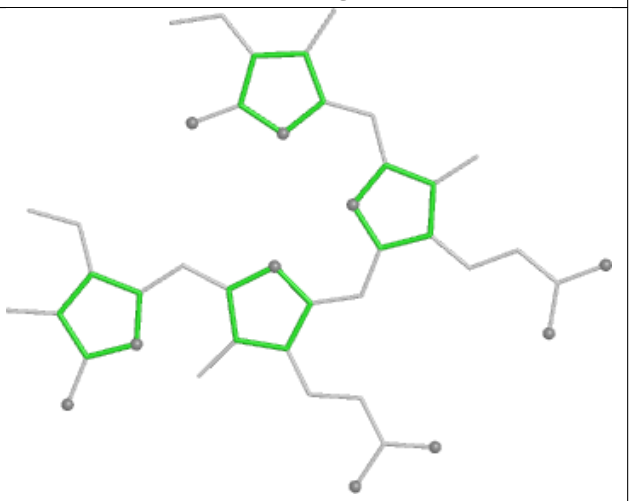

Rings

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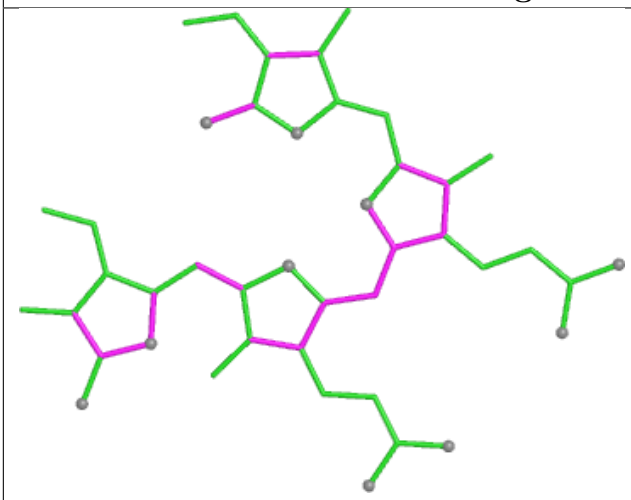

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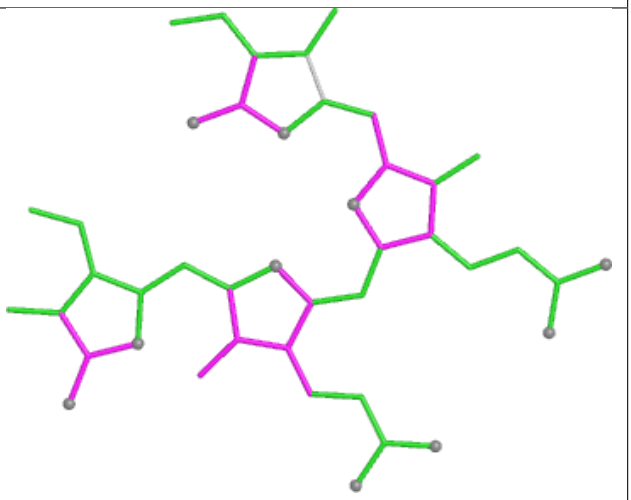

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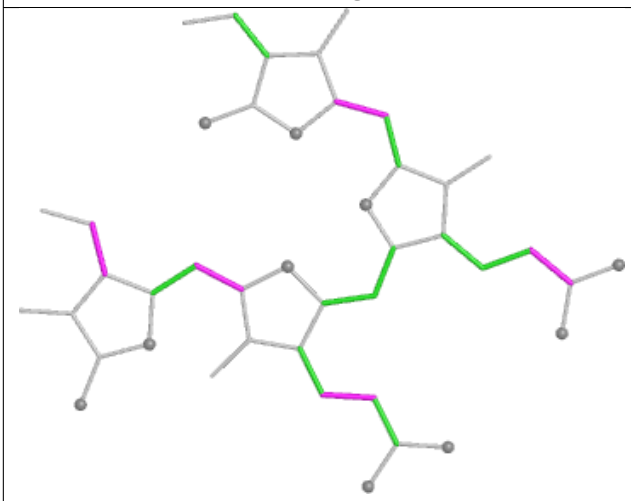

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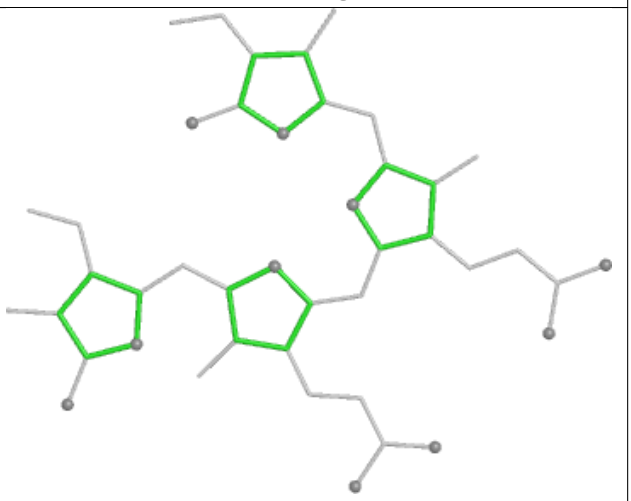

Rings

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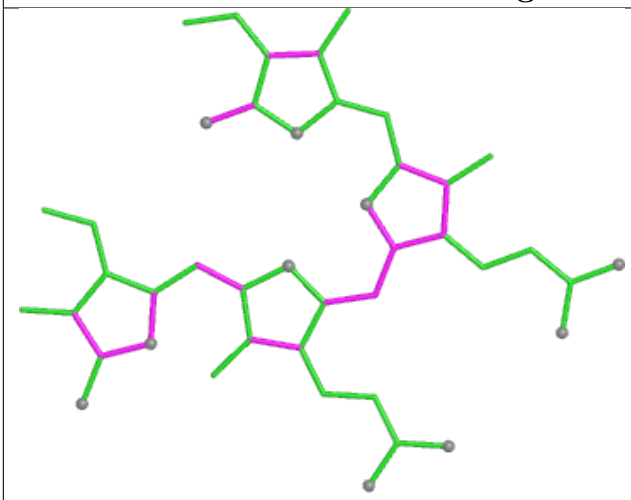

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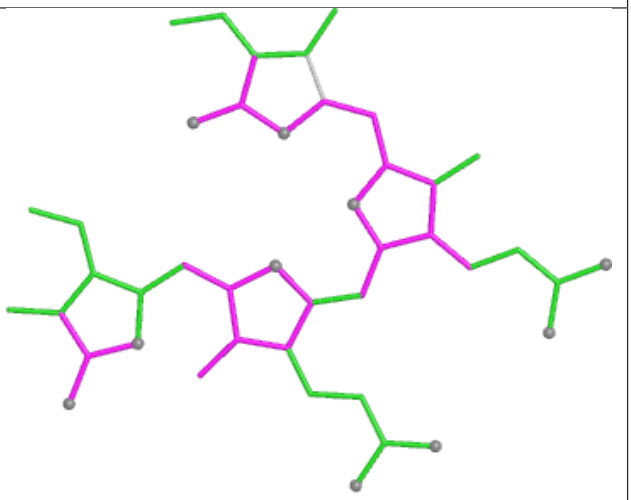

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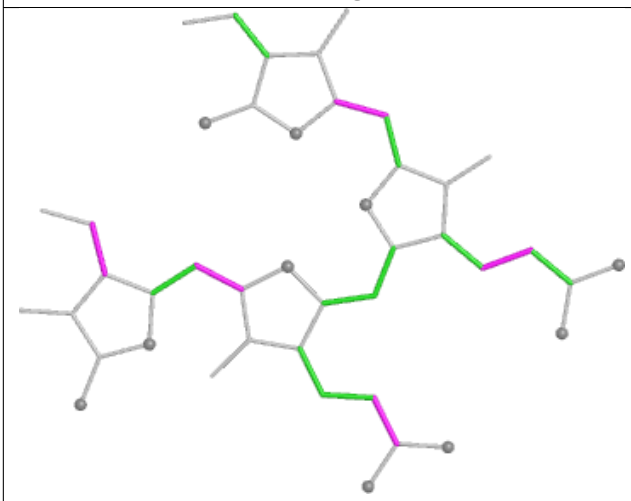

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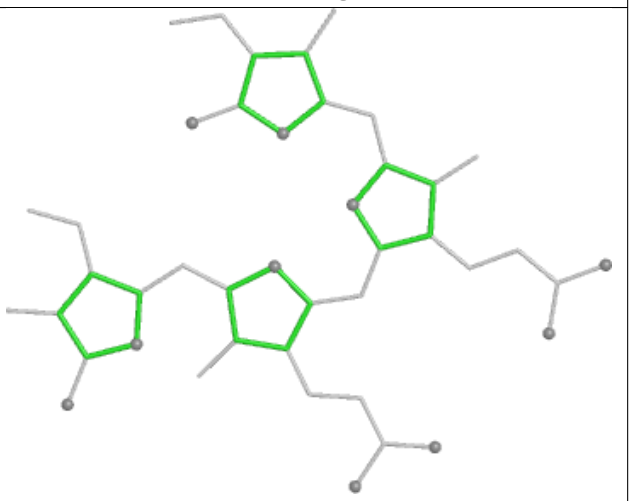

Rings

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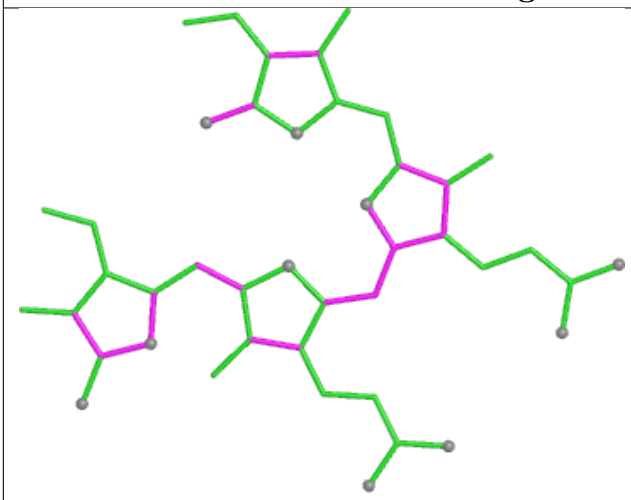

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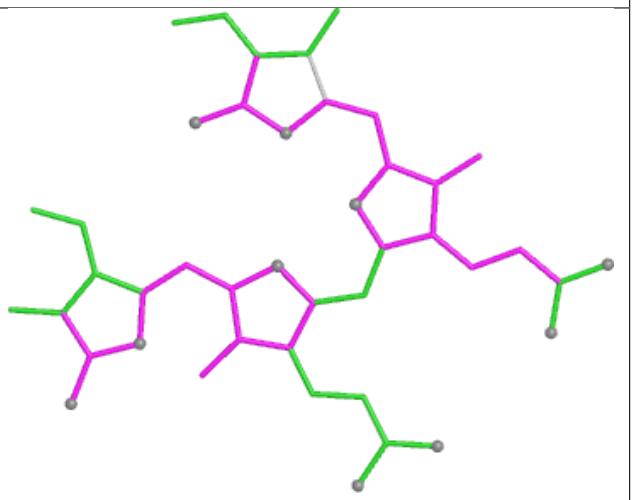

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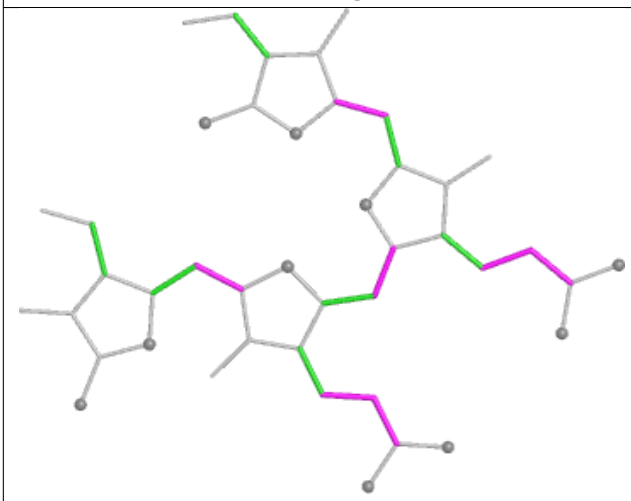

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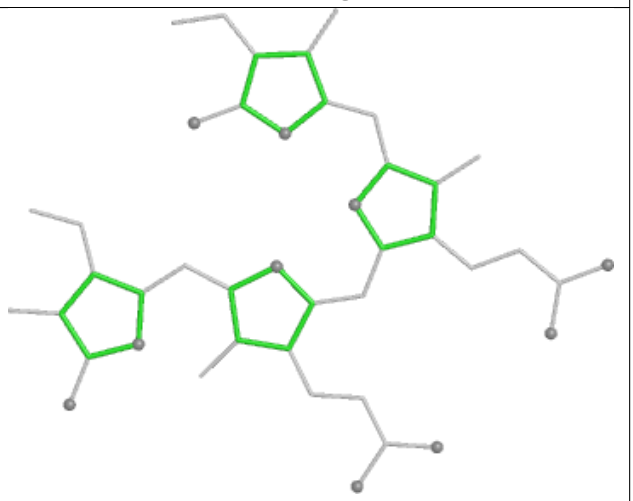

Rings

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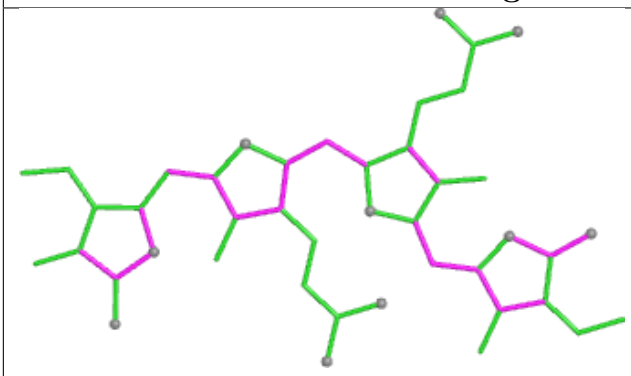

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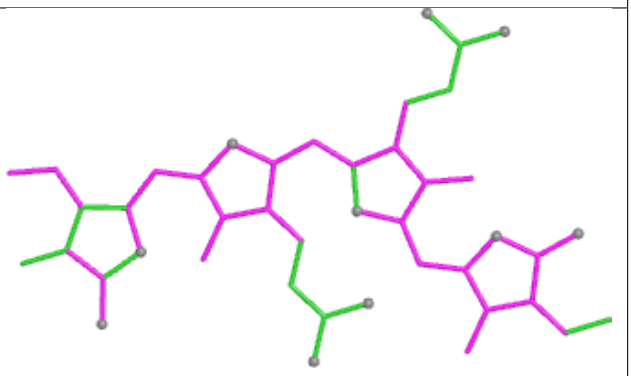

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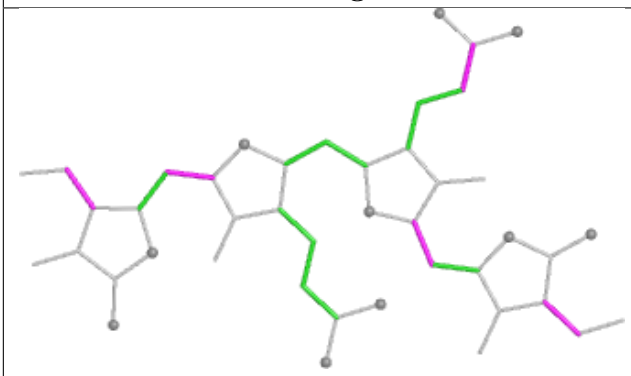

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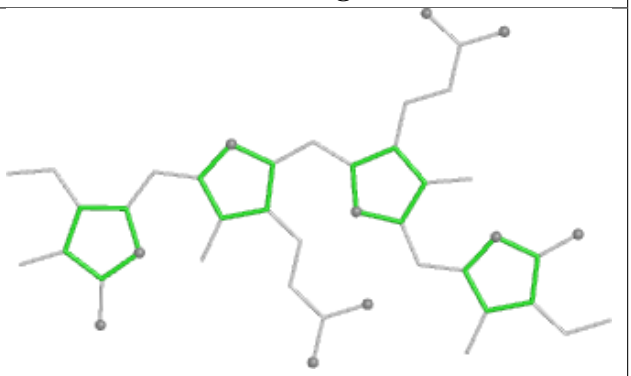

Rings

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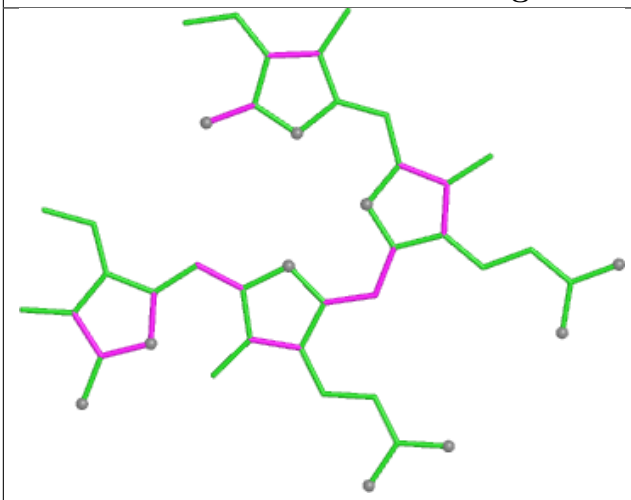

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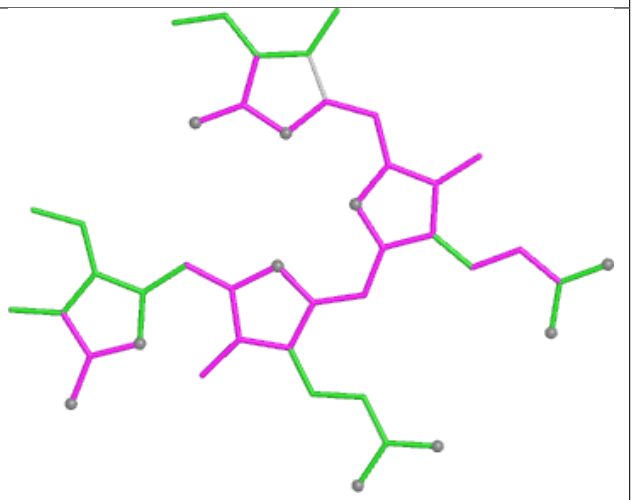

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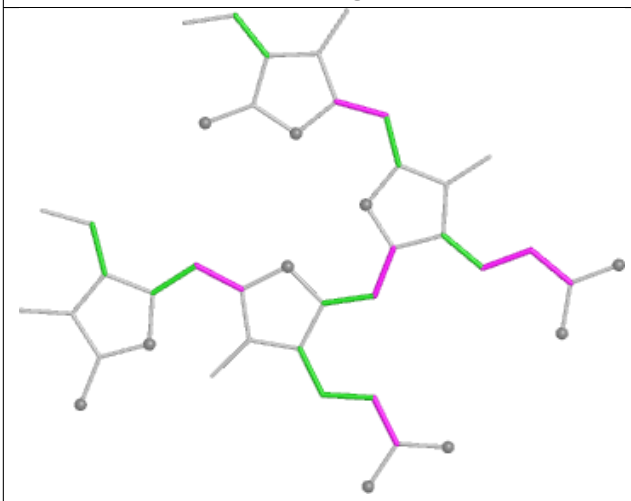

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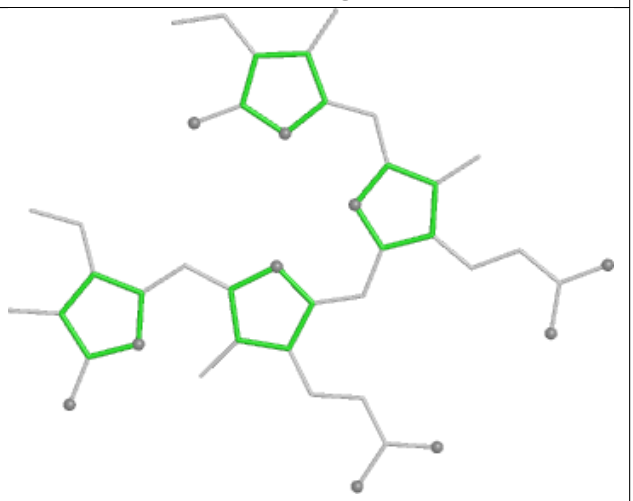

Rings

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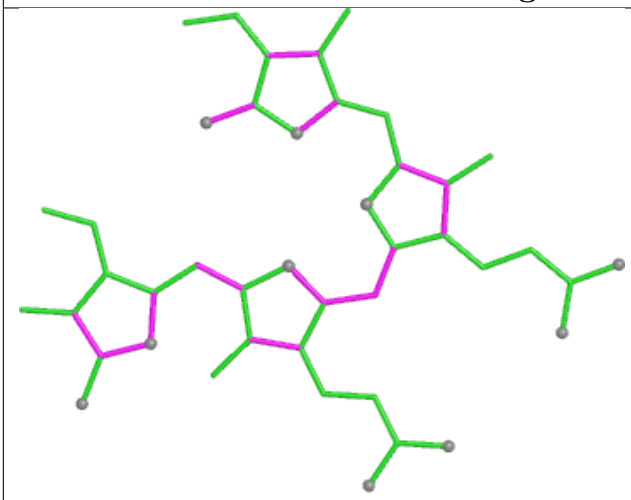

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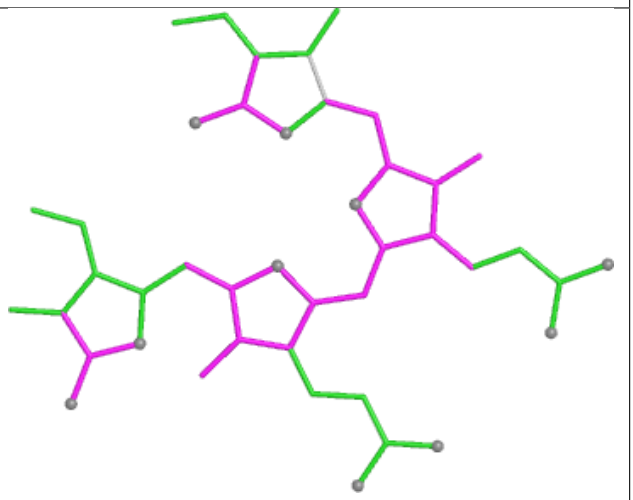

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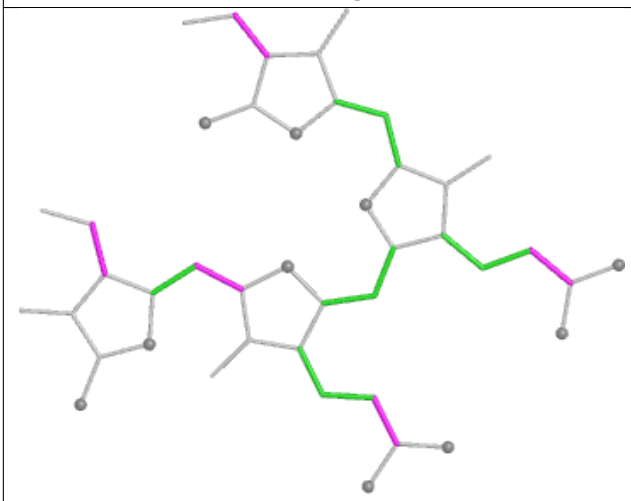

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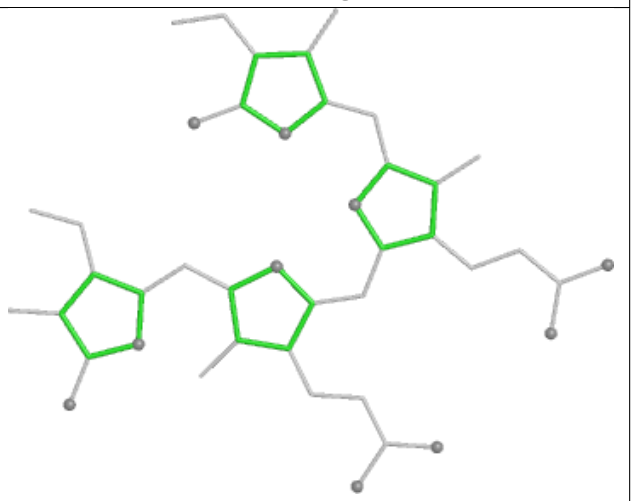

Rings

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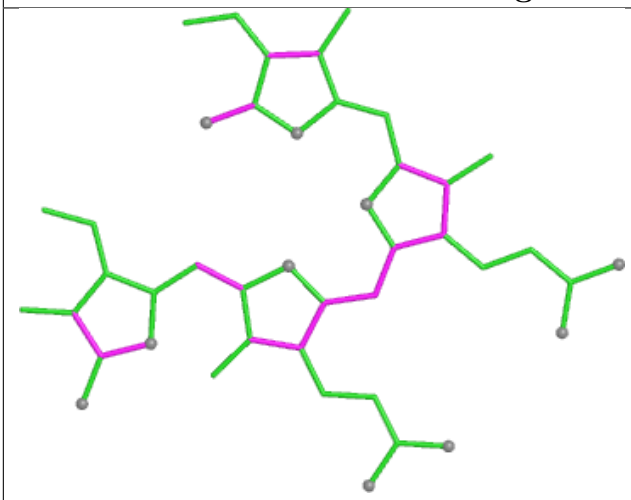

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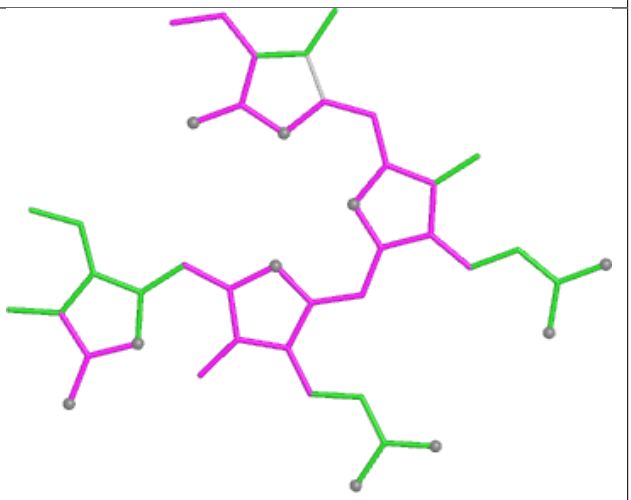

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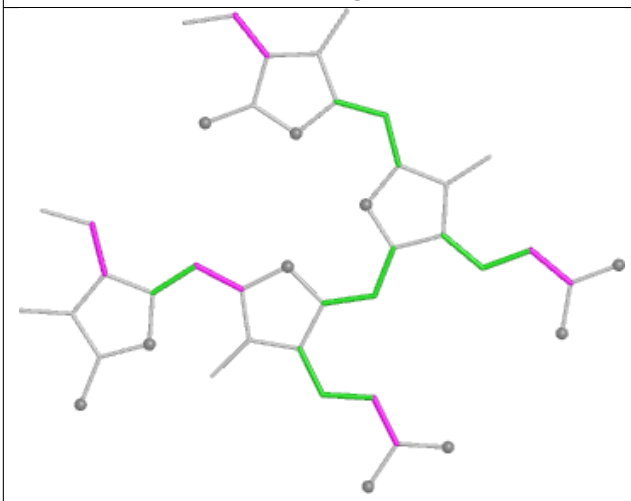

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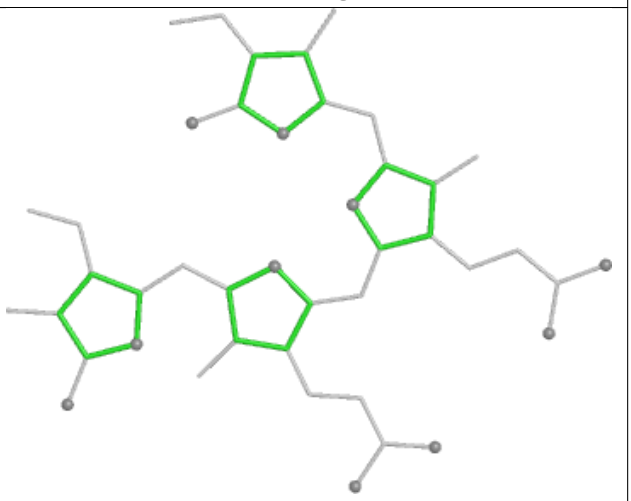

Rings

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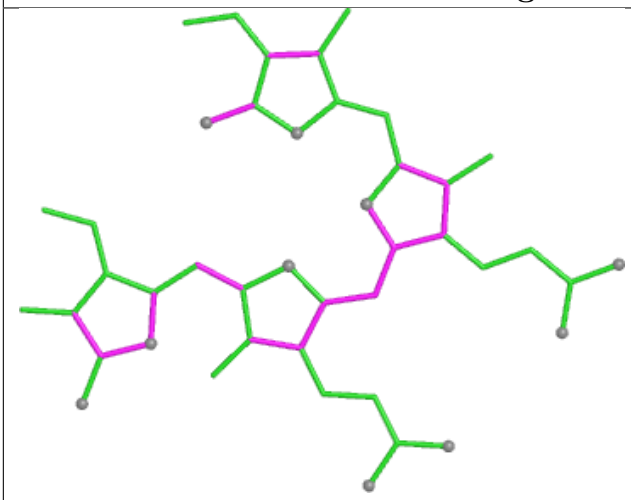

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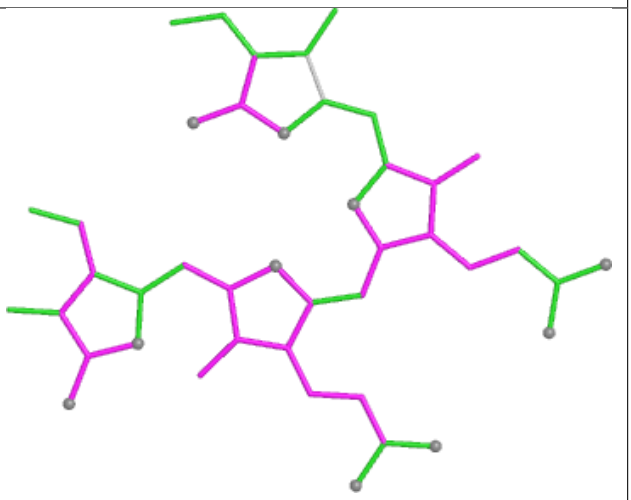

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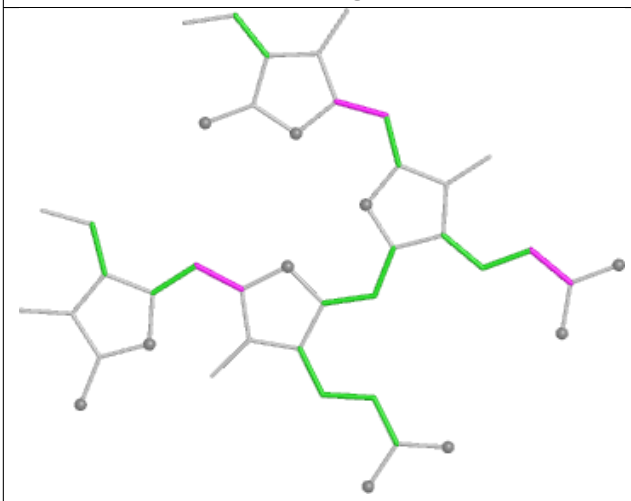

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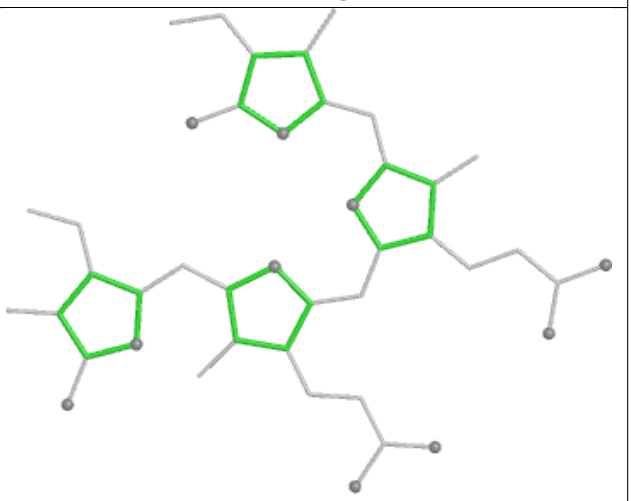

Rings

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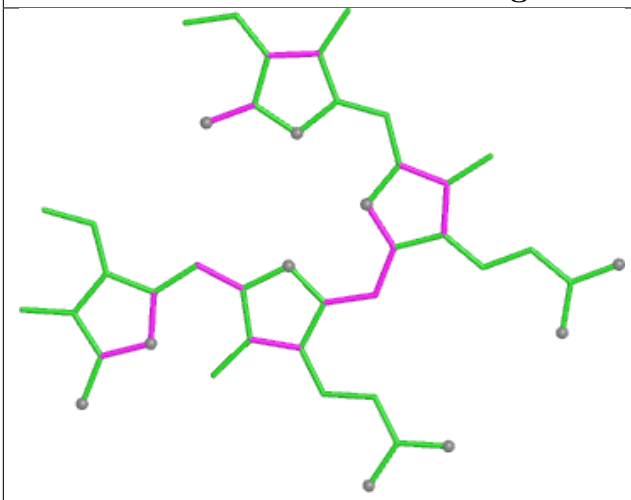

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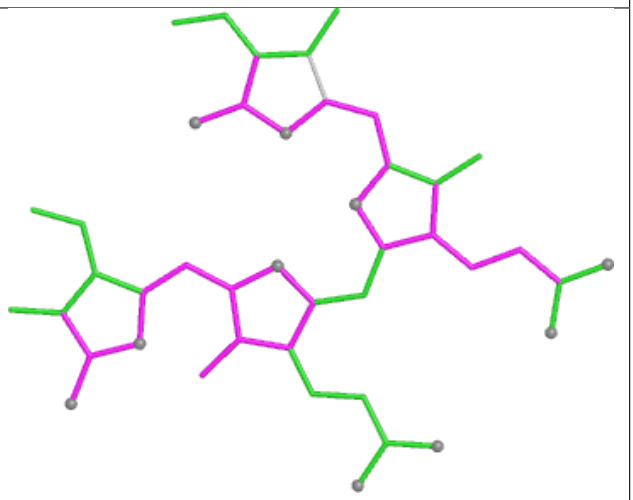

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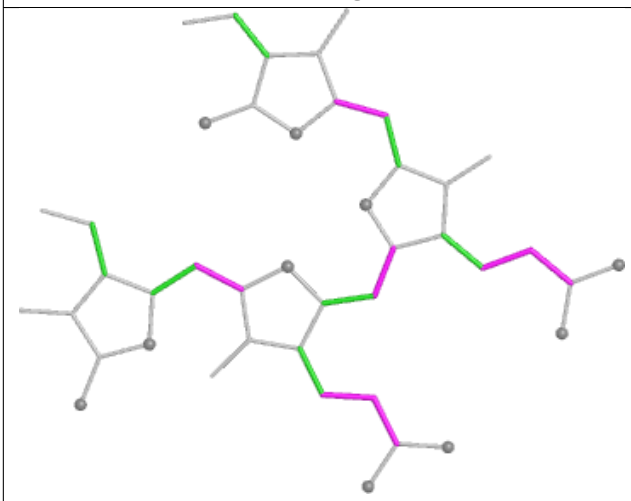

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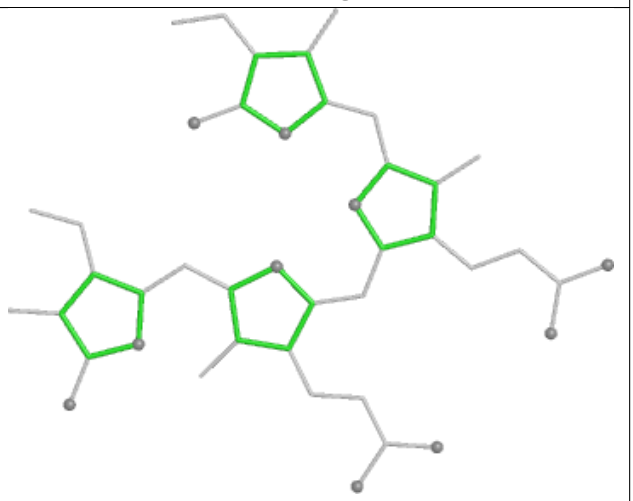

Rings

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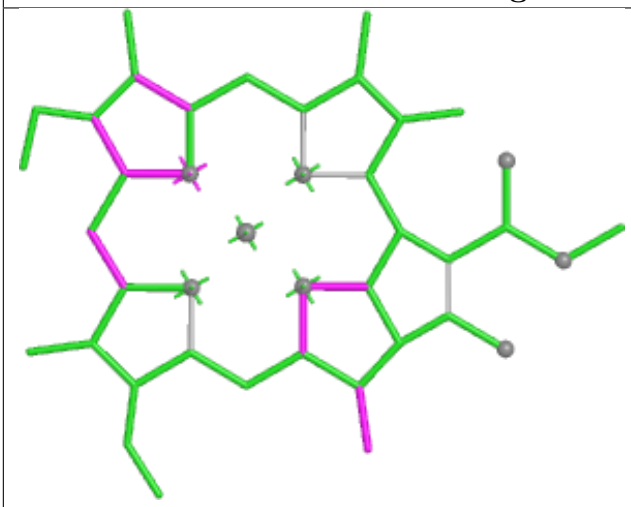

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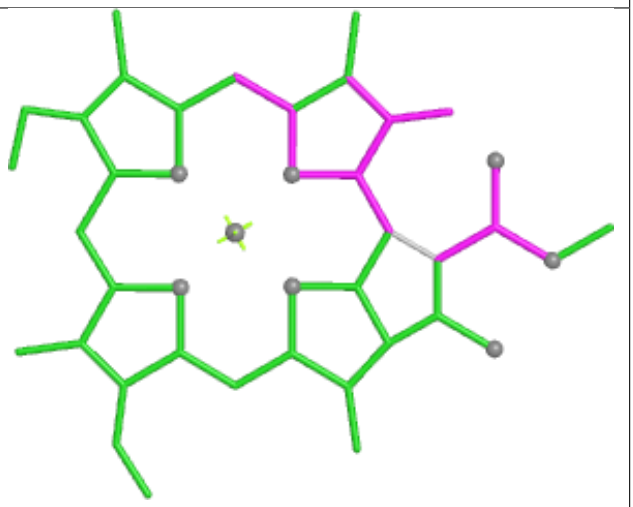

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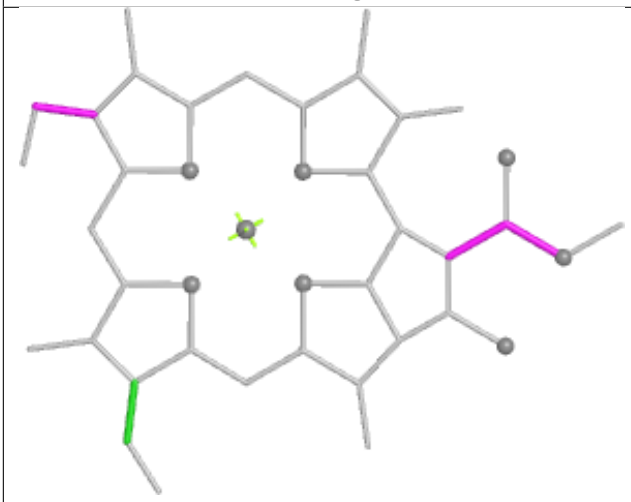

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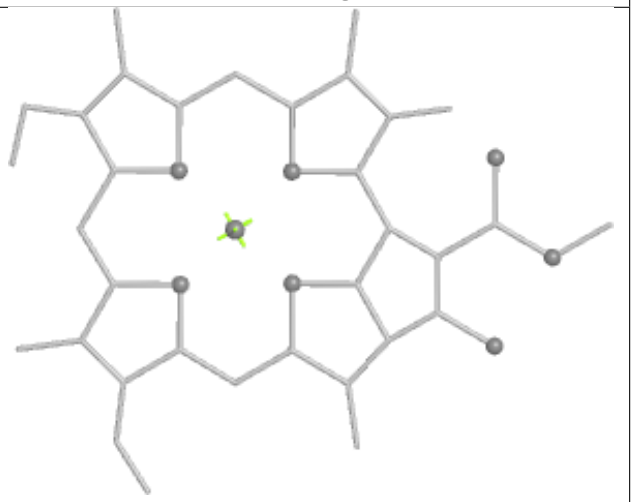

Rings

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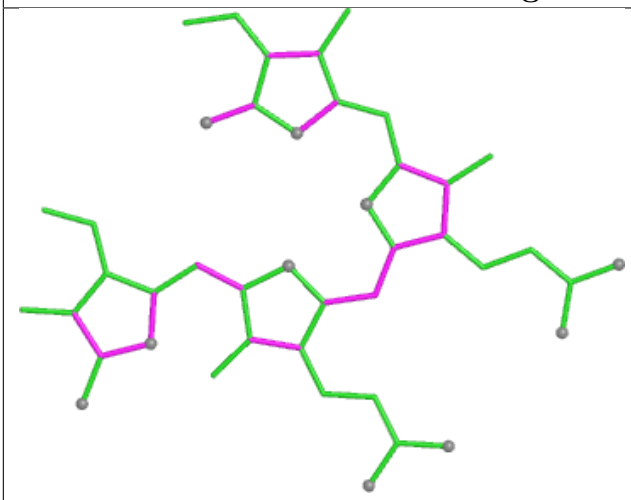

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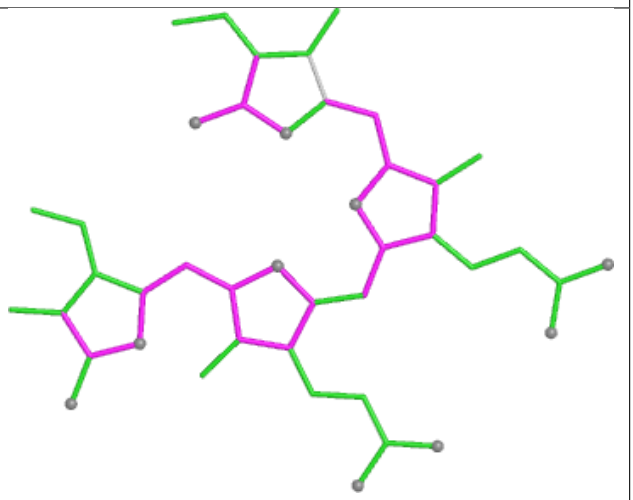

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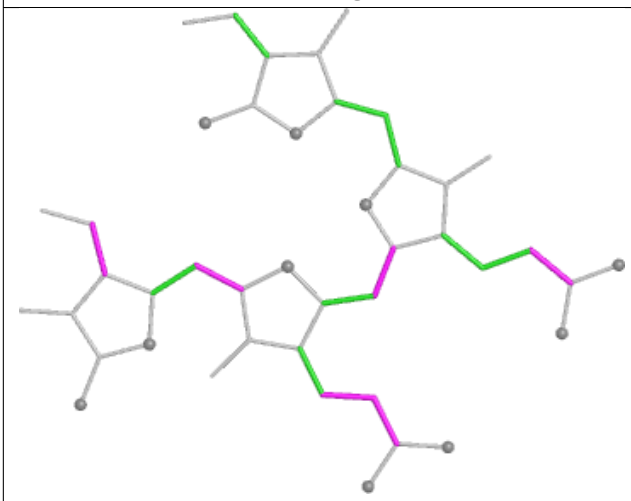

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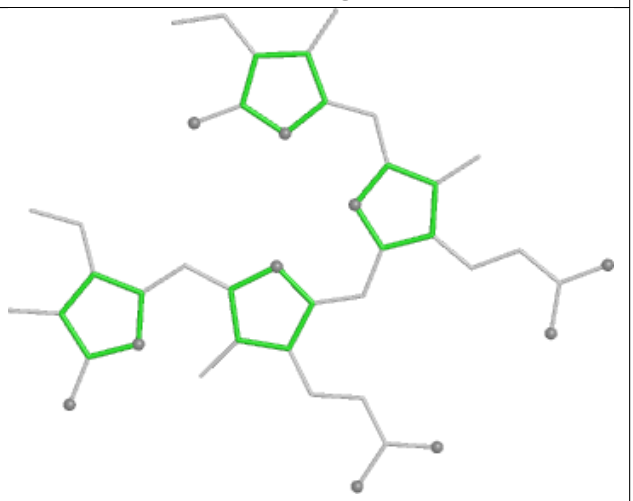
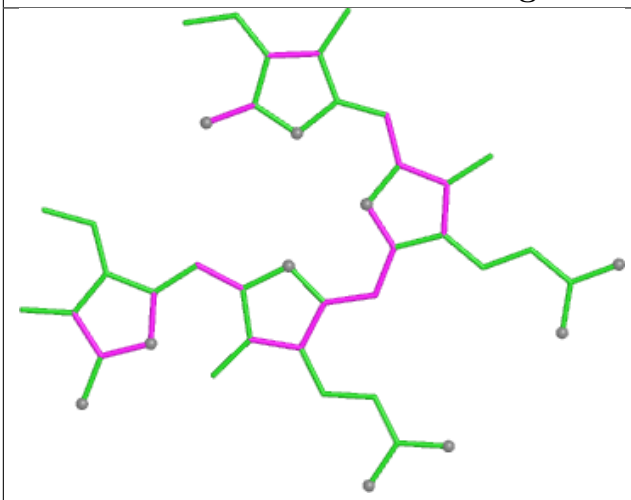


Rings

Ligand PEB kJ 201



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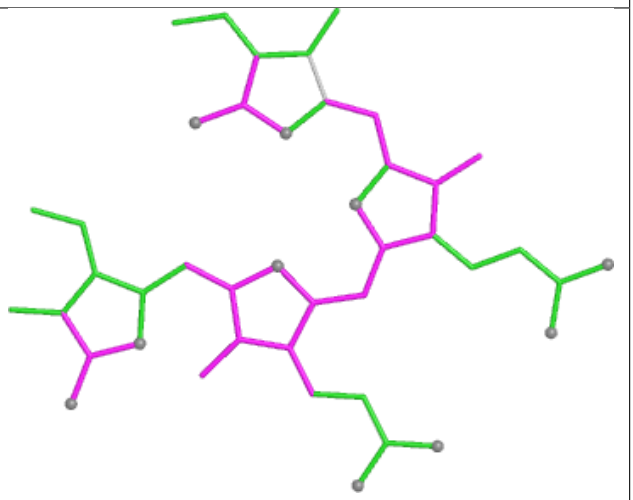

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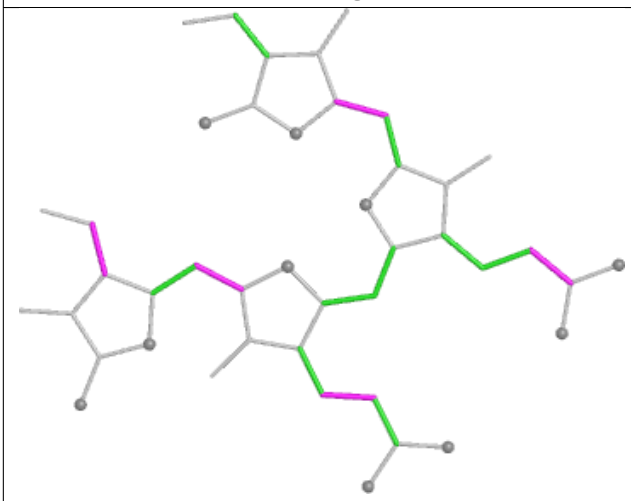

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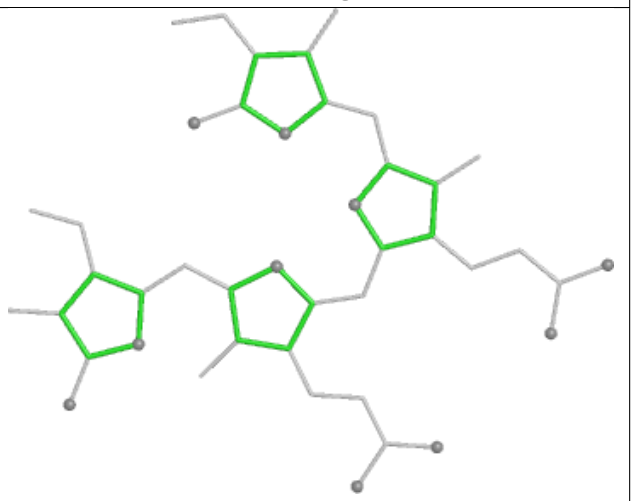

Rings

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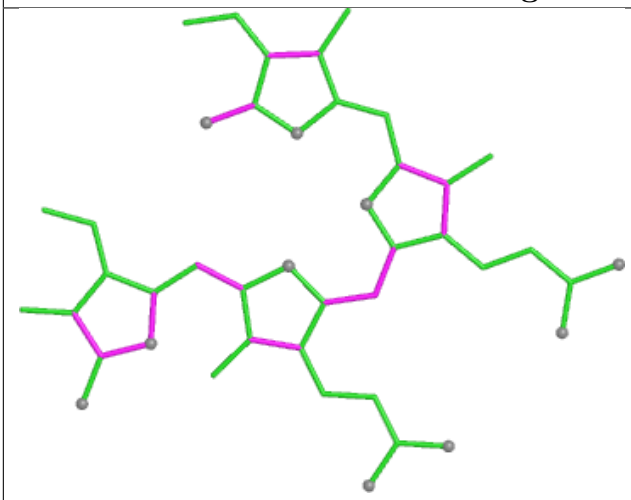
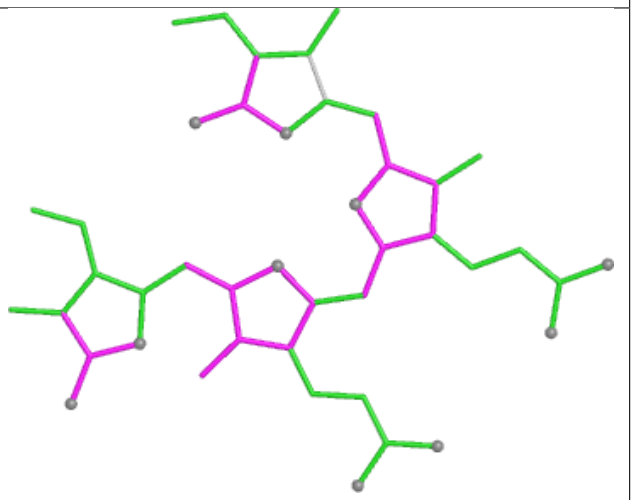
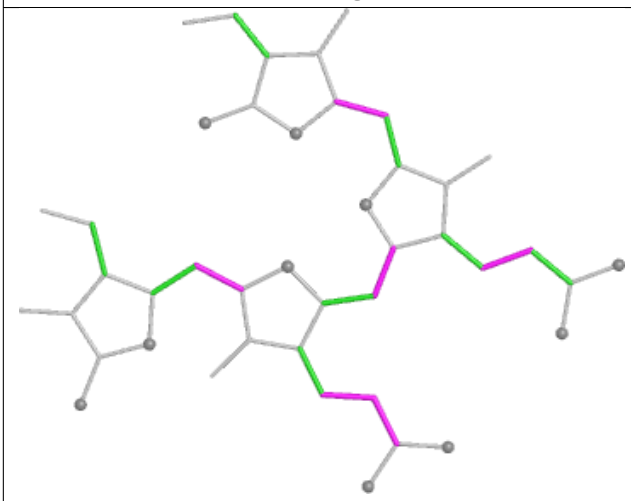


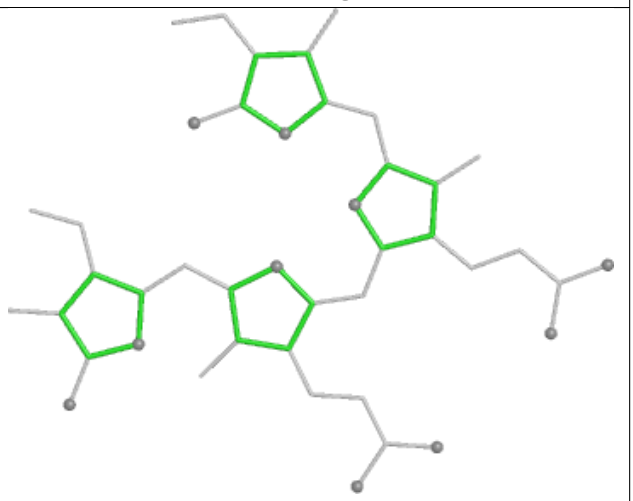
Bond lengths



Bond angles

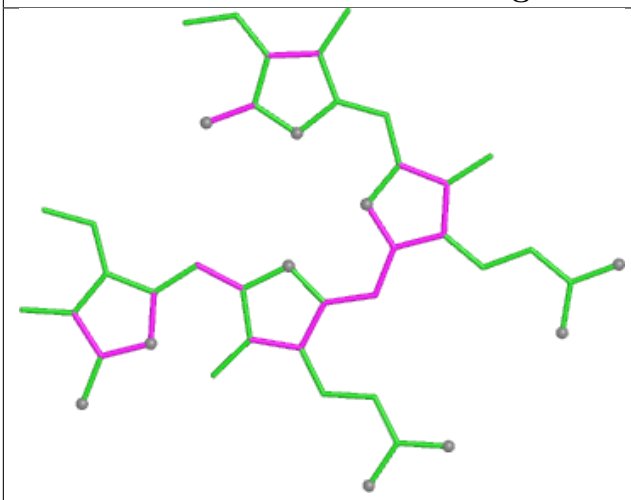


Torsions



Rings

Ligand PEB VE 201



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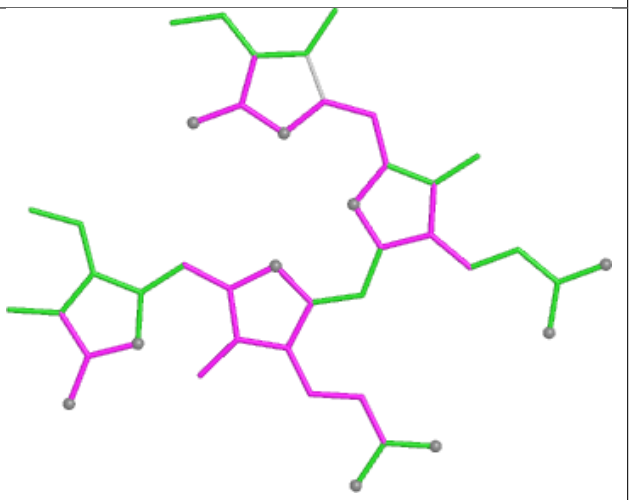

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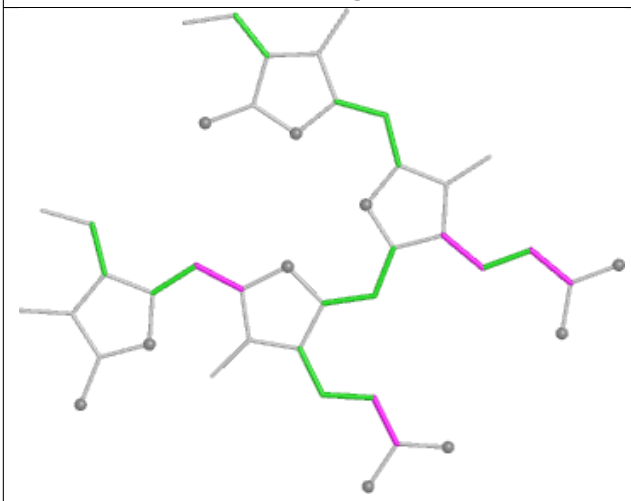

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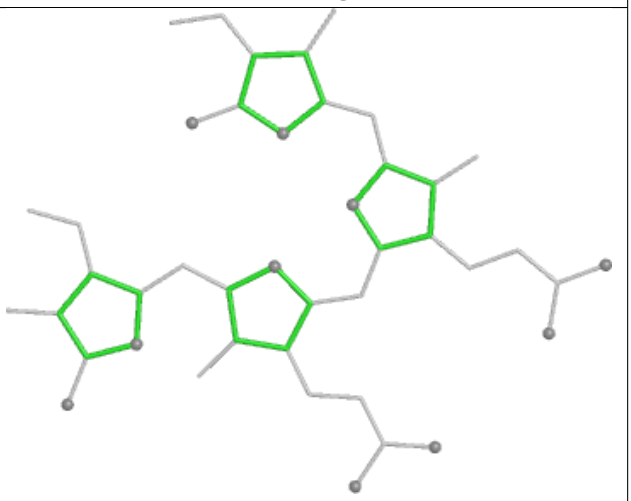
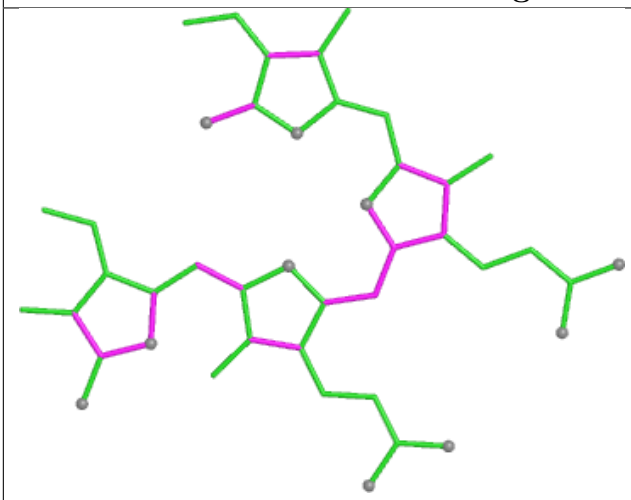


Rings

Ligand PEB ZG 202



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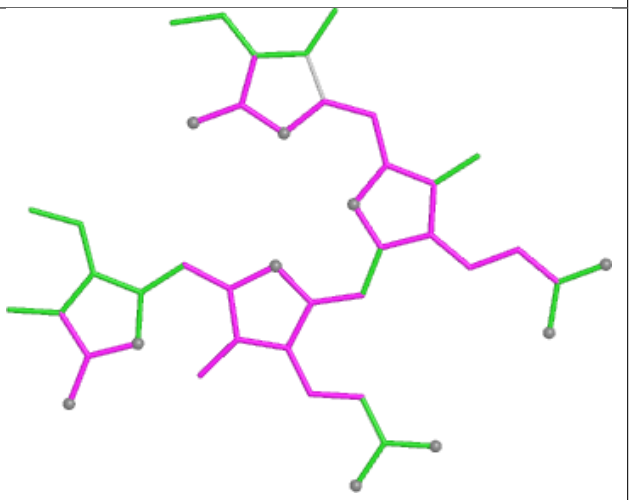

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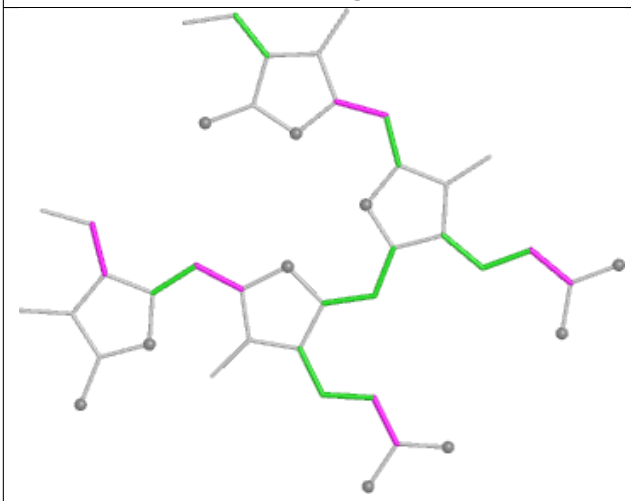

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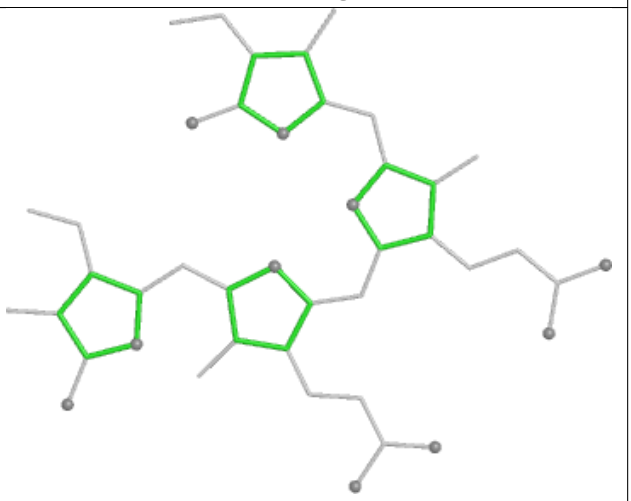
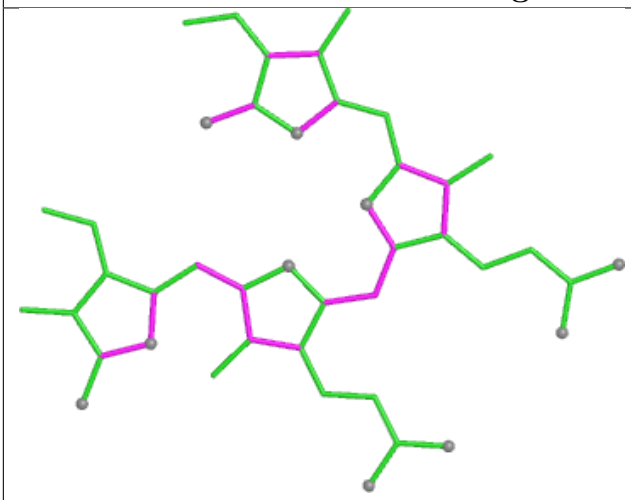


Rings

Ligand PEB M9 305



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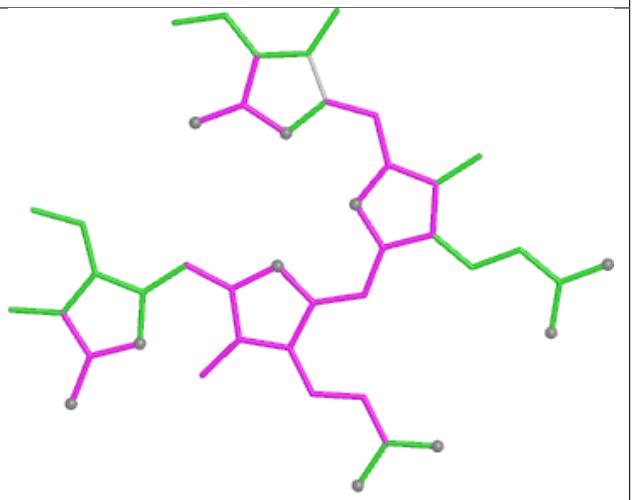

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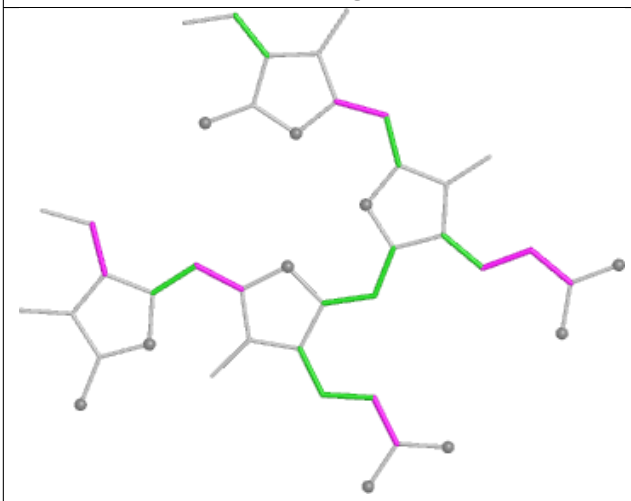

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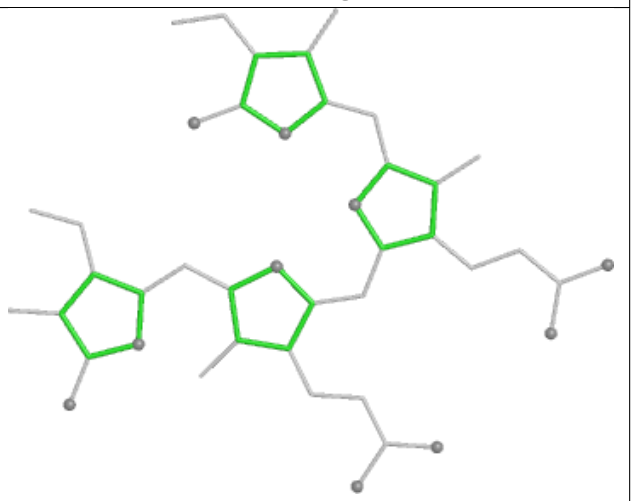
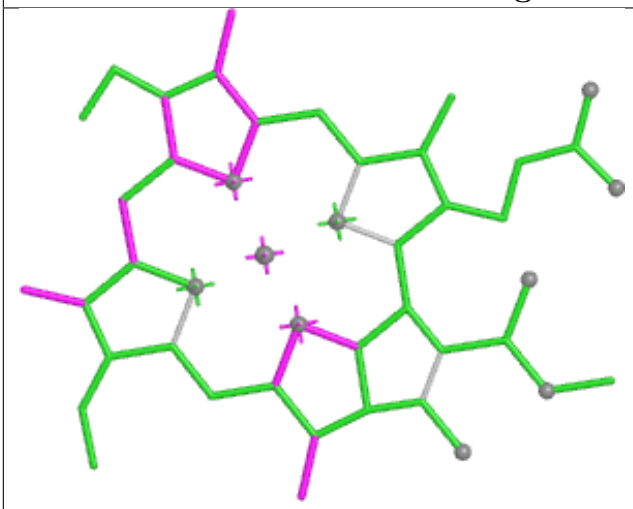


Rings

Ligand CLA K2 103



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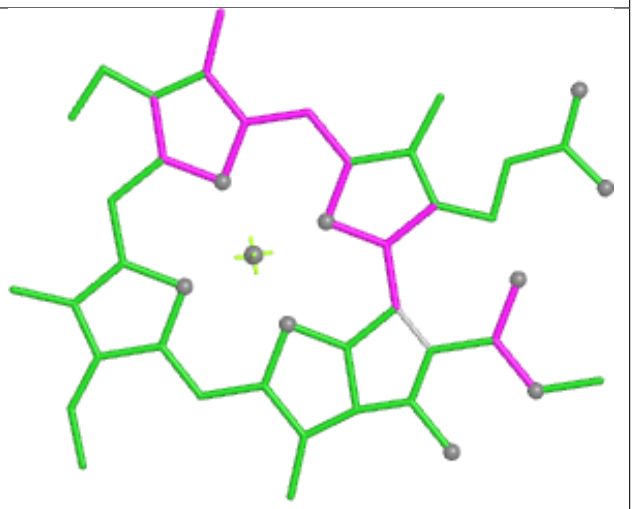

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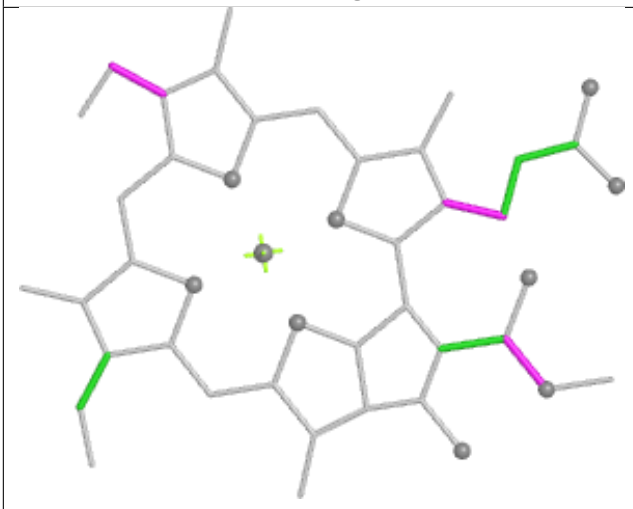
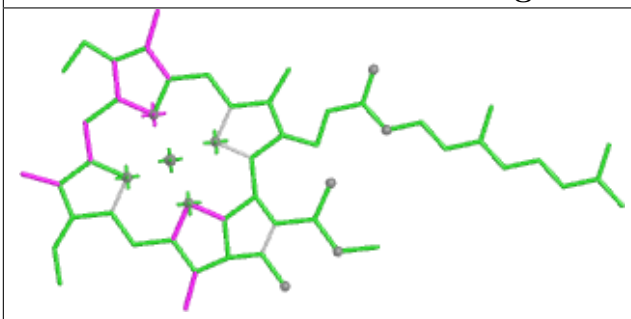


Torsions



Rings

Ligand CLA A2 806



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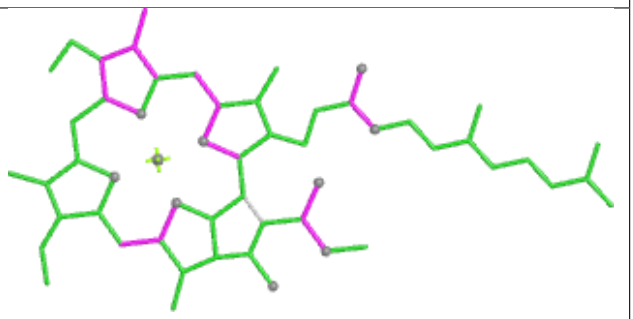

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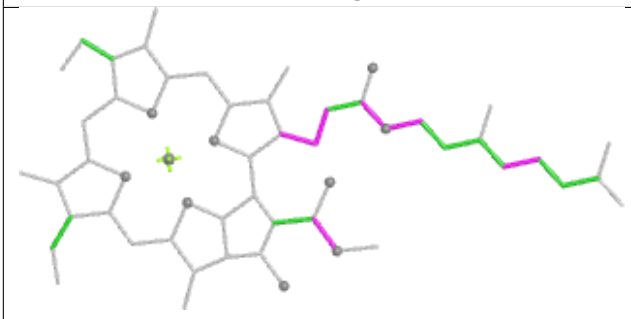

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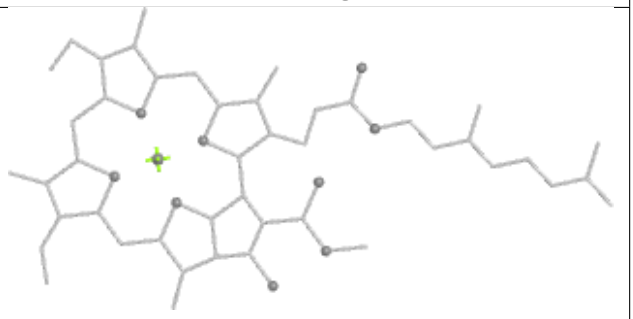
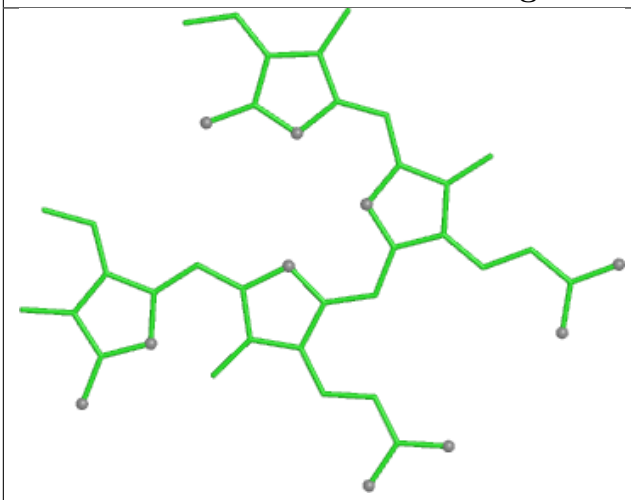


Rings

Ligand PEB IF 202



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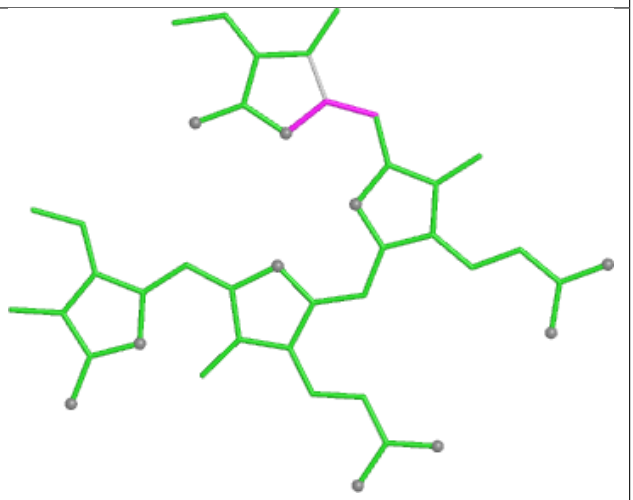

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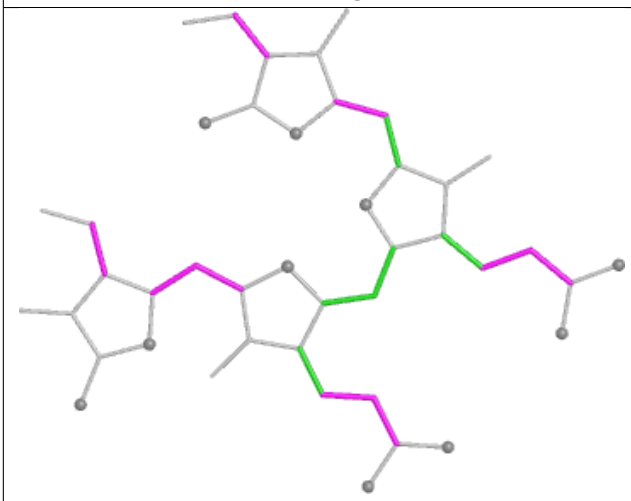

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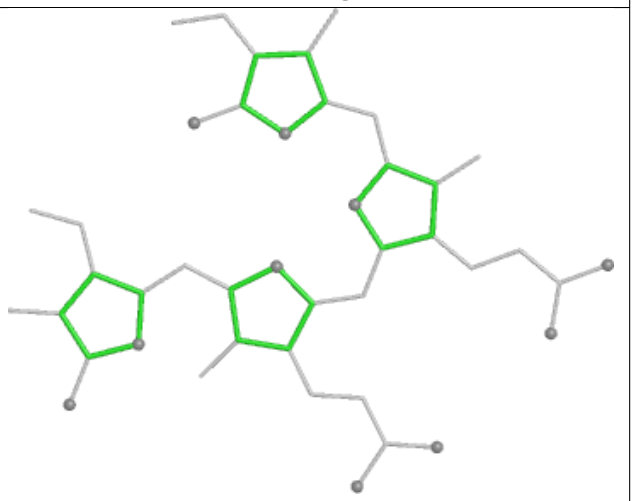
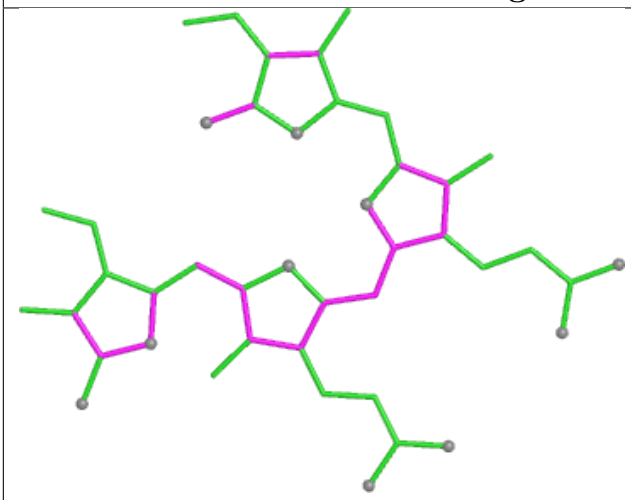


Rings

Ligand PEB mH 201



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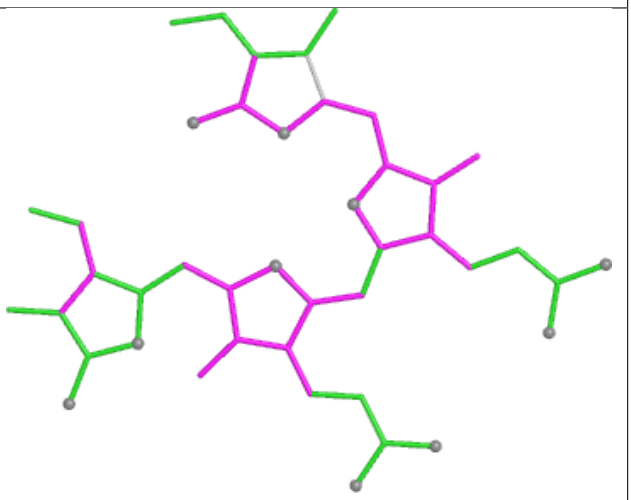
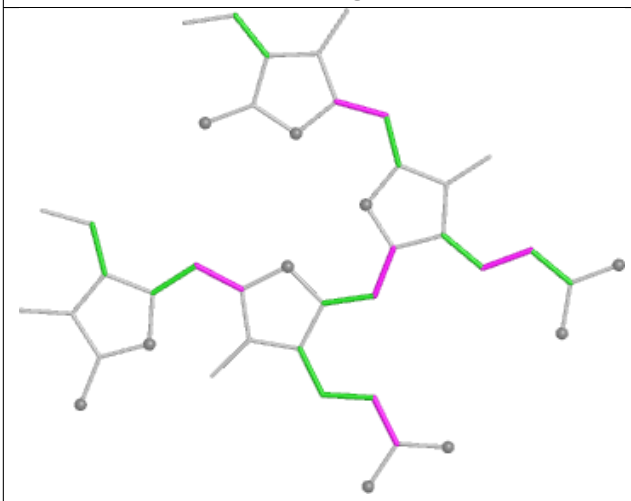


Bond angles



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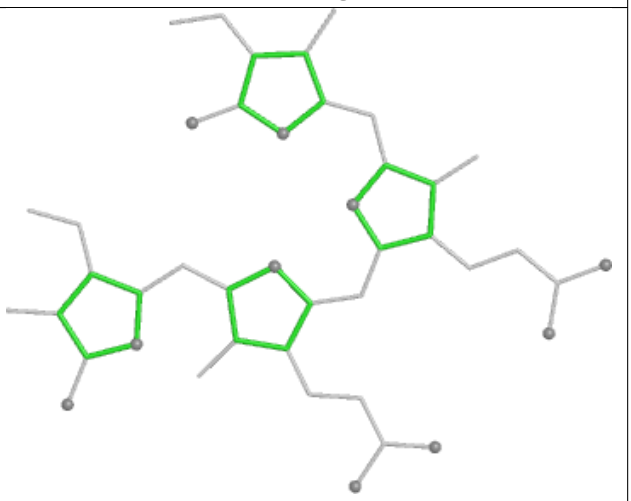
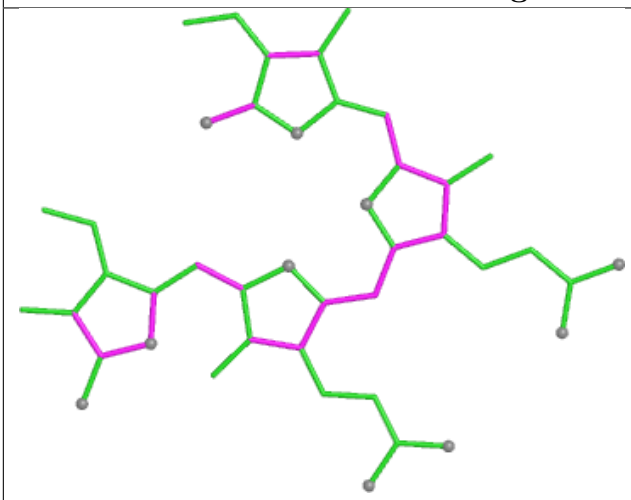


Rings

Ligand PEB W1 203



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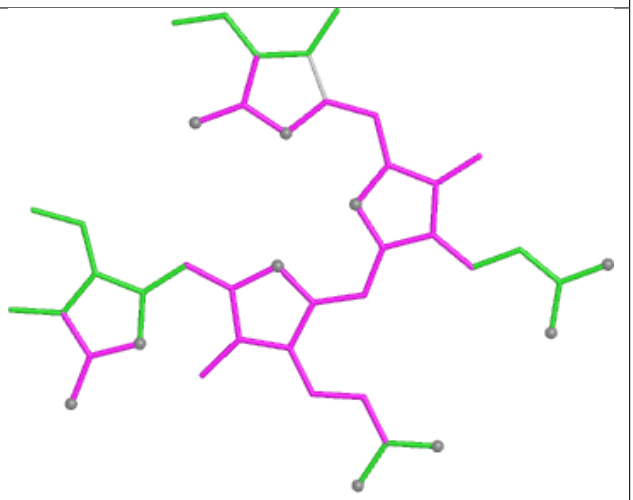

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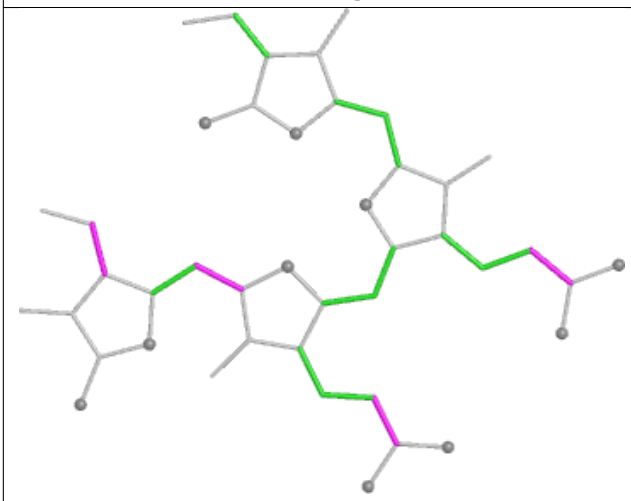

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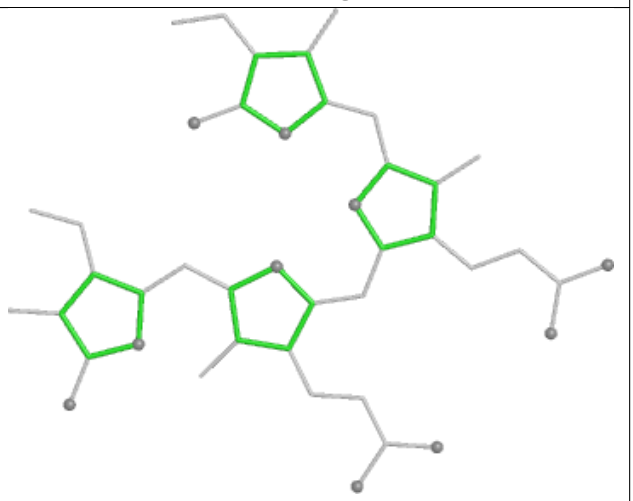
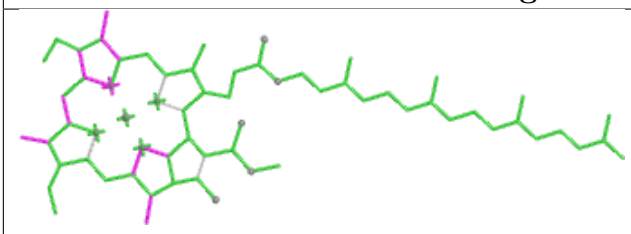


Rings

Ligand CLA a6 607



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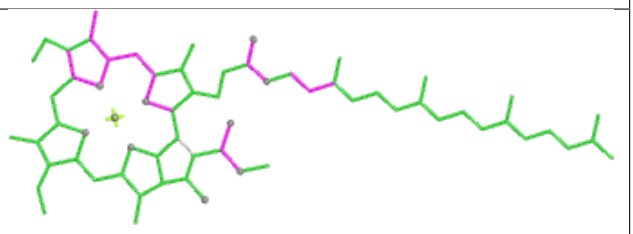
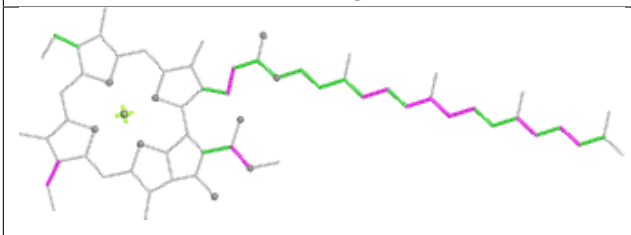


Bond angles



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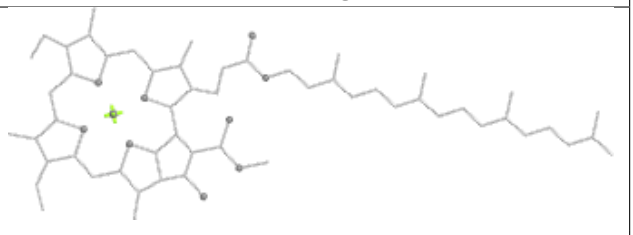
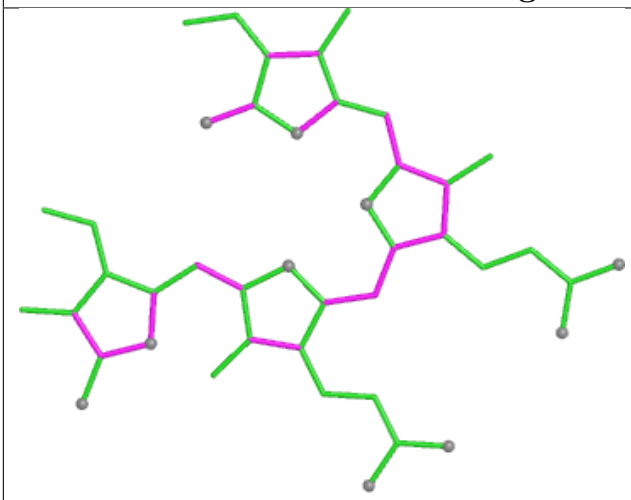


Rings

Ligand PEB h1 202



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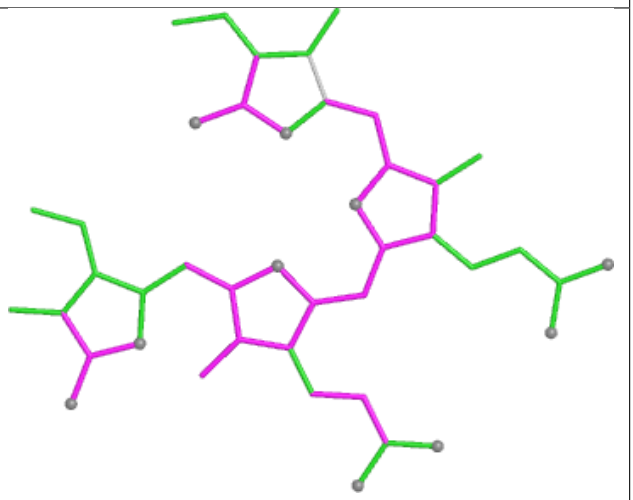
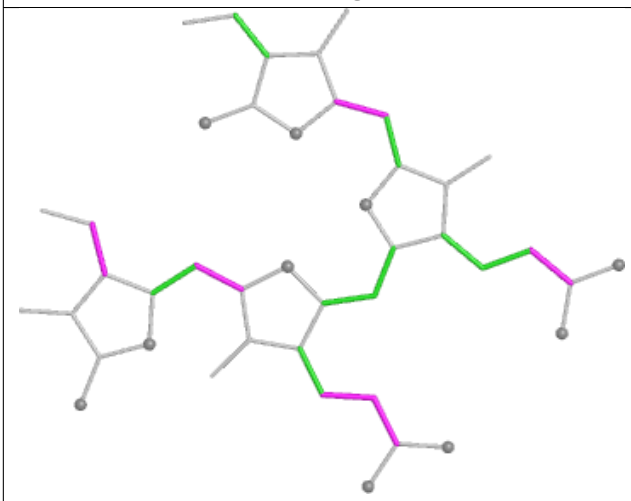


Bond angles



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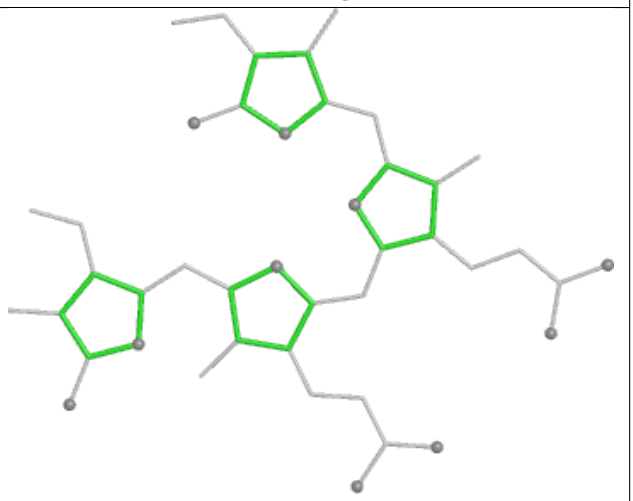
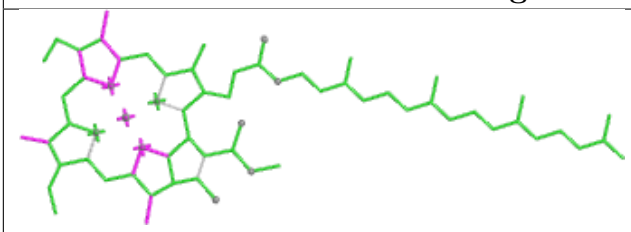


Rings

Ligand CLA AN 841



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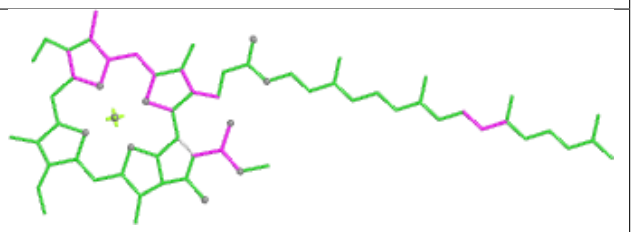
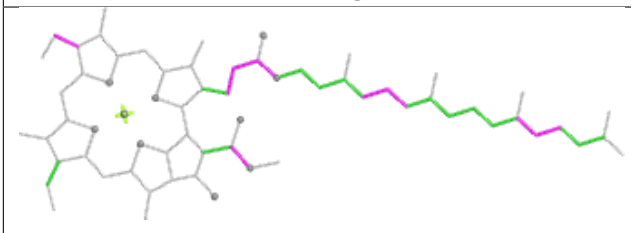


Bond angles



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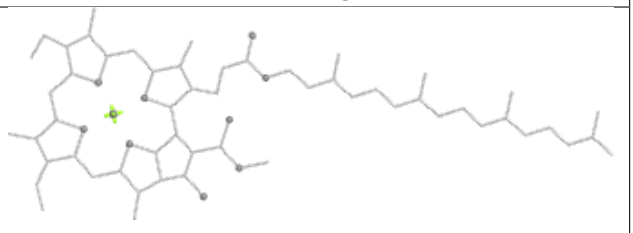
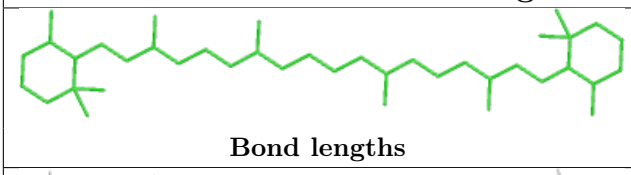


Rings

Ligand BCR cL 518



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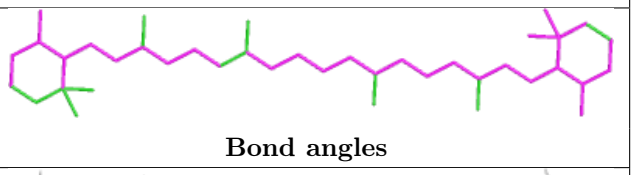
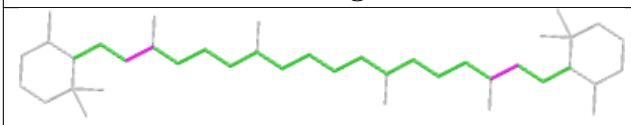


Bond angles



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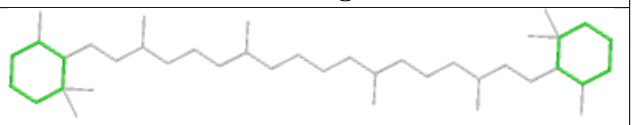
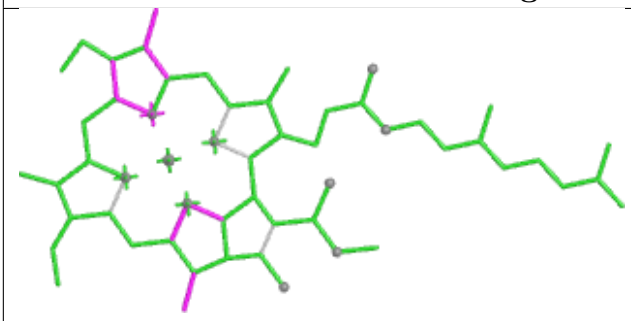


Rings

Ligand CLA c6 615



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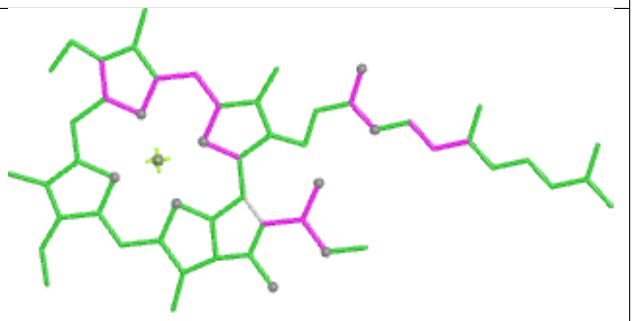
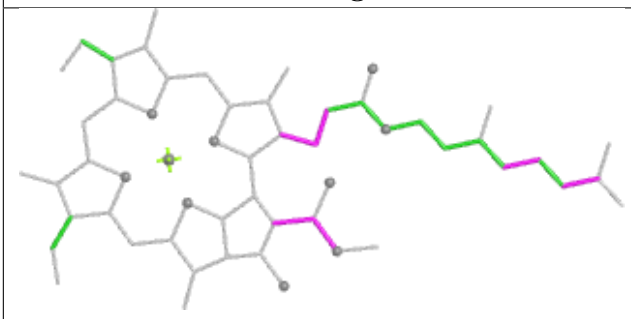


Bond angles



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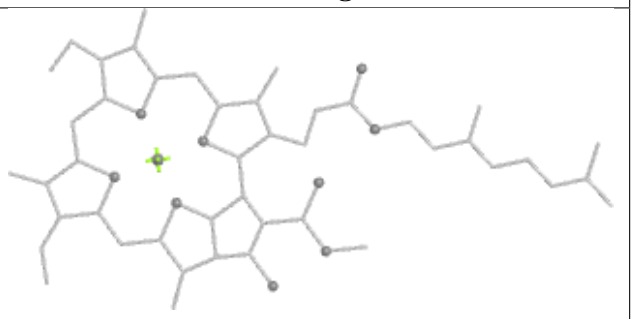
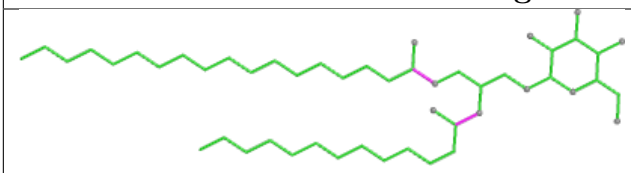


Rings

Ligand LMG x6 601



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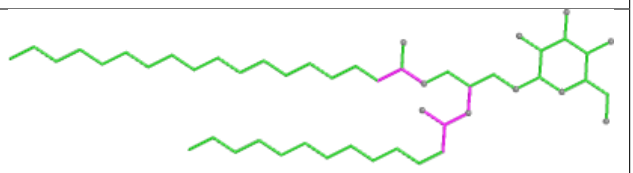
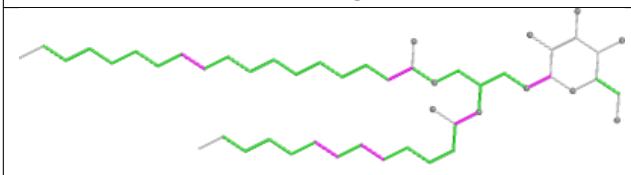


Bond angles



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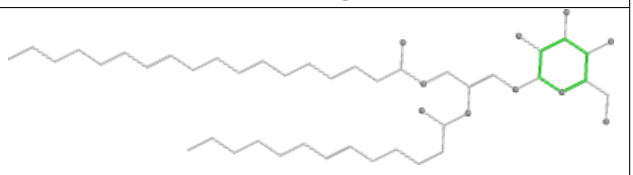
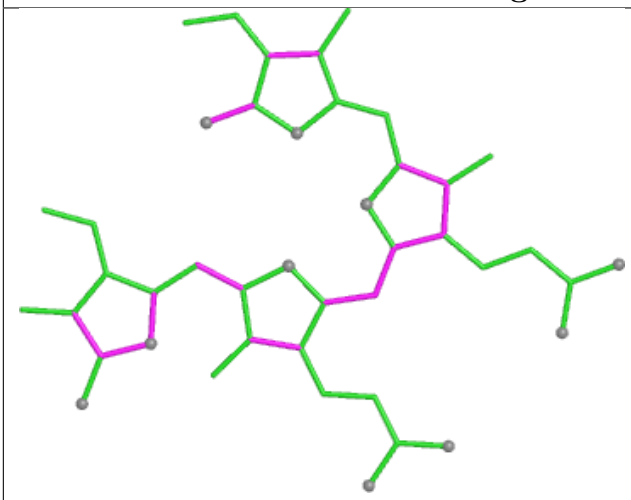


Rings

Ligand PEB W9 203



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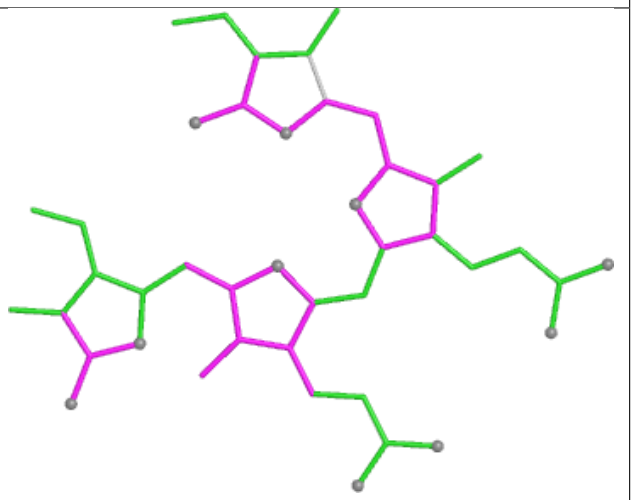

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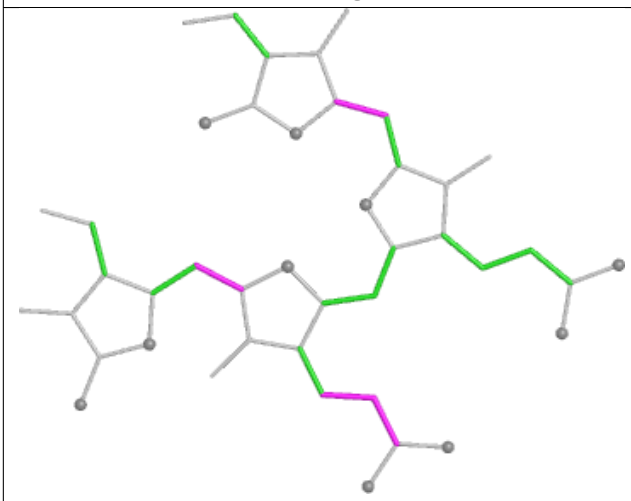
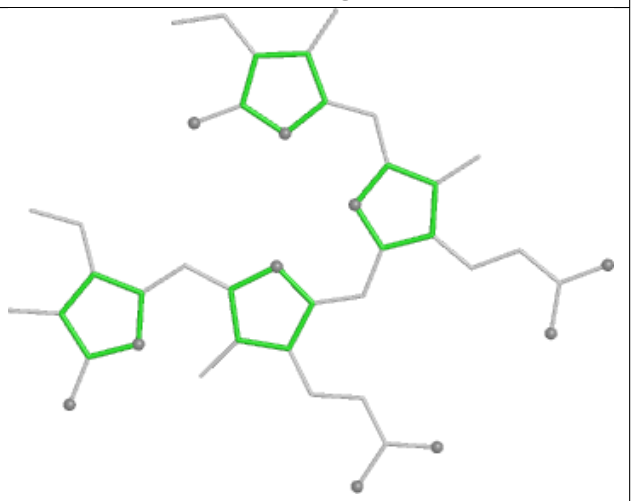
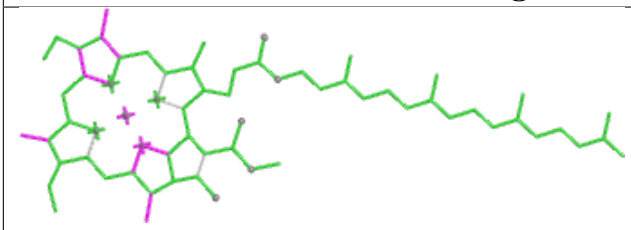


Torsions



Rings

Ligand CLA BN 825



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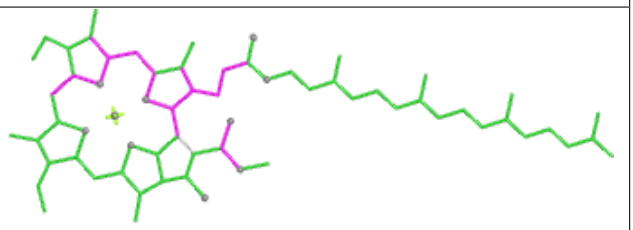

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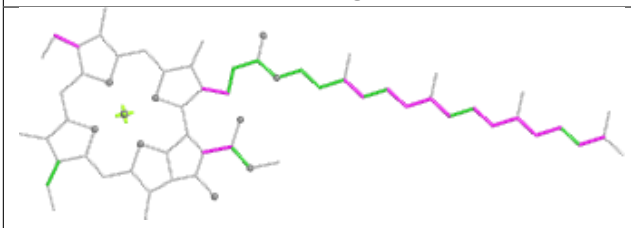

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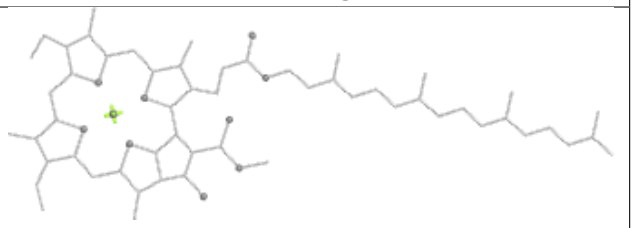

Rings

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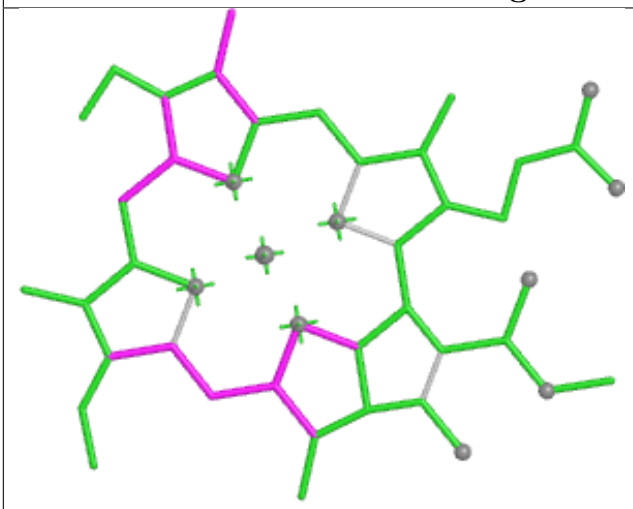

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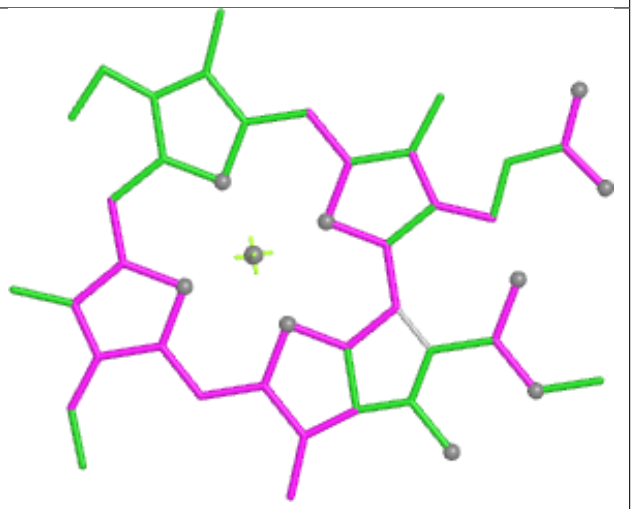

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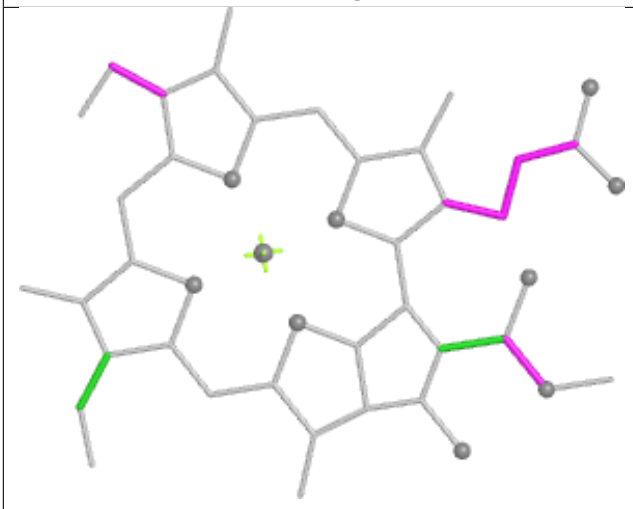
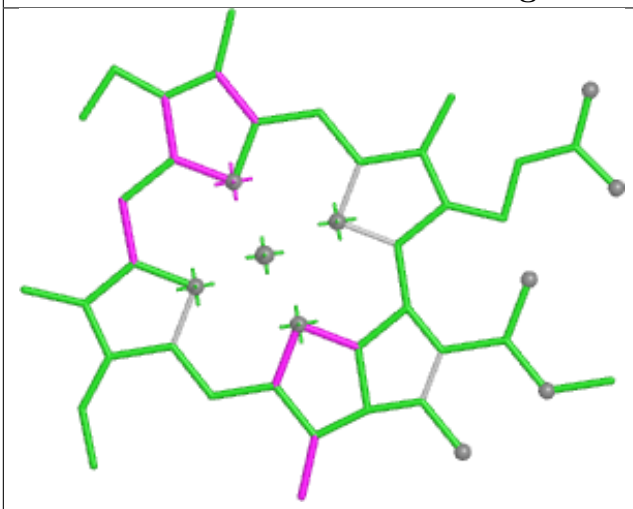


Torsions



Rings

Ligand CLA 62 306



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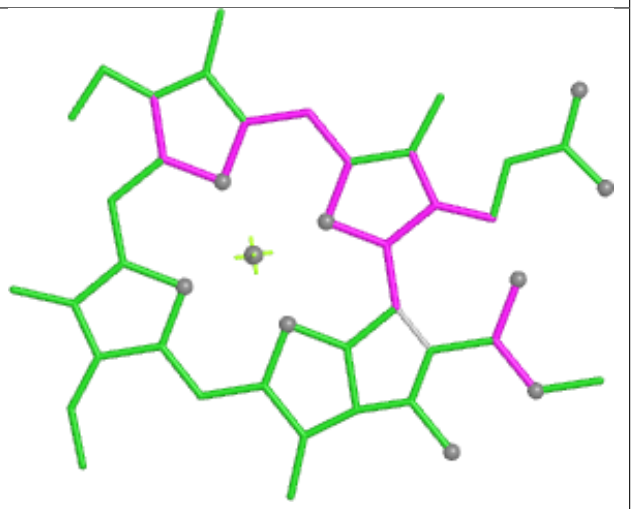

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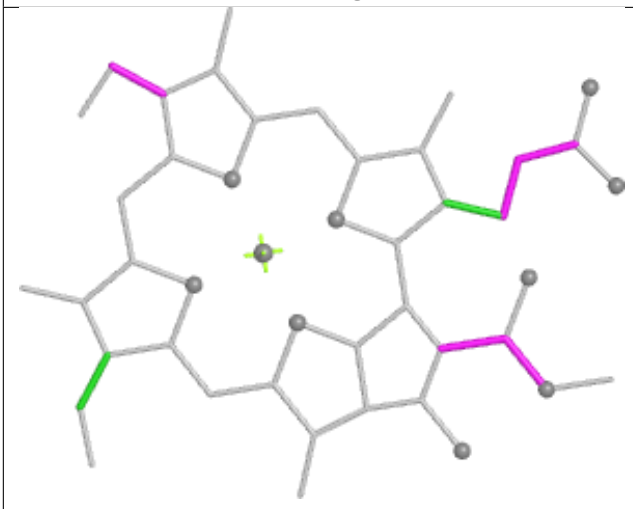
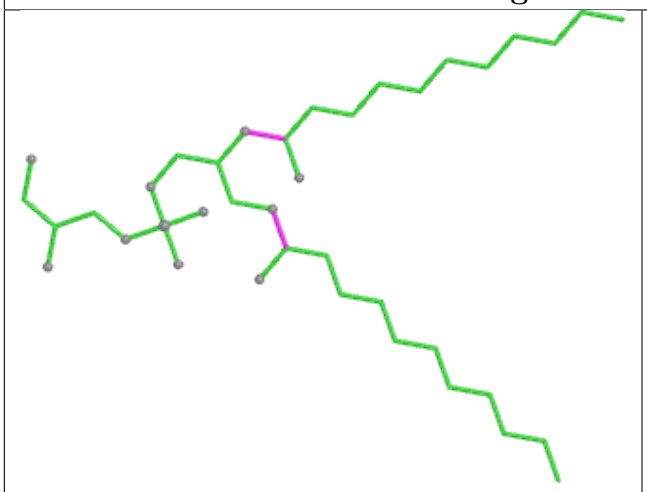


Torsions



Rings

Ligand LHG M6 101



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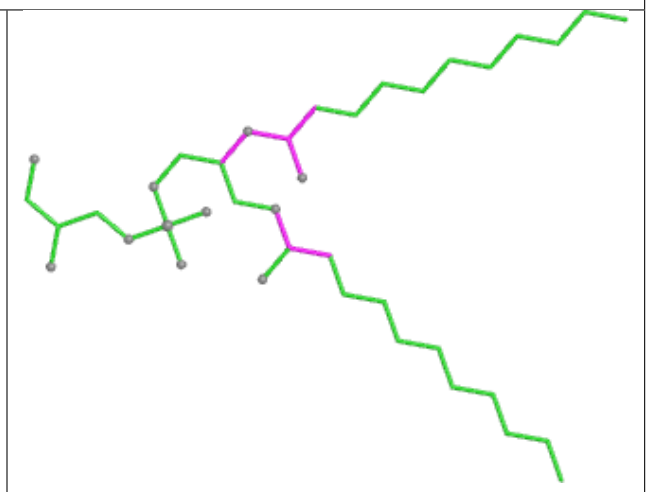

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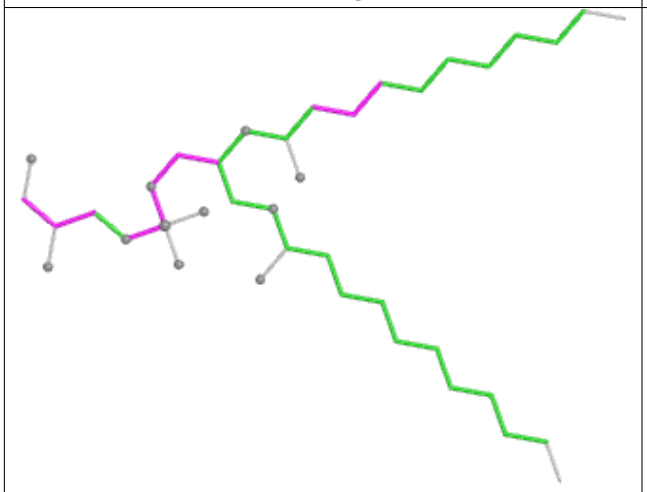

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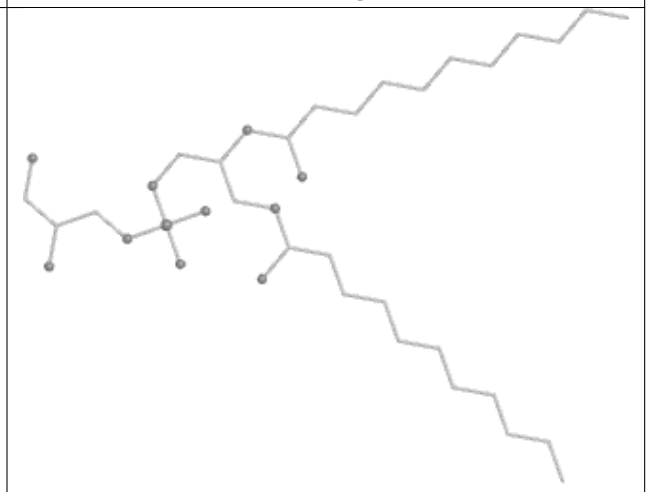
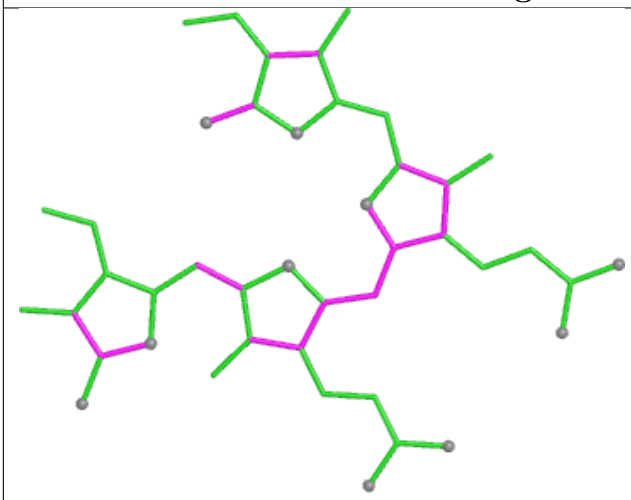


Rings

Ligand PEB pC 202



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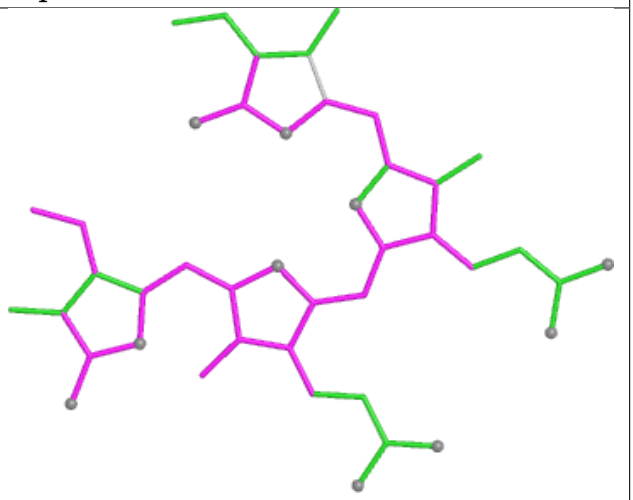

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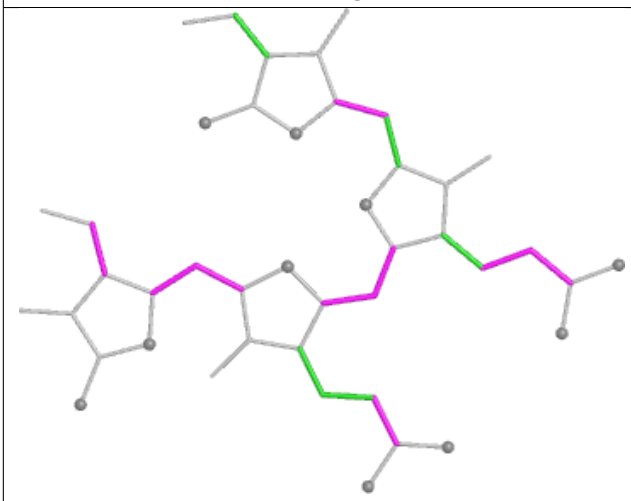

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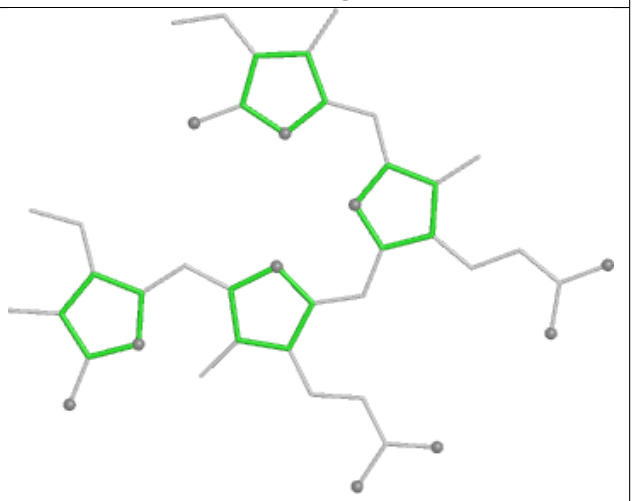
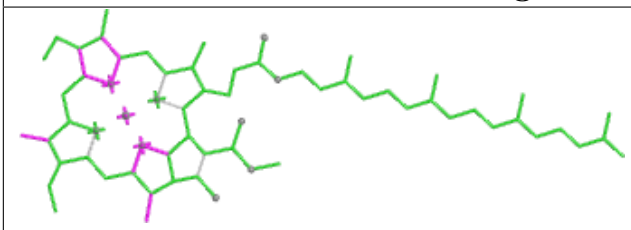


Rings

Ligand CLA BL 603



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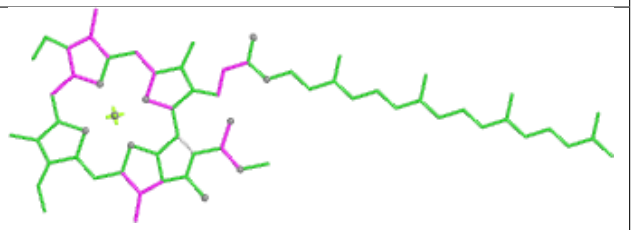

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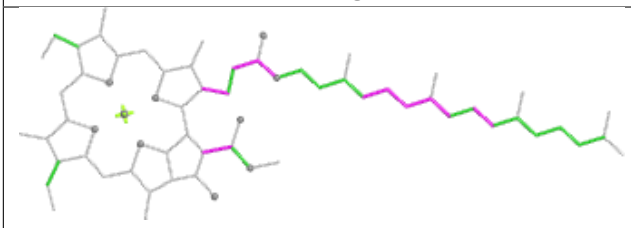

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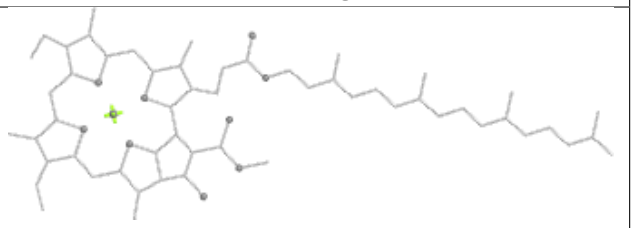
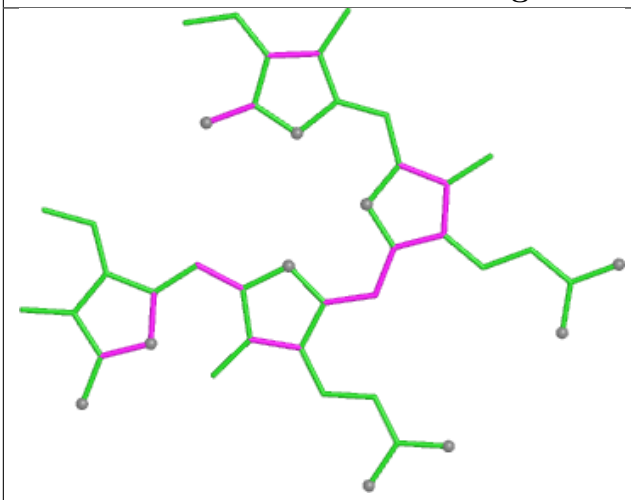


Rings

Ligand PEB BD 203



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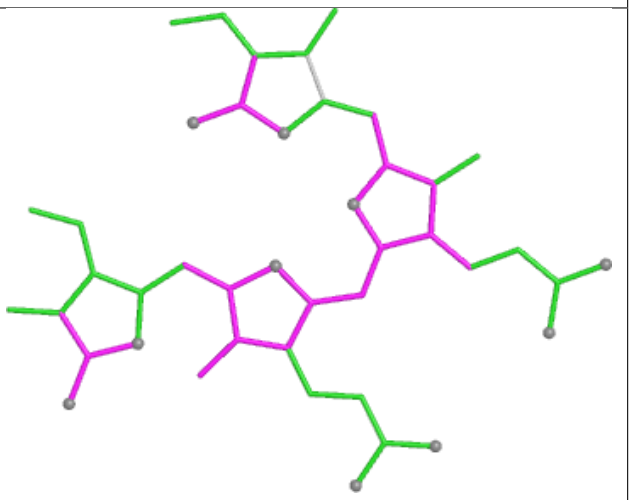

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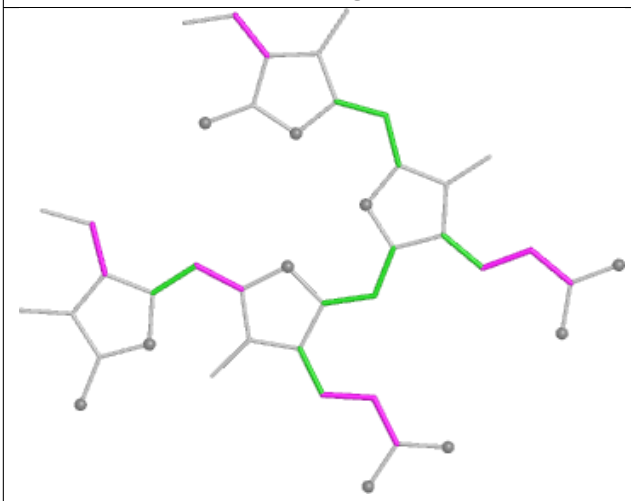

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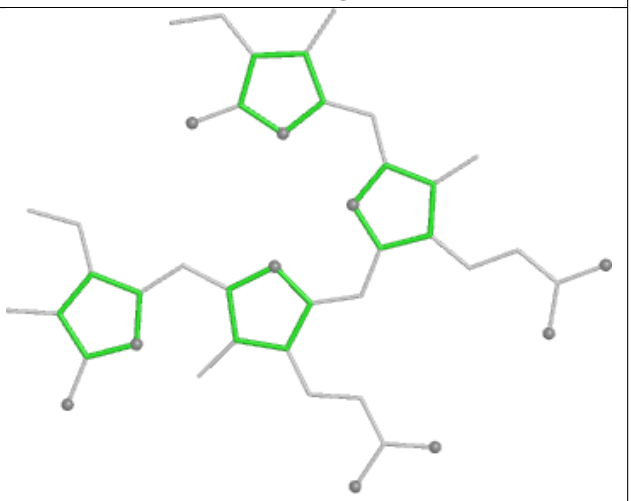
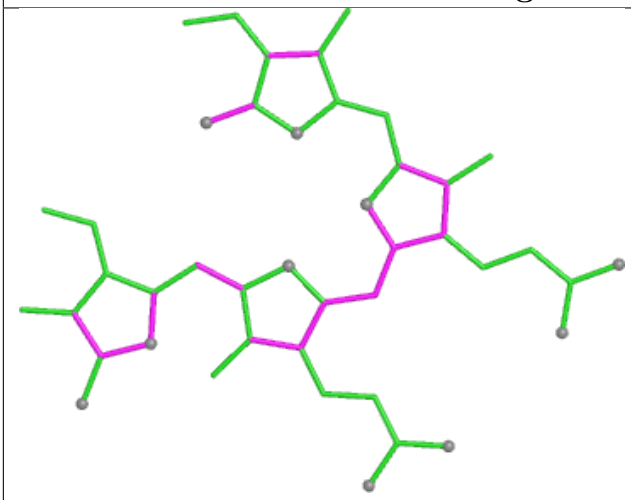


Rings

Ligand PEB B5 201



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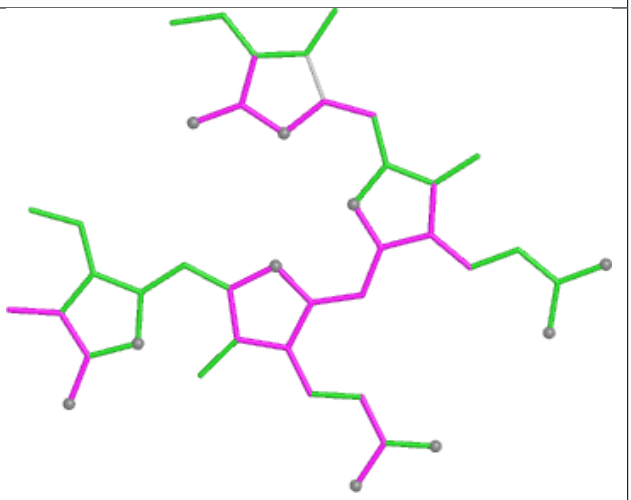

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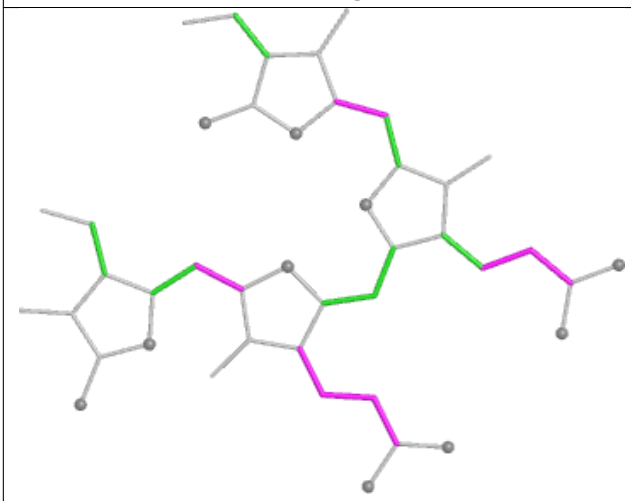

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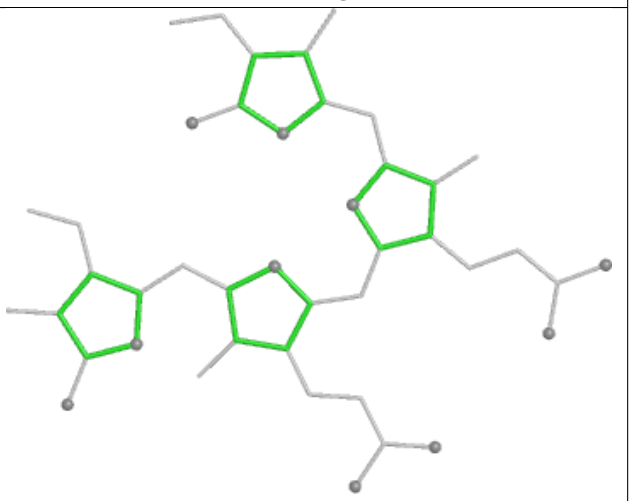
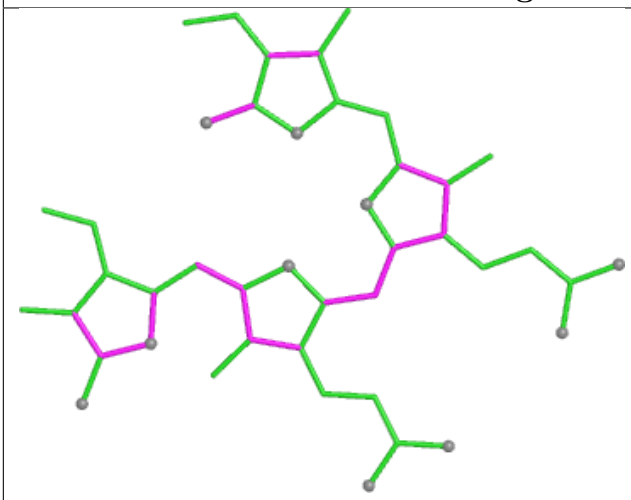


Rings

Ligand PEB B7 201



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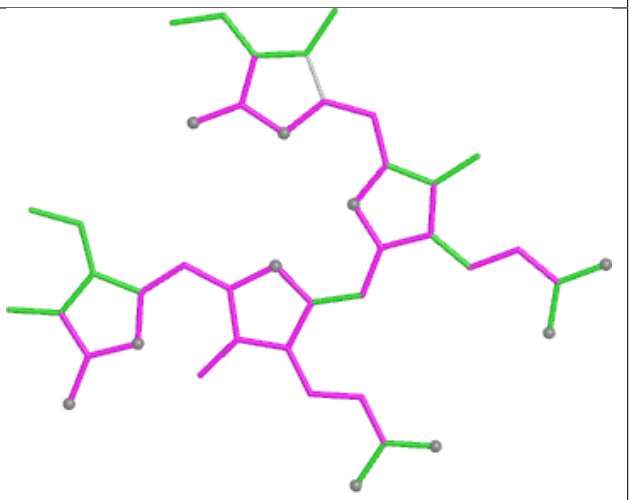

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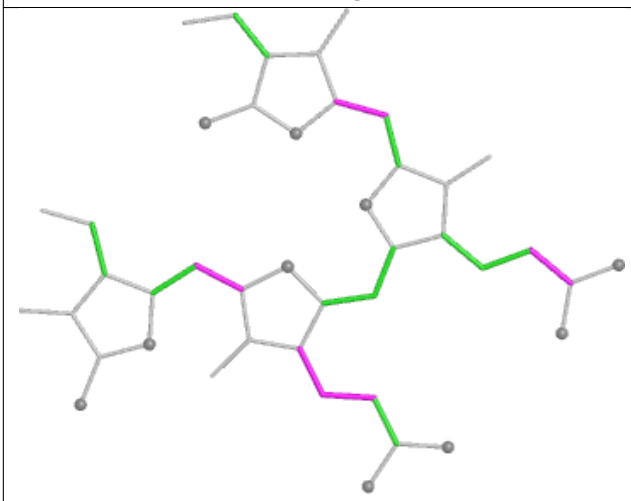

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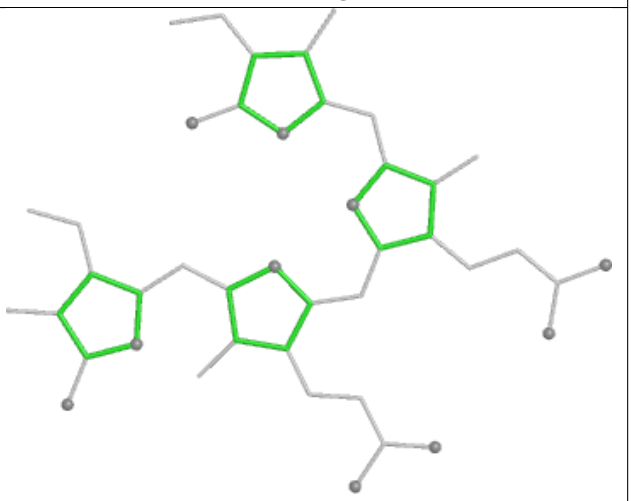
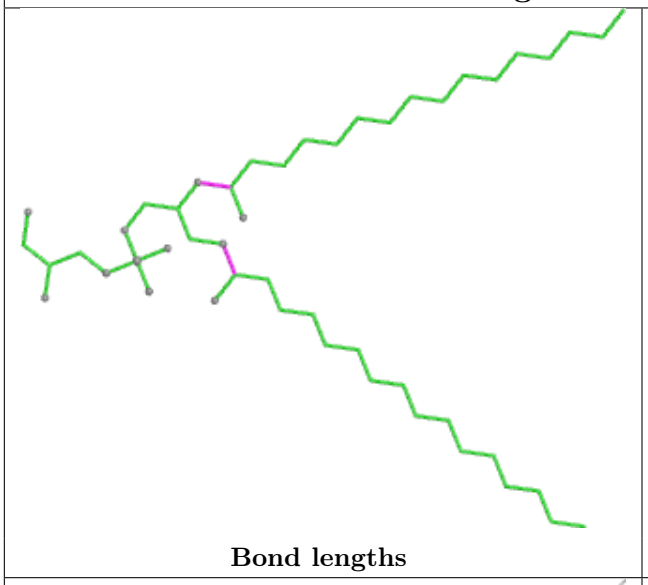


Rings

Ligand LHG A2 843



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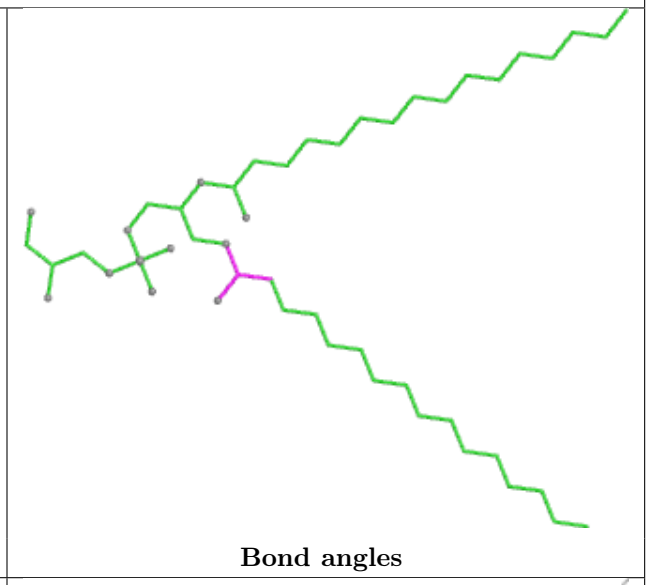

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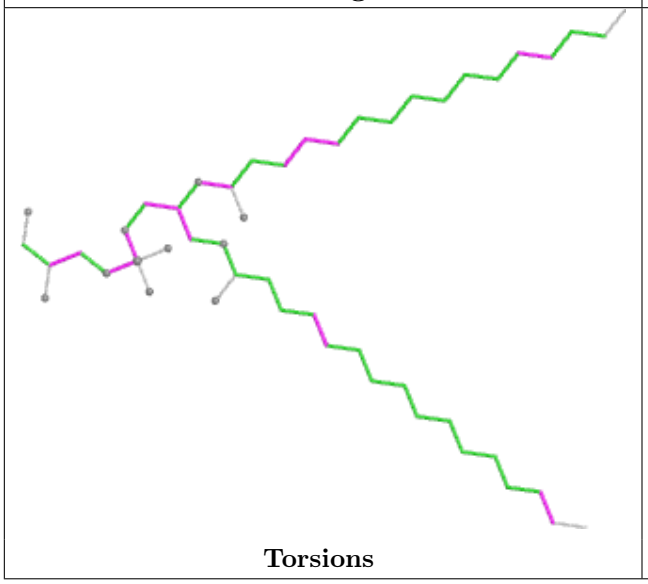

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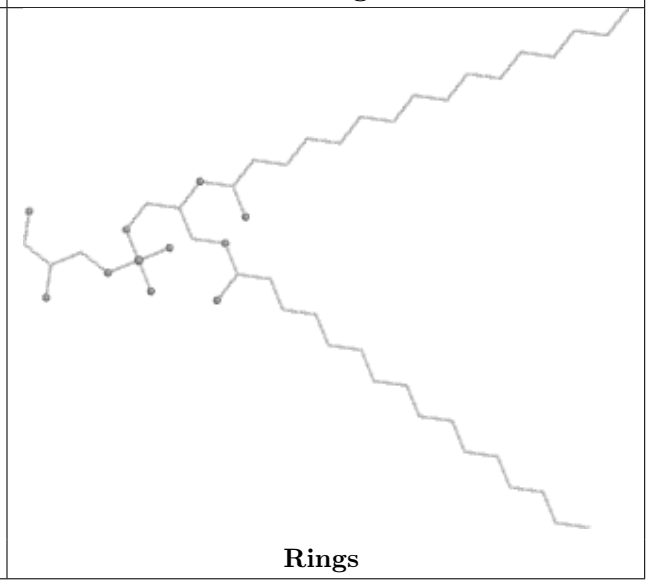
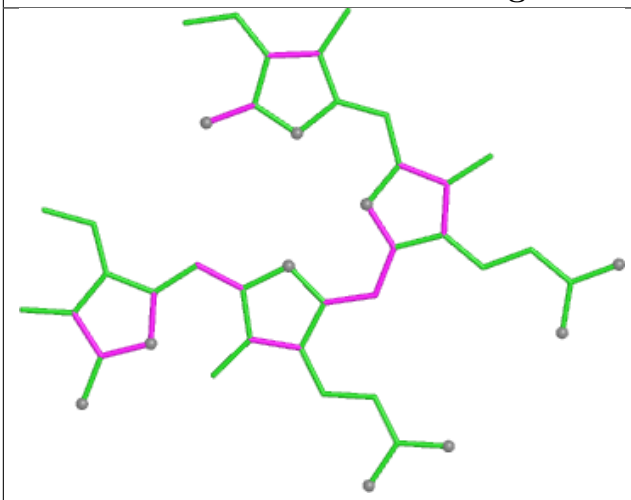


Rings

Ligand PEB MP 201



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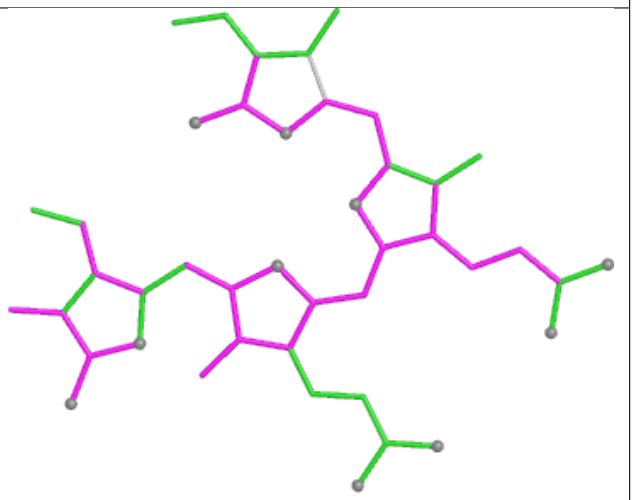

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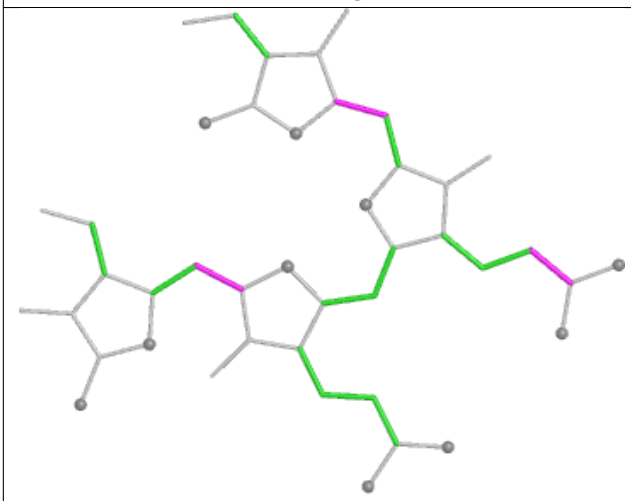

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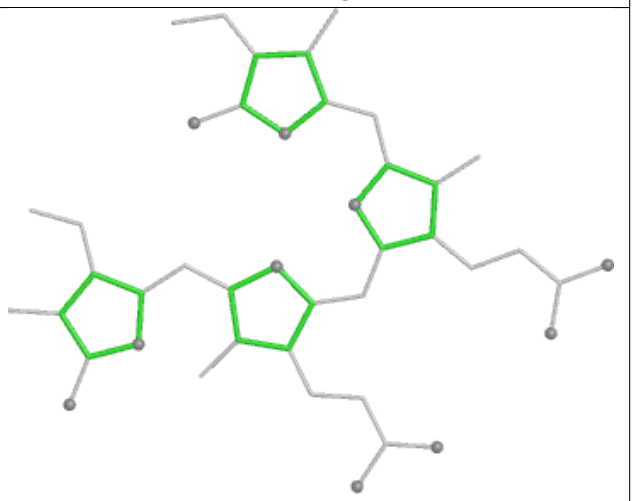
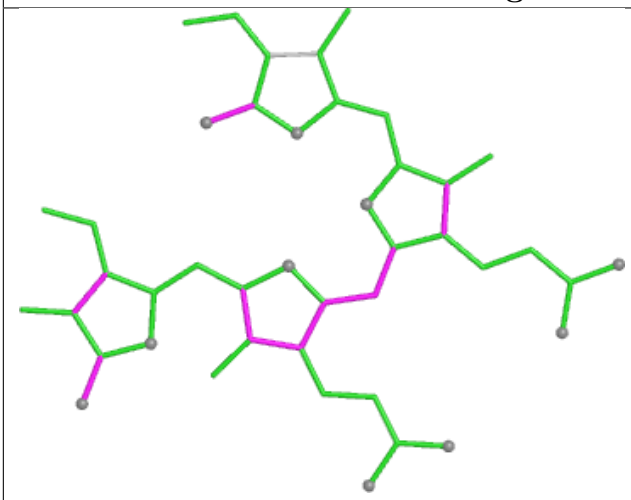


Rings

Ligand PUB BM 302



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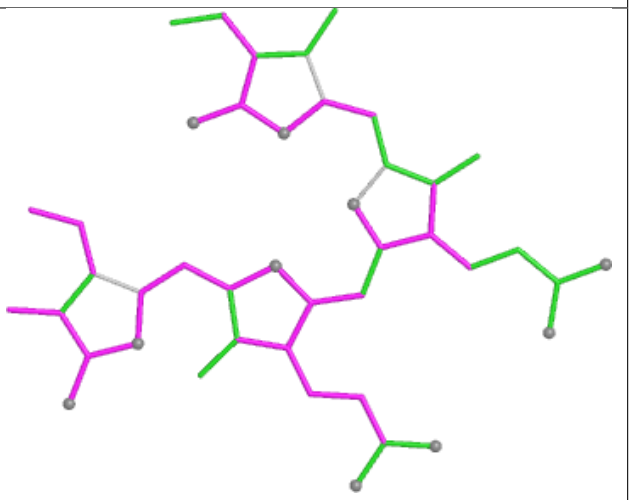
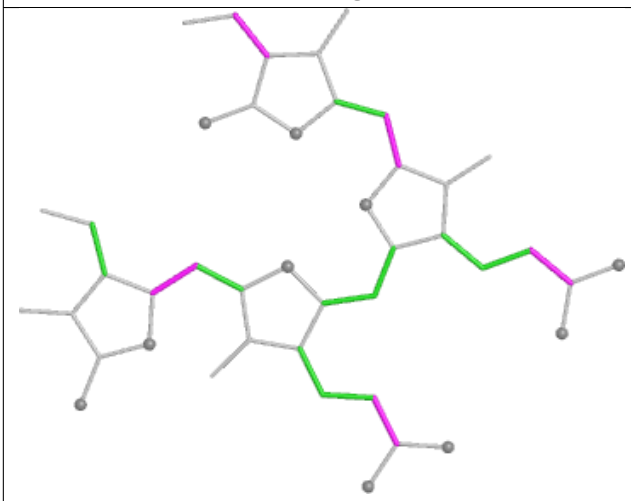


Bond angles



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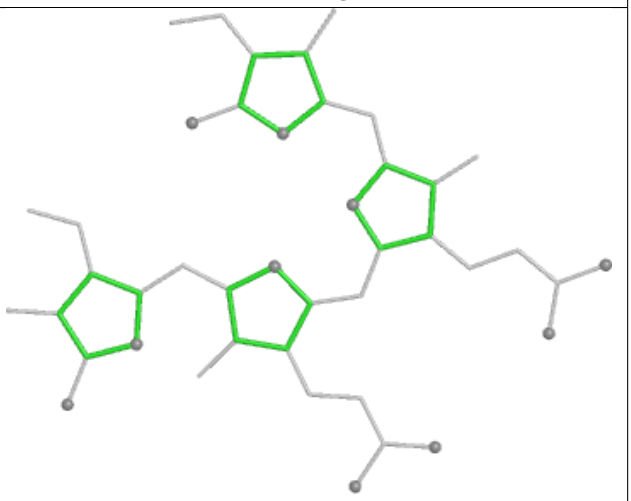
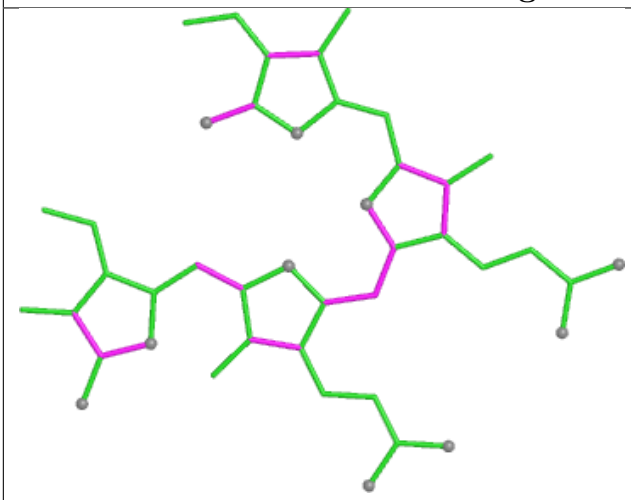


Rings

Ligand PEB IP 202



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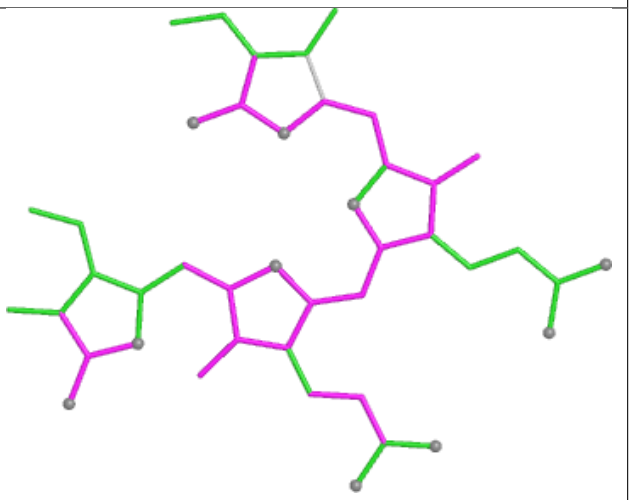
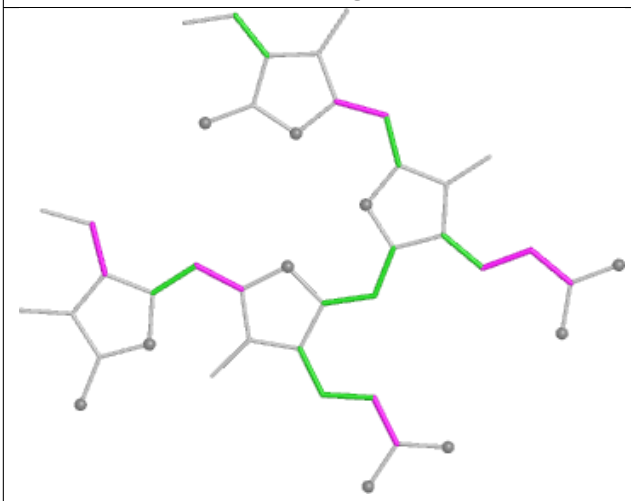


Bond angles



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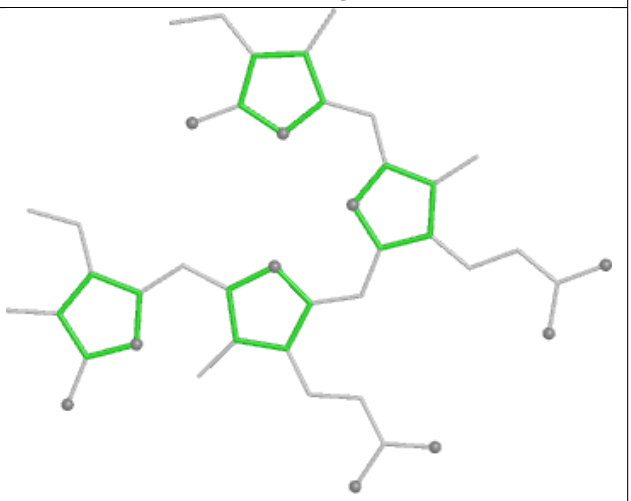
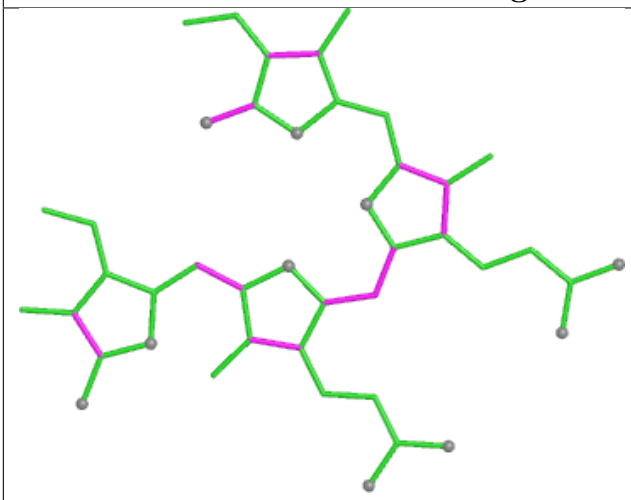


Rings

Ligand PEB RK 201



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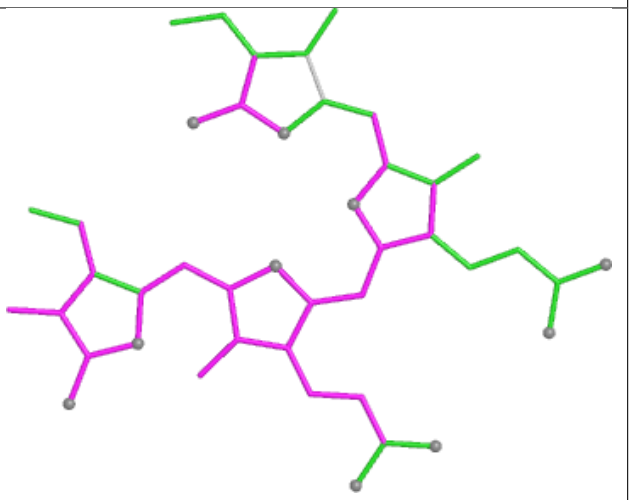
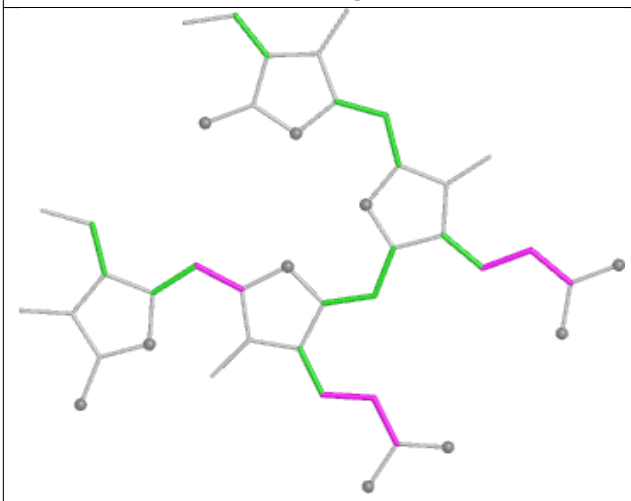


Bond angles



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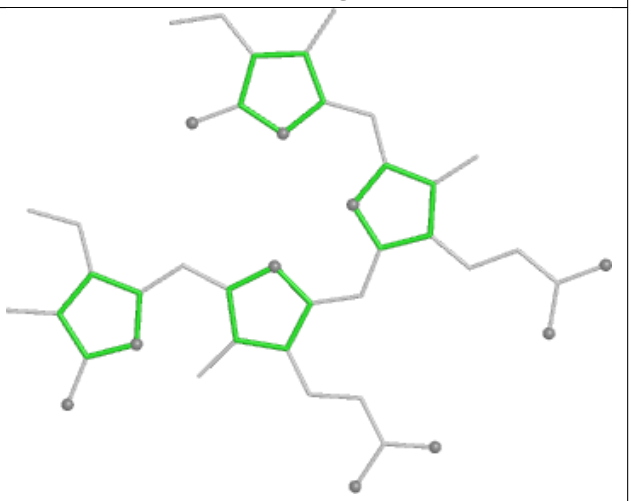
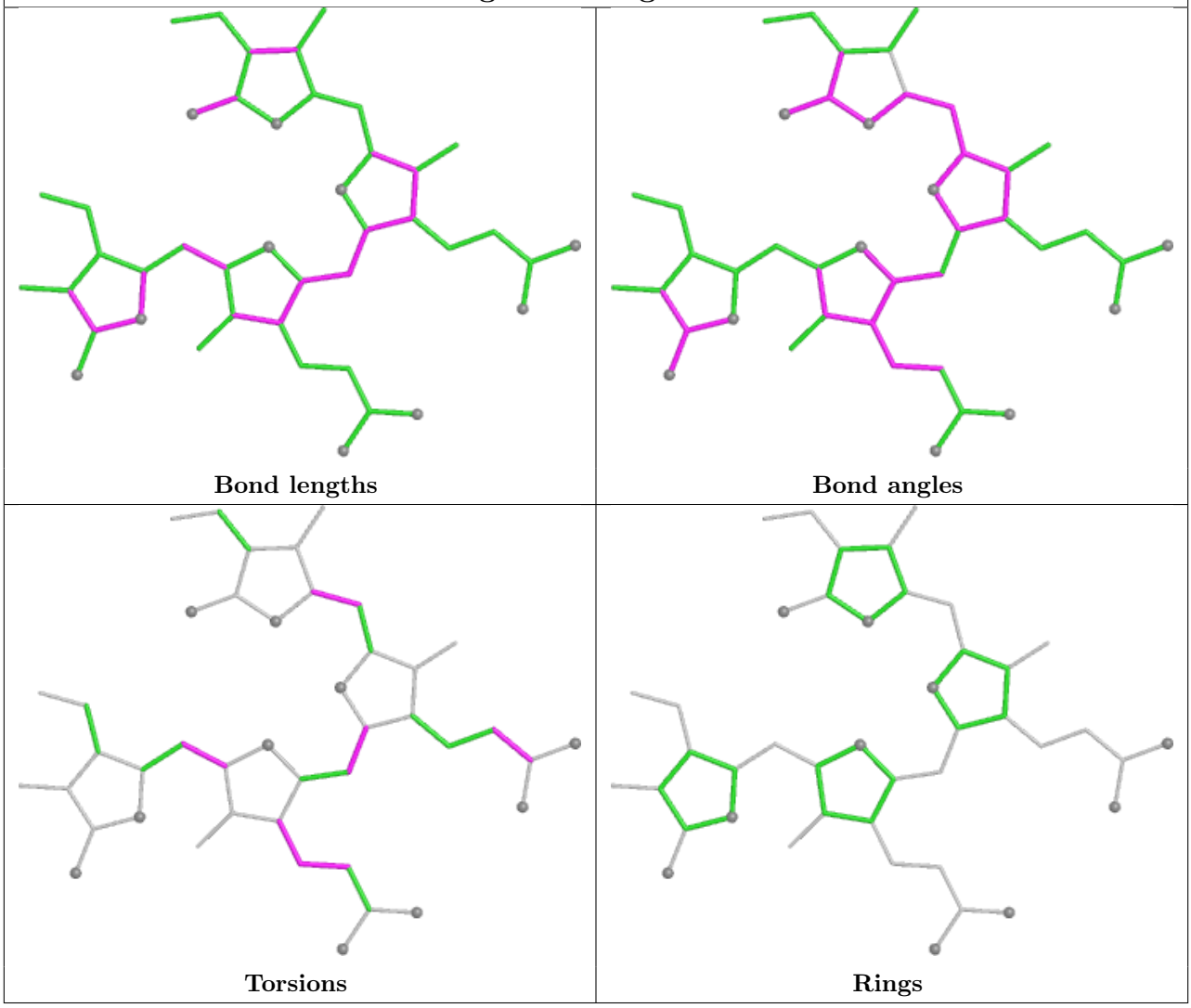
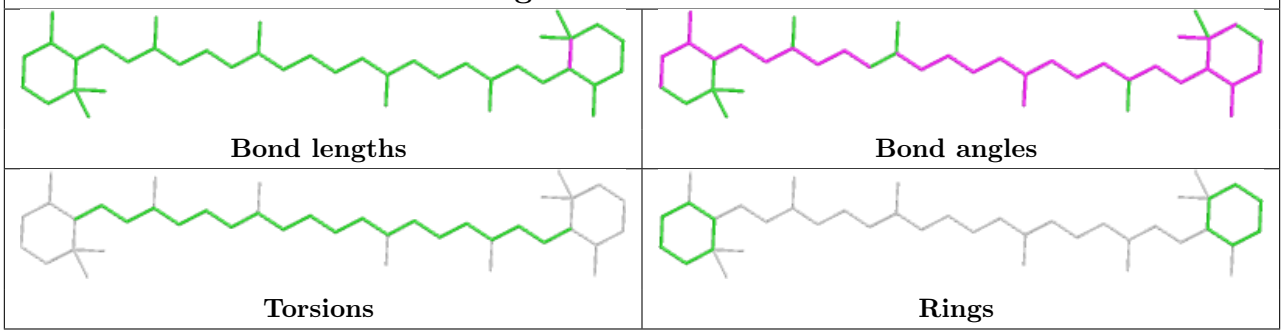


Rings

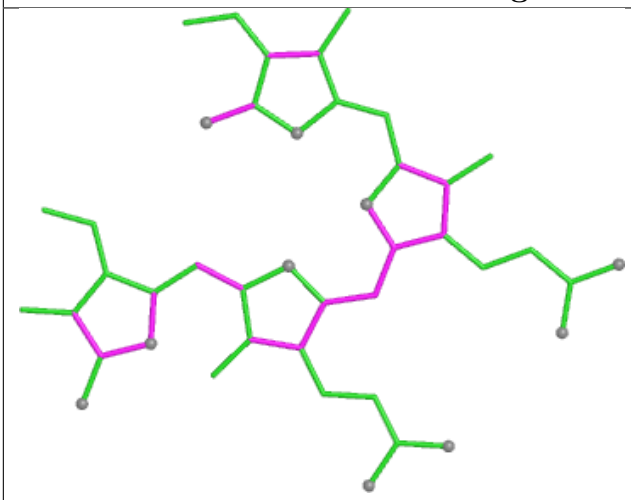
Ligand PEB gO 203



Ligand BCR B6 601



Ligand PEB YQ 201



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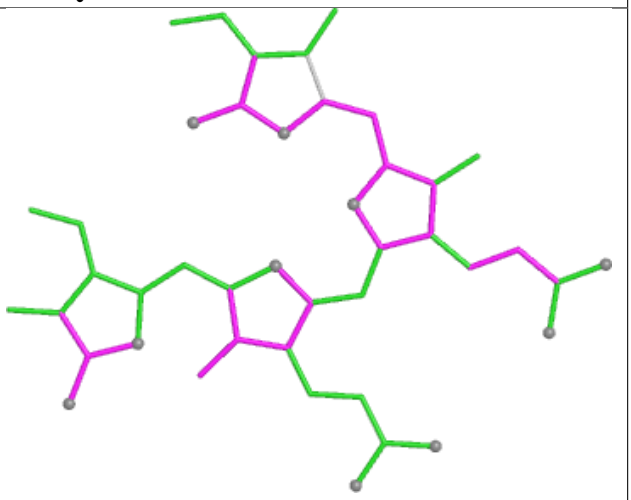
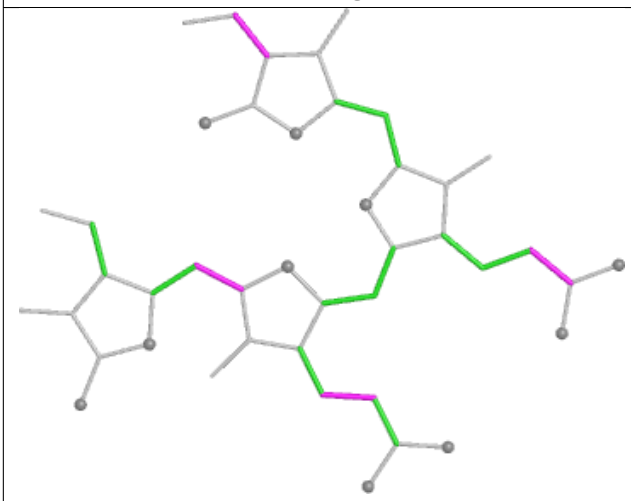
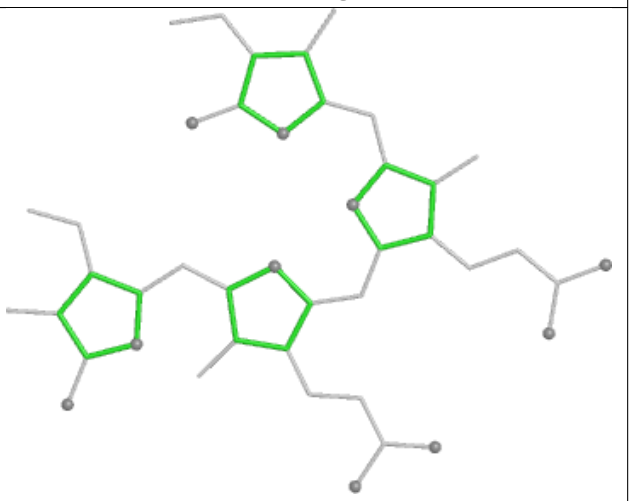


Bond angles

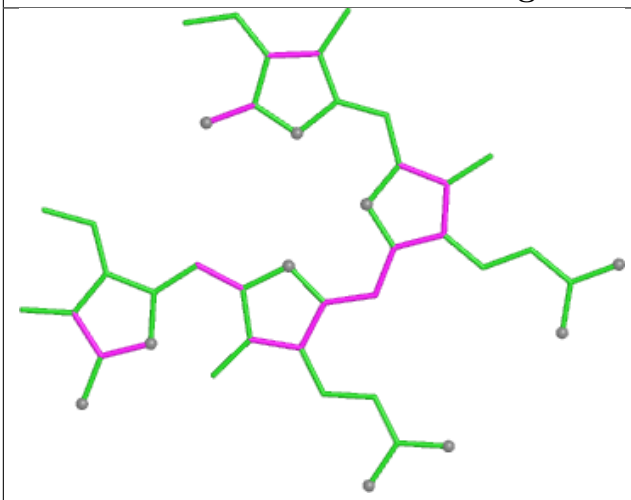


Torsions



Rings

Ligand PEB L7 202



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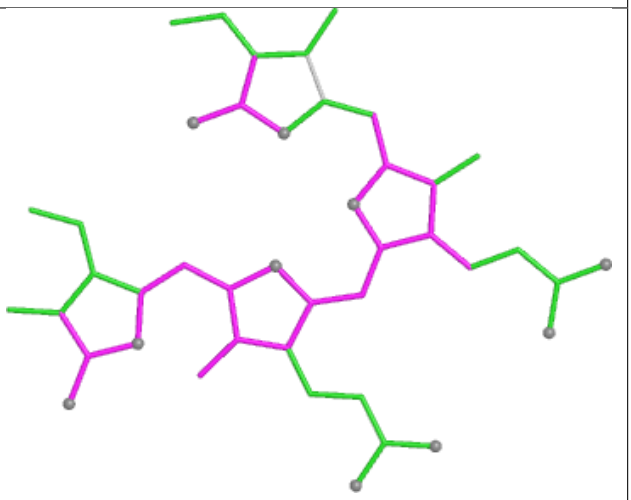

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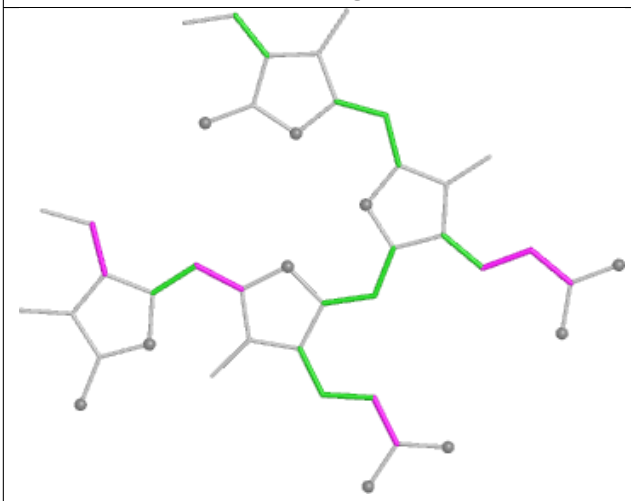

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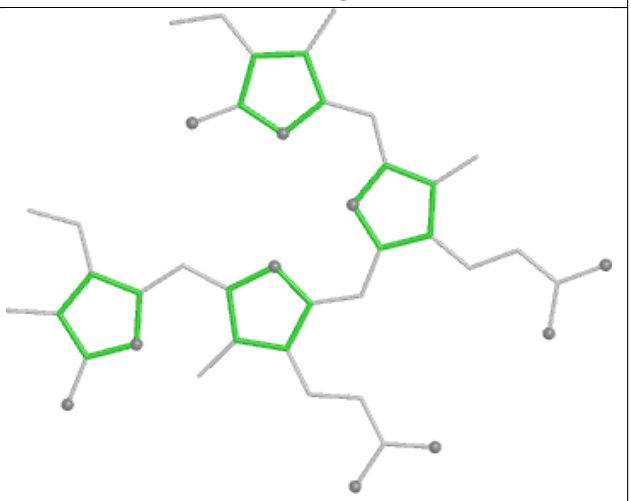
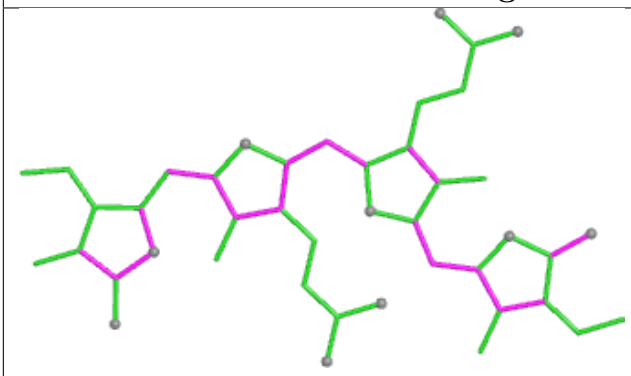


Rings

Ligand CYC DH 1003



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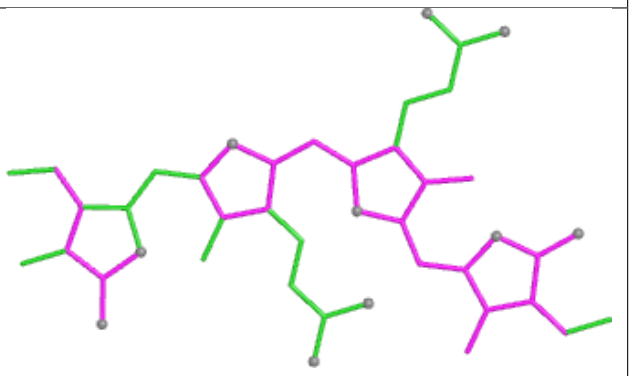

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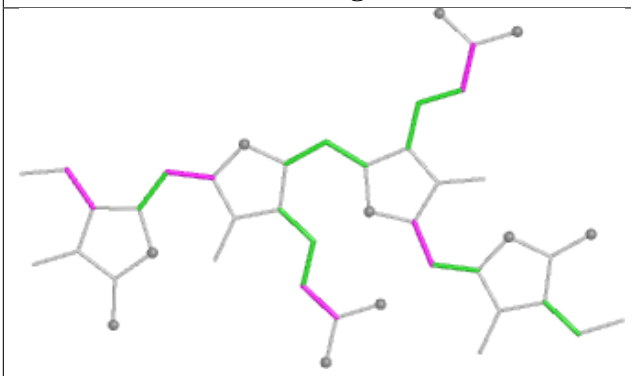

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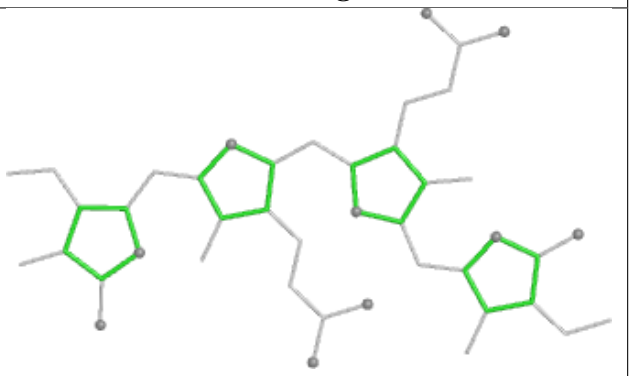
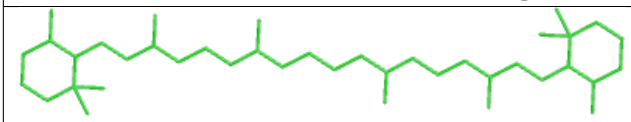


Rings

Ligand BCR L2 201



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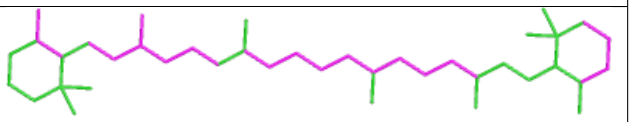

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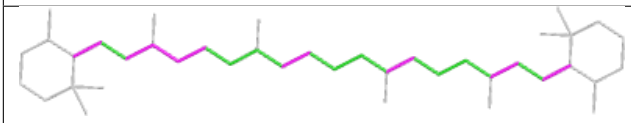

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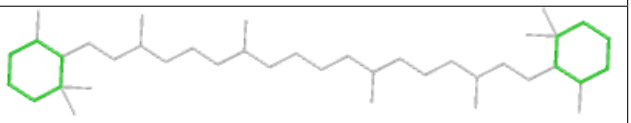
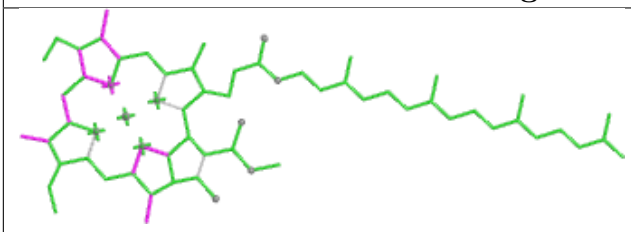


Rings

Ligand CLA c6 612



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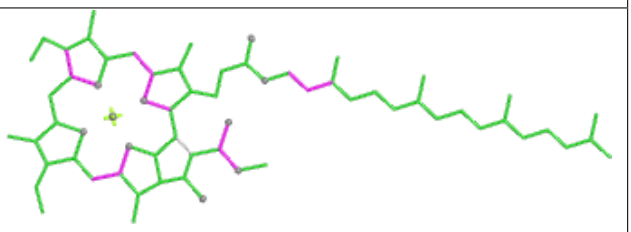

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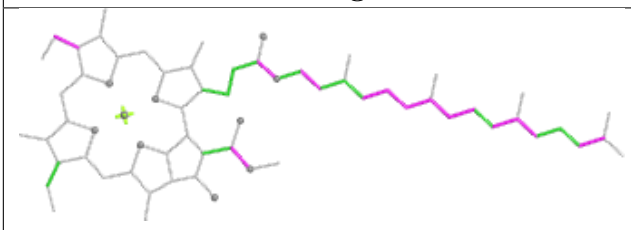

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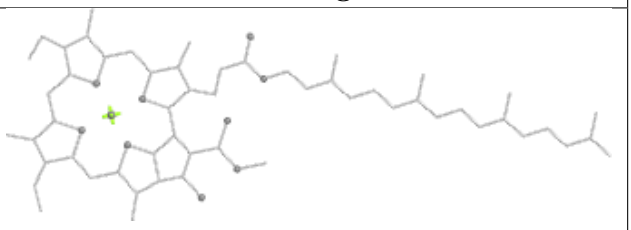
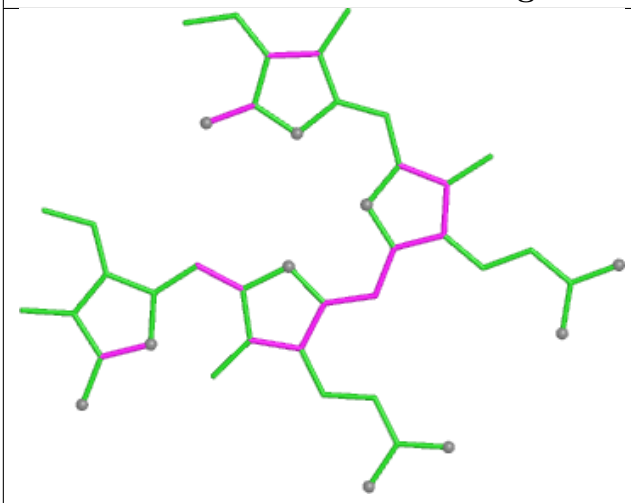


Rings

Ligand PEB F9 202



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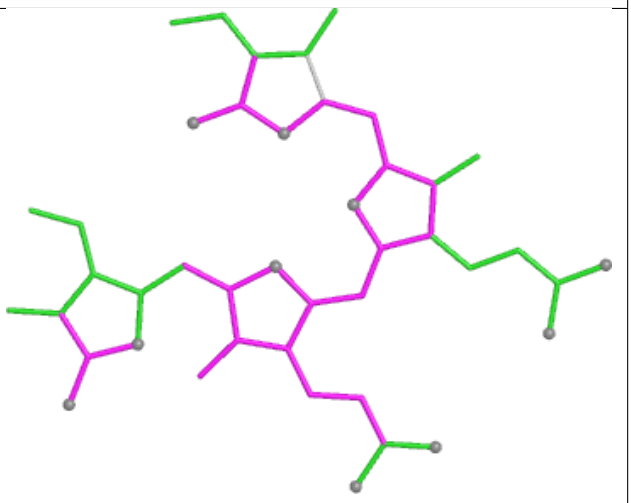

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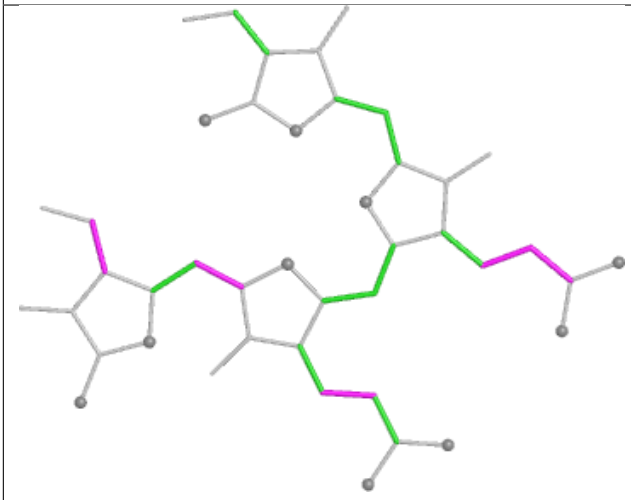

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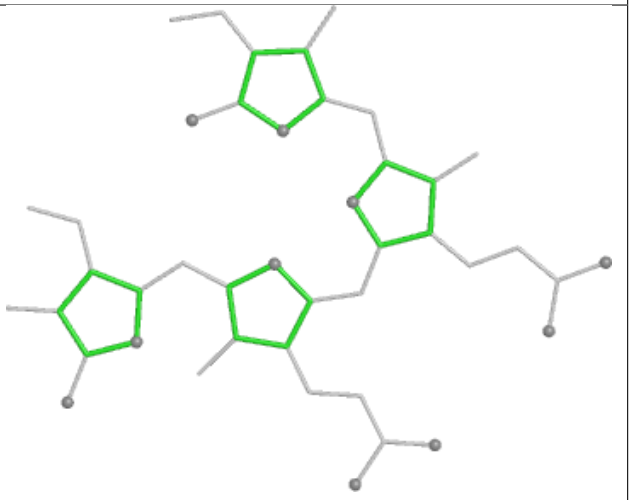
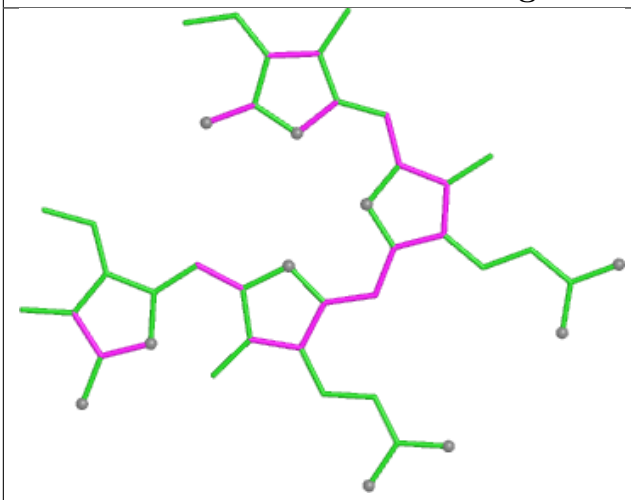


Rings

Ligand PEB lK 201



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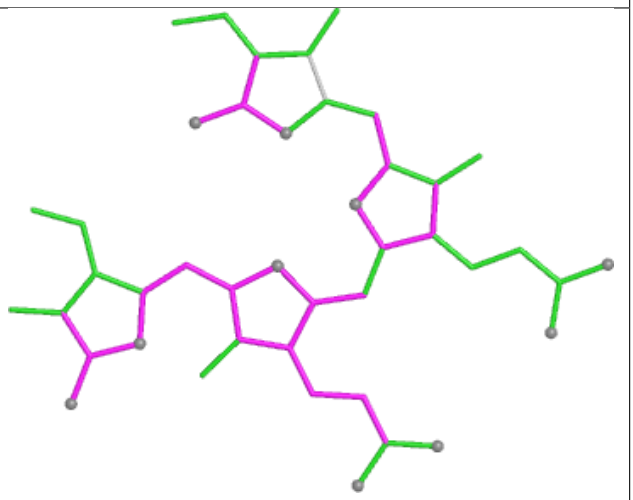
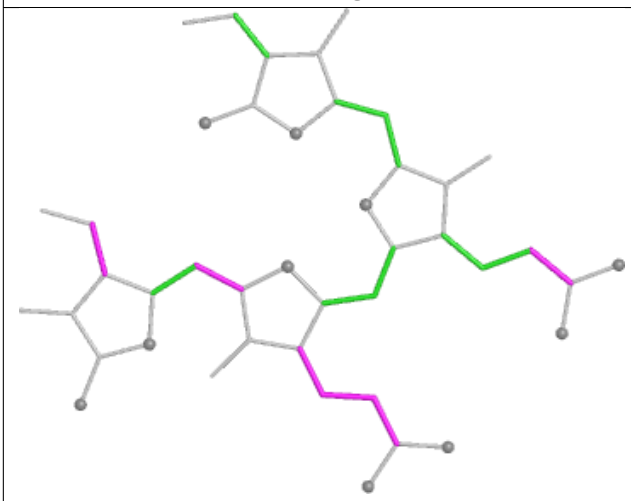


Bond angles



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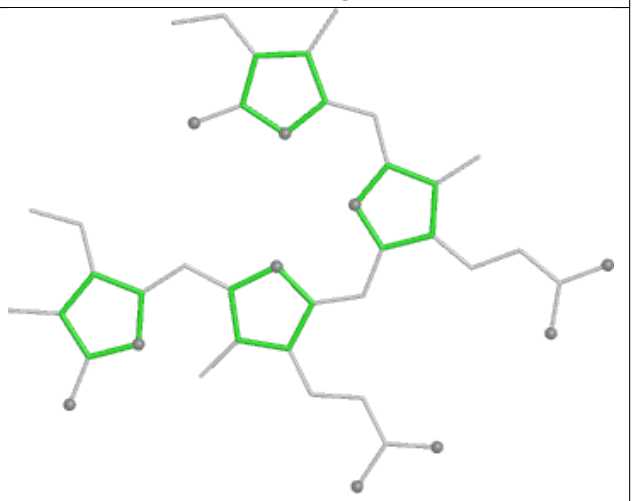
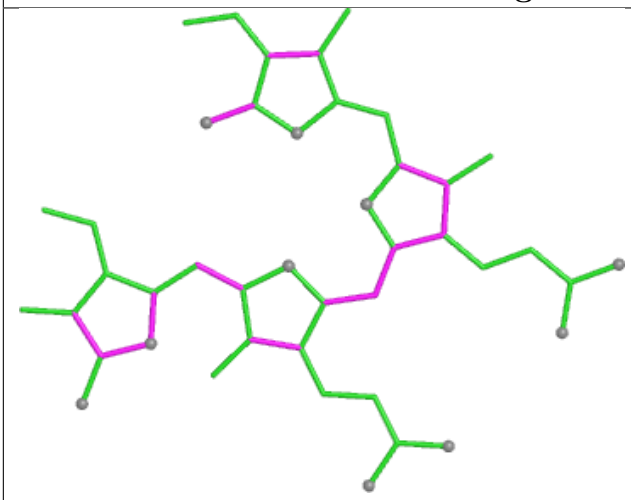


Rings

Ligand PEB AJ 301



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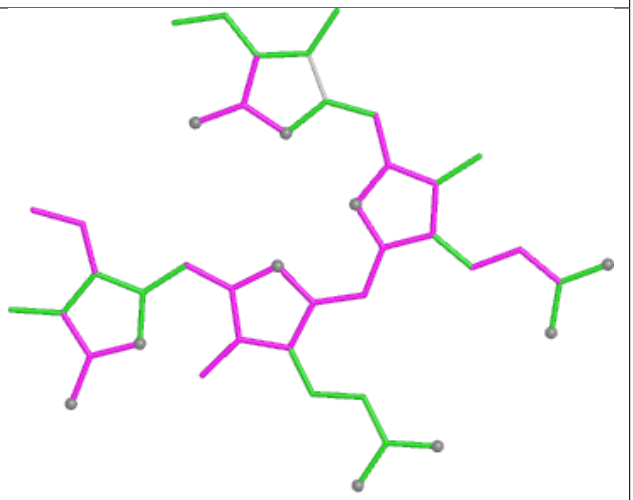

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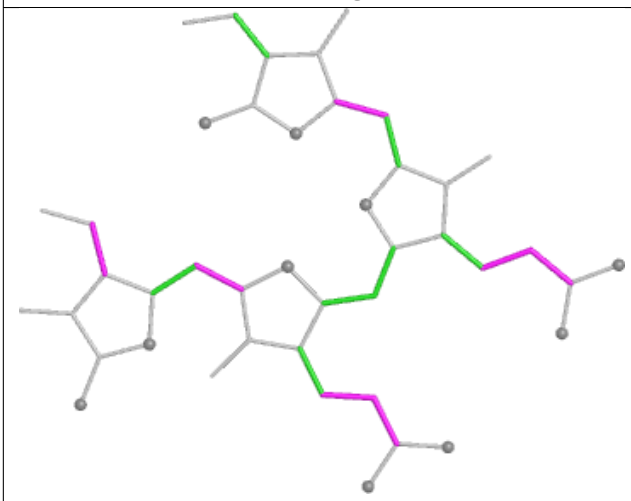

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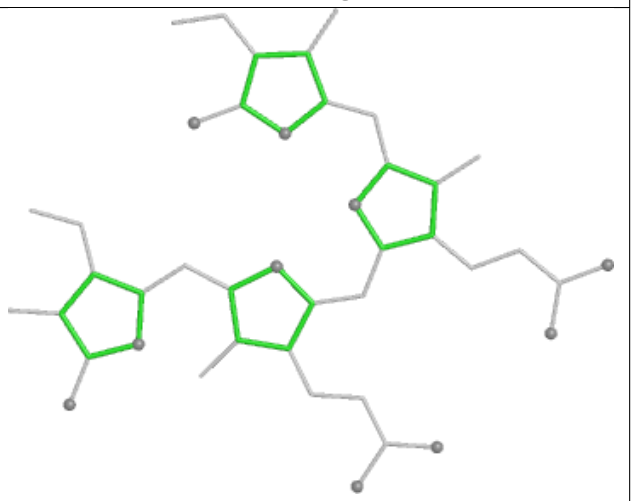
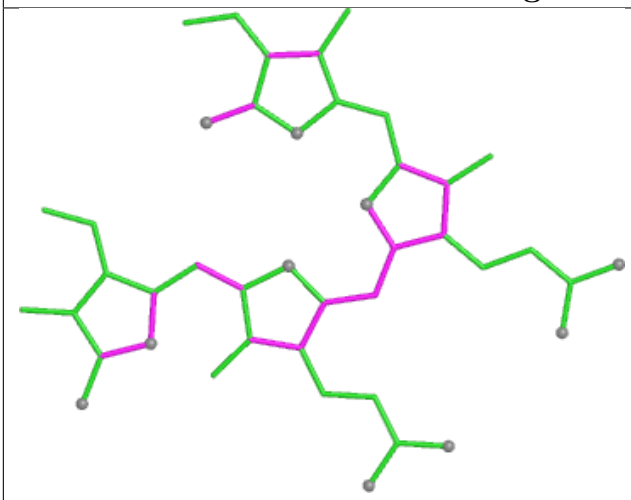


Rings

Ligand PEB lJ 203



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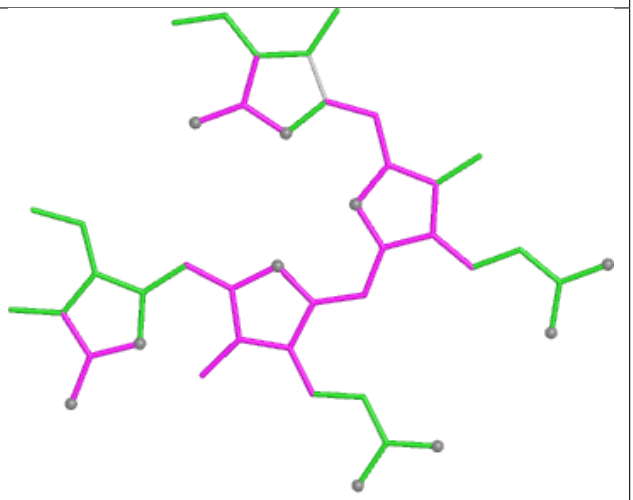

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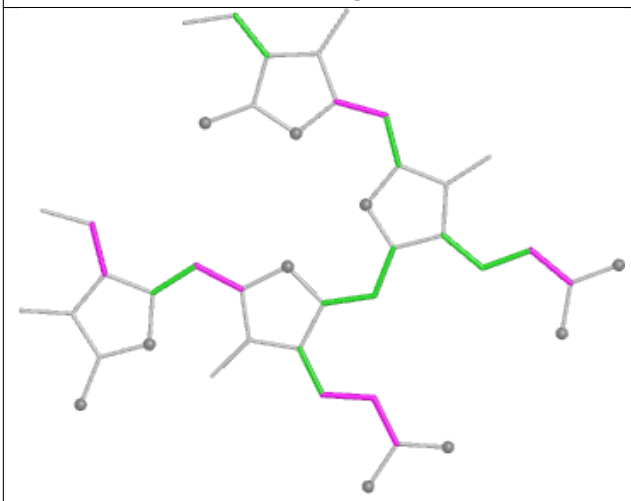

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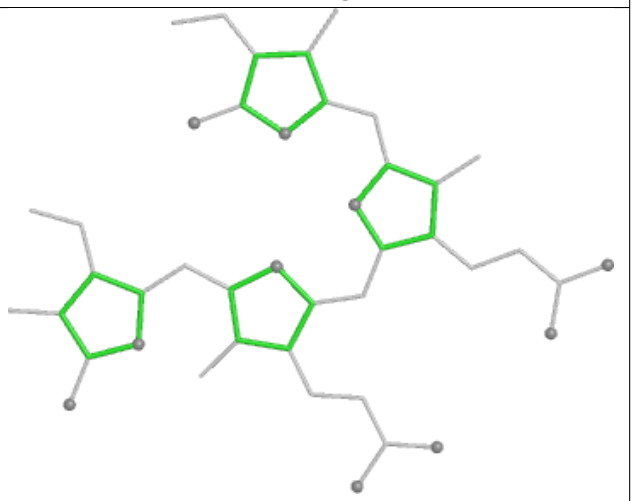
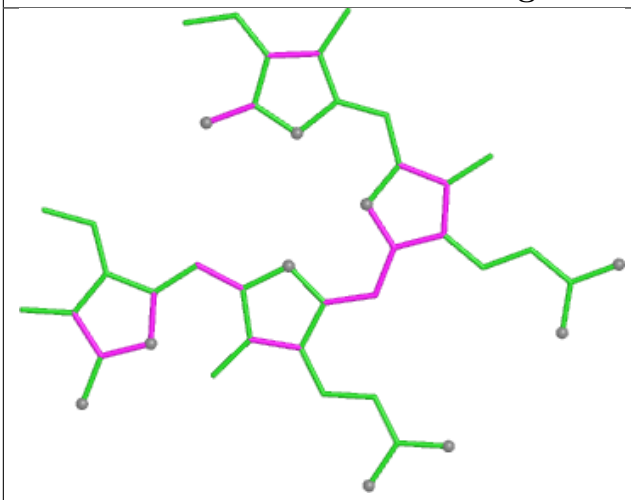


Rings

Ligand PEB fG 201



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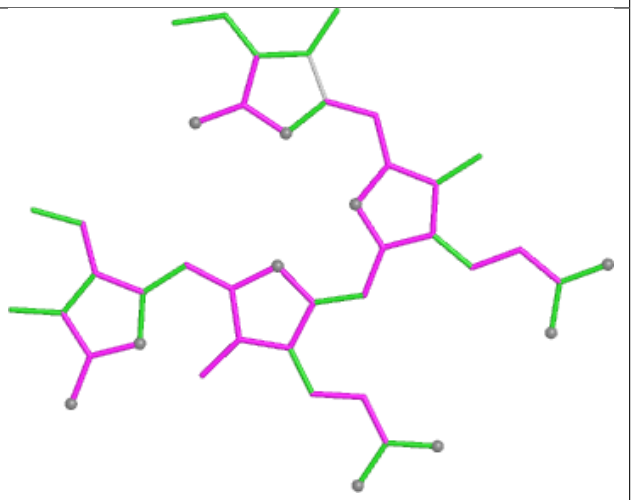
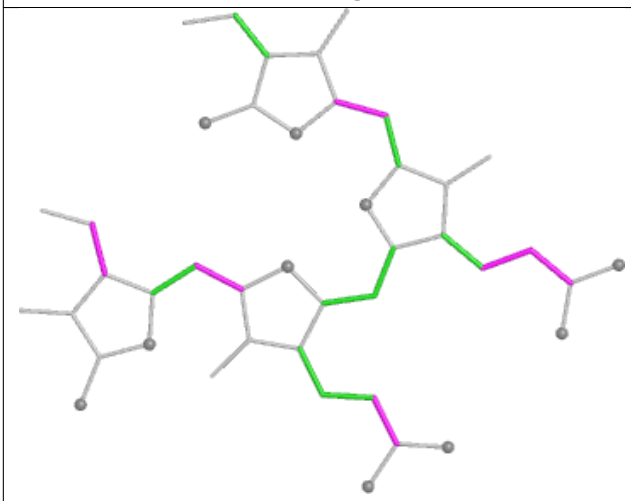


Bond angles



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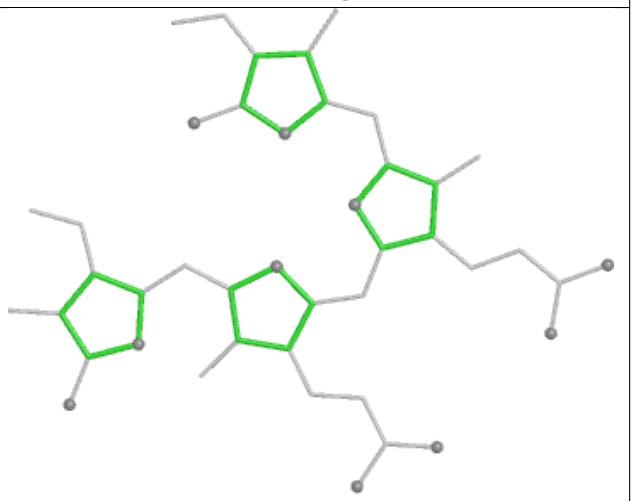
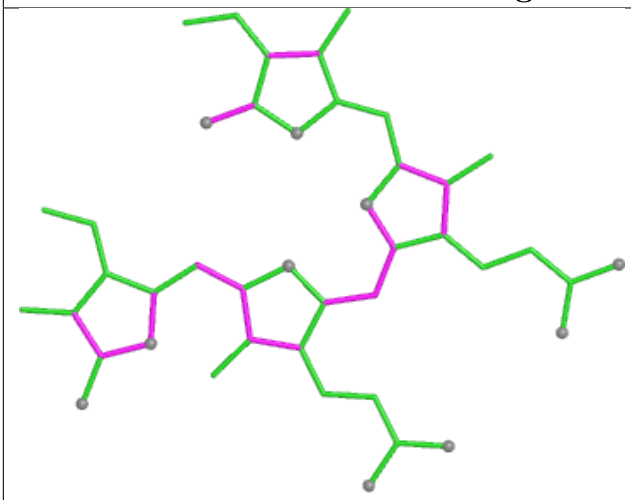


Rings

Ligand PEB R5 201



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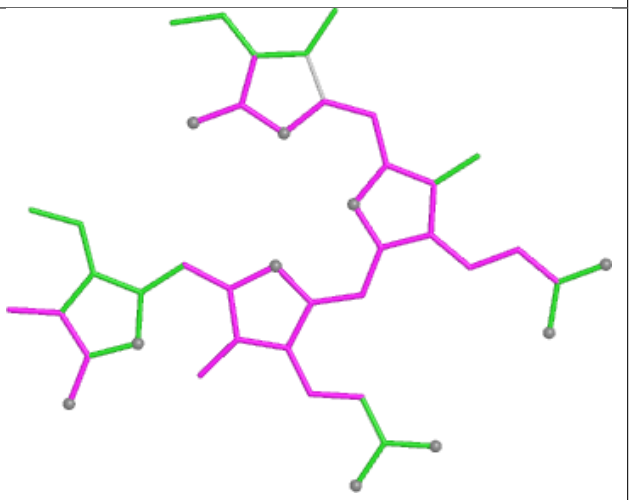

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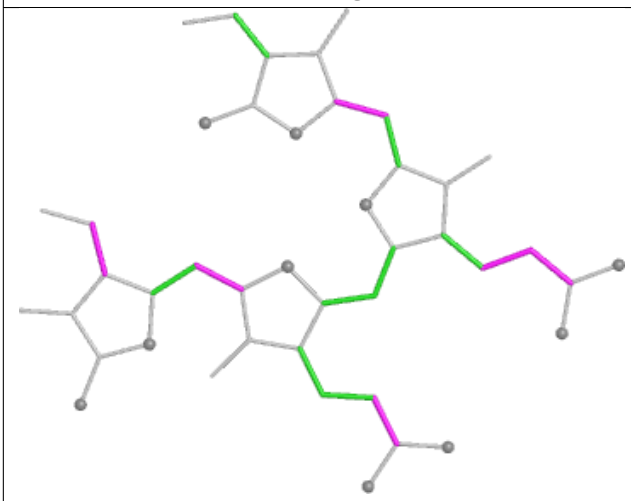

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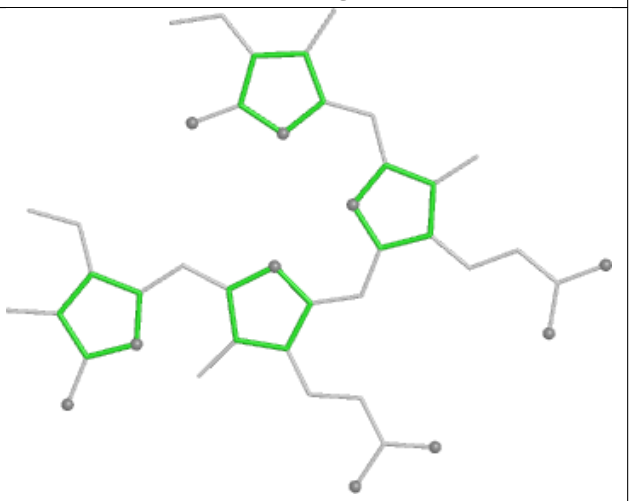
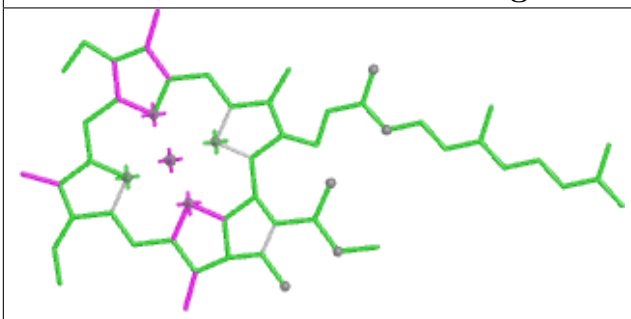


Rings

Ligand CLA BN 812



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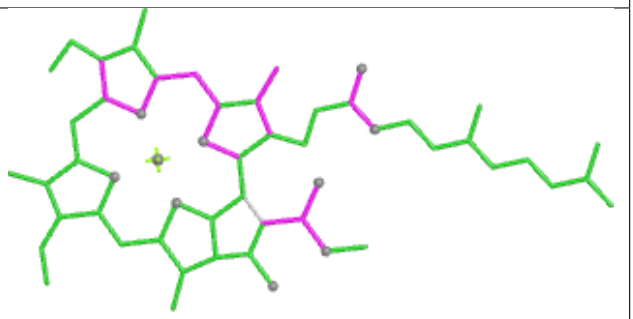
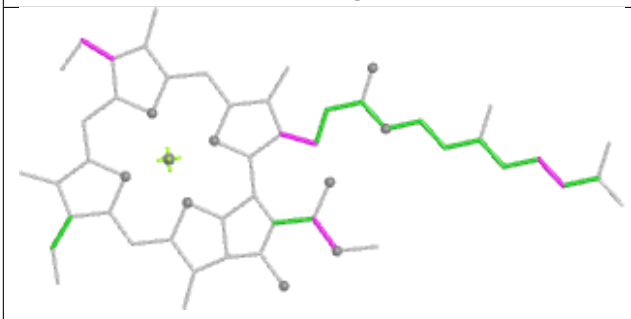


Bond angles



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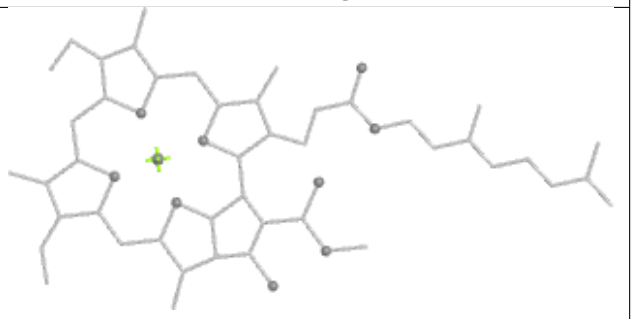
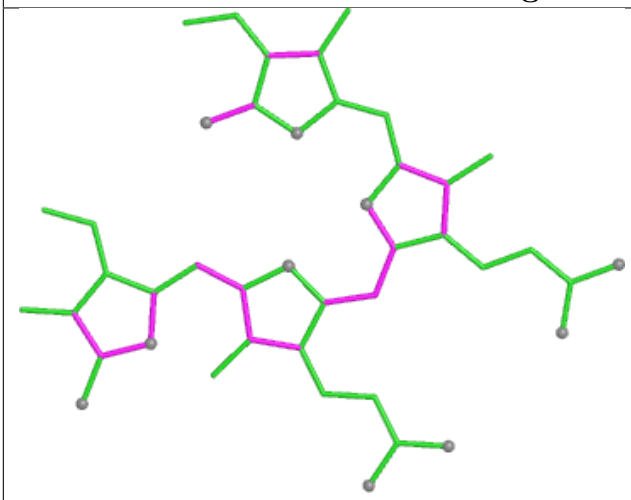


Rings

Ligand PEB IJ 202



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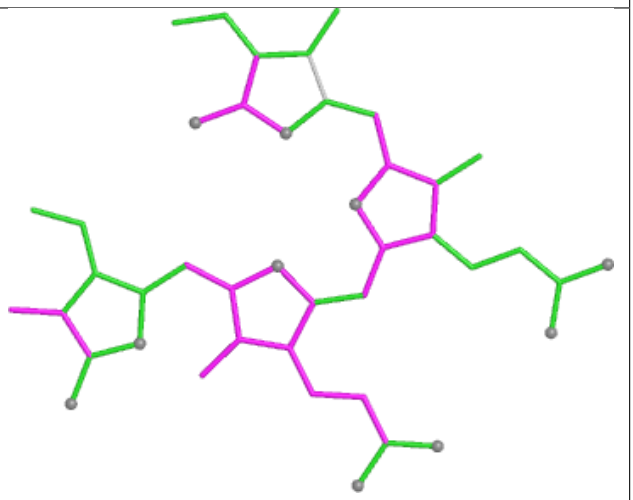
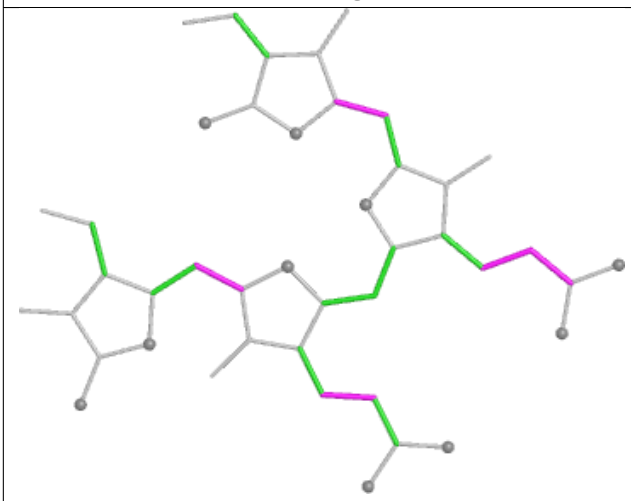


Bond angles



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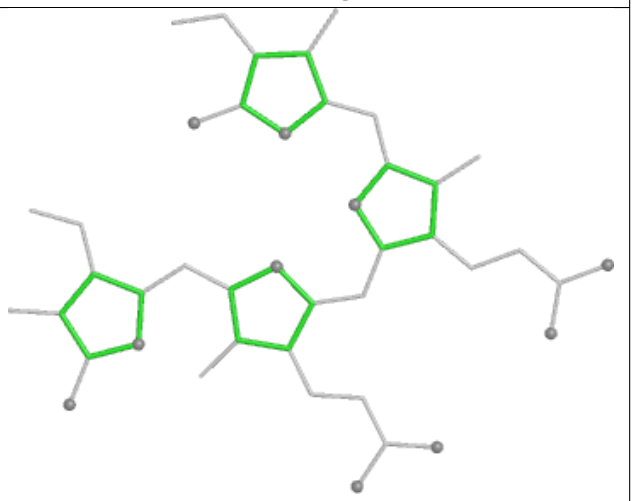
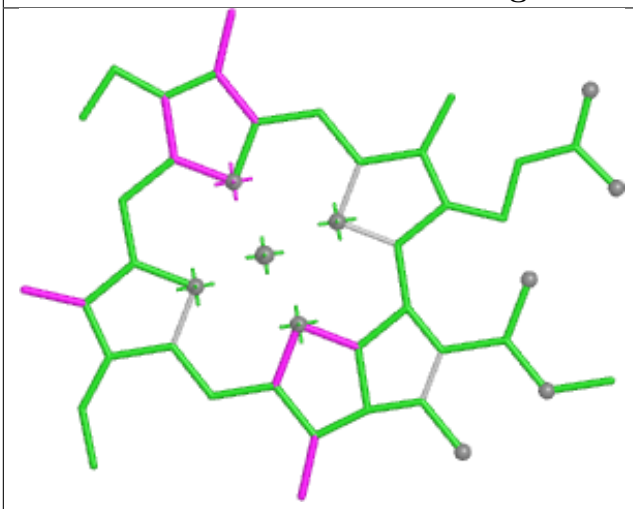


Rings

Ligand CLA AN 818



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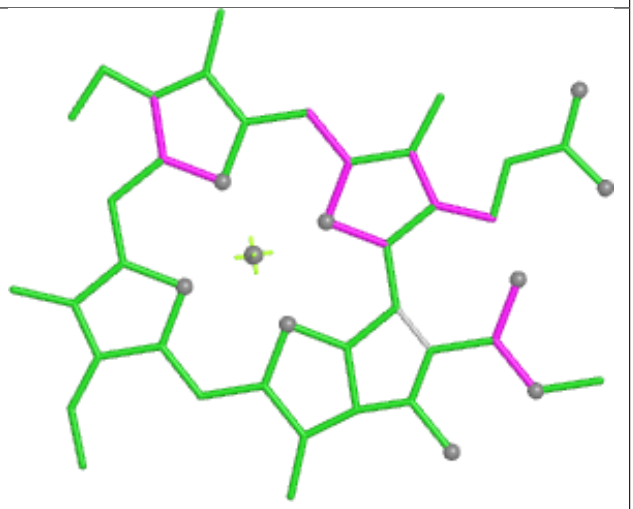
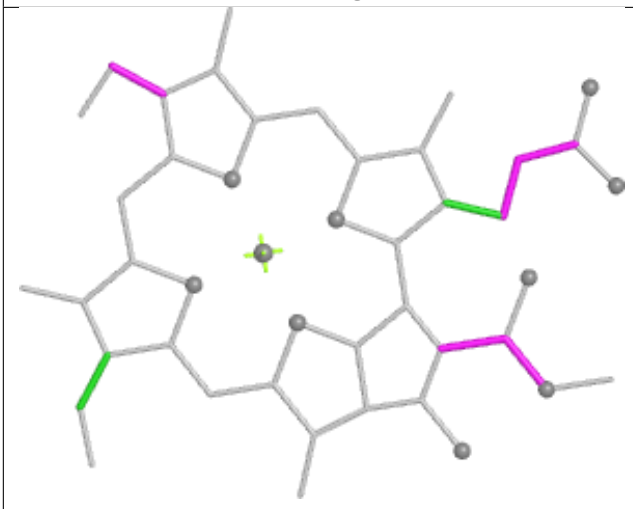


Bond angles

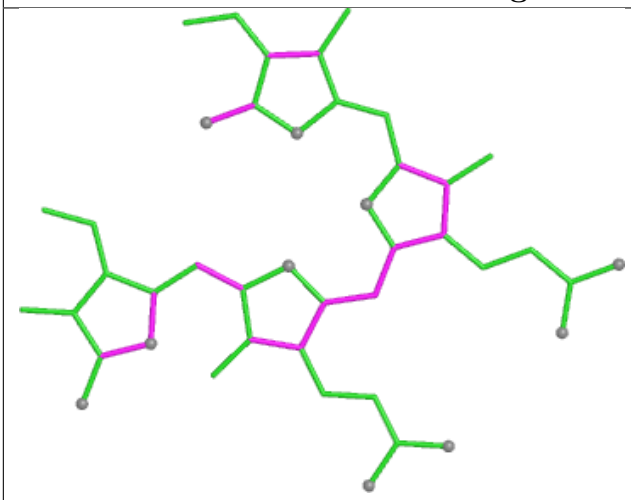


Torsions



Rings

Ligand PEB UH 203



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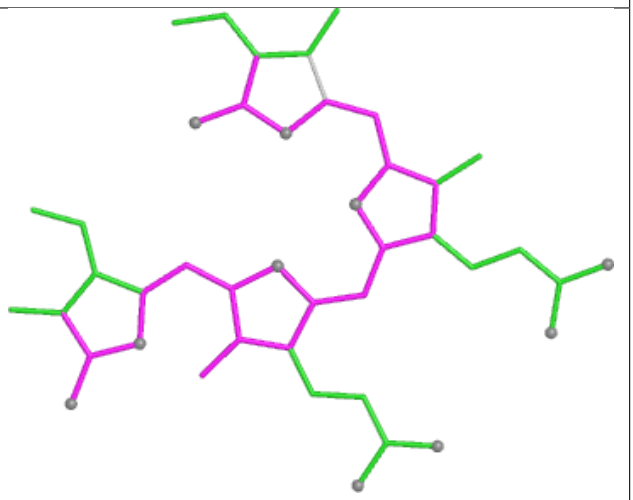
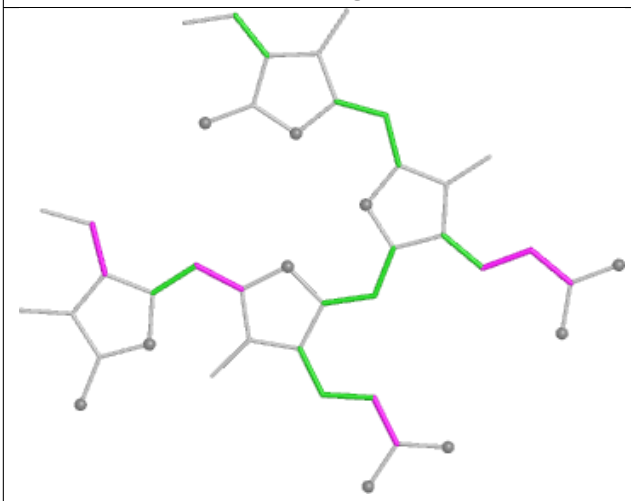


Bond angles



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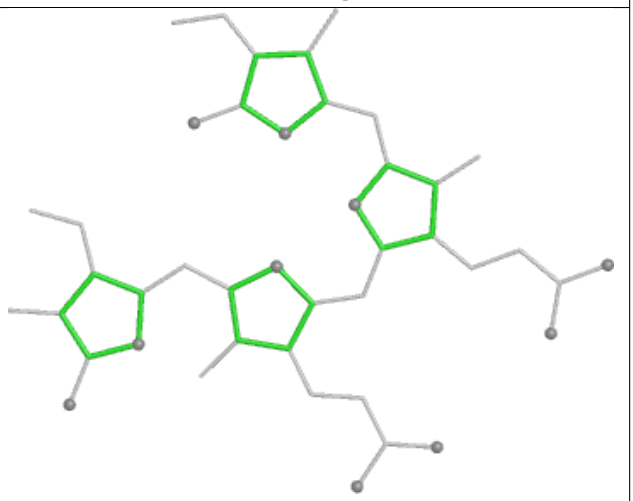
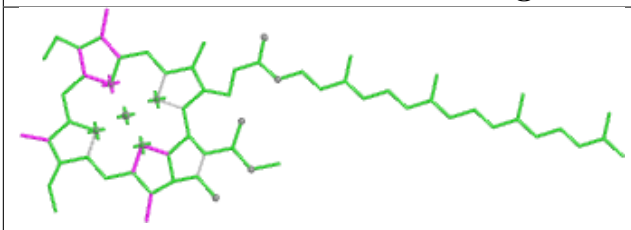


Rings

Ligand CLA B6 606



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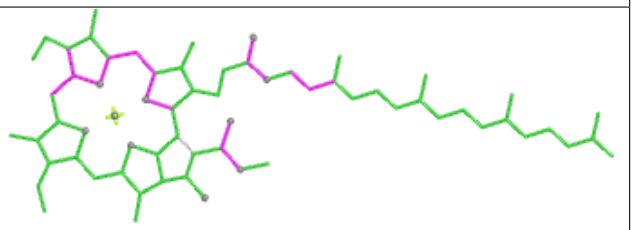

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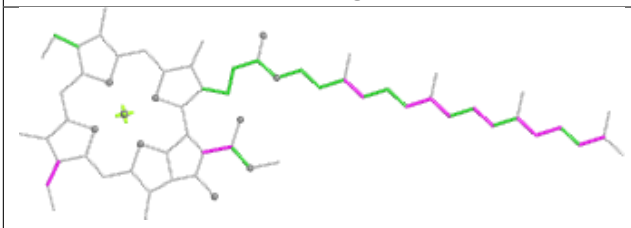

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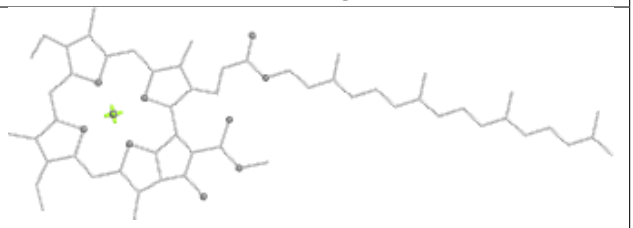
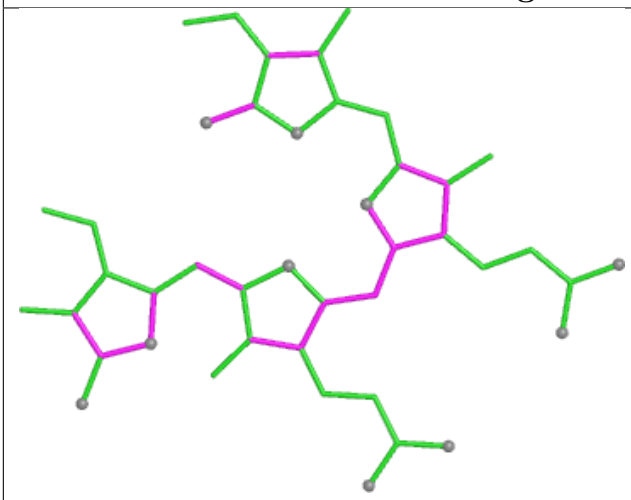


Rings

Ligand PEB AI 202



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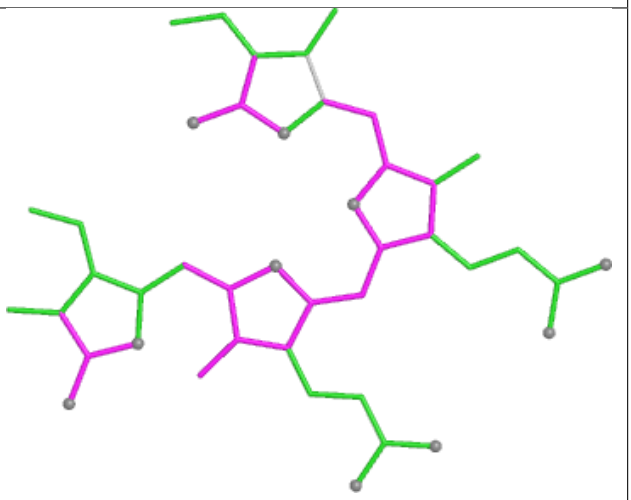

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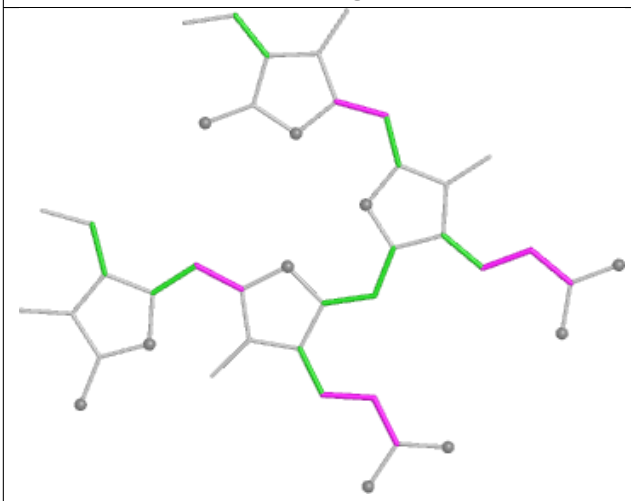

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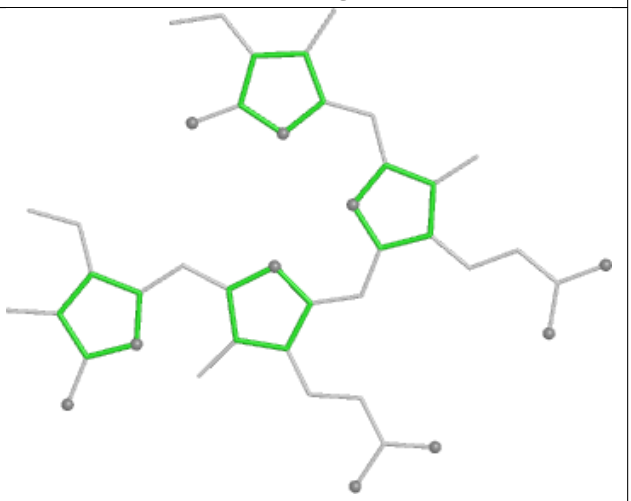
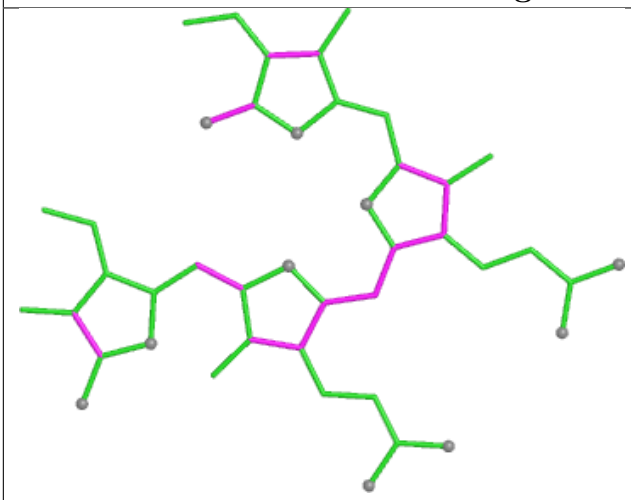


Rings

Ligand PEB JK 201



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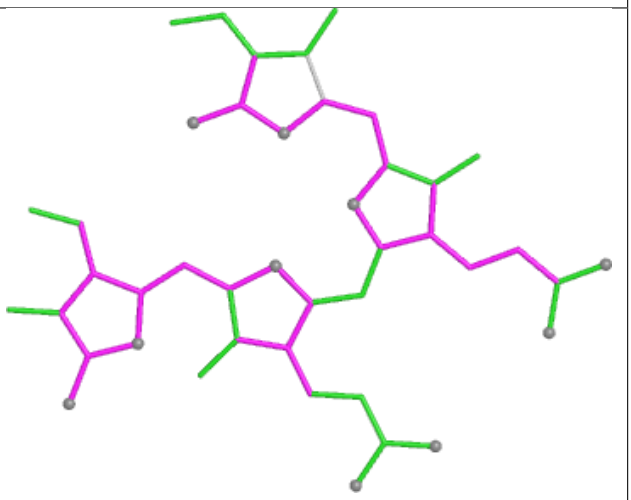

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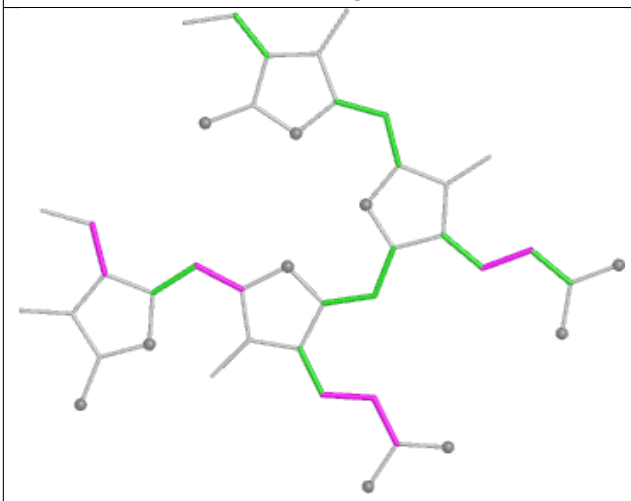

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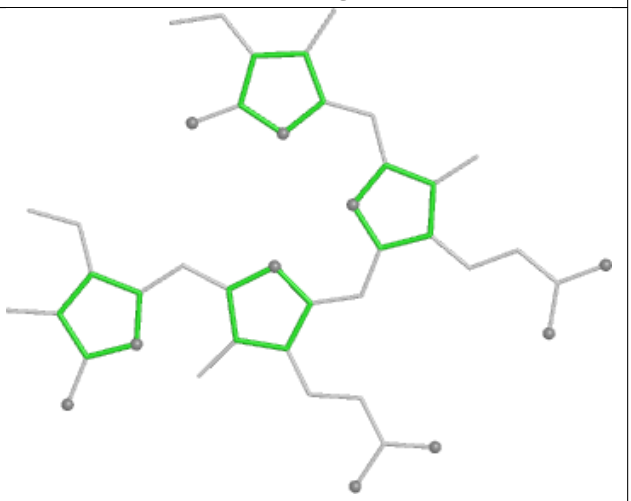
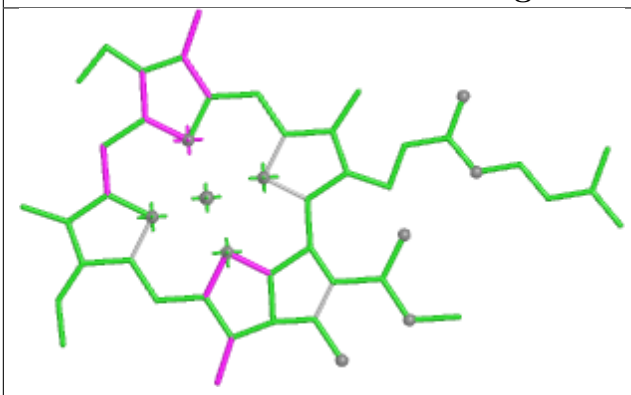


Rings

Ligand CLA 7N 607



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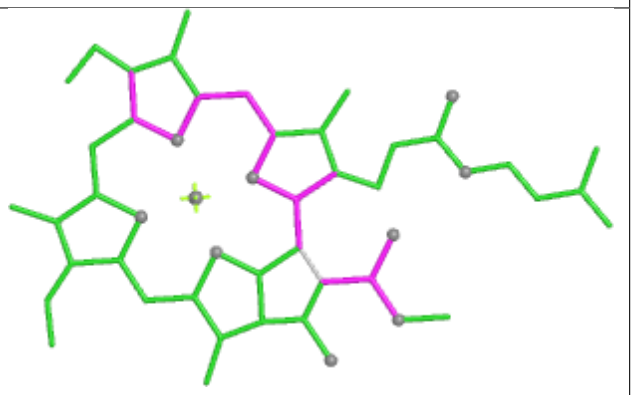

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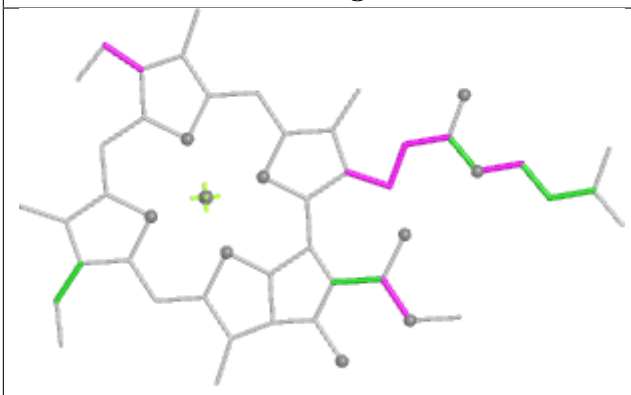

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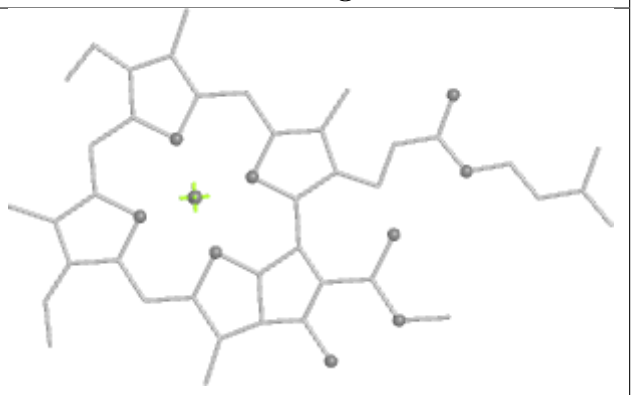
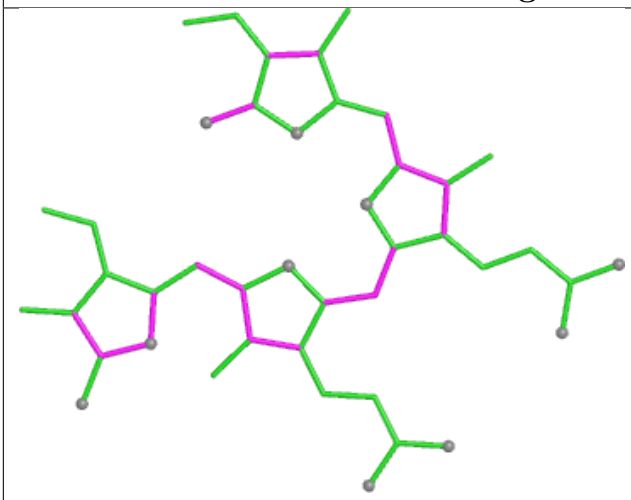


Rings

Ligand PEB d1 202



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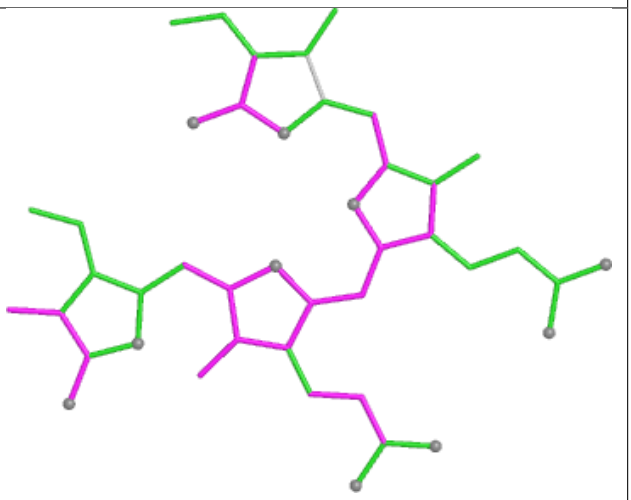

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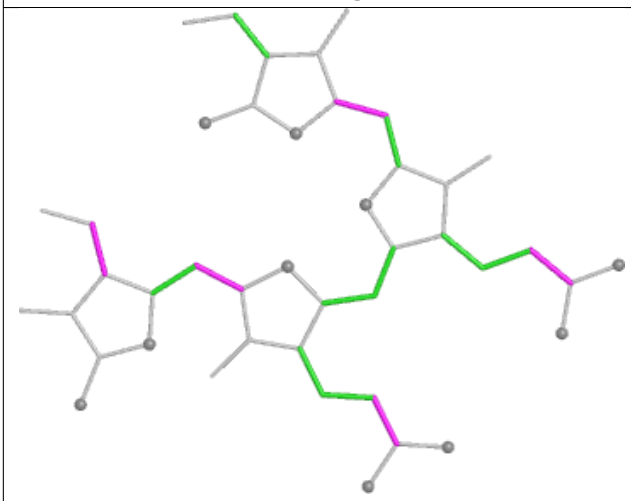

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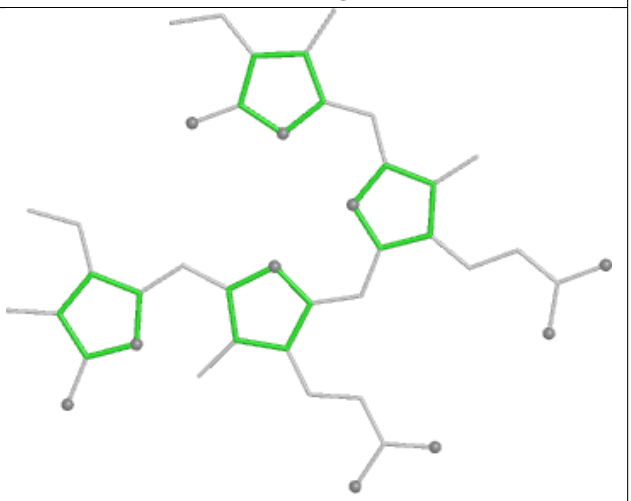

Rings

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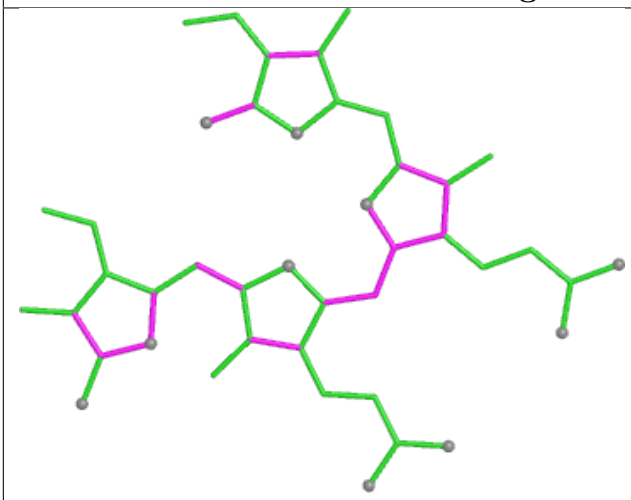

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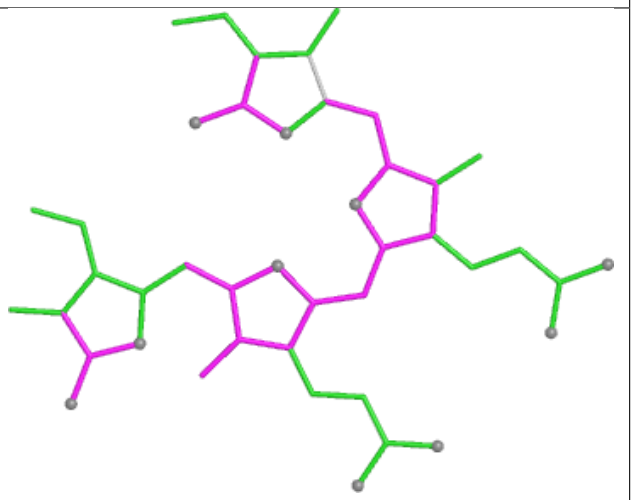
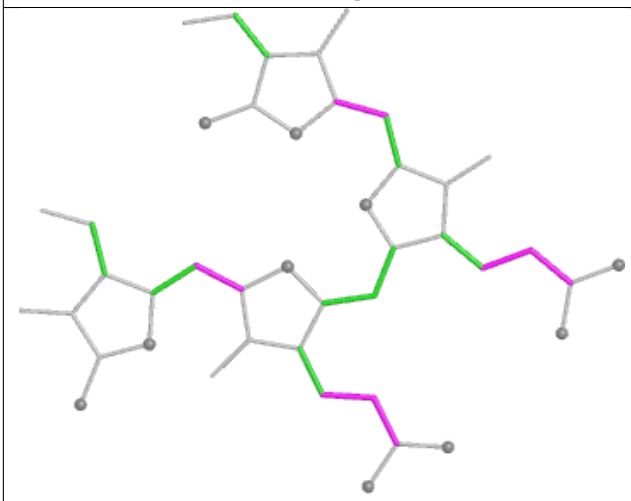


Bond angles



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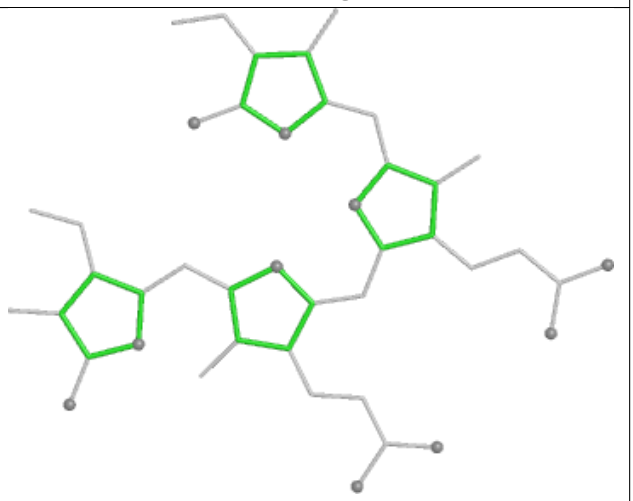
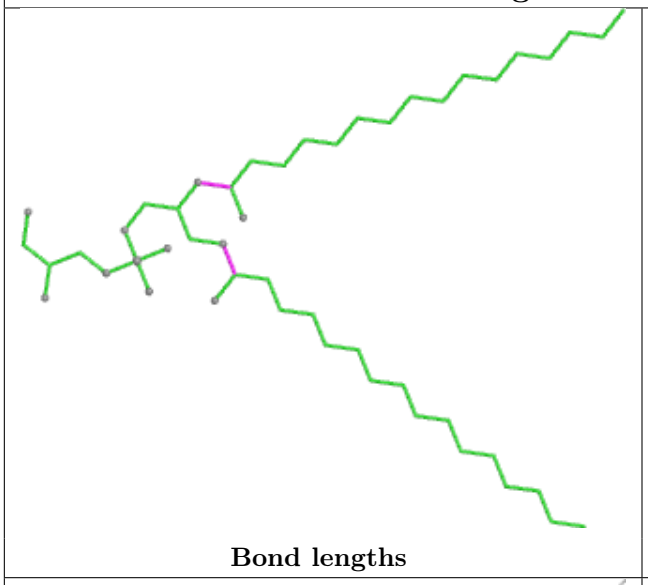


Rings

Ligand LHG DL 407



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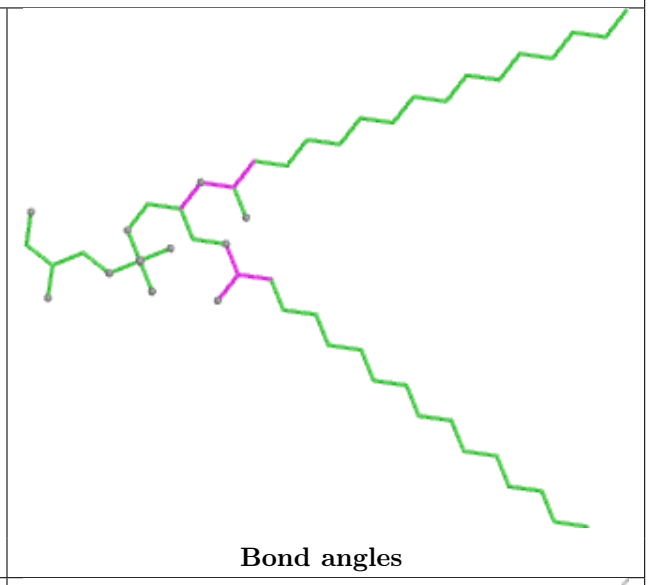

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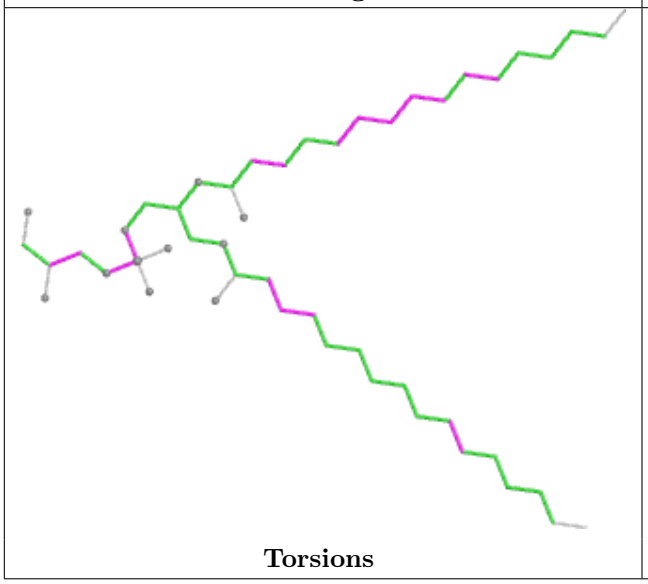

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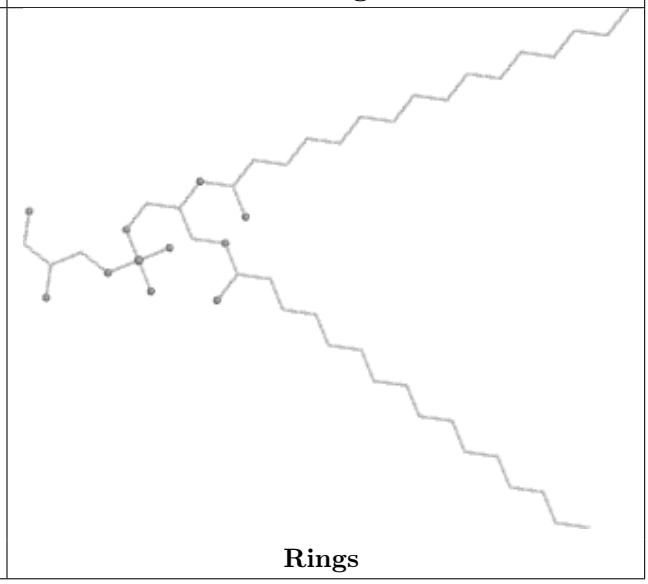
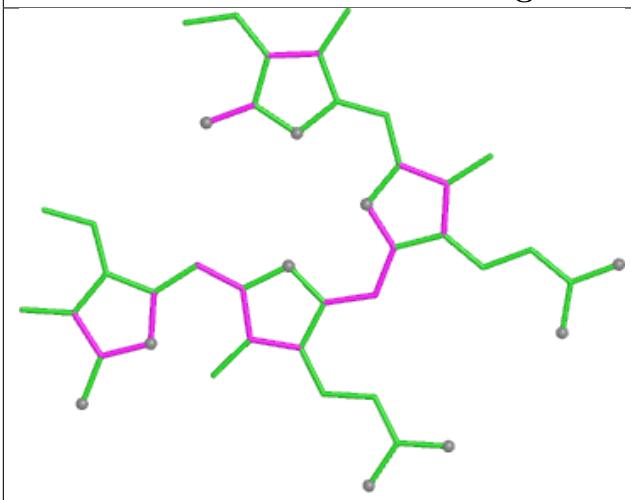


Rings

Ligand PEB C5 201



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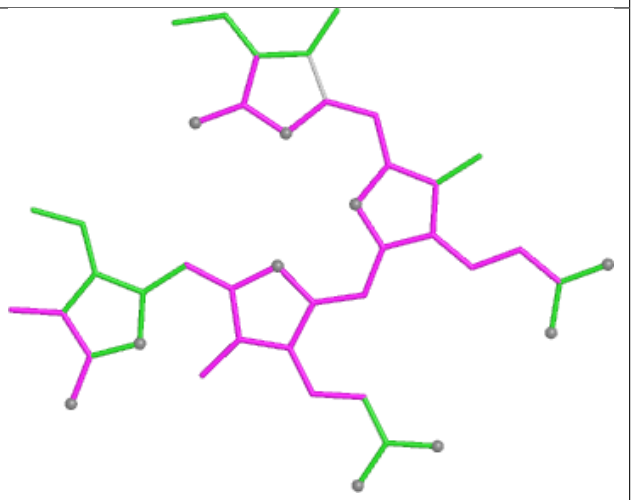

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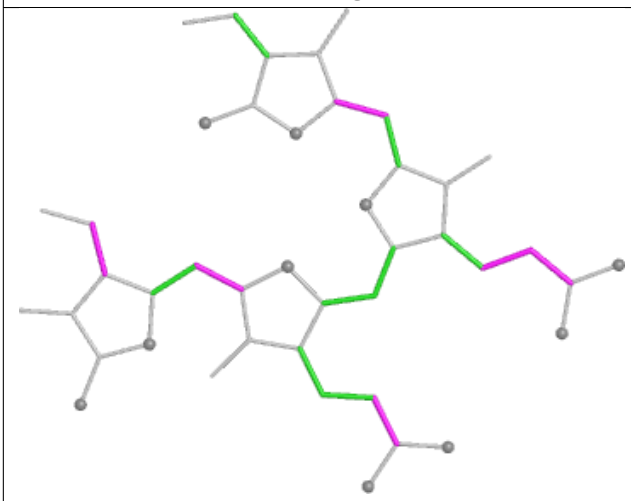

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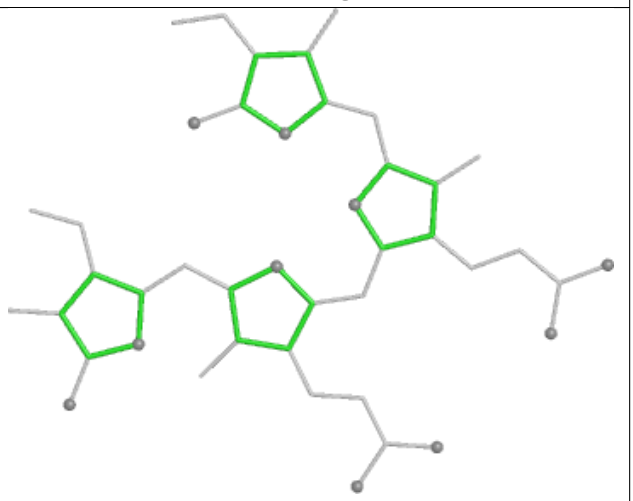
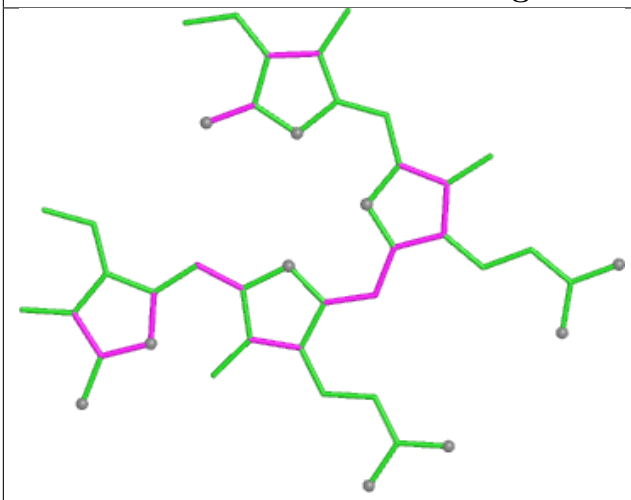


Rings

Ligand PEB aM 204



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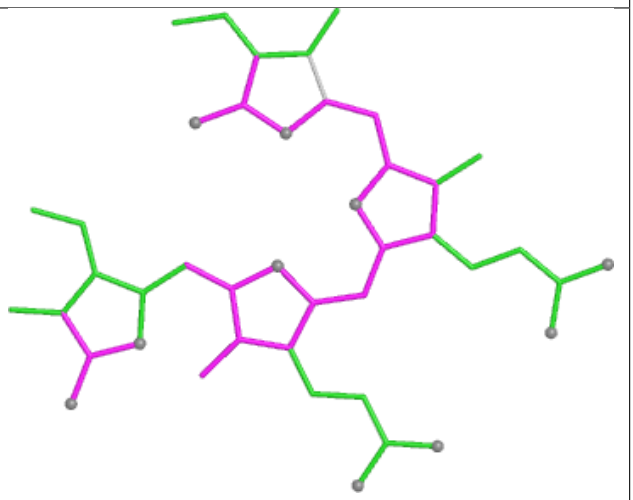
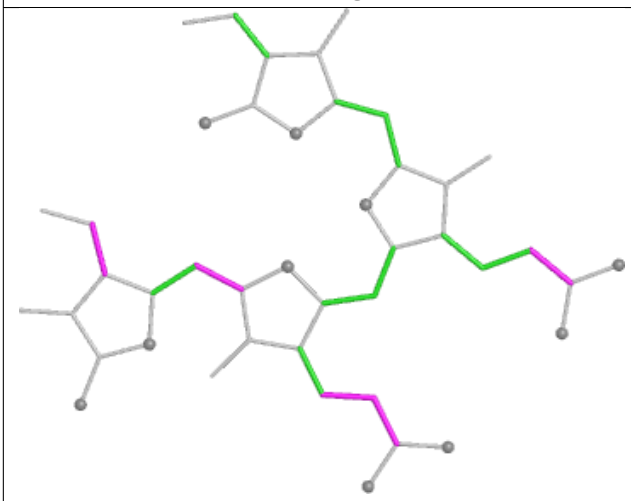


Bond angles



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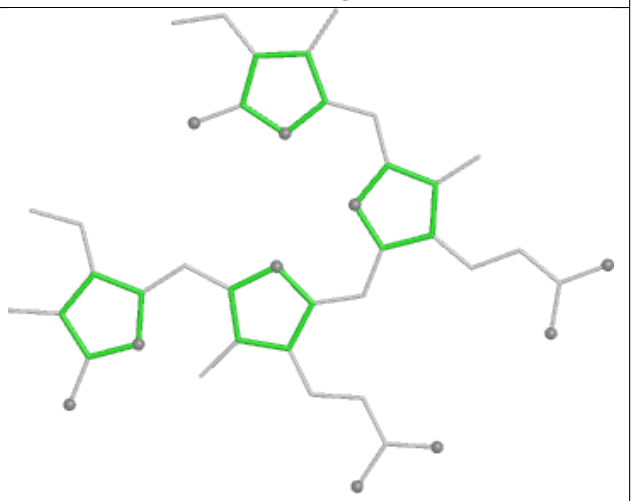
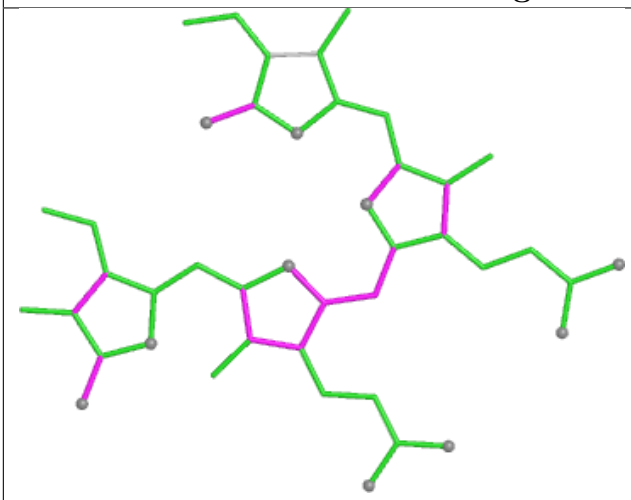


Rings

Ligand PUB Y7 302



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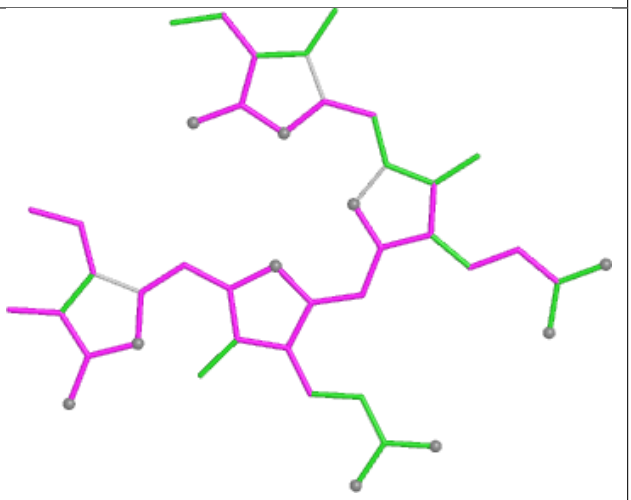

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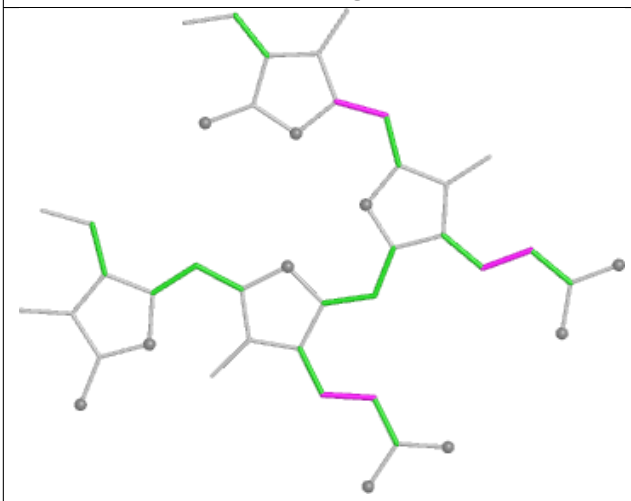

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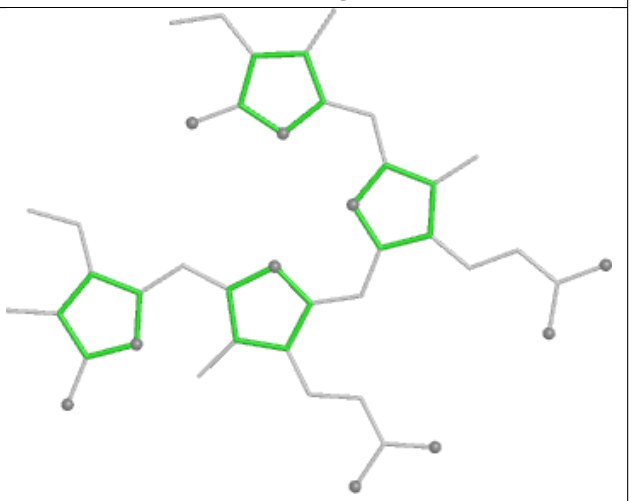
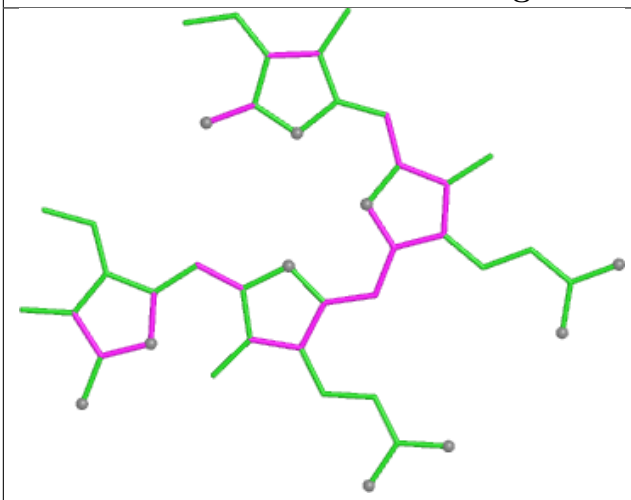


Rings

Ligand PEB XF 203



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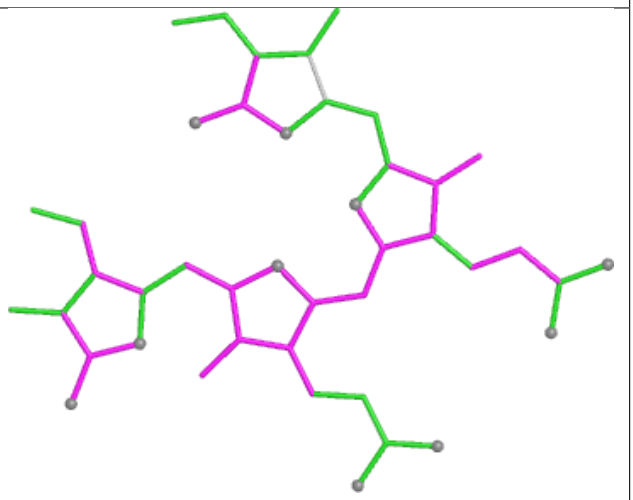

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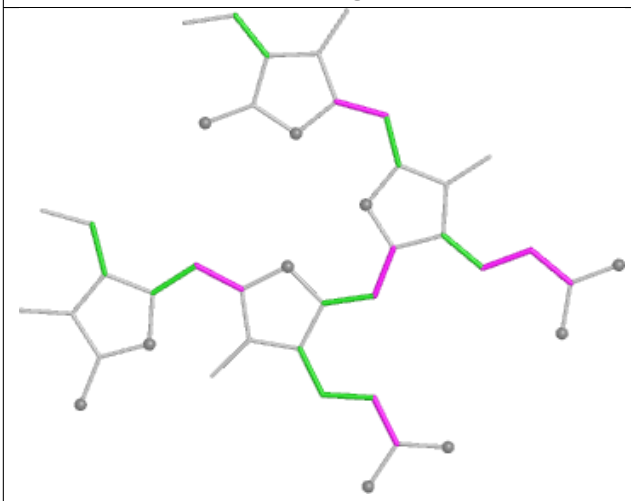

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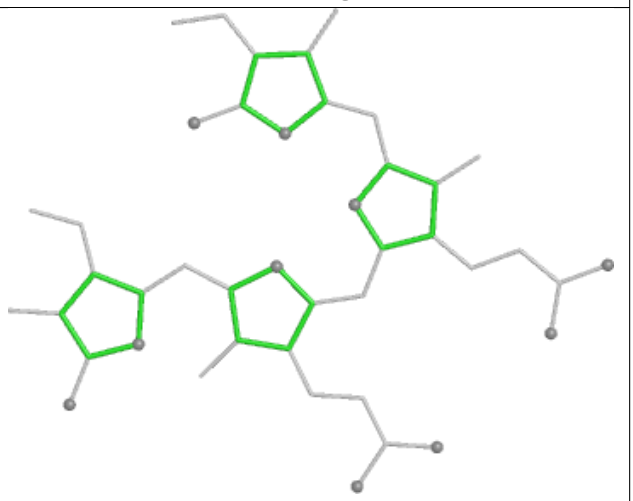
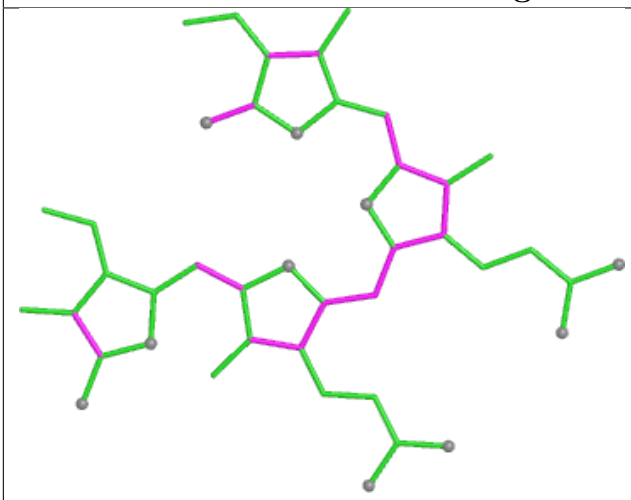


Rings

Ligand PEB nK 201



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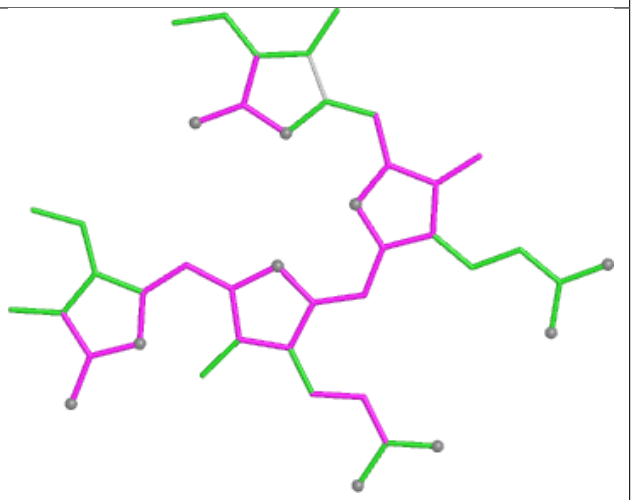

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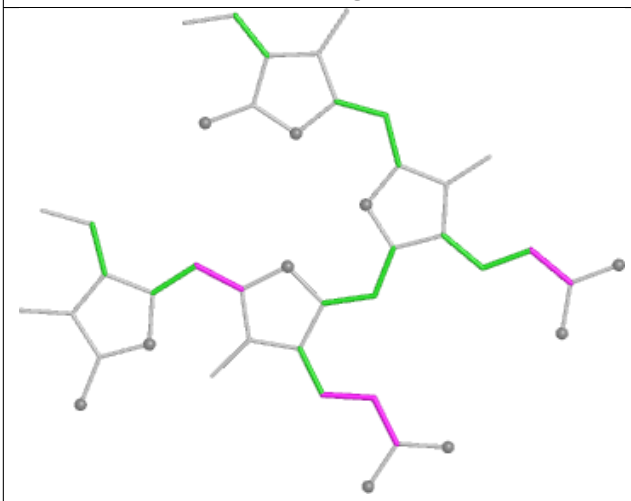

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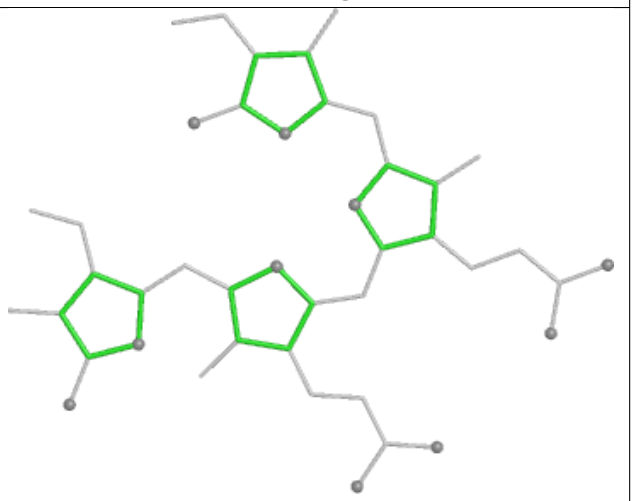
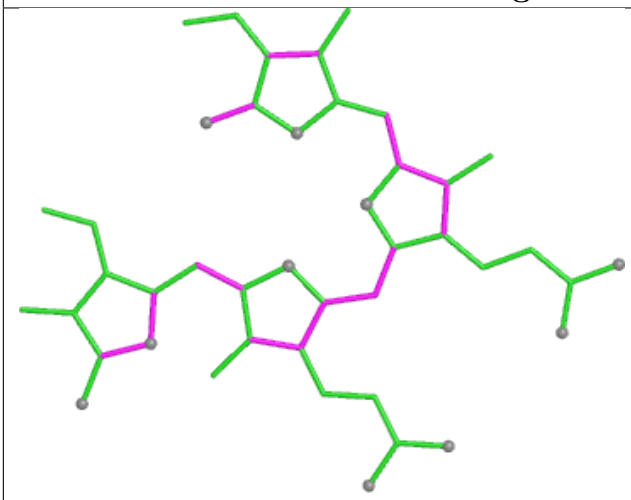


Rings

Ligand PEB ZH 202



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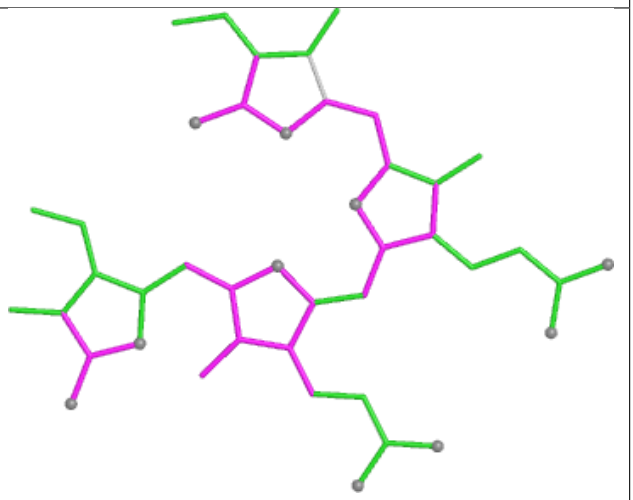

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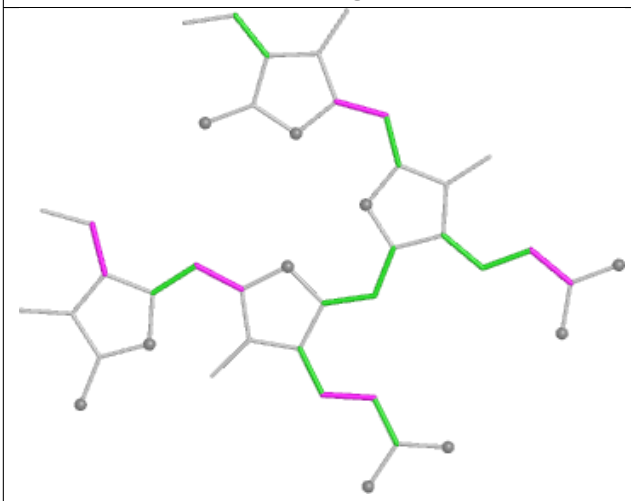

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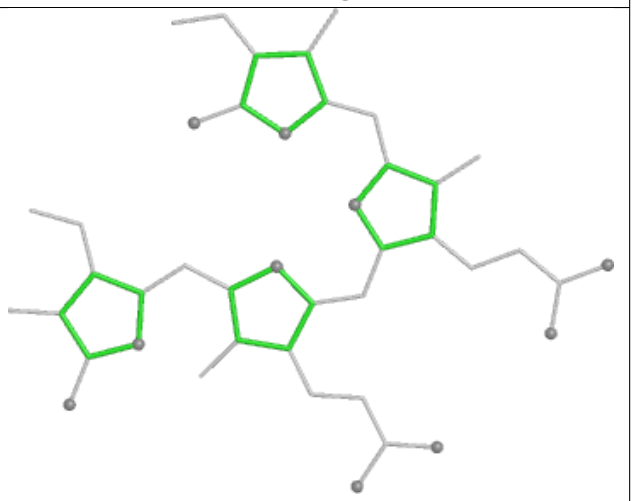
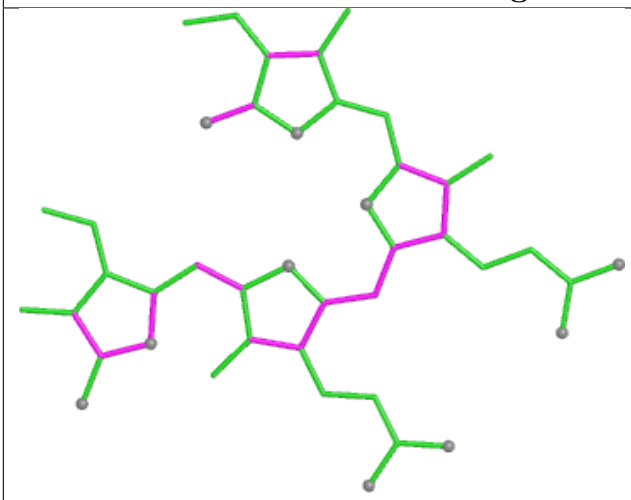


Rings

Ligand PEB DQ 201



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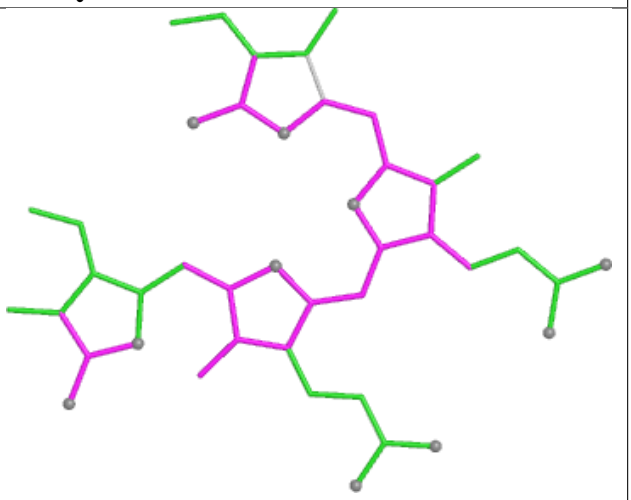
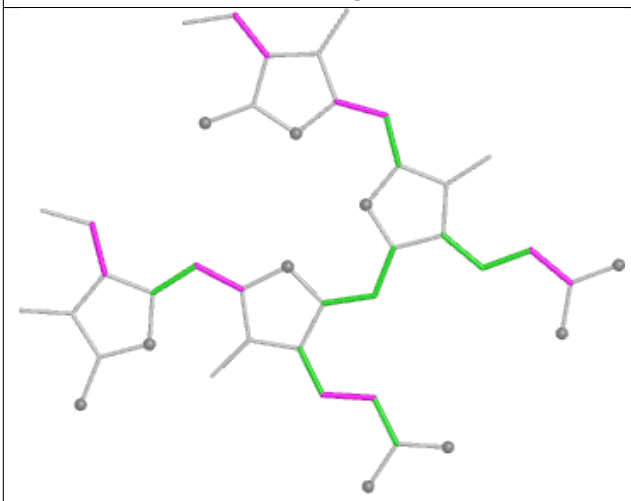


Bond angles



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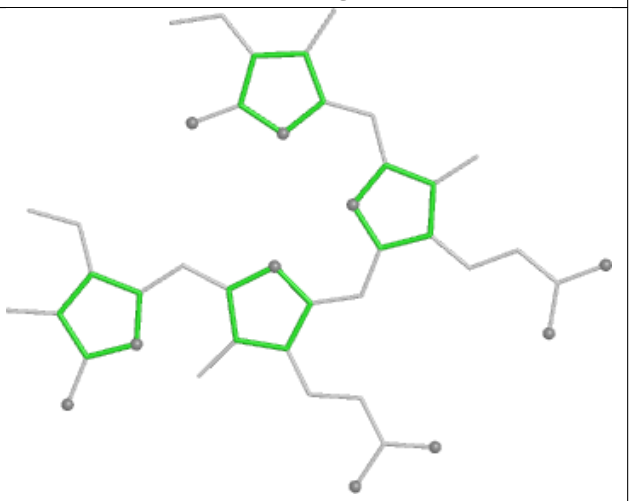
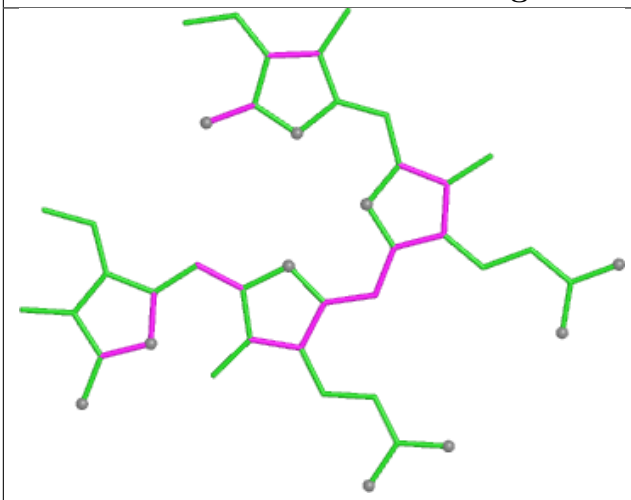
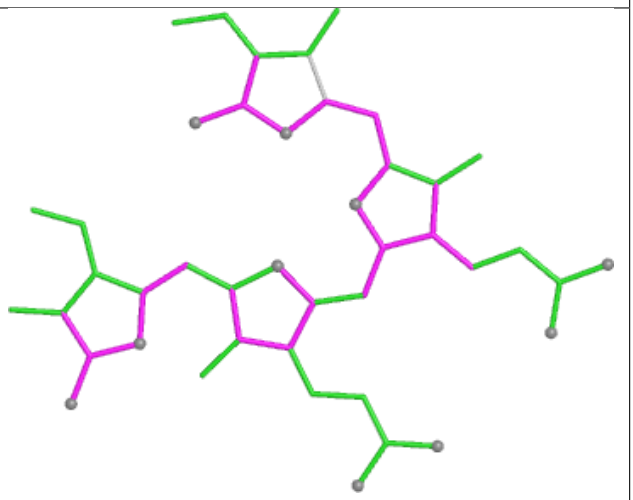


Rings

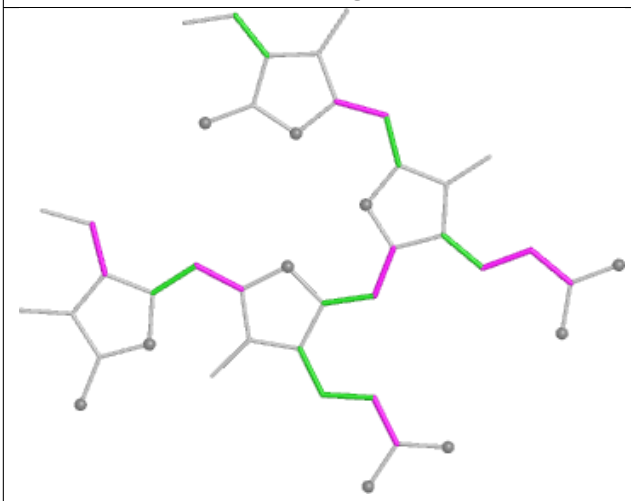
Ligand PEB dM 203



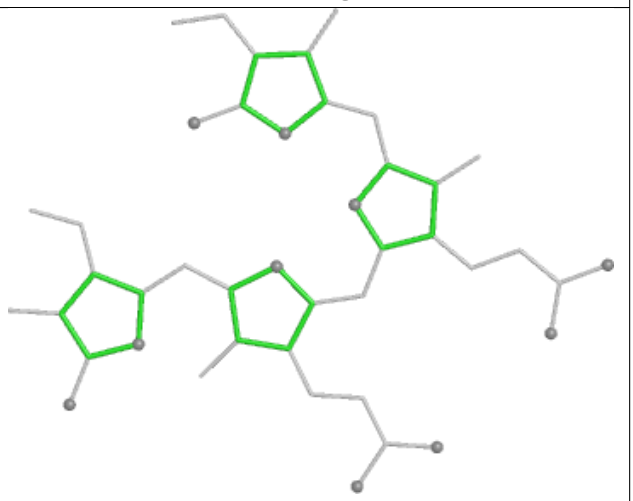
Bond lengths



Bond angles

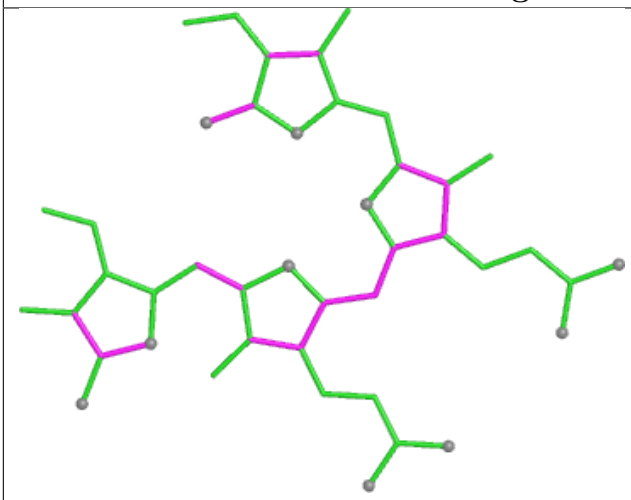


Torsions



Rings

Ligand PEB wC 203



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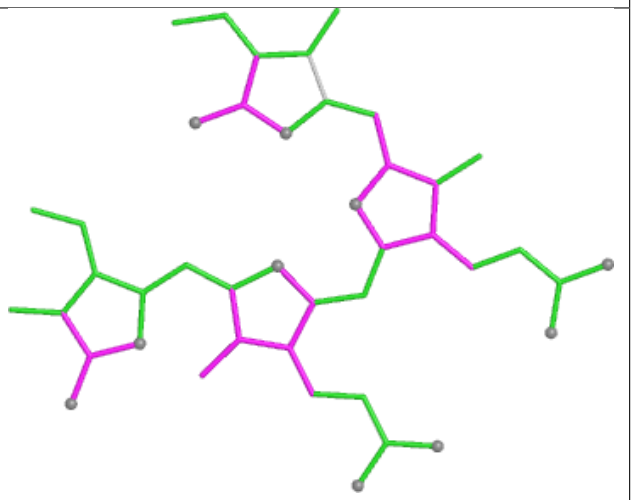

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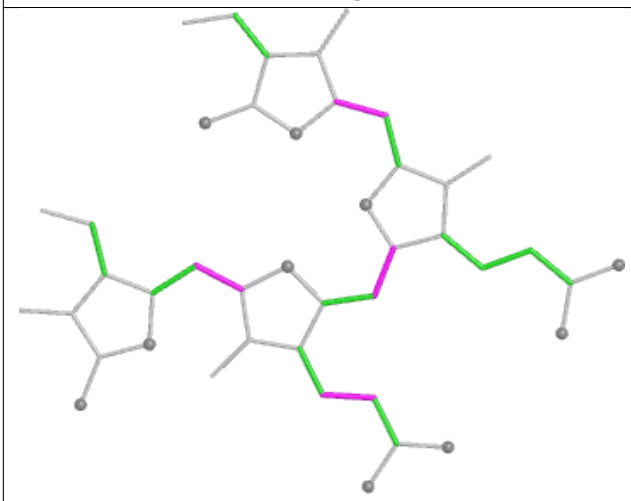

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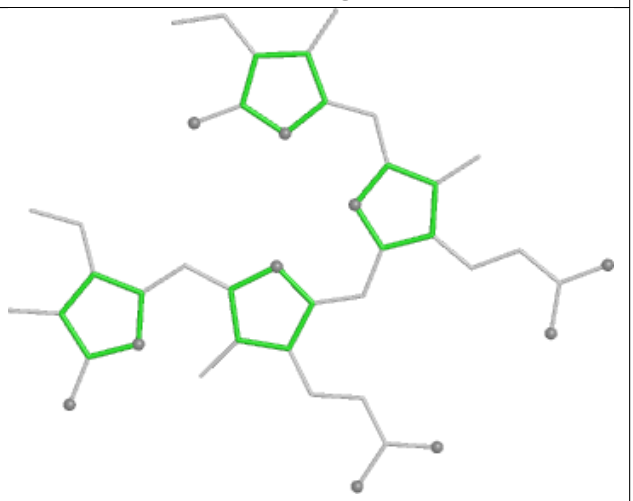
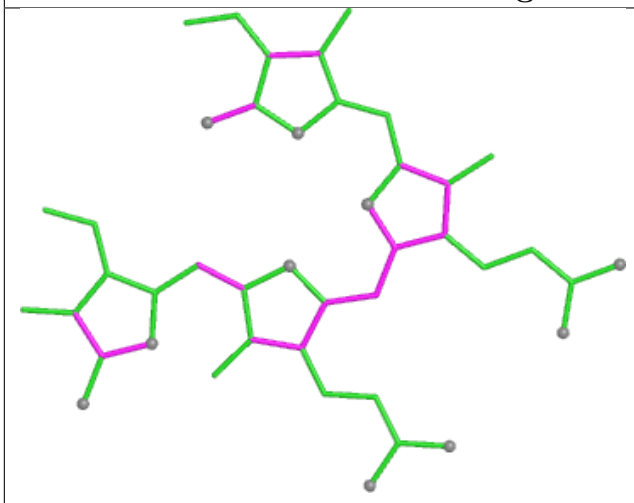


Rings

Ligand PEB xC 202



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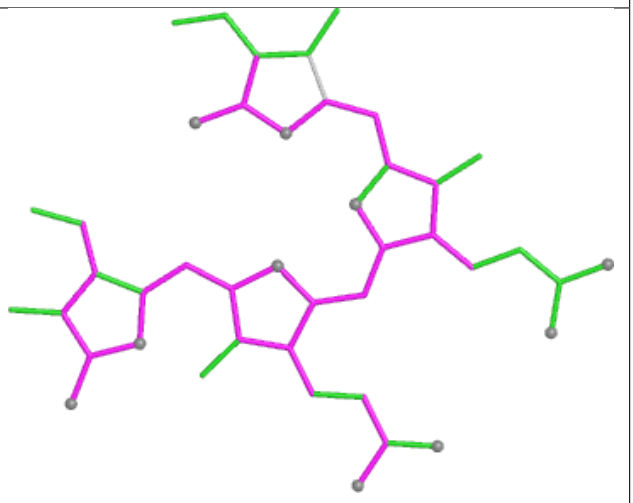

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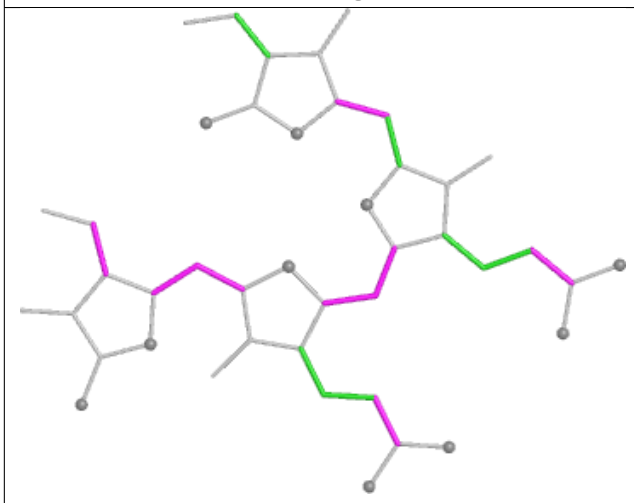

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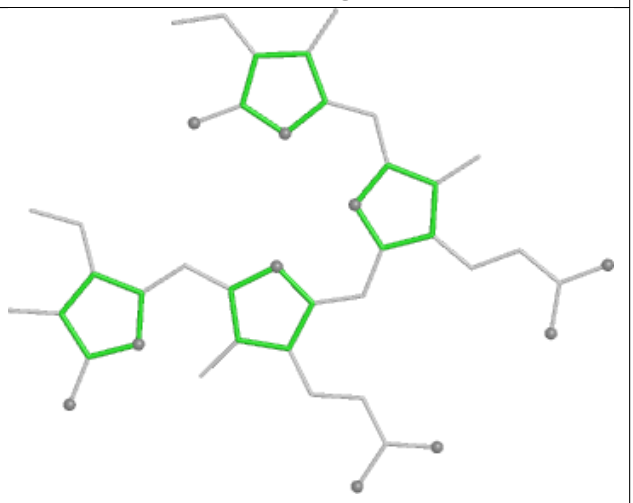
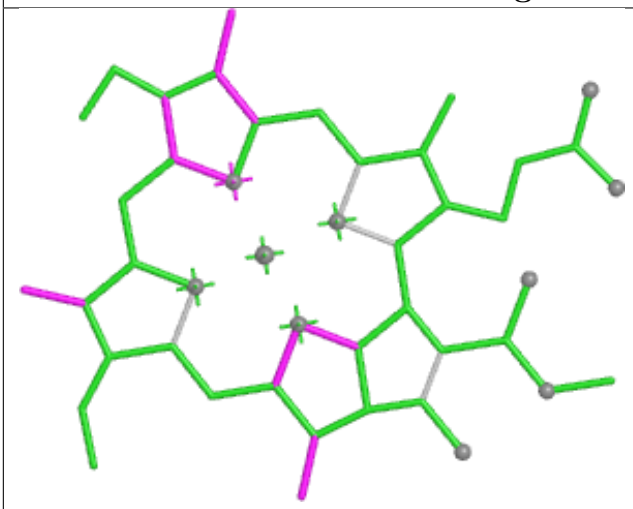


Rings

Ligand CLA 3N 313



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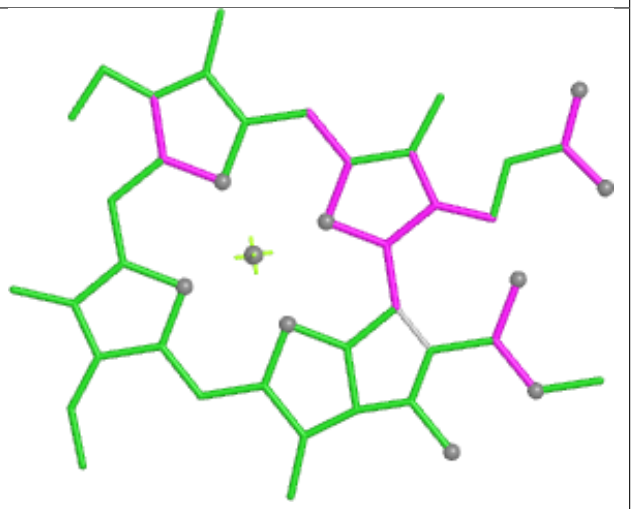

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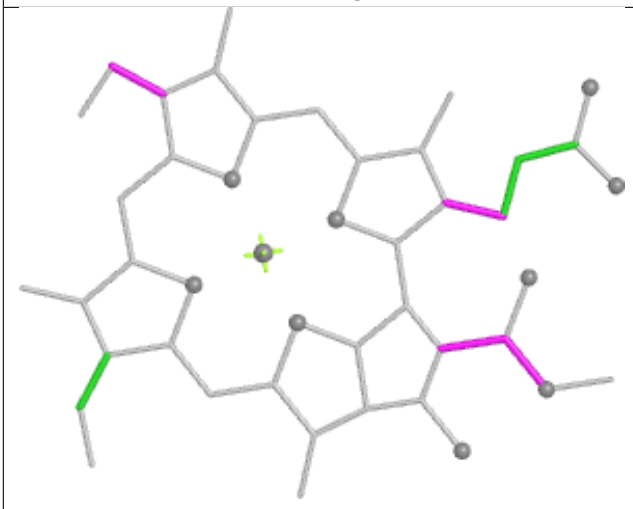
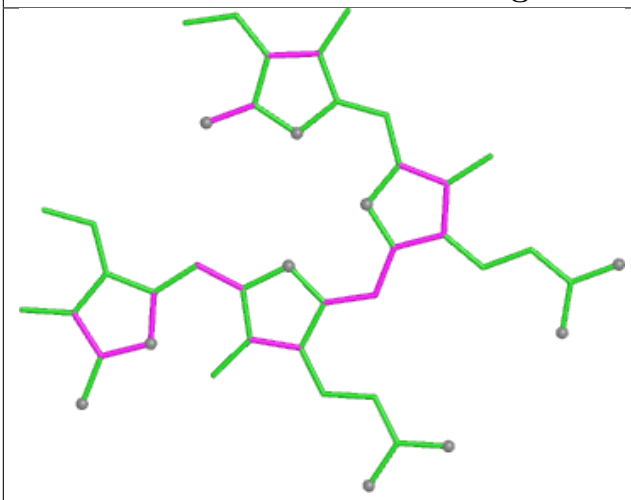


Torsions



Rings

Ligand PEB HP 202



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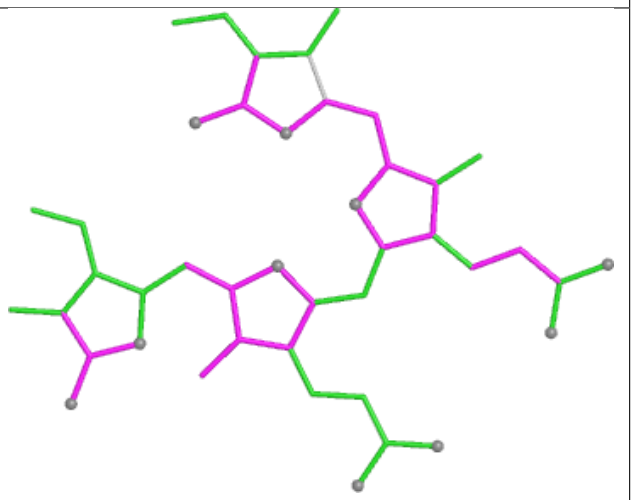

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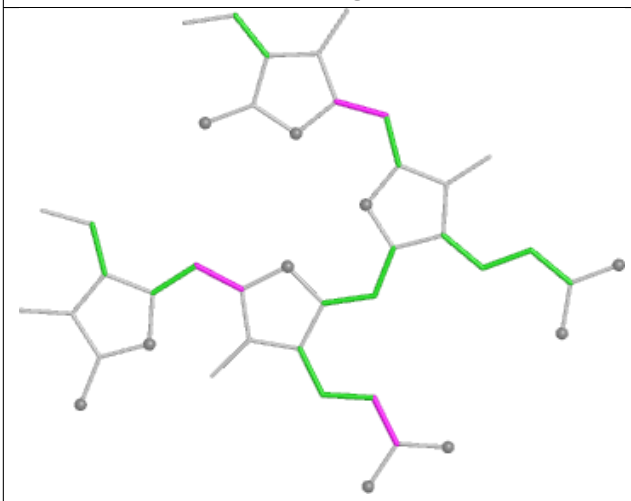

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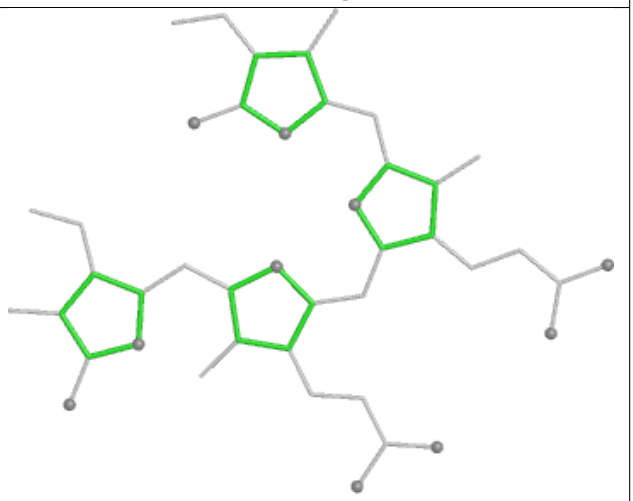
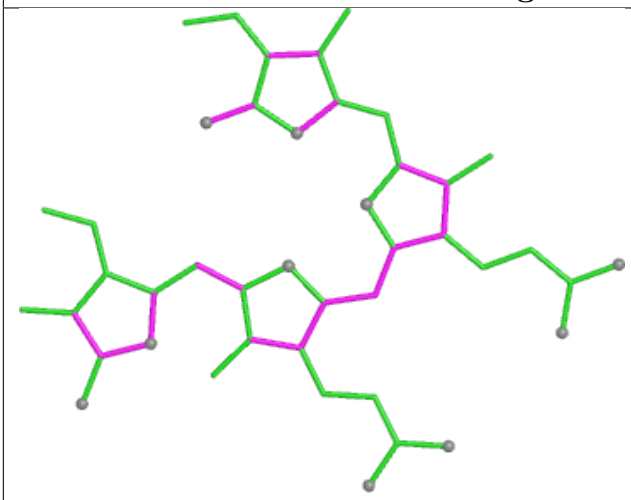


Rings

Ligand PEB E7 202



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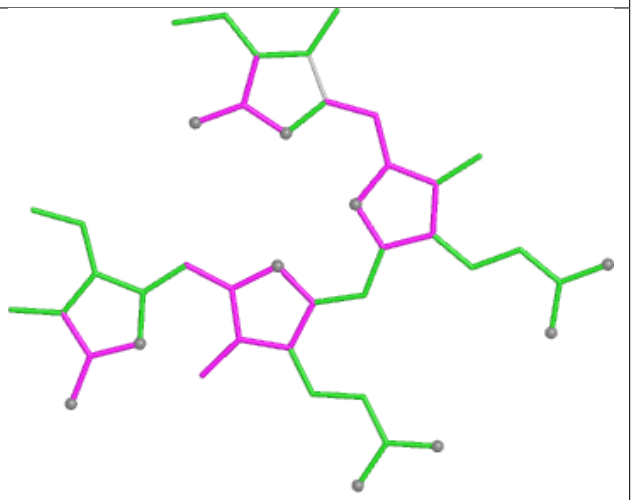

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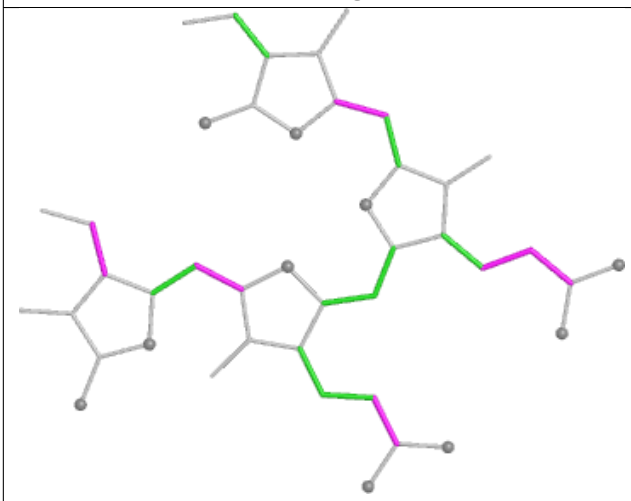

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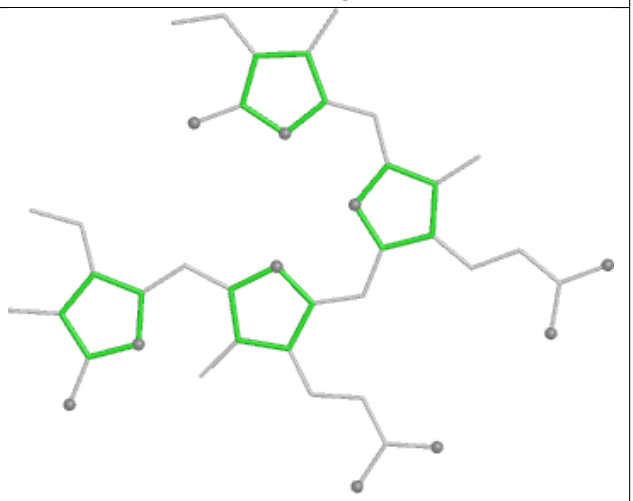
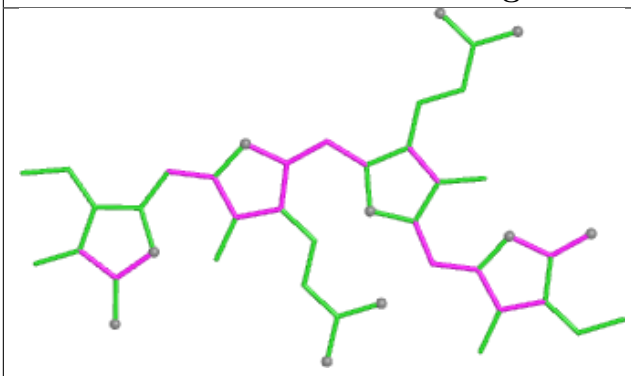


Rings

Ligand CYC JH 1003



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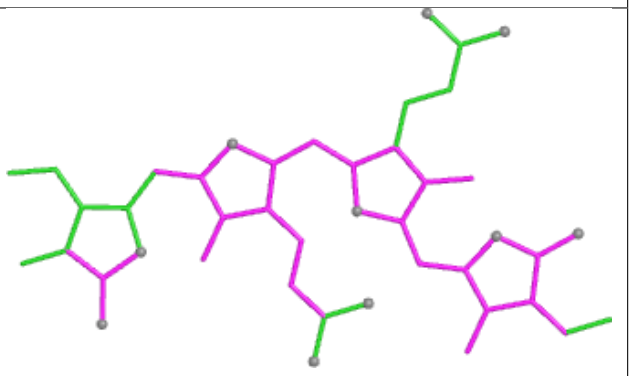
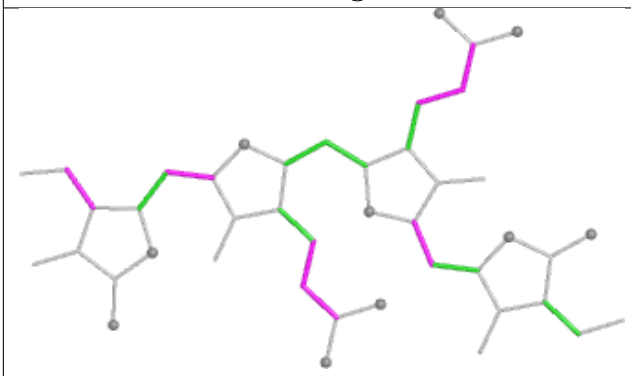


Bond angles



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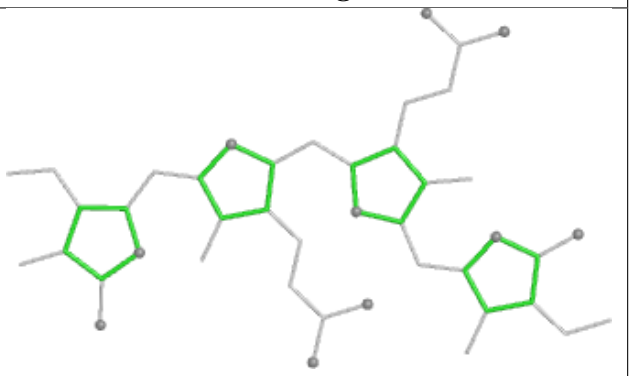
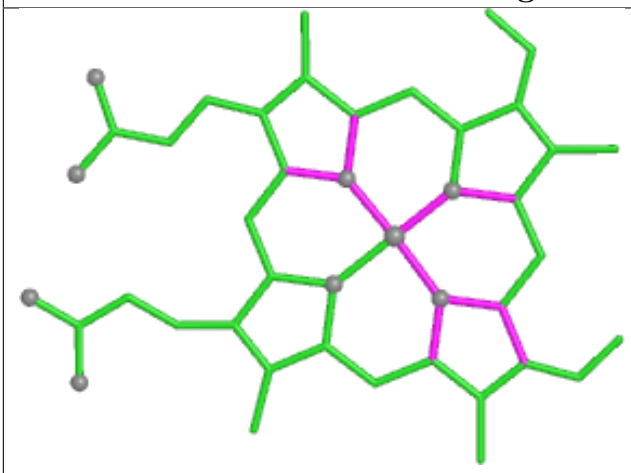


Rings

Ligand HEM f6 101



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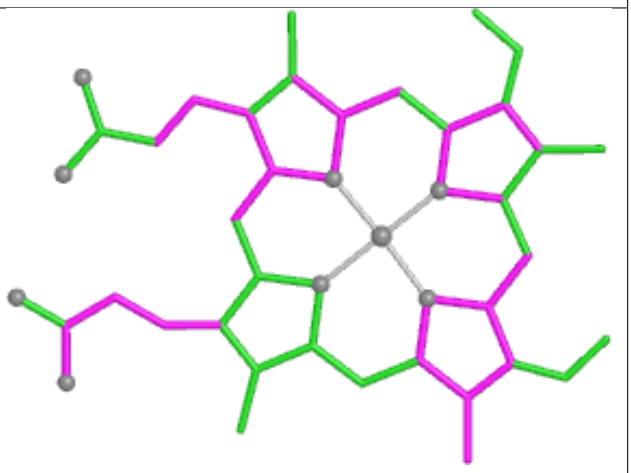

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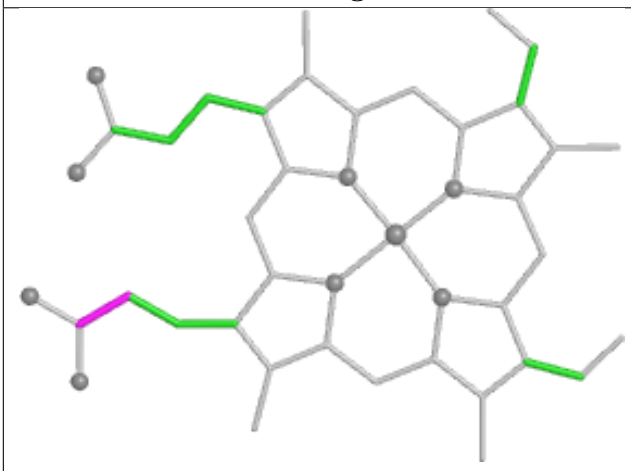

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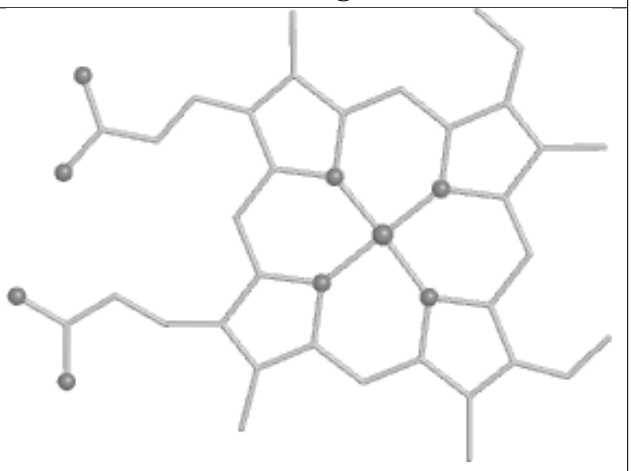
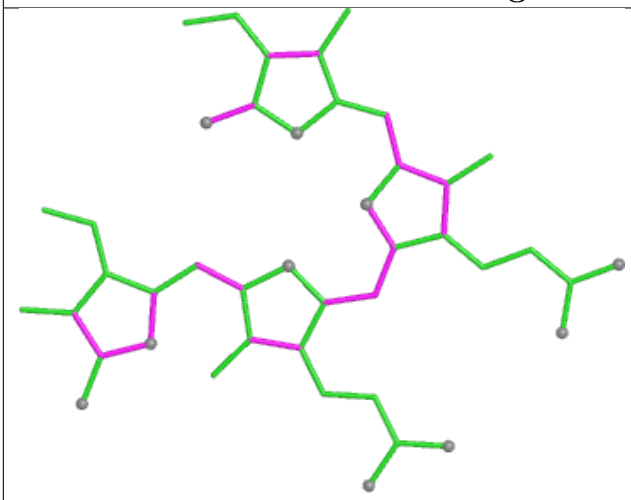


Rings

Ligand PEB MP 203



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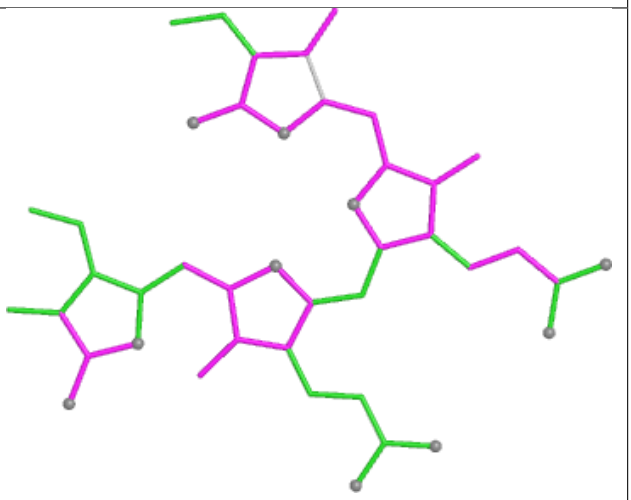
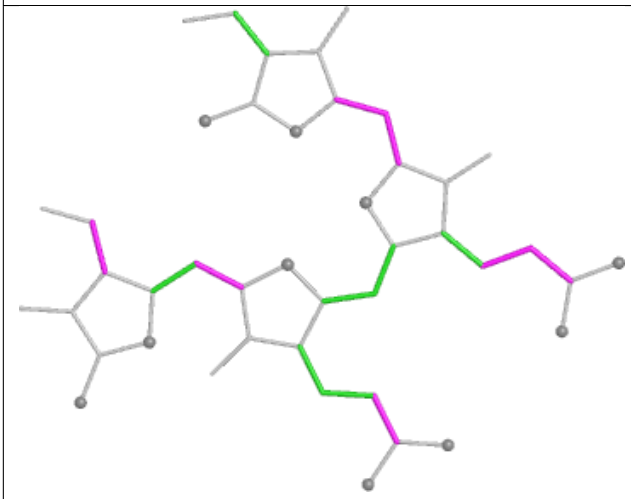


Bond angles



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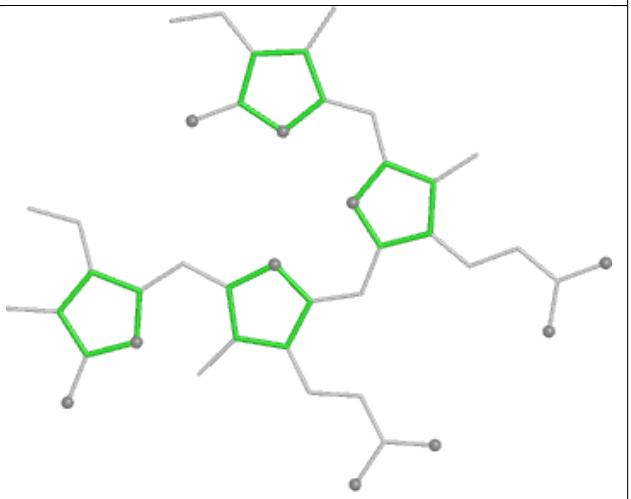
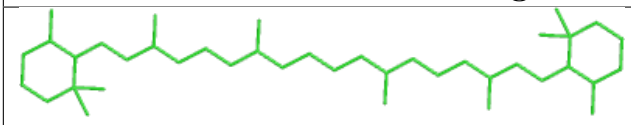


Rings

Ligand BCR LN 205



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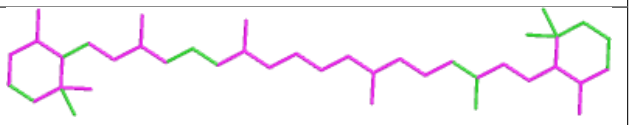
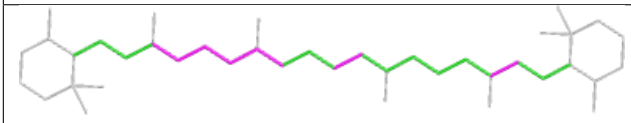


Bond angles



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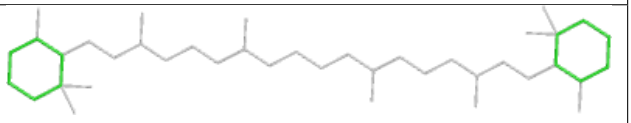
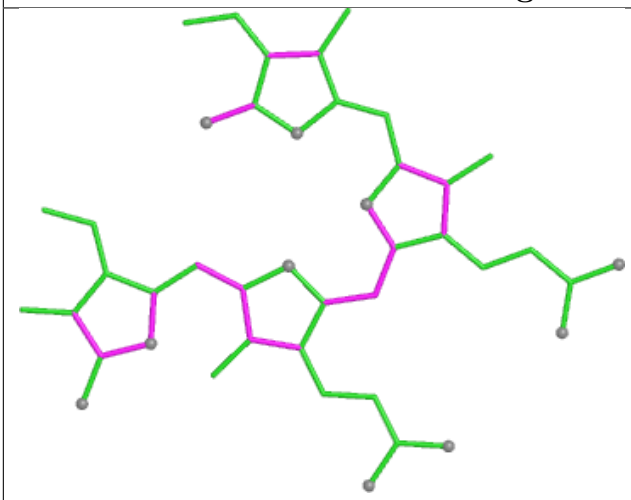


Rings

Ligand PEB P5 201



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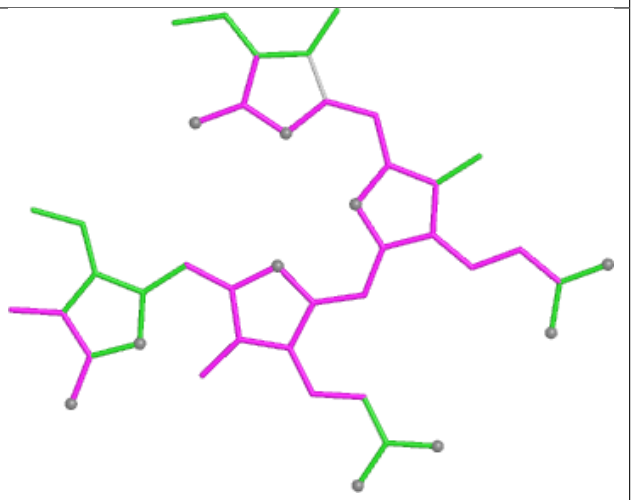
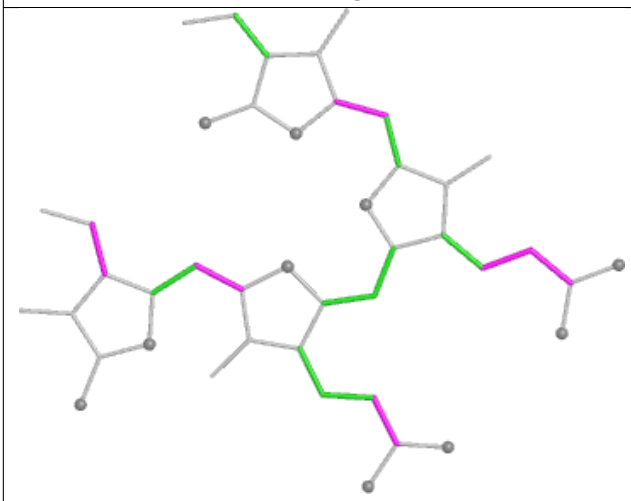


Bond angles



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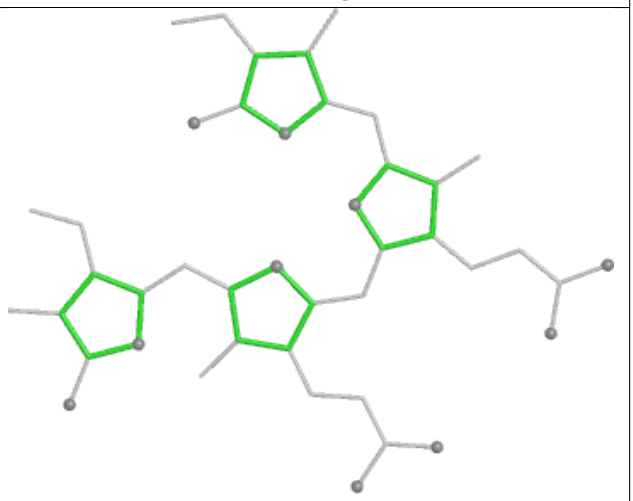
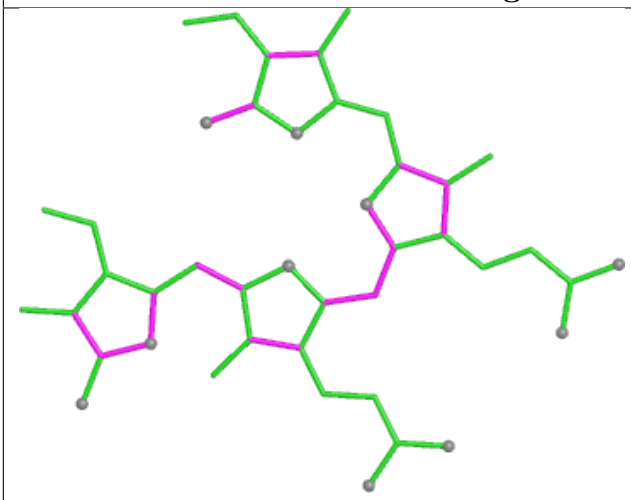


Rings

Ligand PEB GE 1002



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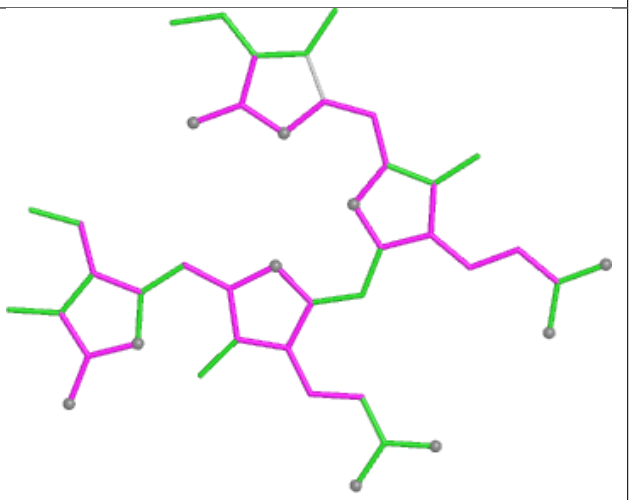
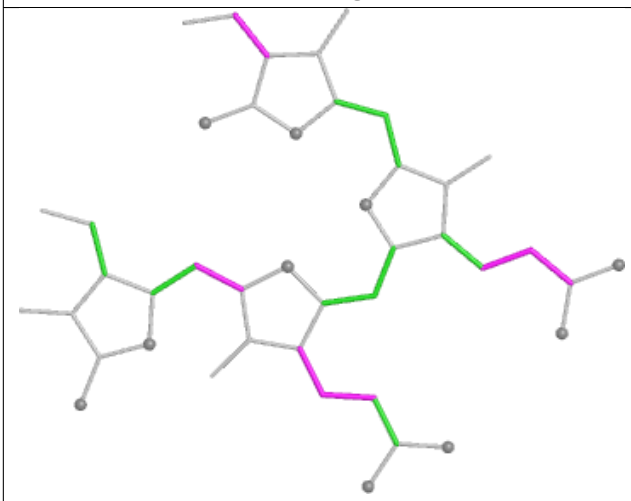


Bond angles



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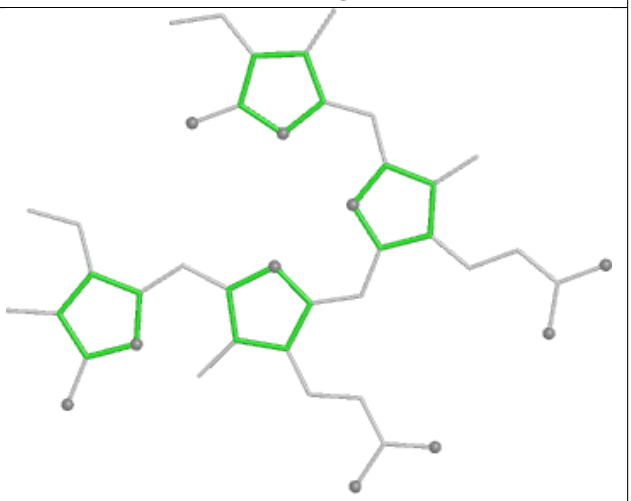
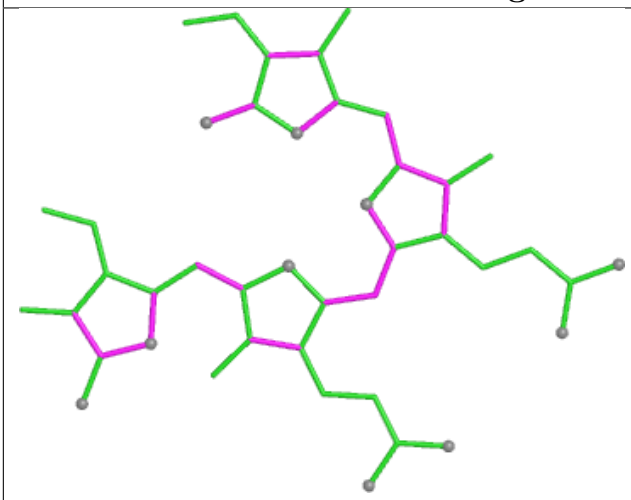


Rings

Ligand PEB TM 201



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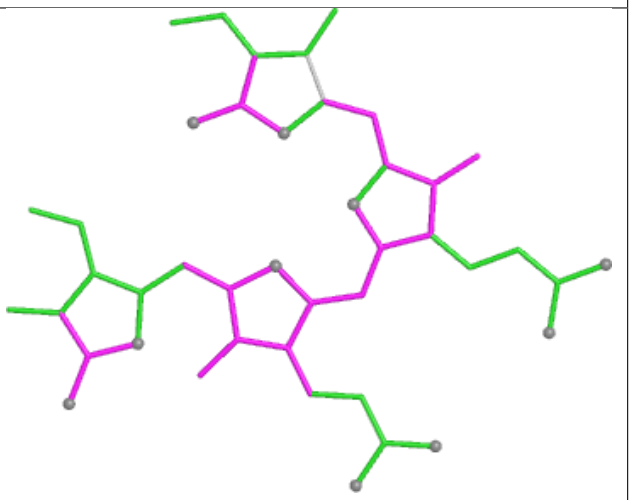
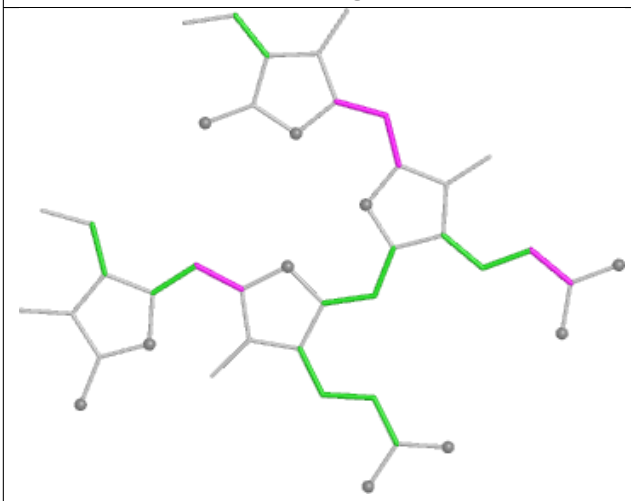


Bond angles



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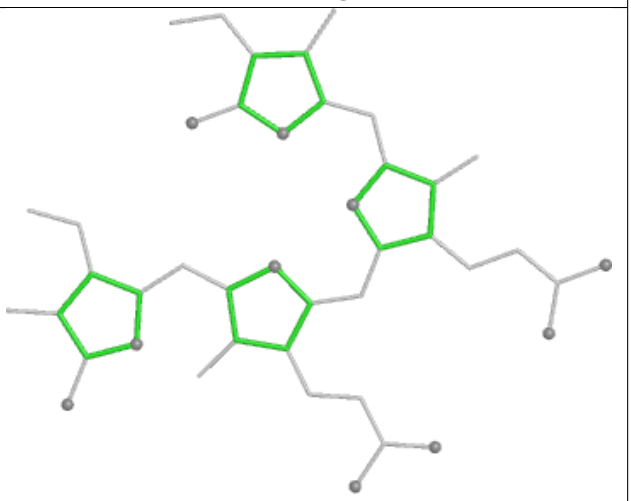
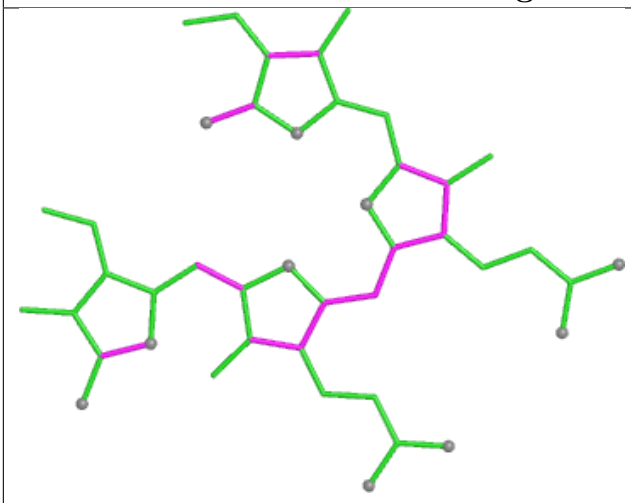


Rings

Ligand PEB hE 203



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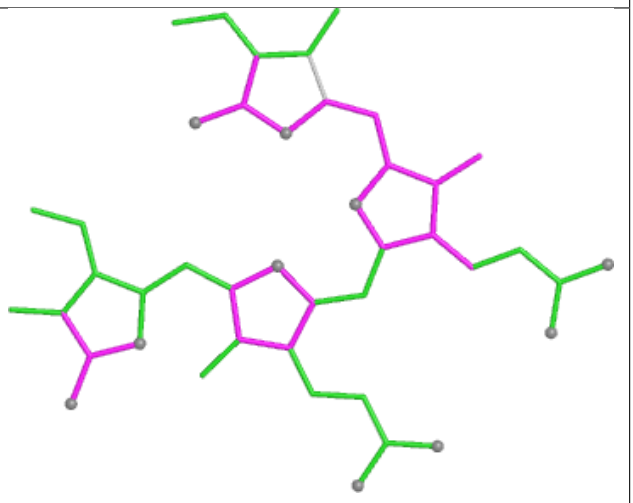
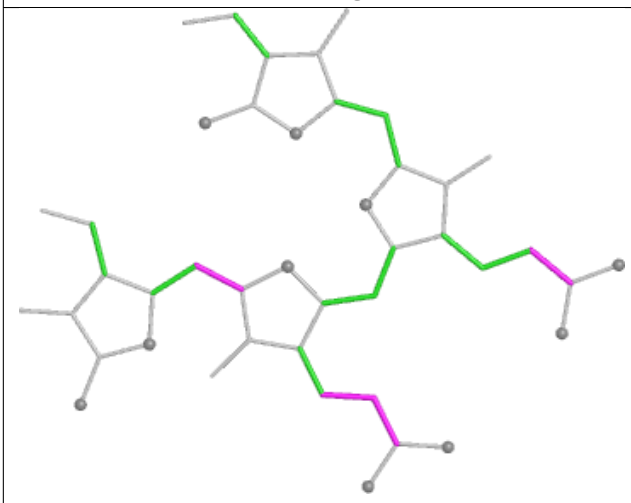


Bond angles



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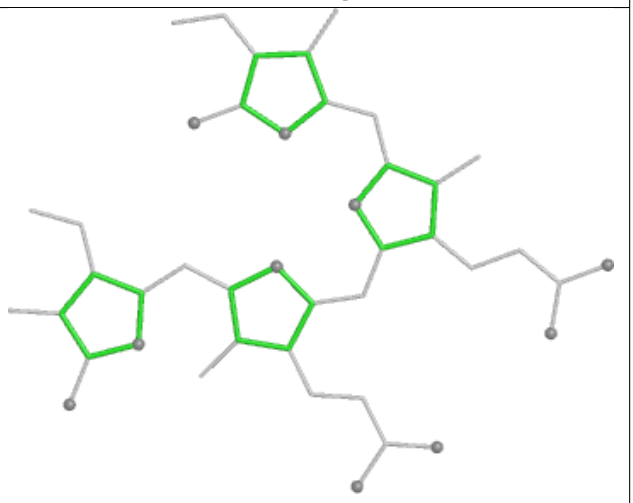
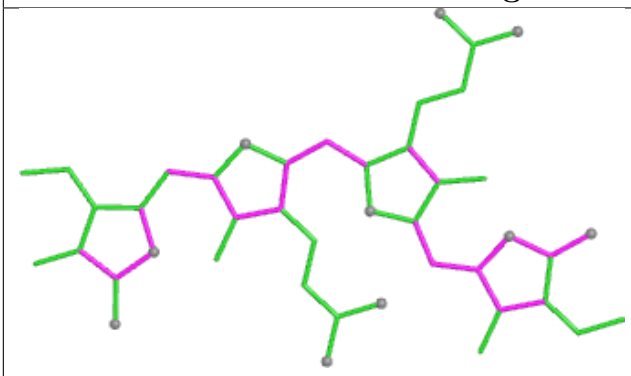


Rings

Ligand CYC H1 1001



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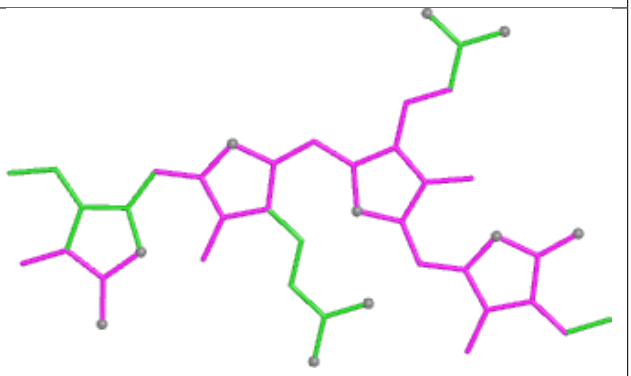
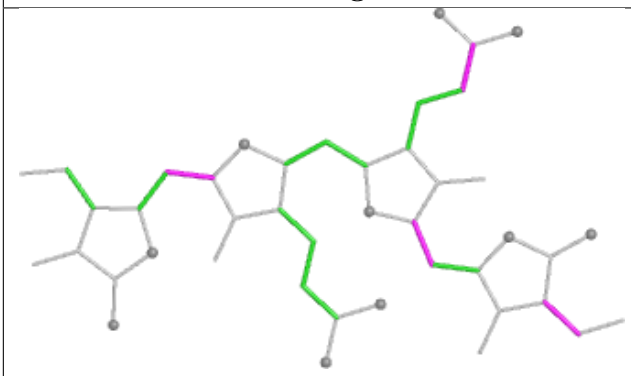


Bond angles



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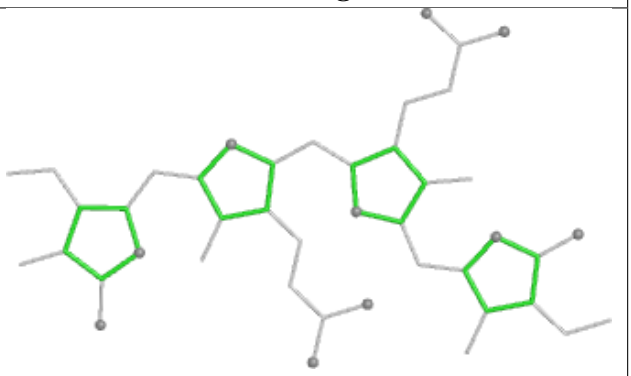
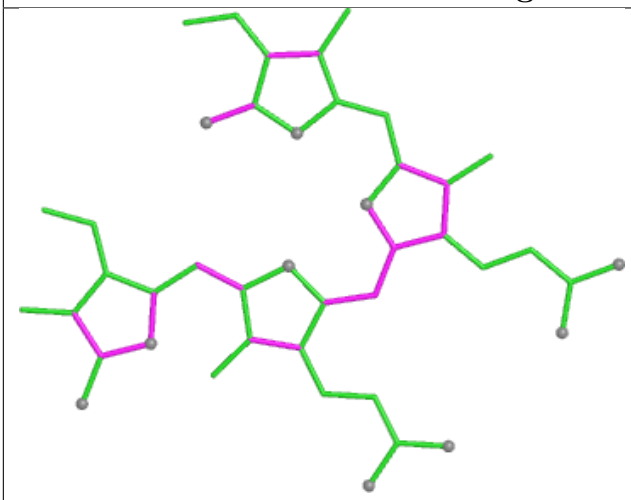


Rings

Ligand PEB P7 201



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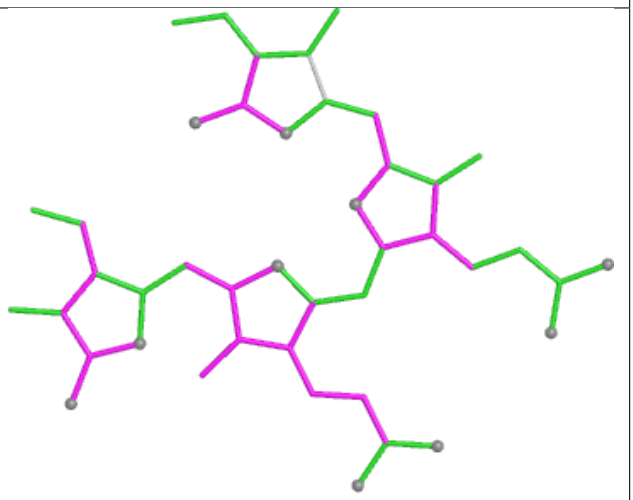

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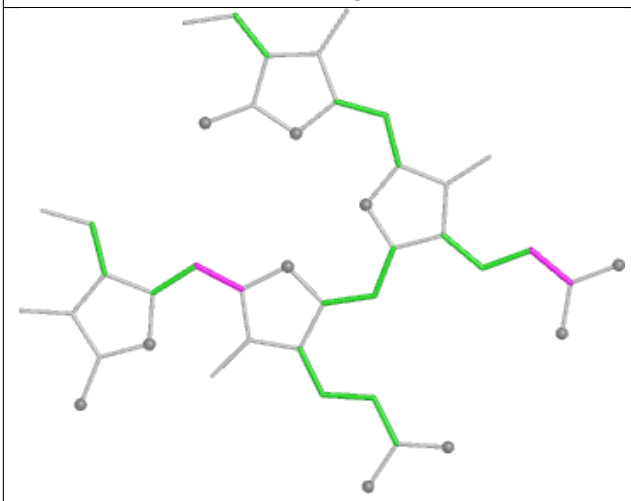
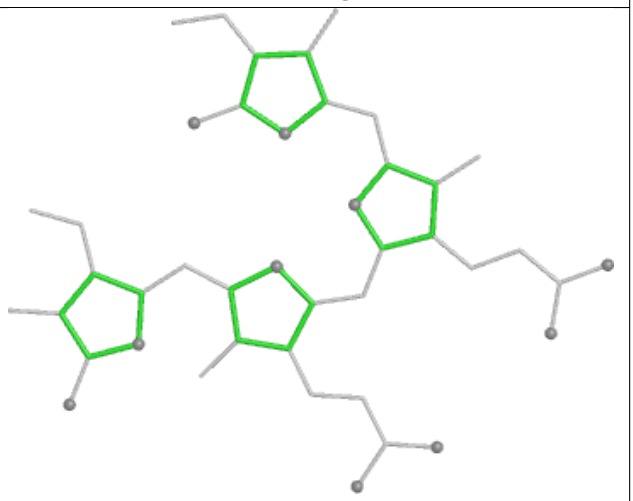
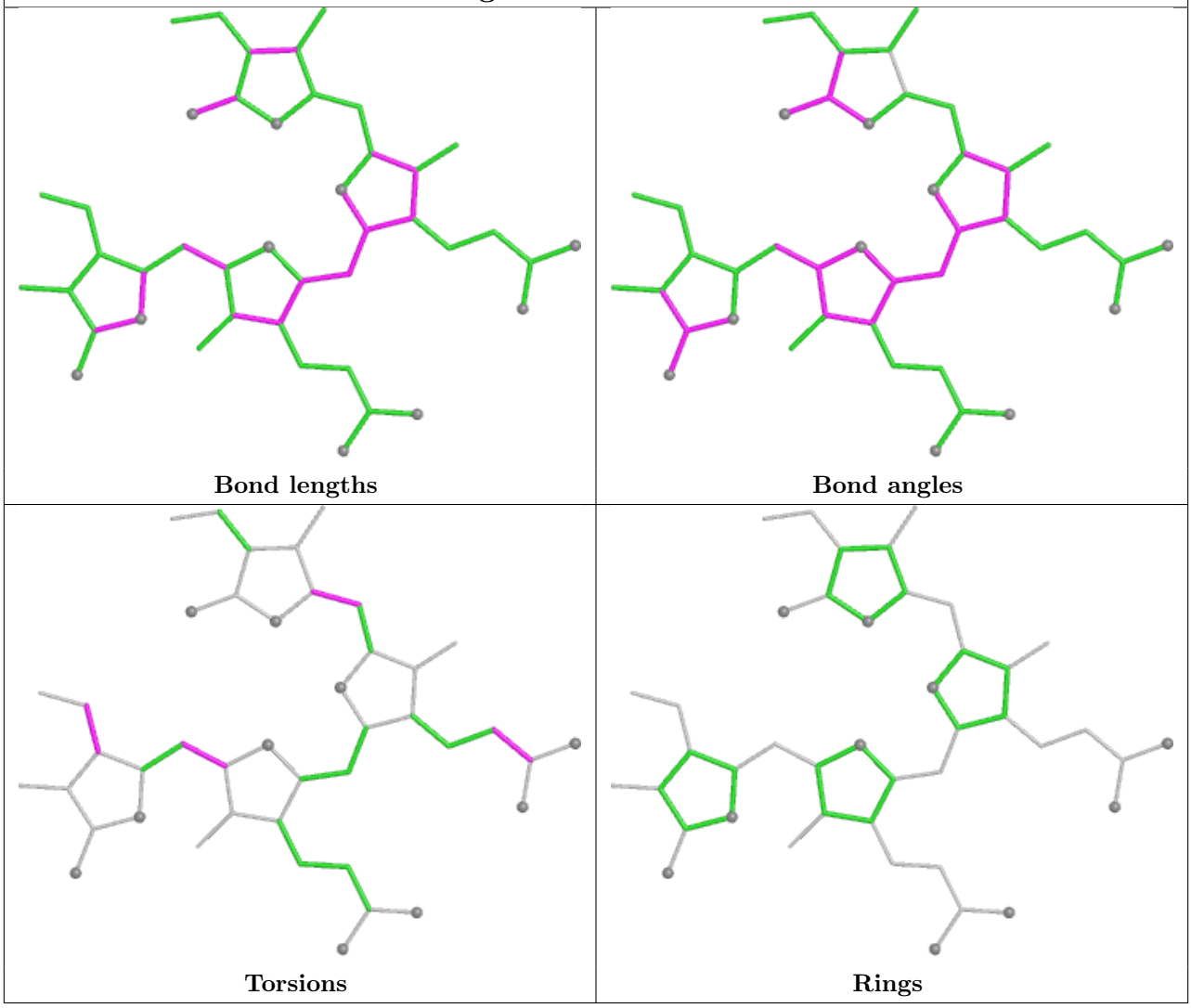


Torsions

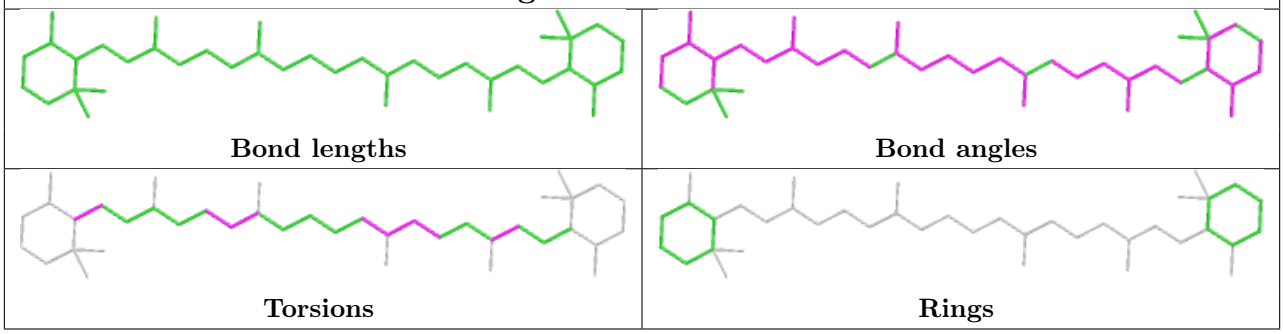


Rings

Ligand PEB U9 204



Ligand BCR k6 102



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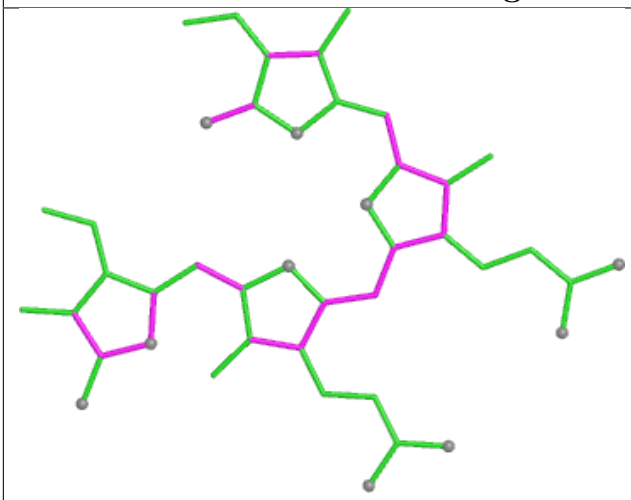

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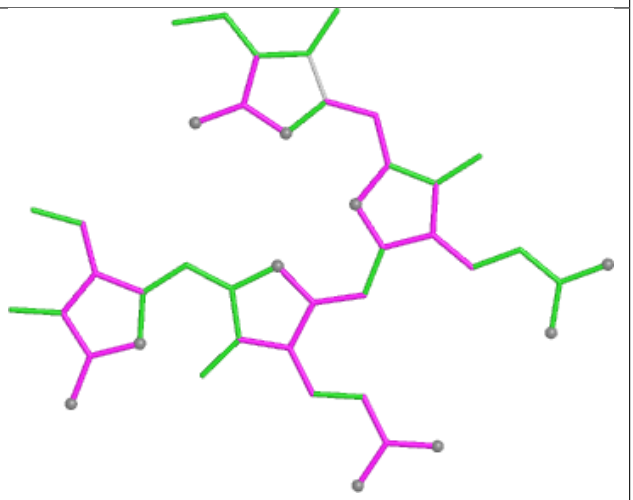

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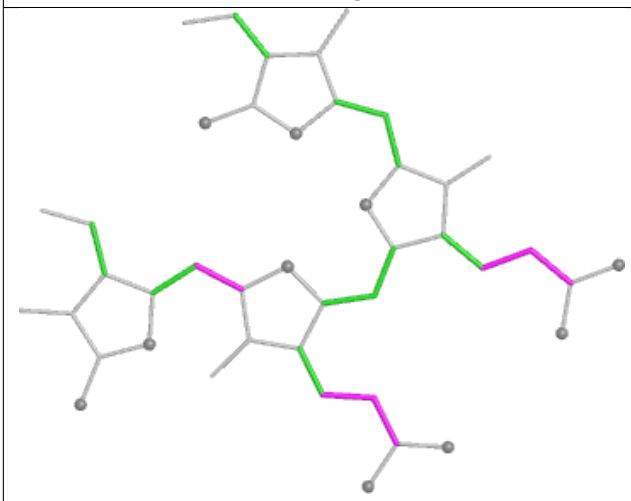

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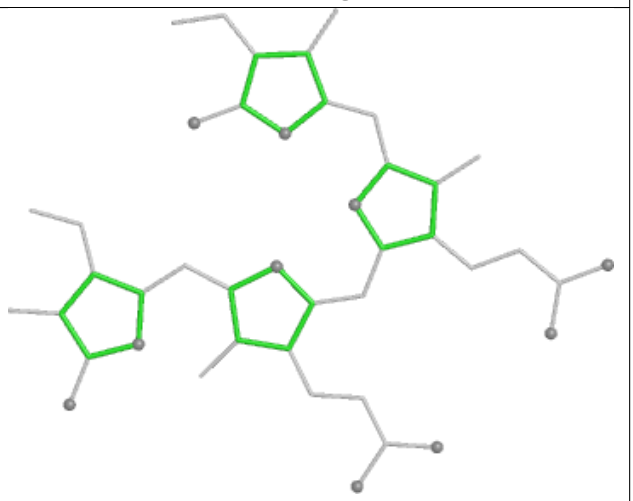
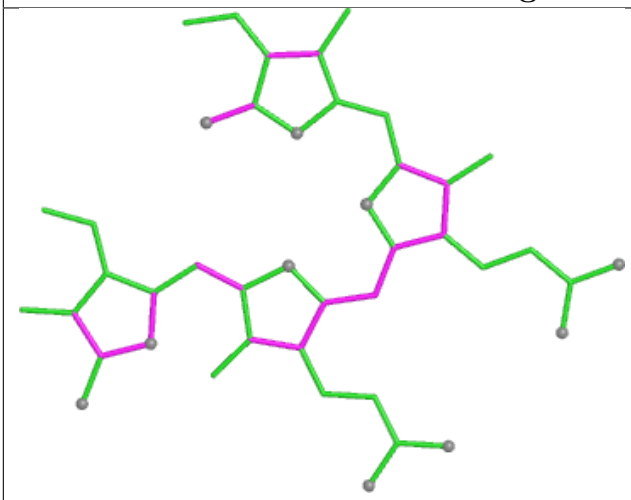


Rings

Ligand PEB gJ 202



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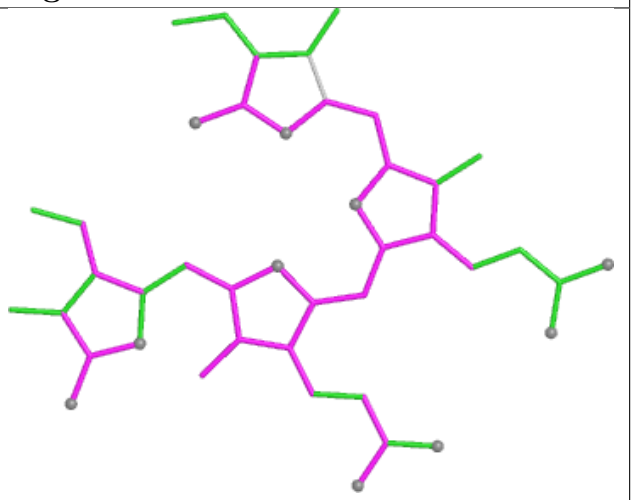

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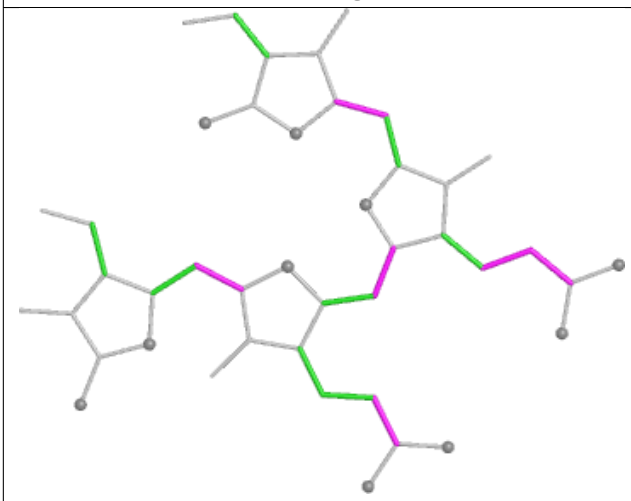

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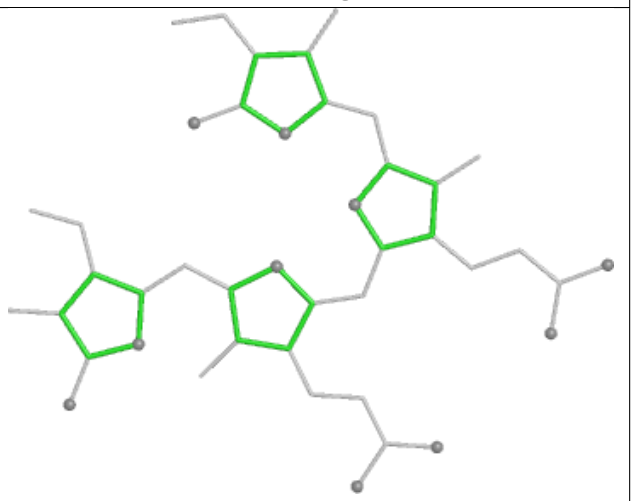
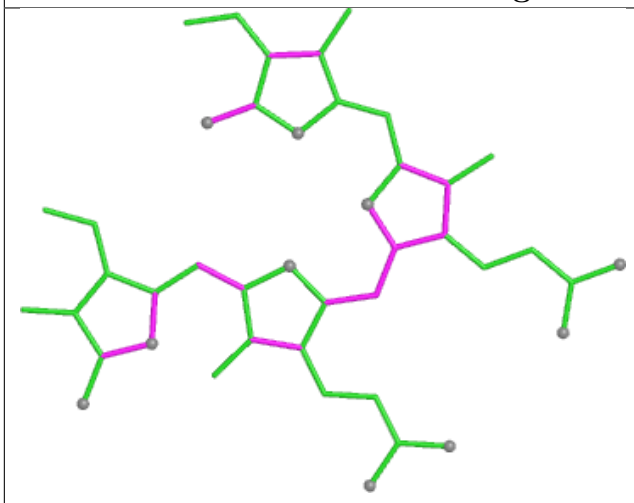


Rings

Ligand PEB PQ 203



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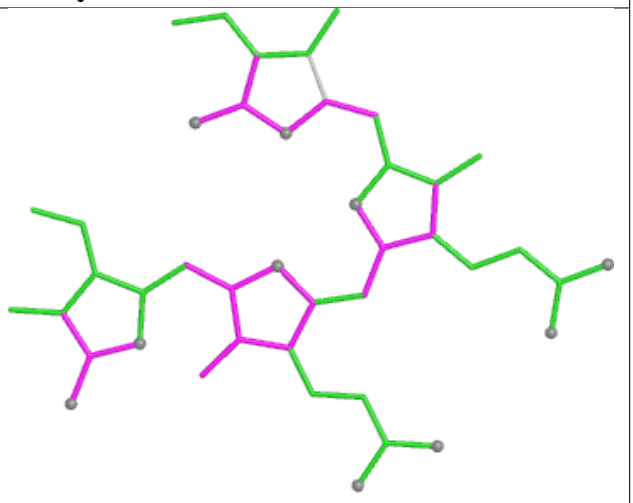

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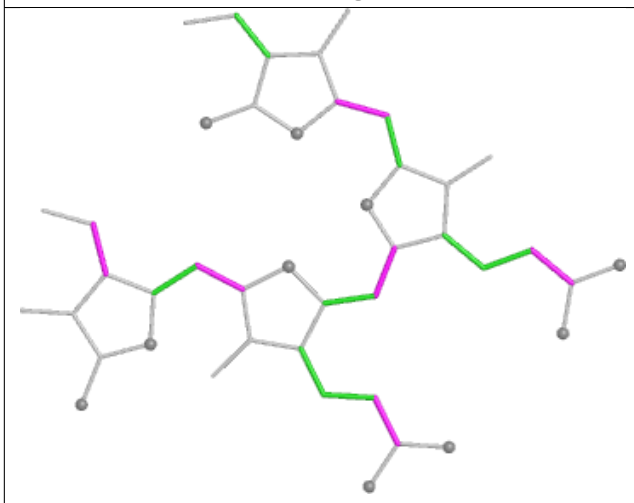

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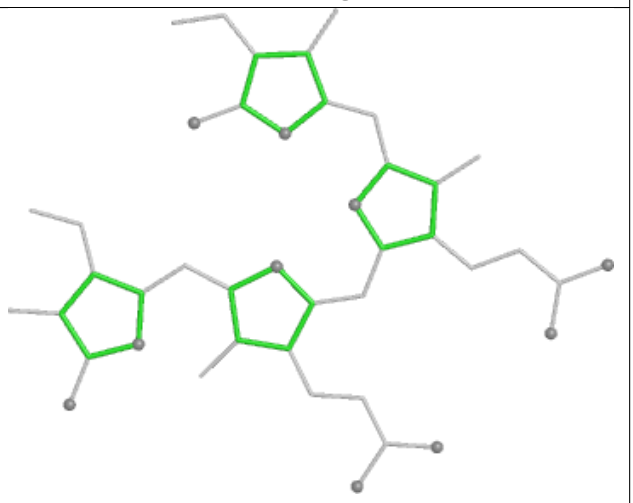

Rings

Ligand BCR b6 603



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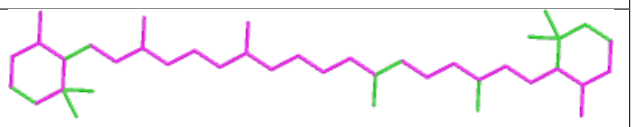

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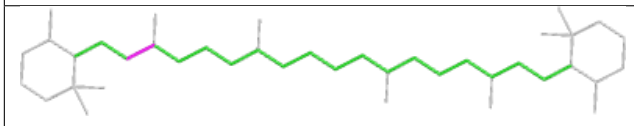

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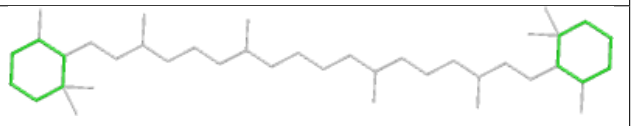
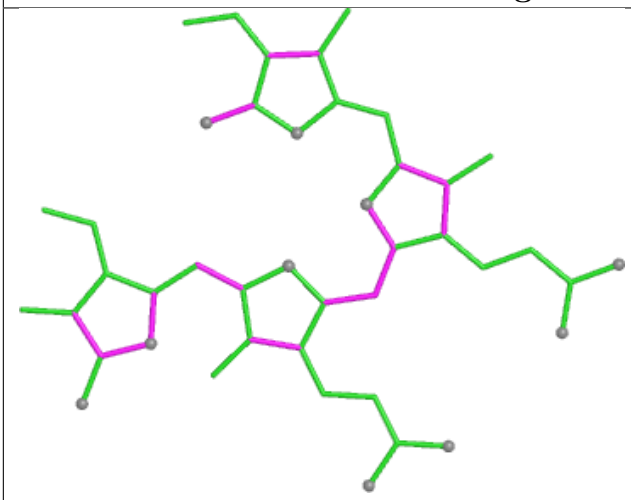


Rings

Ligand PEB dQ 401



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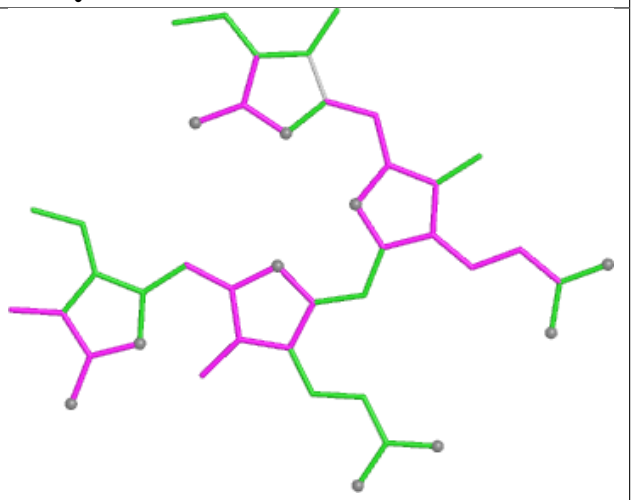

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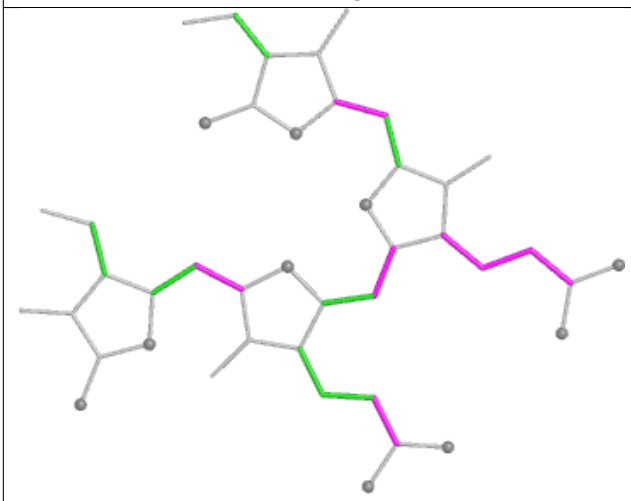

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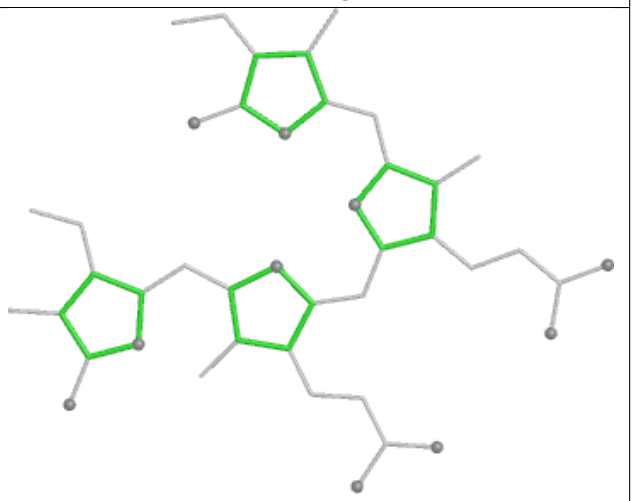
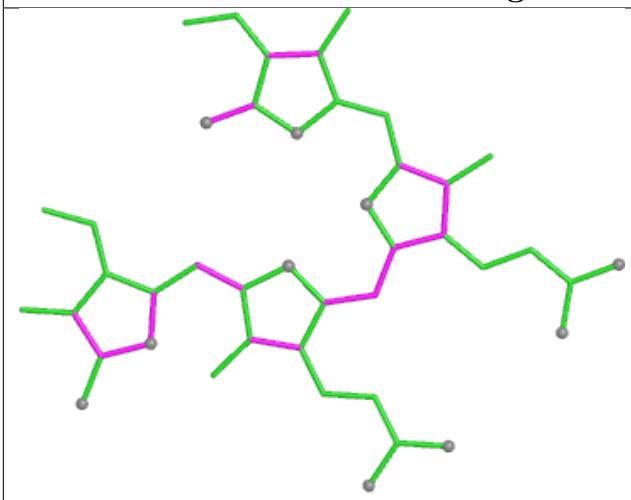


Rings

Ligand PEB YM 201



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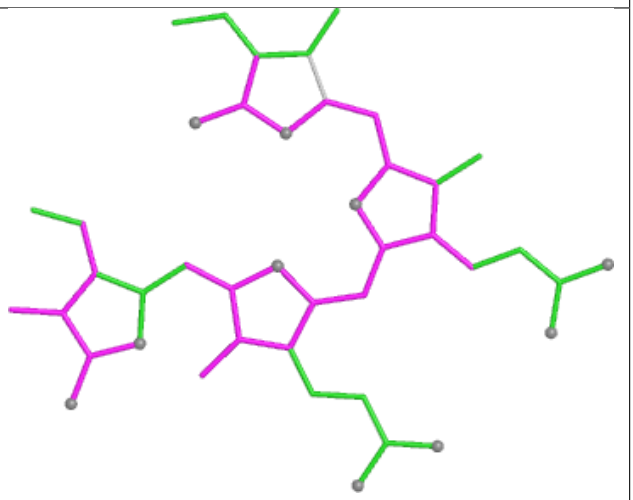

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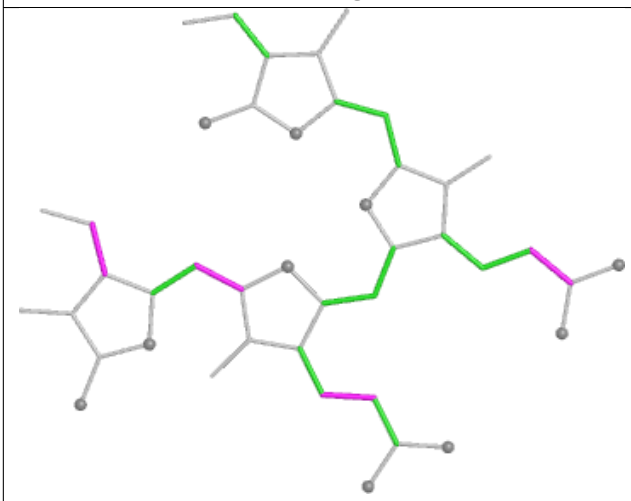

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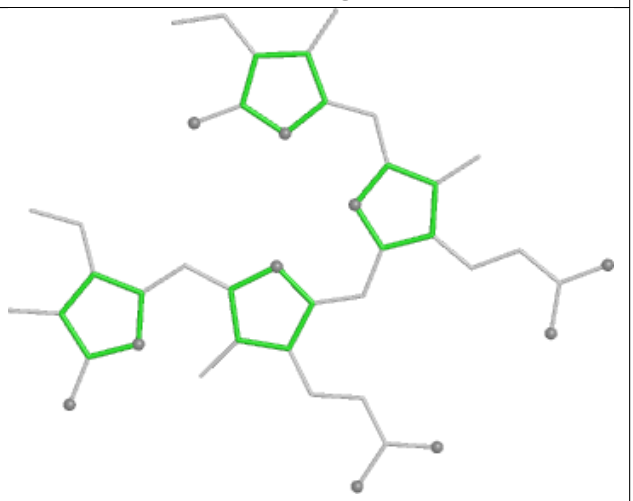

Rings

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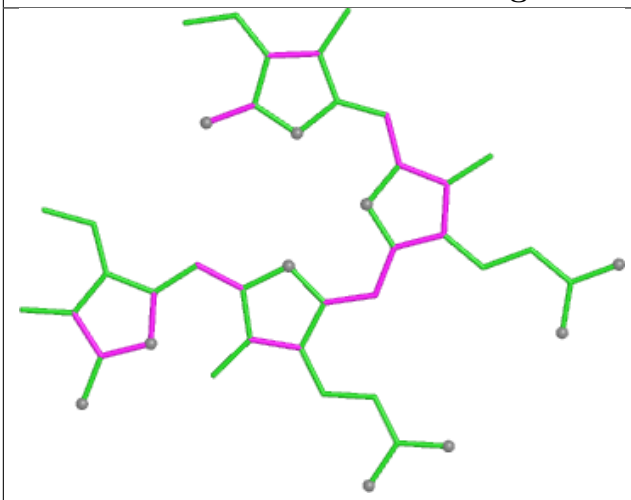

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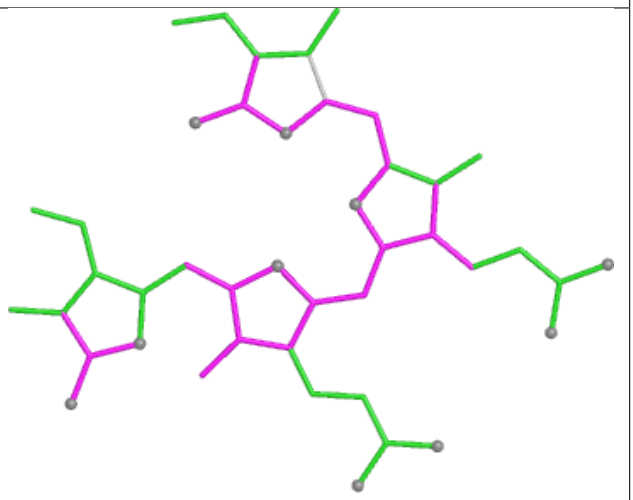

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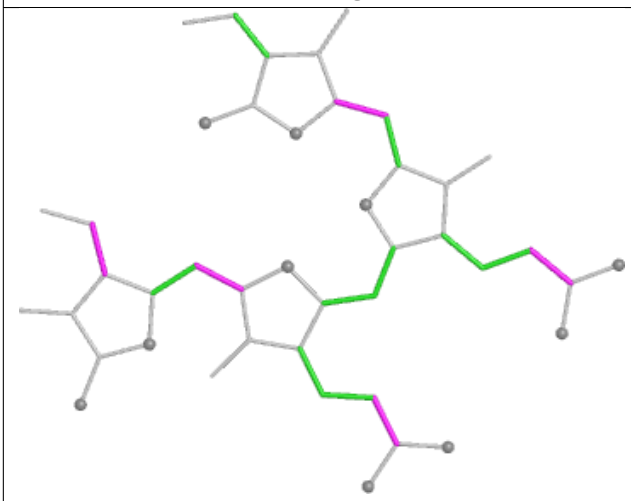

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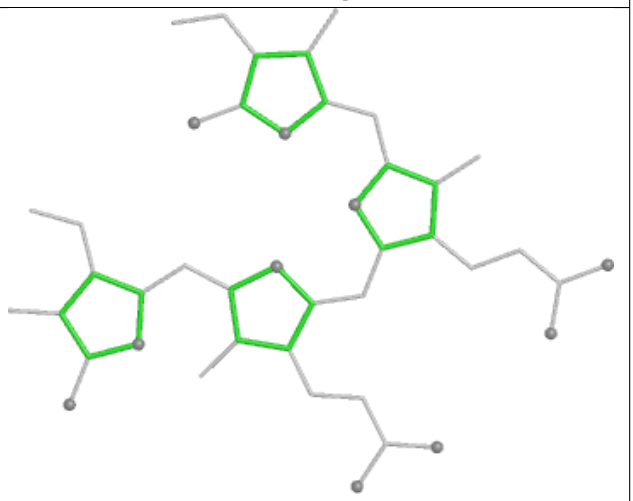
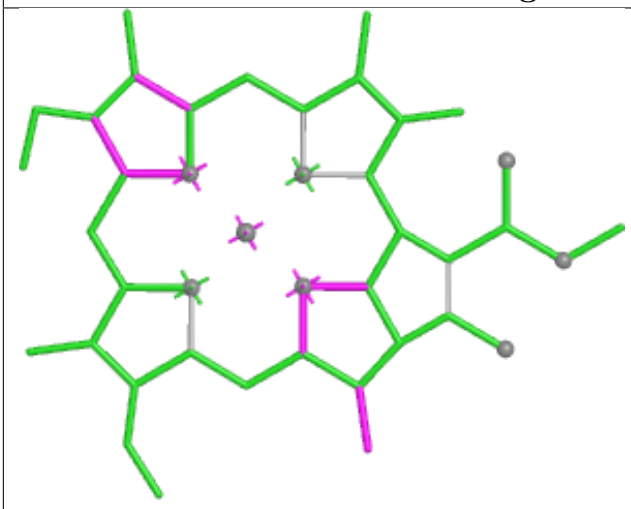


Rings

Ligand CLA 42 609



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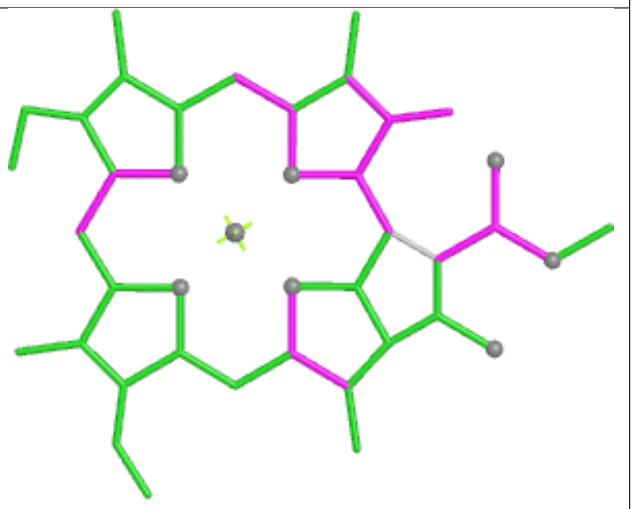

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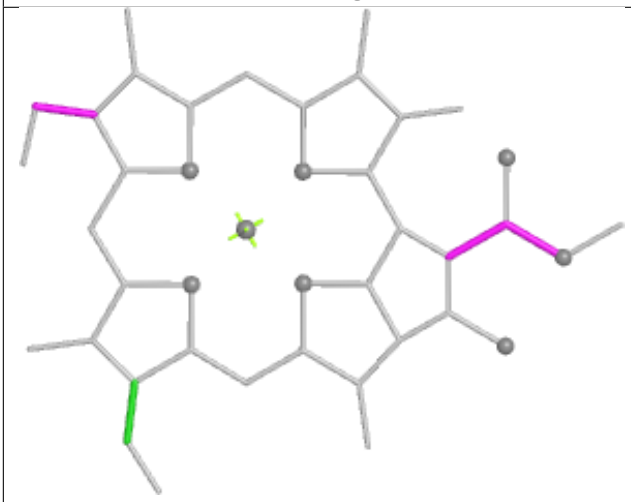

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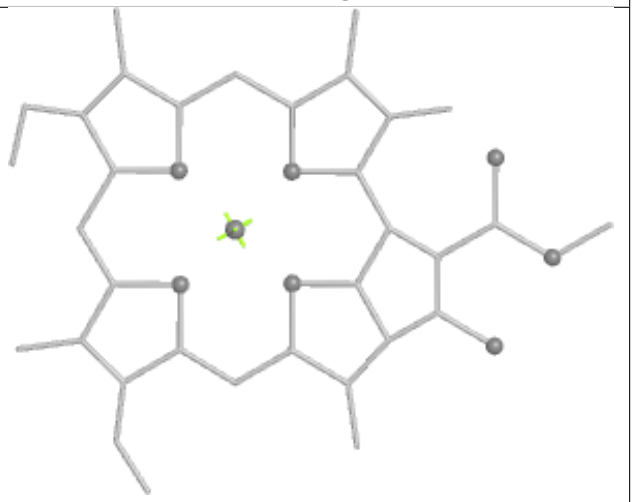
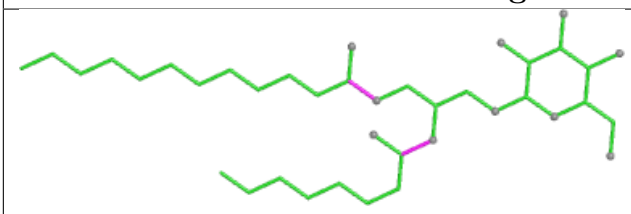


Rings

Ligand LMG BL 612



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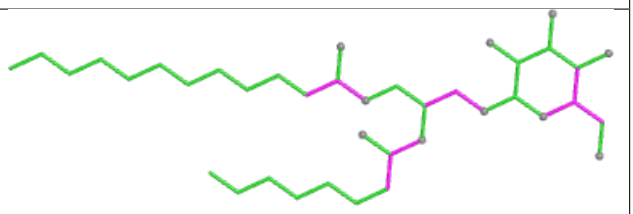

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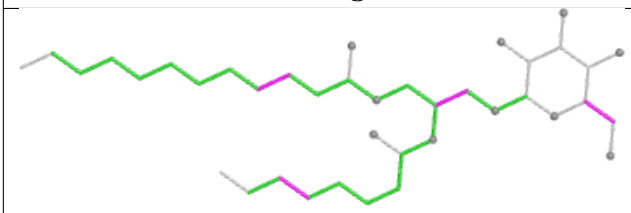

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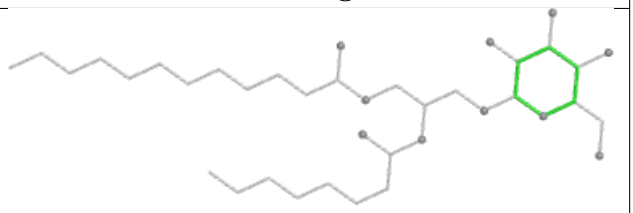
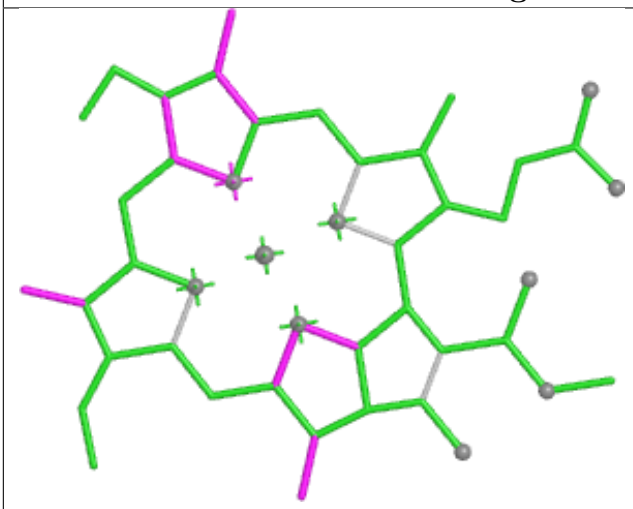


Rings

Ligand CLA AN 836



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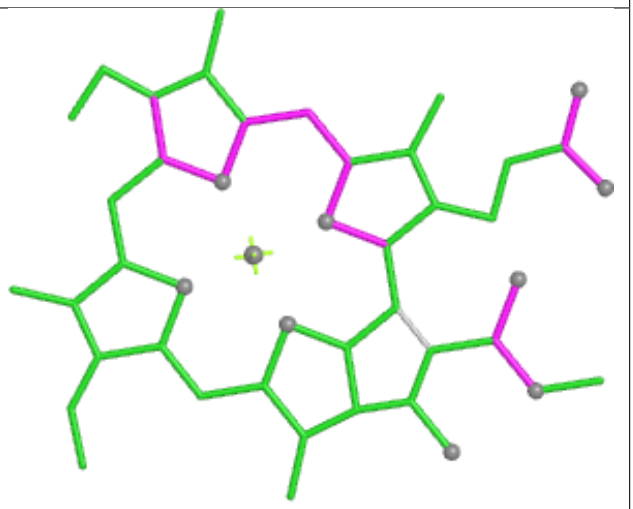

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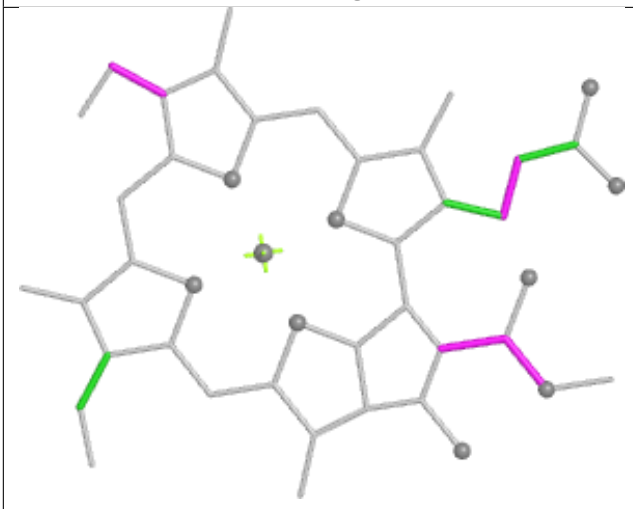
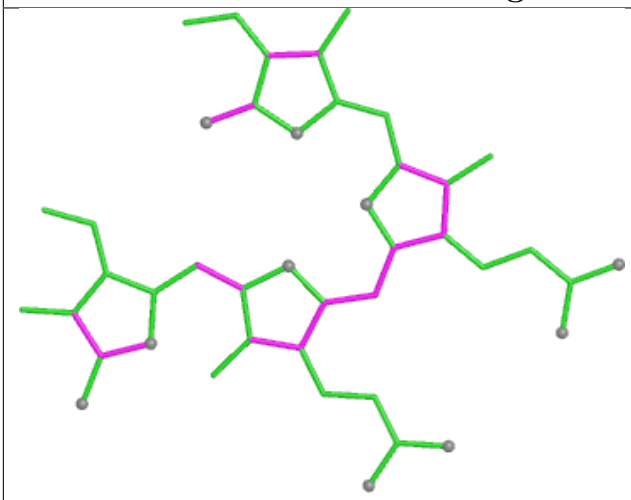


Torsions



Rings

Ligand PEB MK 202



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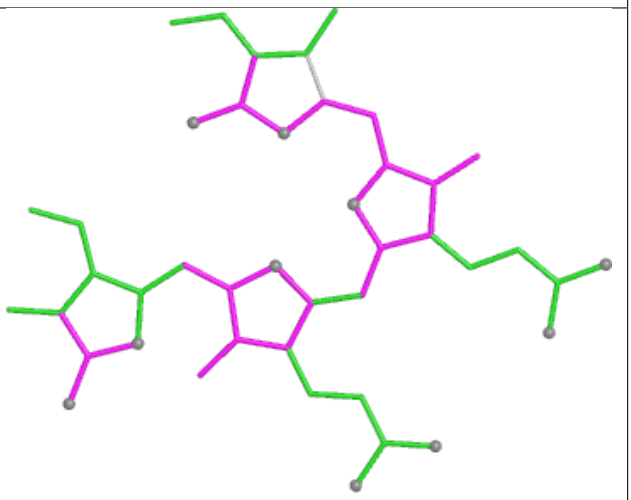

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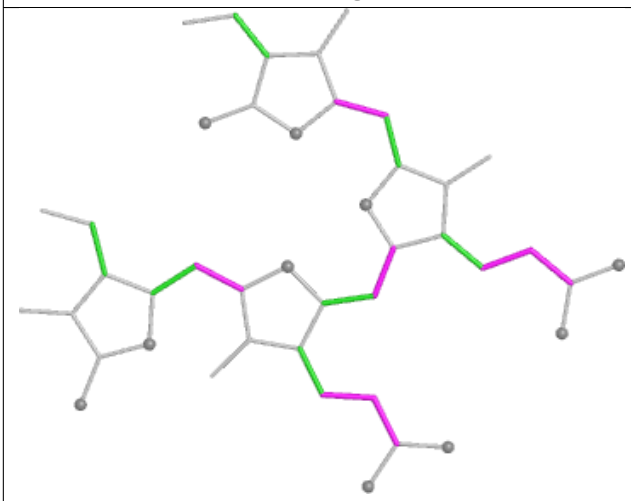

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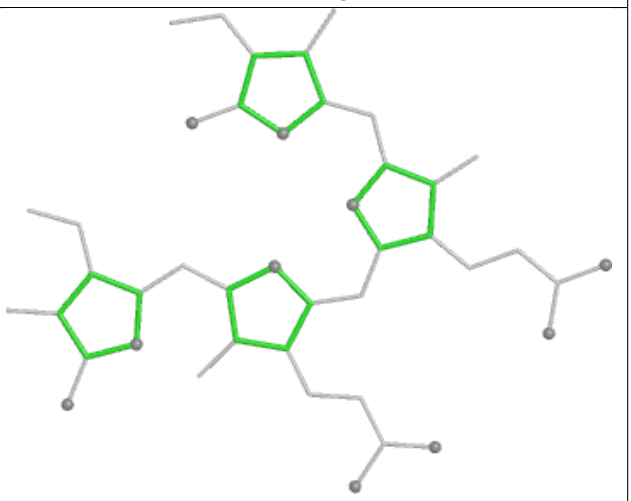
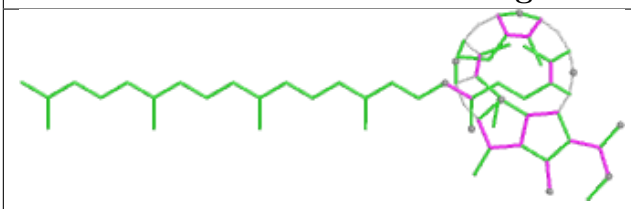


Rings

Ligand PHO aL 610



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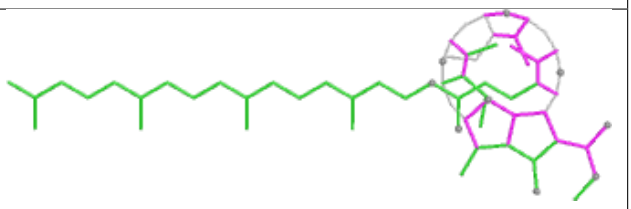
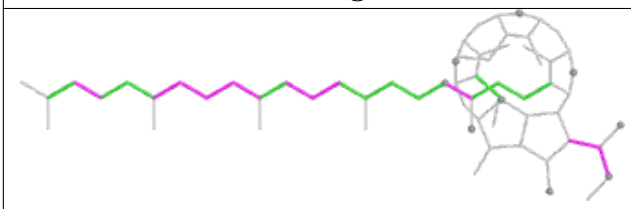


Bond angles



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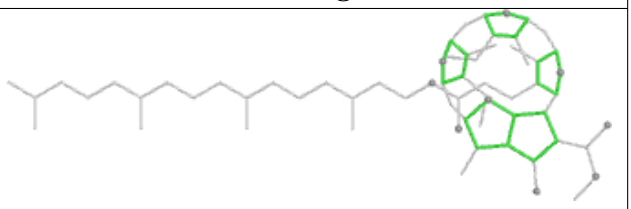
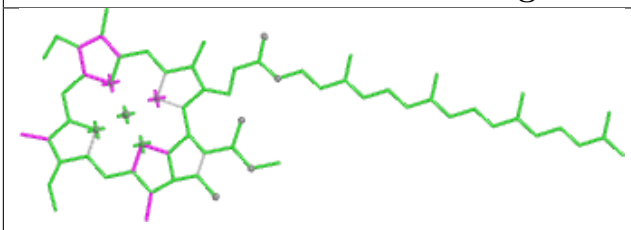


Rings

Ligand CLA b6 605



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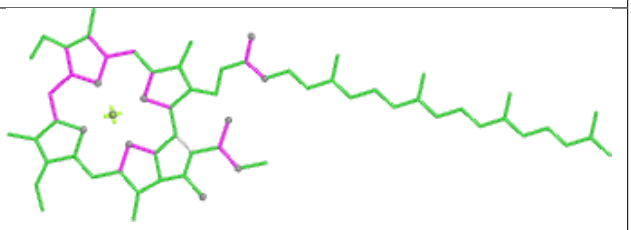
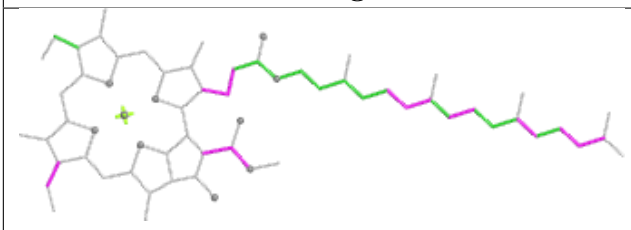


Bond angles



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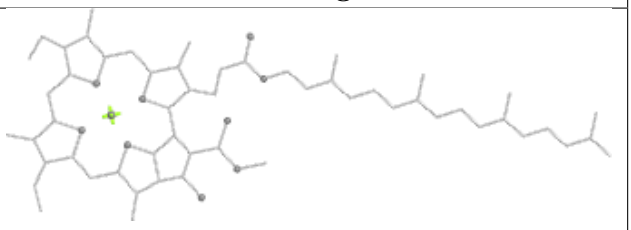
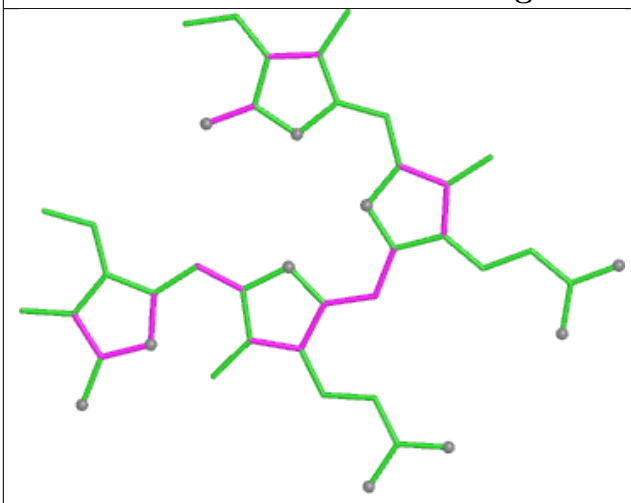


Rings

Ligand PEB D5 202



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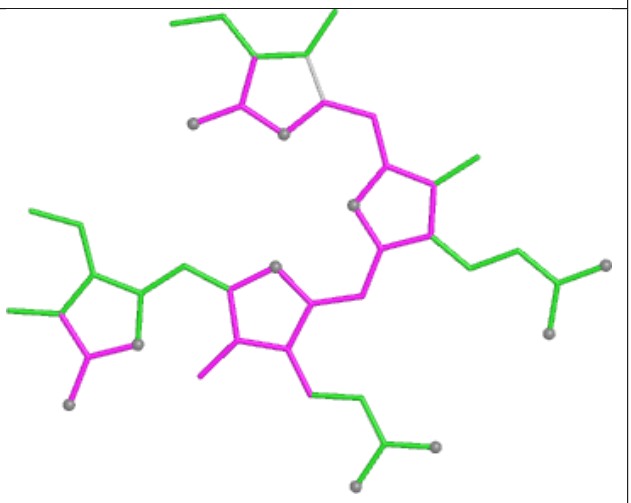
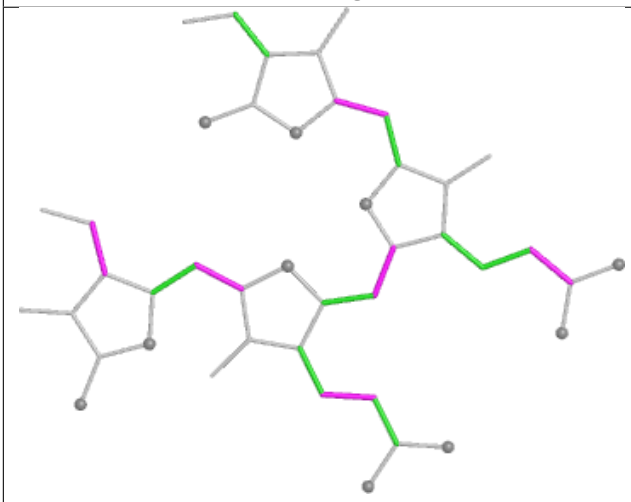
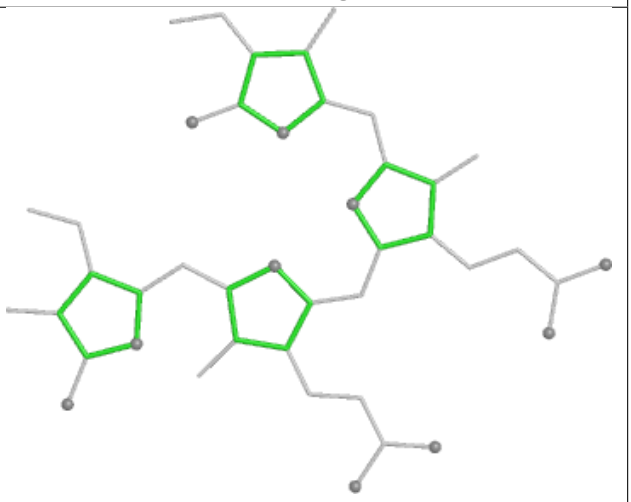


Bond angles

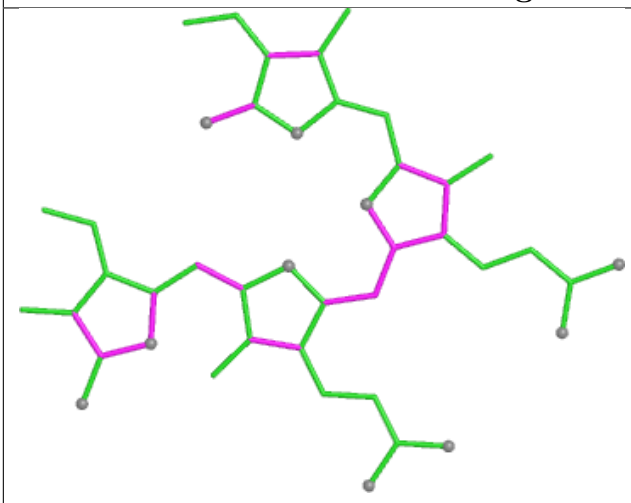


Torsions



Rings

Ligand PEB R7 203



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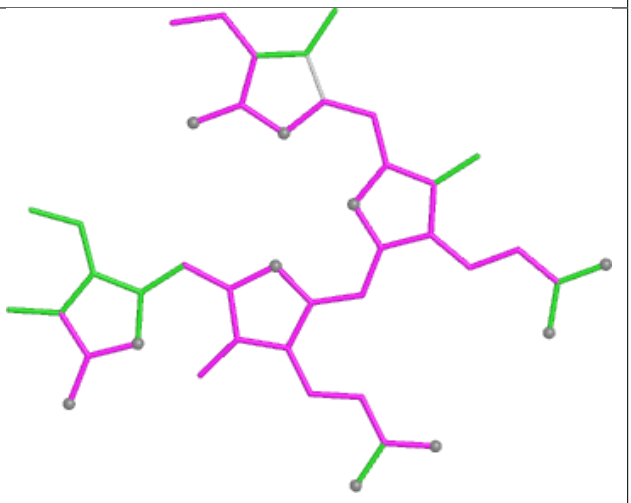
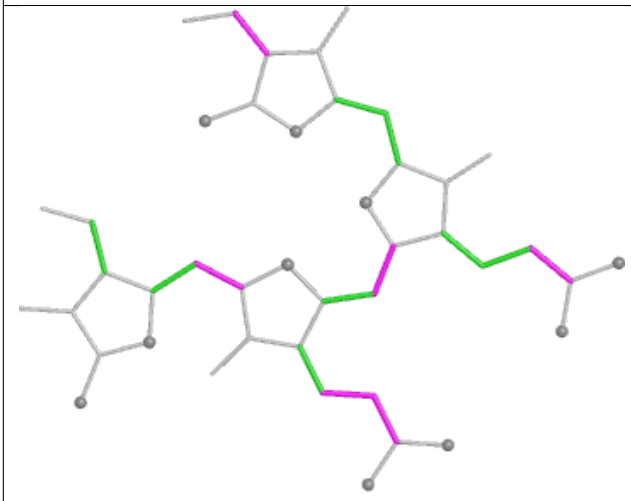


Bond angles



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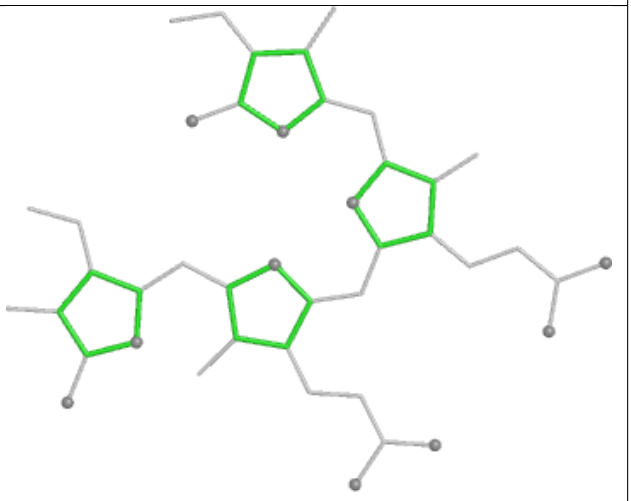
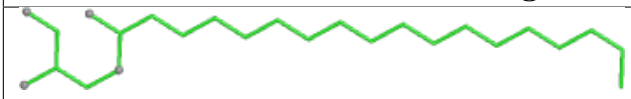


Rings

Ligand 3XQ J2 104



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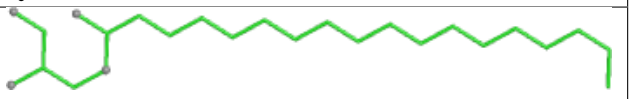

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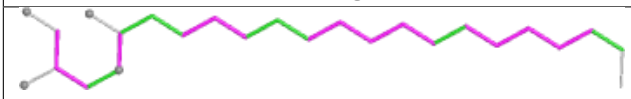

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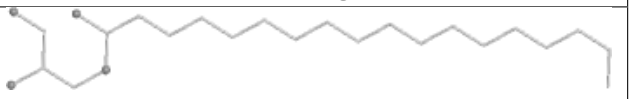
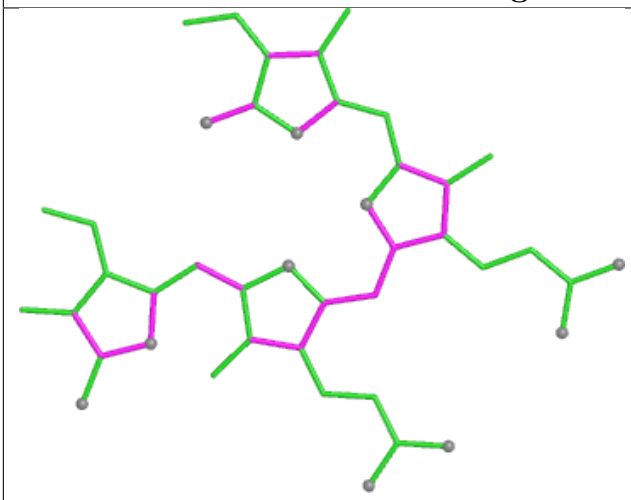


Rings

Ligand PEB QQ 202



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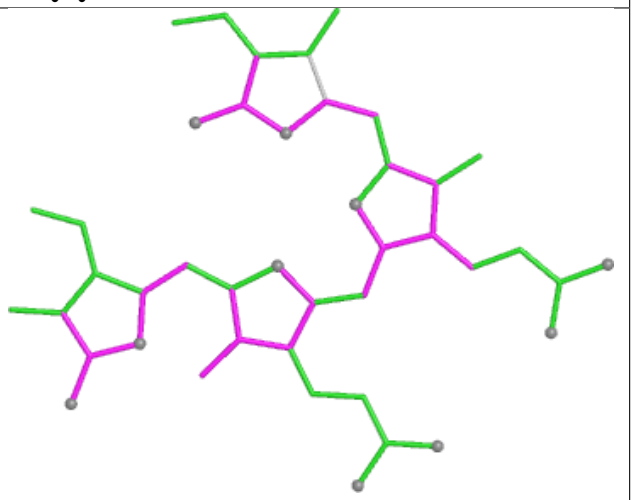

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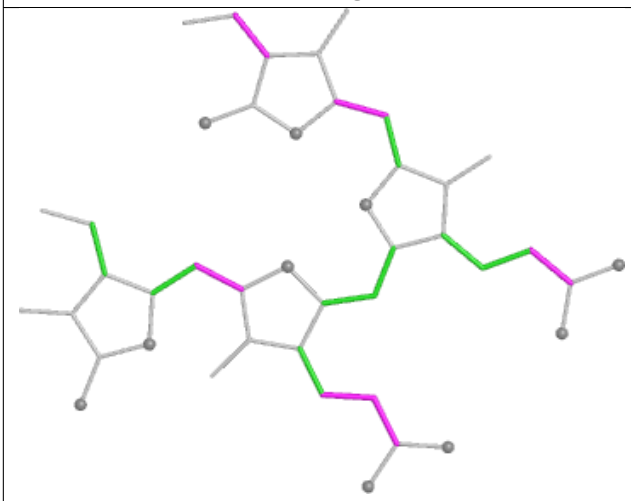

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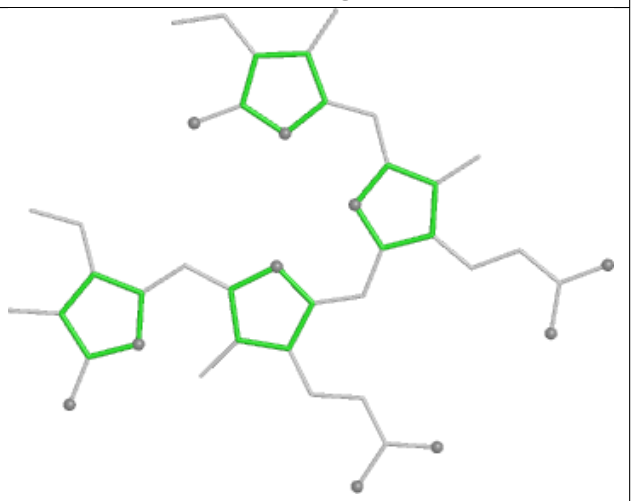
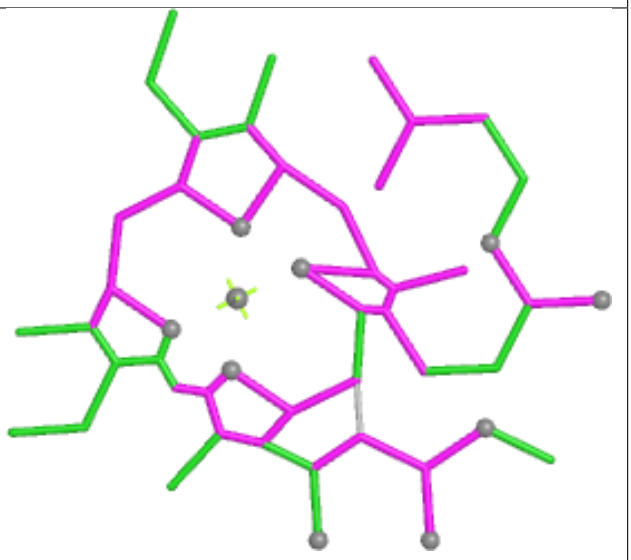


Rings

Ligand CLA 62 309



Bond lengths



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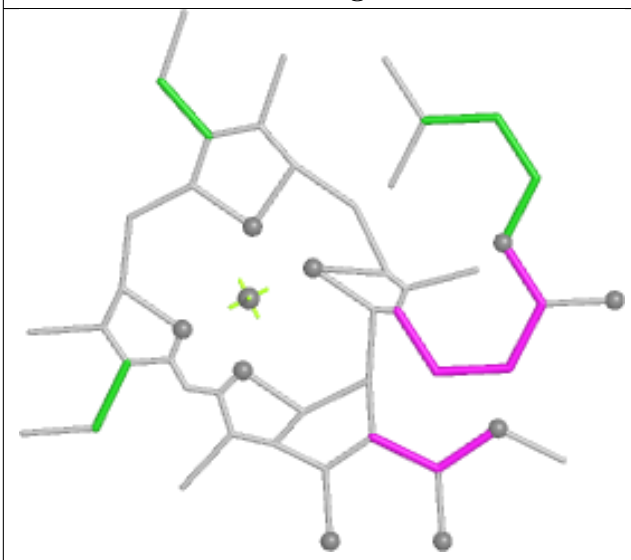

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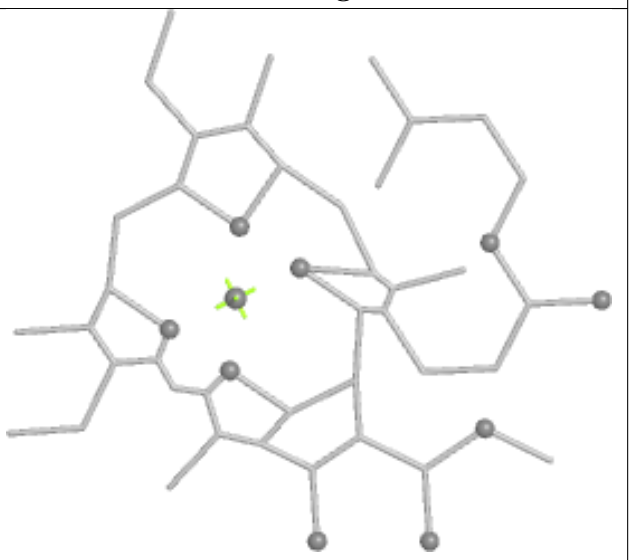
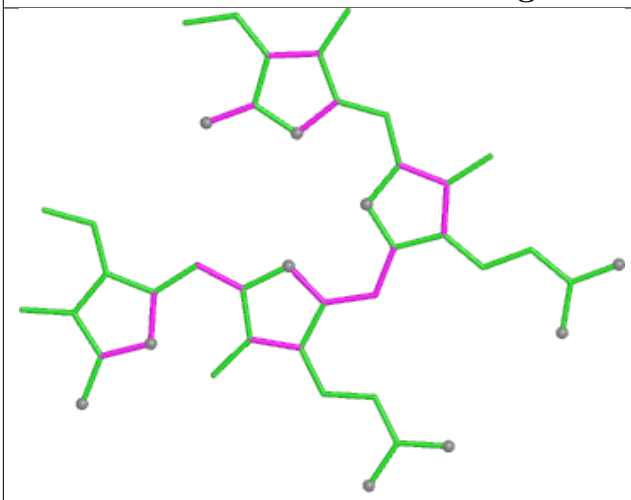


Rings

Ligand PEB OI 202



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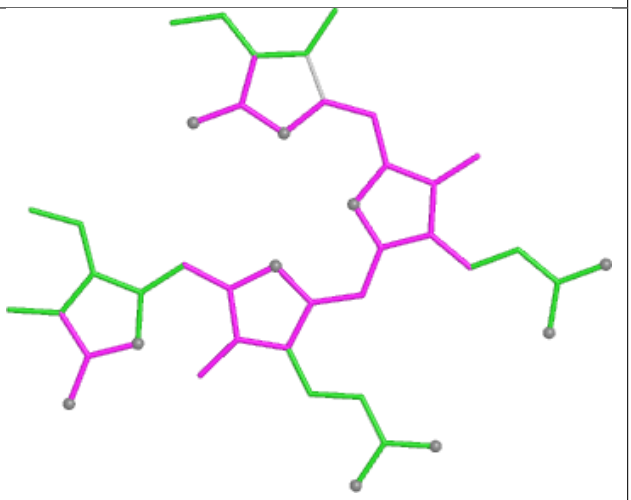

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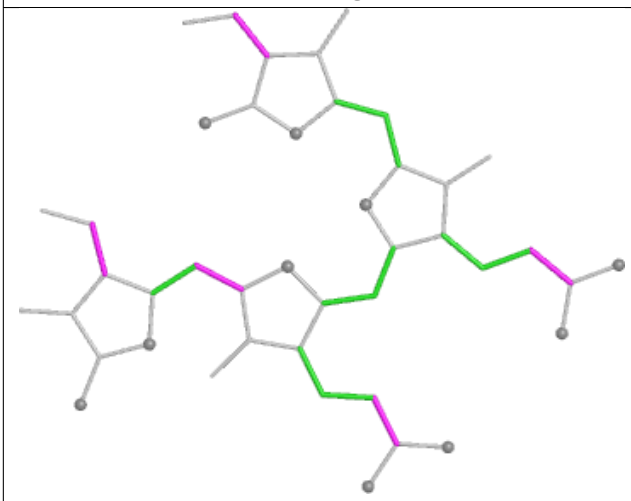

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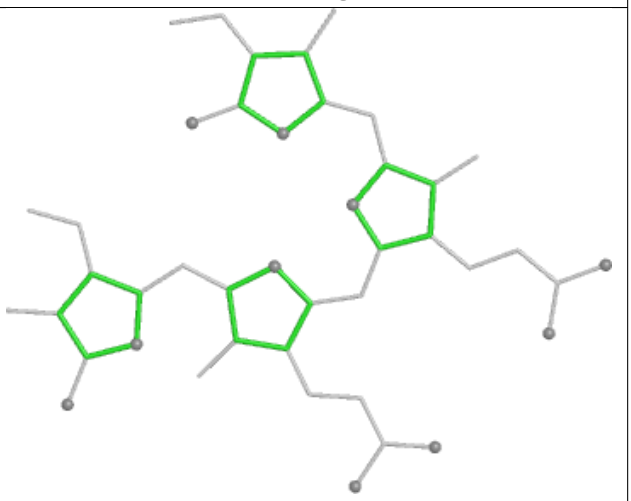
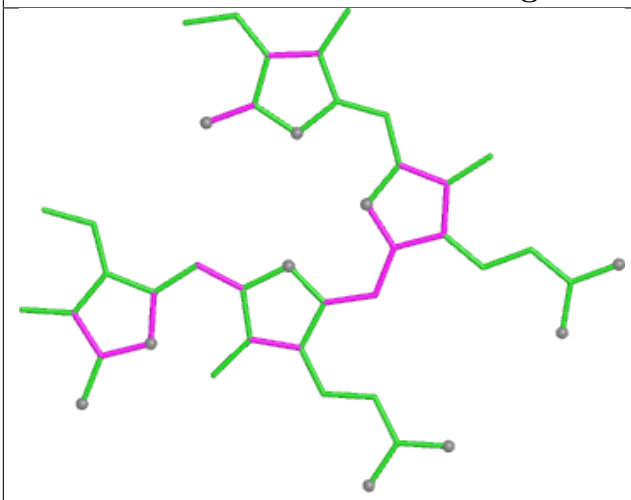


Rings

Ligand PEB c1 201



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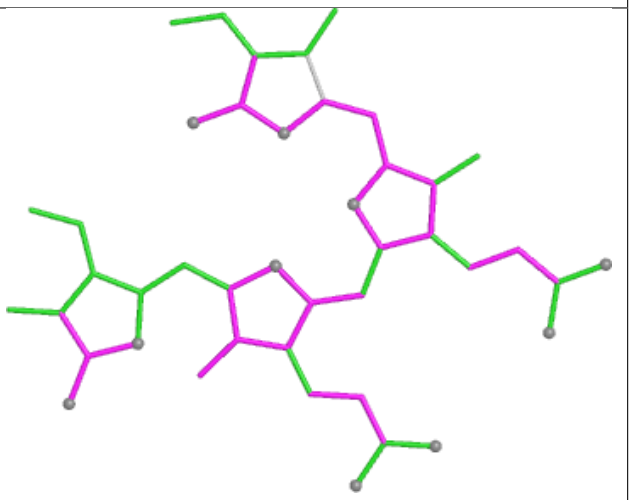

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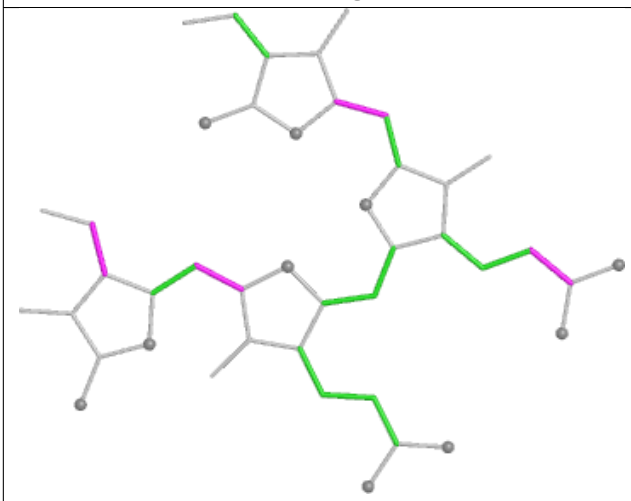

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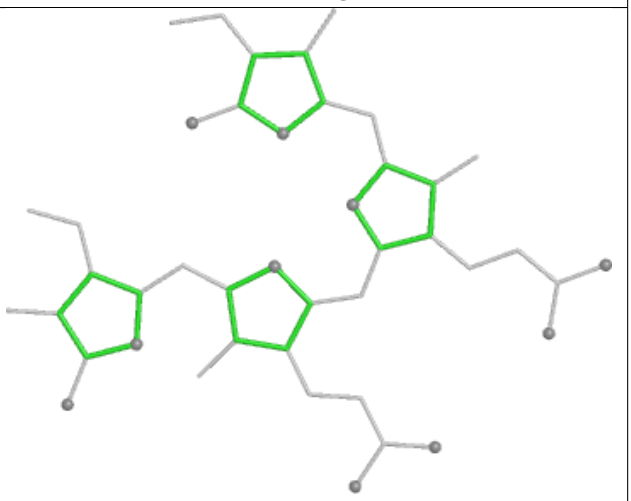
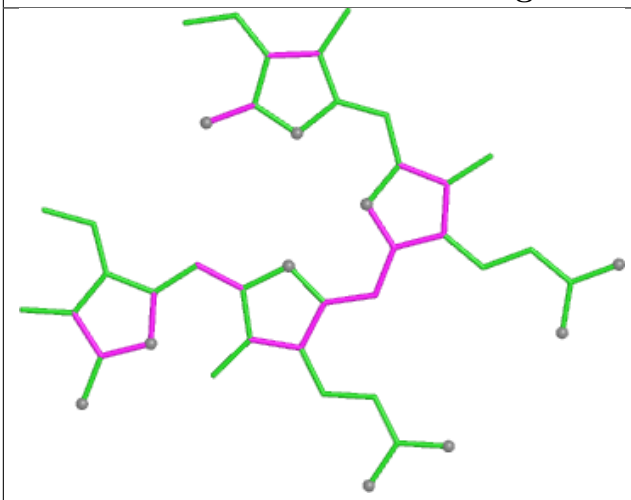


Rings

Ligand PEB lM 203



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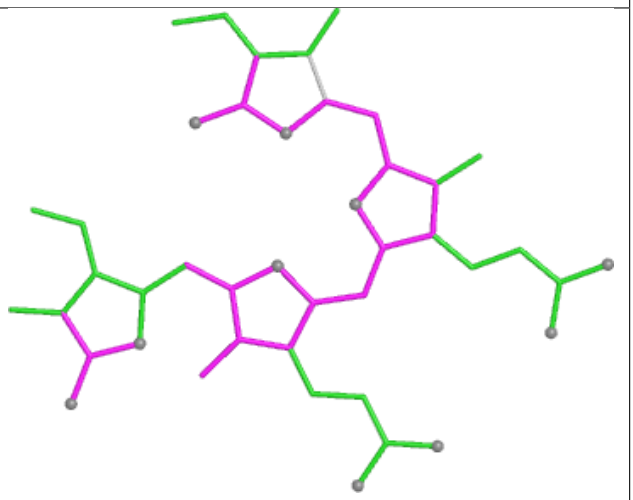

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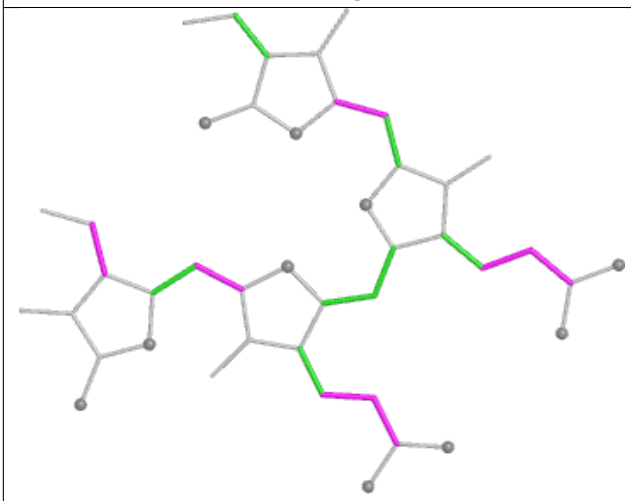

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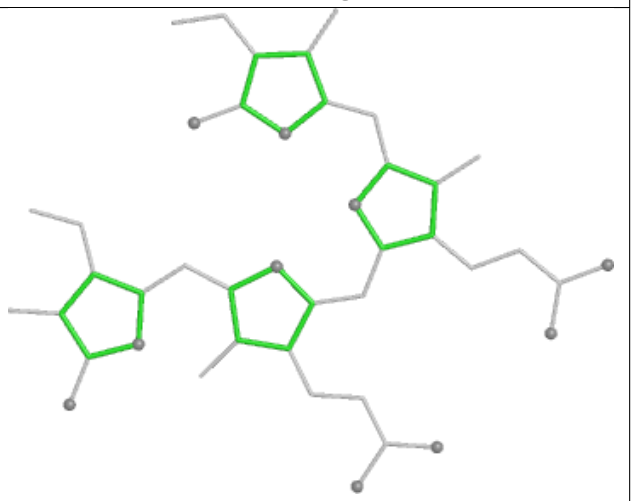
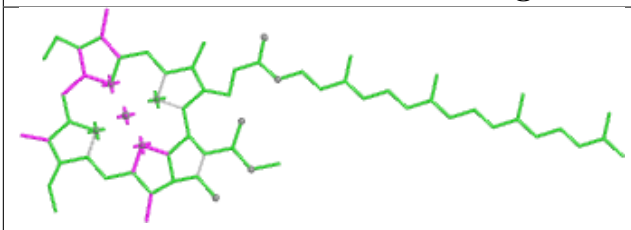


Rings

Ligand CLA A2 811



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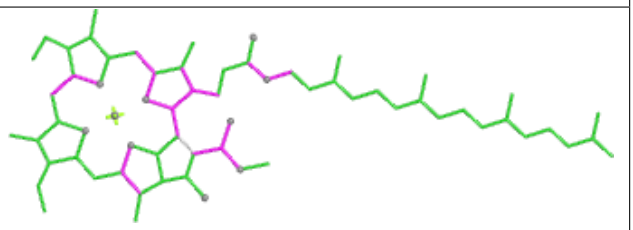

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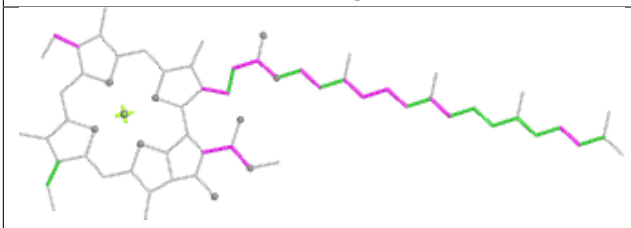

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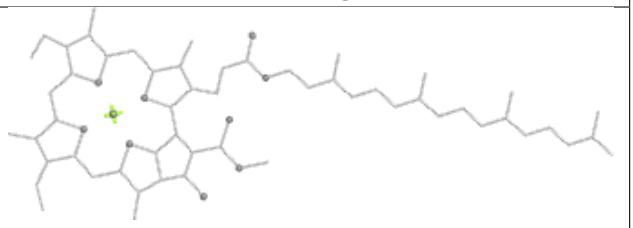
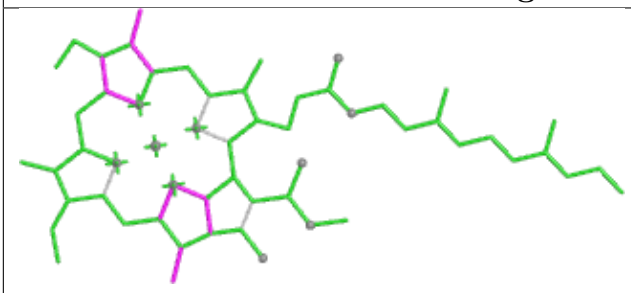


Rings

Ligand CLA L2 202



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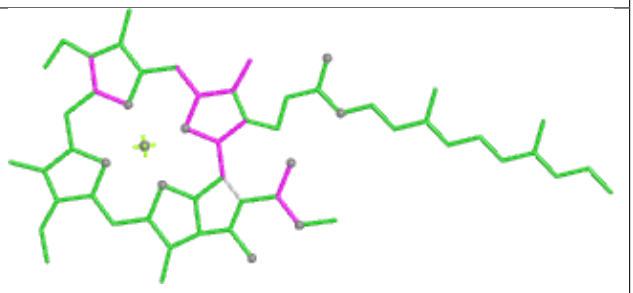
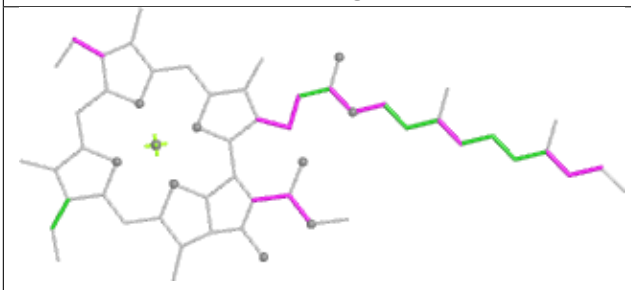


Bond angles



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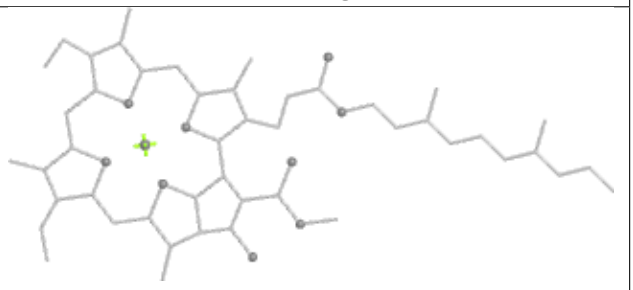
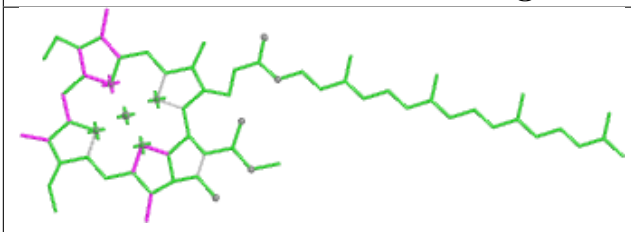


Rings

Ligand CLA bL 608



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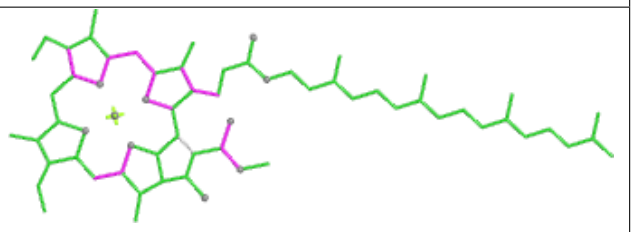
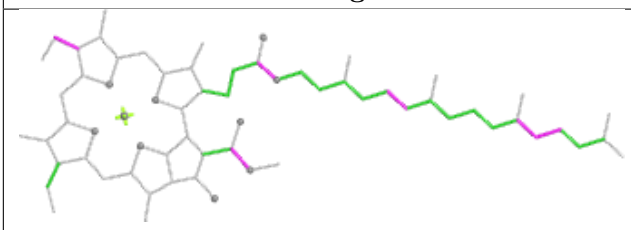


Bond angles



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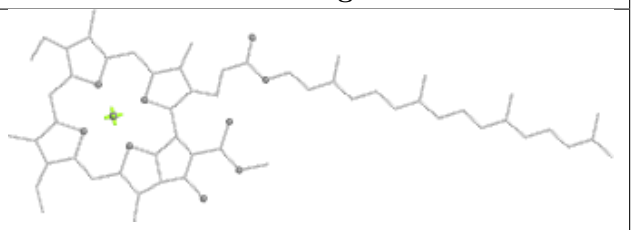
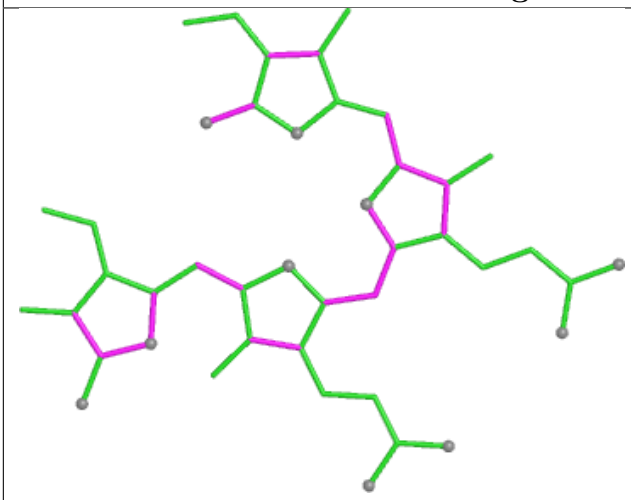


Rings

Ligand PEB QB 201



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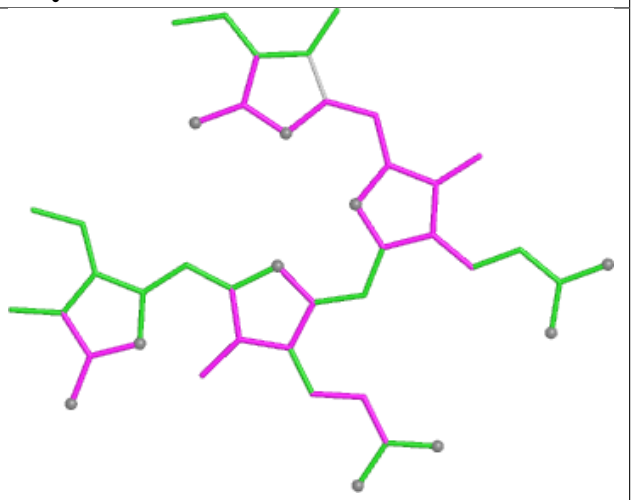
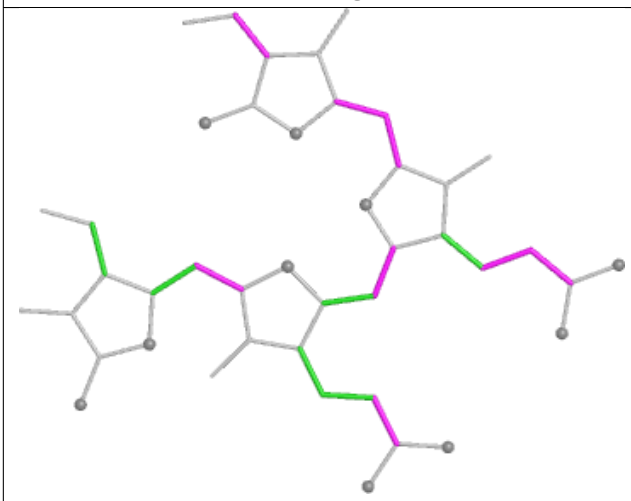


Bond angles



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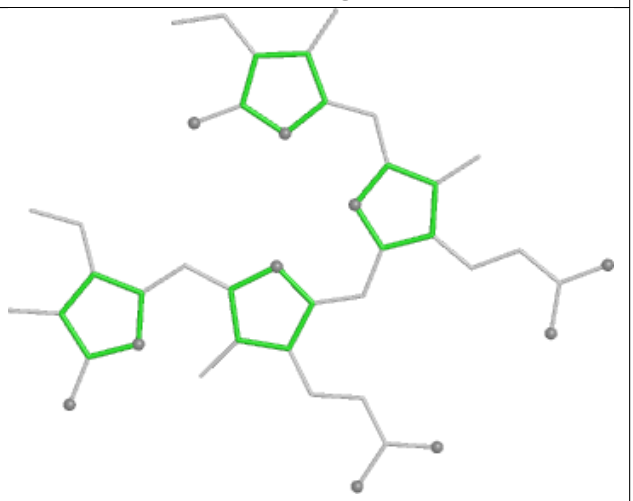
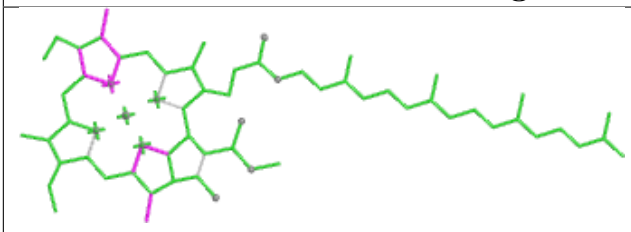


Rings

Ligand CLA BN 835



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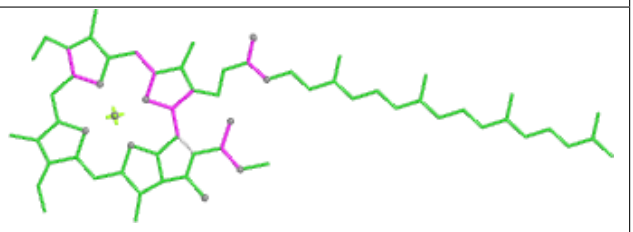
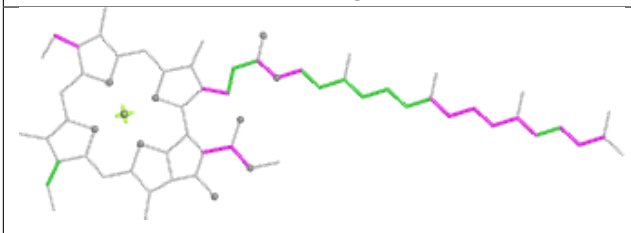


Bond angles



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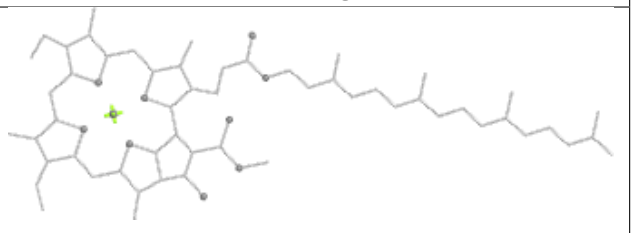
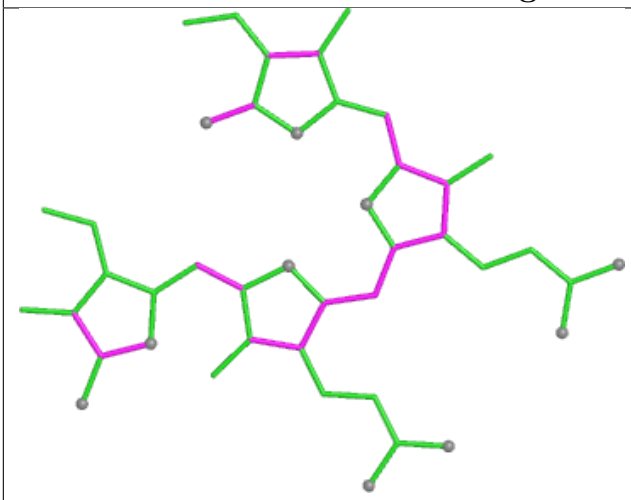


Rings

Ligand PEB J9 202



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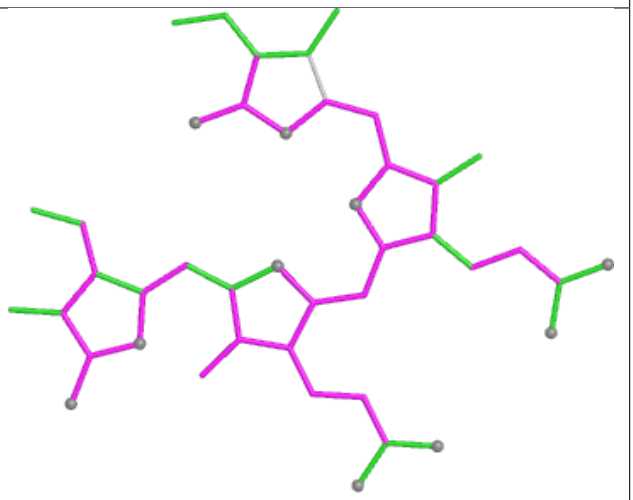
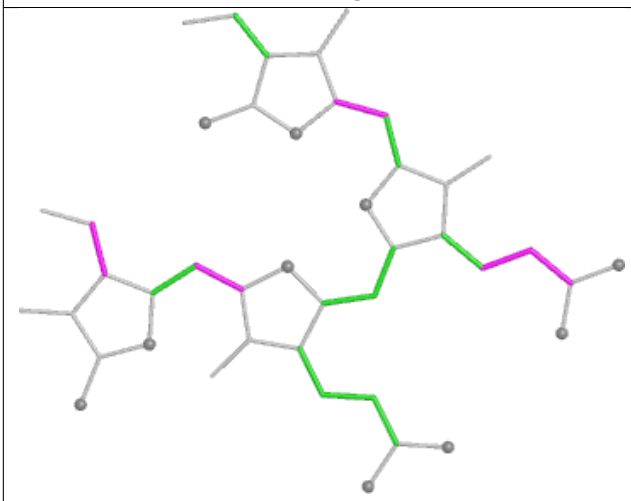


Bond angles



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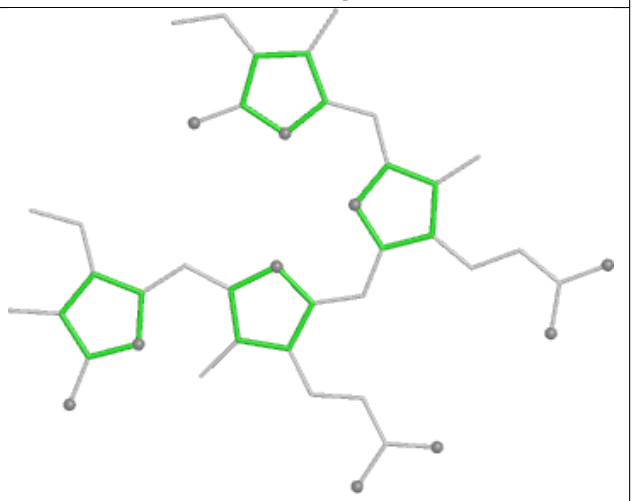
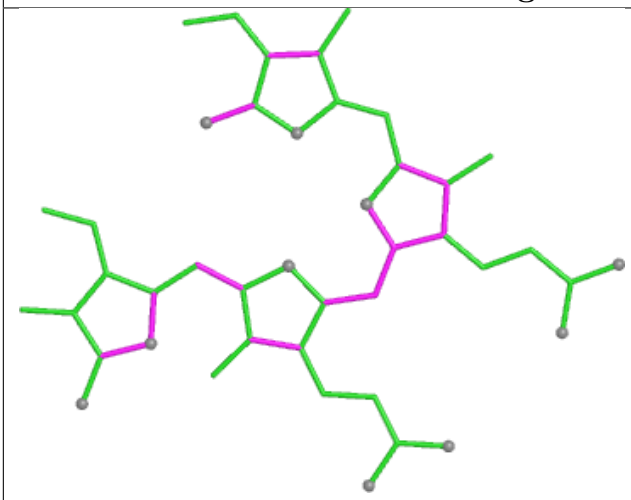


Rings

Ligand PEB RI 201



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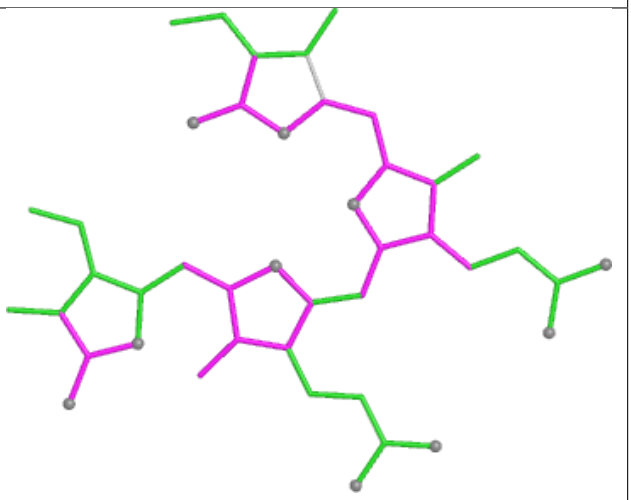
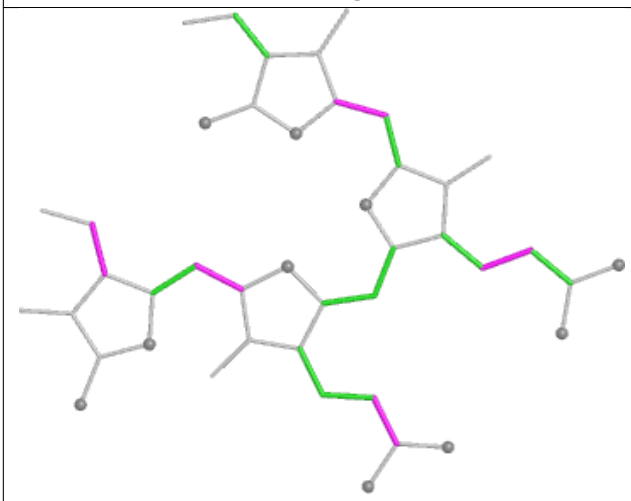


Bond angles



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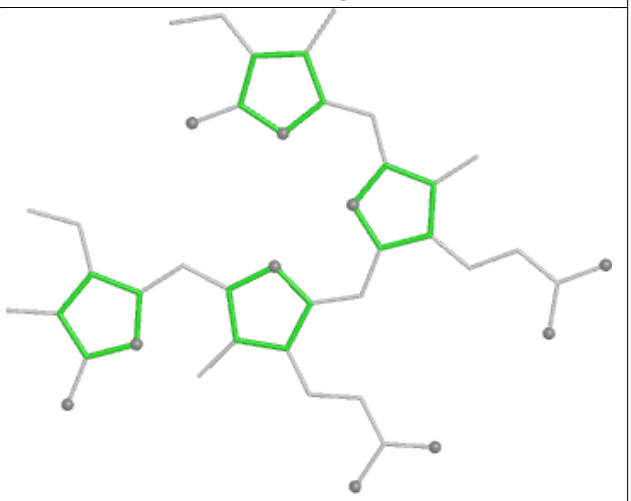
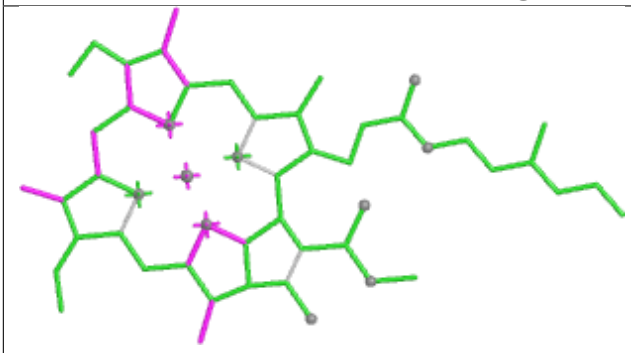
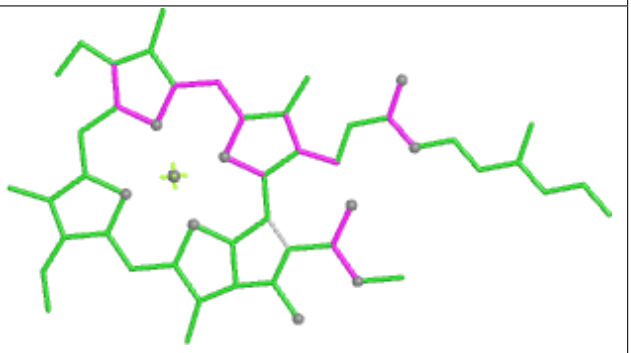


Rings

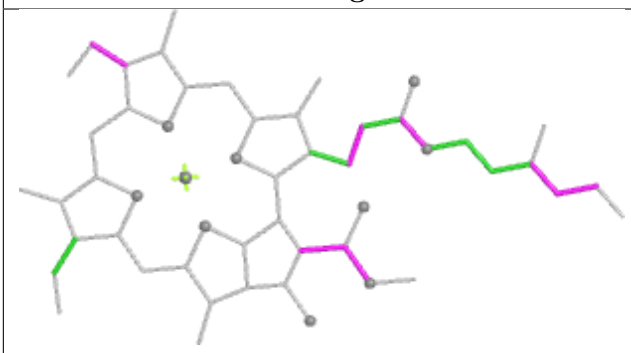
Ligand CLA A2 803



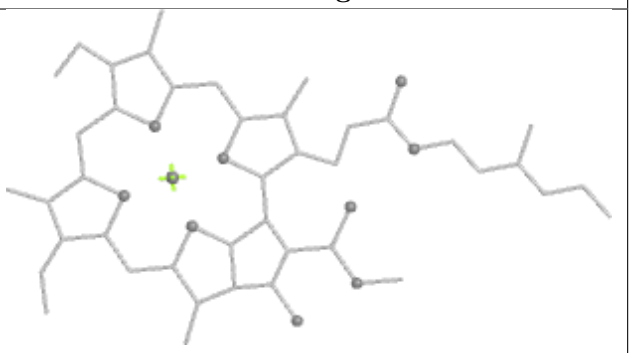
Bond lengths



Bond angles

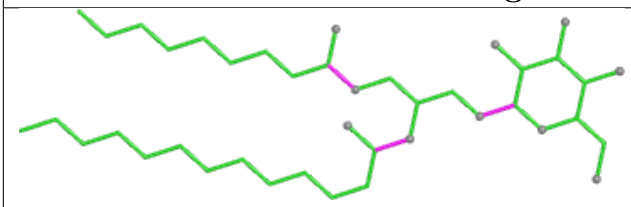


Torsions



Rings

Ligand LMG ML 101



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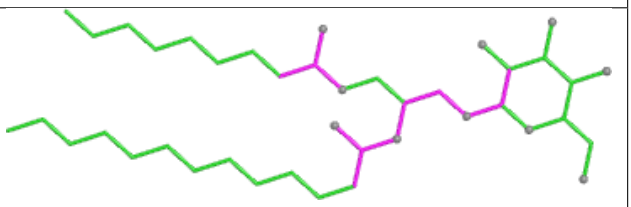

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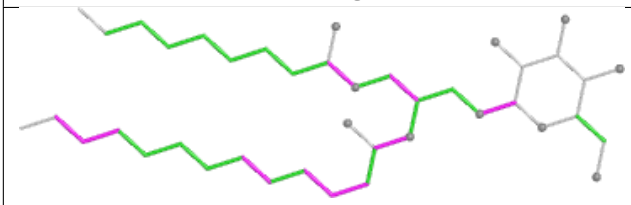

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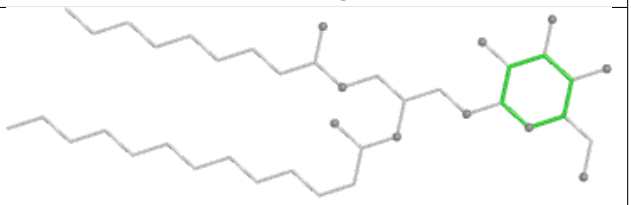
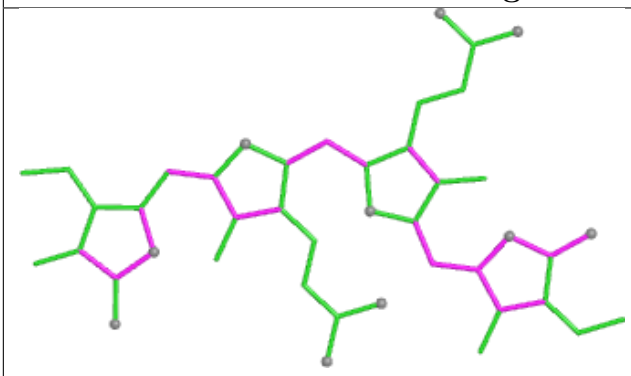


Rings

Ligand CYC FE 1002



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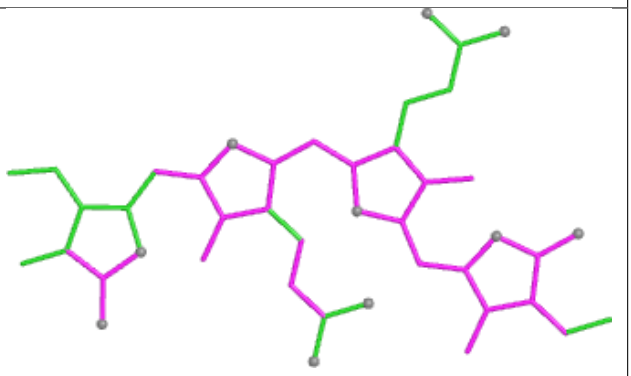

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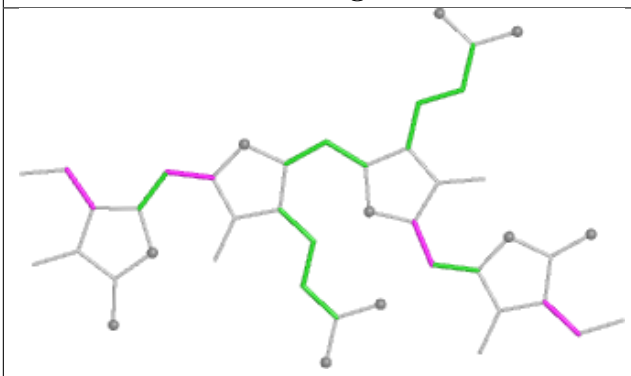

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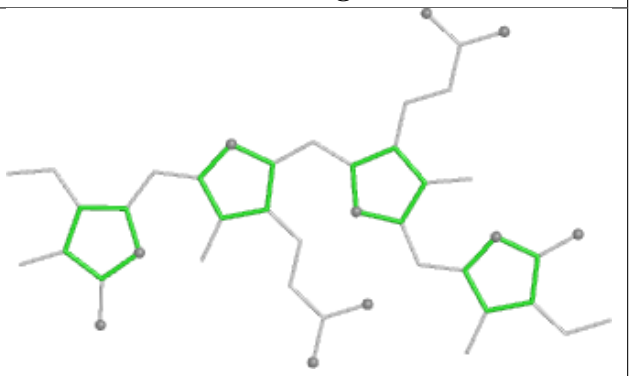
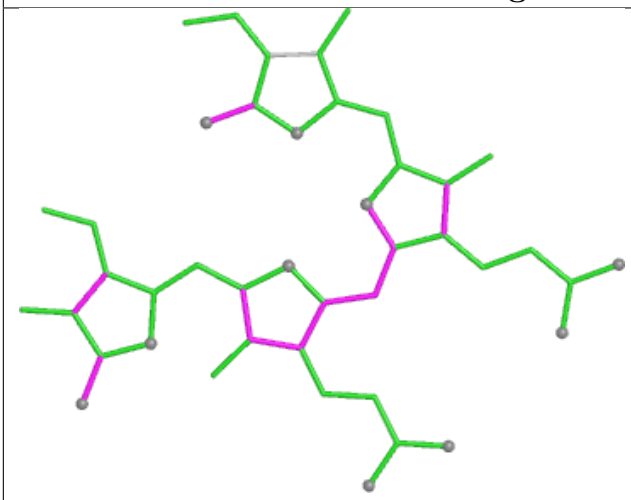


Rings

Ligand PUB AG 302



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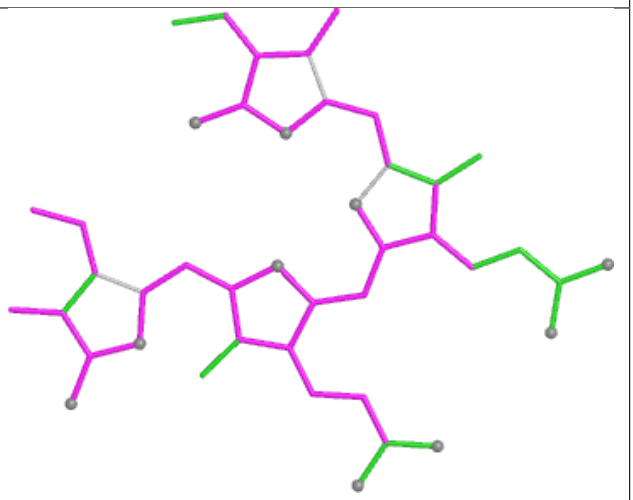

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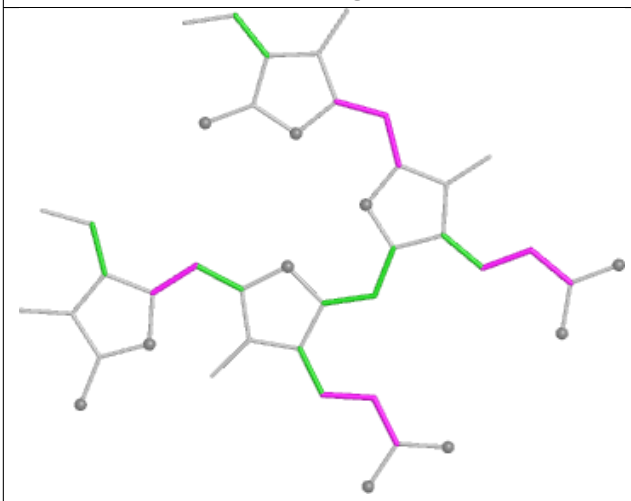

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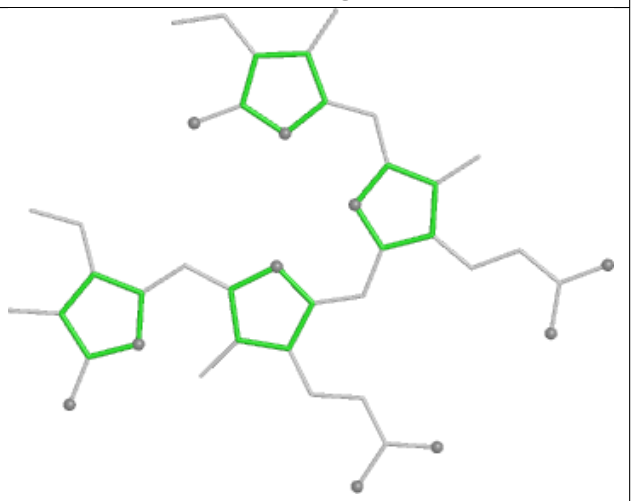
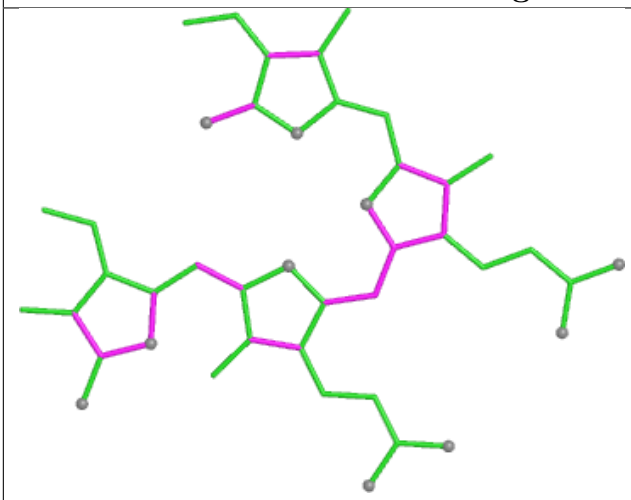


Rings

Ligand PEB VE 202



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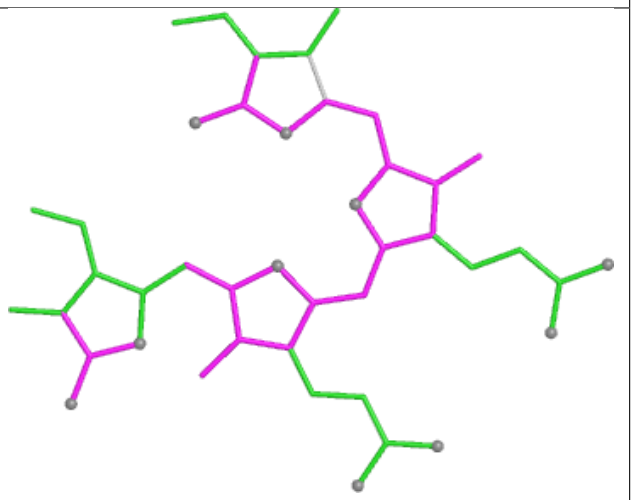

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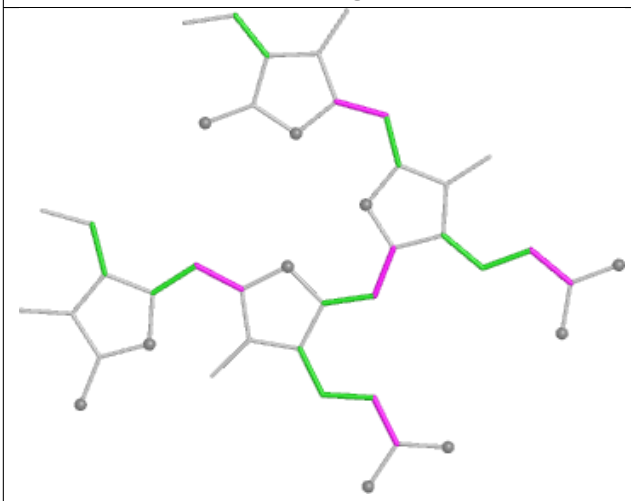

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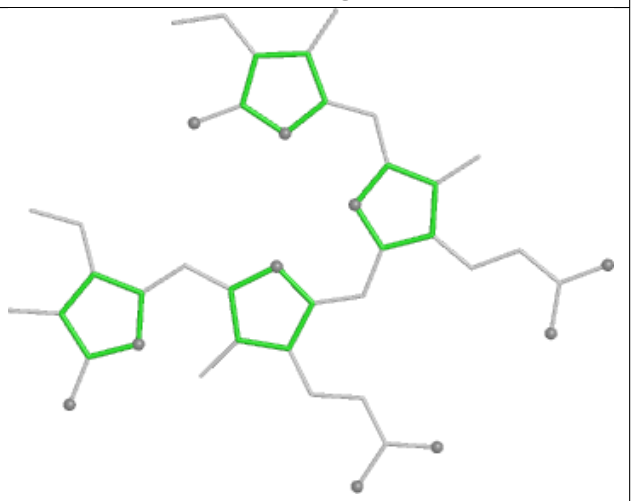
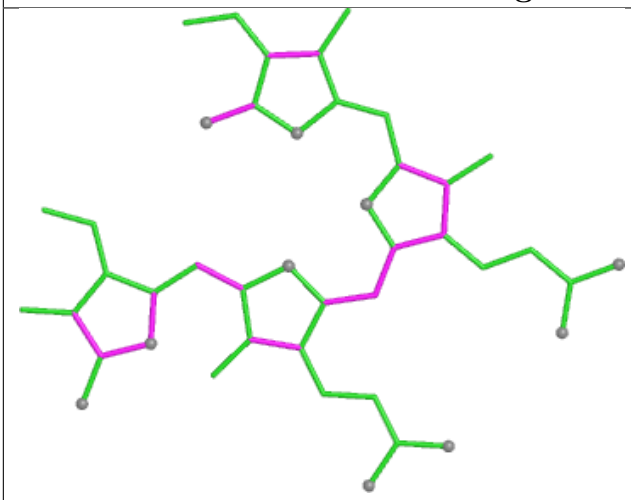


Rings

Ligand PEB OJ 203



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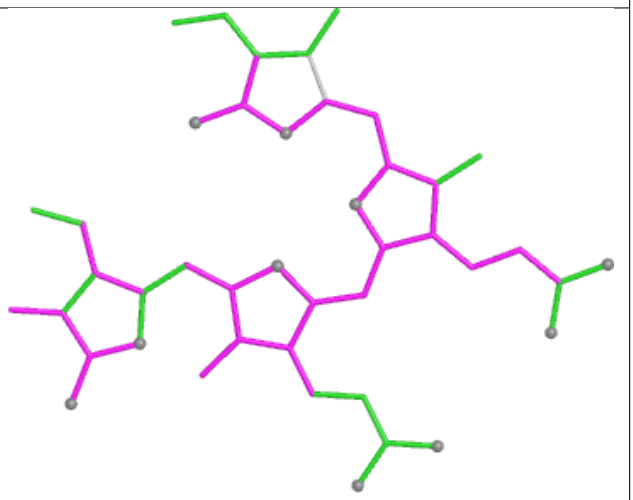

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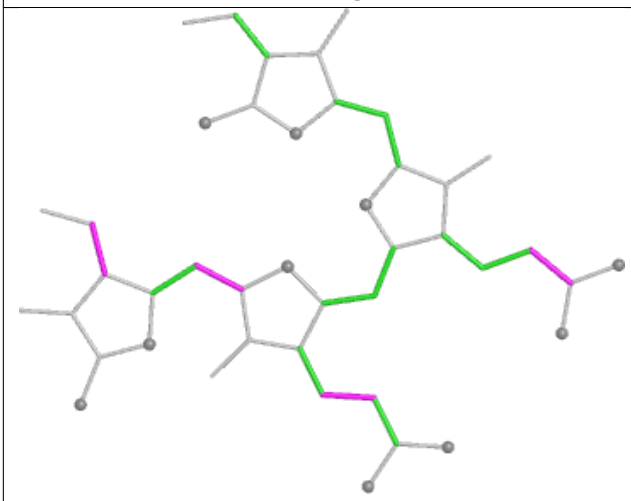

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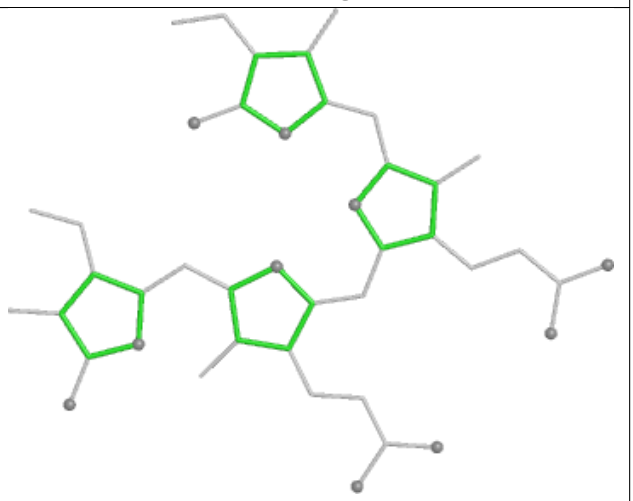
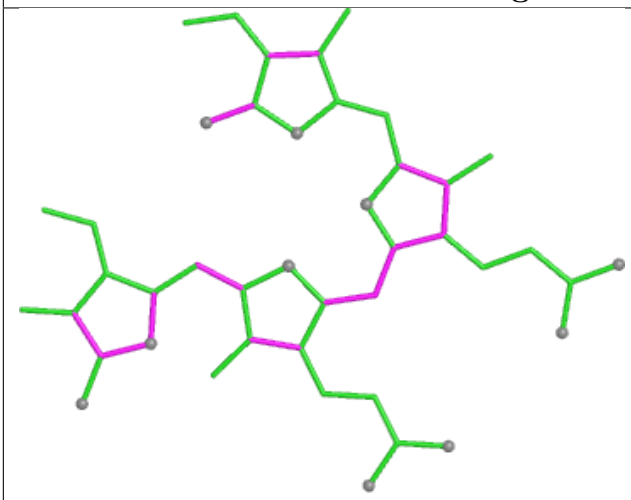


Rings

Ligand PEB M7 202



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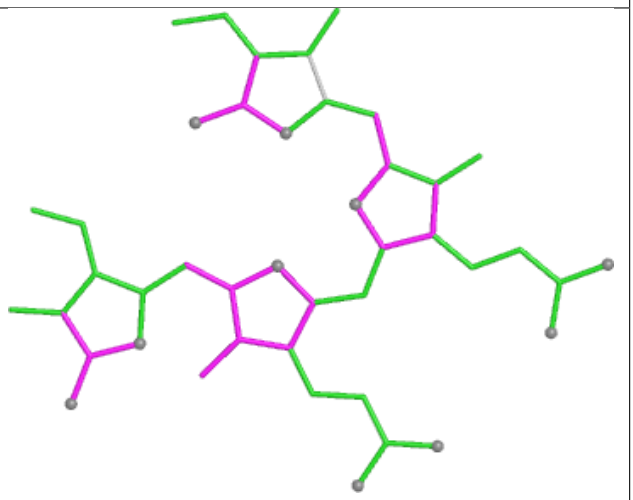
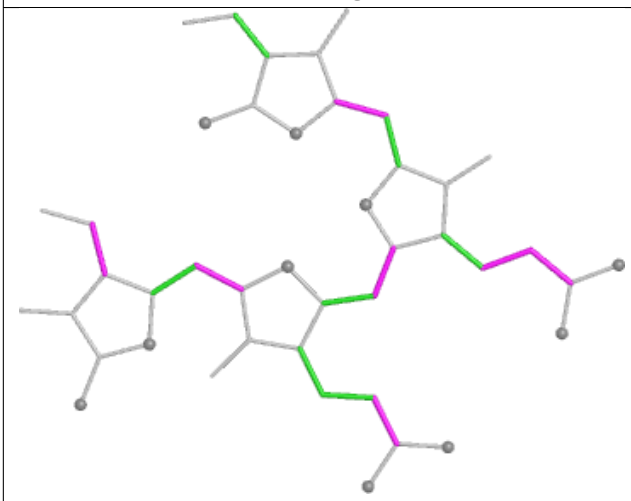


Bond angles



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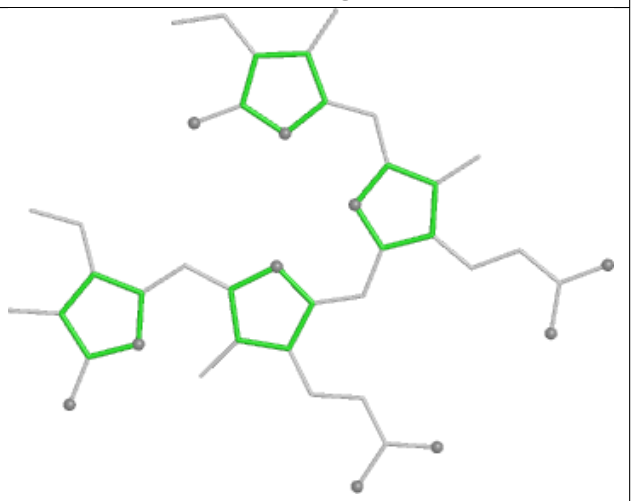
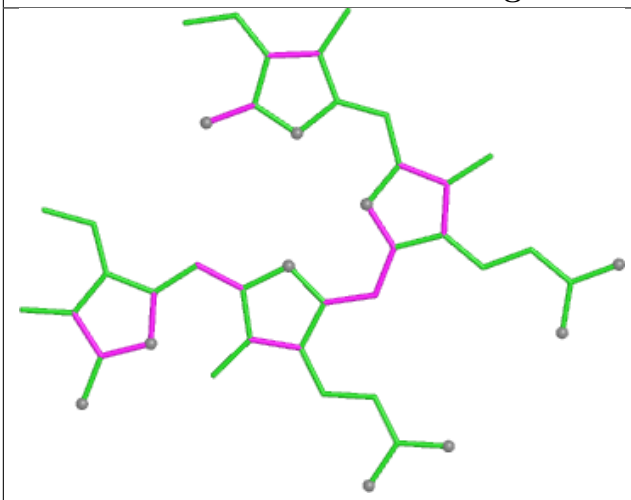


Rings

Ligand PEB LH 1003



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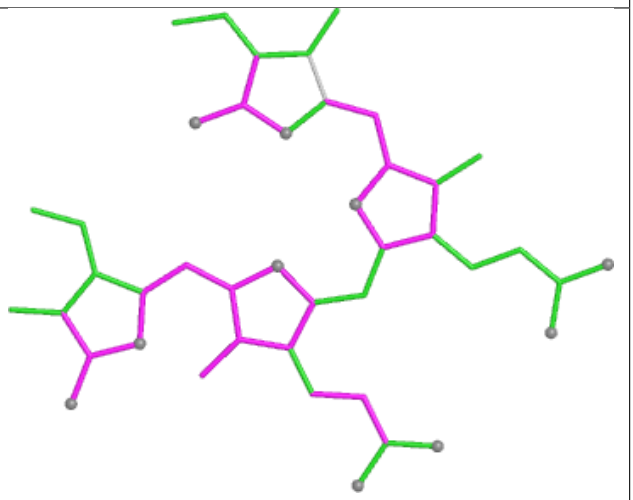

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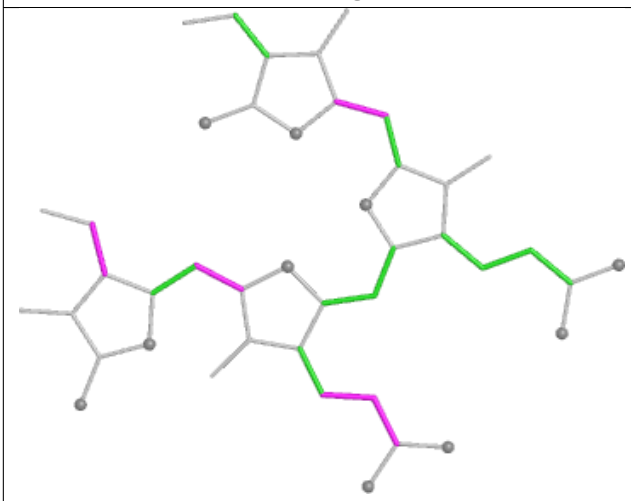

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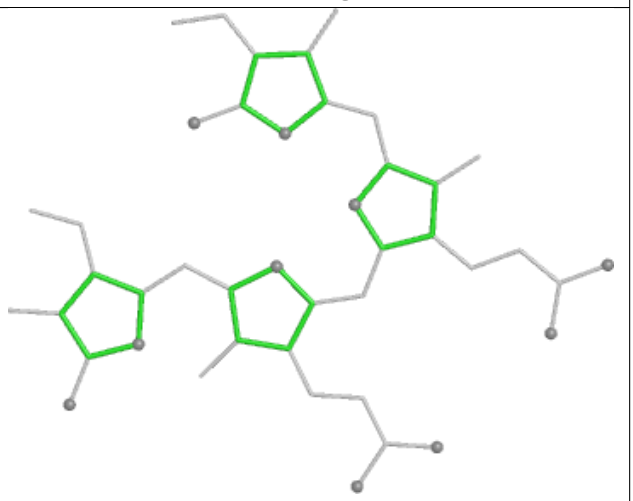
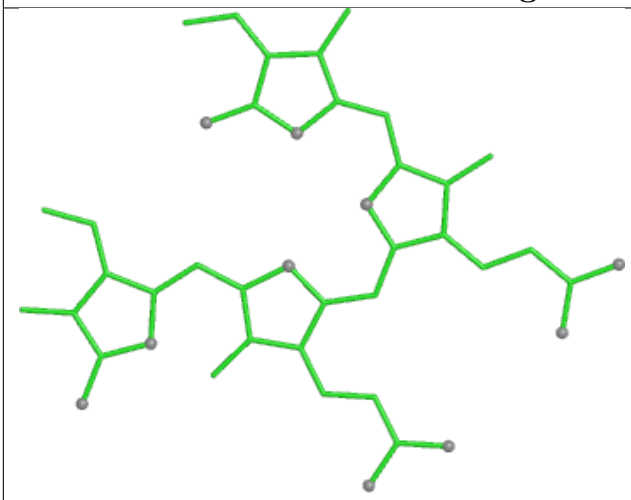


Rings

Ligand PEB y8 201



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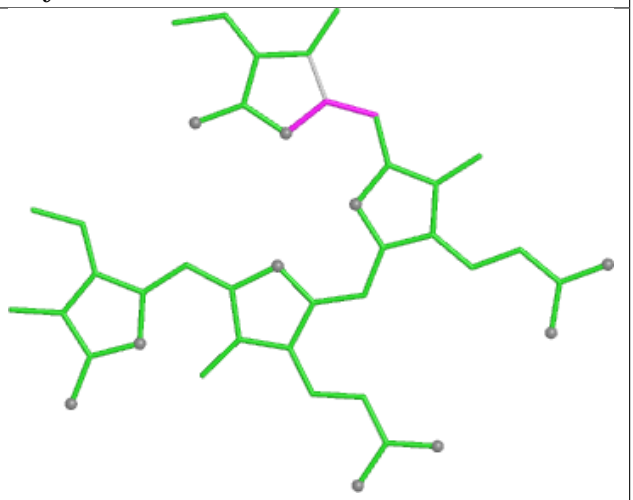

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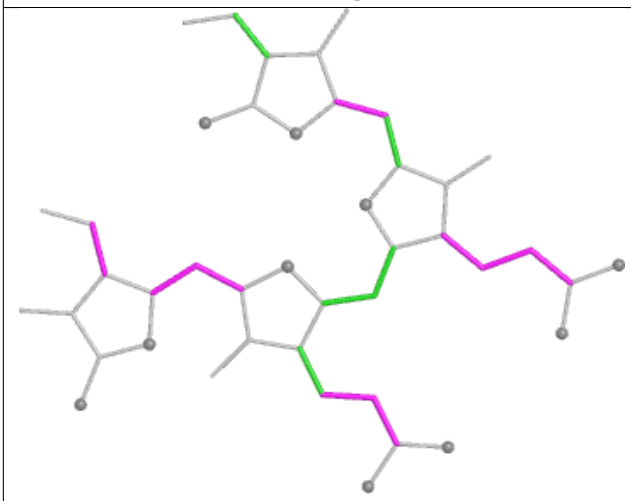

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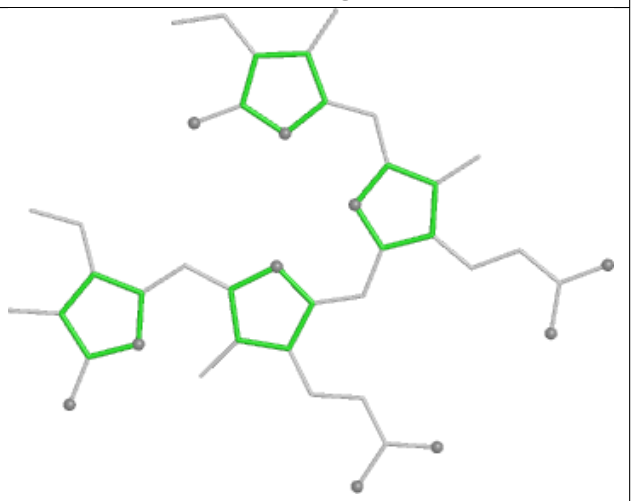
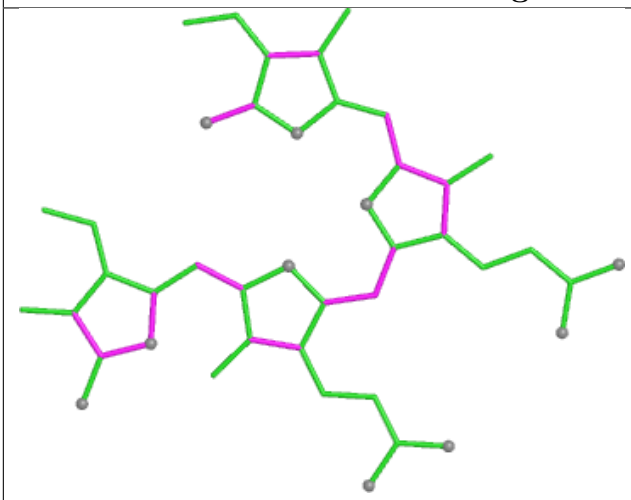


Rings

Ligand PEB OB 201



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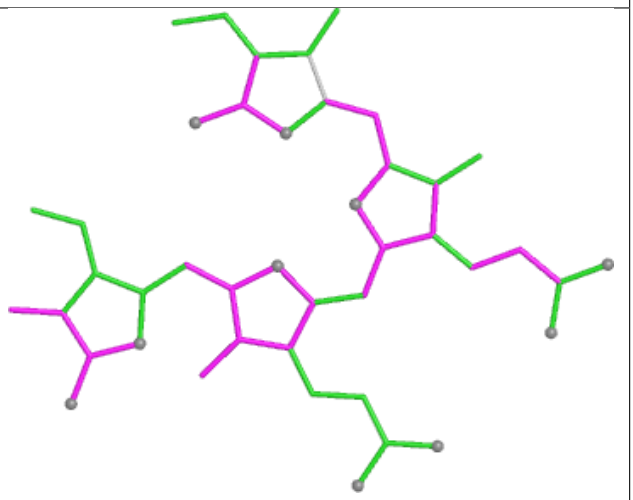

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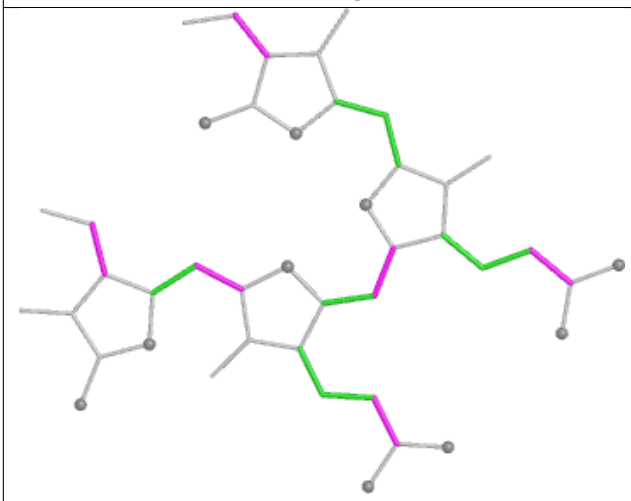

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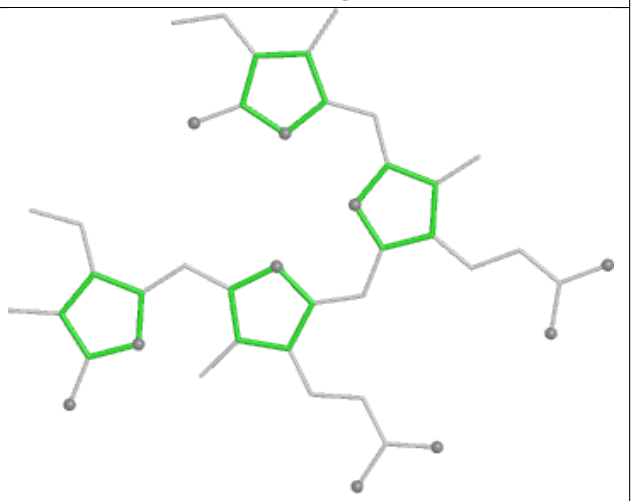
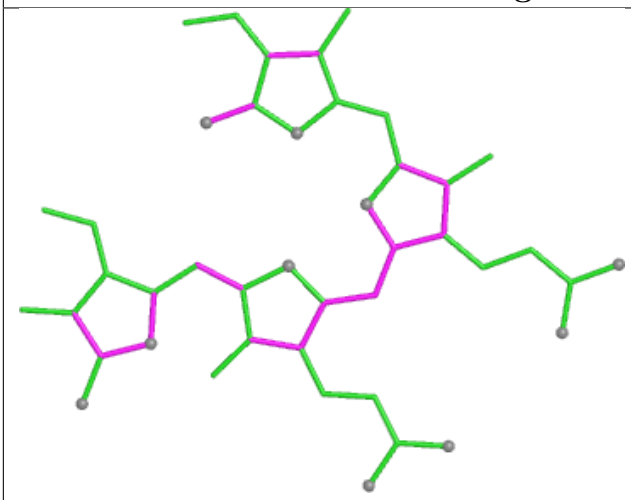


Rings

Ligand PEB FP 201



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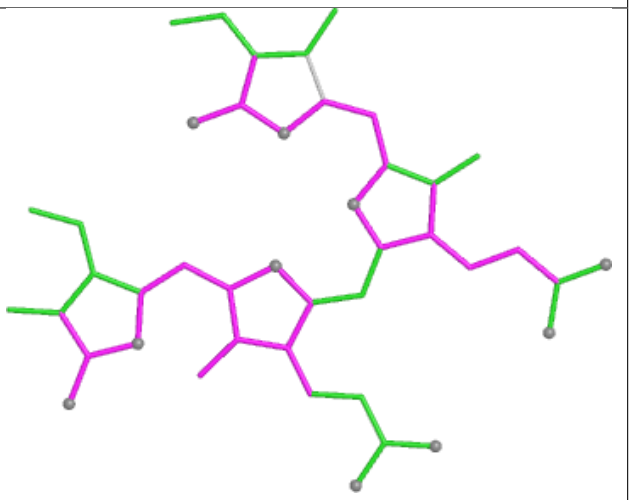
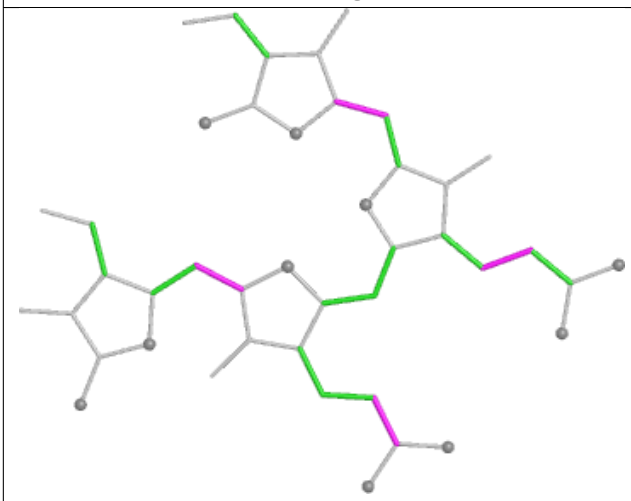


Bond angles



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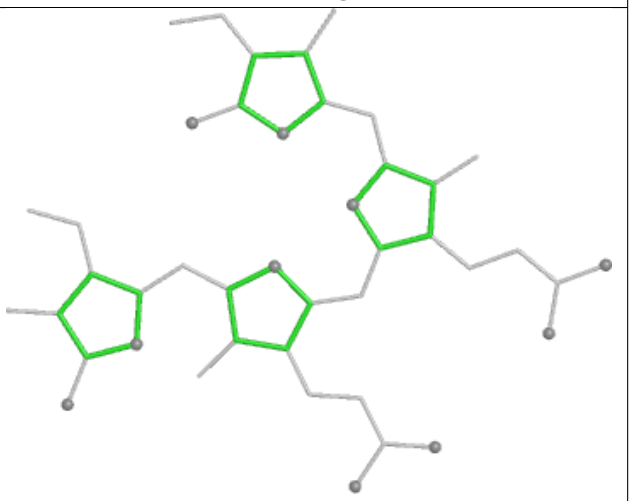
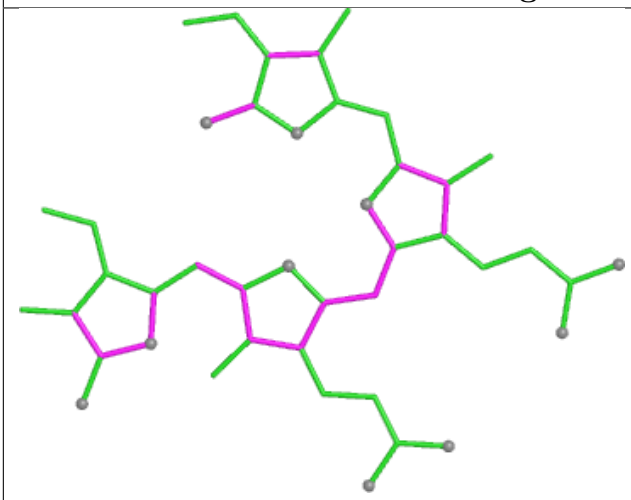


Rings

Ligand PEB FI 201



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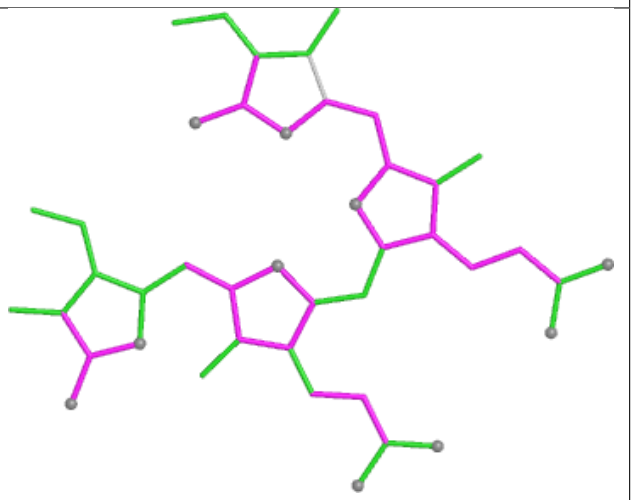
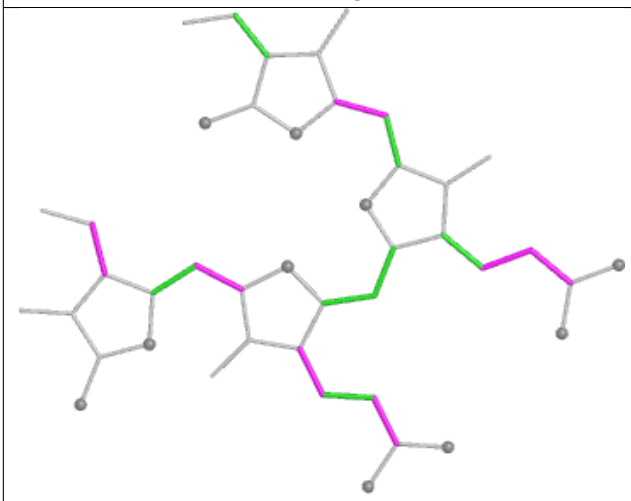


Bond angles



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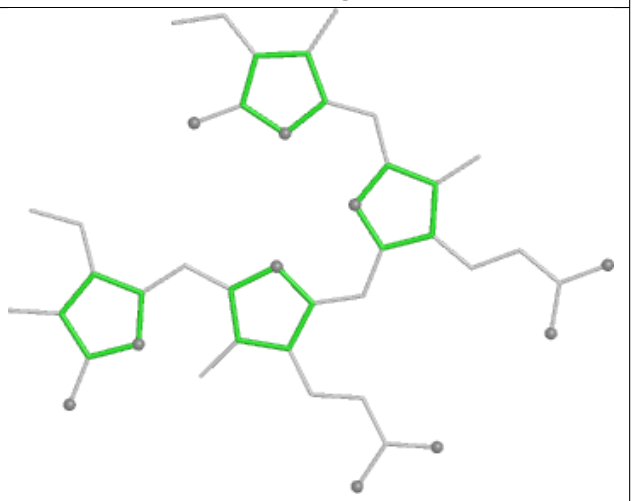
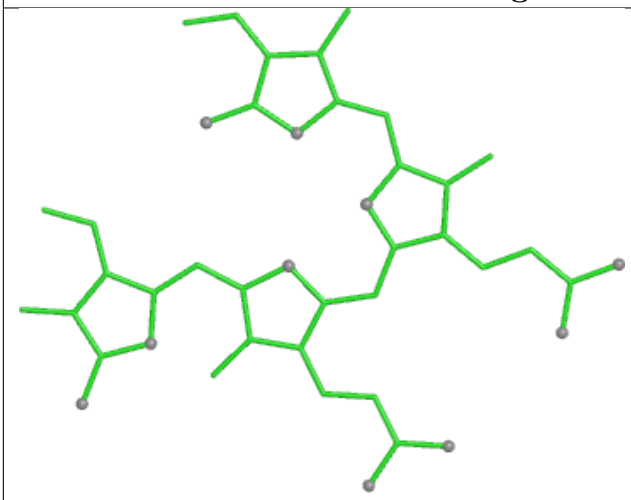


Rings

Ligand PEB KB 303



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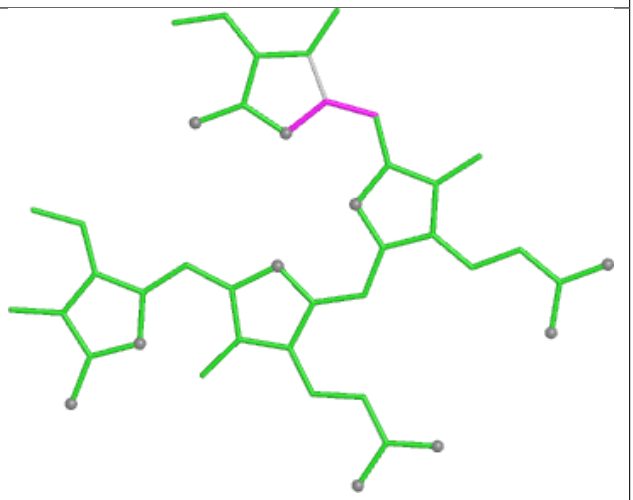
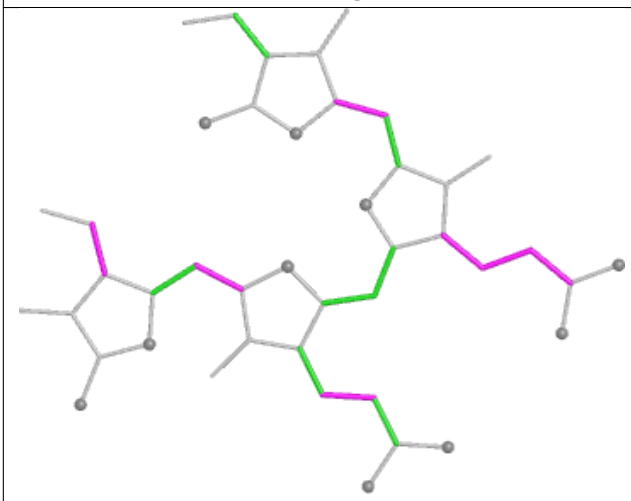


Bond angles



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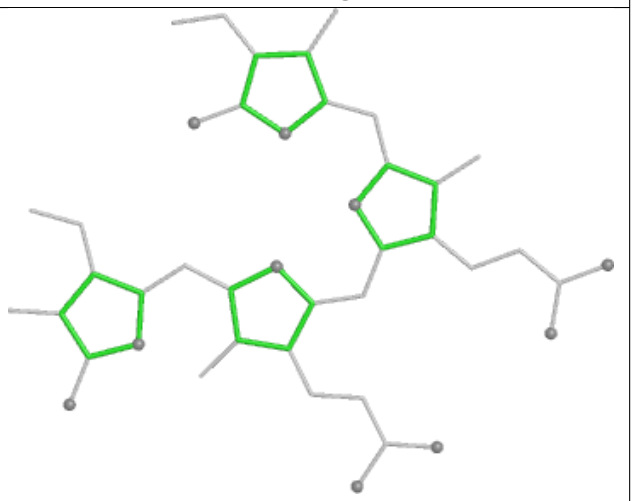
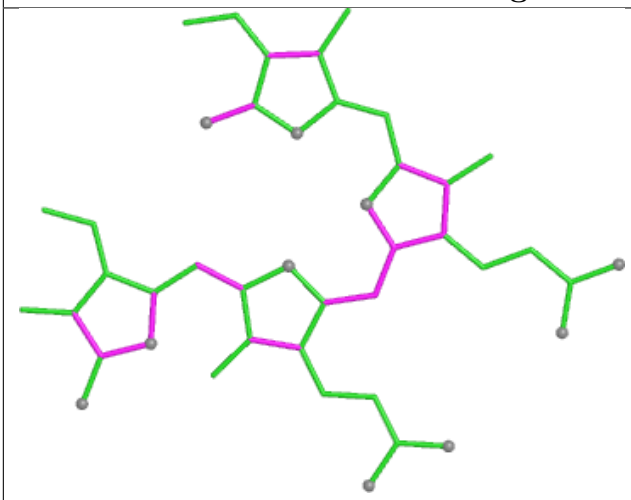


Rings

Ligand PEB OG 201



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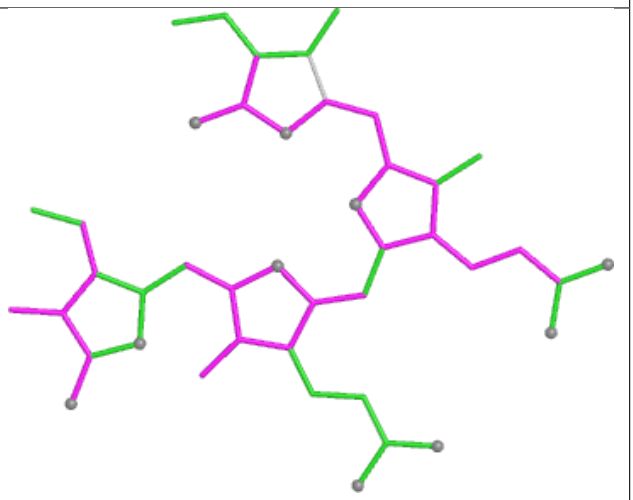
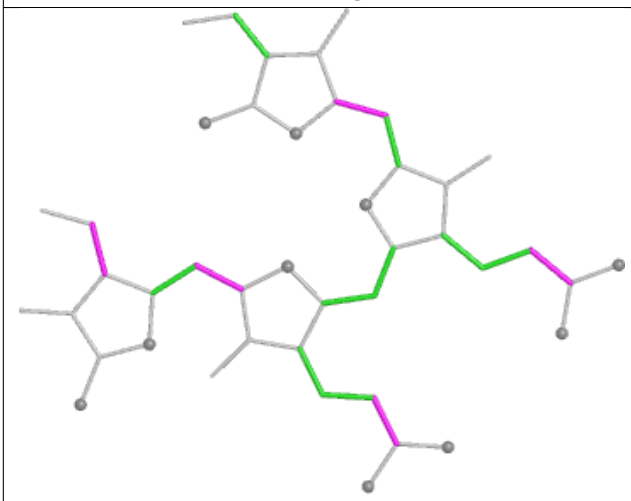


Bond angles



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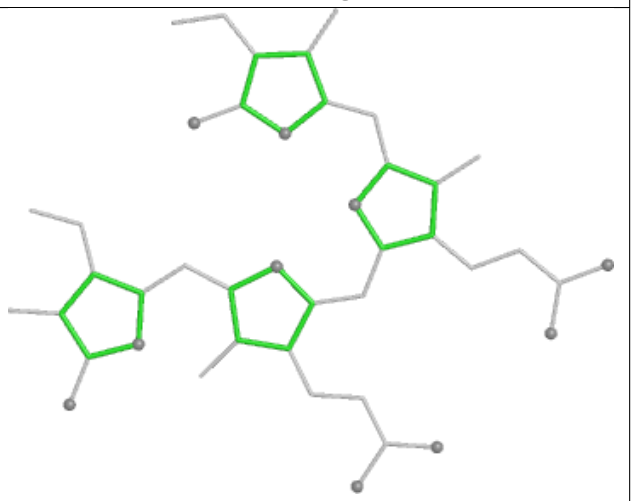
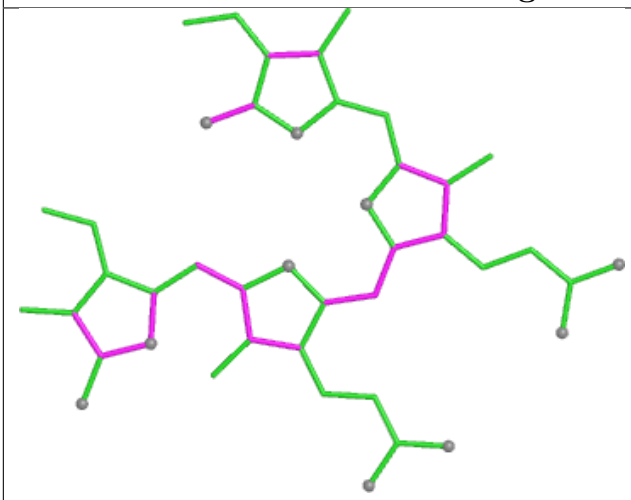


Rings

Ligand PEB cF 203



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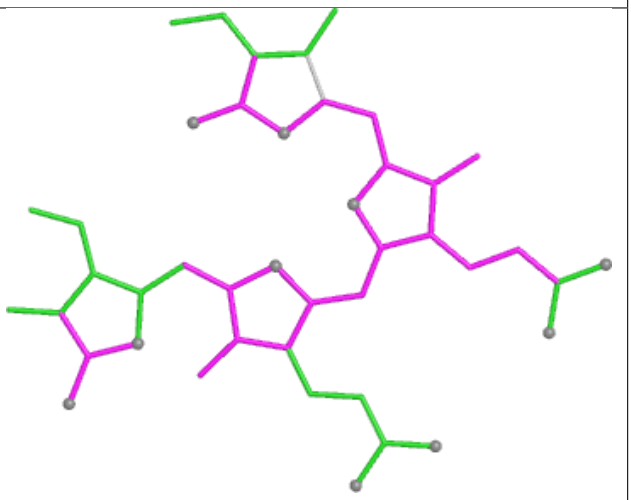
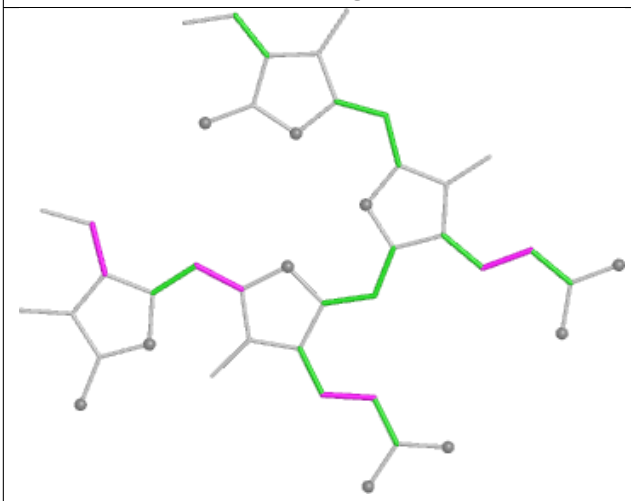


Bond angles



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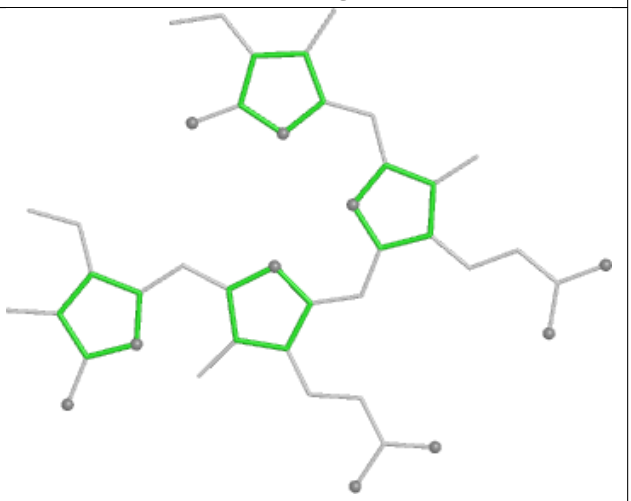
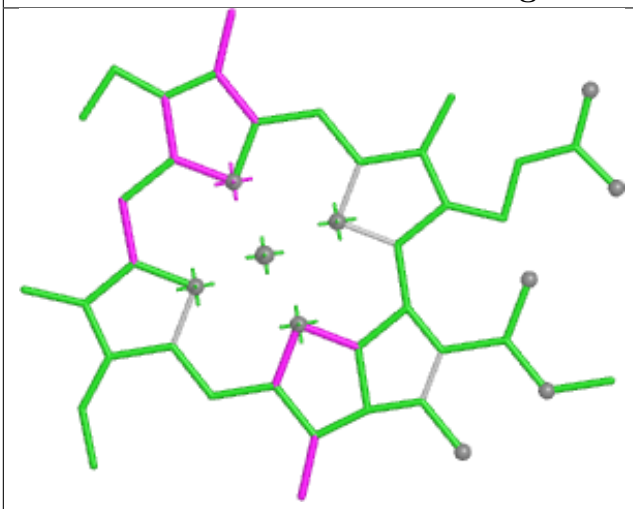
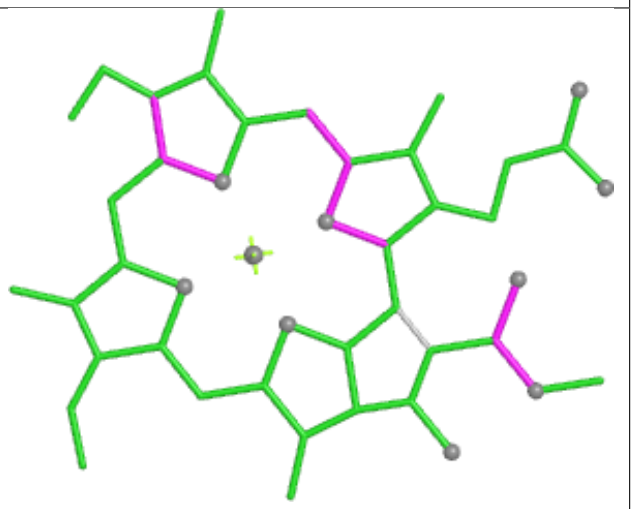


Rings

Ligand CLA 62 302



Bond lengths



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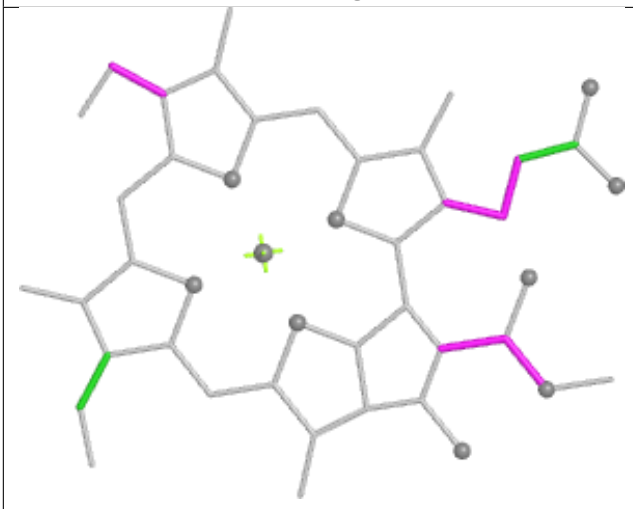
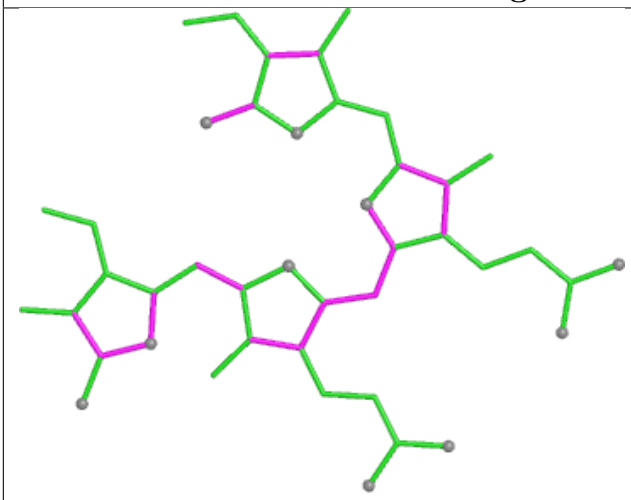


Torsions



Rings

Ligand PEB AK 202



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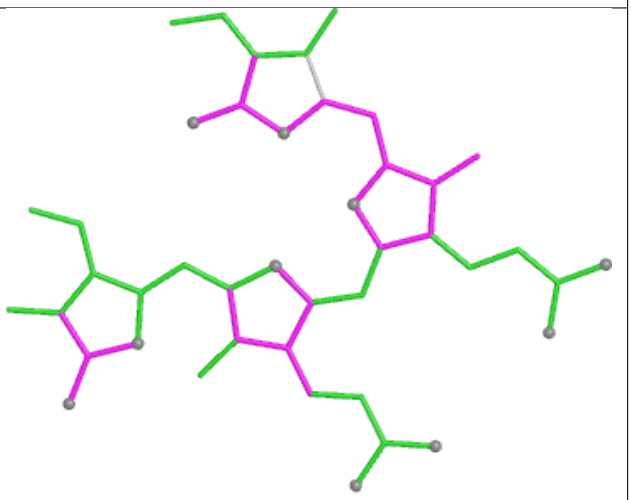

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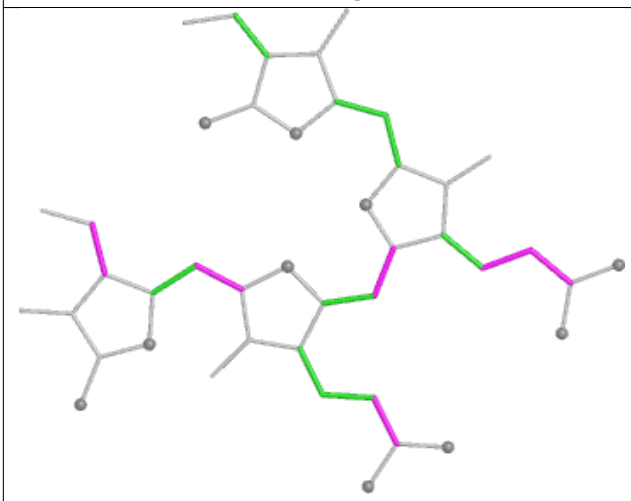

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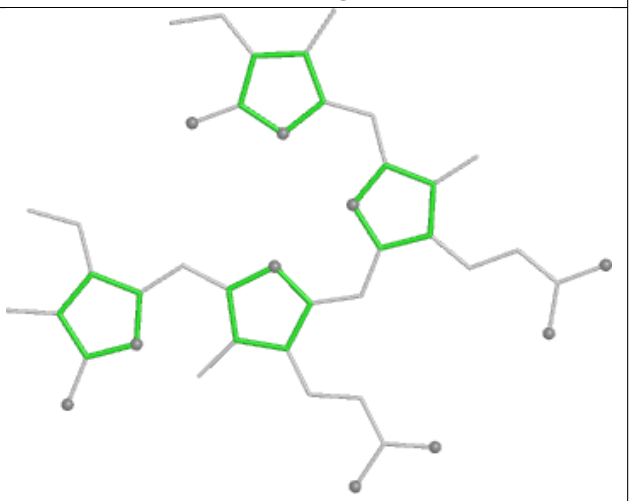

Rings

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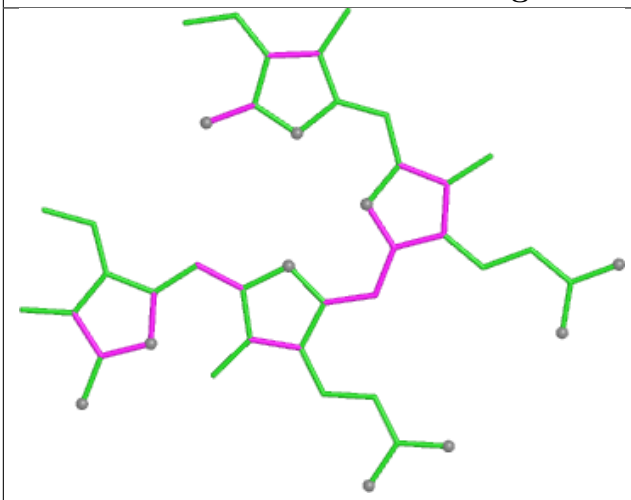

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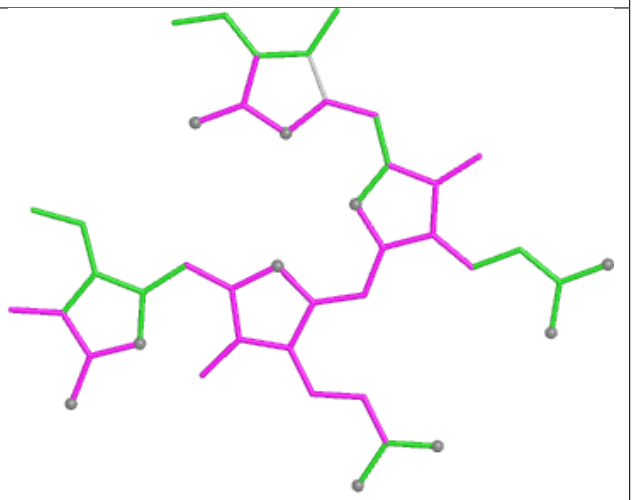

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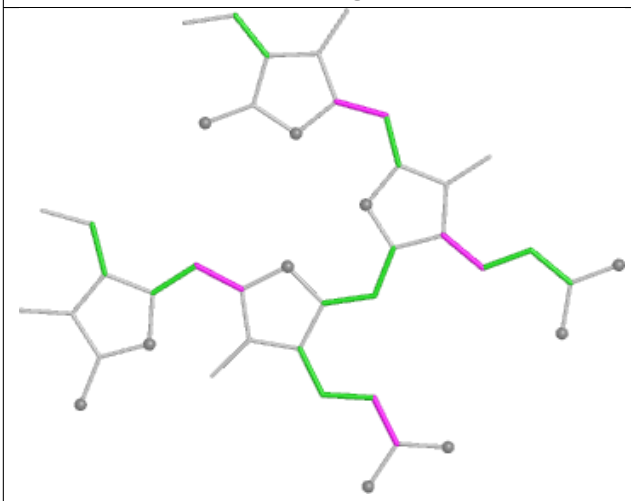

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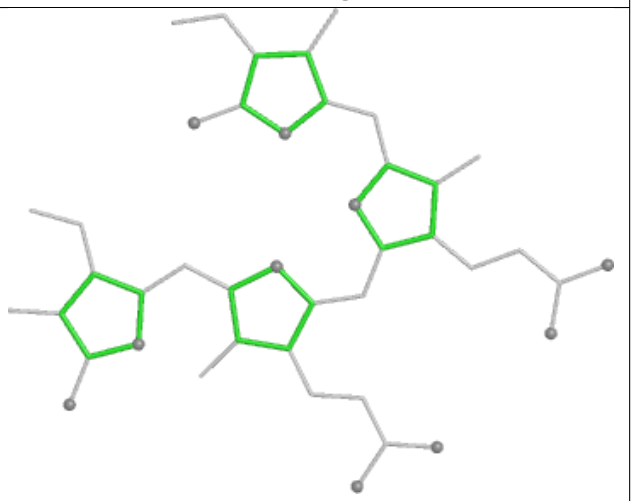
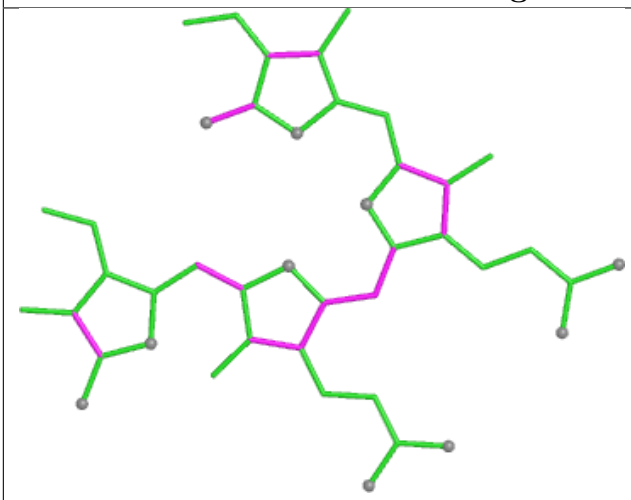


Rings

Ligand PEB XK 201



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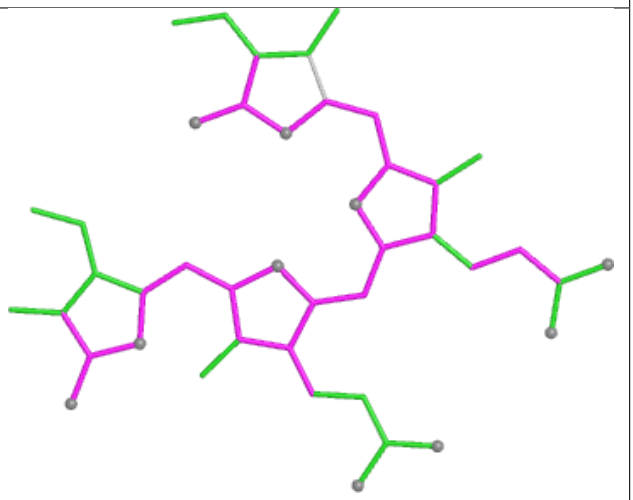

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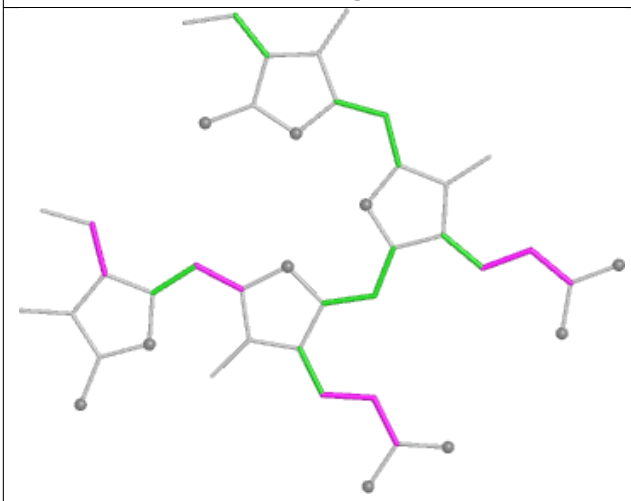

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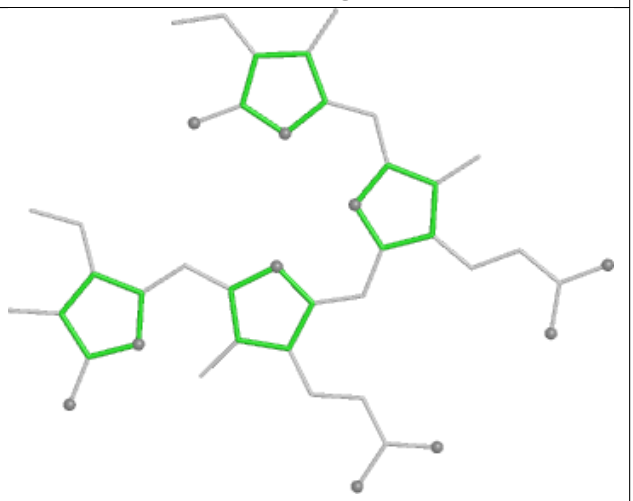
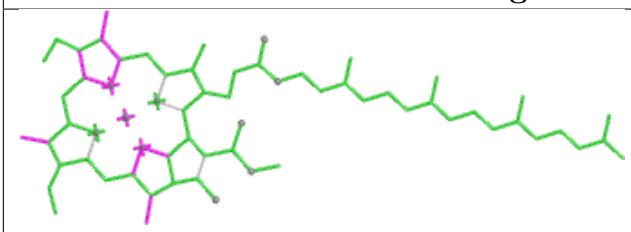


Rings

Ligand CLA AN 815



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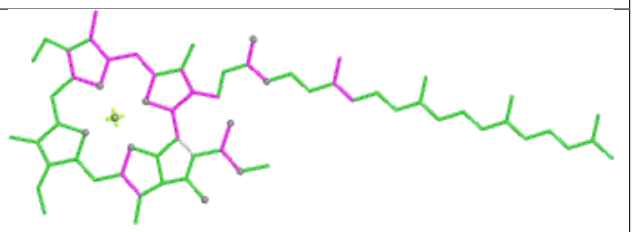
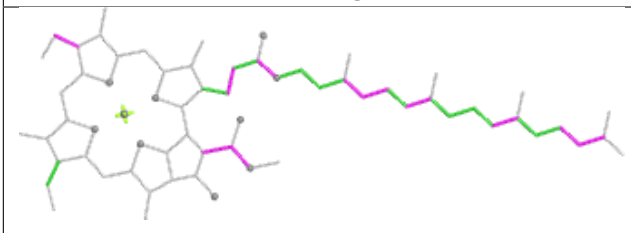


Bond angles



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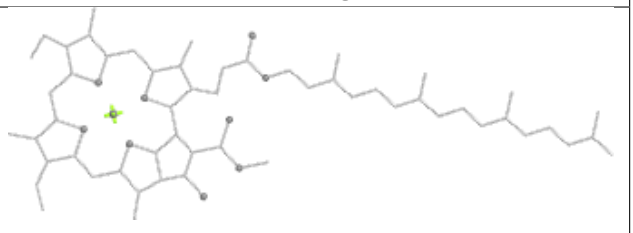
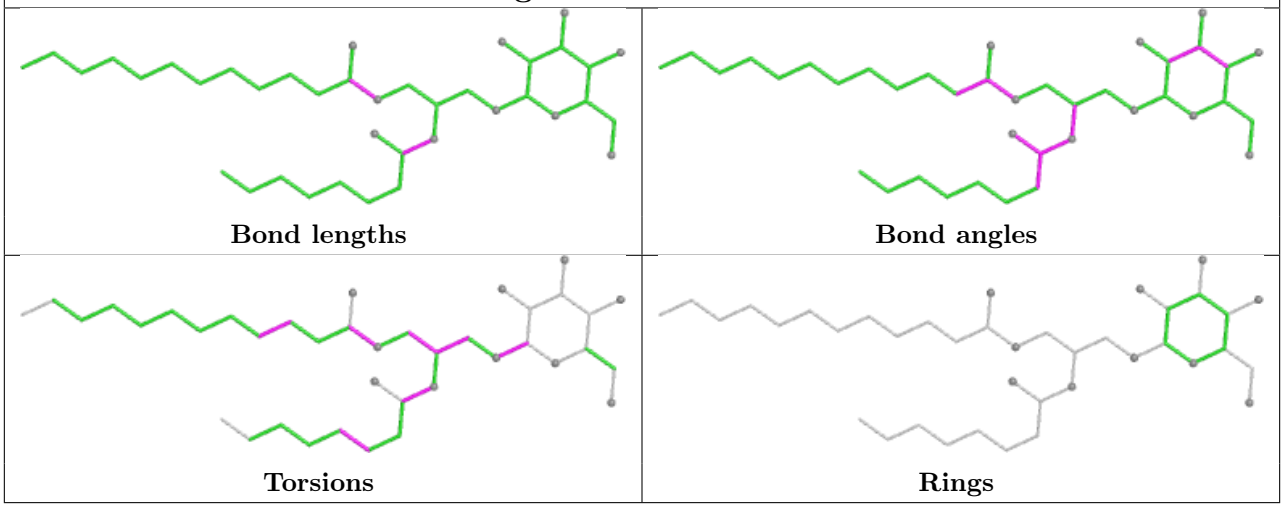
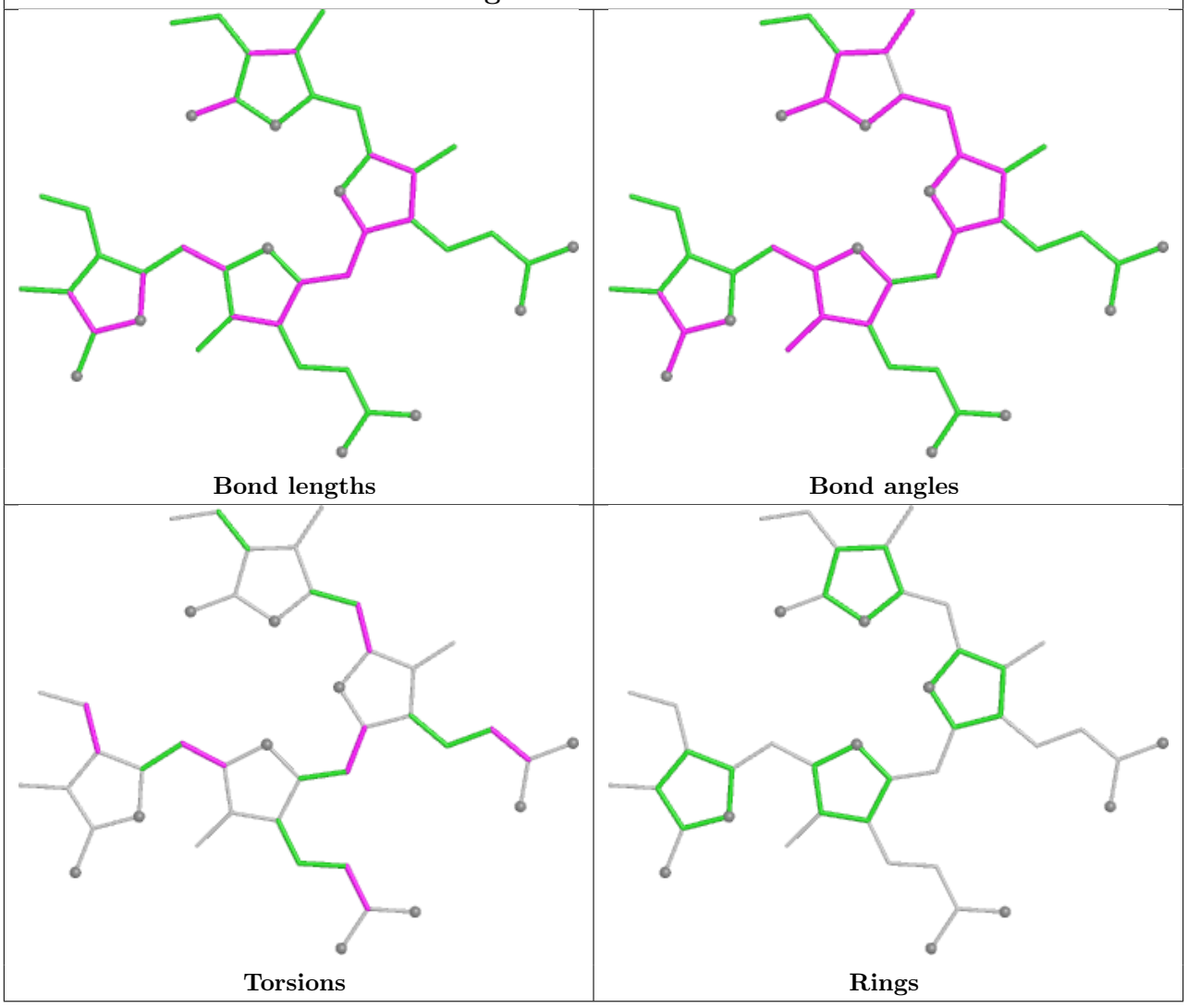


Rings

Ligand LMG b6 620



Ligand PEB fJ 202



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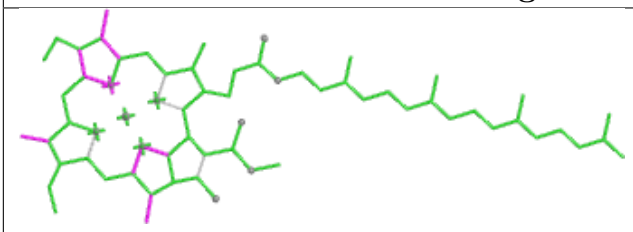

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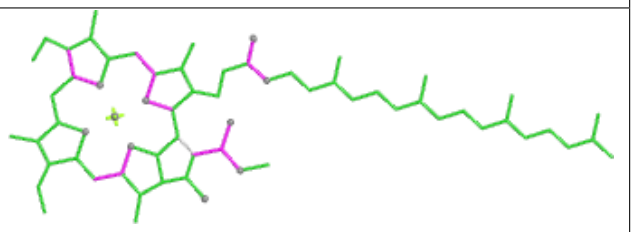

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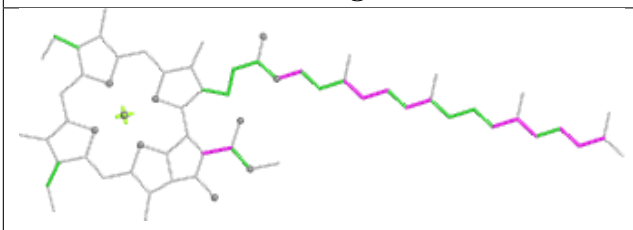

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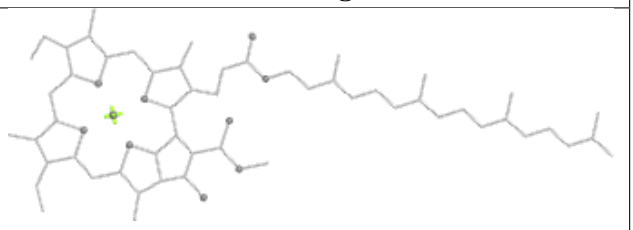
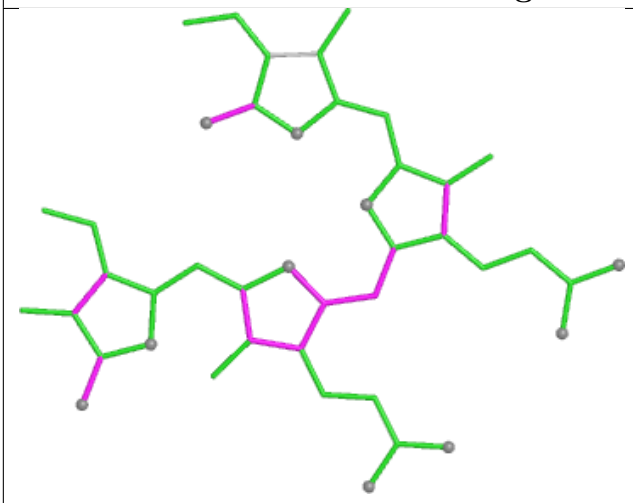


Rings

Ligand PUB xF 306



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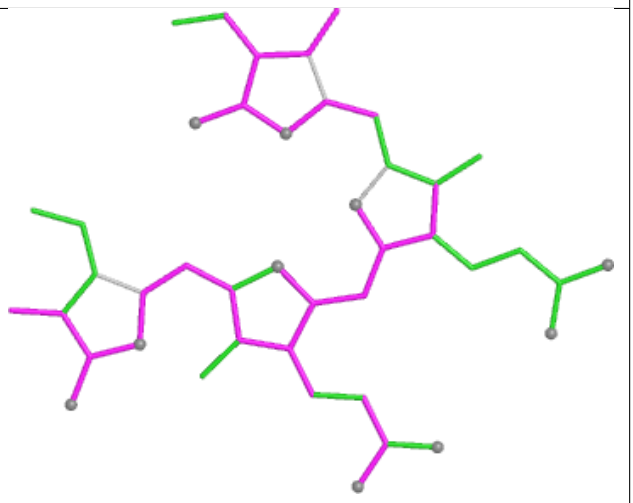

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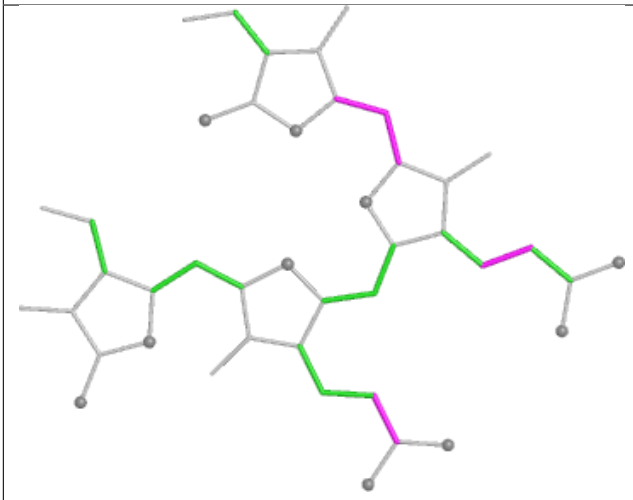

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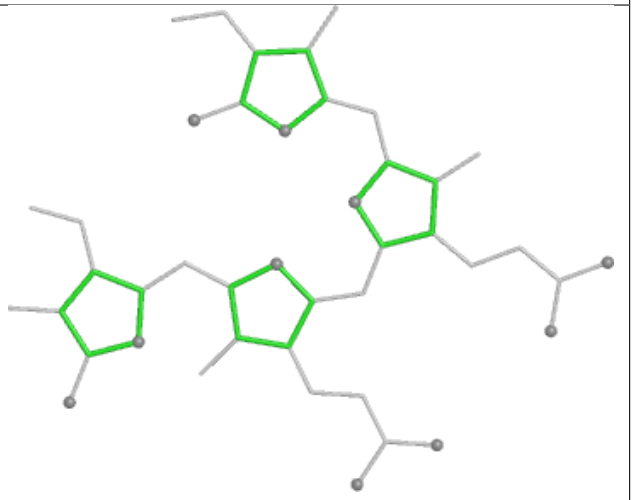
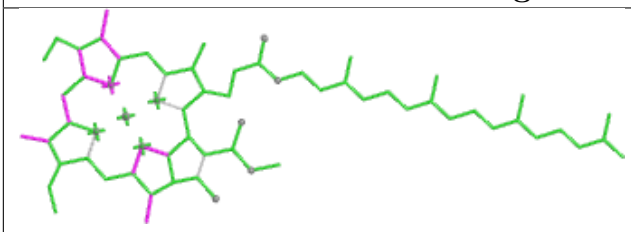


Rings

Ligand CLA CL 515



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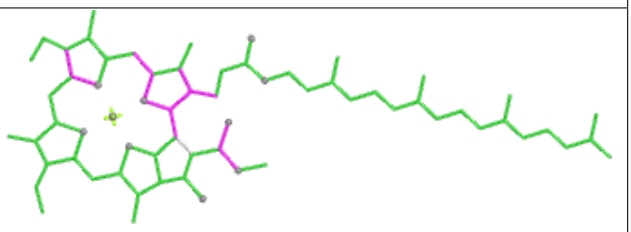

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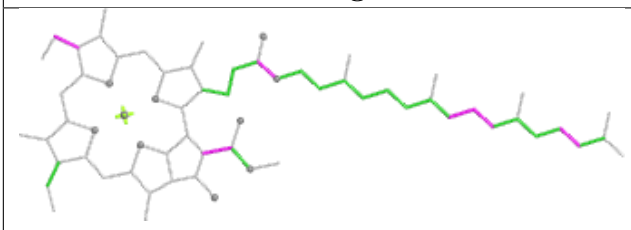

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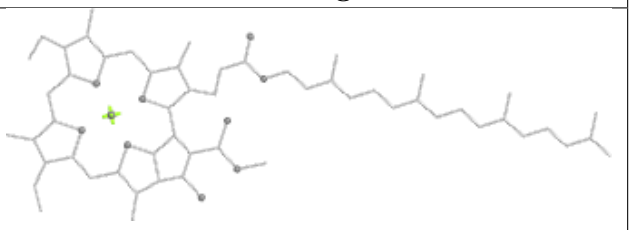
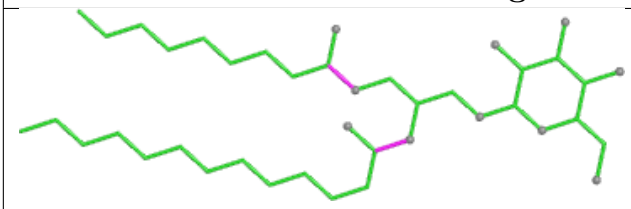


Rings

Ligand LMG m6 101



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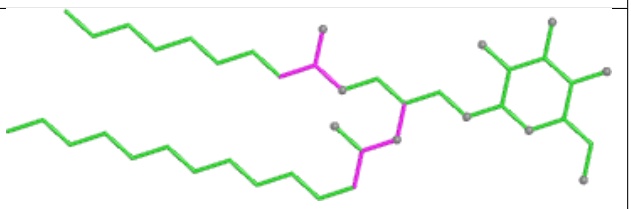
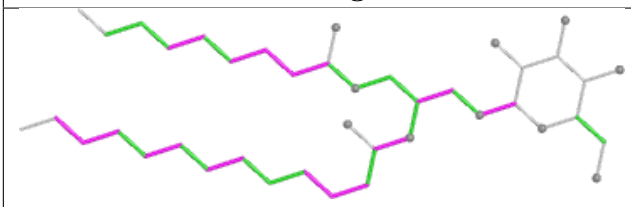


Bond angles



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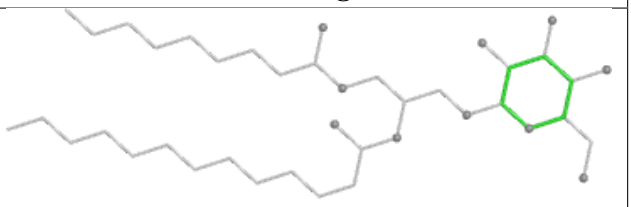
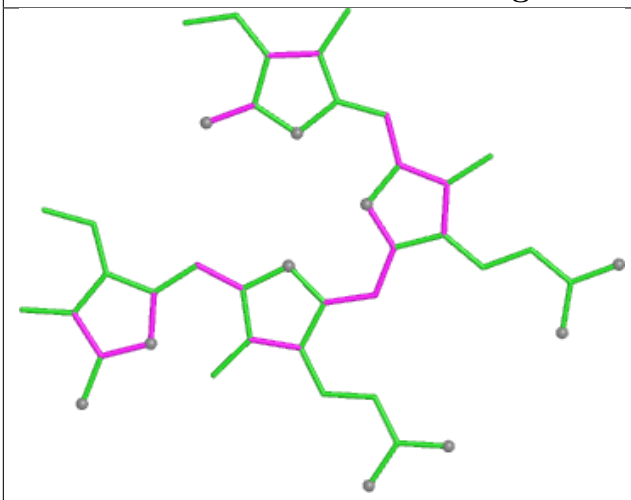


Rings

Ligand PEB AP 203



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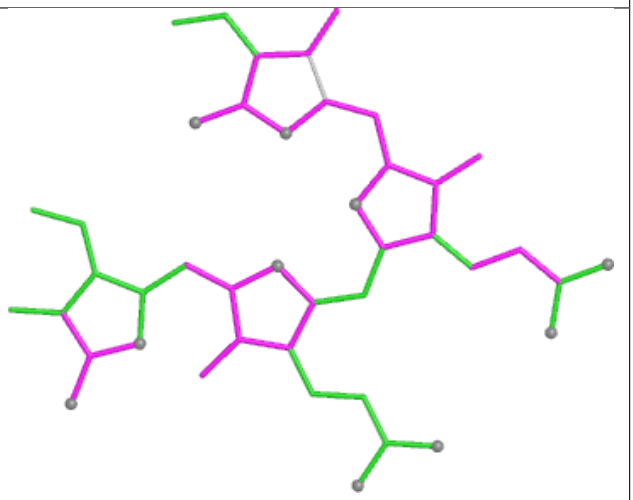

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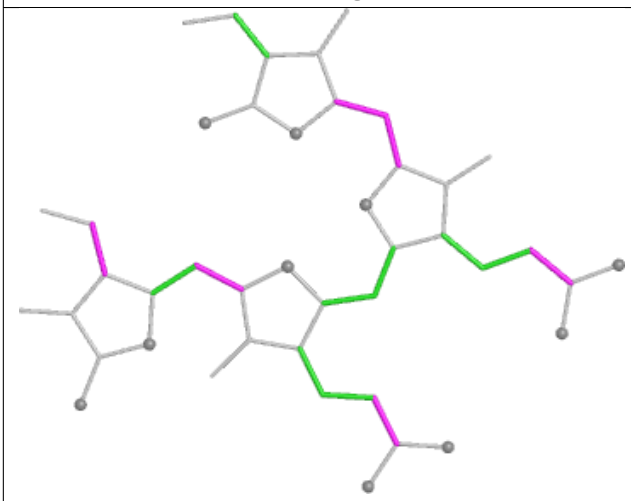

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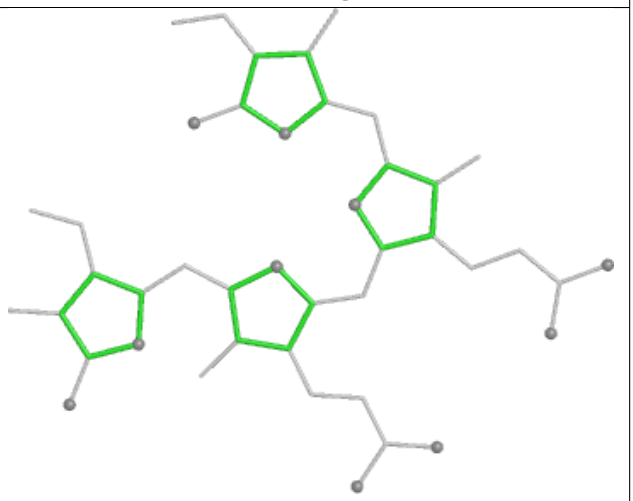
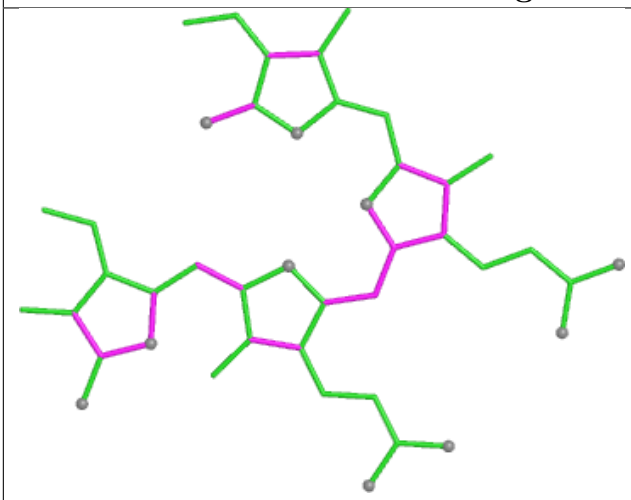


Rings

Ligand PEB V9 201



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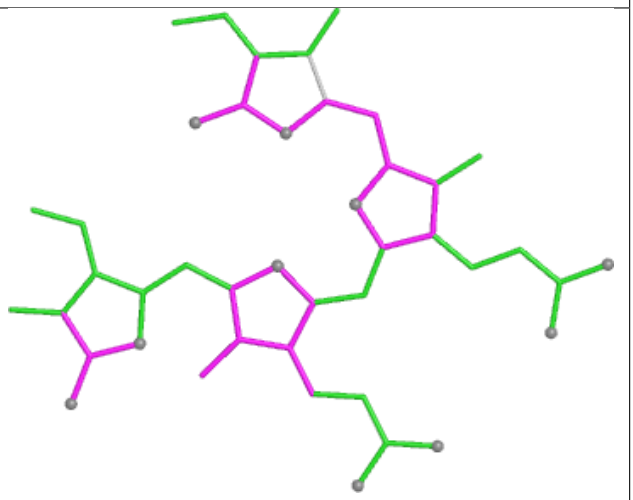
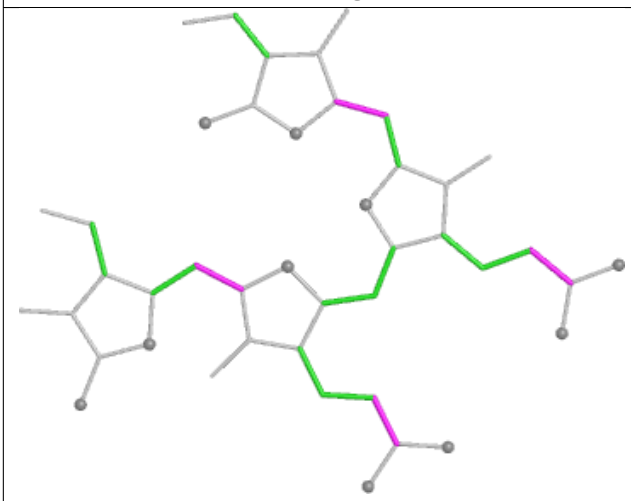


Bond angles



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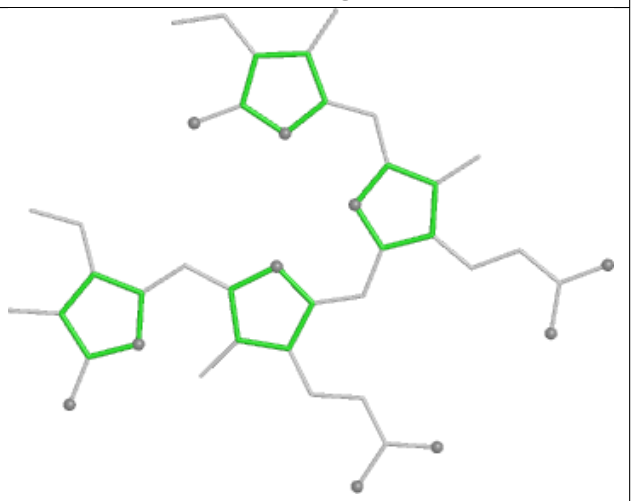
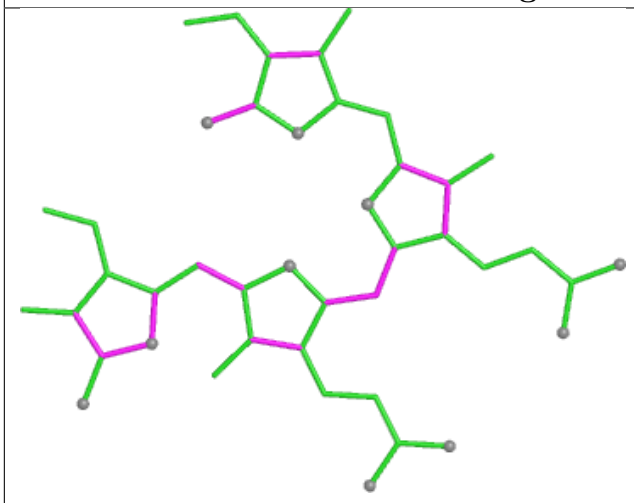


Rings

Ligand PEB SJ 203



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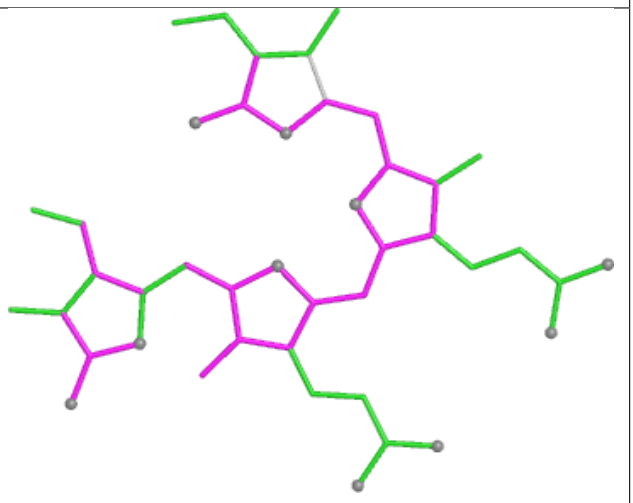

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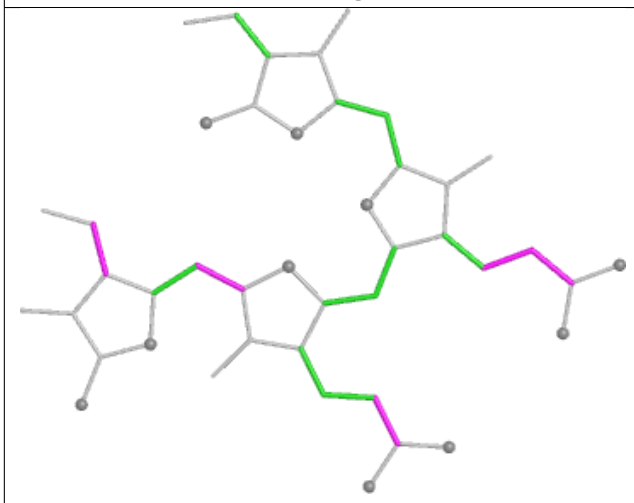

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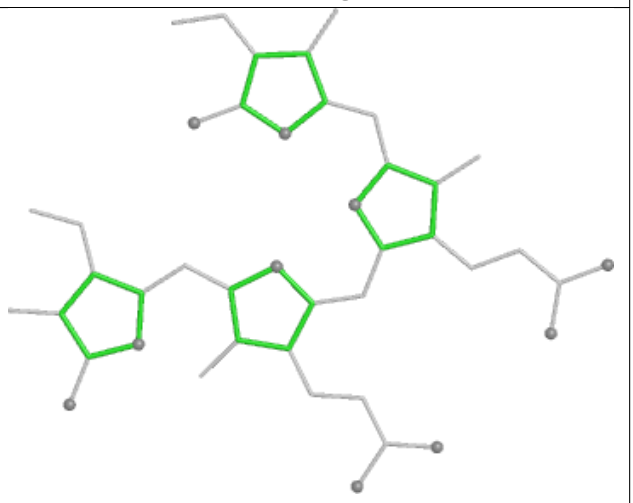

Rings

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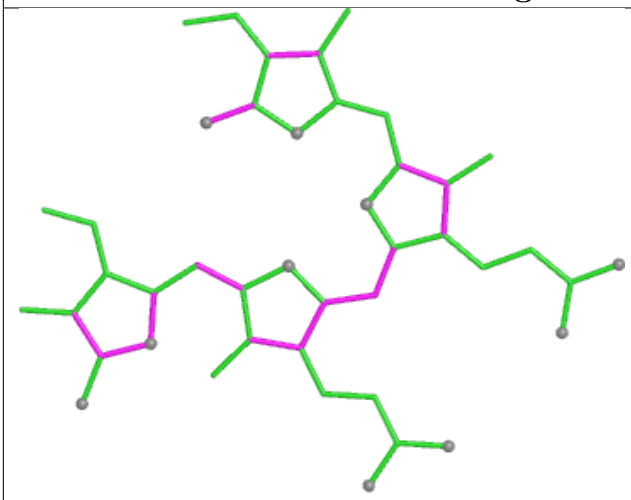

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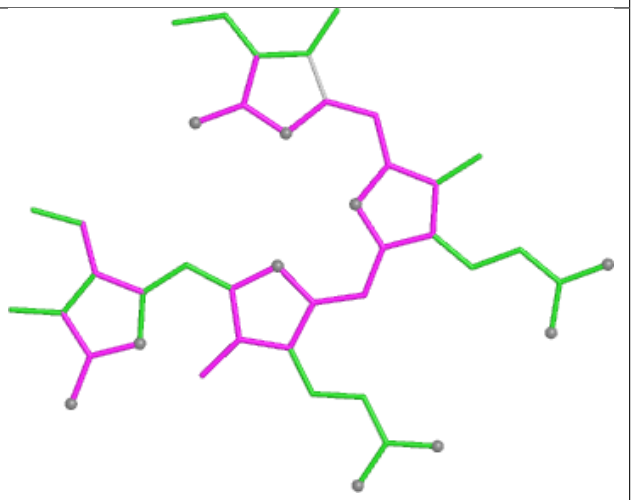

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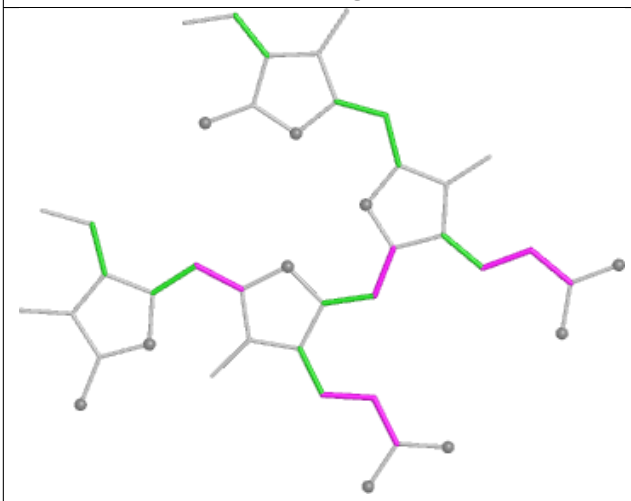

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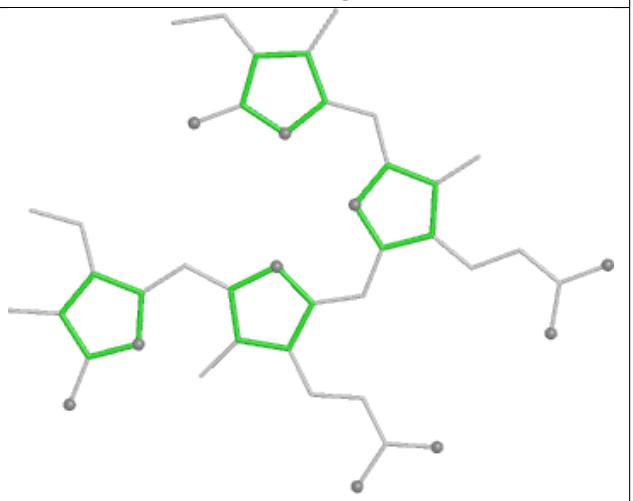
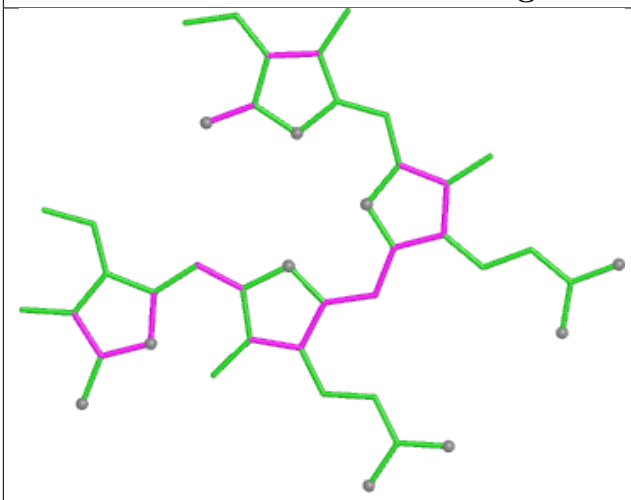


Rings

Ligand PEB eE 201



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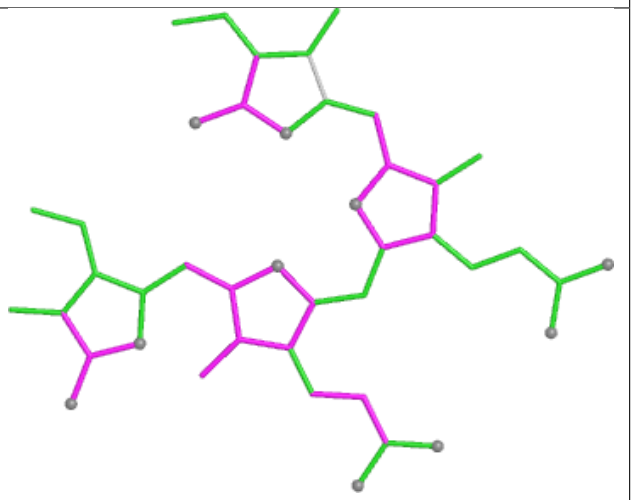
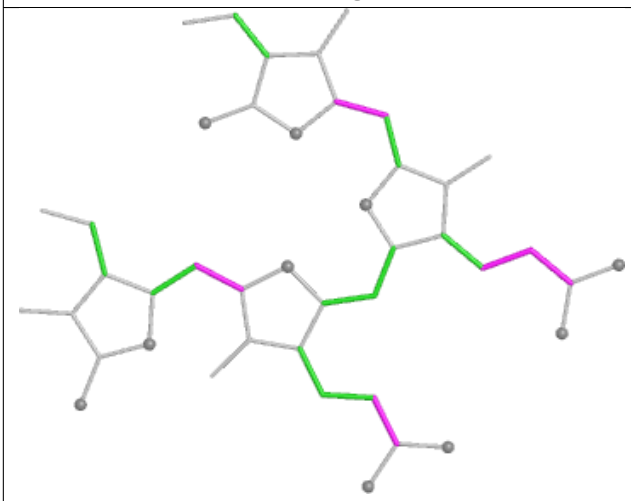


Bond angles



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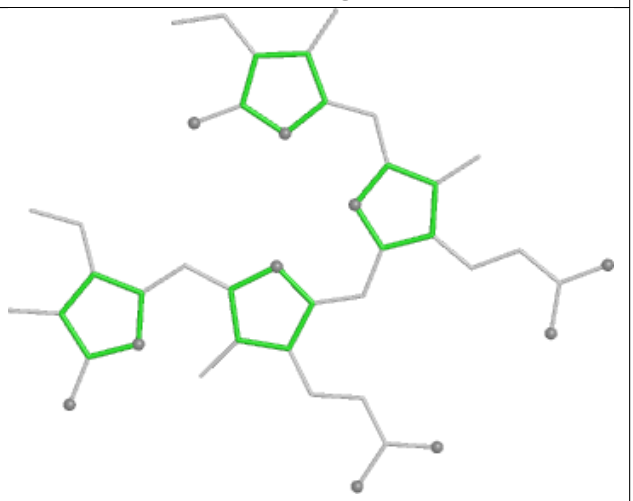
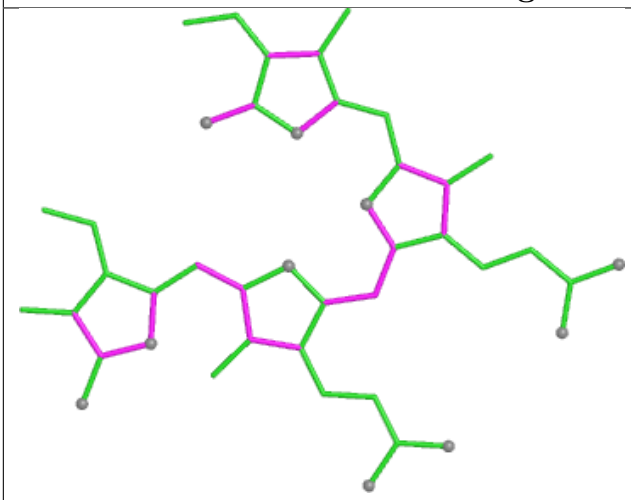


Rings

Ligand PEB Z9 304



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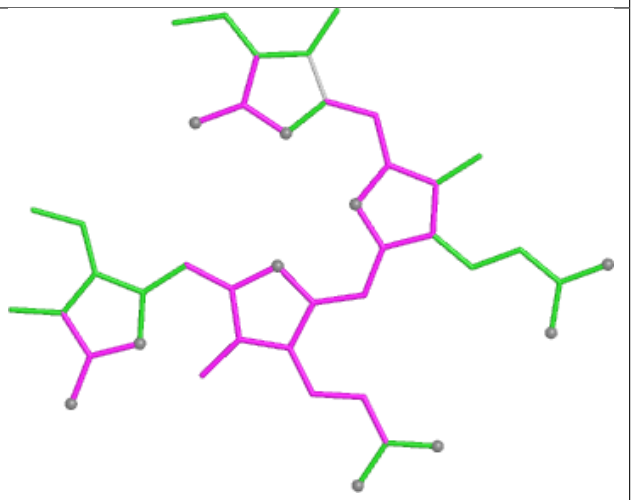
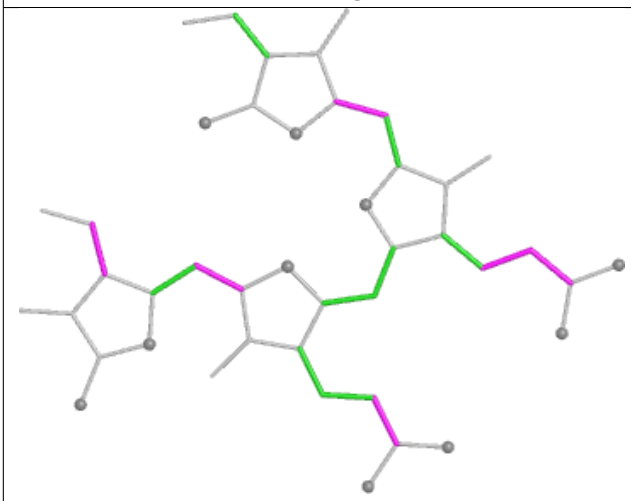
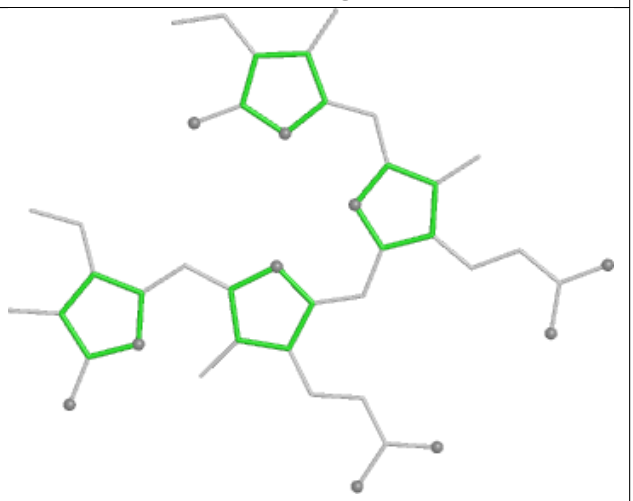


Bond angles

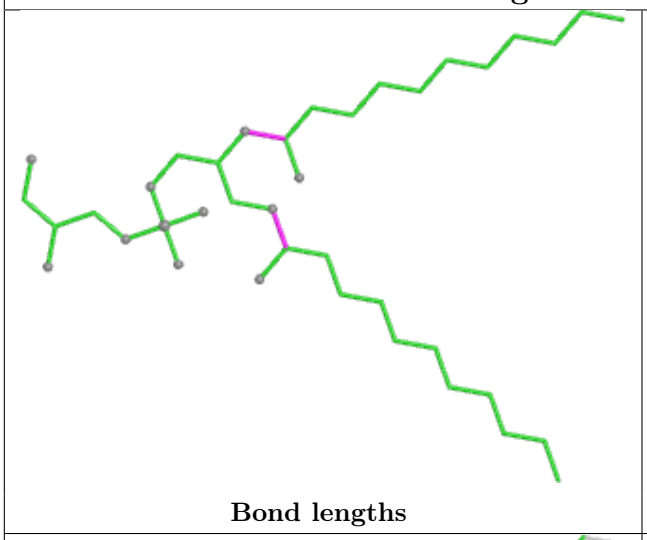


Torsions



Rings

Ligand LHG mL 102



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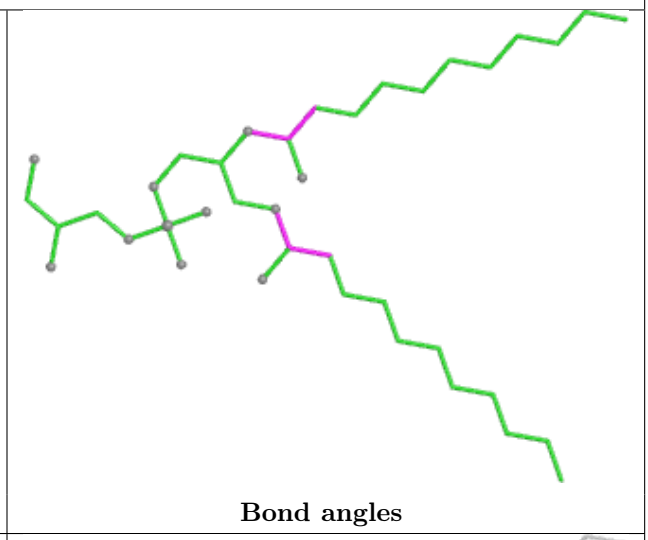

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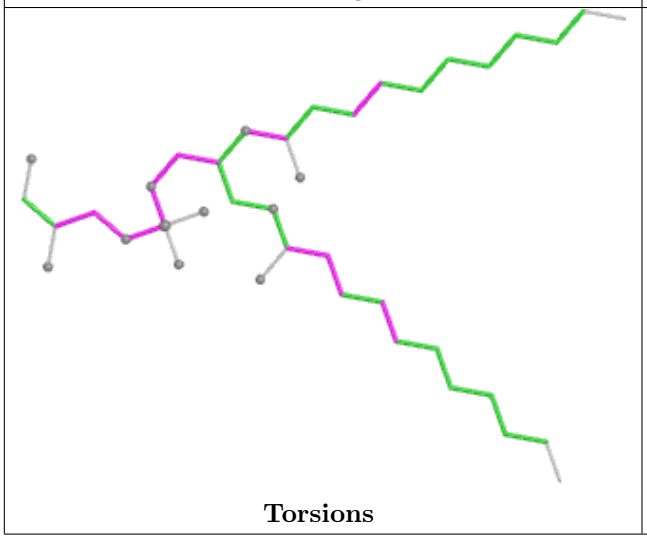

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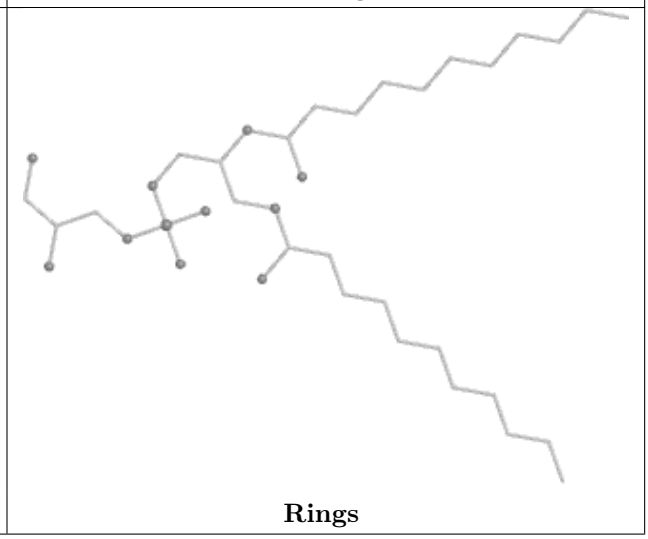
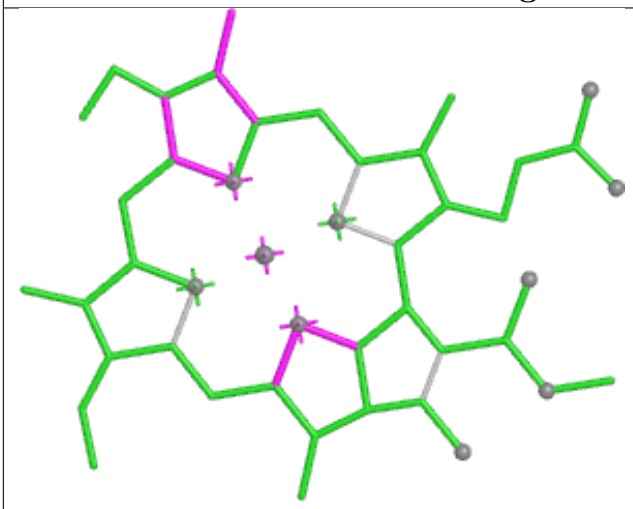


Rings

Ligand CLA 52 601



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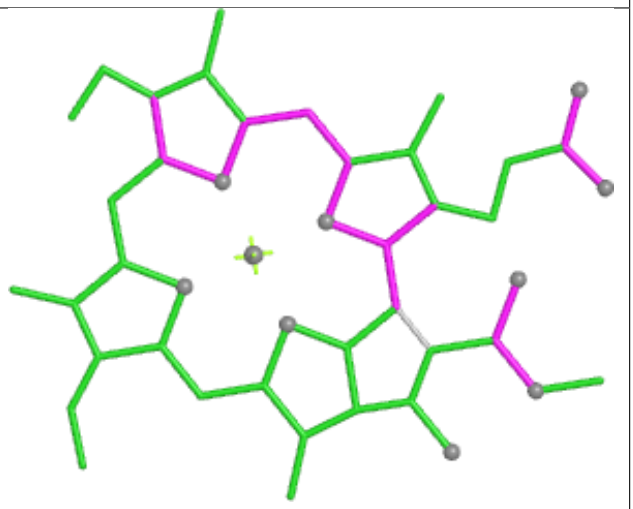

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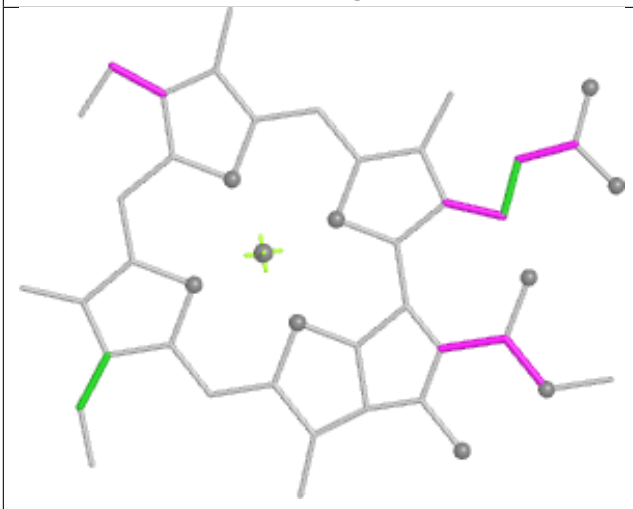
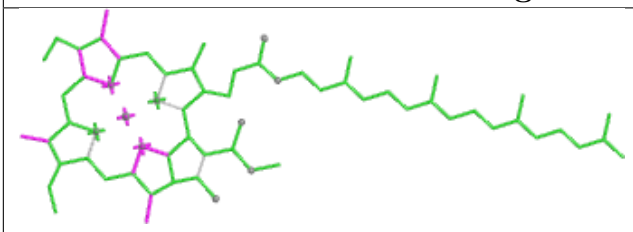


Torsions



Rings

Ligand CLA A2 840



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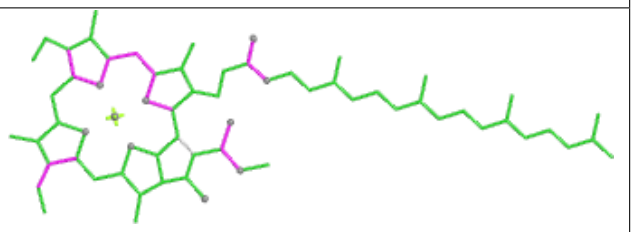
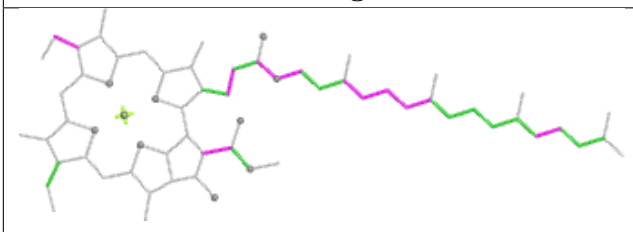


Bond angles



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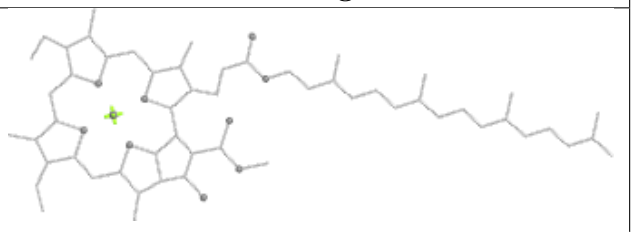
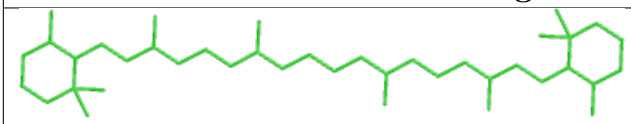


Rings

Ligand BCR bL 602



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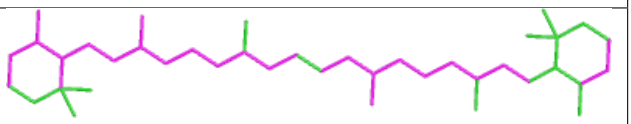
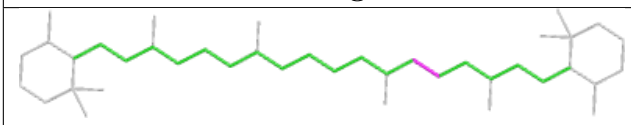


Bond angles



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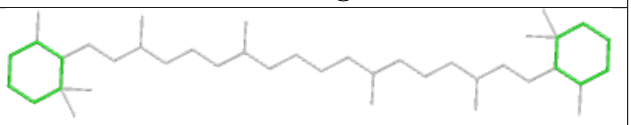
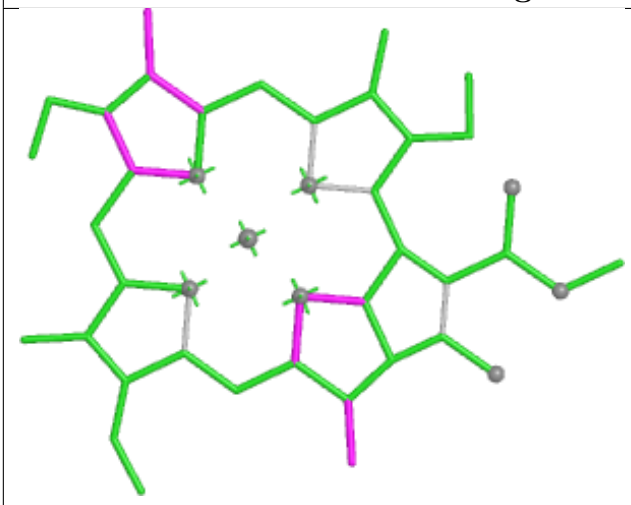


Rings

Ligand CLA 4N 610



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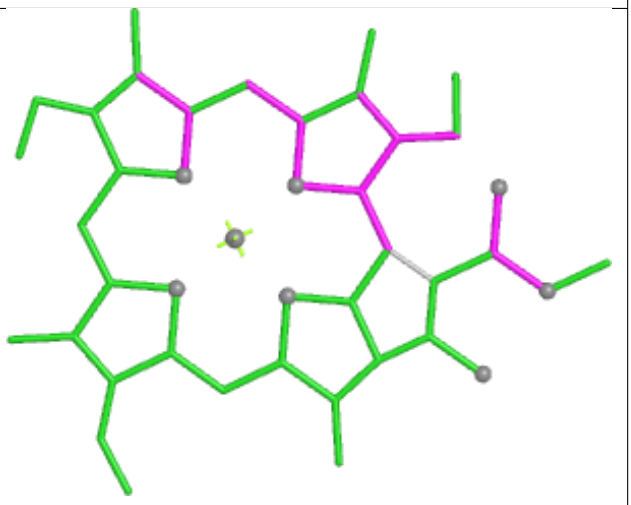
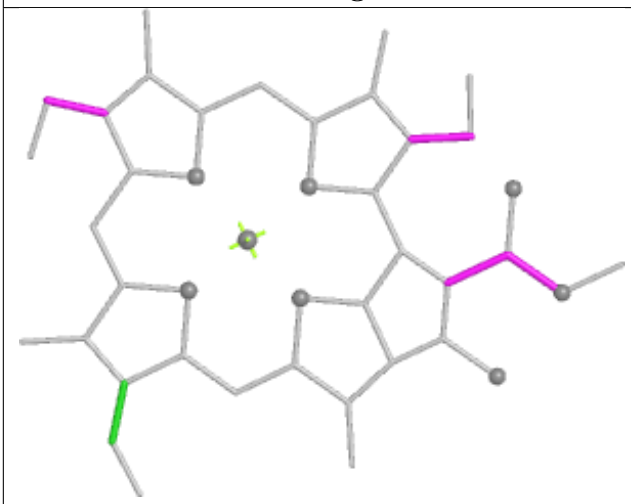


Bond angles



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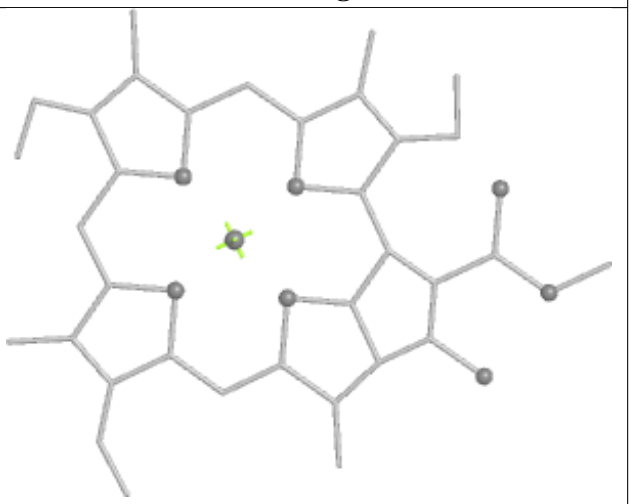
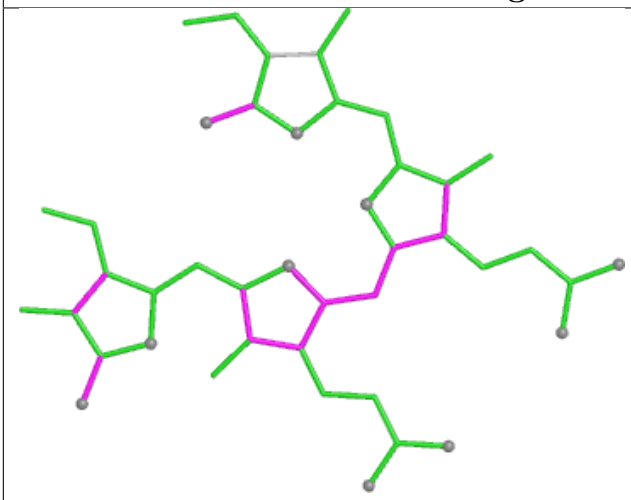


Rings

Ligand PUB AH 304



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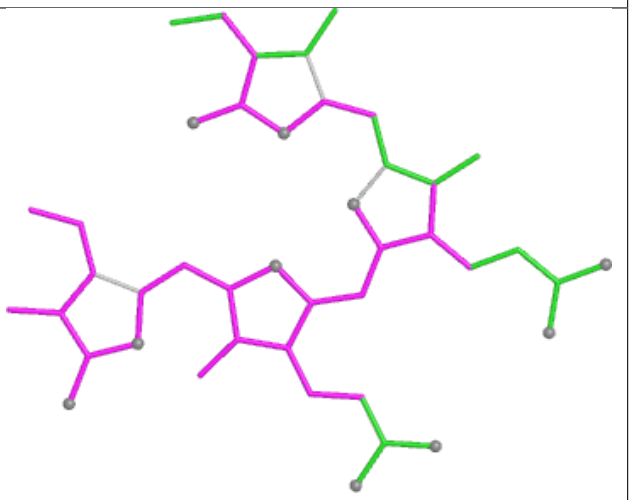
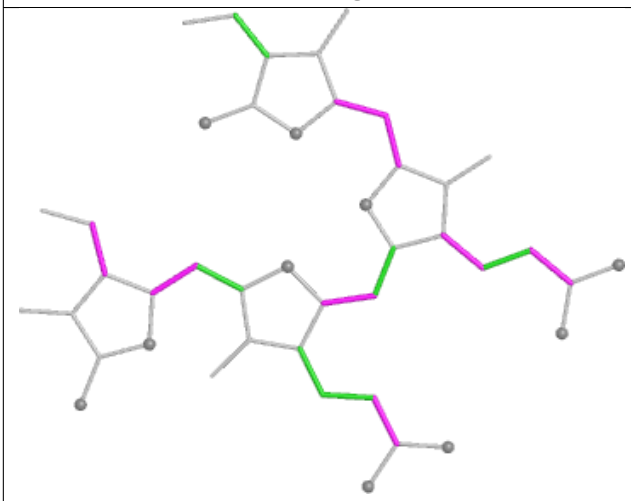


Bond angles



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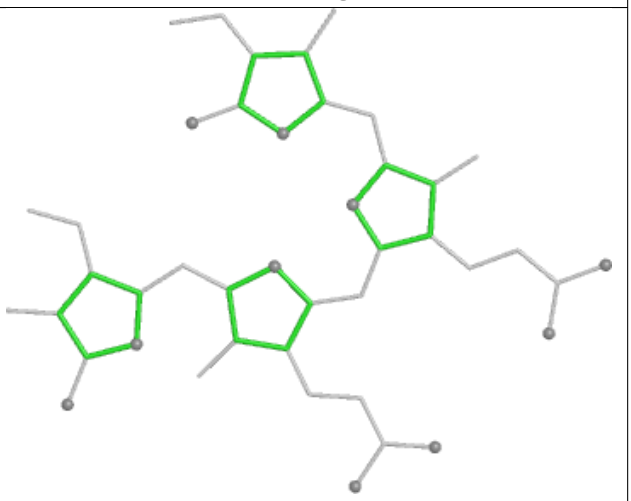
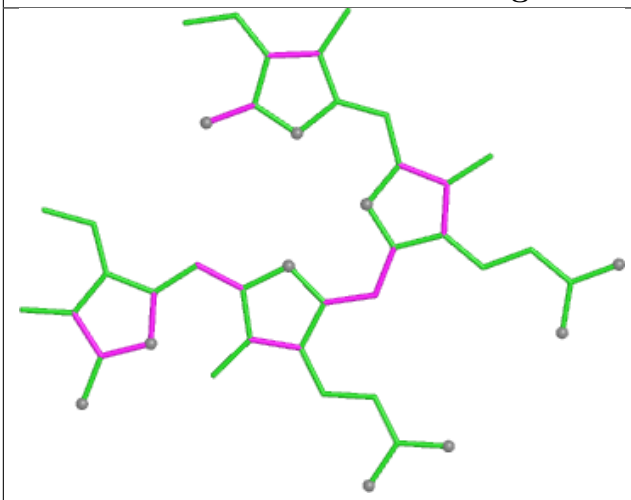


Rings

Ligand PEB QB 203



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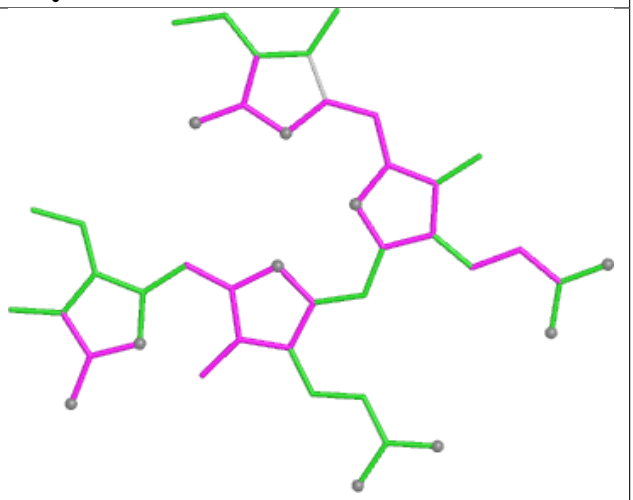
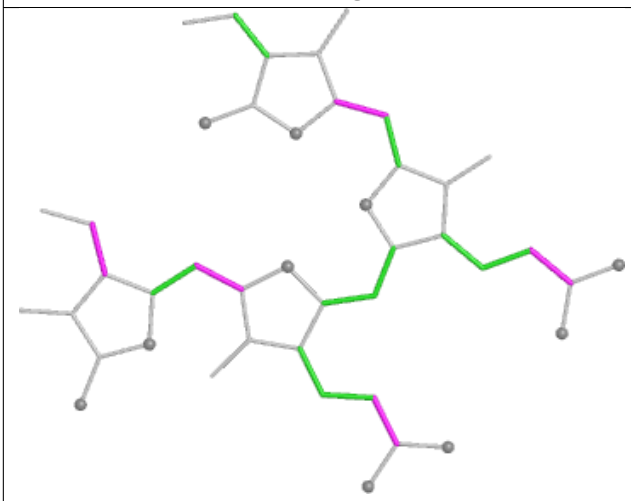


Bond angles



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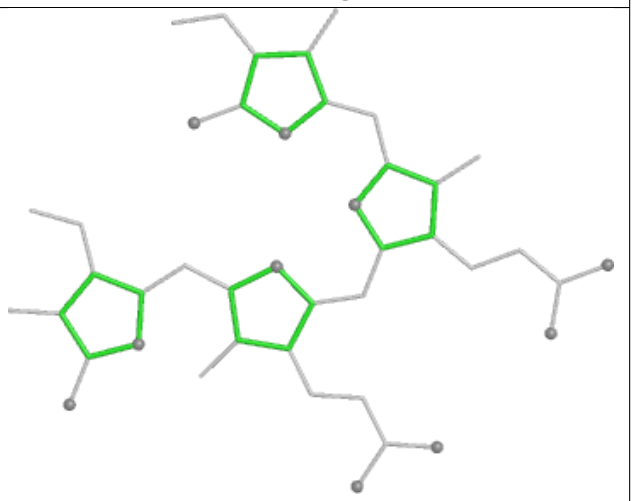
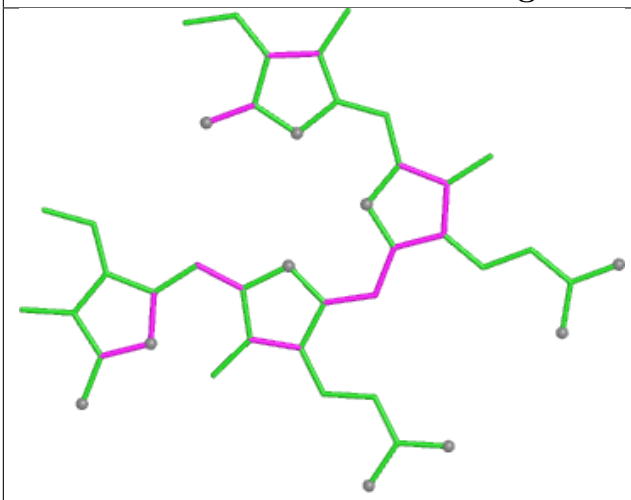


Rings

Ligand PEB cE 202



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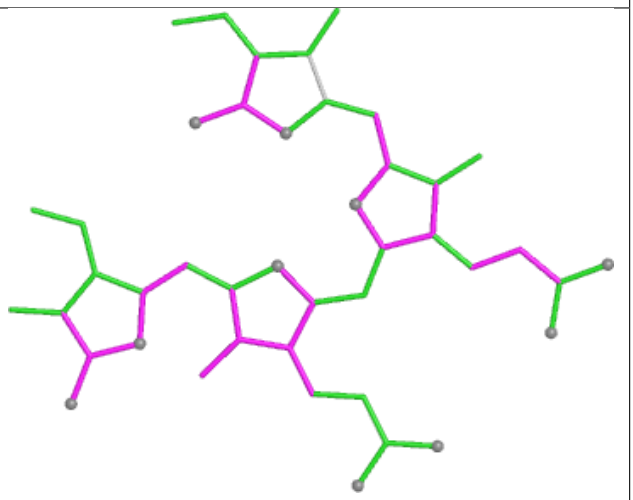
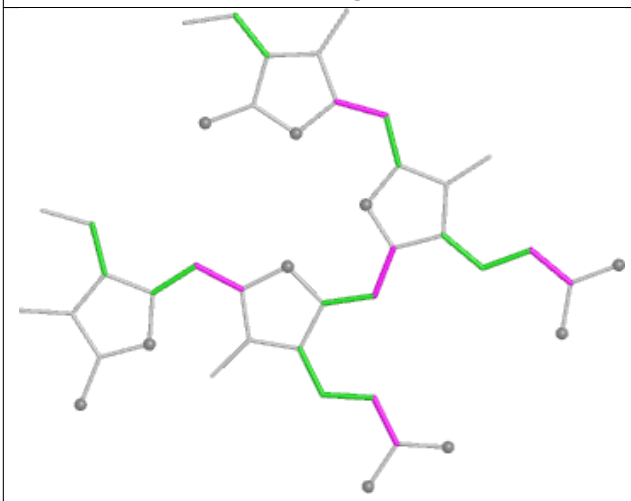


Bond angles



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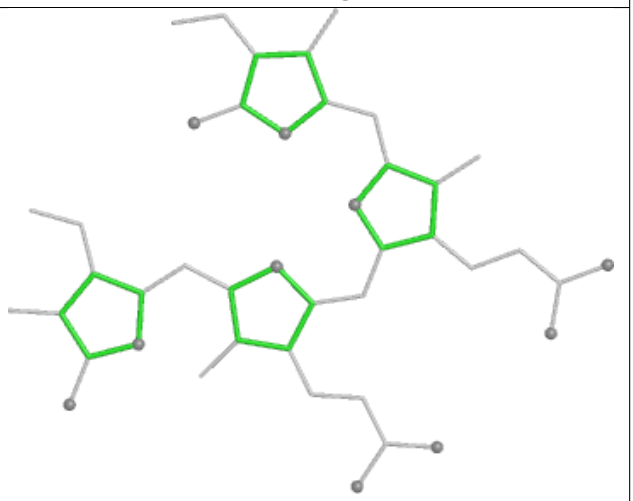
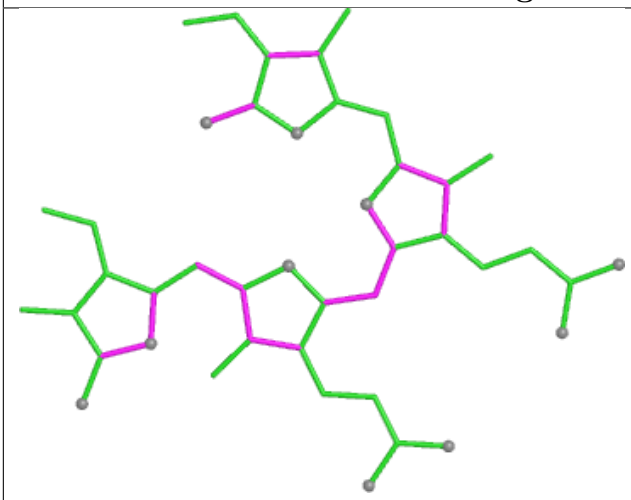


Rings

Ligand PEB B5 203



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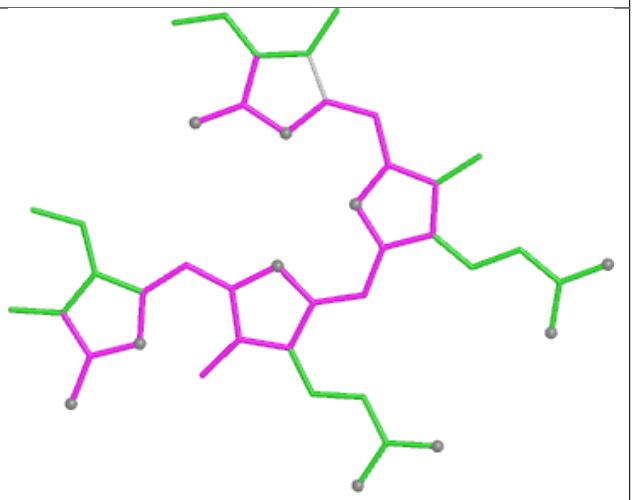
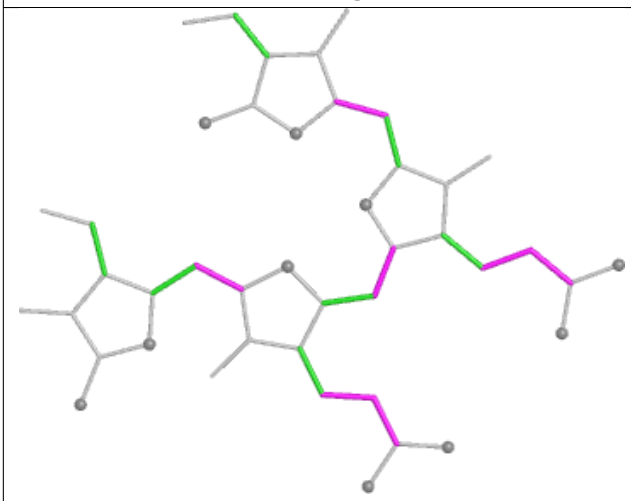


Bond angles



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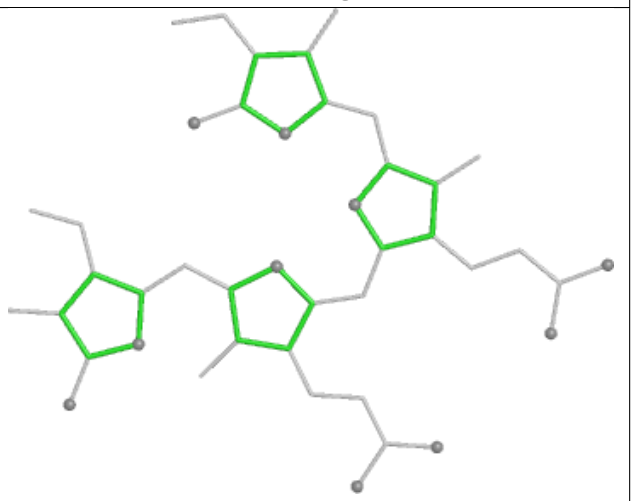
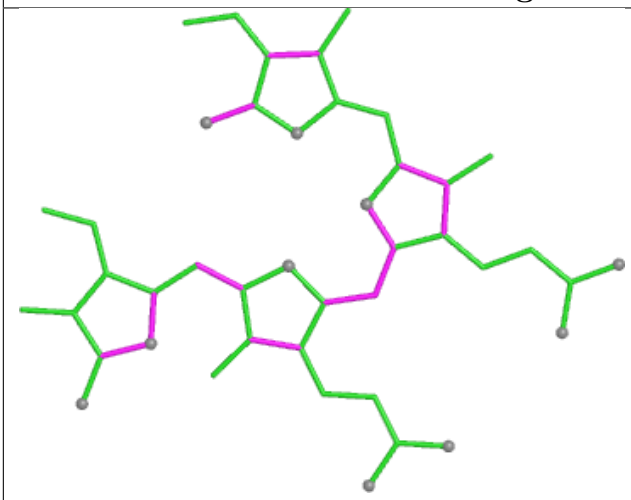


Rings

Ligand PEB B7 203



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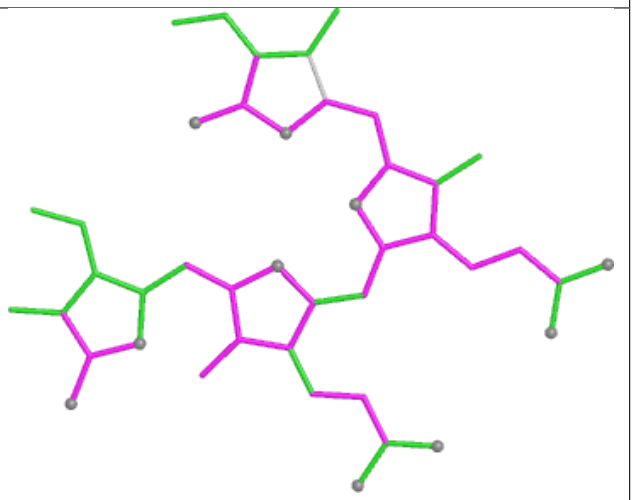

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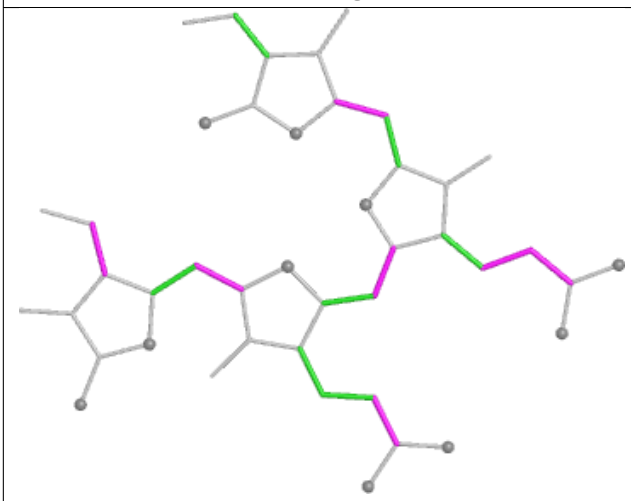

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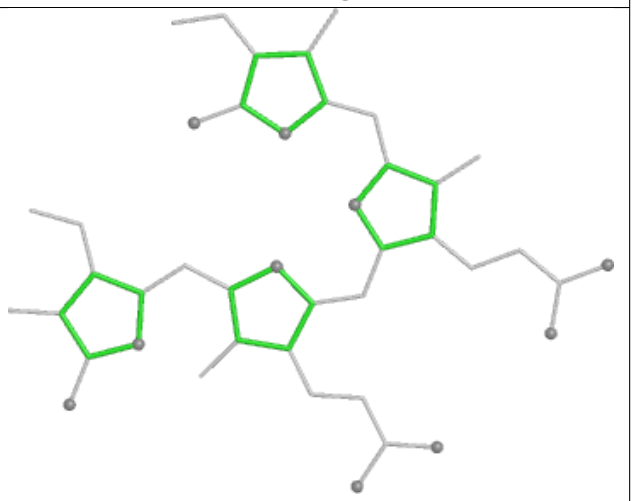
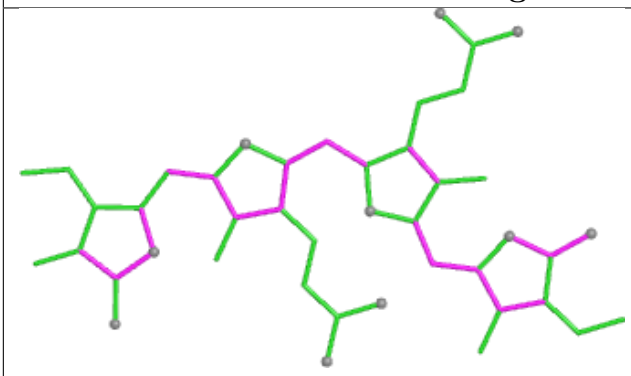


Rings

Ligand CYC c3 1001



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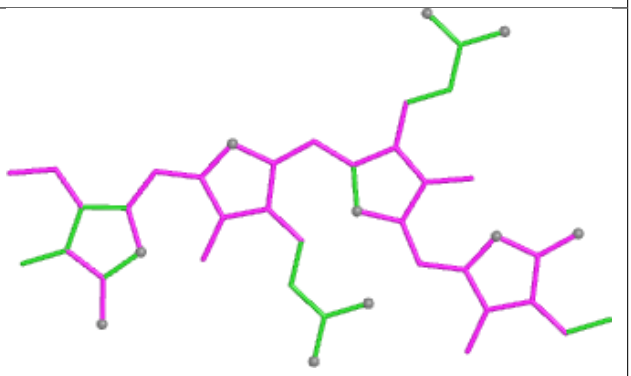

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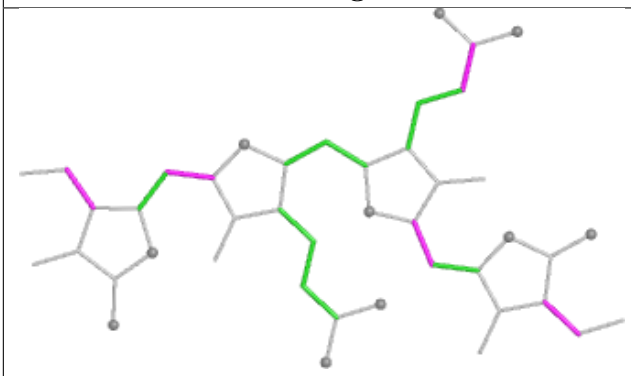

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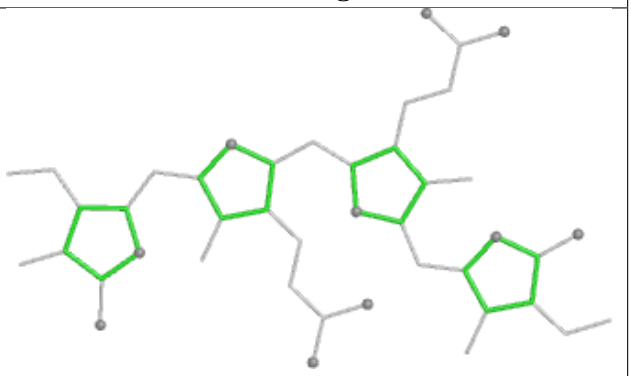
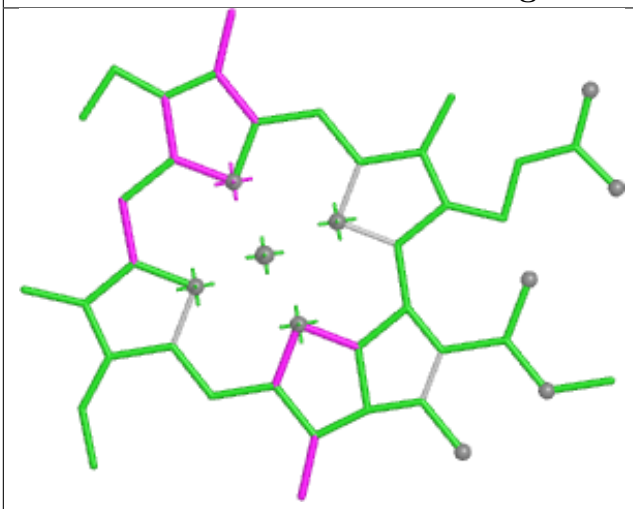


Rings

Ligand CLA 12 603



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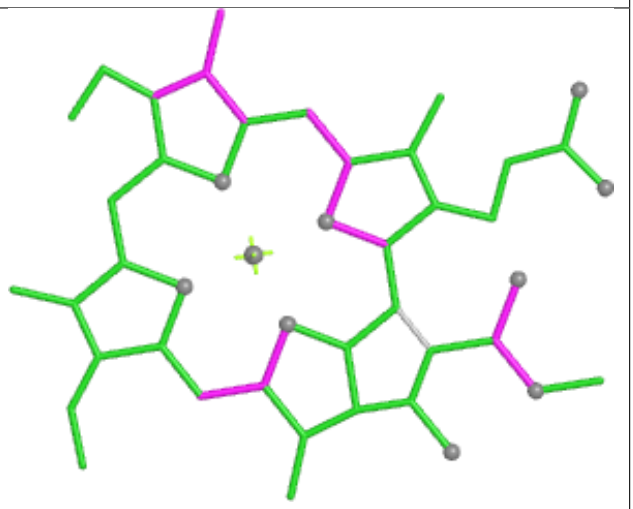
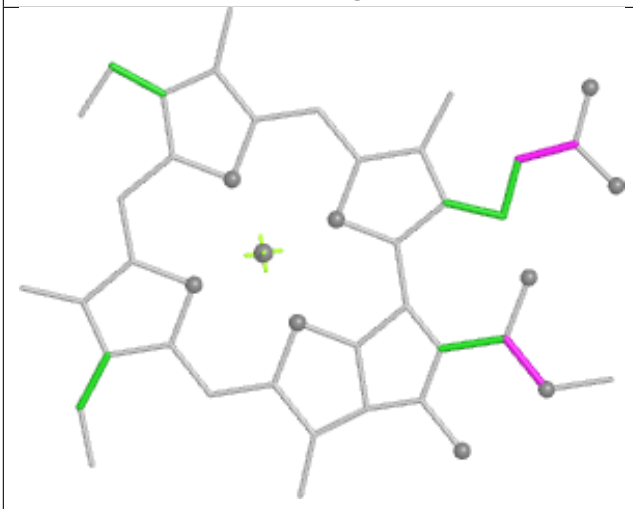


Bond angles

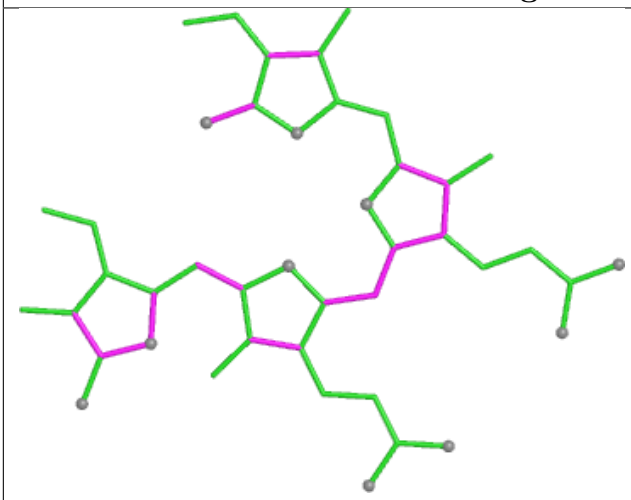


Torsions



Rings

Ligand PEB fE 201



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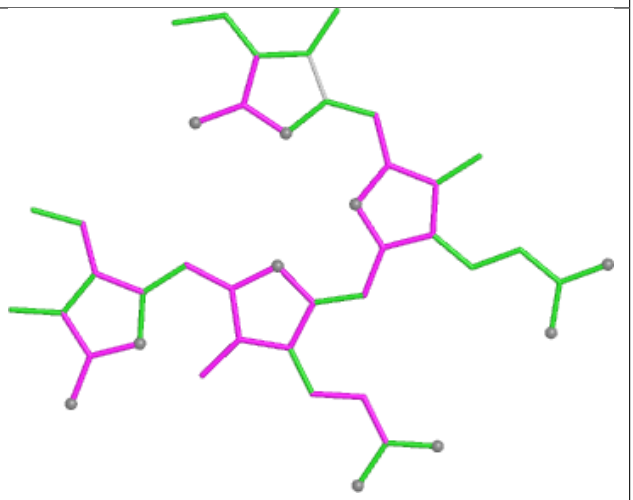
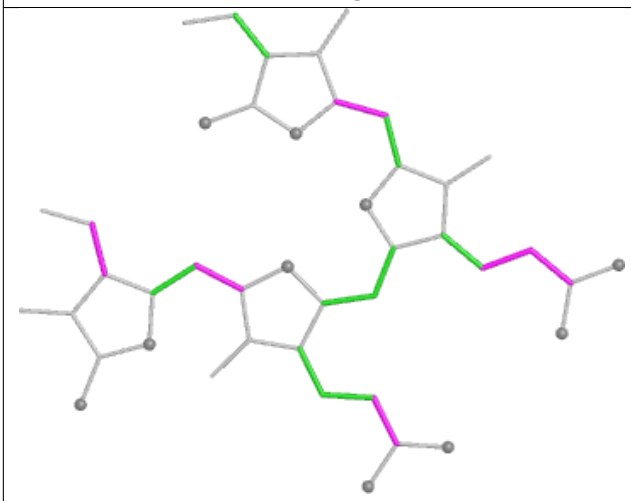


Bond angles



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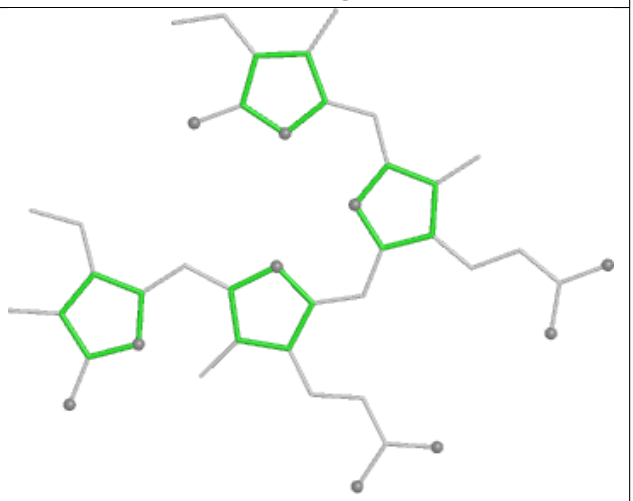
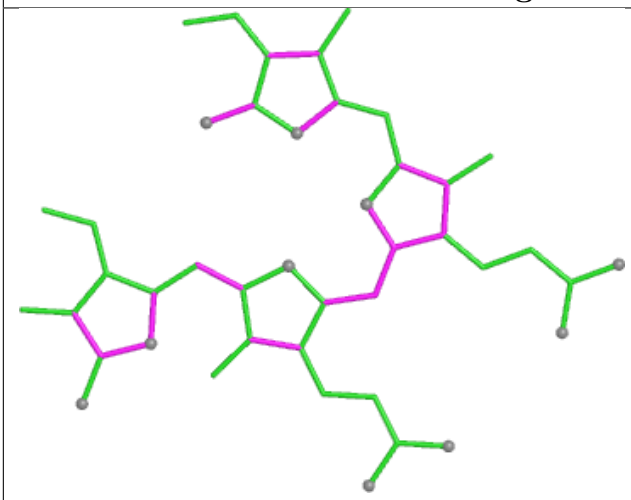


Rings

Ligand PEB eG 203



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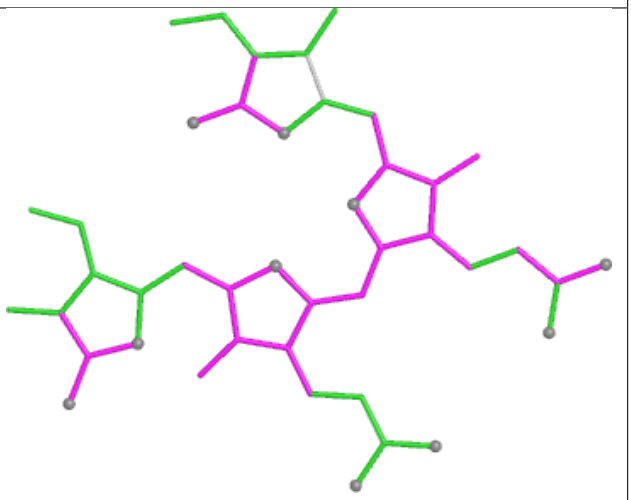
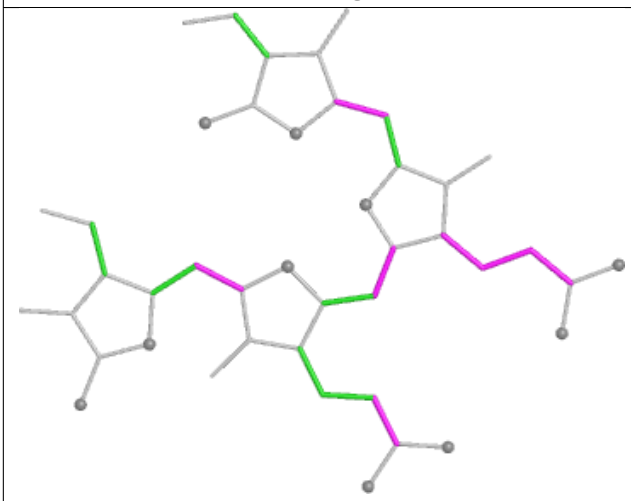


Bond angles



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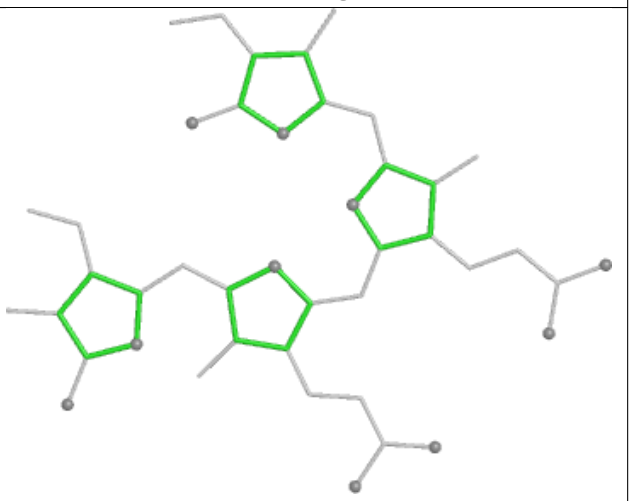
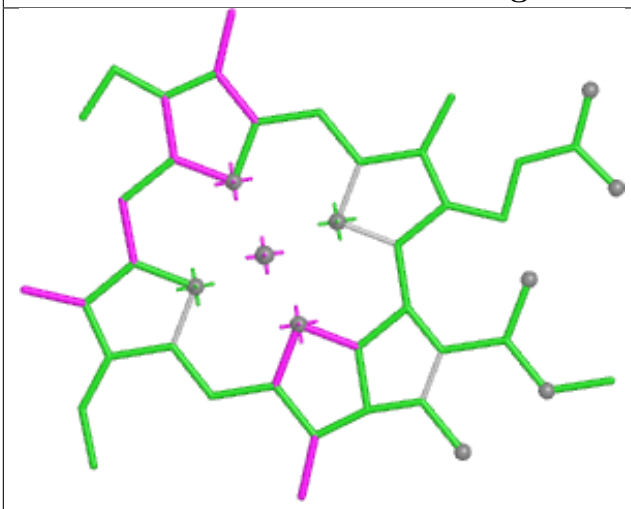


Rings

Ligand CLA BN 828



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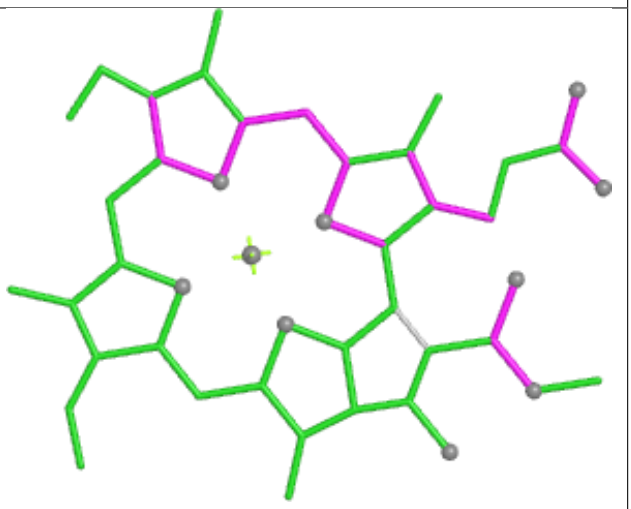
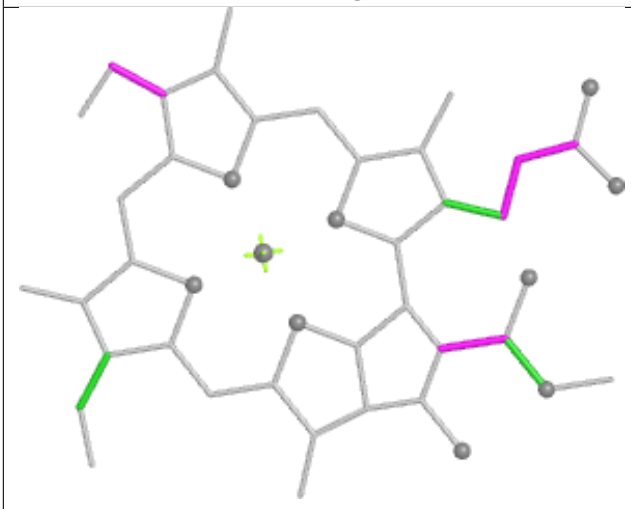


Bond angles

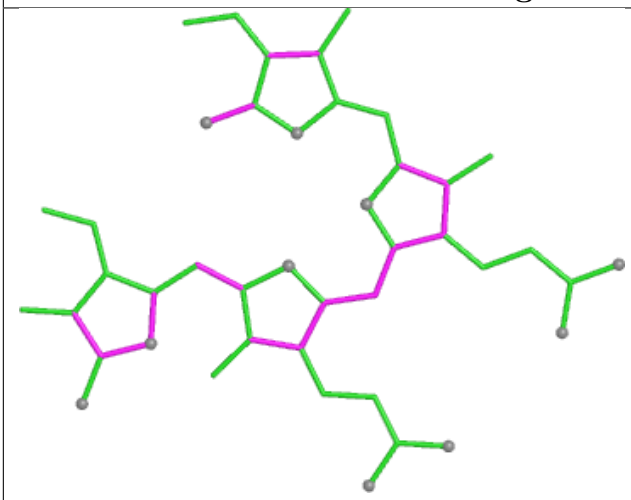


Torsions



Rings

Ligand PEB qC 201



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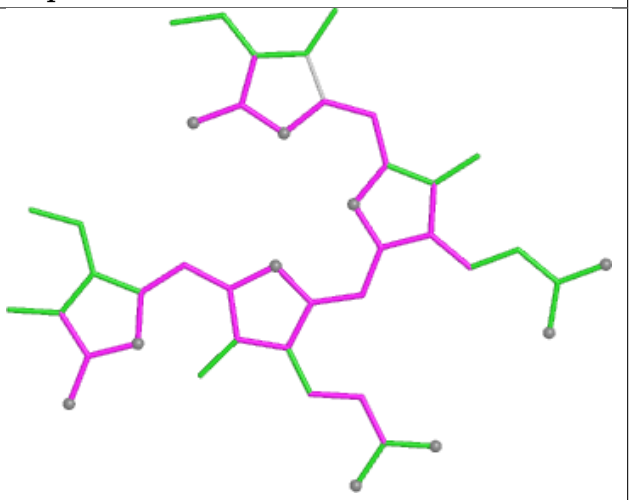

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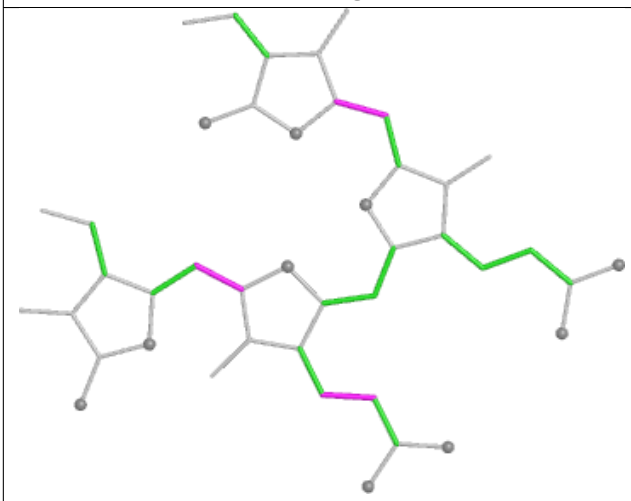

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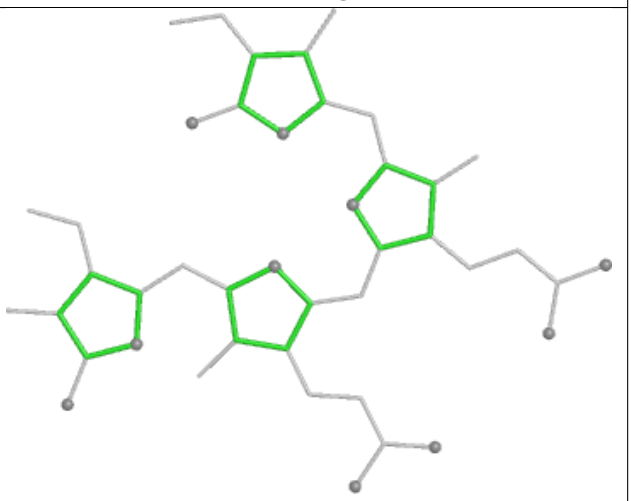
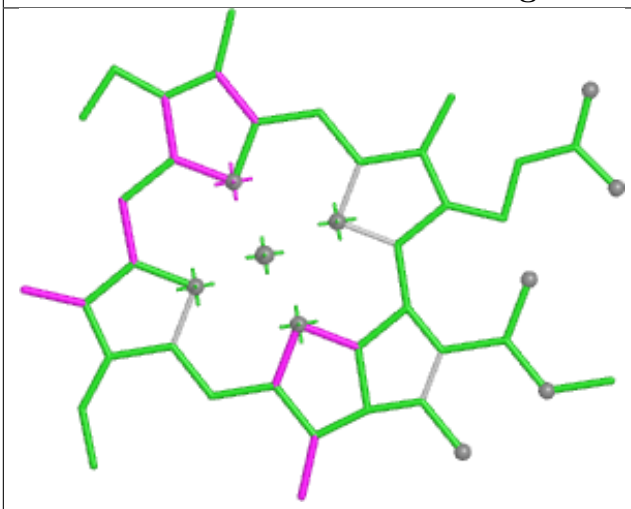


Rings

Ligand CLA 12 601



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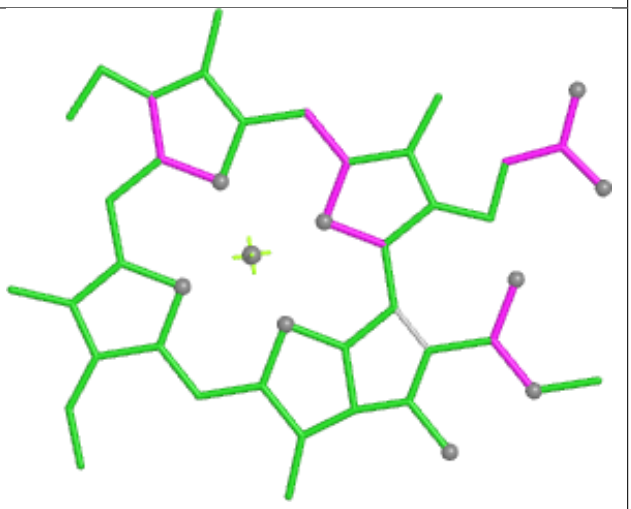

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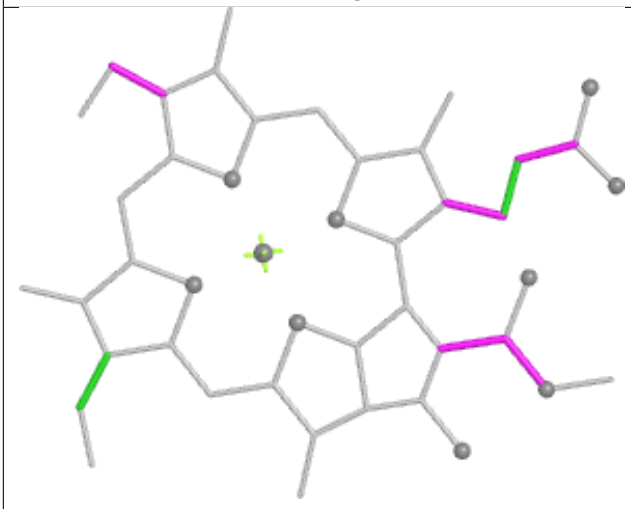
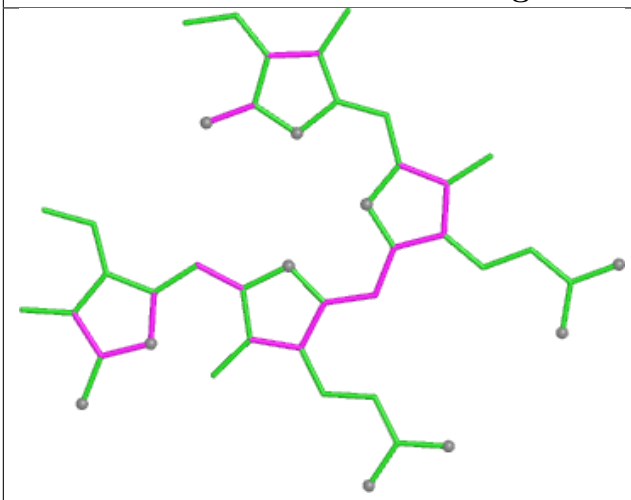


Torsions



Rings

Ligand PEB aM 201



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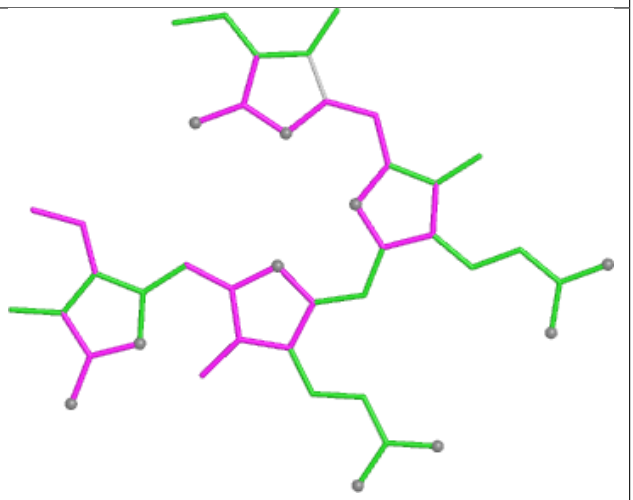

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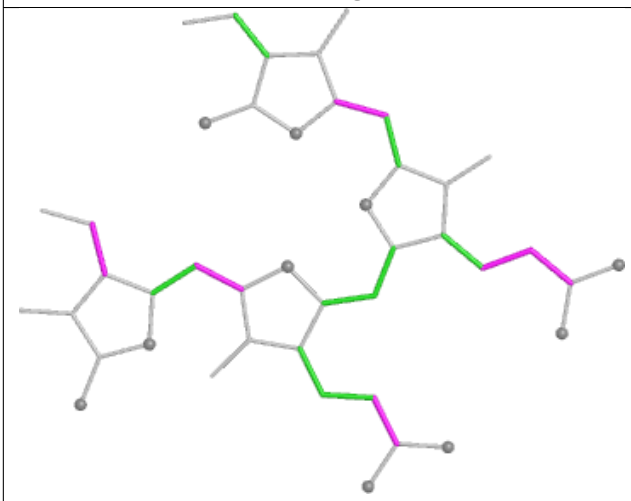

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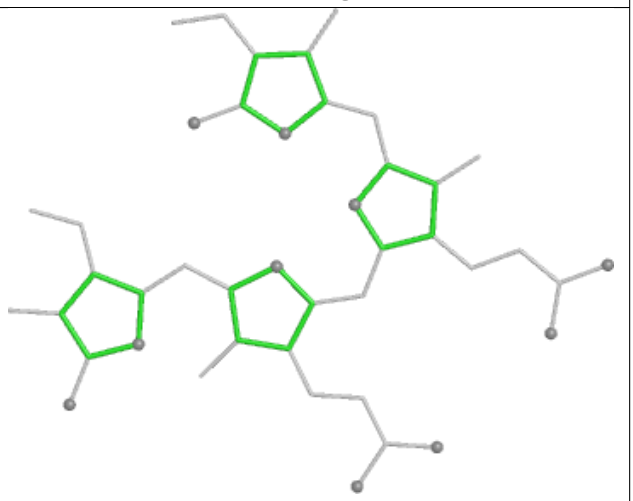

Rings

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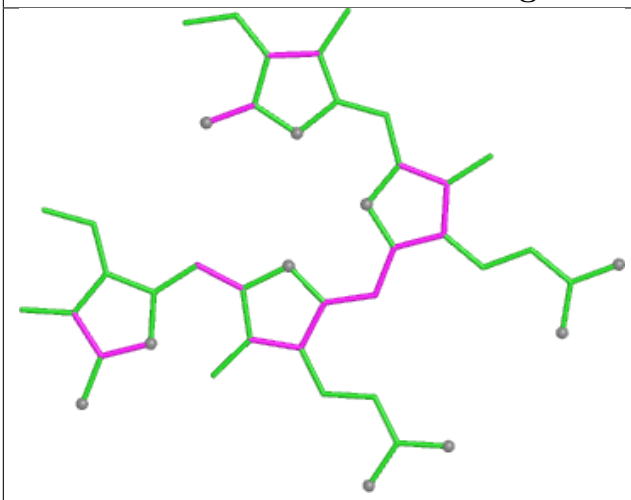

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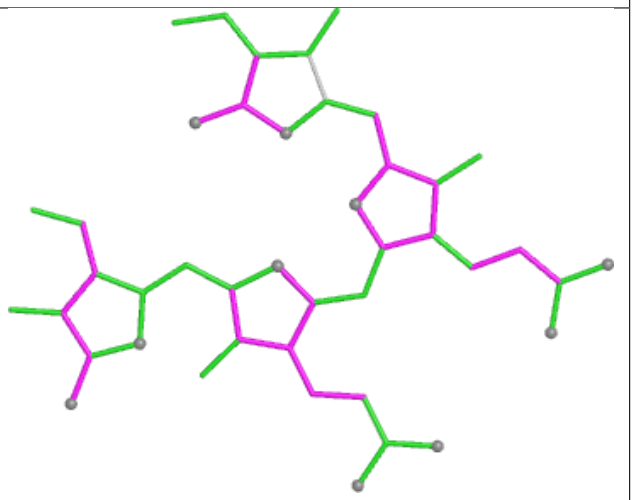

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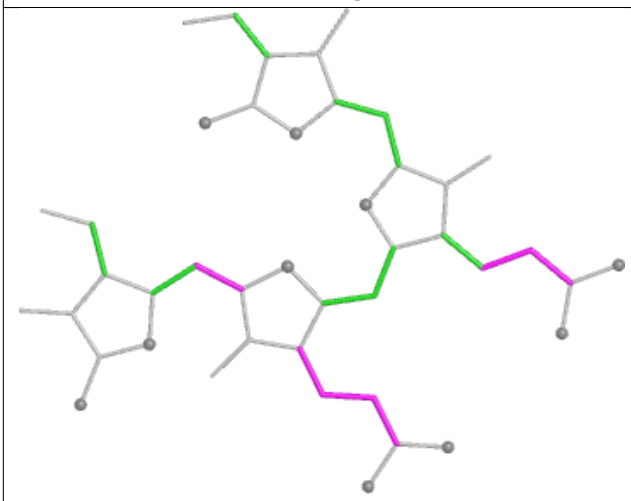

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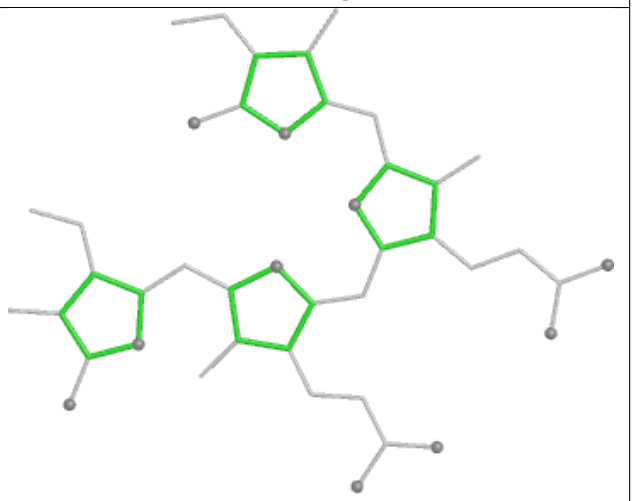
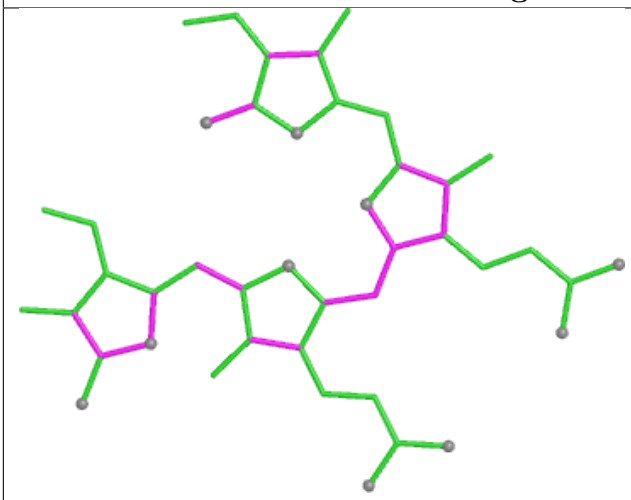


Rings

Ligand PEB VG 202



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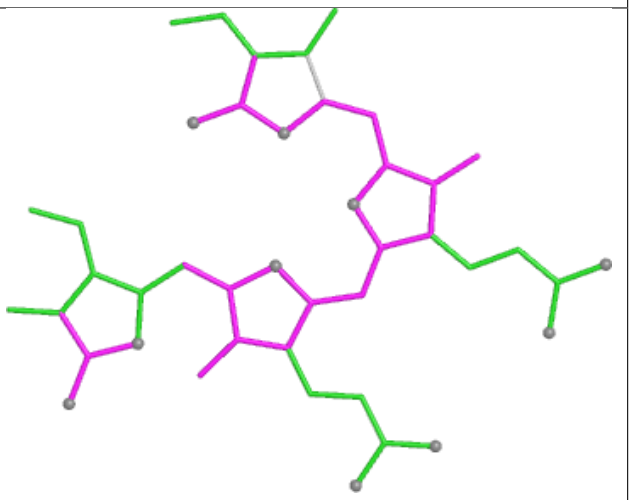

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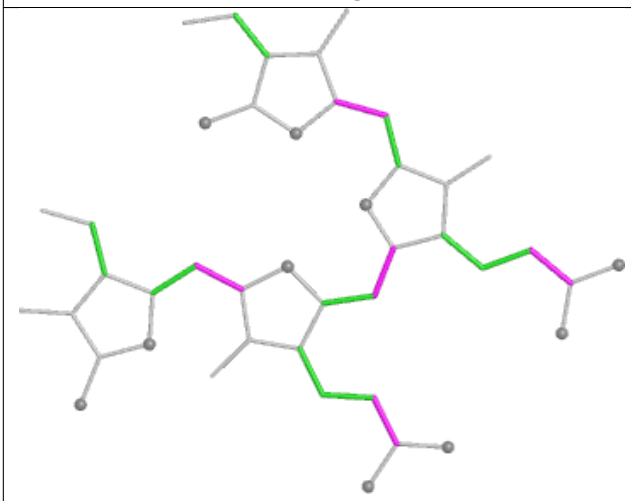

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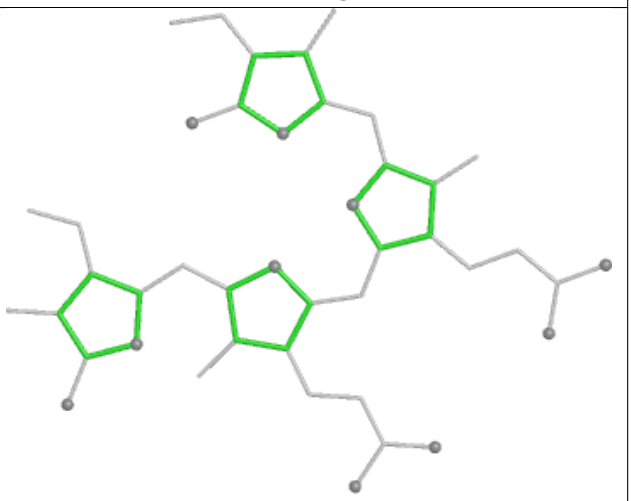

Rings

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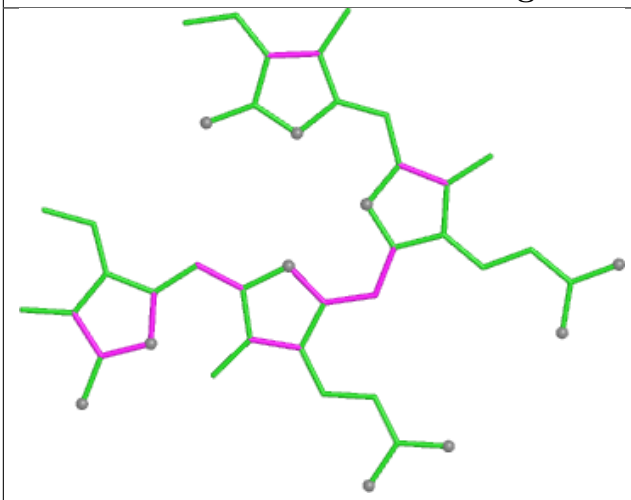

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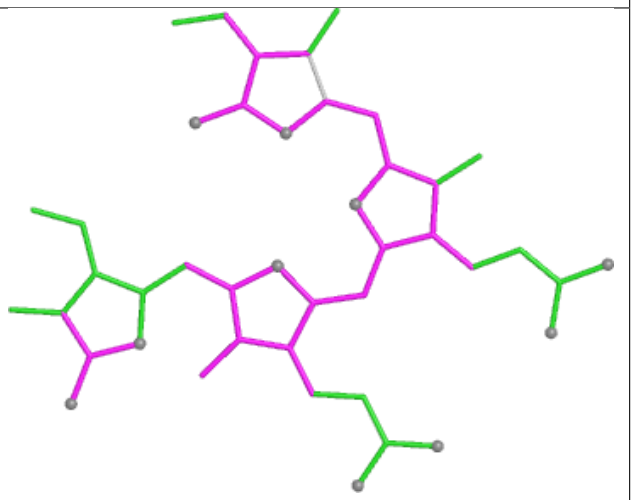

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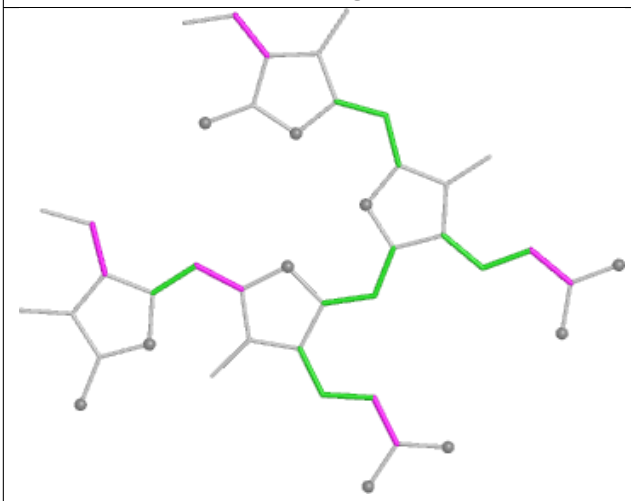

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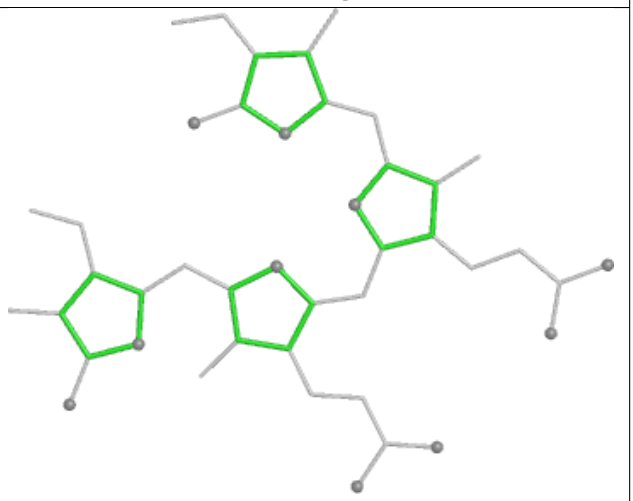
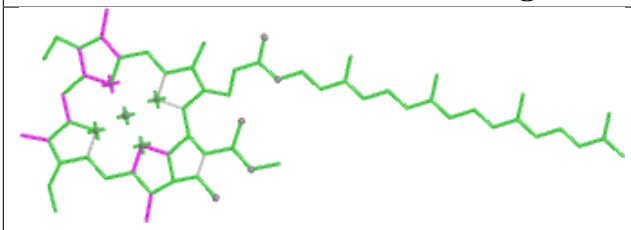


Rings

Ligand CLA b6 610



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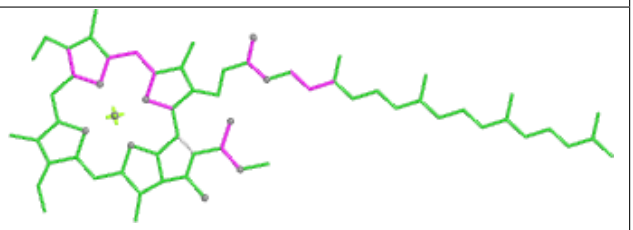

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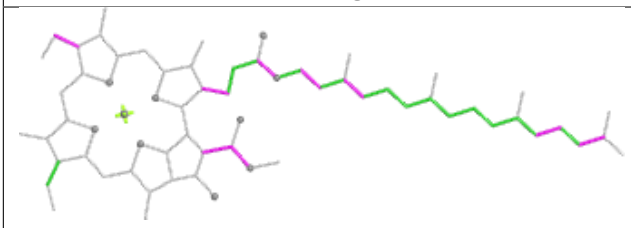

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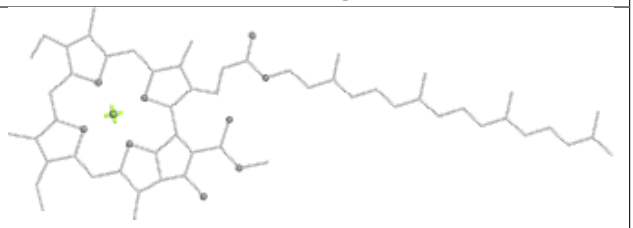
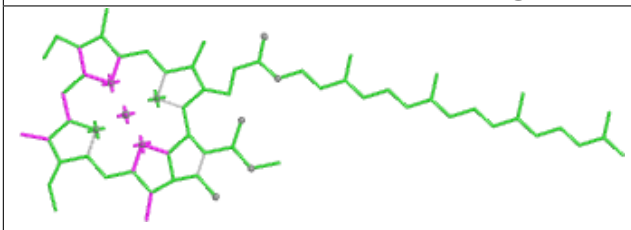


Rings

Ligand CLA AN 849



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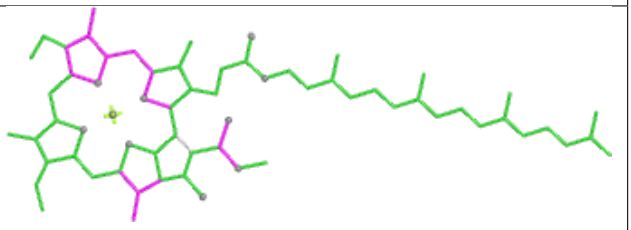

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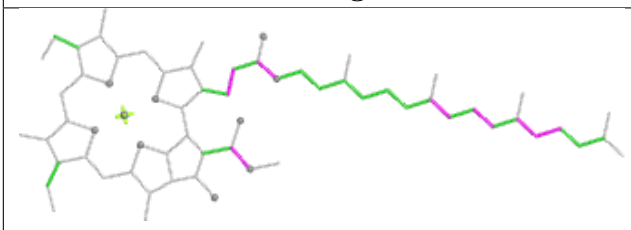

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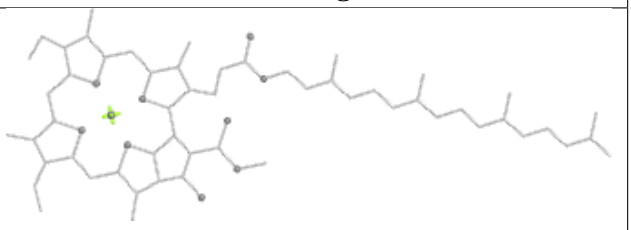
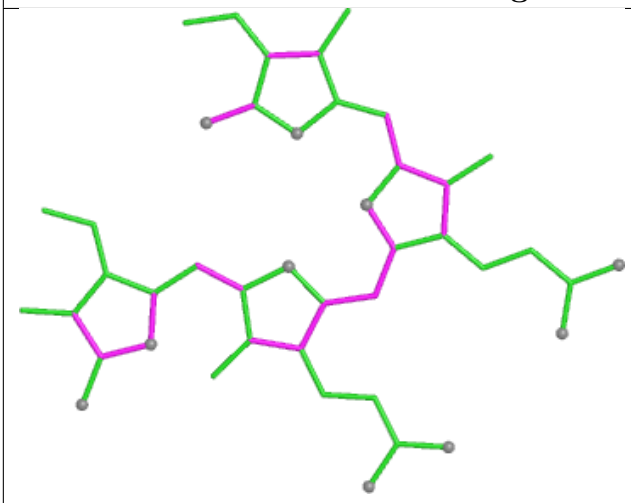


Rings

Ligand PEB J4 1002



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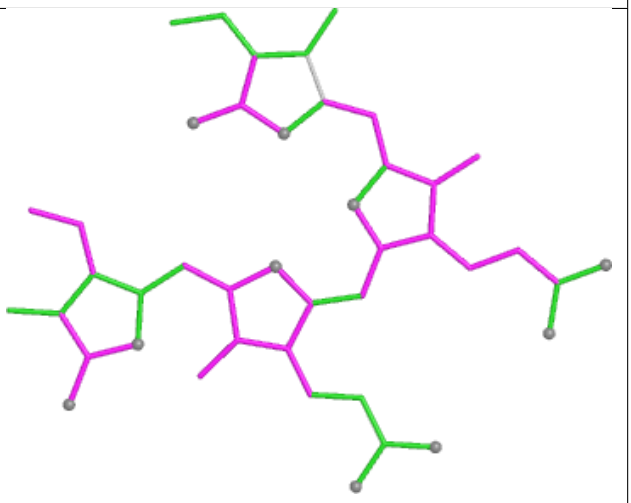

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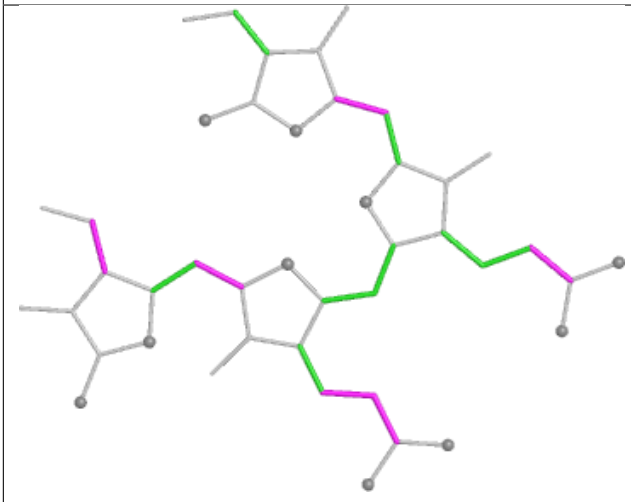

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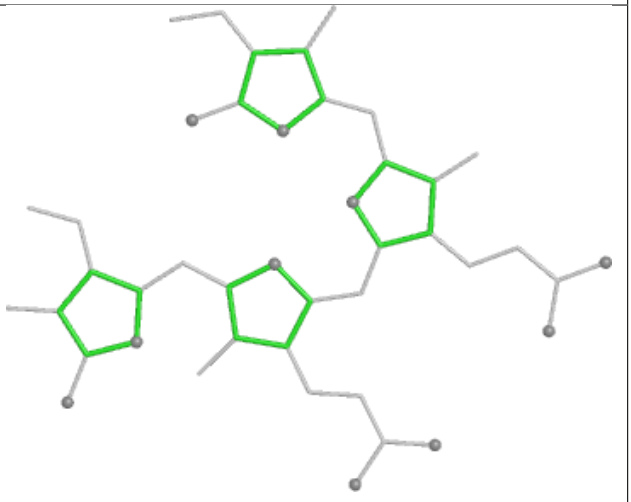
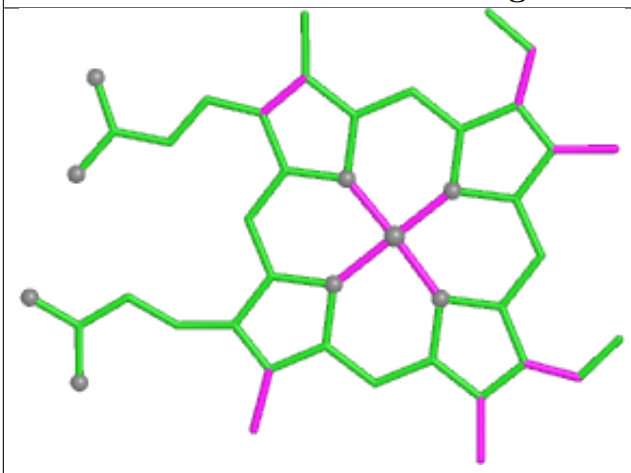


Rings

Ligand HEM G2 201



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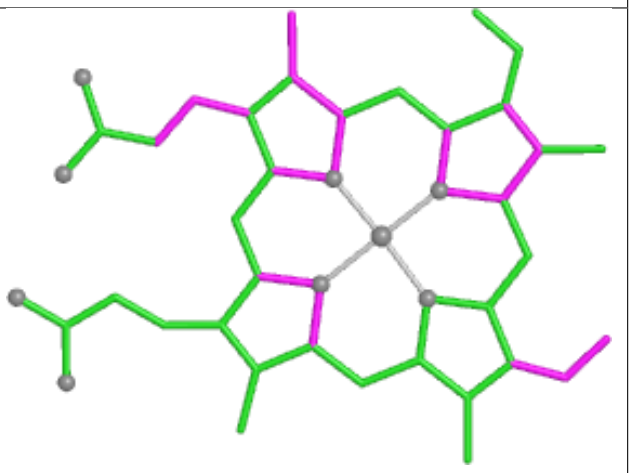

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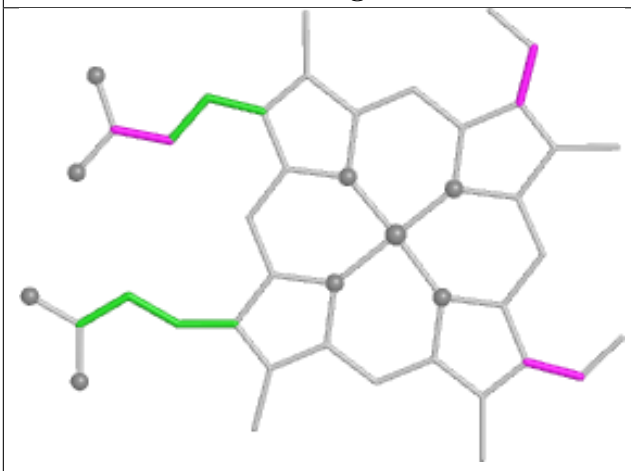

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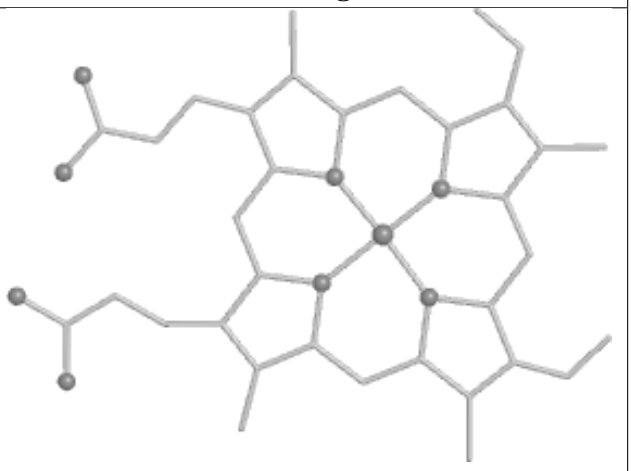
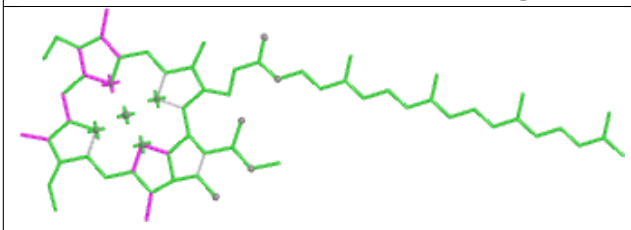


Rings

Ligand CLA A2 835



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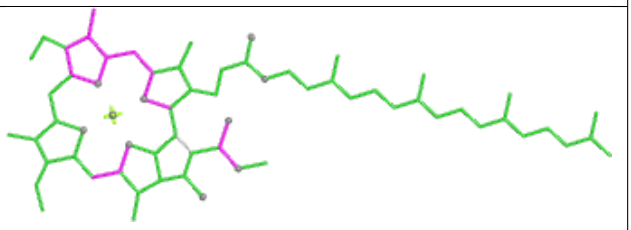

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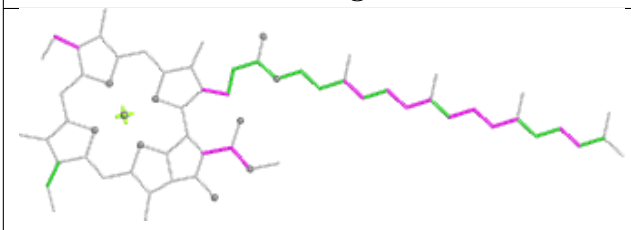

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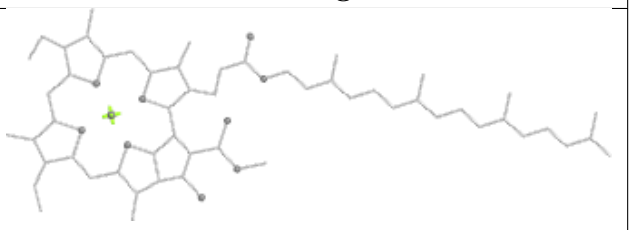
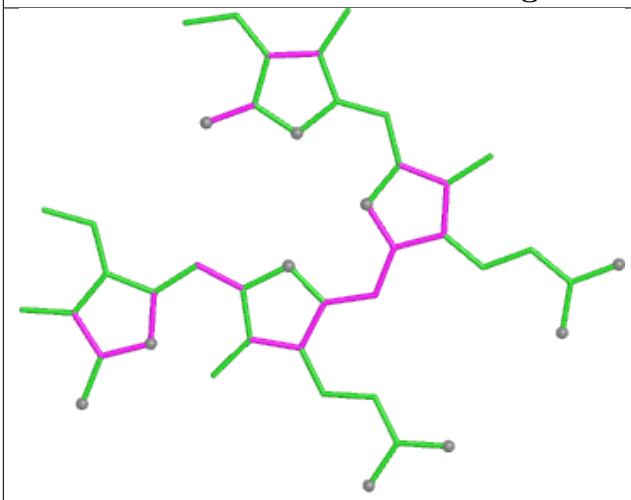


Rings

Ligand PEB lE 203



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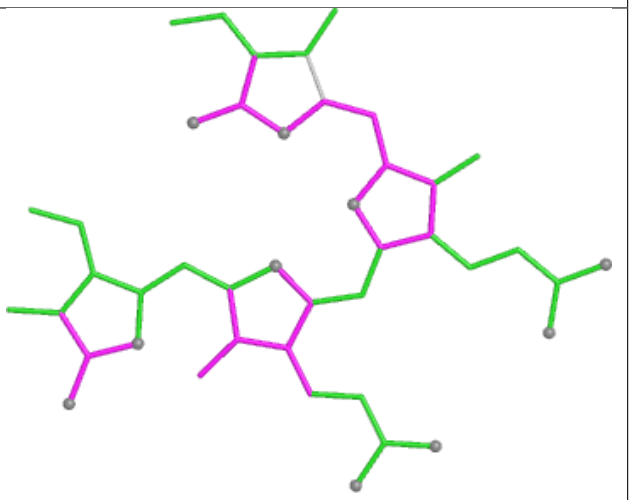

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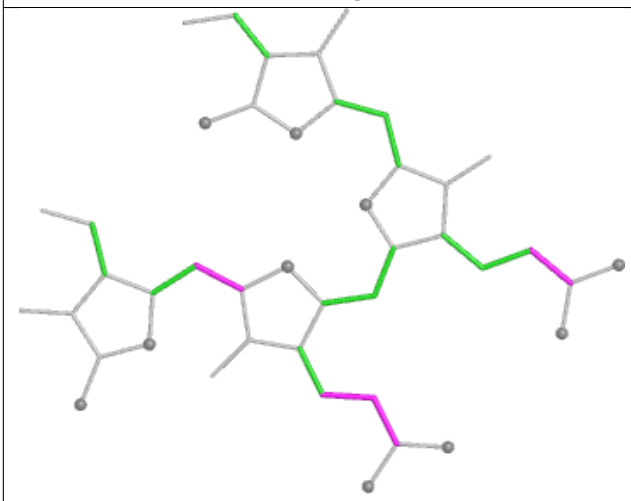

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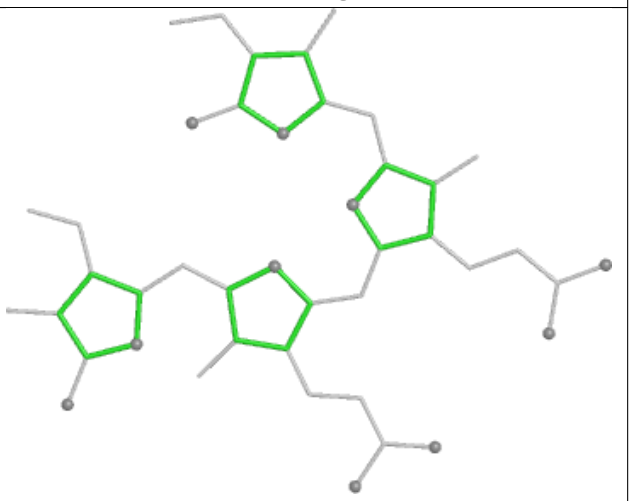
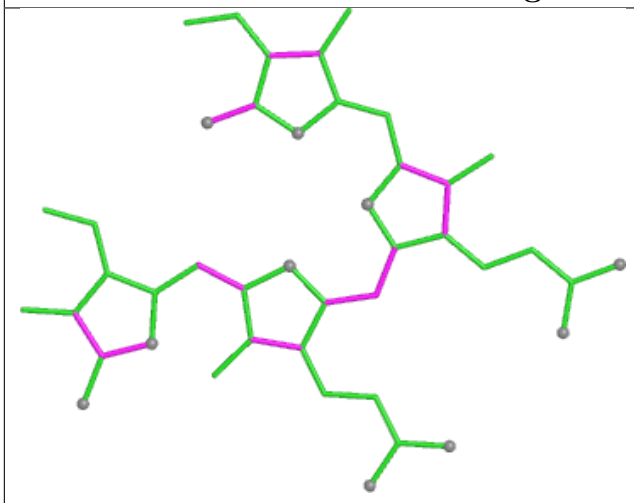


Rings

Ligand PEB fJ 201



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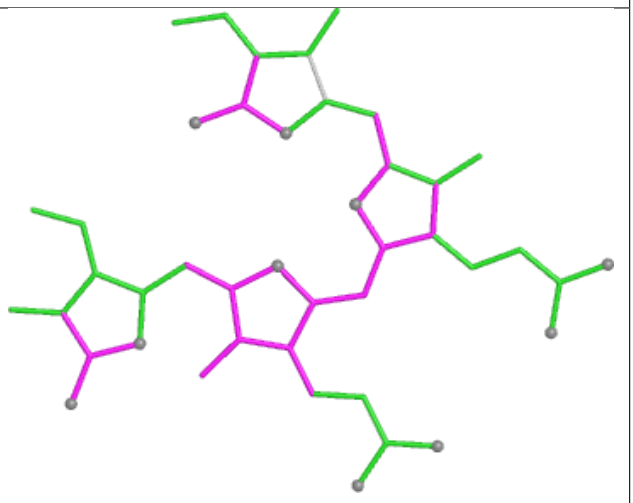
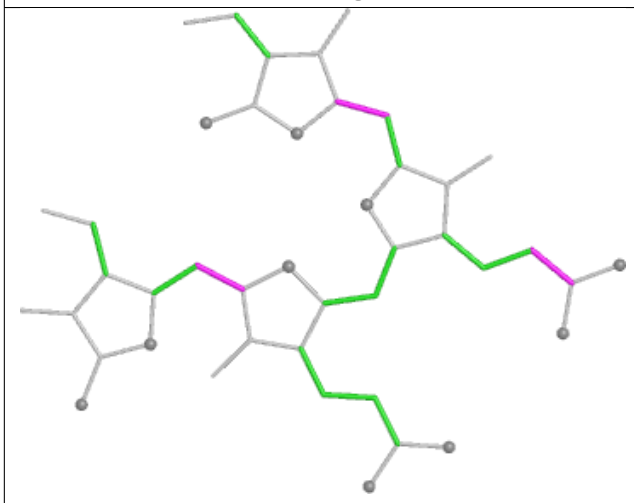


Bond angles



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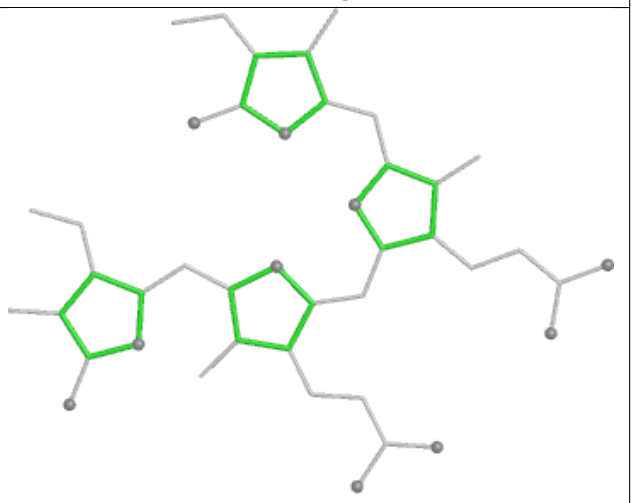
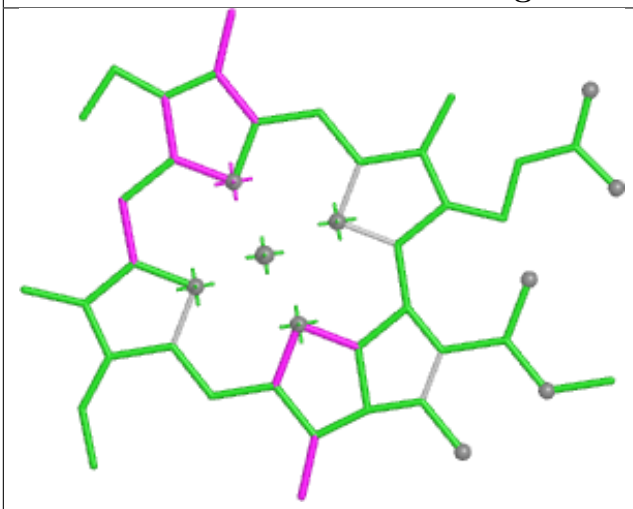


Rings

Ligand CLA 6N 607



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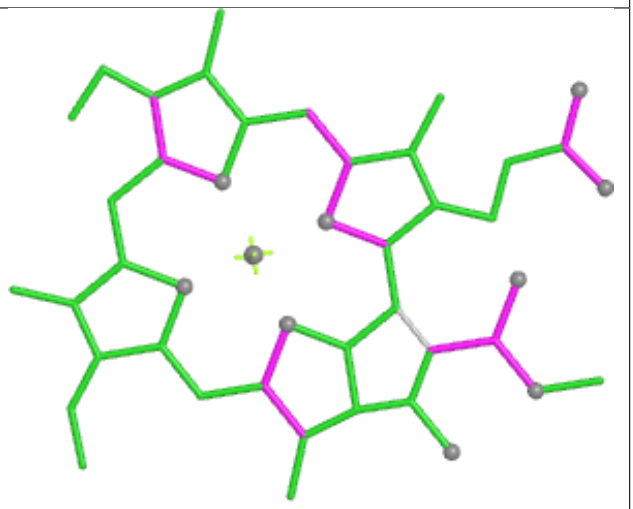
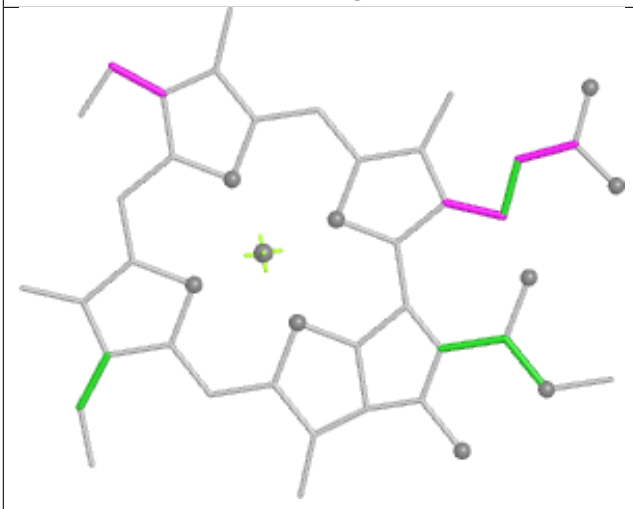


Bond angles

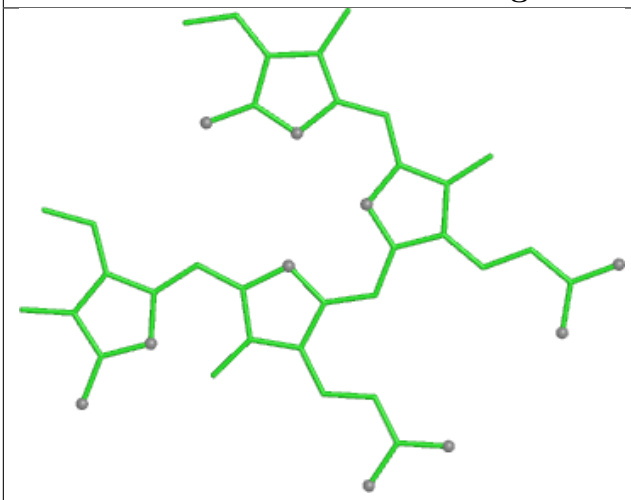


Torsions



Rings

Ligand PEB QO 202



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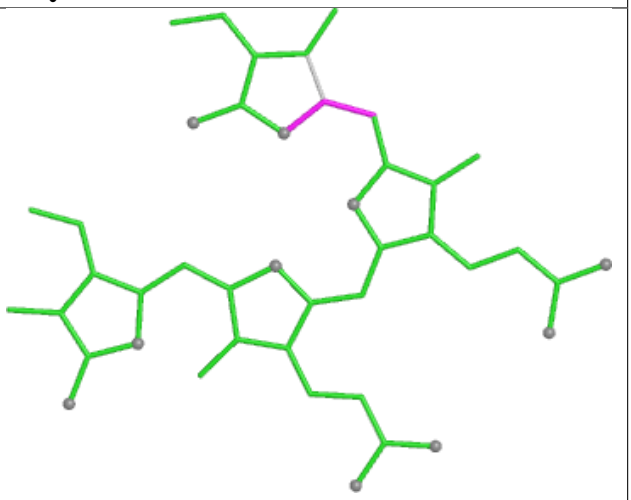
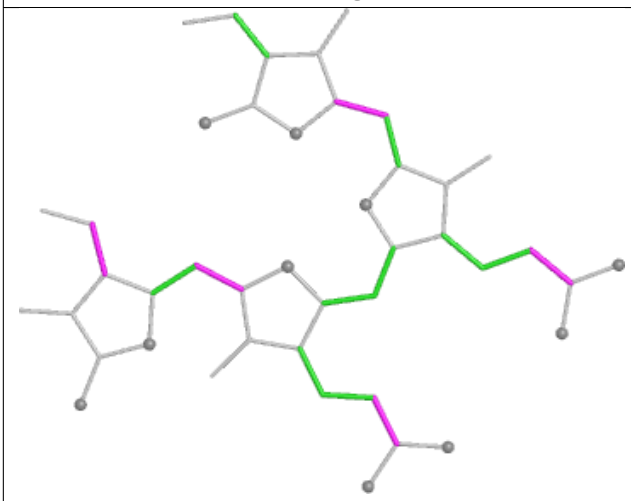
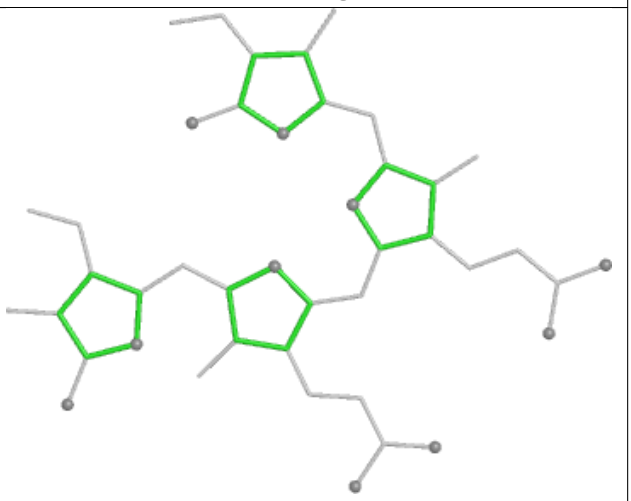


Bond angles

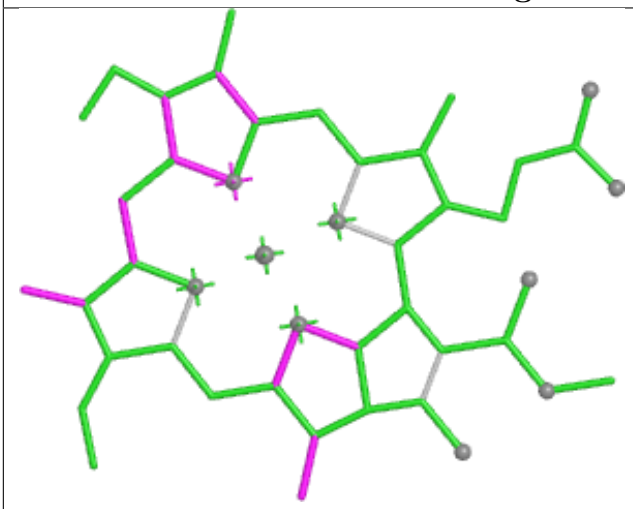


Torsions



Rings

Ligand CLA 4N 607



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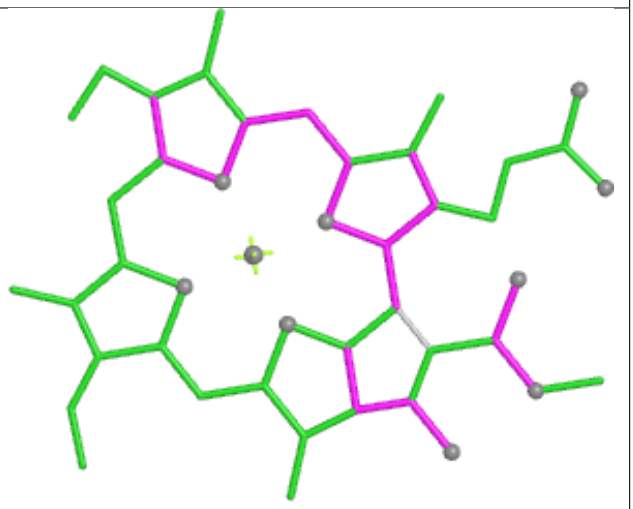
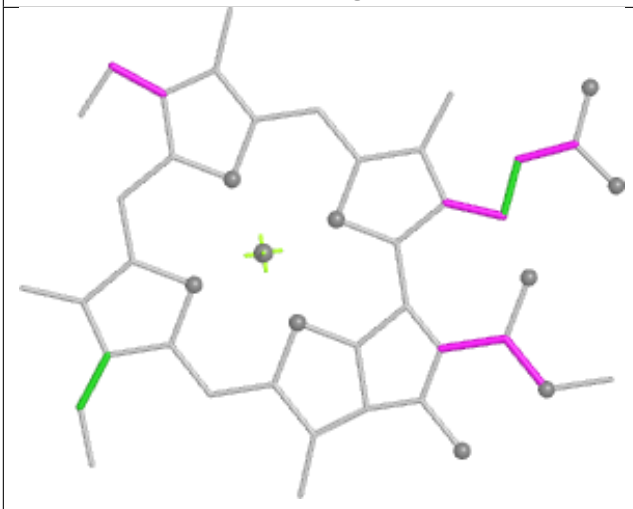


Bond angles

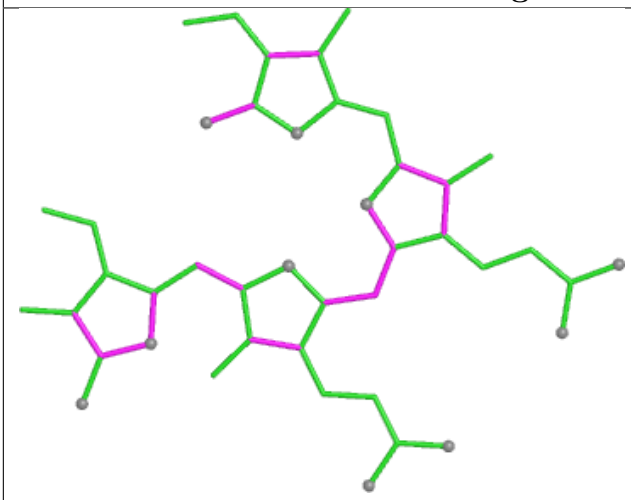


Torsions



Rings

Ligand PEB DB 201



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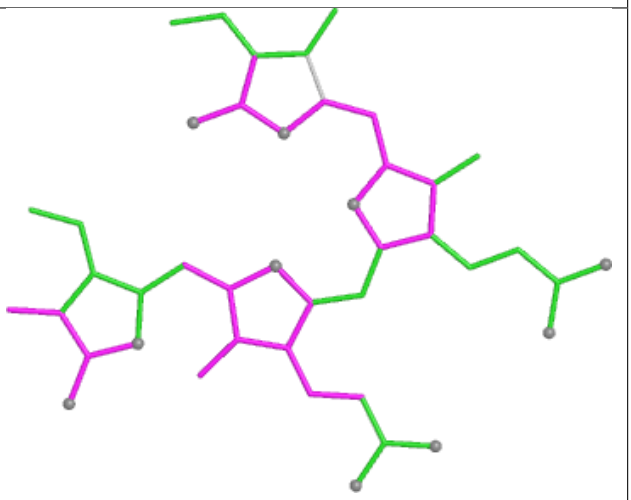

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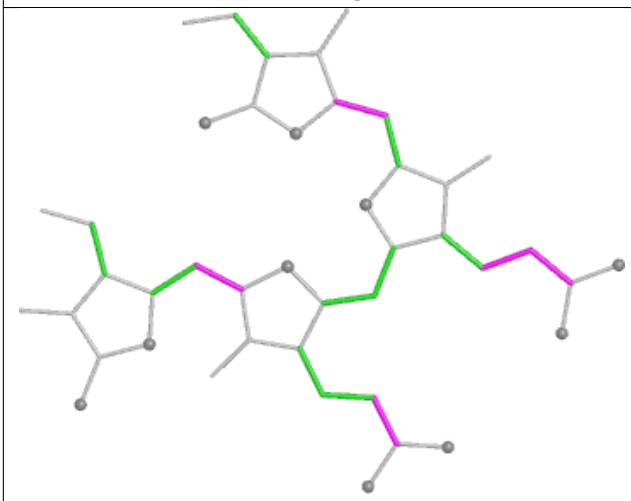

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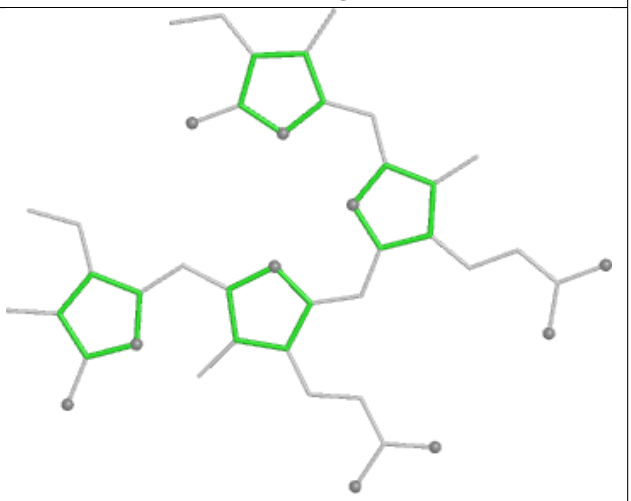
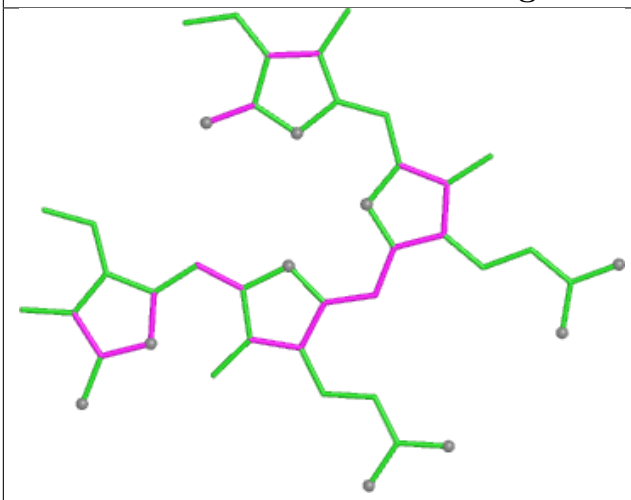


Rings

Ligand PEB S5 202



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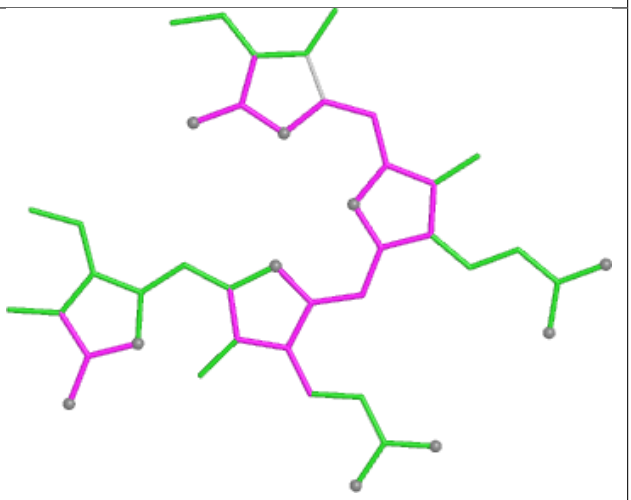

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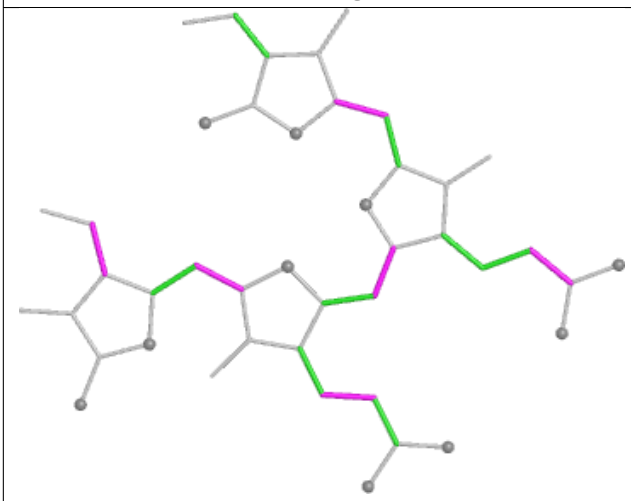

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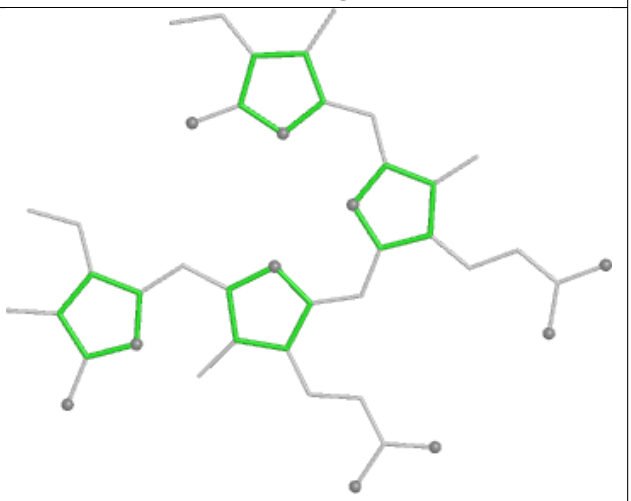
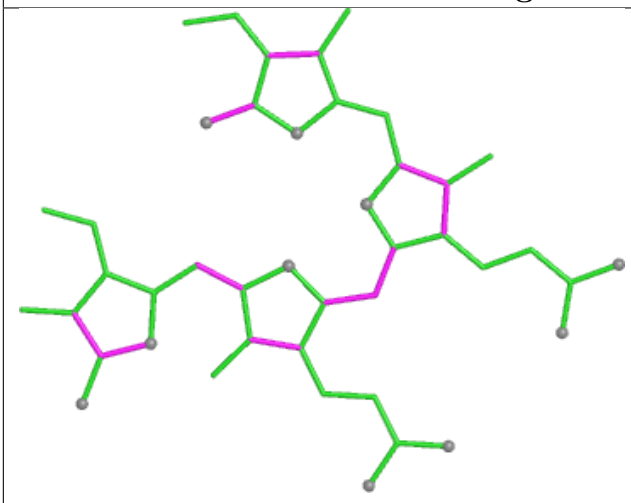


Rings

Ligand PEB 1C 203



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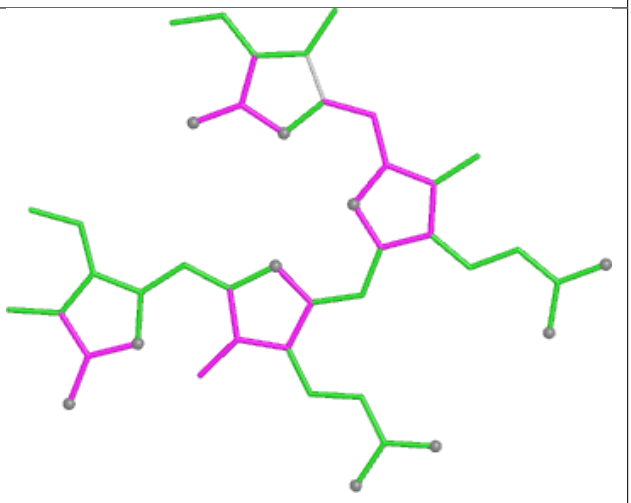

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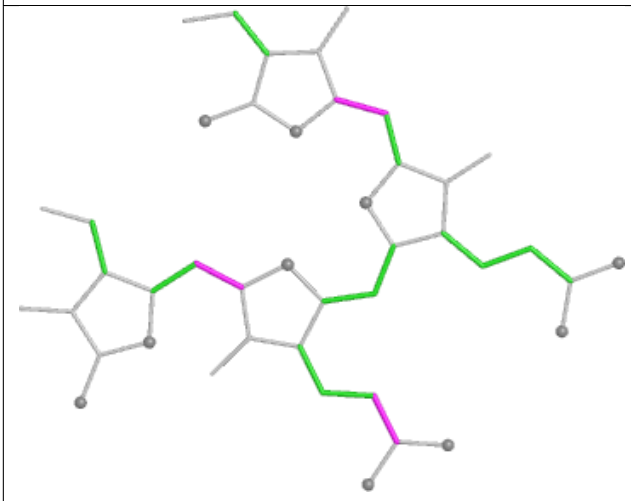

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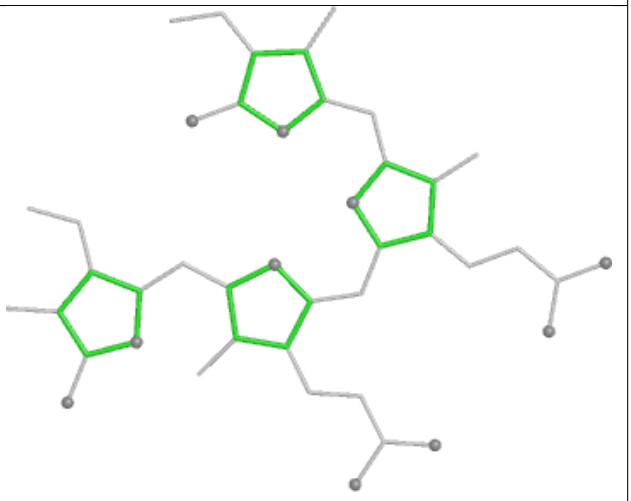
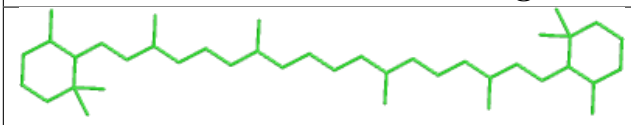


Rings

Ligand BCR F2 203



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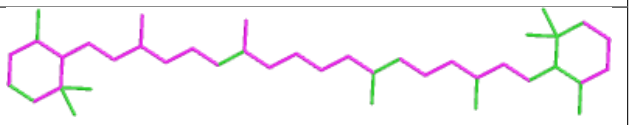

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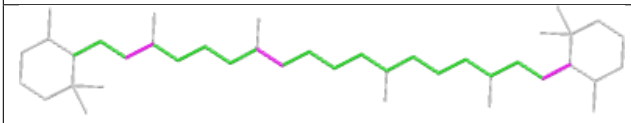

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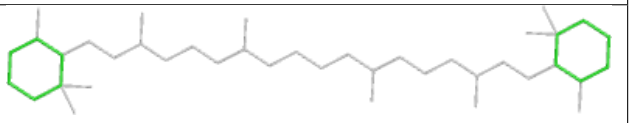
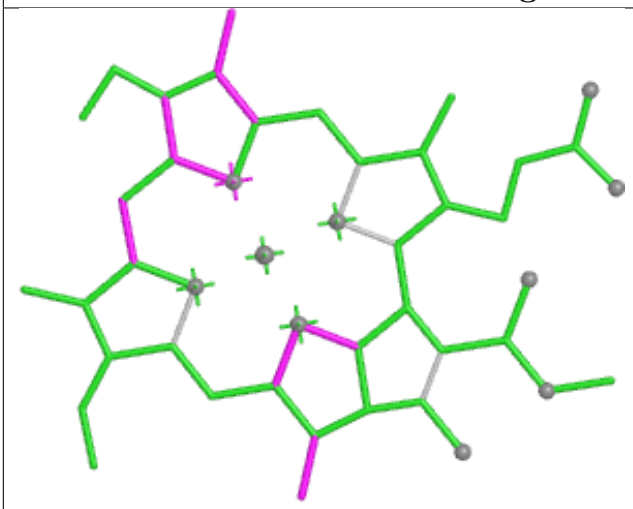


Rings

Ligand CLA 72 605



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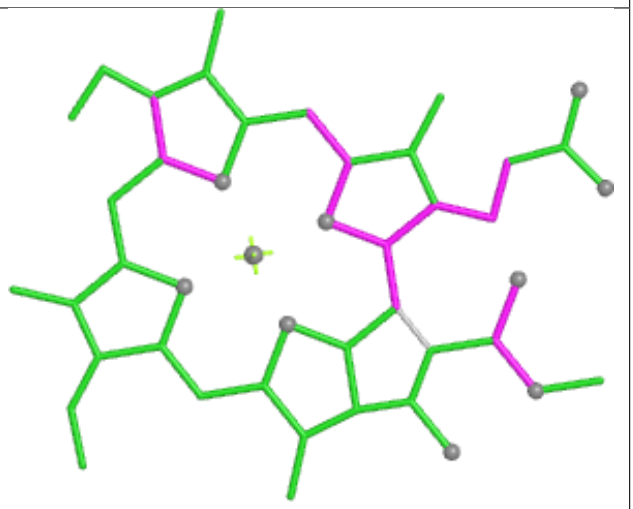
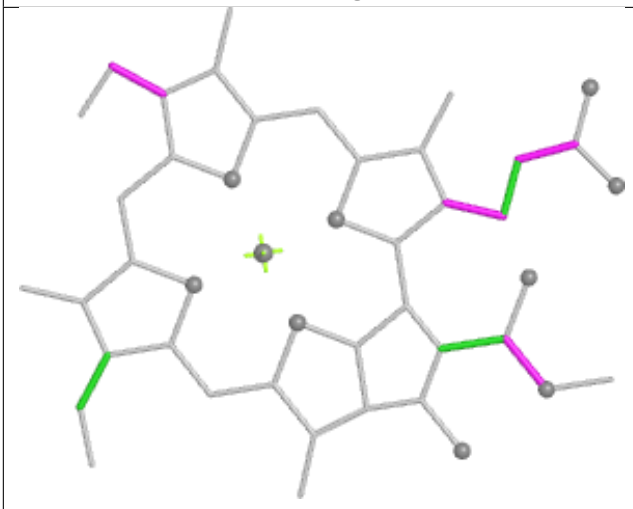


Bond angles

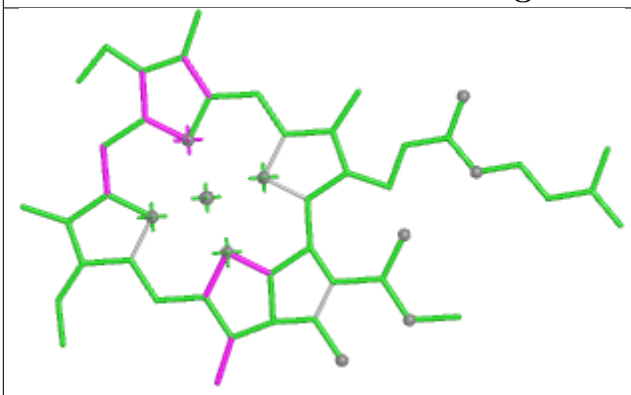


Torsions



Rings

Ligand CLA 5N 607



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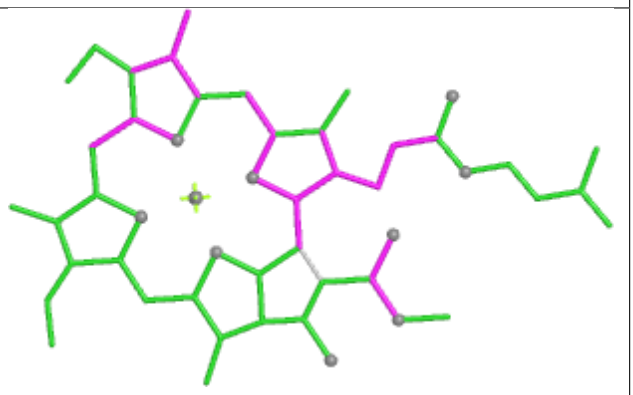

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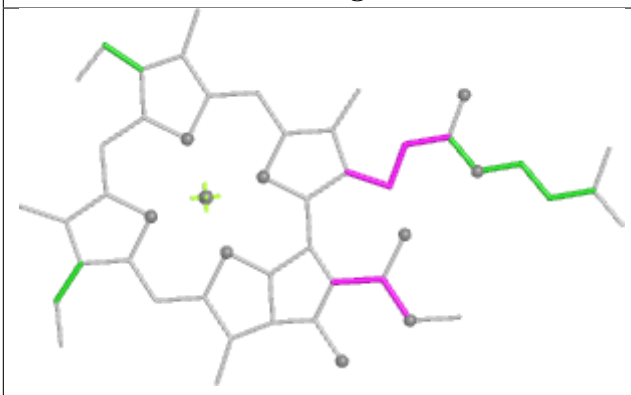

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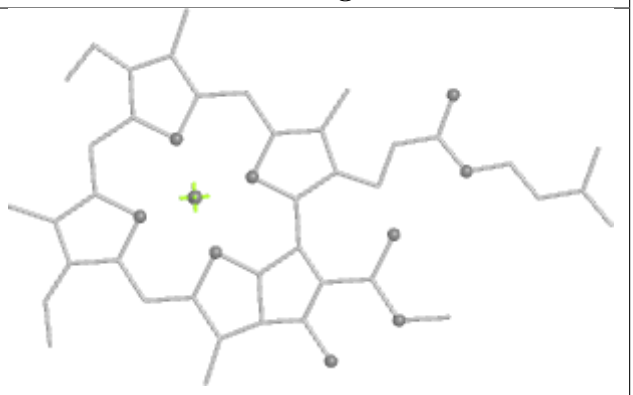
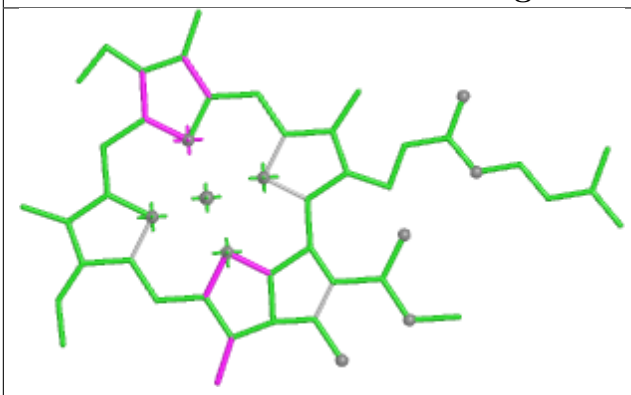


Rings

Ligand CLA 3N 309



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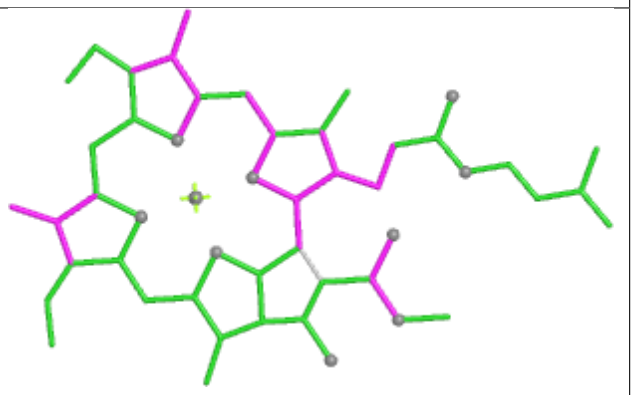

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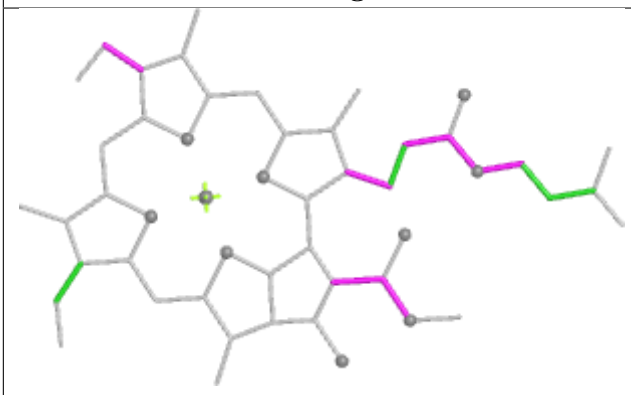

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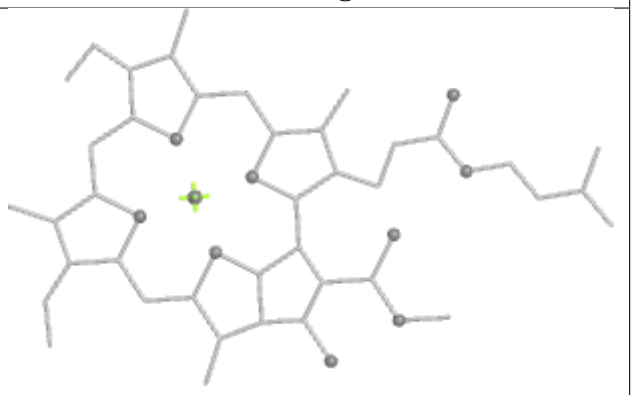
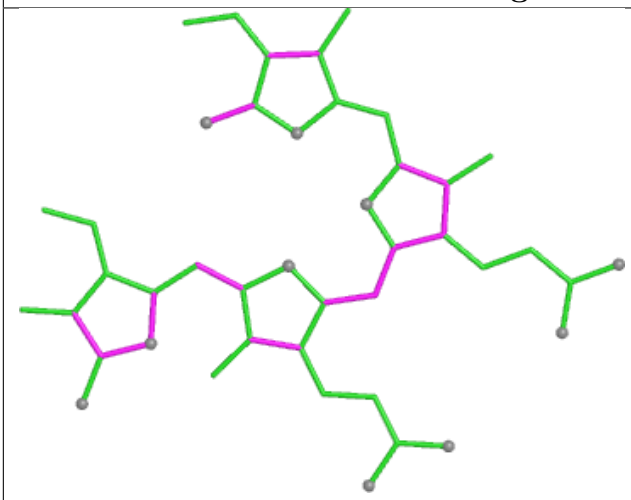


Rings

Ligand PEB RD 202



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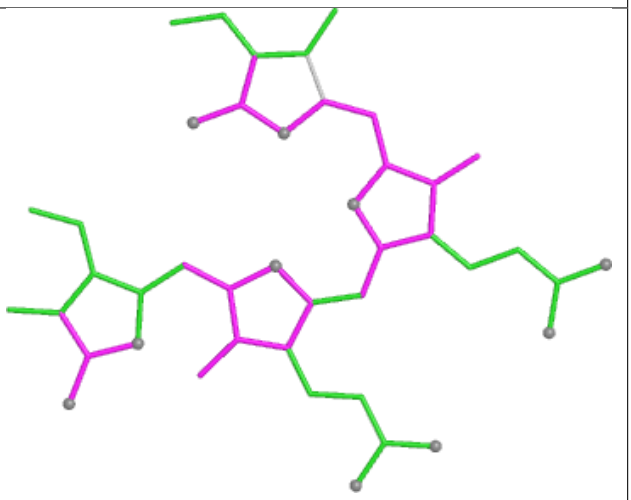
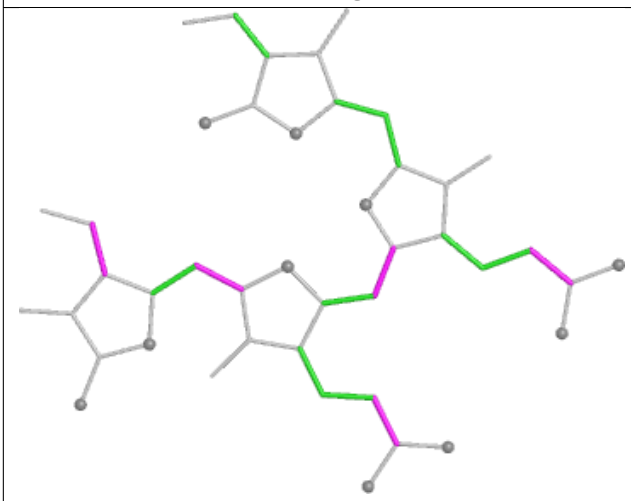


Bond angles



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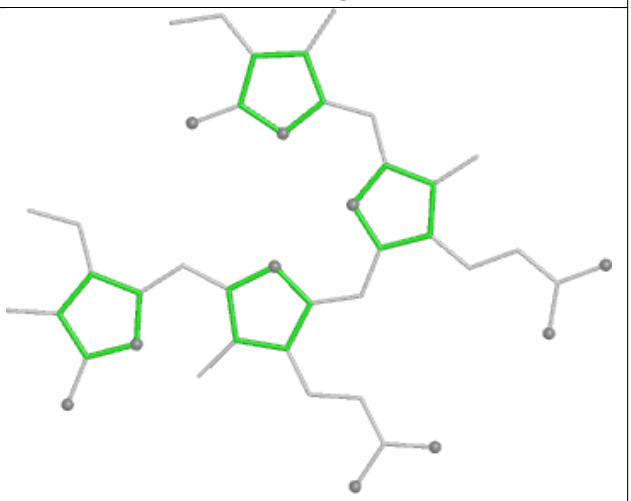
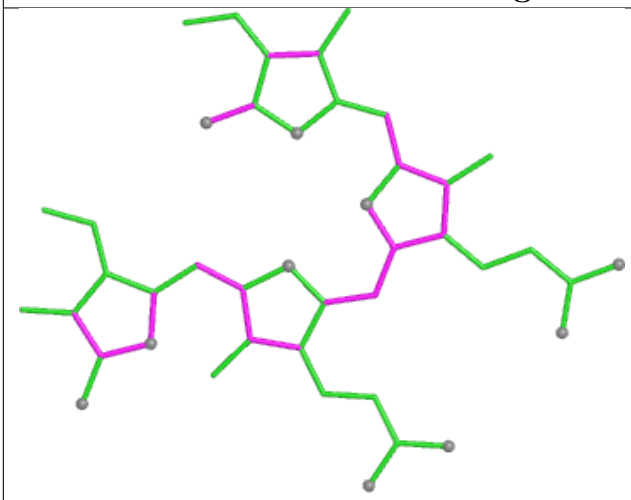


Rings

Ligand PEB dK 202



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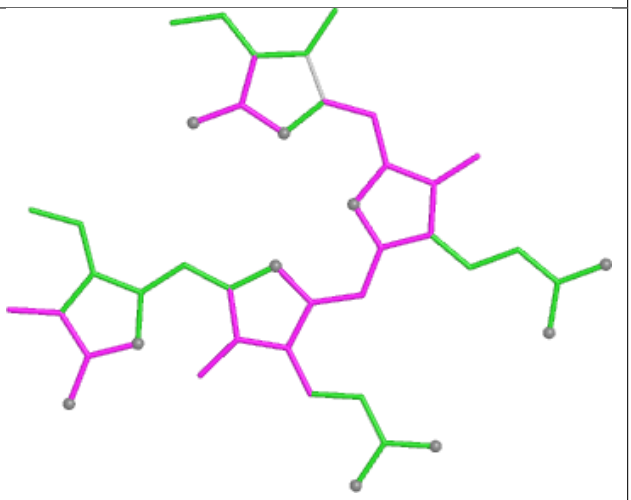

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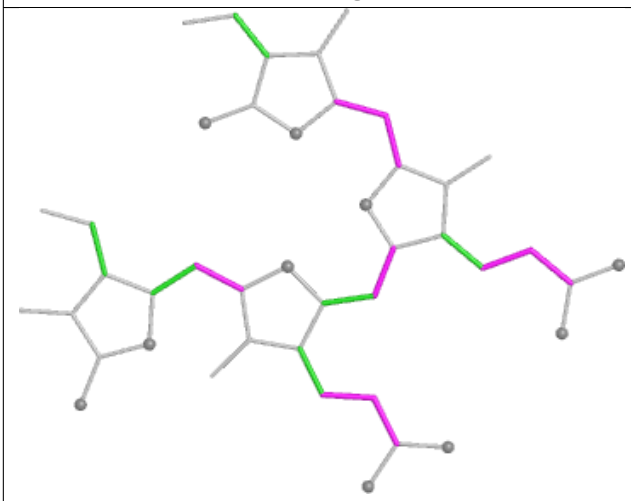

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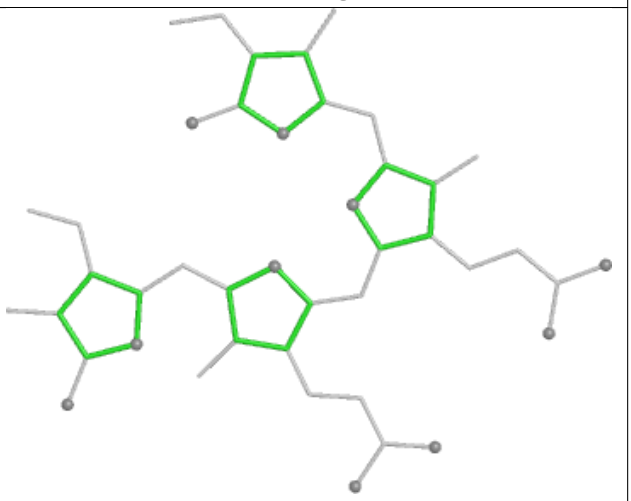
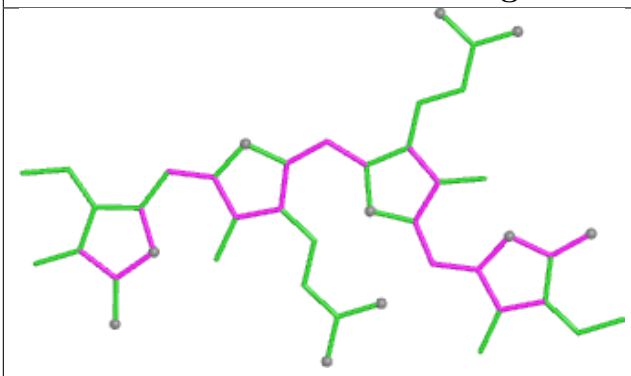


Rings

Ligand CYC EO 1001



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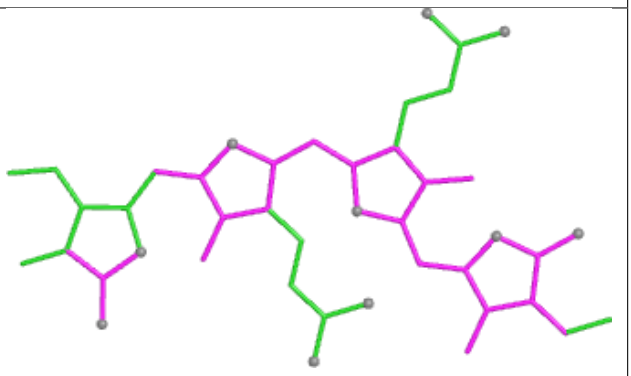

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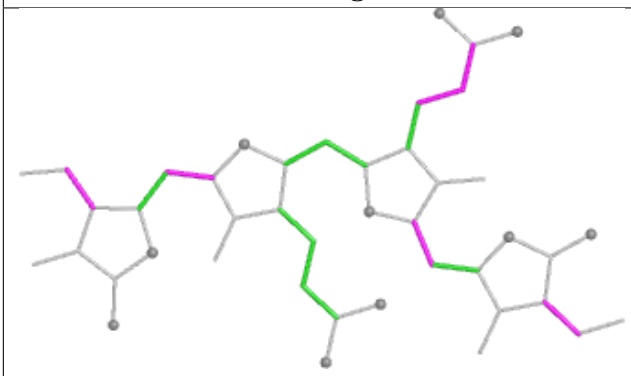

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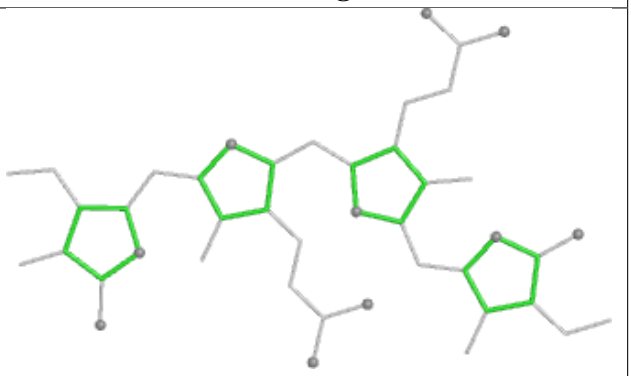
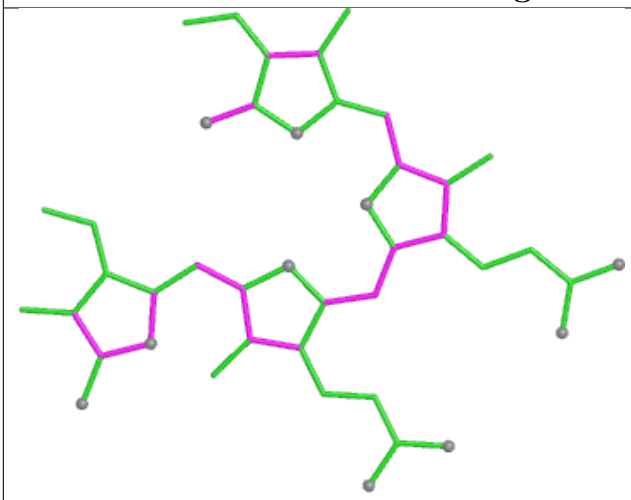


Rings

Ligand PEB dH 202



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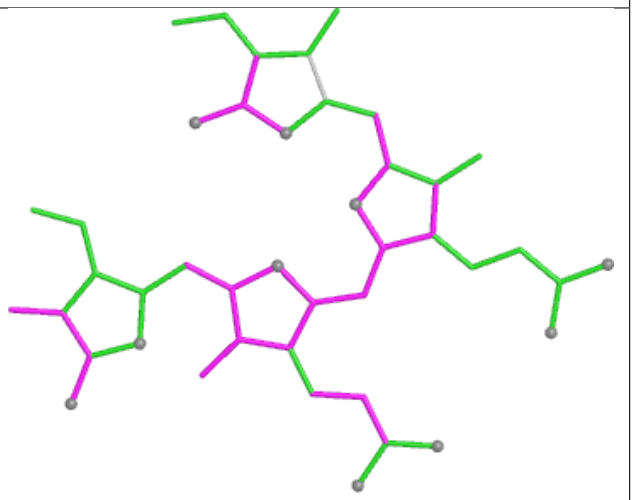

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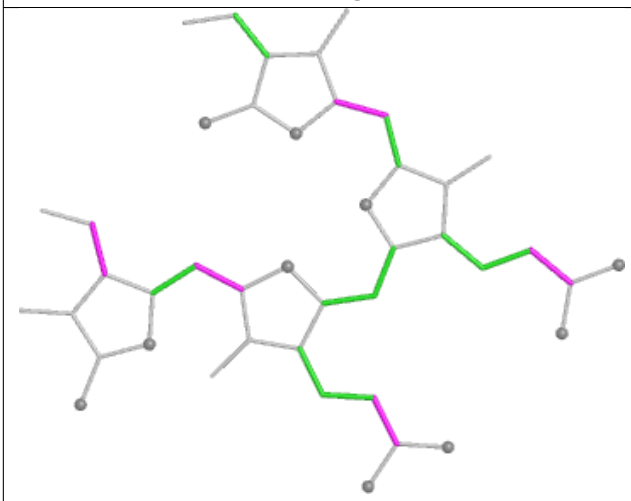

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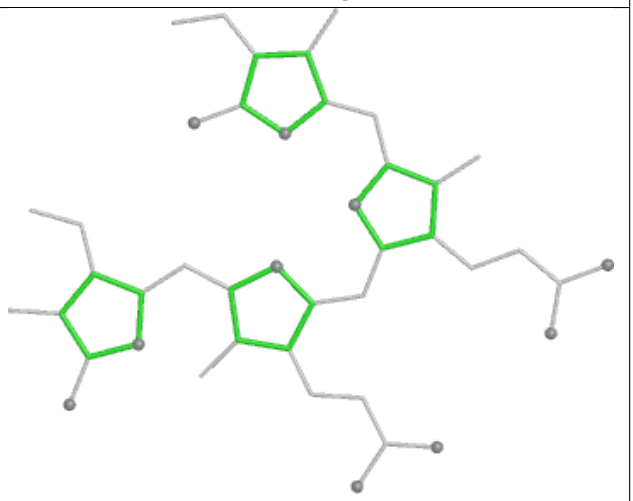
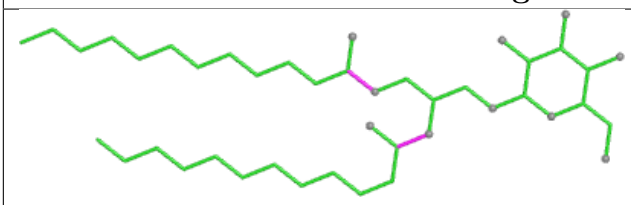


Rings

Ligand LMG qL 301



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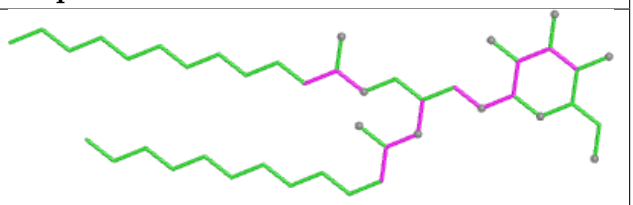

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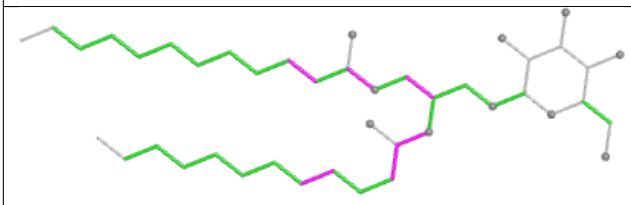

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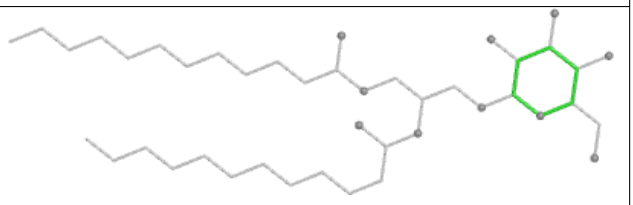
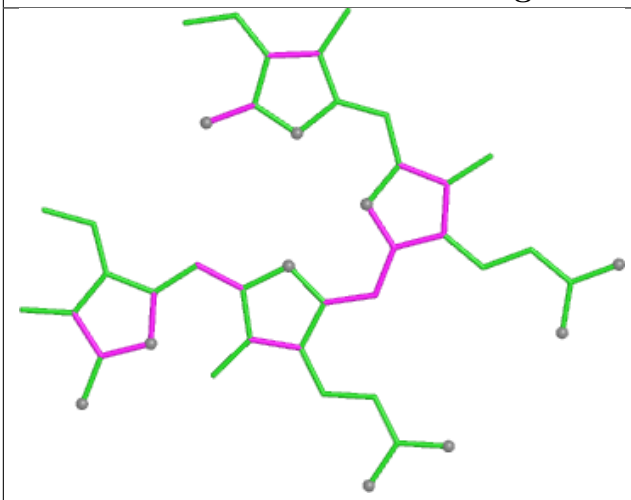


Rings

Ligand PEB KJ 202



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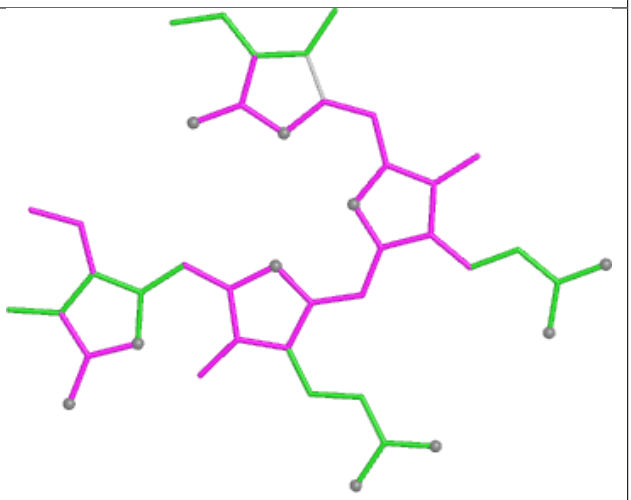
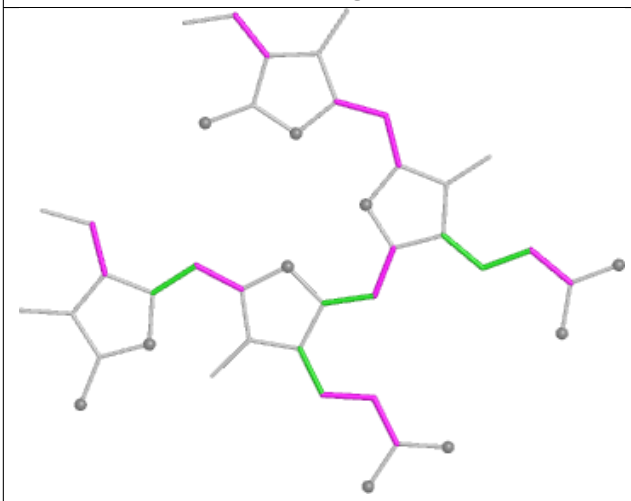


Bond angles



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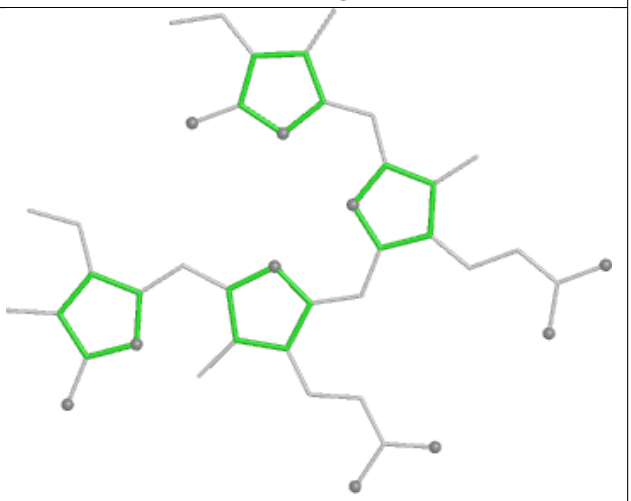
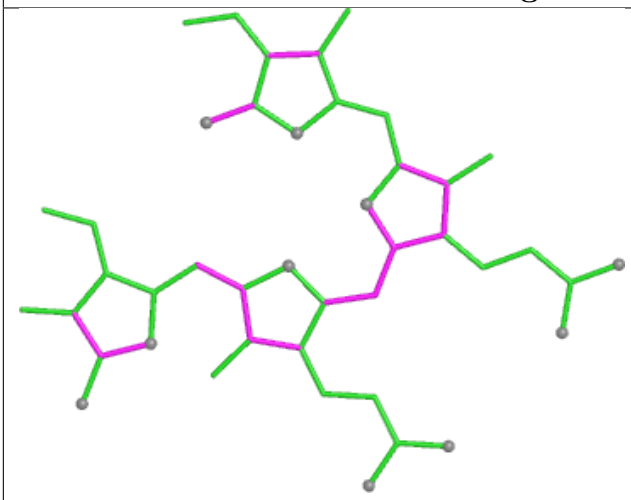


Rings

Ligand PEB c1 202



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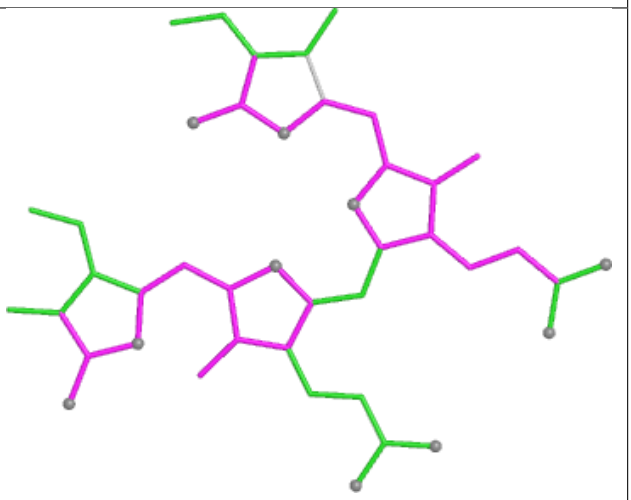
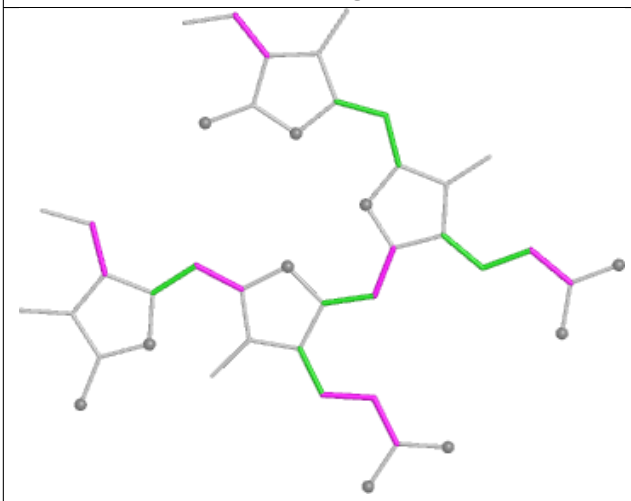
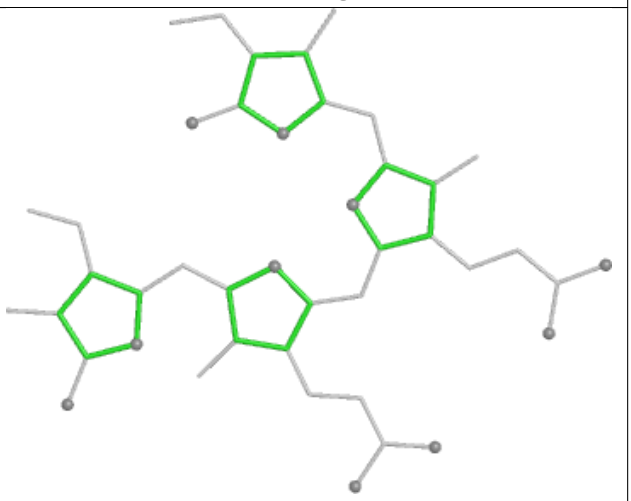


Bond angles

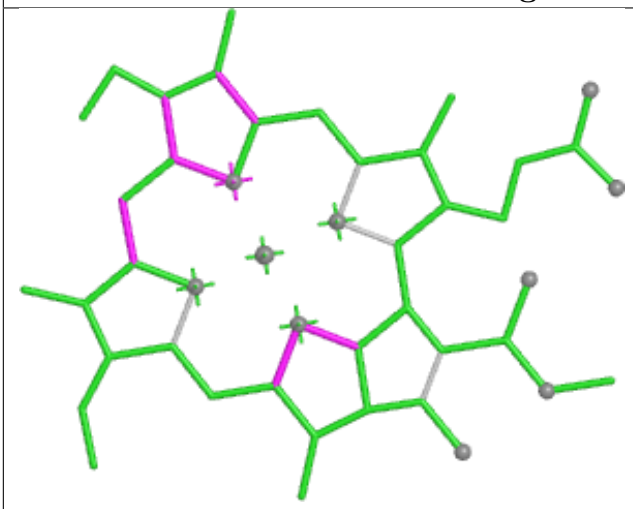


Torsions



Rings

Ligand CLA 72 601



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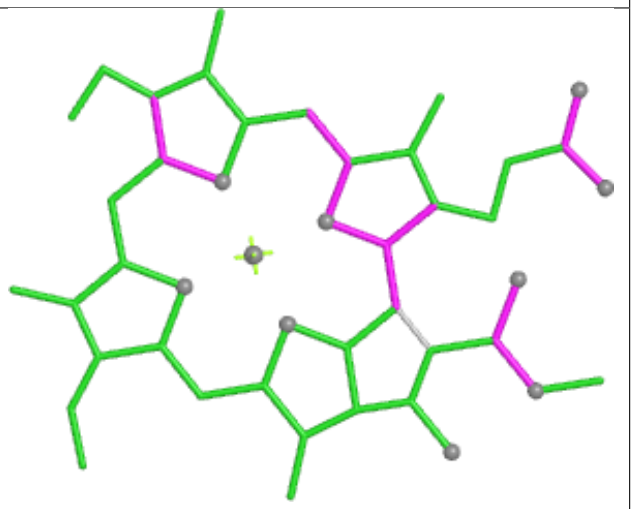

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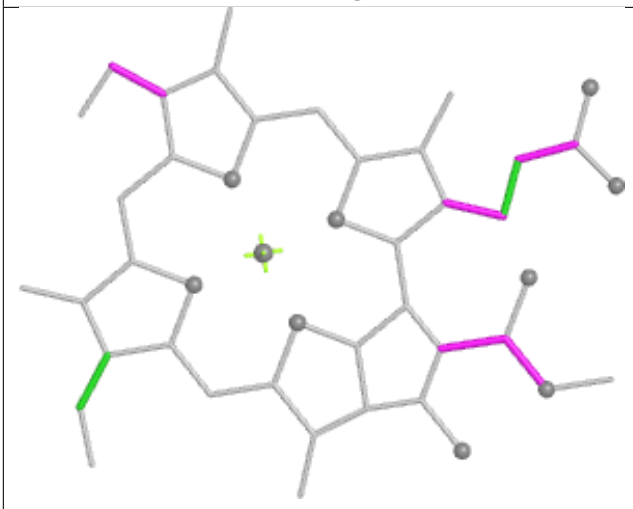
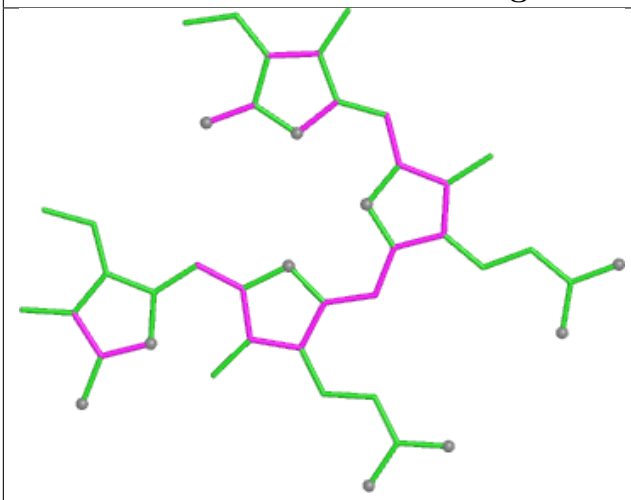


Torsions



Rings

Ligand PEB YK 203



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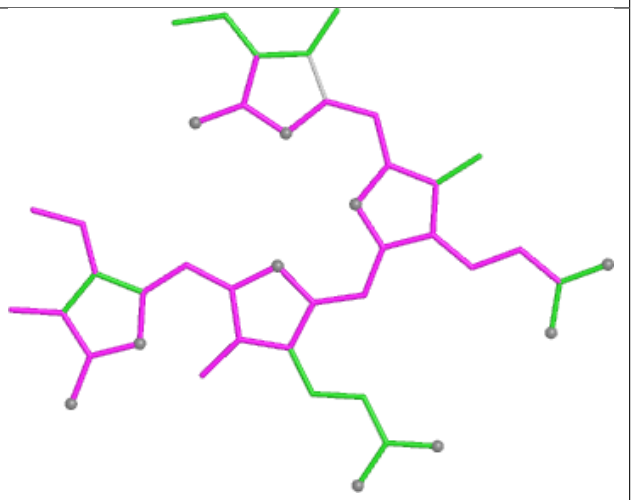

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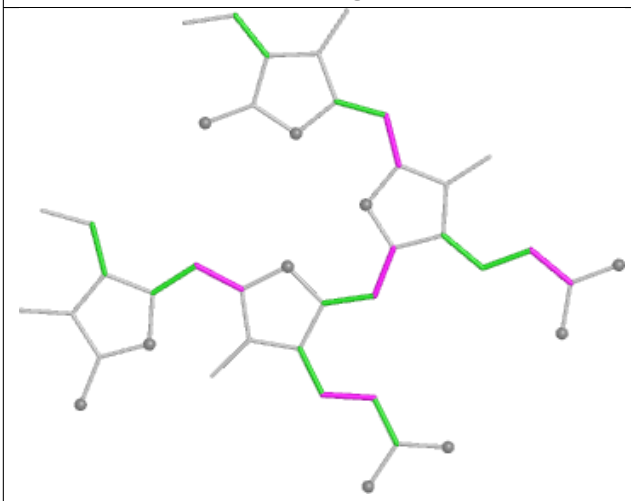

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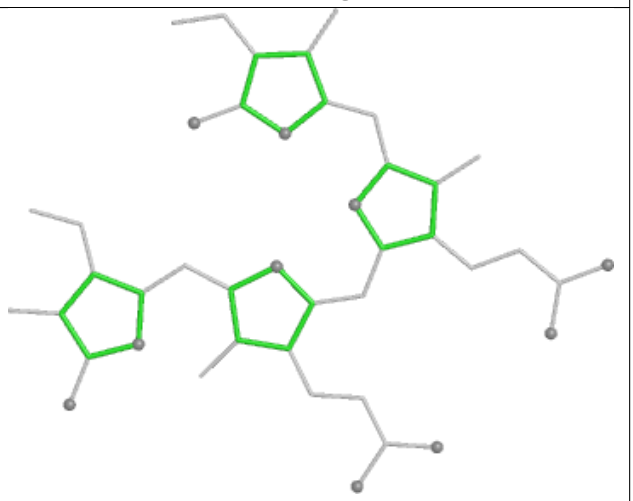
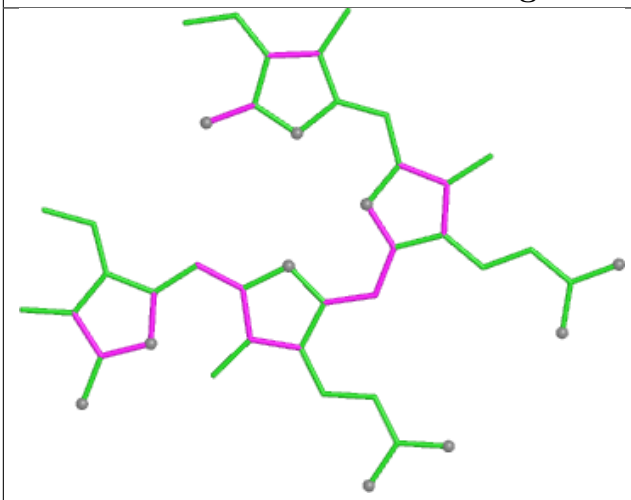


Rings

Ligand PEB J9 203



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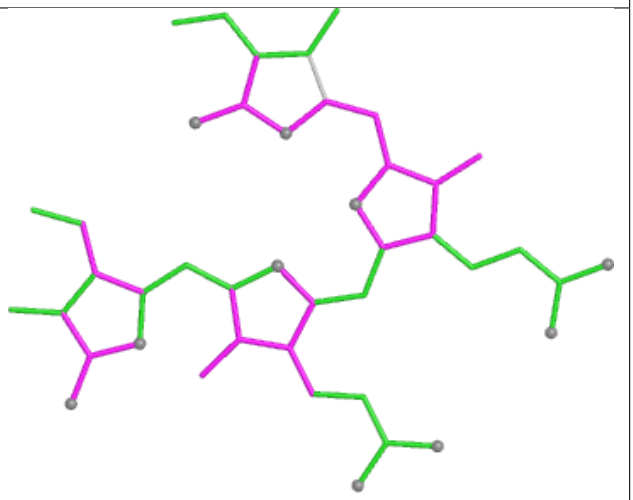

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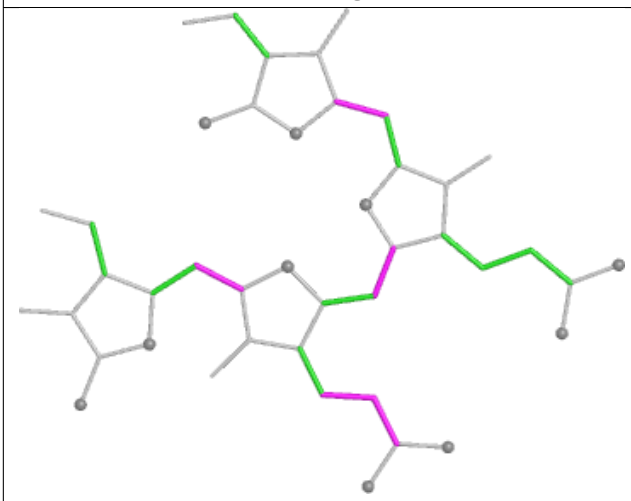

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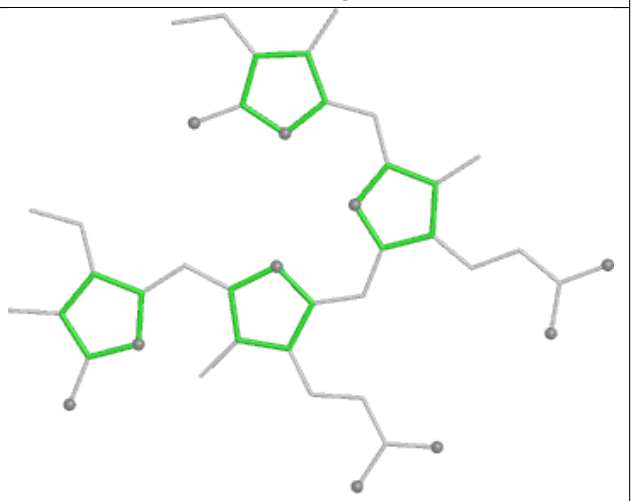

Rings

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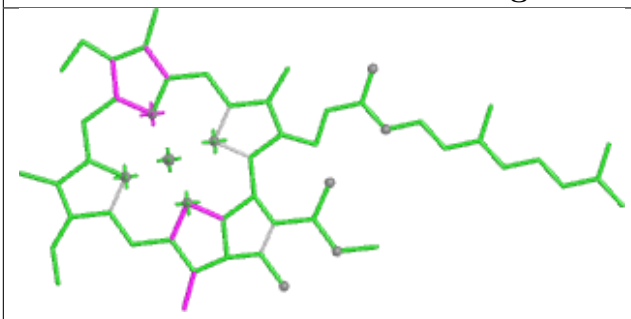

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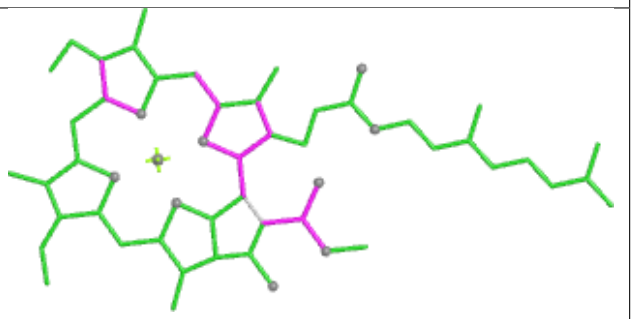

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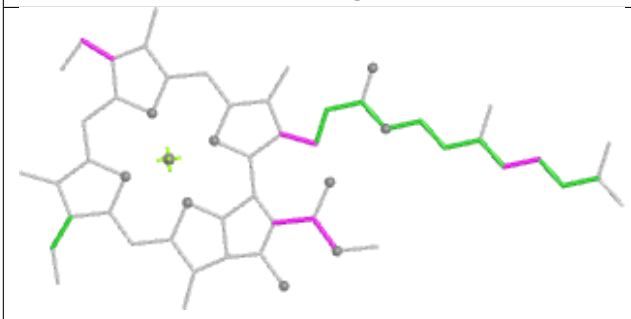

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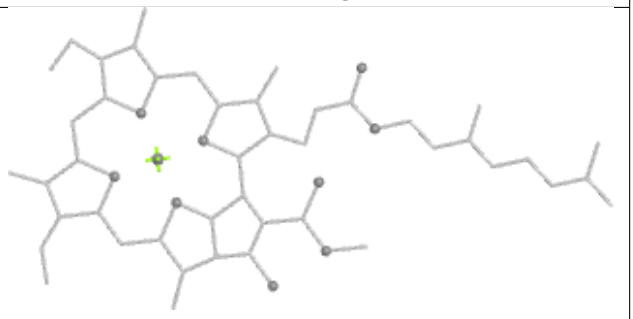
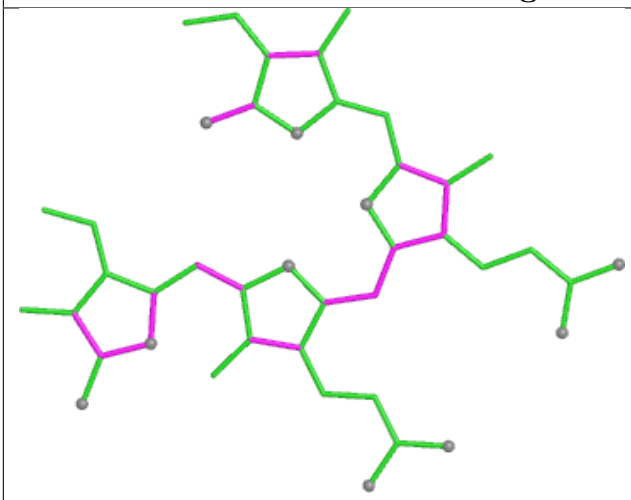


Rings

Ligand PEB aJ 203



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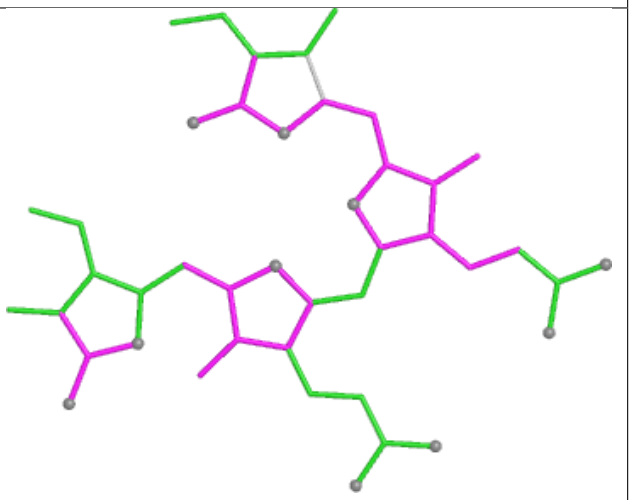

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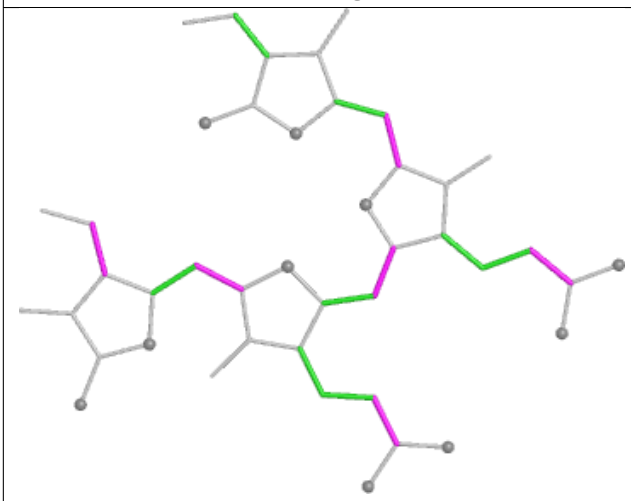

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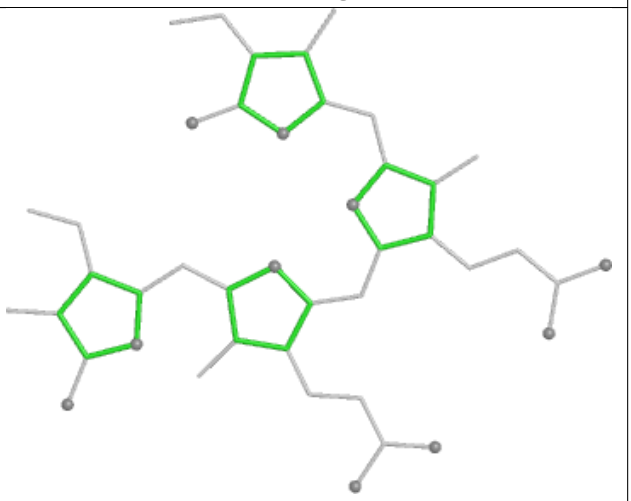

Rings

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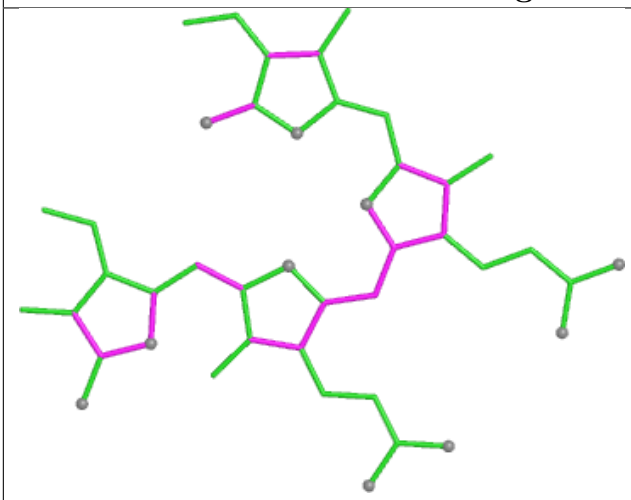

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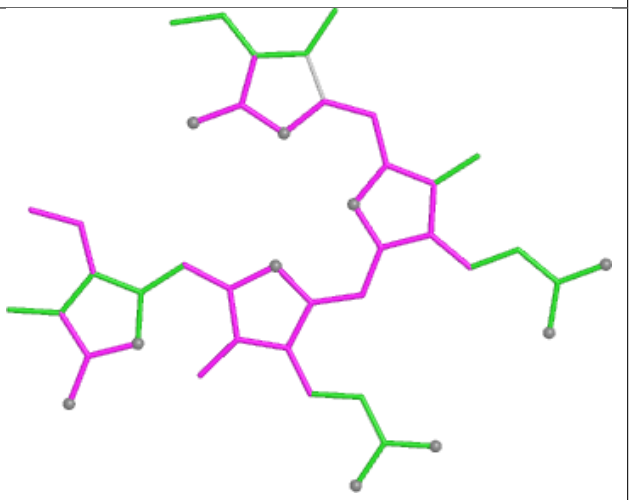

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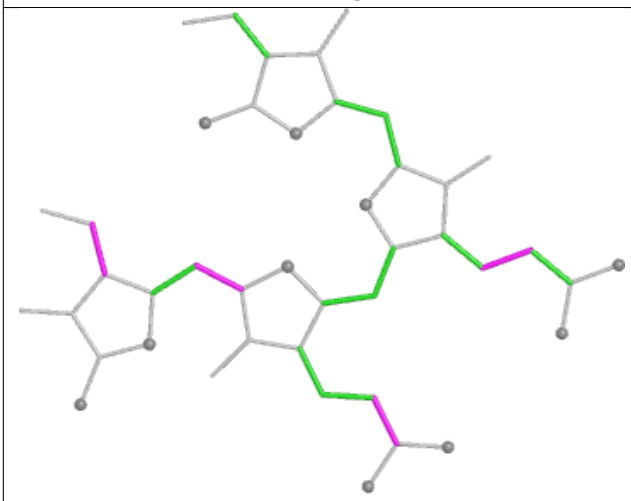

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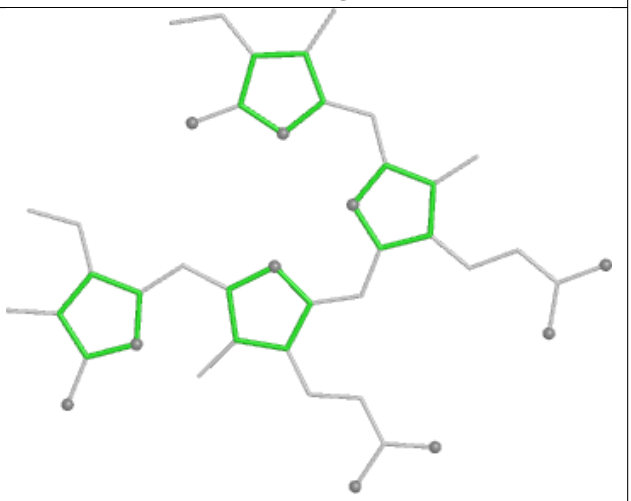

Rings

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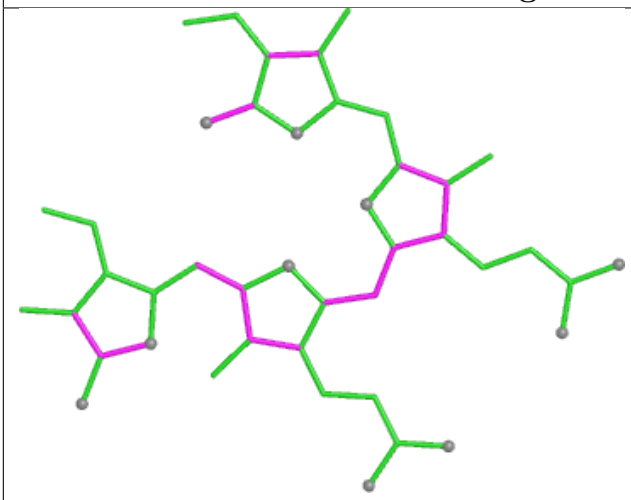

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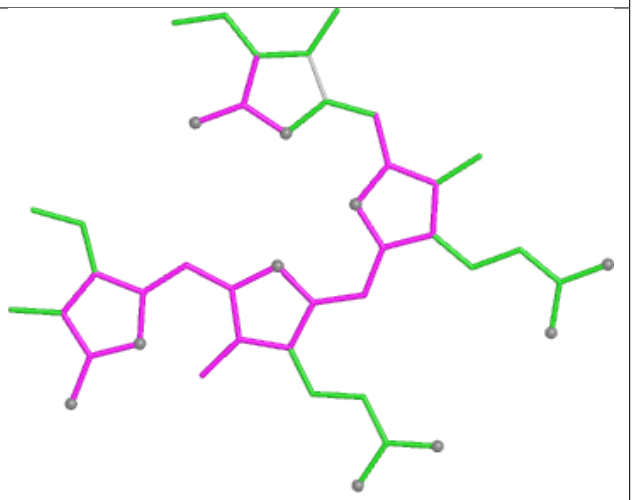

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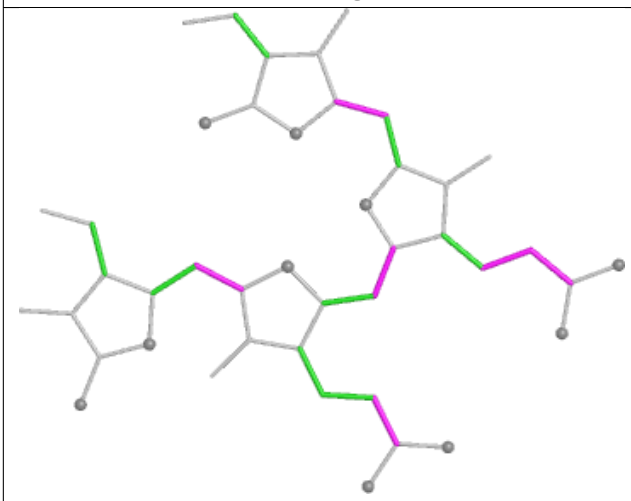

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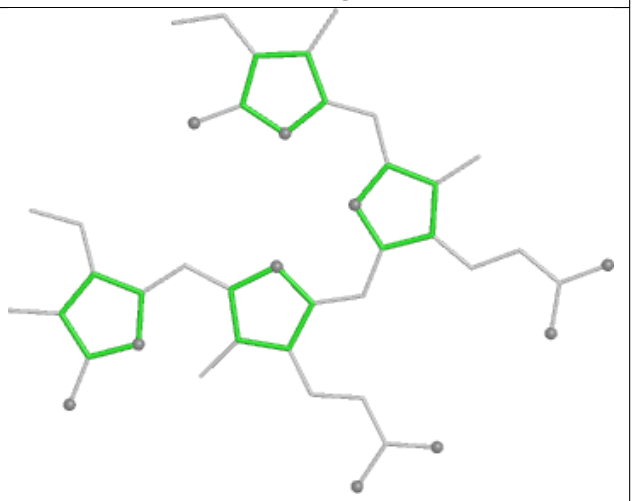
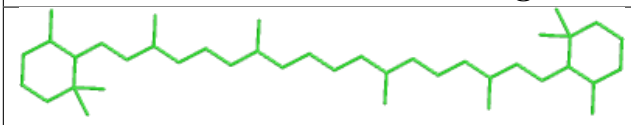


Rings

Ligand BCR bL 601



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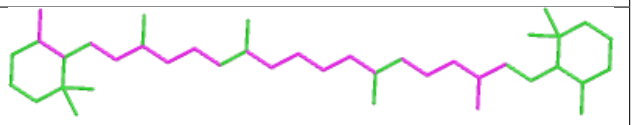

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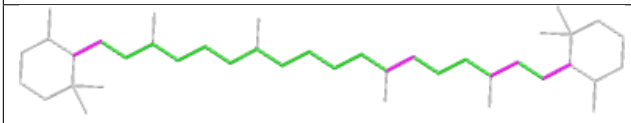

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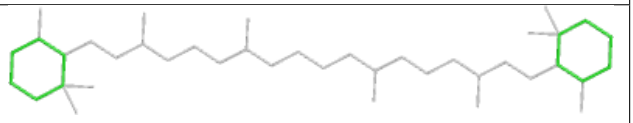
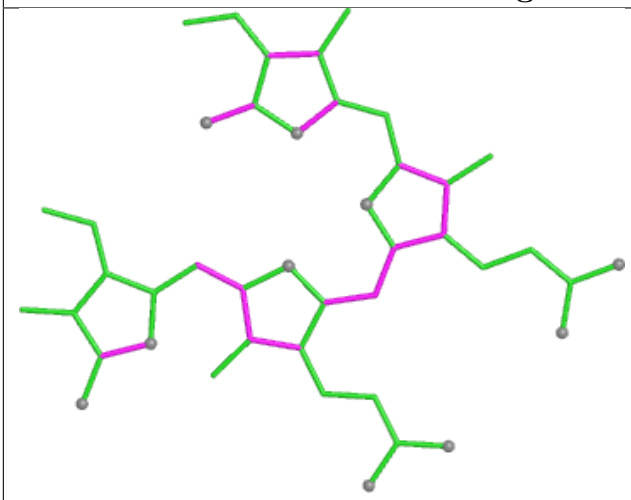


Rings

Ligand PEB uF 202



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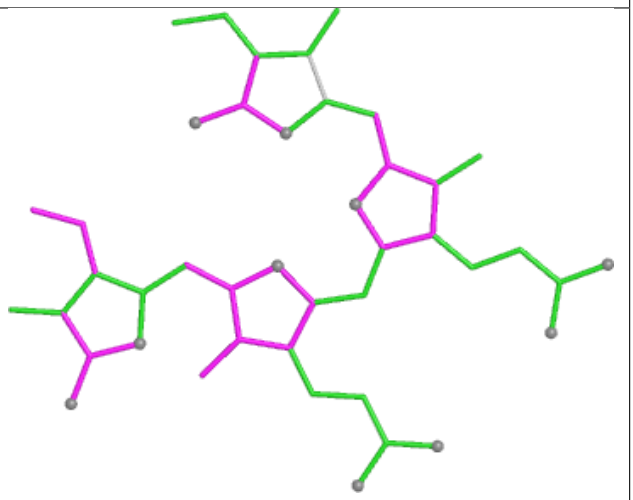

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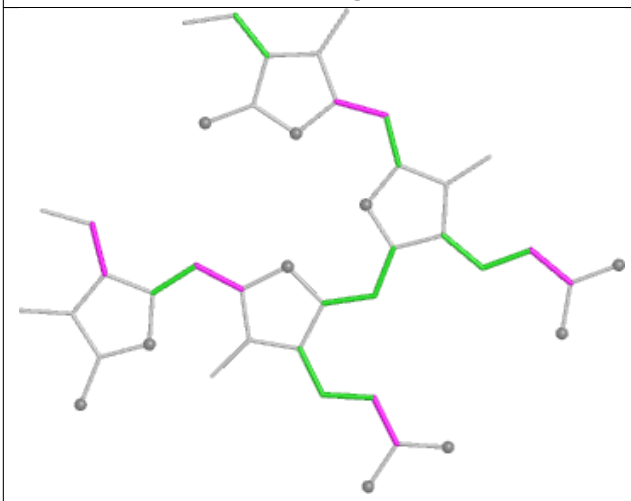

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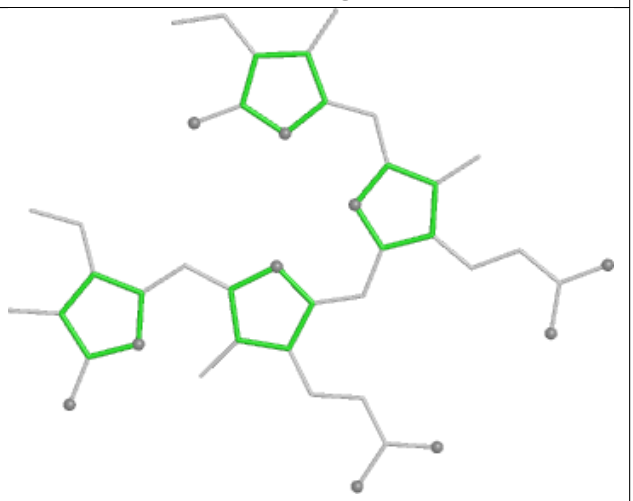

Rings

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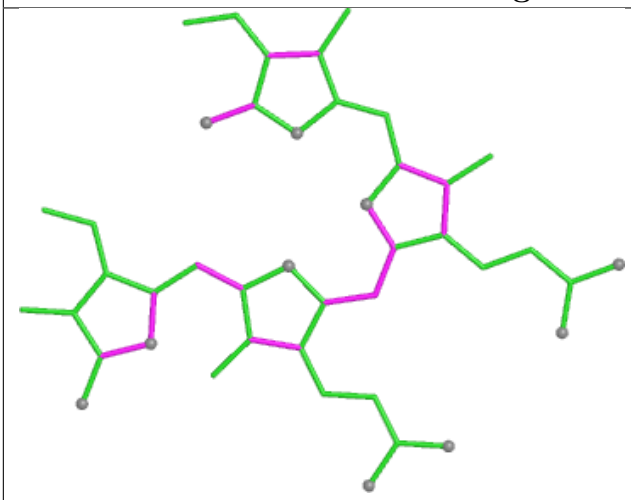

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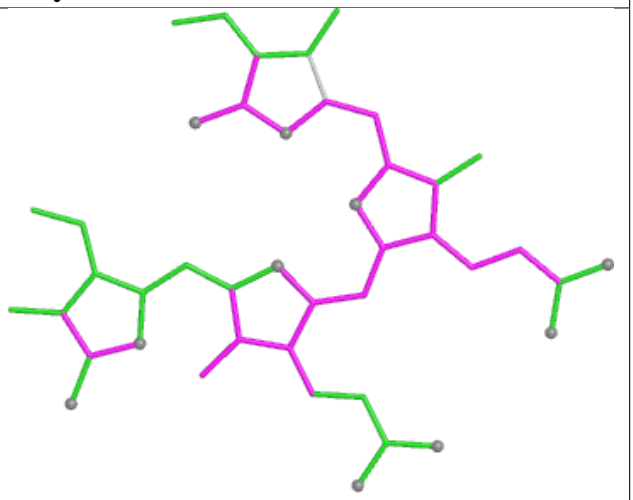

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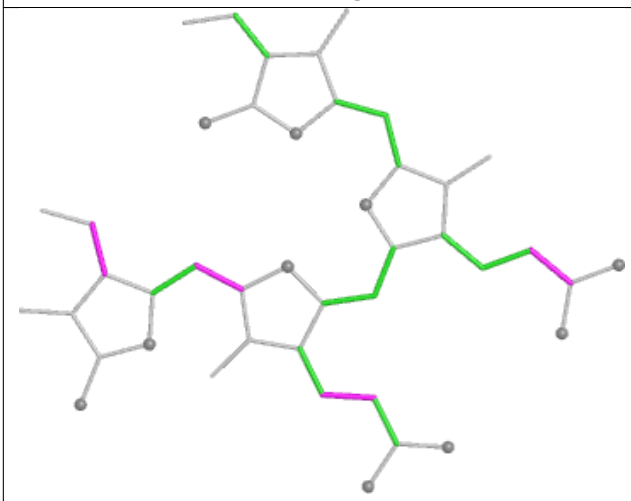

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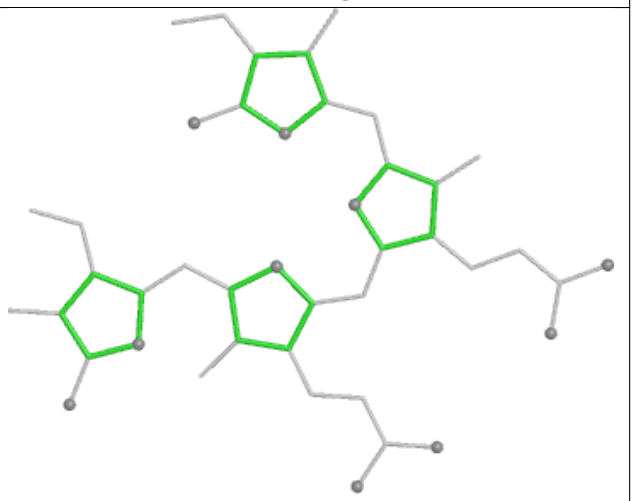
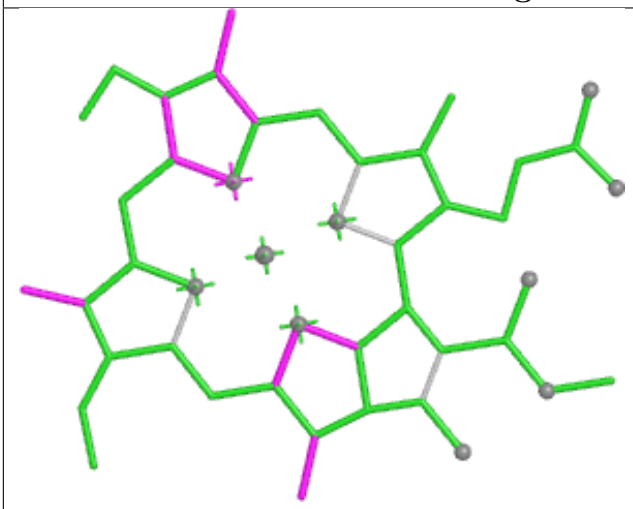


Rings

Ligand CLA 4N 601



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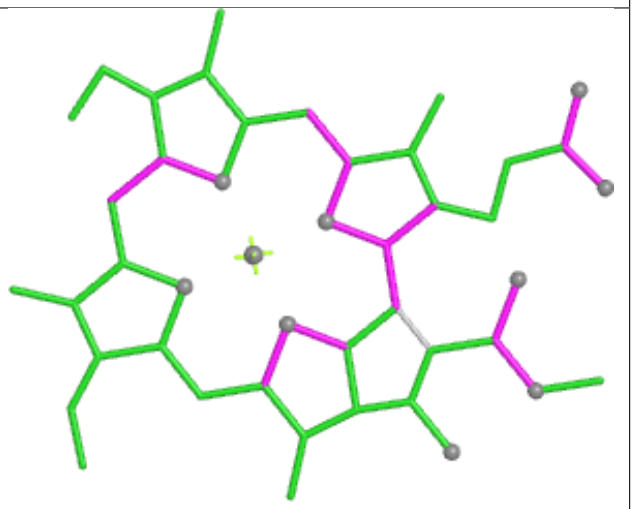

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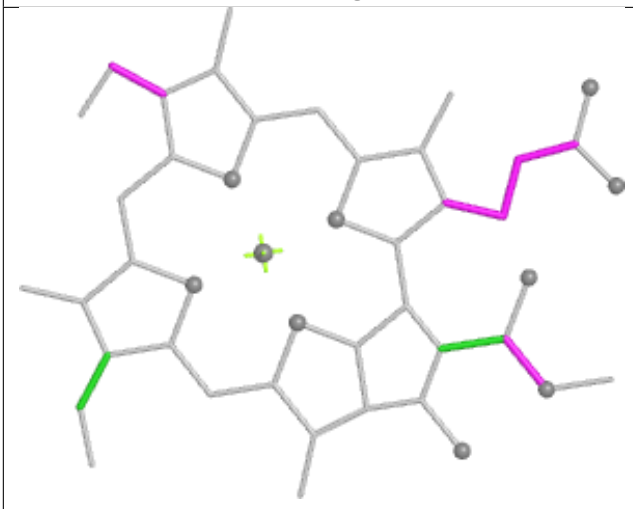
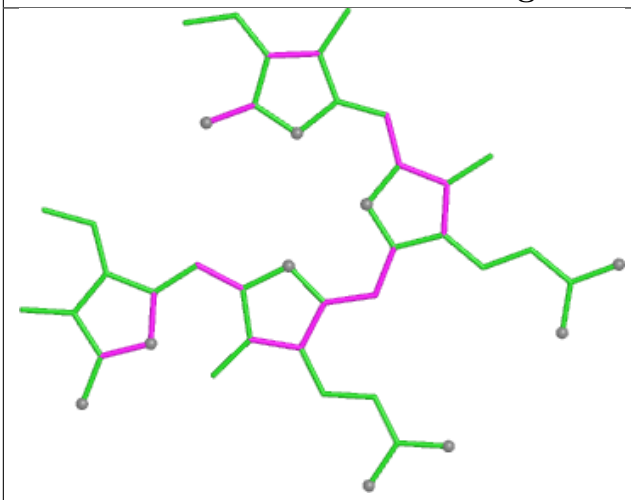


Torsions



Rings

Ligand PEB Z1 202



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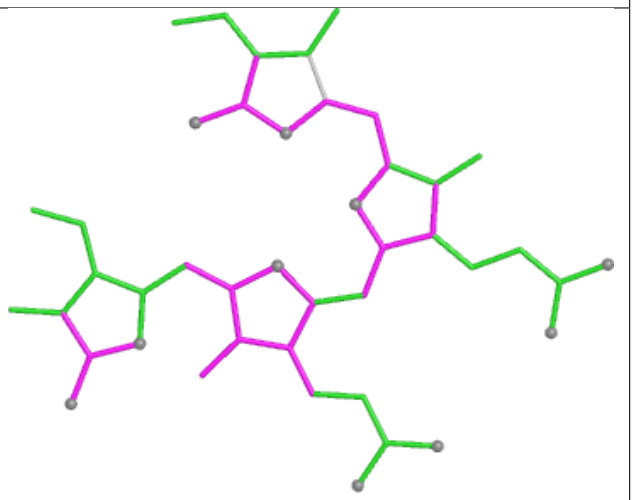

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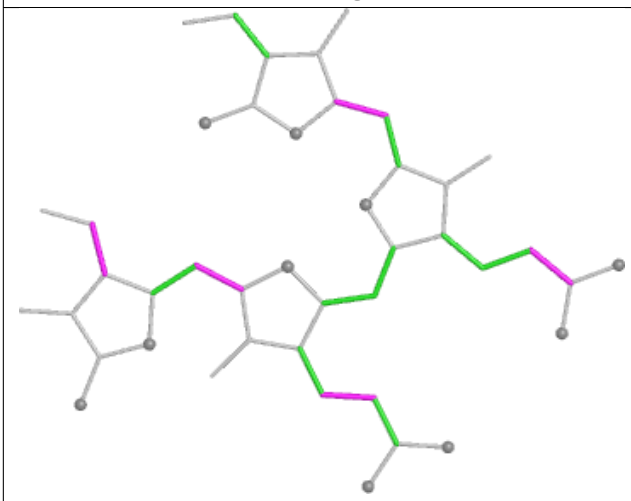

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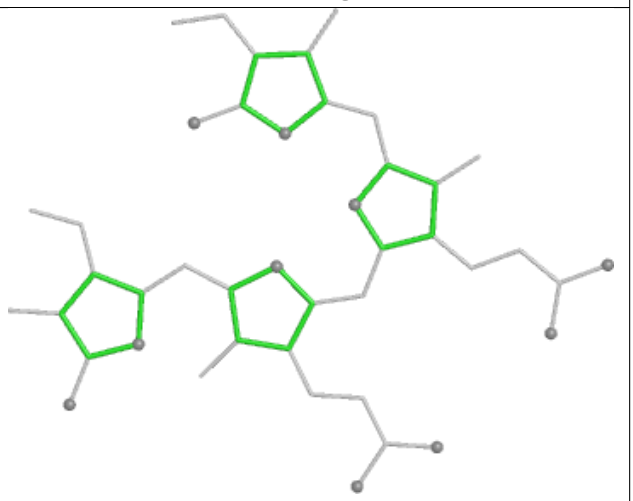
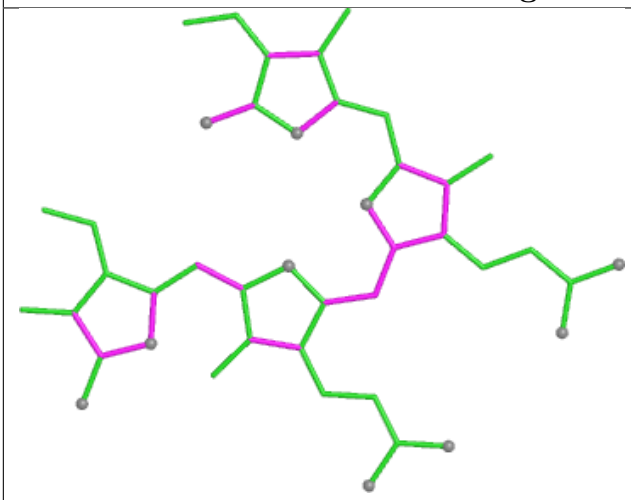


Rings

Ligand PEB g4 201



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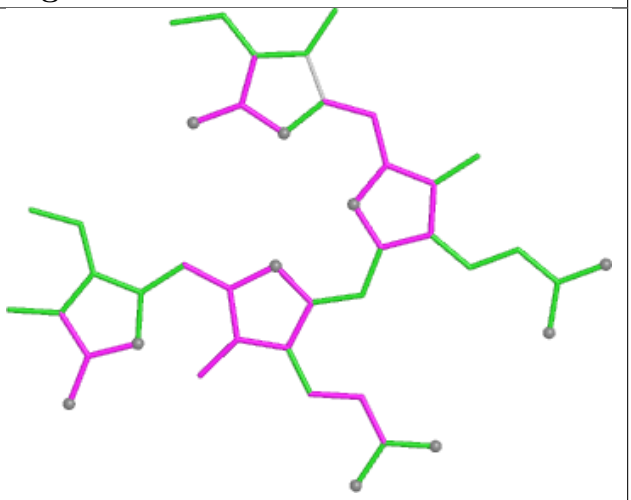
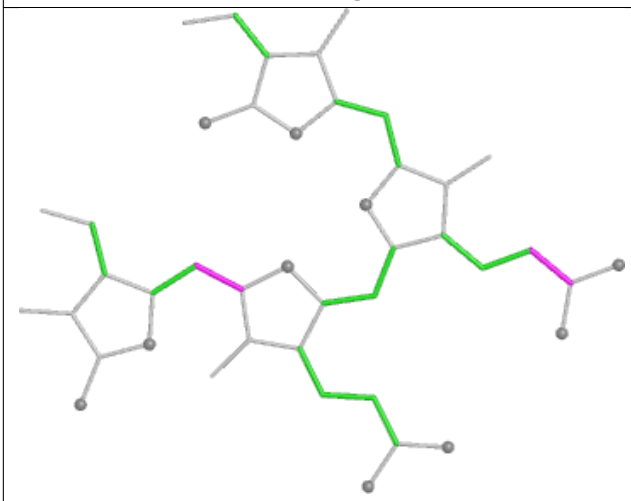


Bond angles



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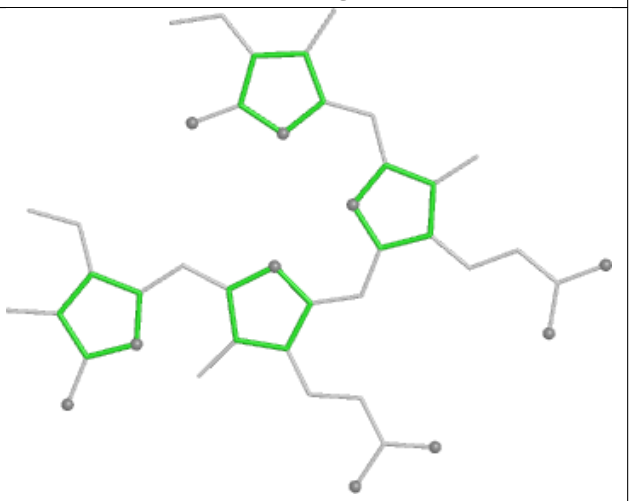

Rings

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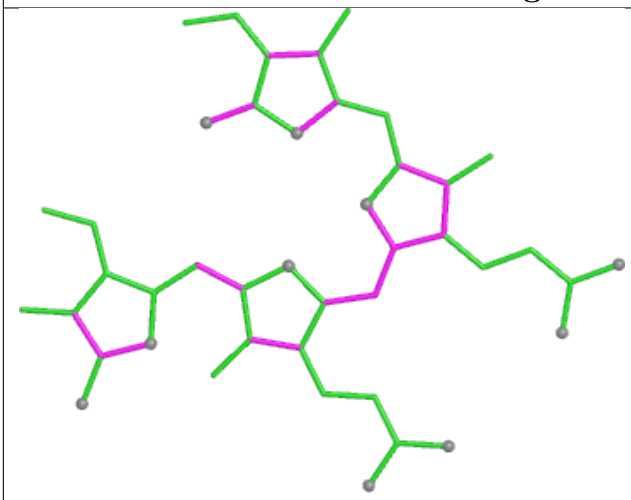

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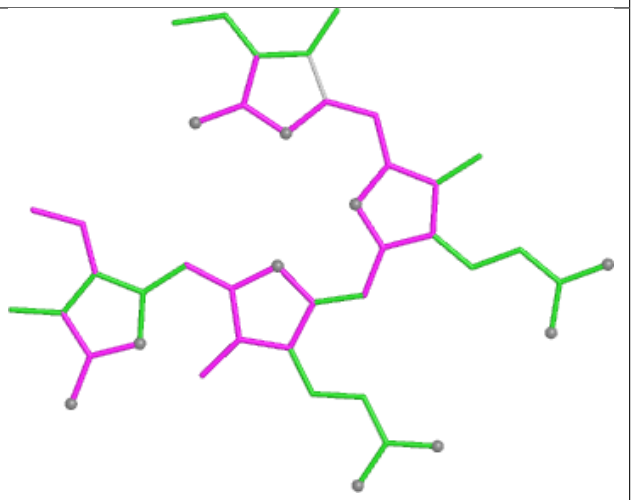
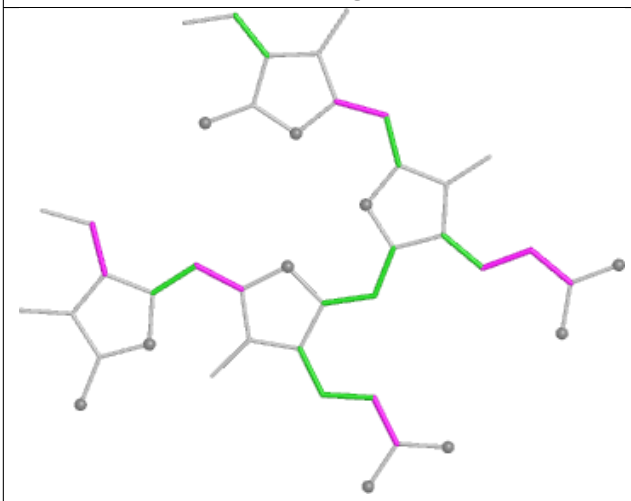


Bond angles



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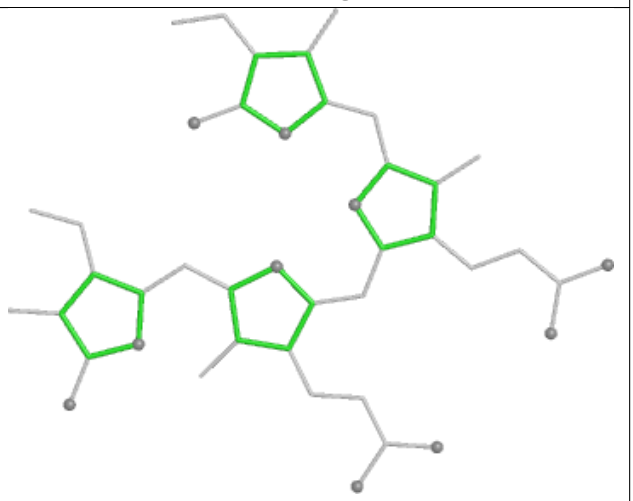

Rings

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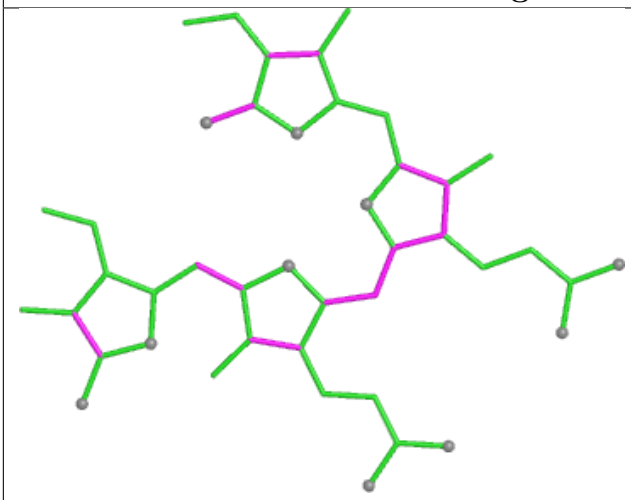

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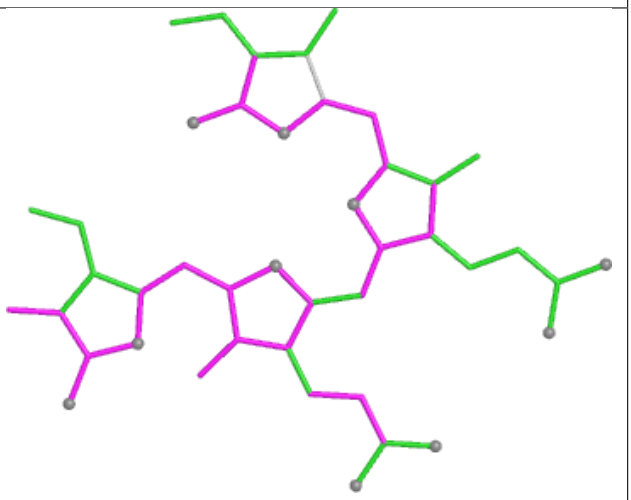
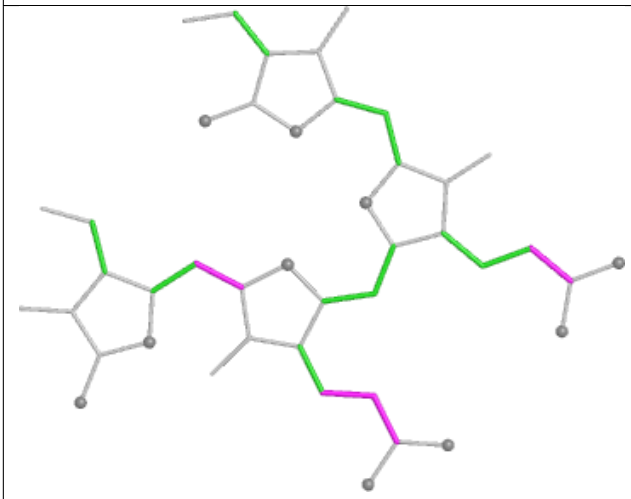
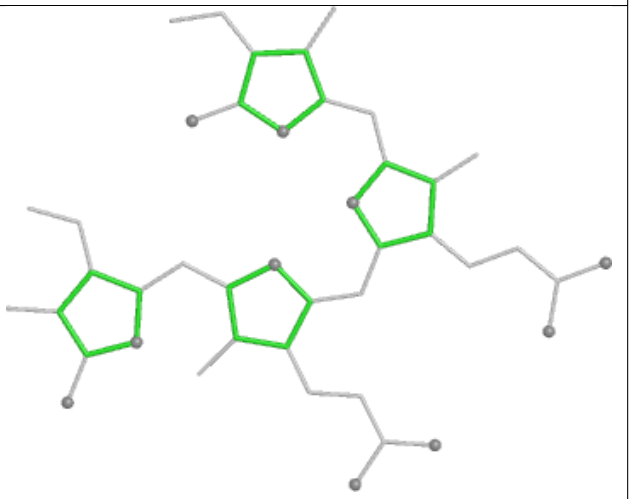


Bond angles

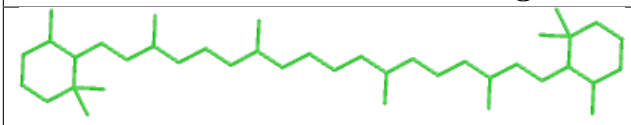


Torsions



Rings

Ligand BCR hL 102



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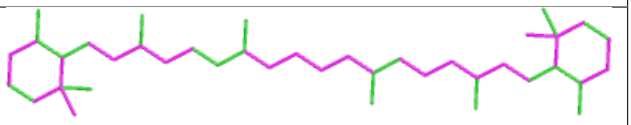
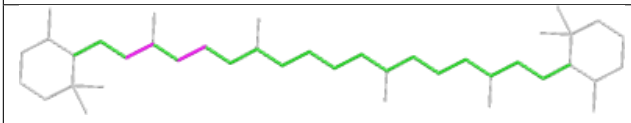


Bond angles



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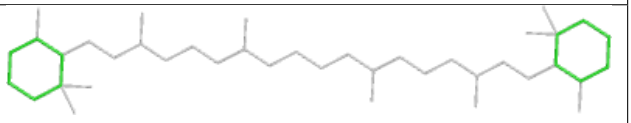
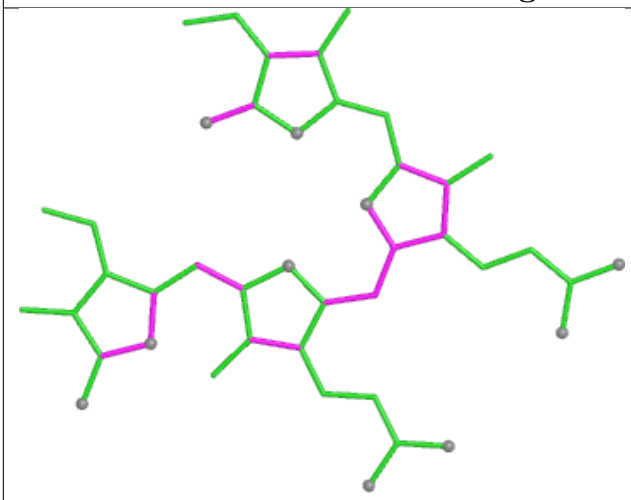


Rings

Ligand PEB TI 203



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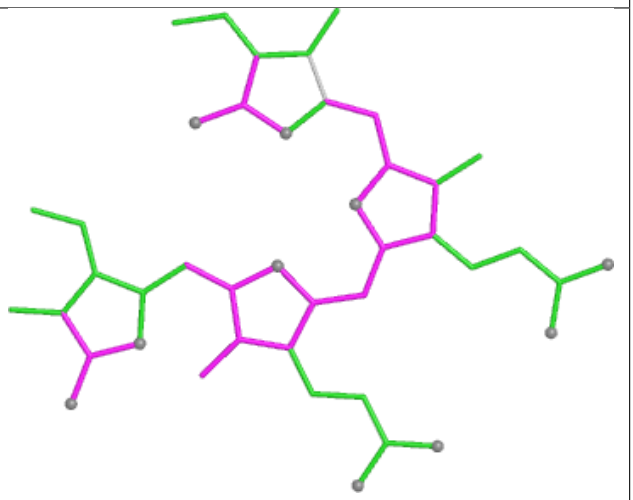

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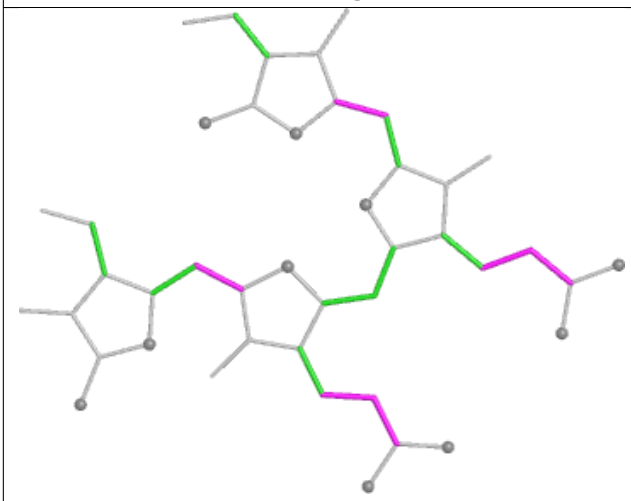

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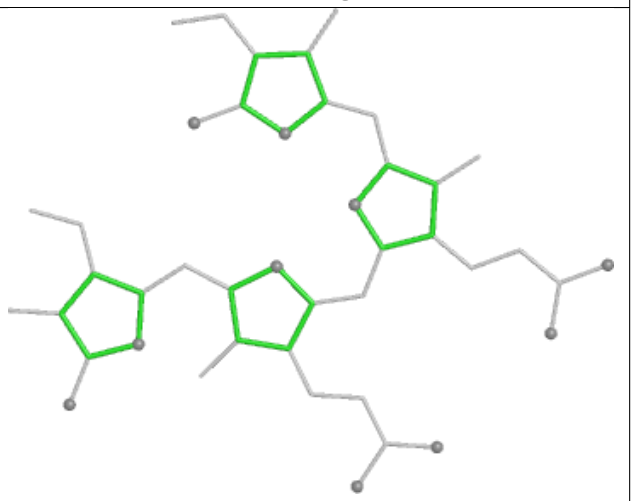
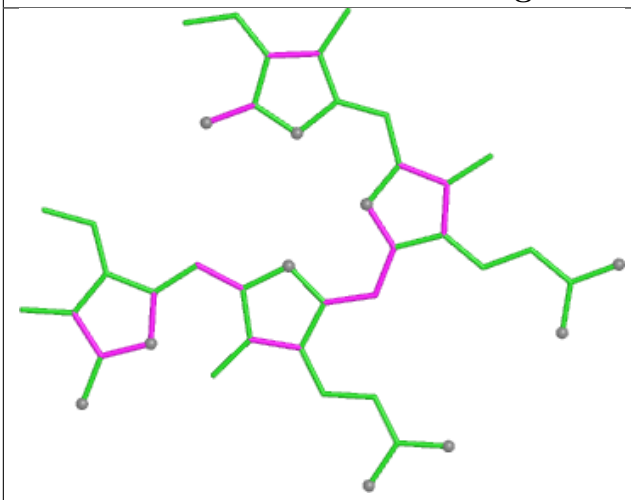


Rings

Ligand PEB gG 202



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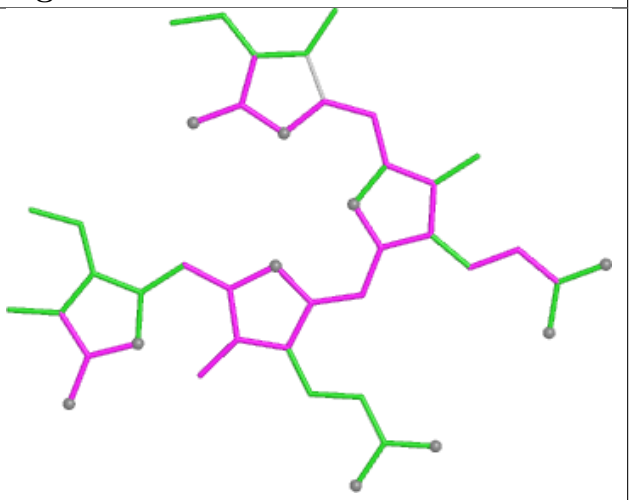

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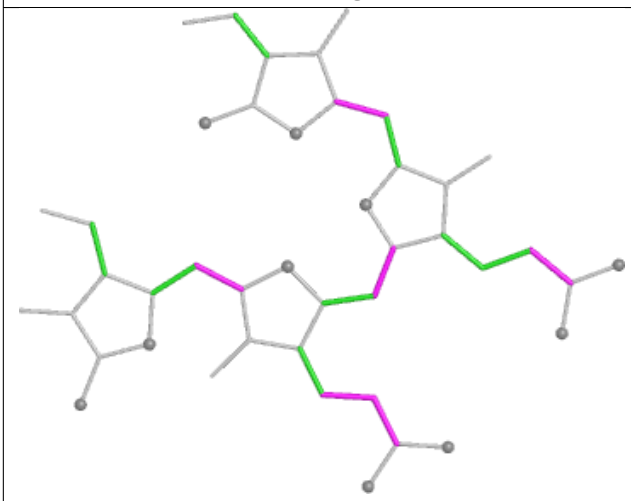

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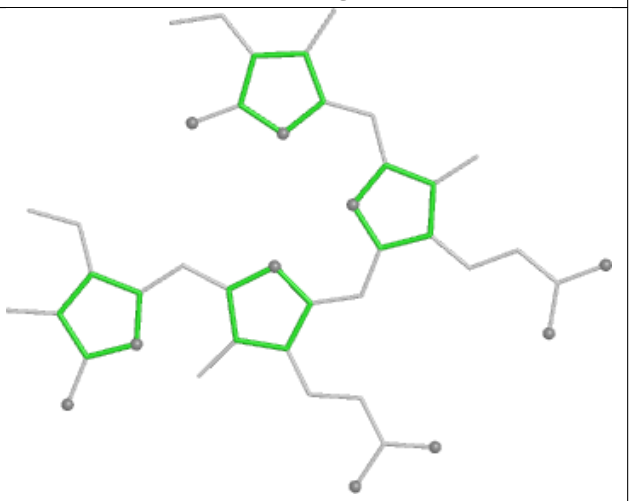
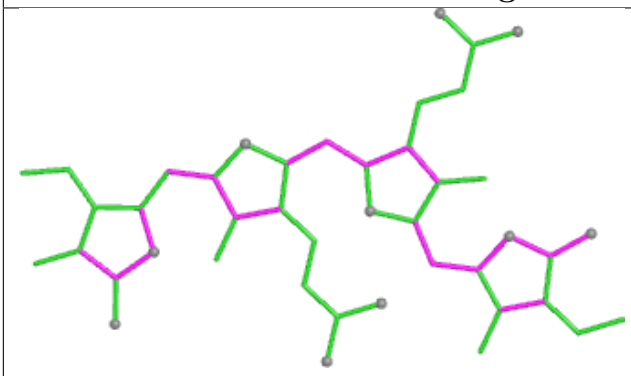


Rings

Ligand CYC DG 1001



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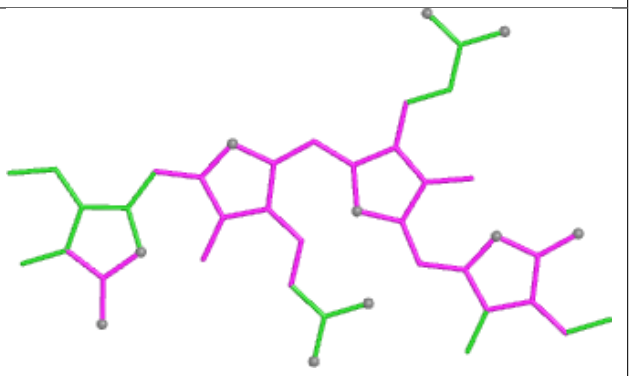

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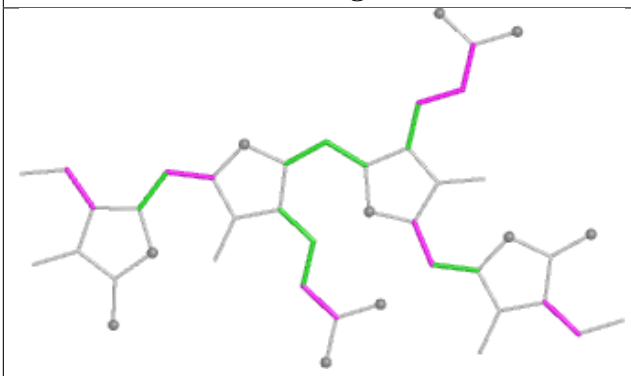

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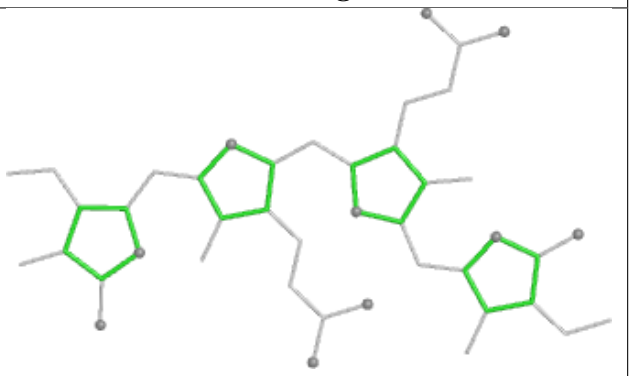
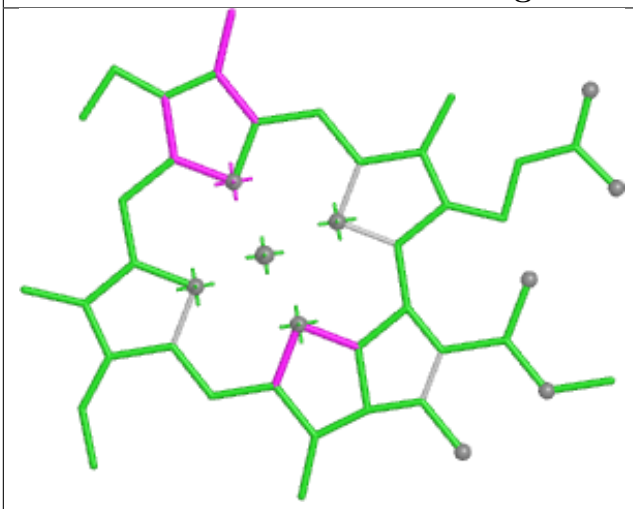


Rings

Ligand CLA 5N 601



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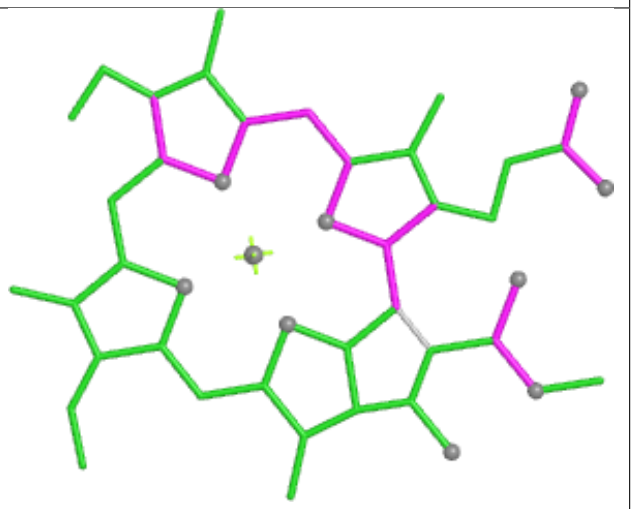

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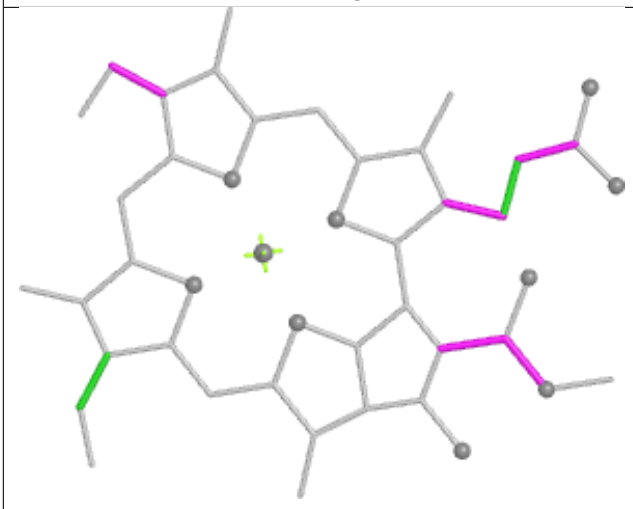
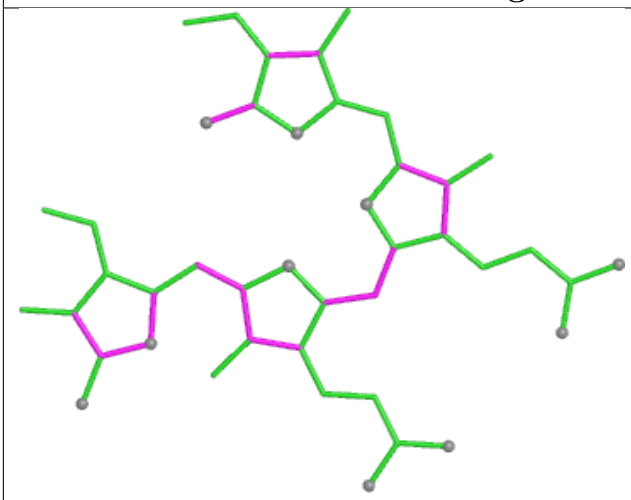


Torsions



Rings

Ligand PEB WF 202



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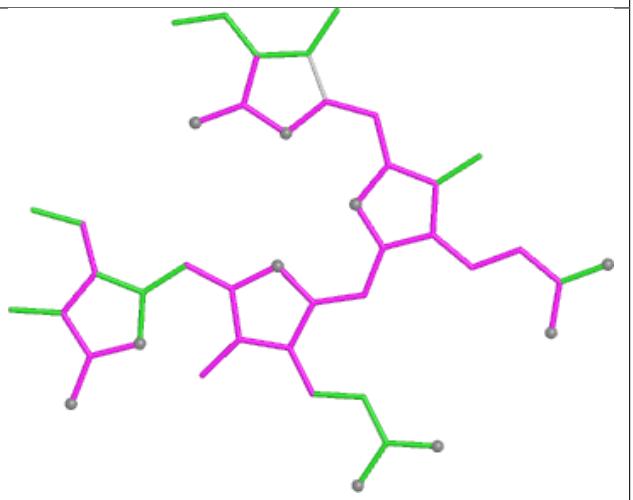

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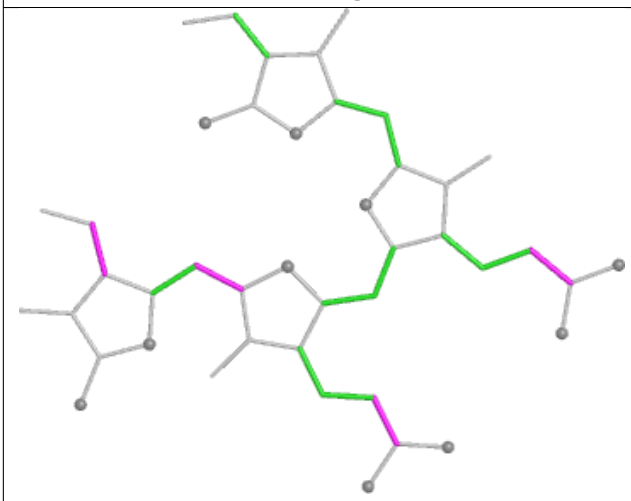

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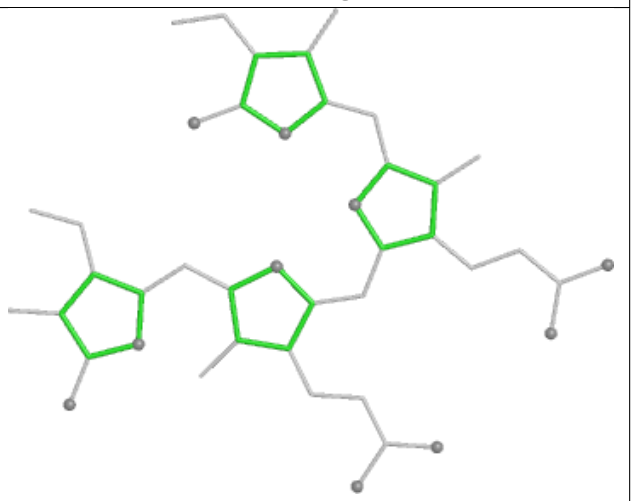
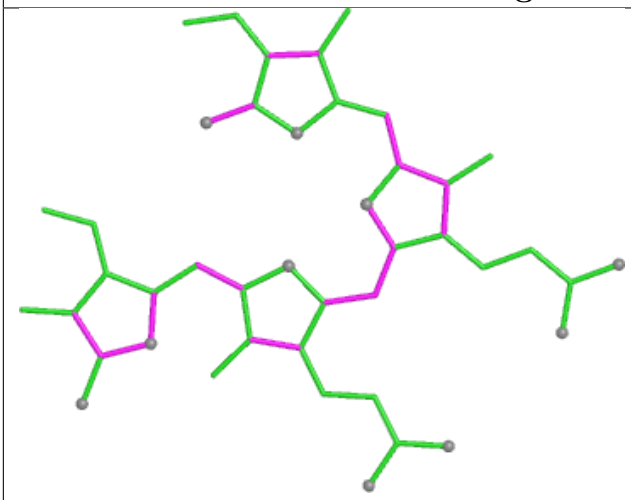


Rings

Ligand PEB Y7 301



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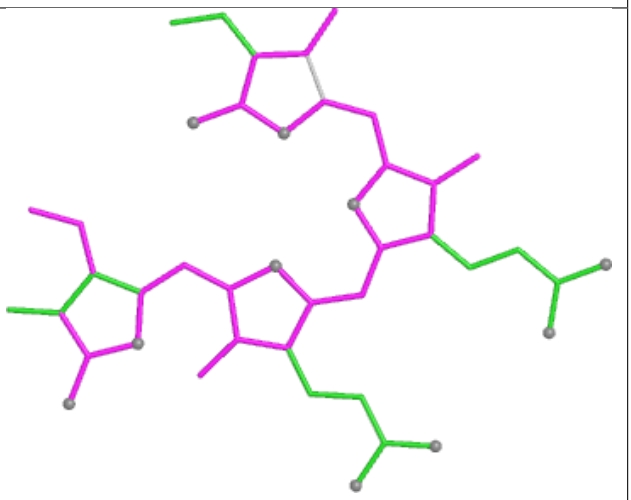

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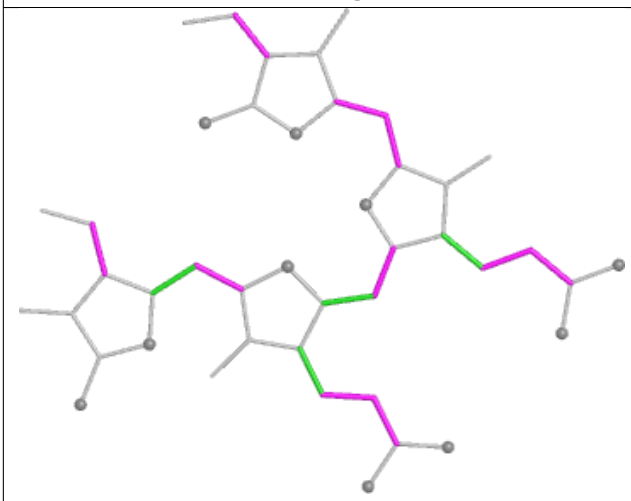

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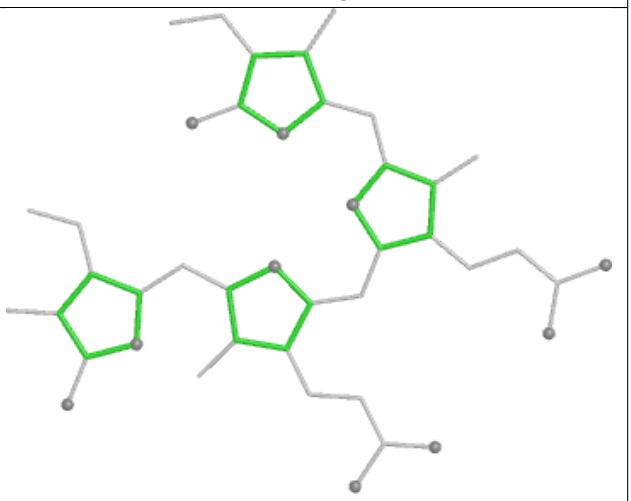
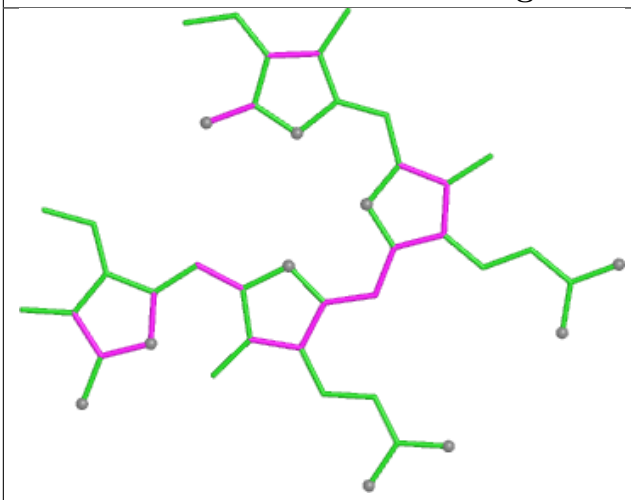


Rings

Ligand PEB kE 201



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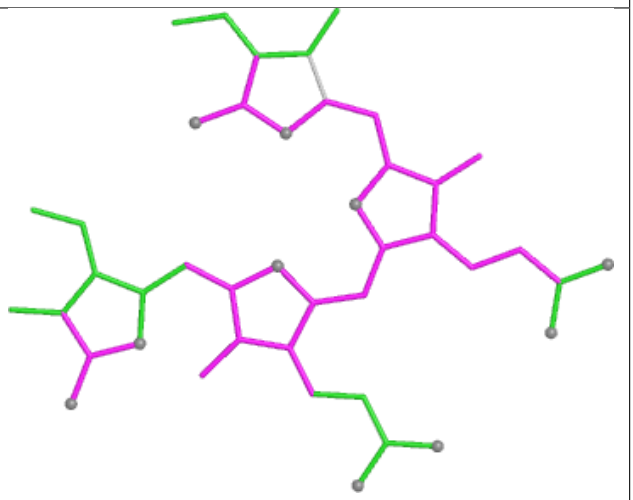

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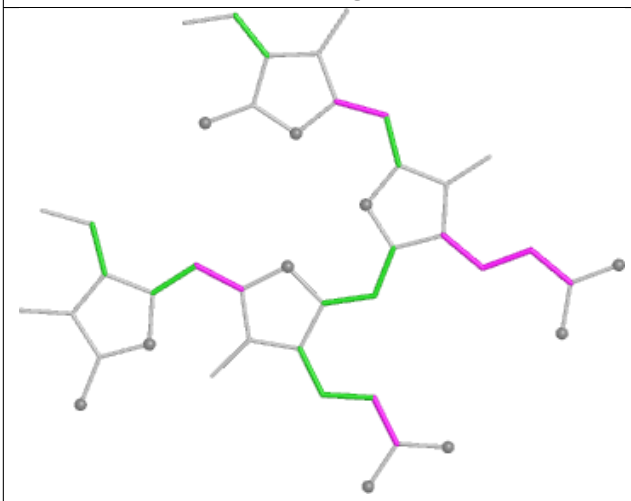

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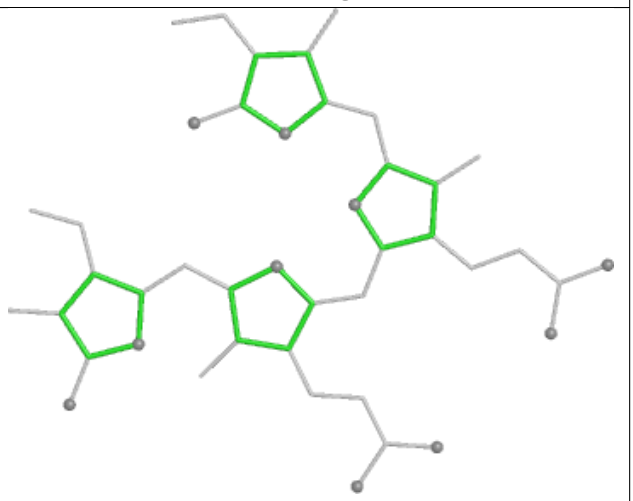
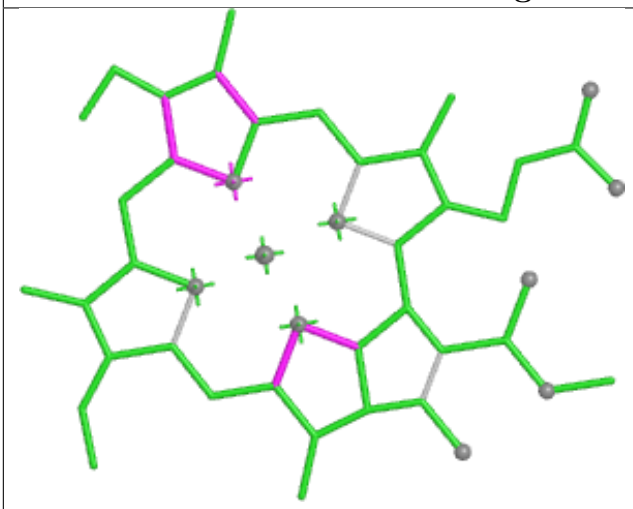


Rings

Ligand CLA 2N 302



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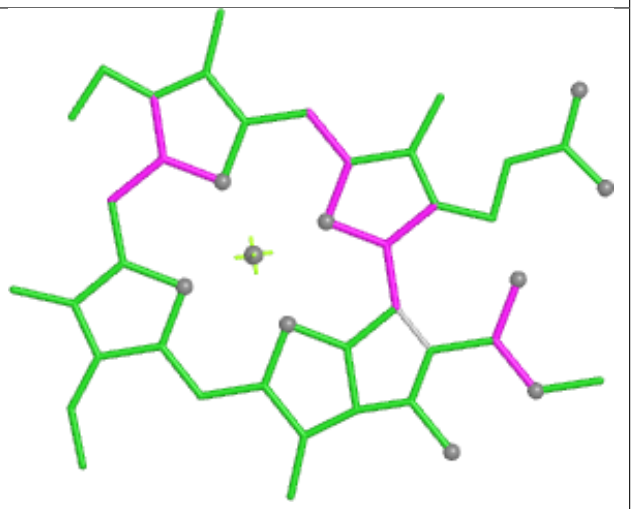
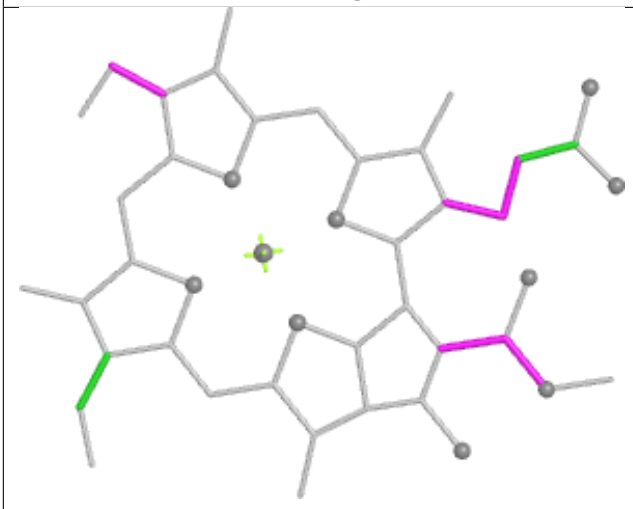


Bond angles

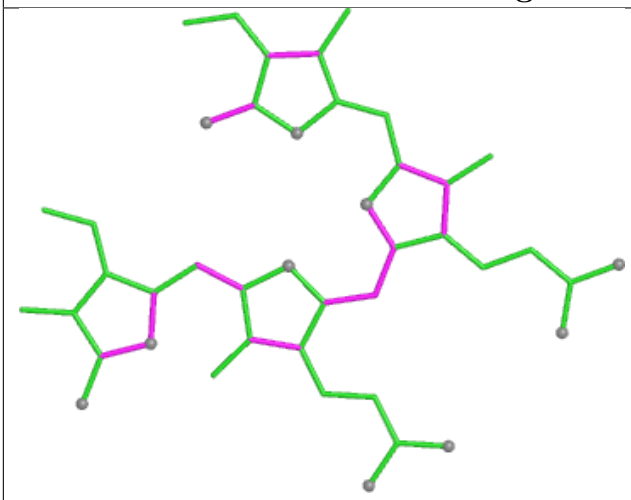


Torsions



Rings

Ligand PEB zK 501



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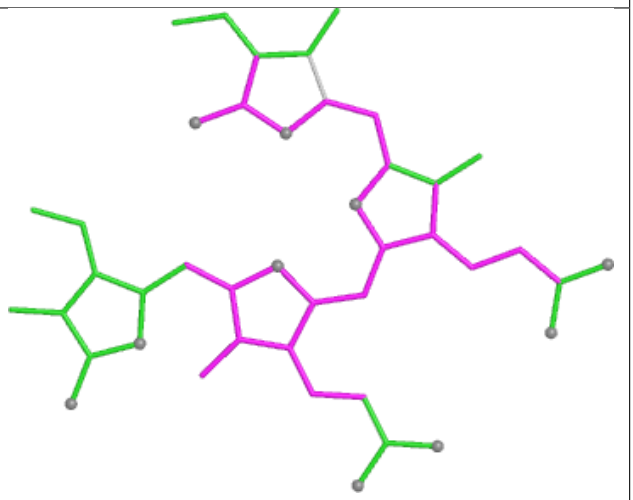

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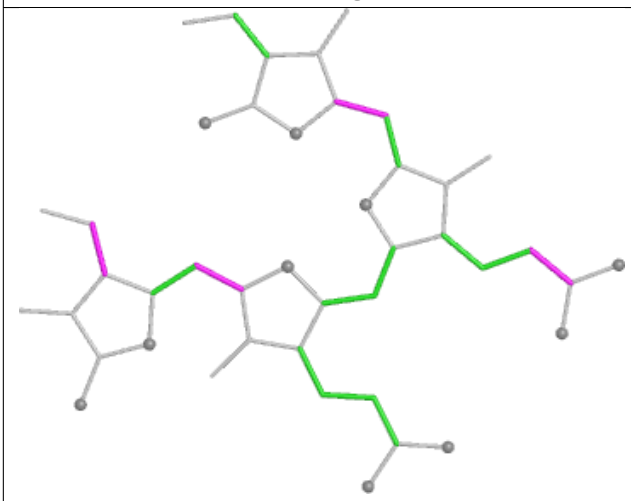

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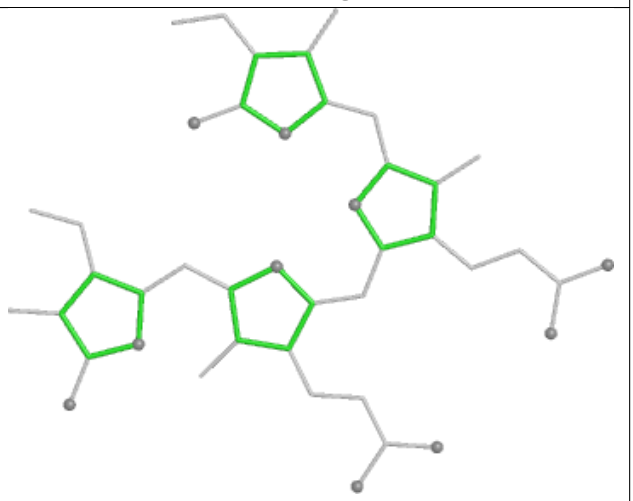
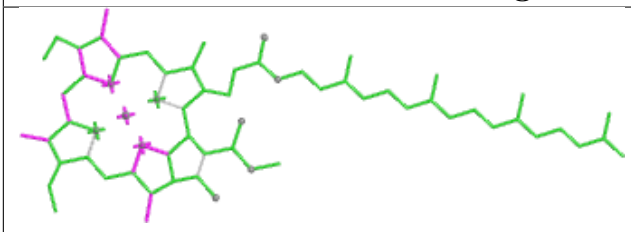


Rings

Ligand CLA BL 605



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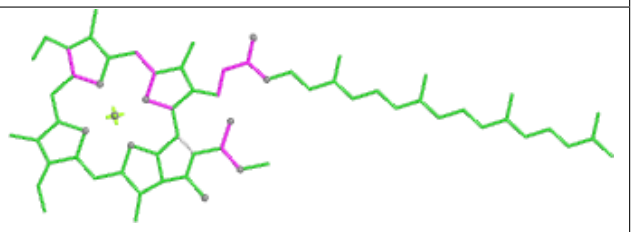
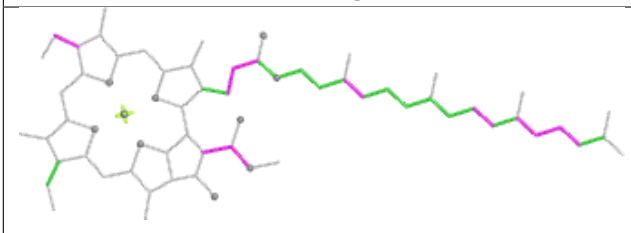


Bond angles



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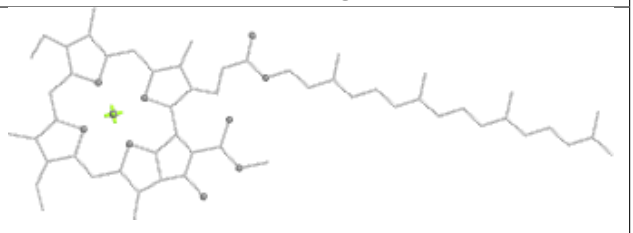
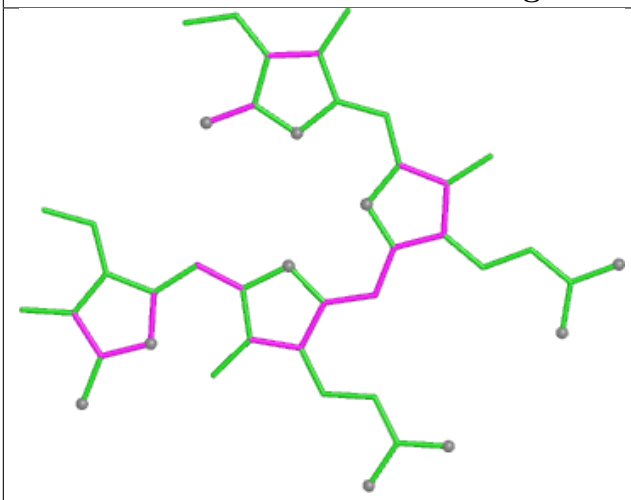


Rings

Ligand PEB fJ 203



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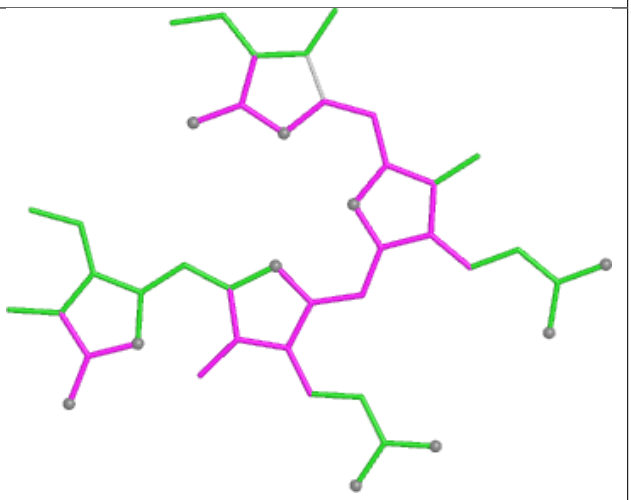

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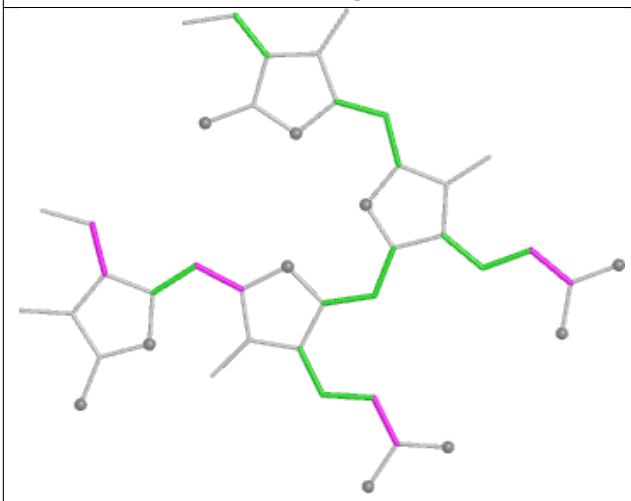

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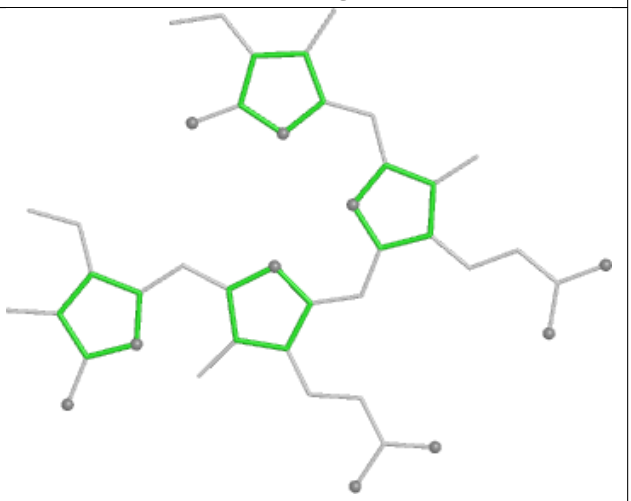
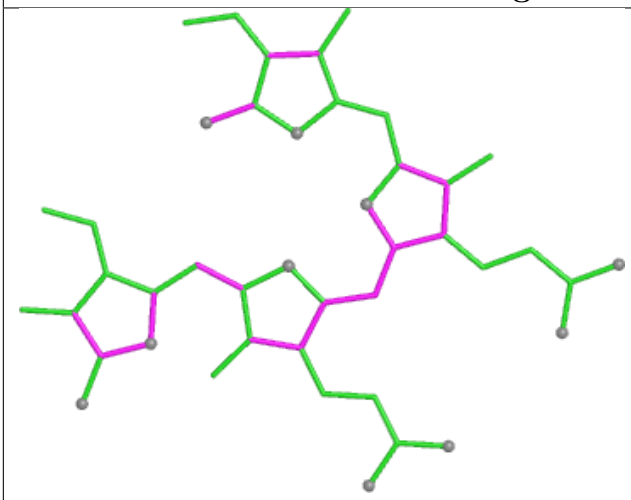


Rings

Ligand PEB LK 202



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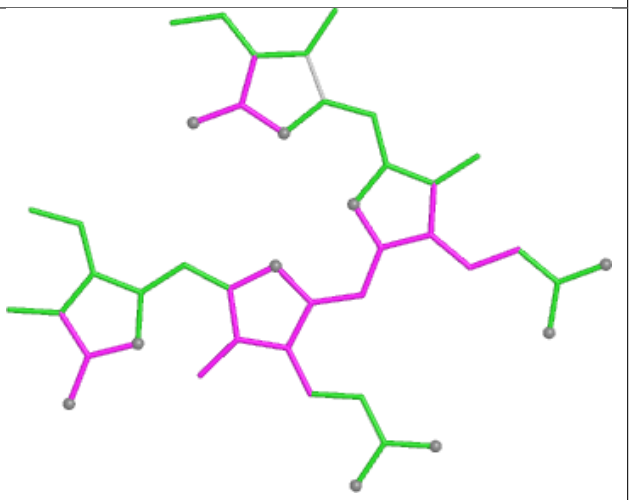
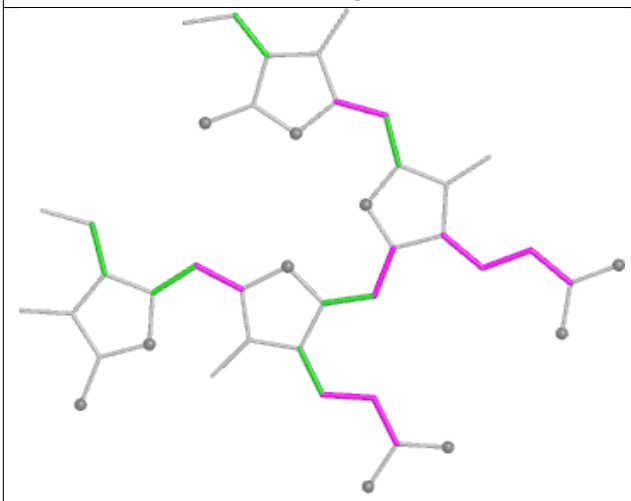


Bond angles



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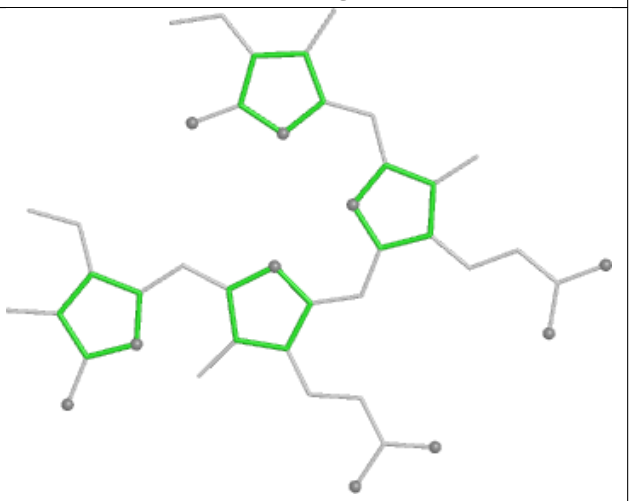
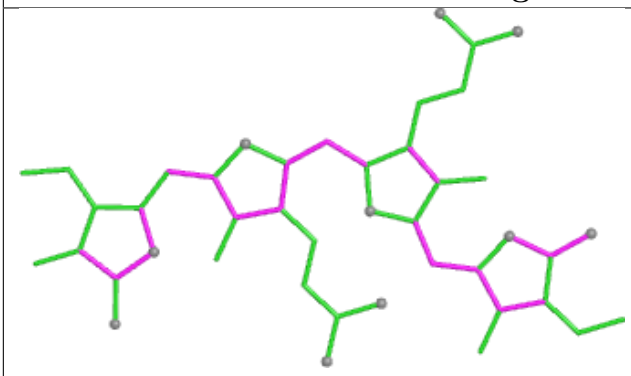


Rings

Ligand CYC i3 1001



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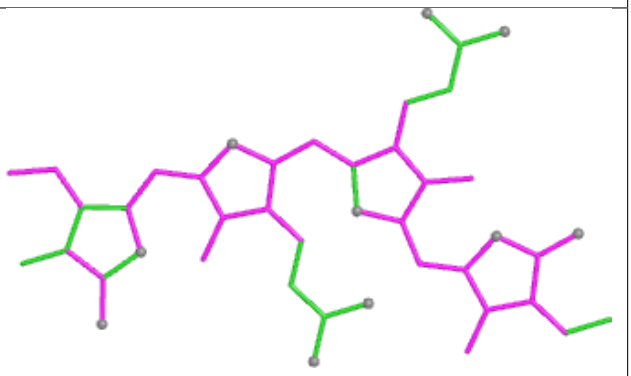
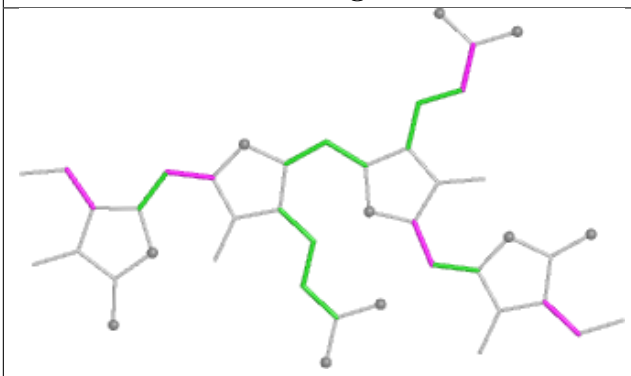


Bond angles



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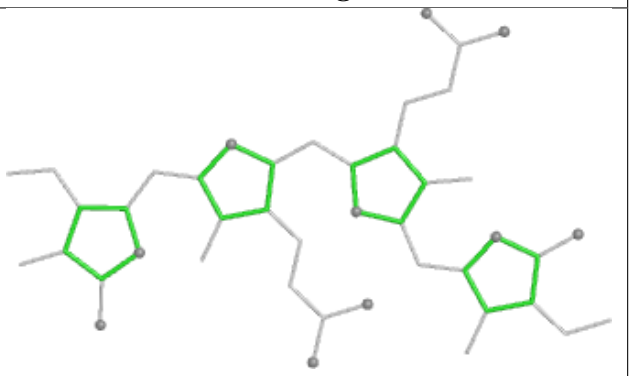
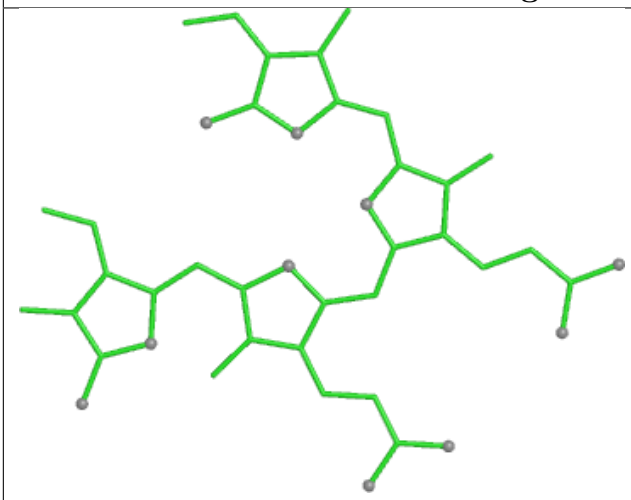


Rings

Ligand PEB lE 202



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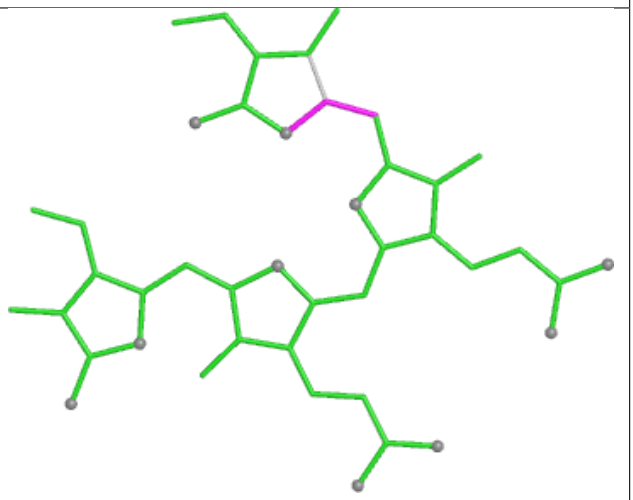
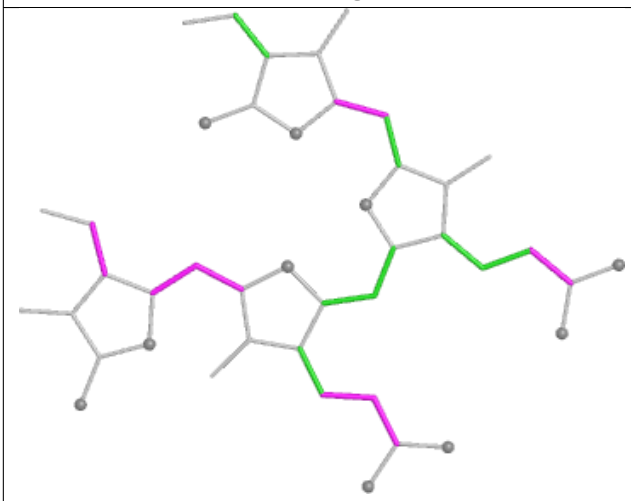
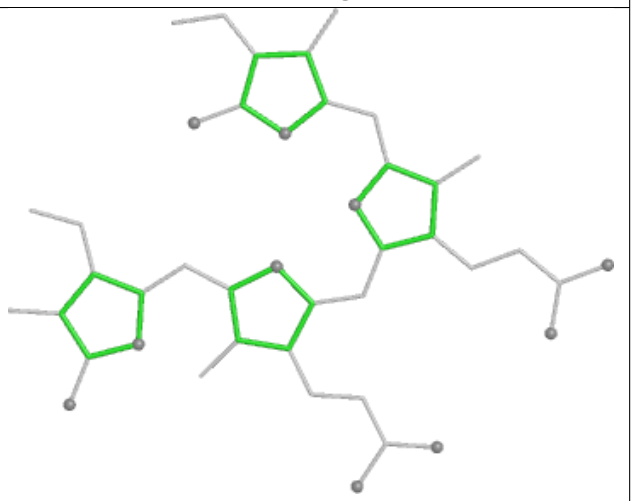


Bond angles

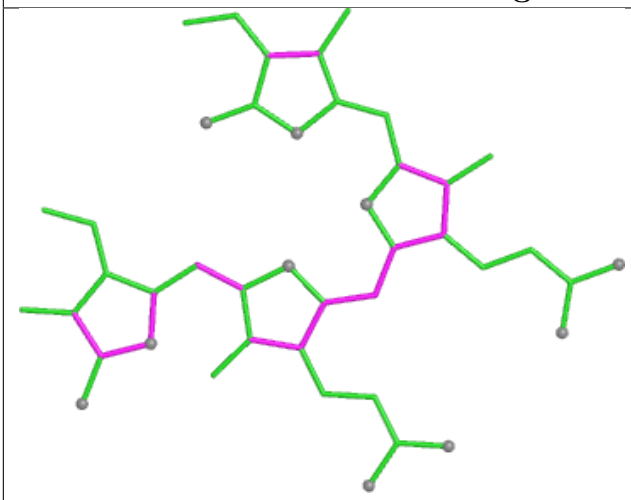


Torsions



Rings

Ligand PEB TA 201



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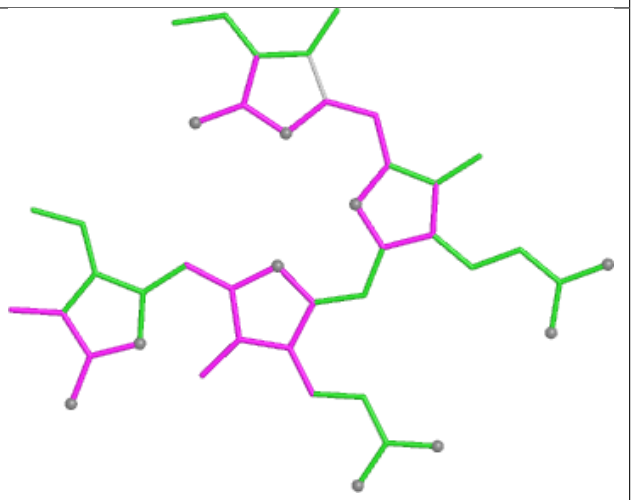
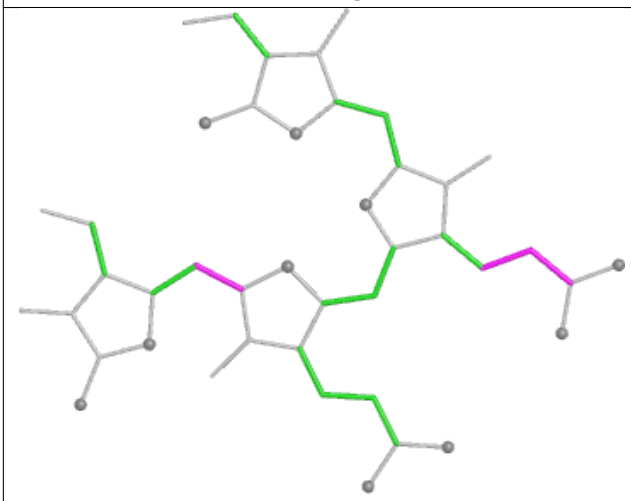


Bond angles



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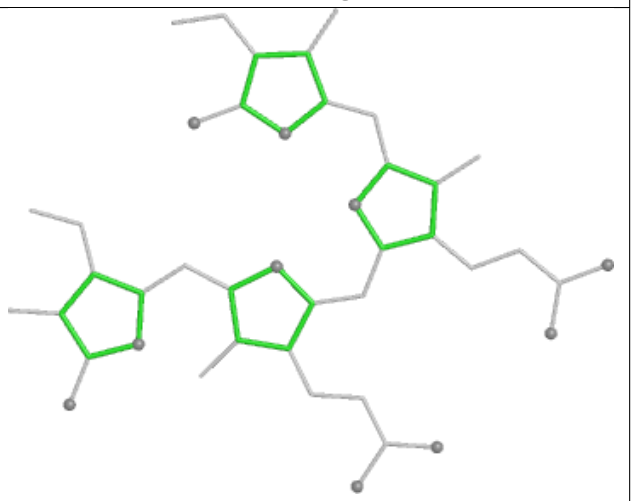
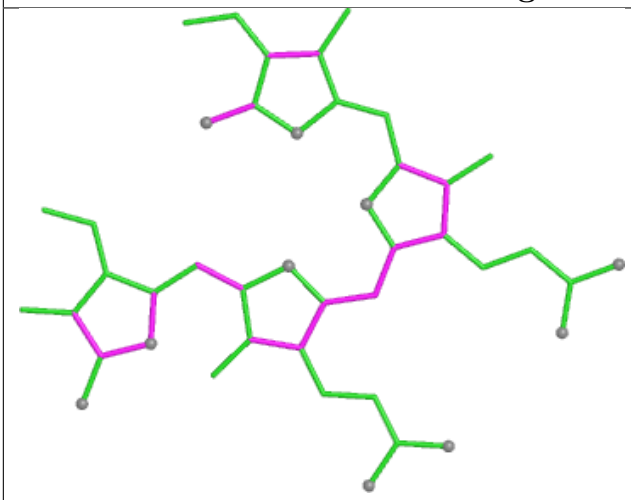


Rings

Ligand PEB cE 201



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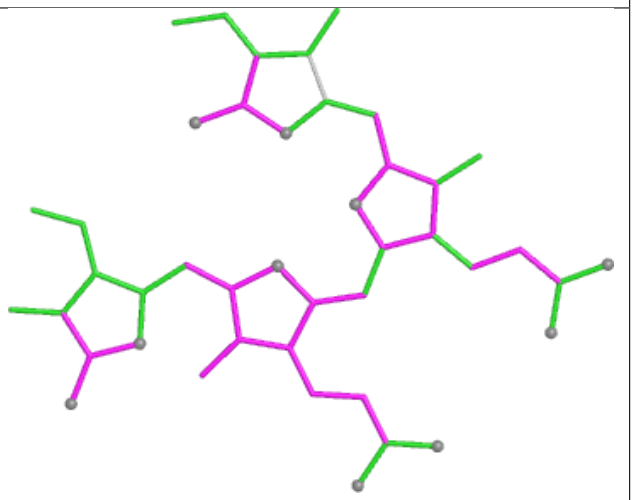

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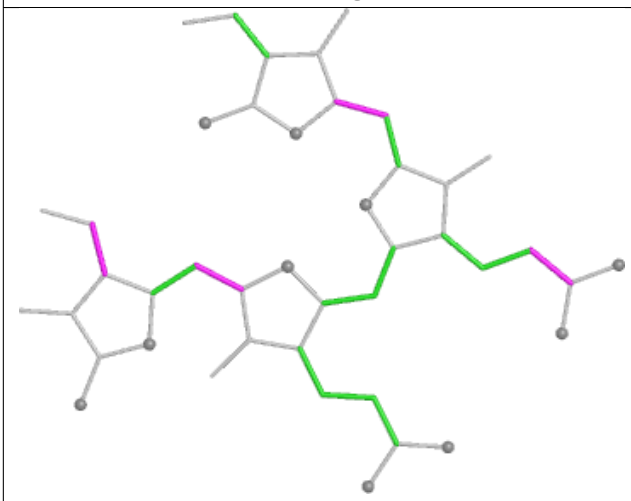

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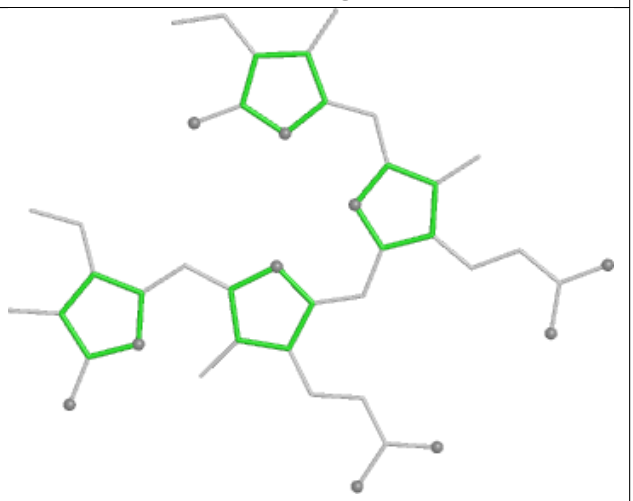
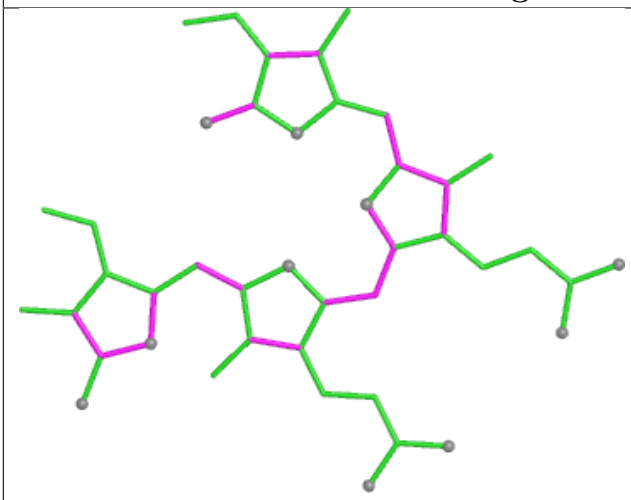


Rings

Ligand PEB KP 201



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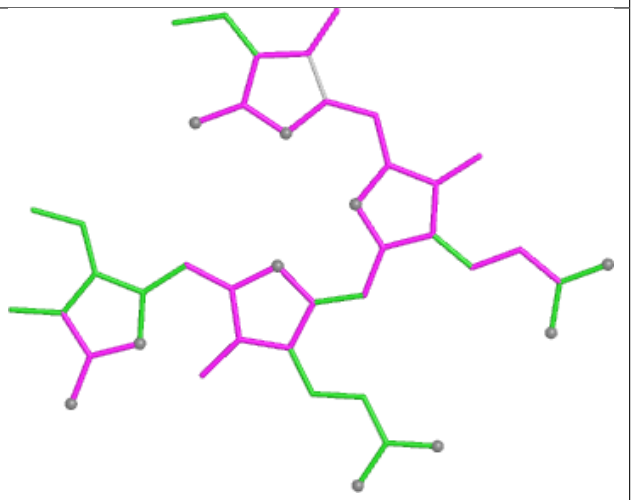

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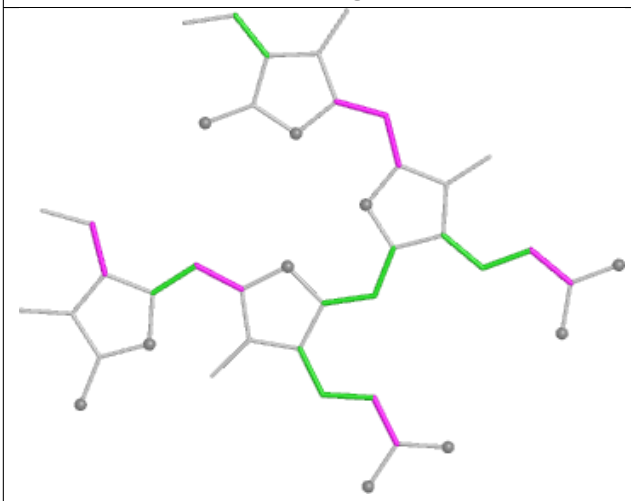

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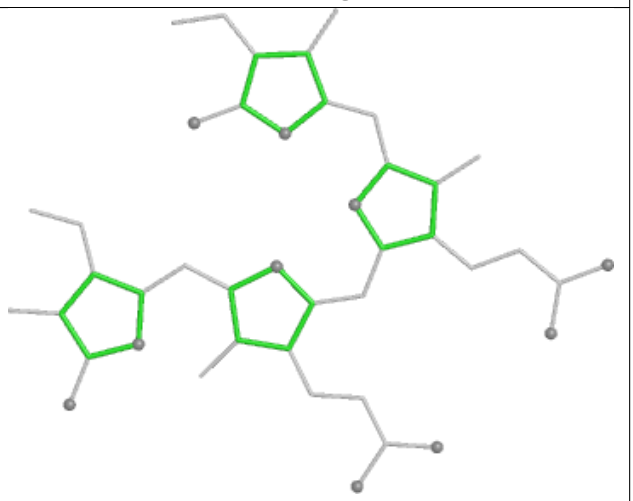
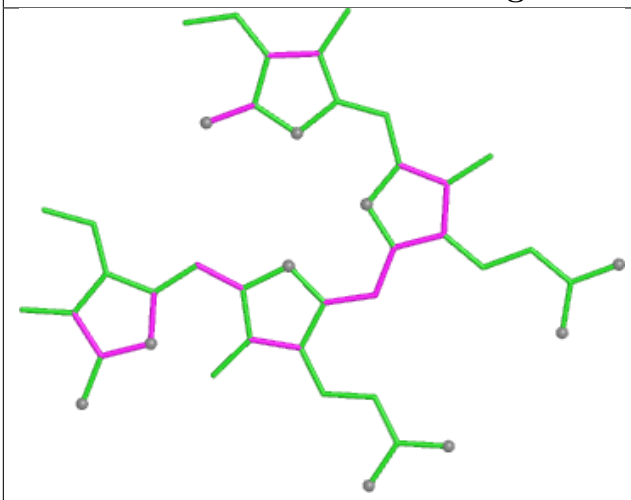


Rings

Ligand PEB UM 201



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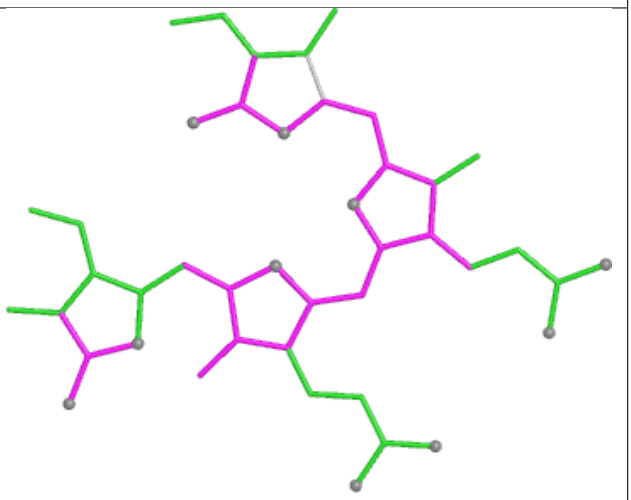

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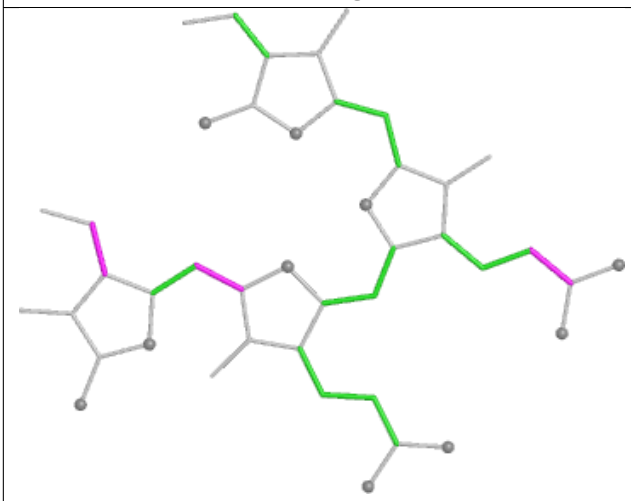

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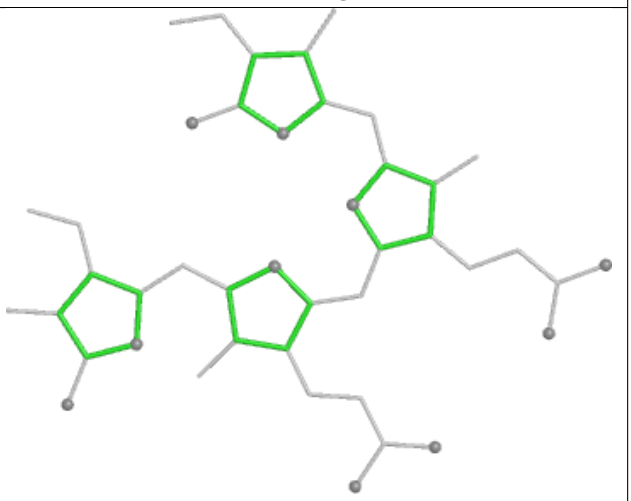
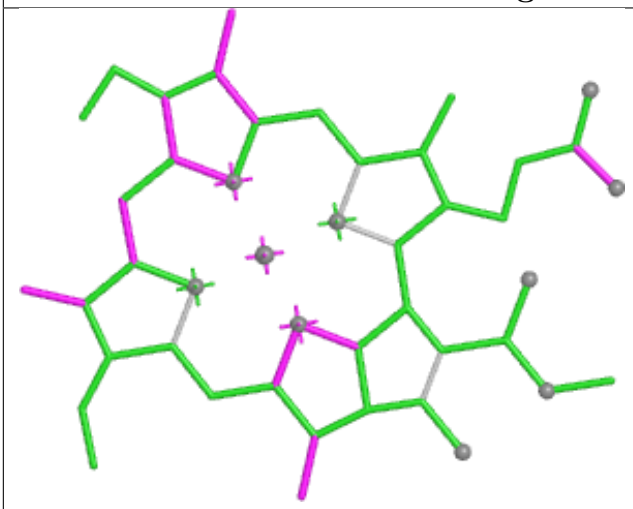


Rings

Ligand CLA F2 201



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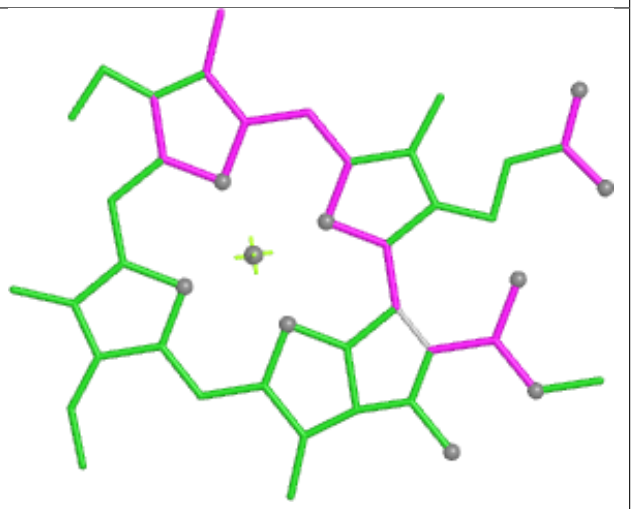

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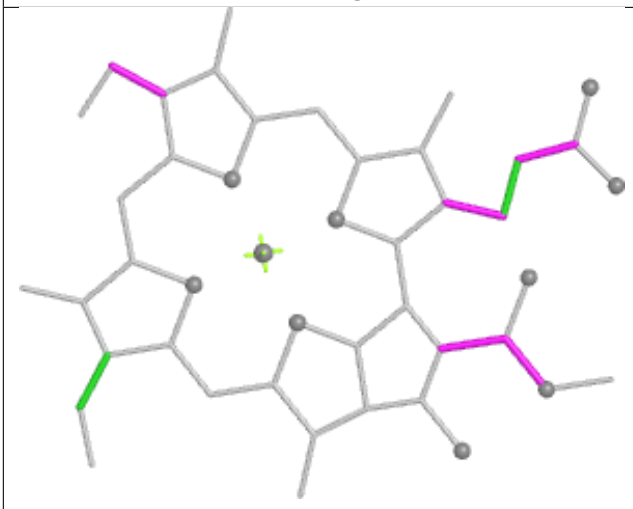
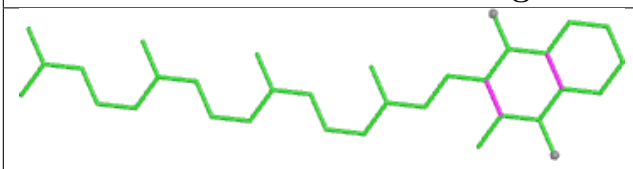


Torsions



Rings

Ligand PQN A2 842



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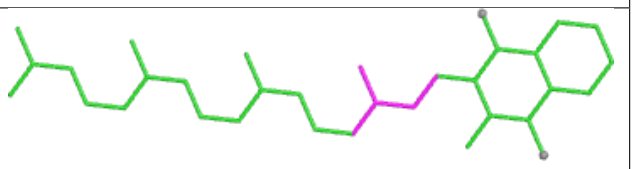

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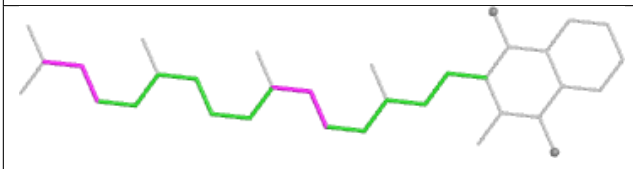

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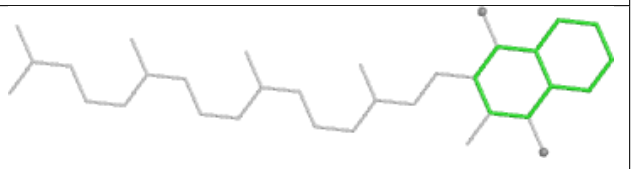
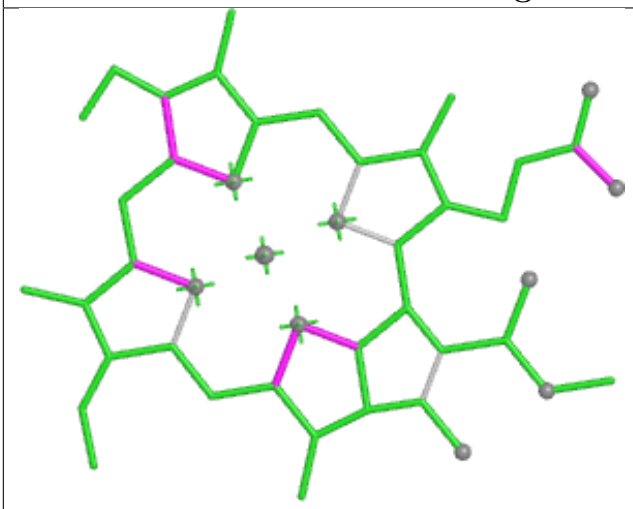


Rings

Ligand CLA 3N 308



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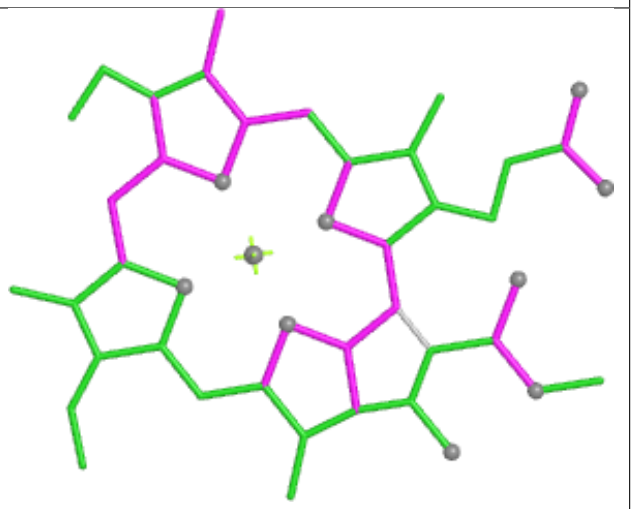

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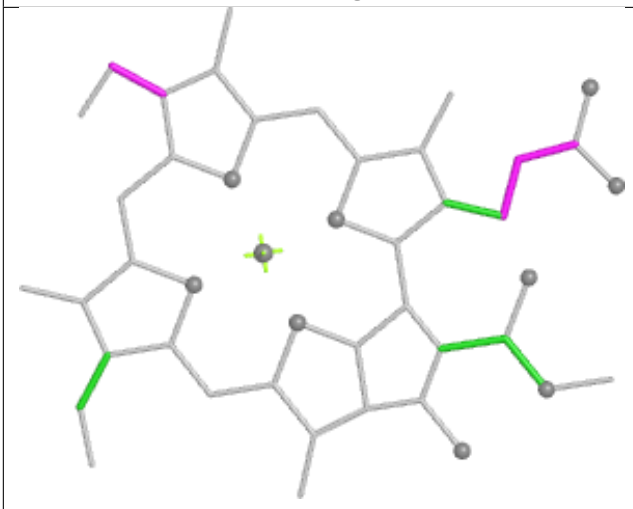
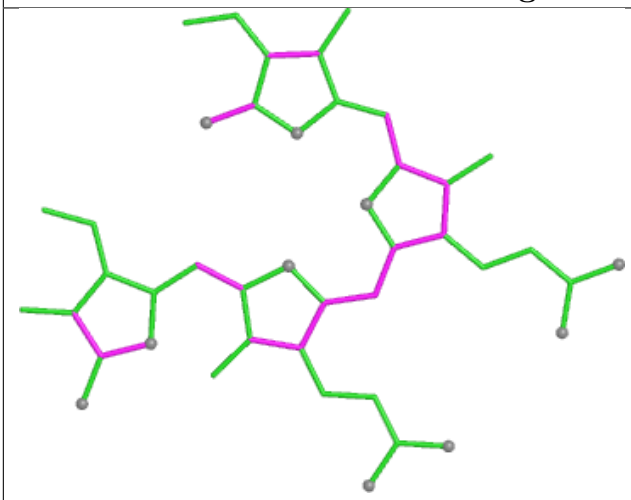


Torsions



Rings

Ligand PEB u8 202



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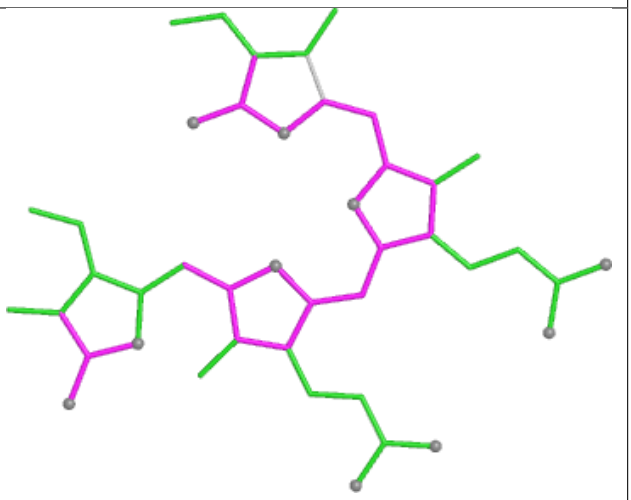

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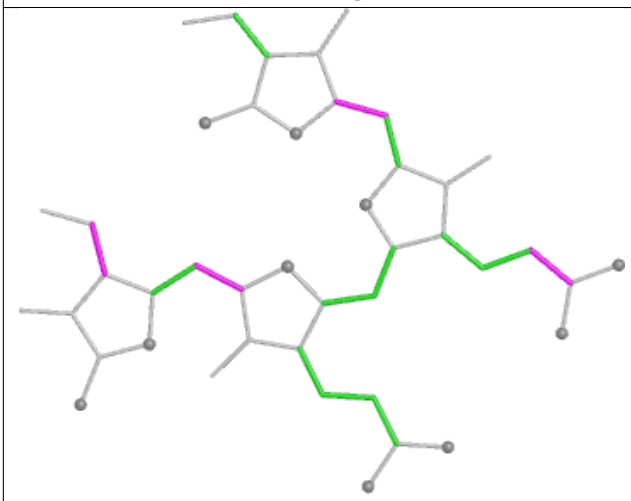

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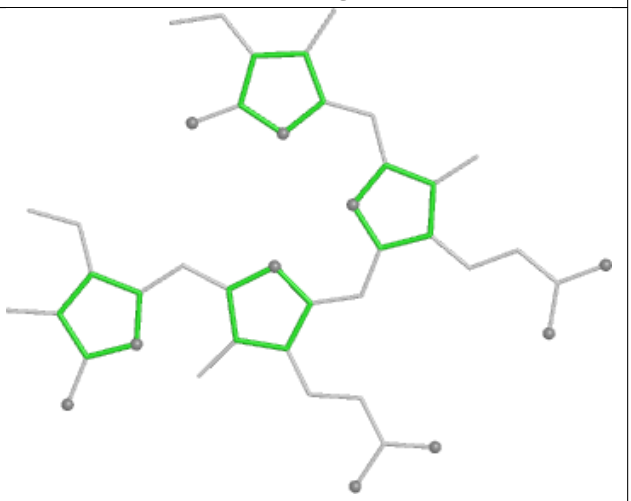
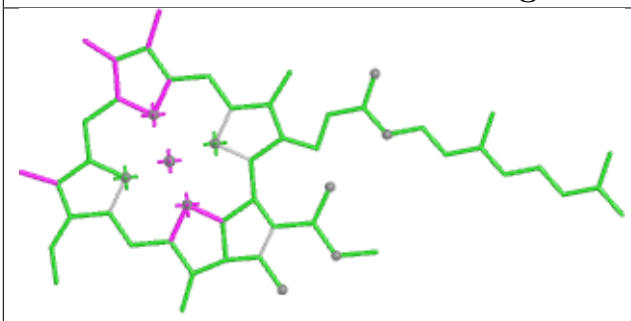


Rings

Ligand CLA 22 605



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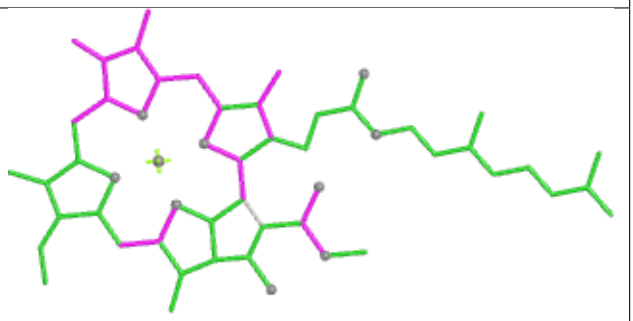

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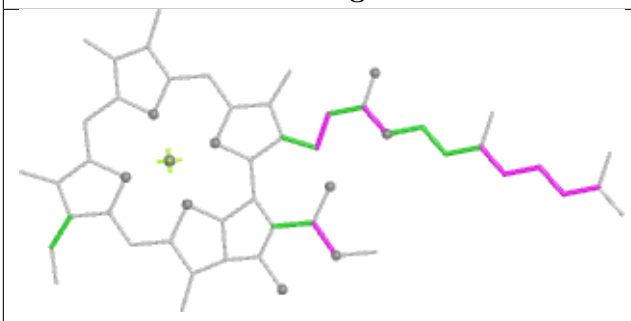

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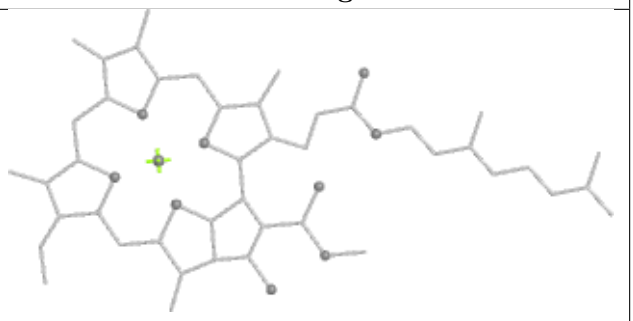
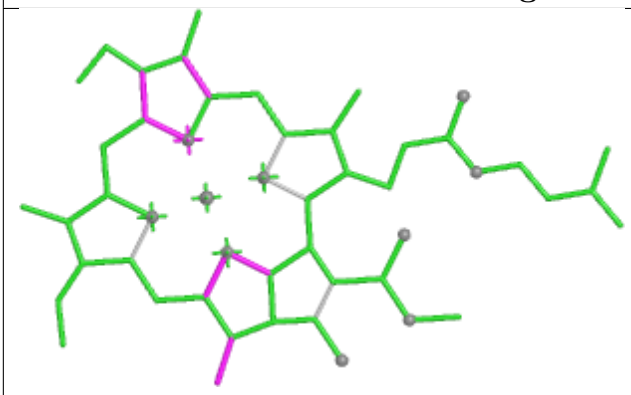


Rings

Ligand CLA 32 309



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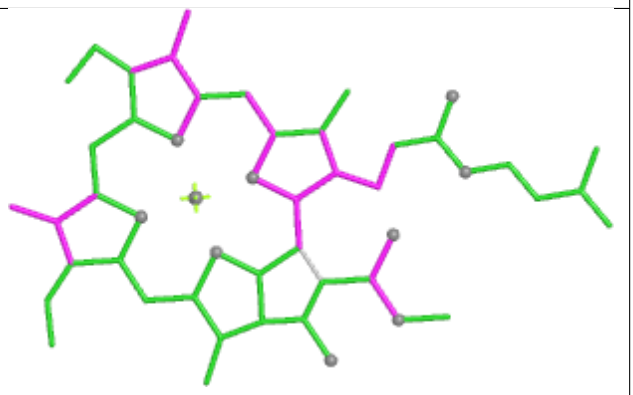

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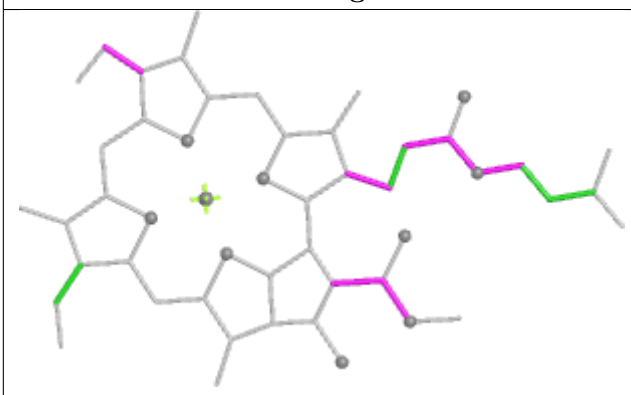

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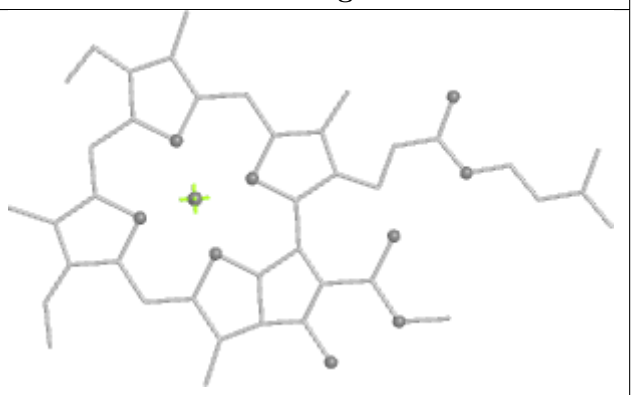
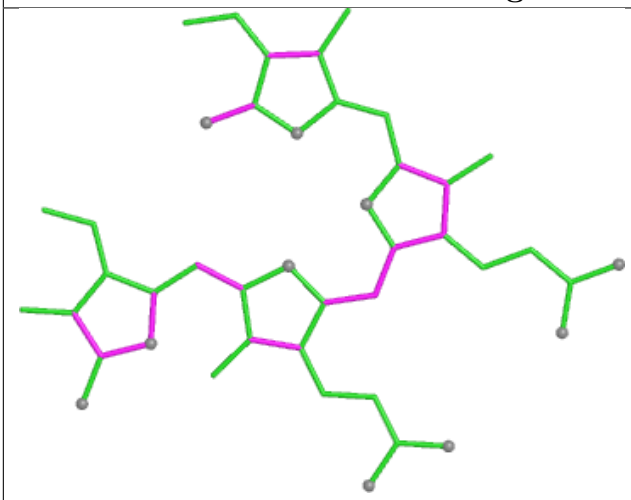


Rings

Ligand PEB WB 401



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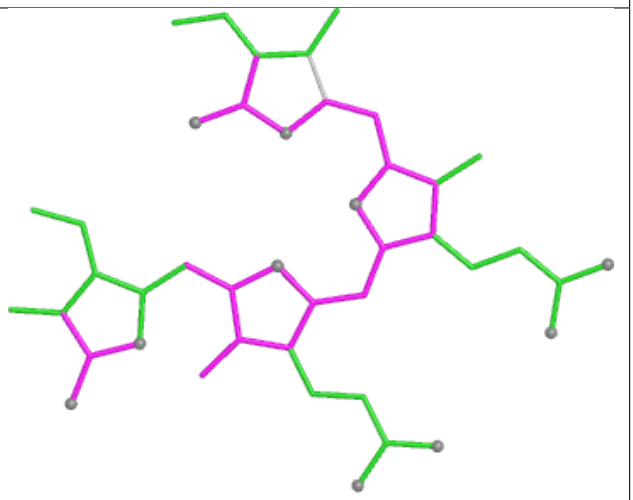
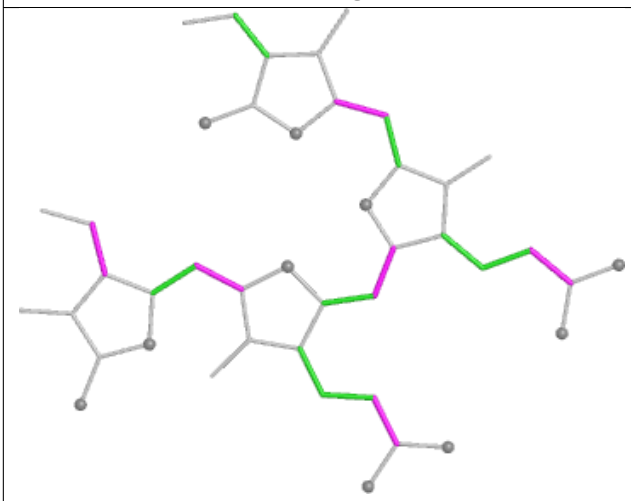


Bond angles



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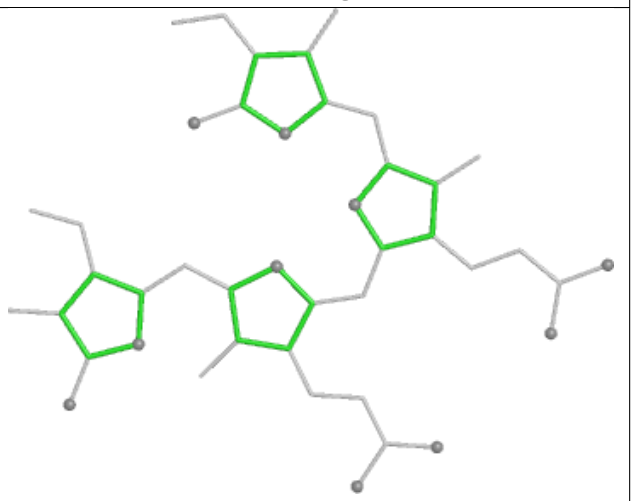
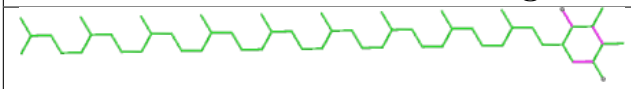


Rings

Ligand PL9 dL 406



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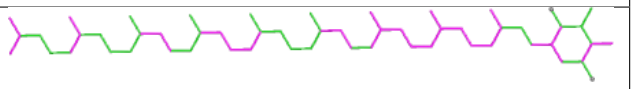

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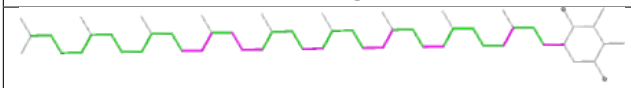

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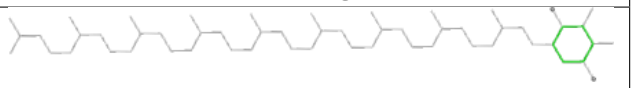
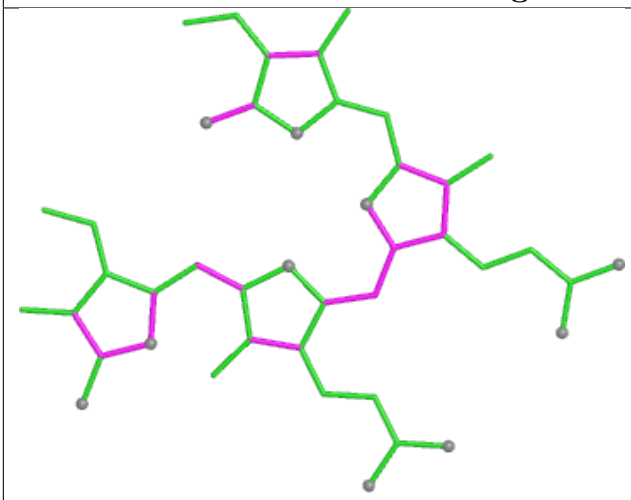


Rings

Ligand PEB DA 203



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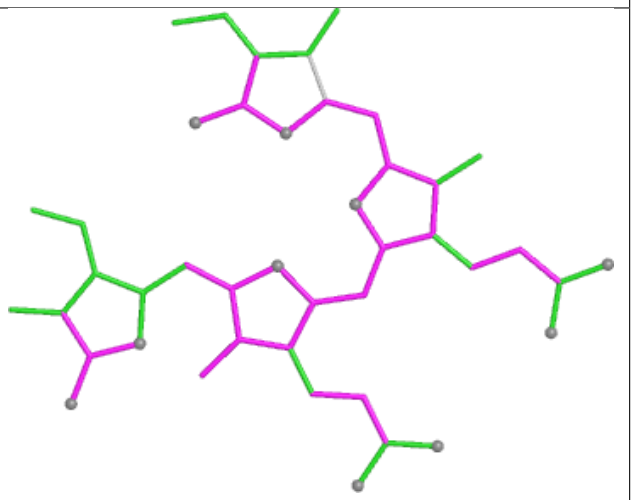
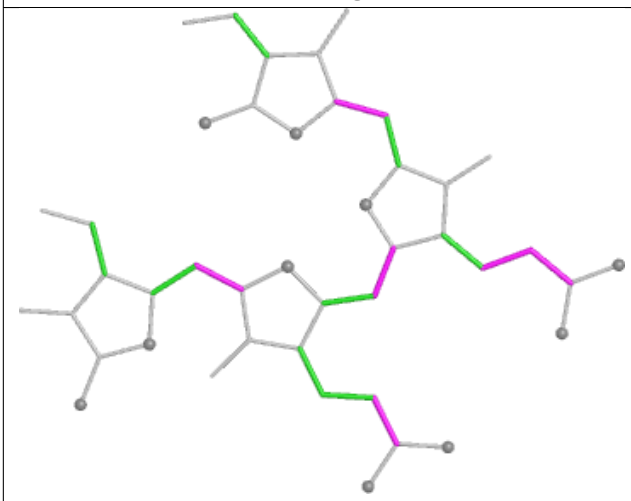


Bond angles



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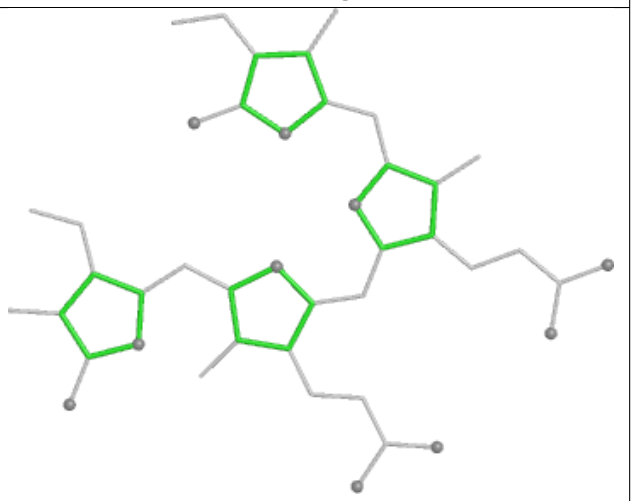
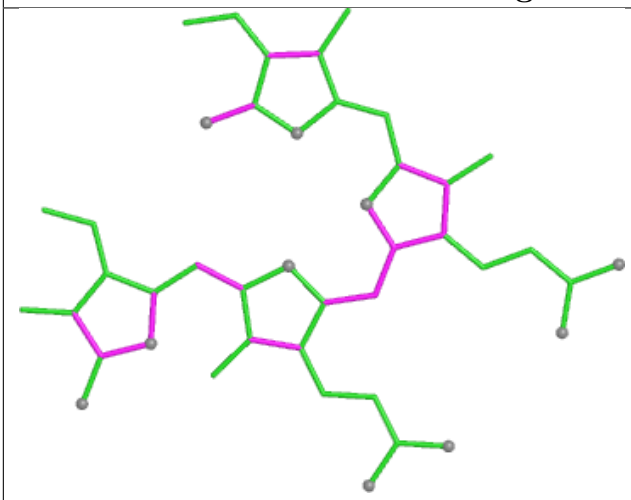


Rings

Ligand PEB C5 202



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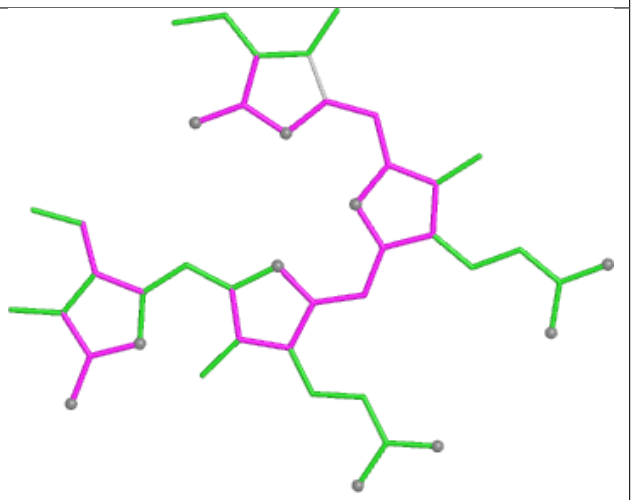
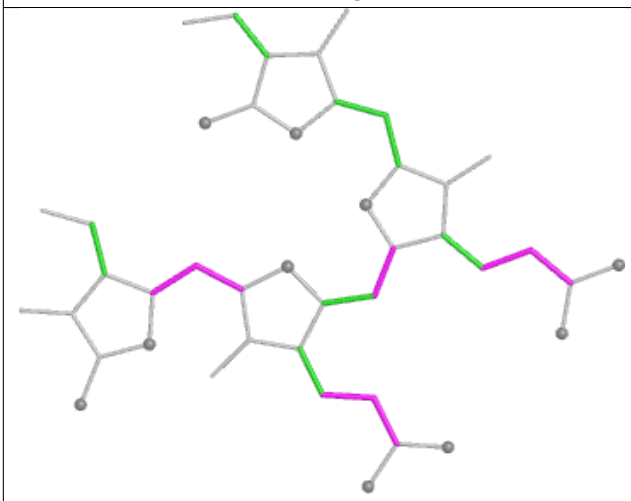


Bond angles



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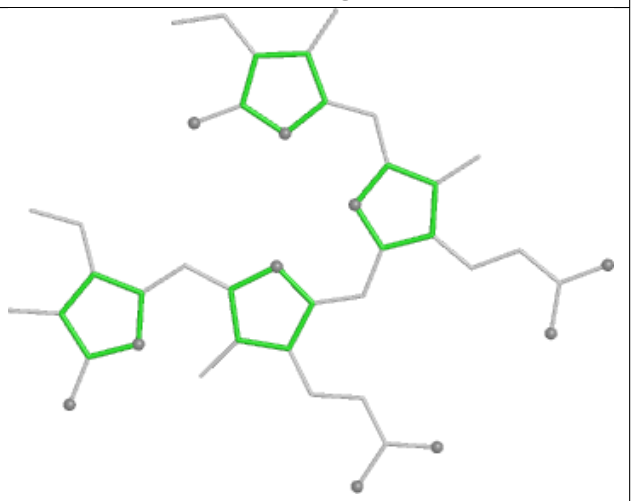
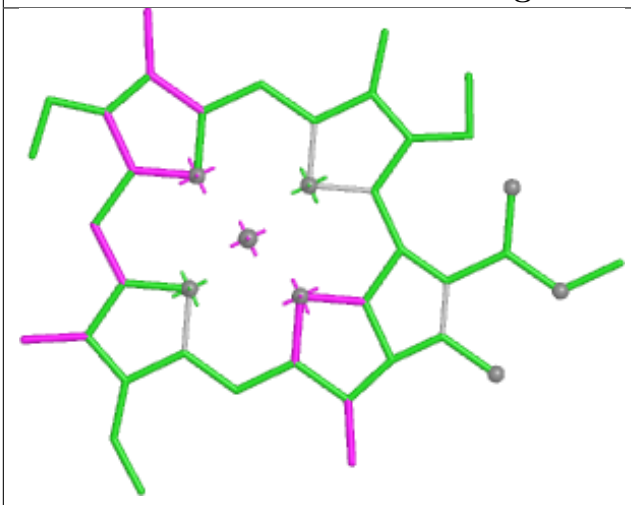


Rings

Ligand CLA JN 101



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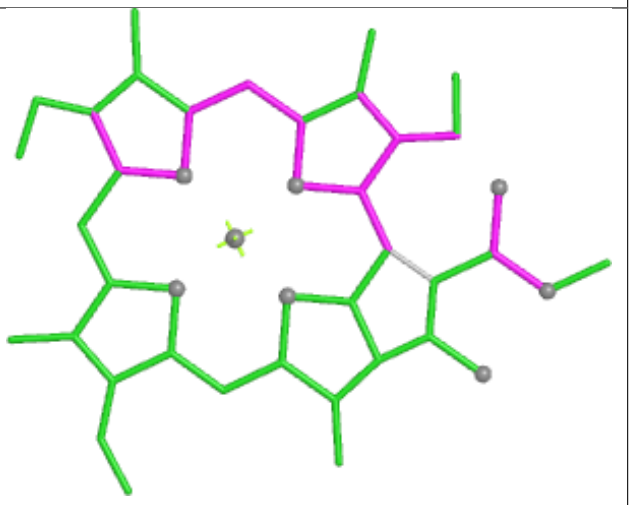

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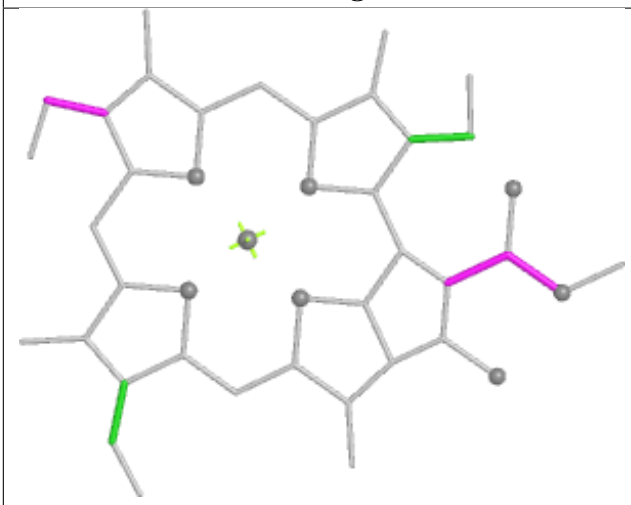


Torsions

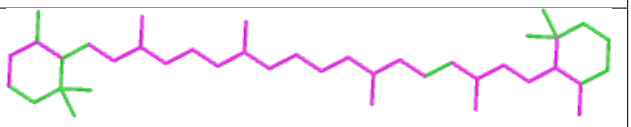


Rings

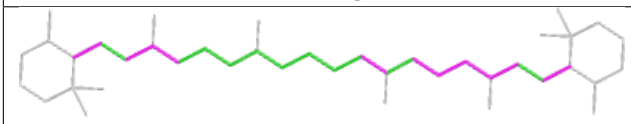
Ligand BCR AN 848



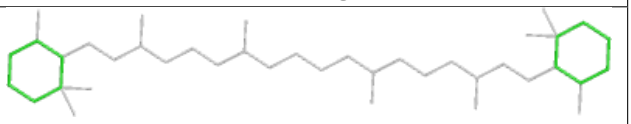
Bond lengths



Bond angles

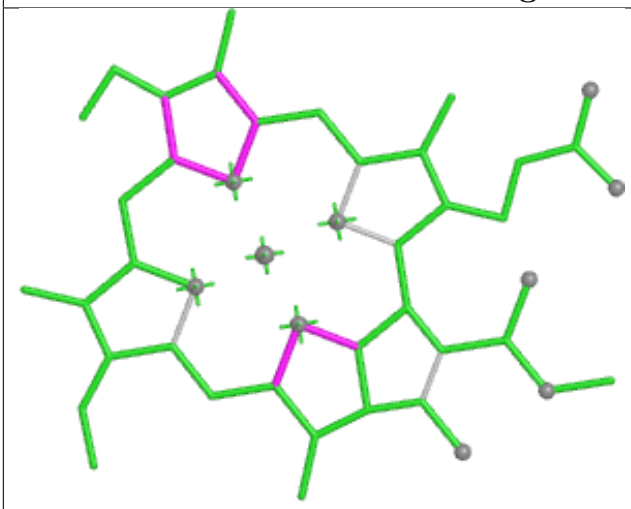


Torsions



Rings

Ligand CLA 32 303



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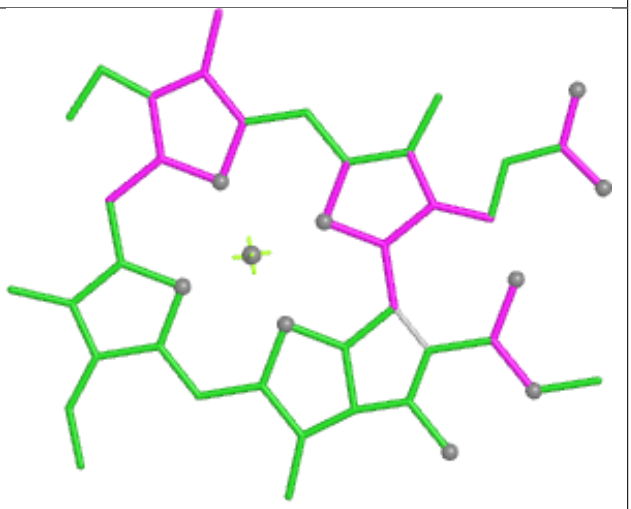

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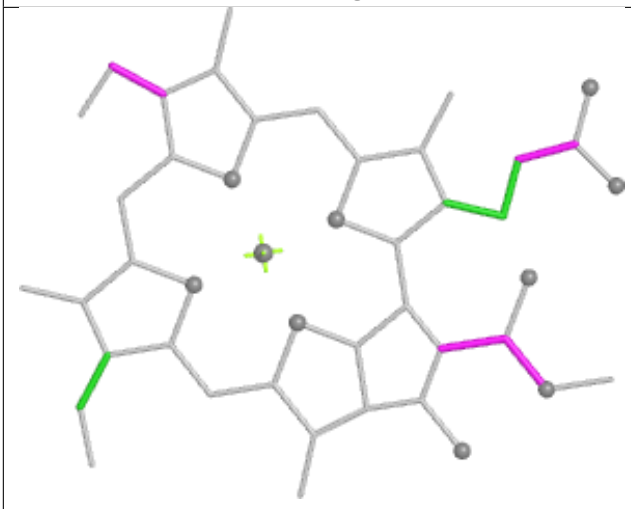
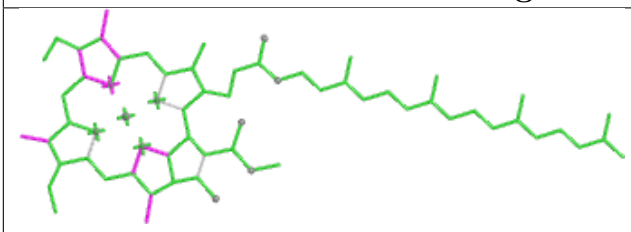


Torsions



Rings

Ligand CLA C6 520



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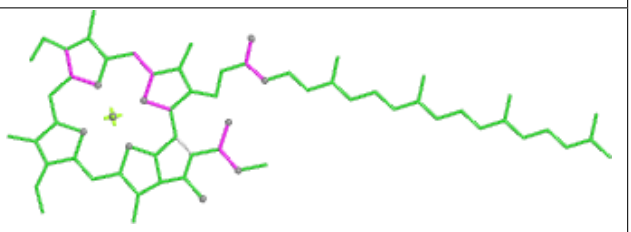

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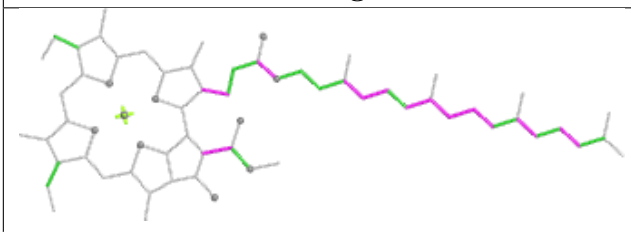

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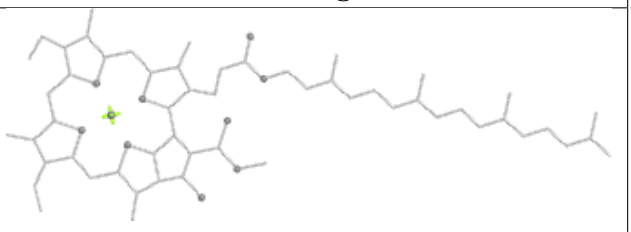
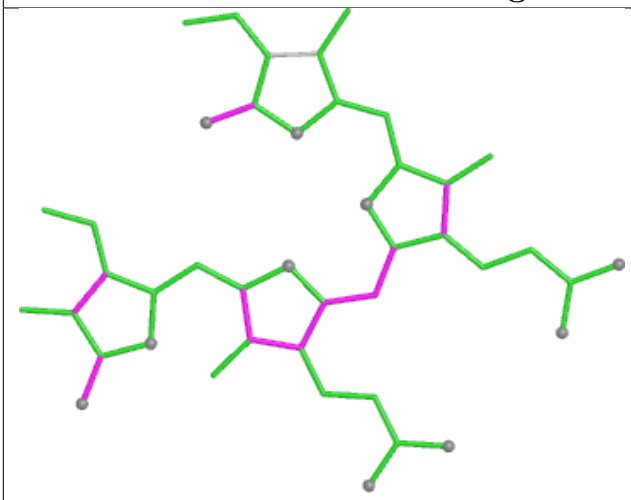


Rings

Ligand PUB AD 302



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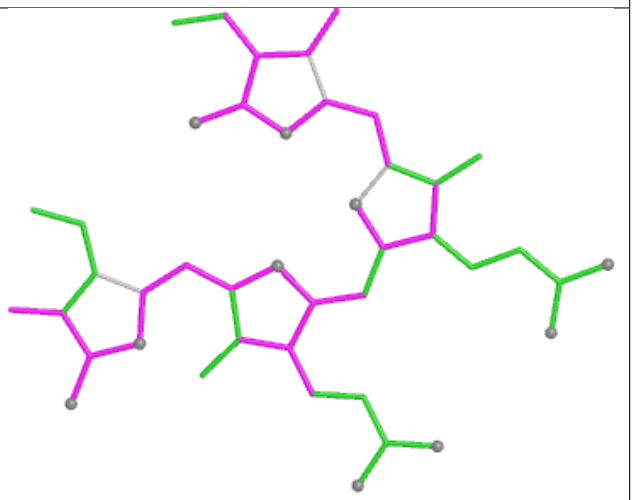

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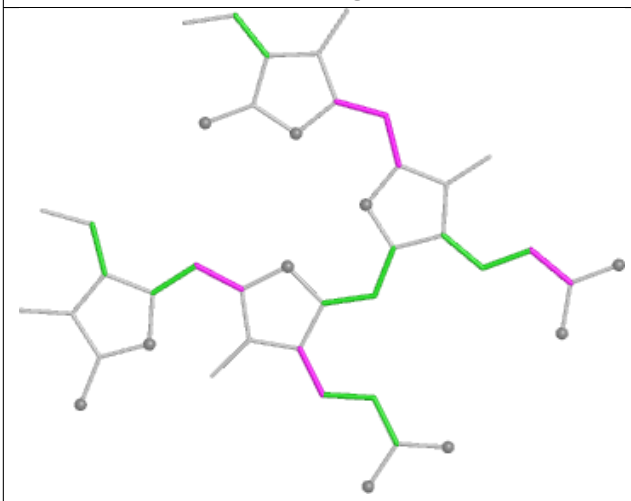

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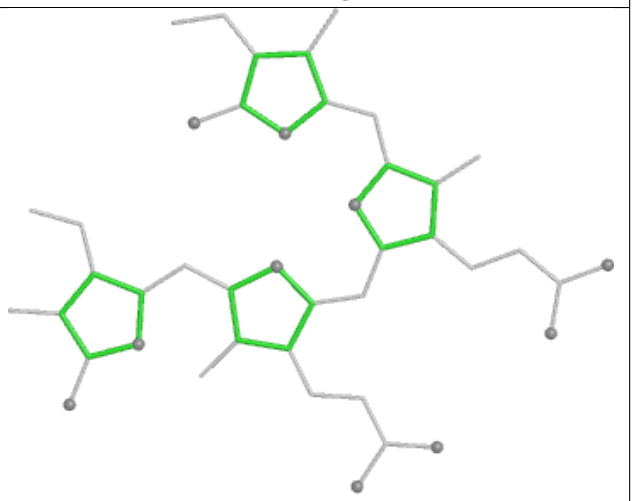
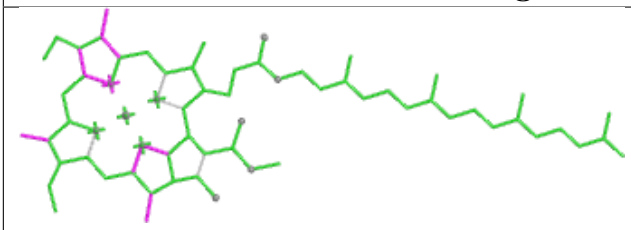


Rings

Ligand CLA K2 101



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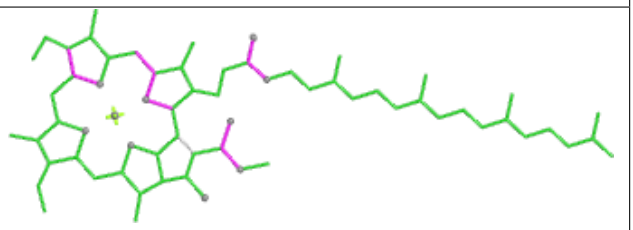

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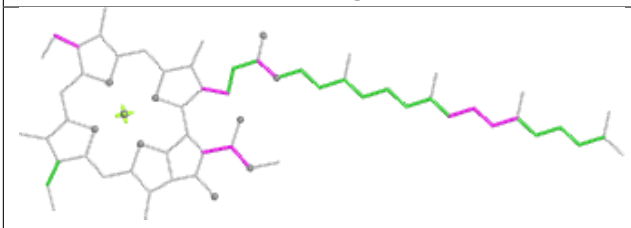

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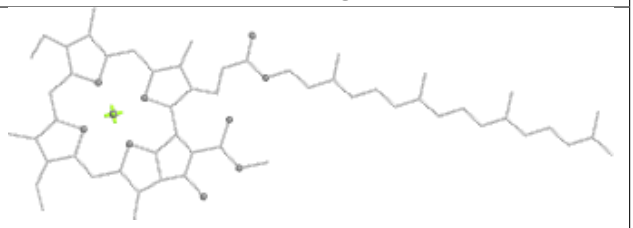
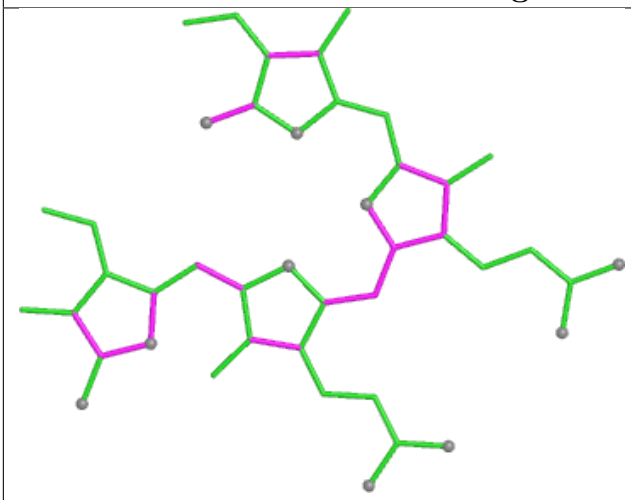


Rings

Ligand PEB AB 501



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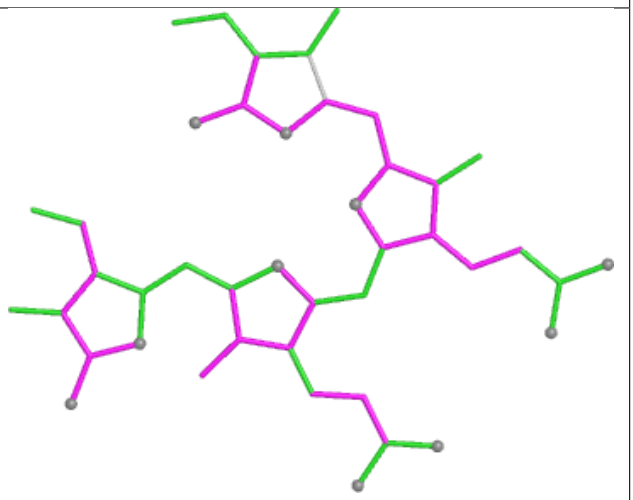

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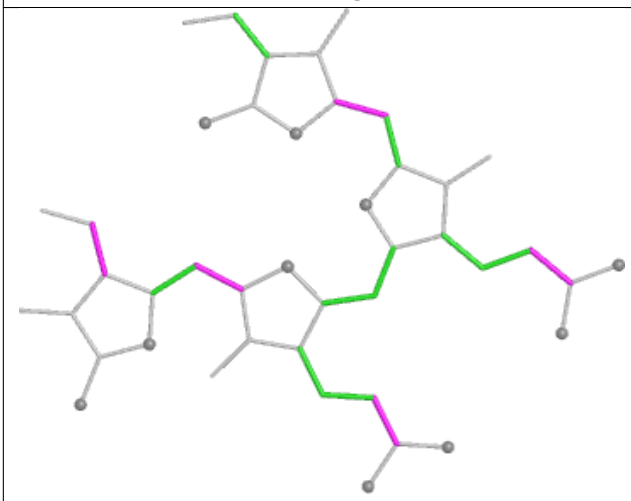

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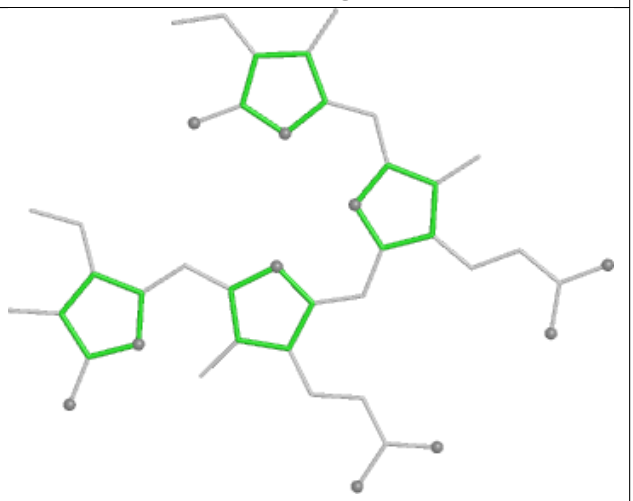
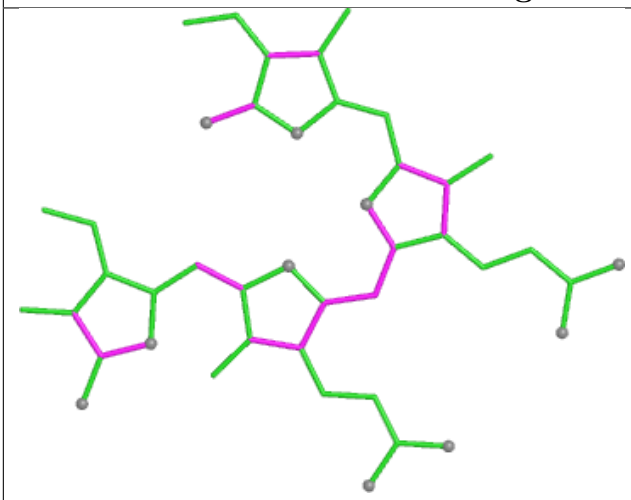


Rings

Ligand PEB JA 203



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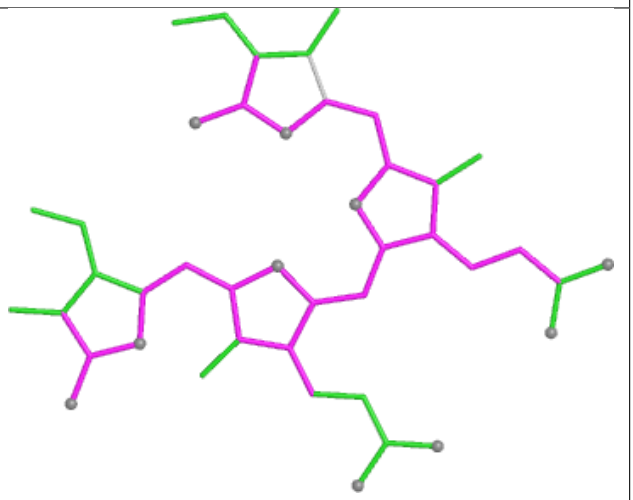

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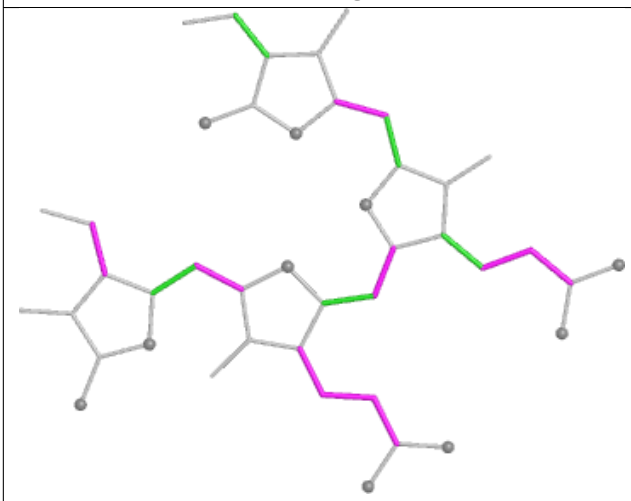

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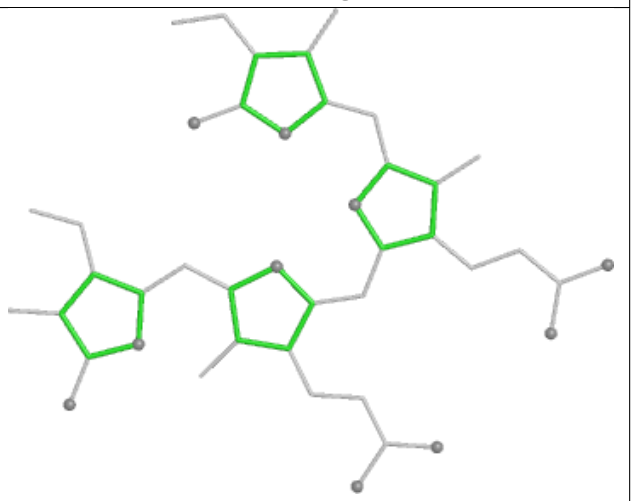
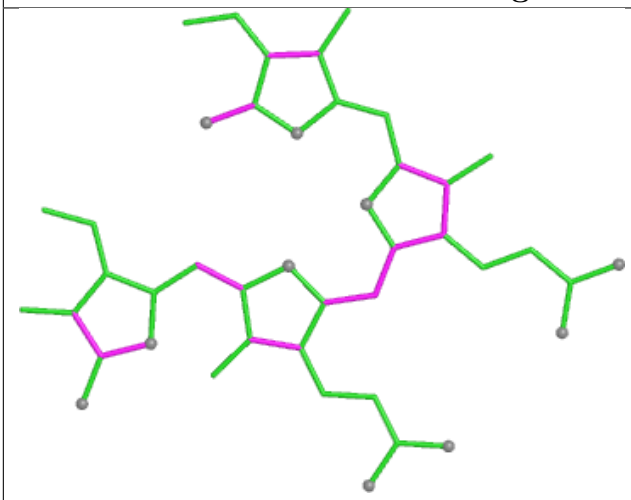


Rings

Ligand PEB gM 202



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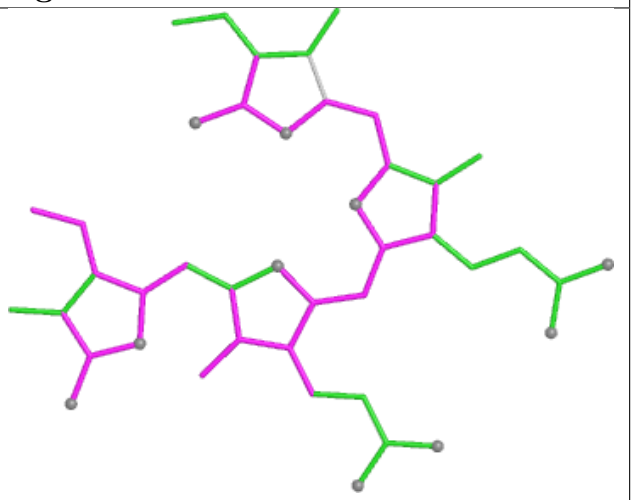

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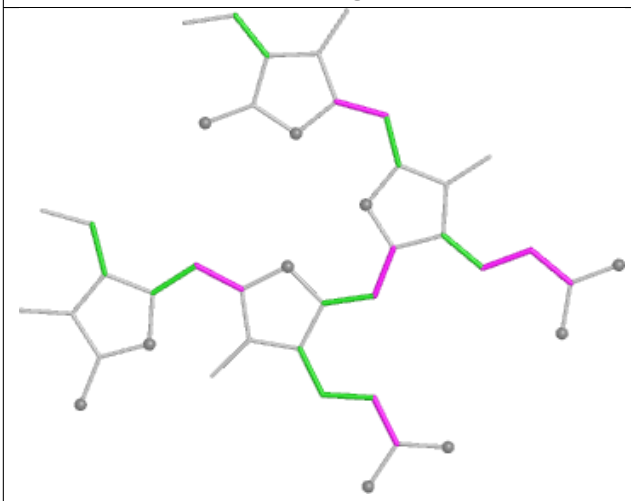

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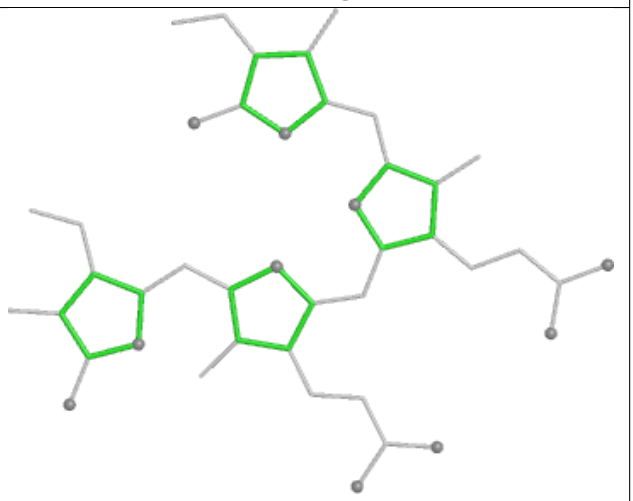
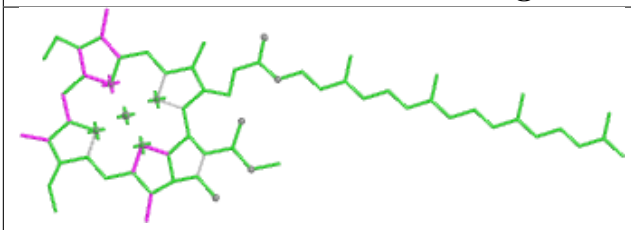


Rings

Ligand CLA B6 613



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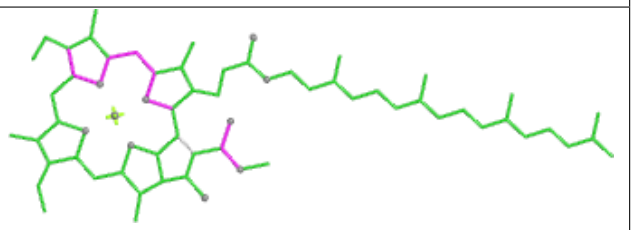

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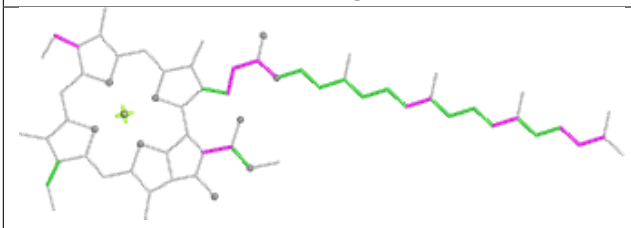

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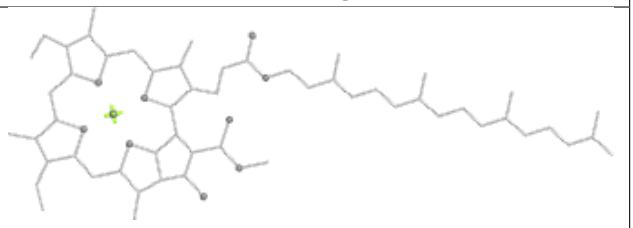
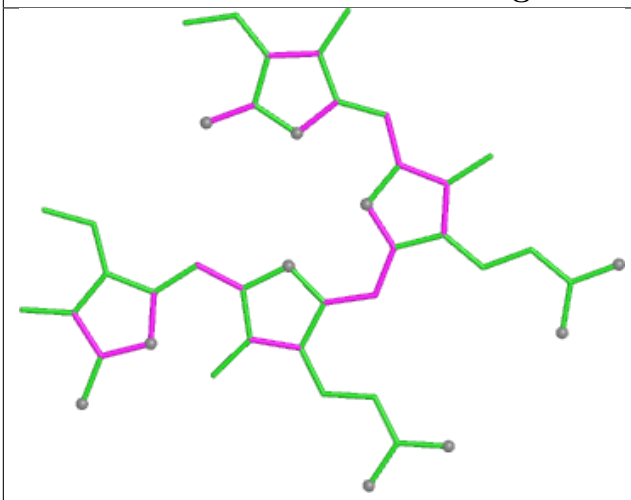


Rings

Ligand PEB eM 201



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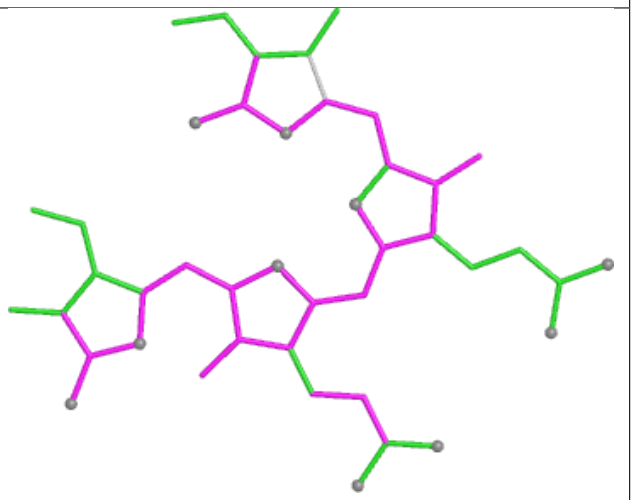

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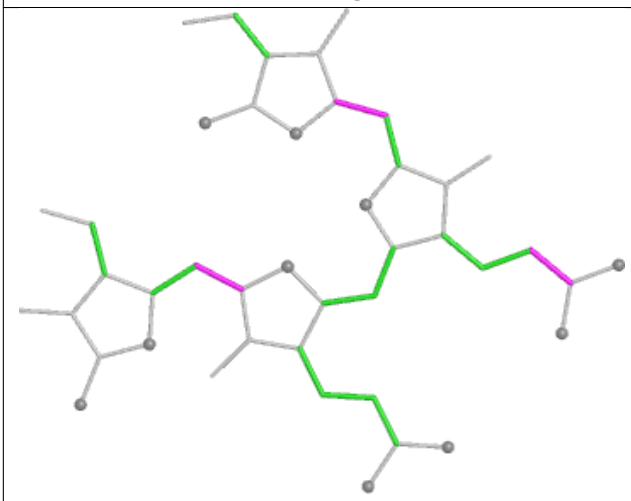

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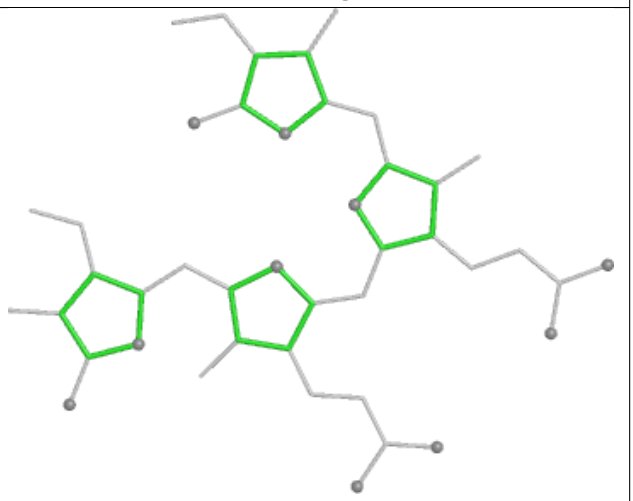

Rings

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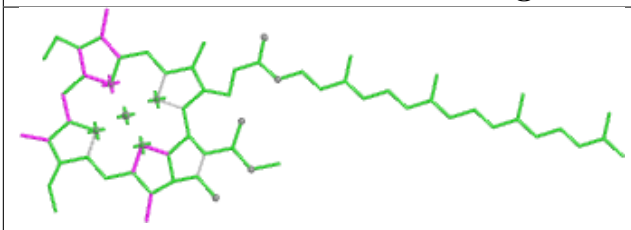

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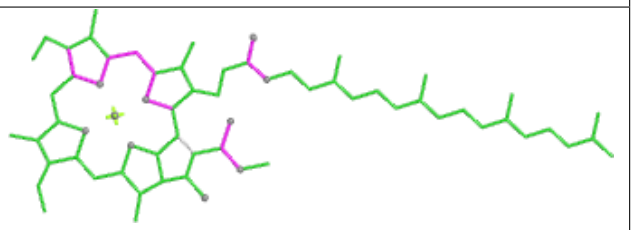

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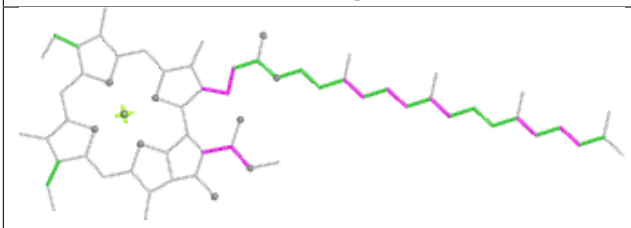

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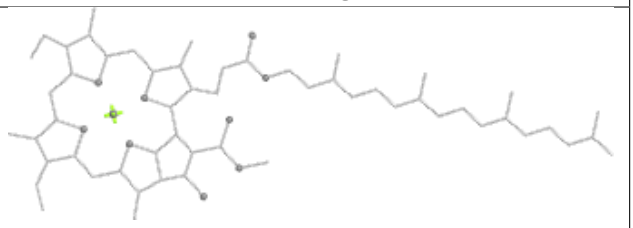
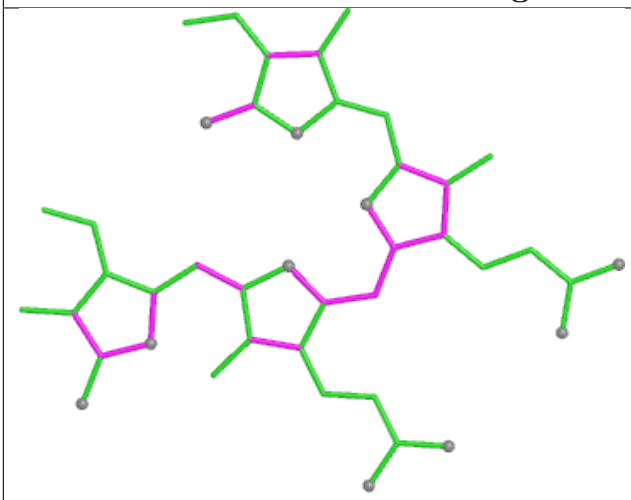


Rings

Ligand PEB YB 201



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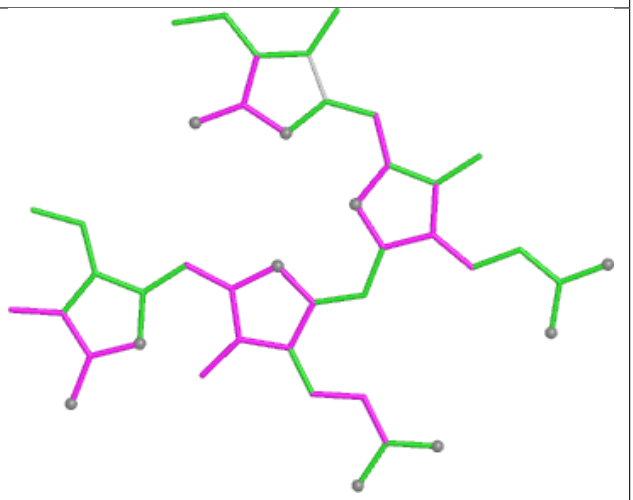

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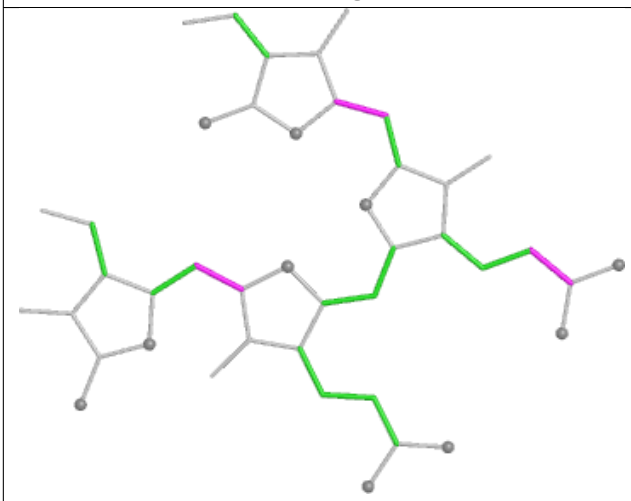

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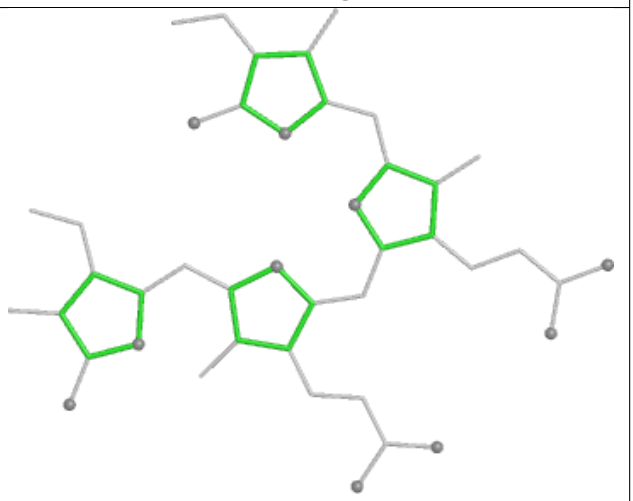
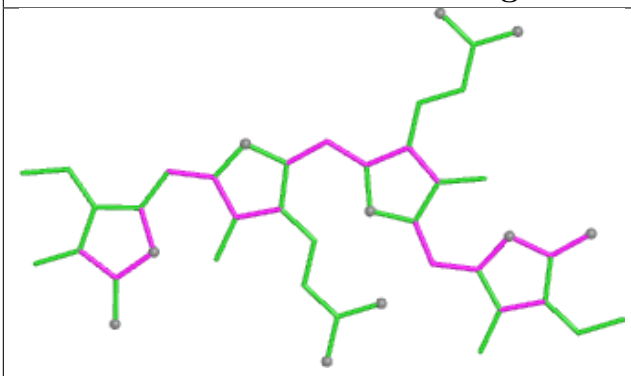


Rings

Ligand CYC DE 1001



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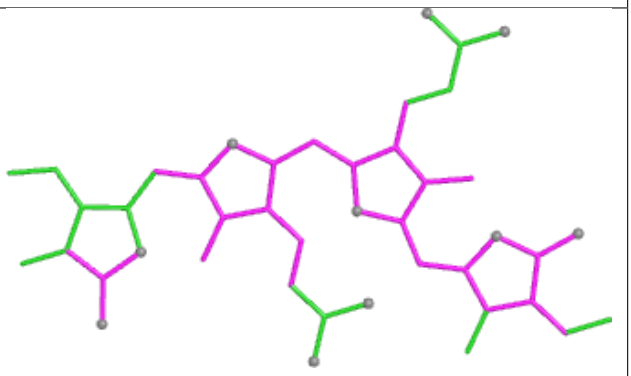
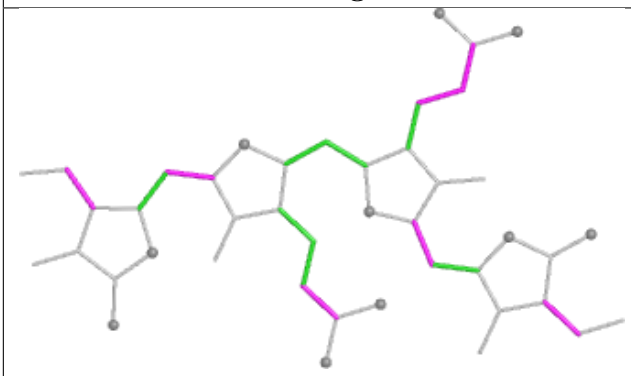


Bond angles



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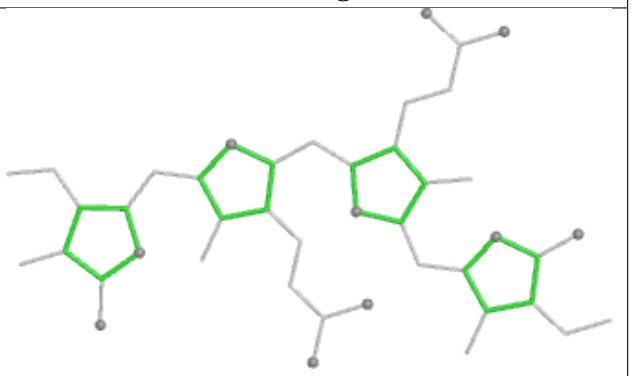
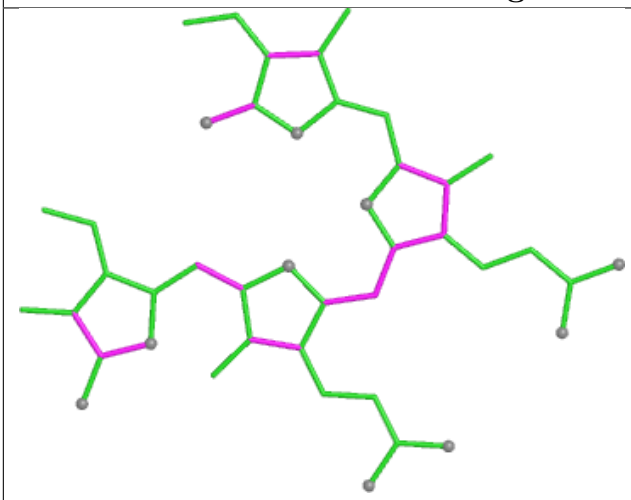


Rings

Ligand PEB QM 202



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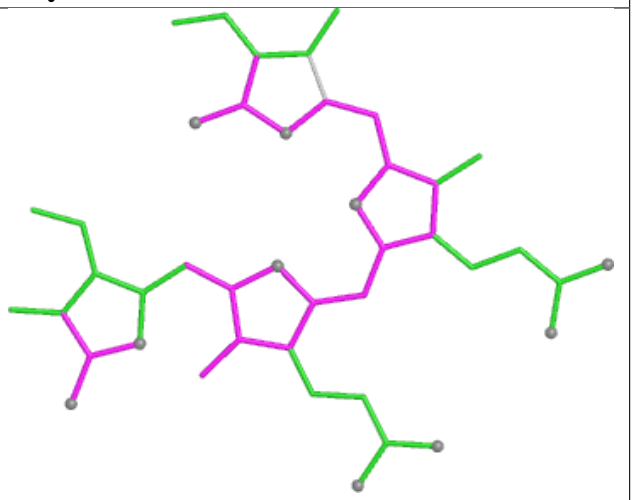

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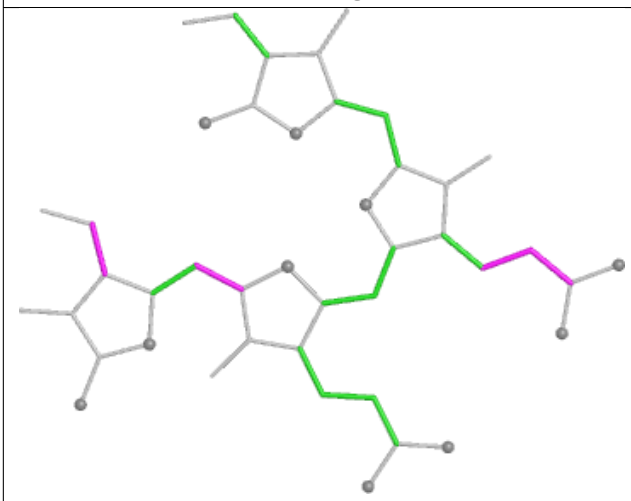

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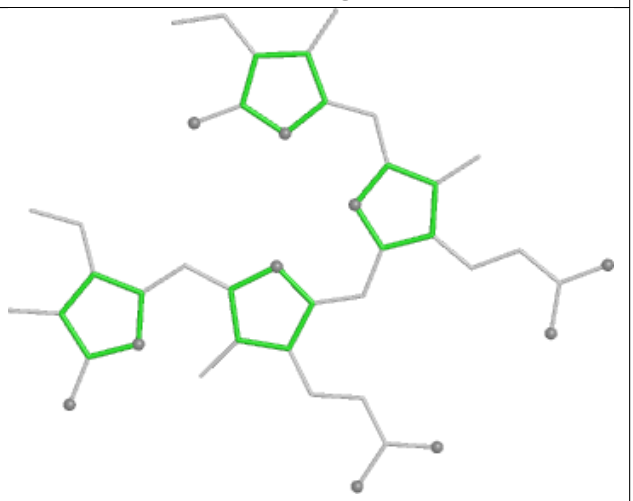
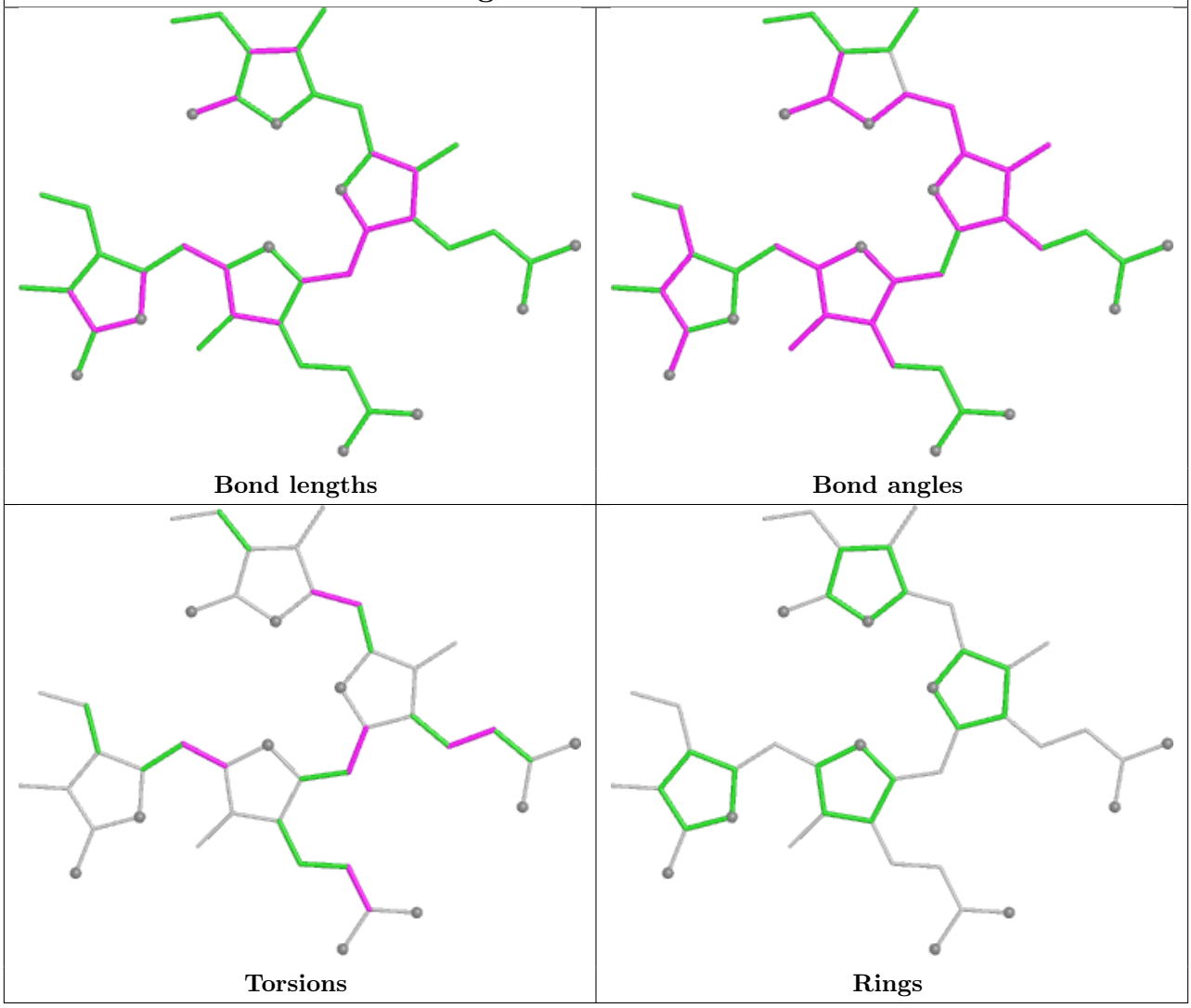
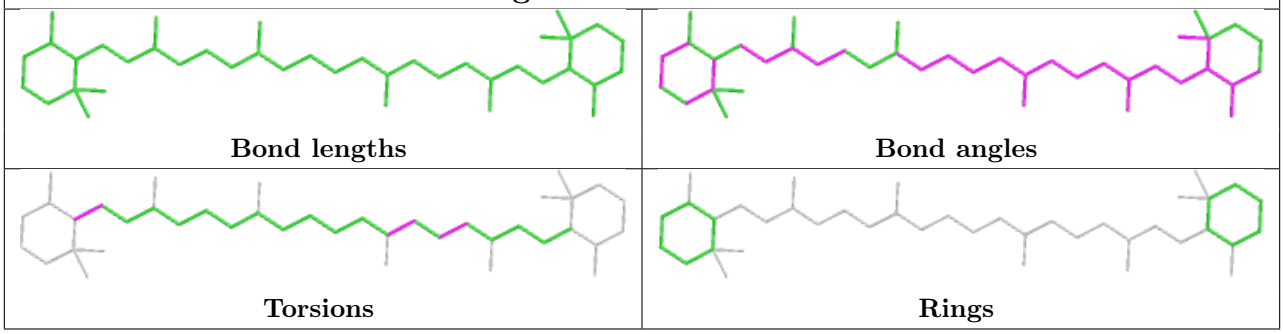


Rings

Ligand PEB m1 201



Ligand BCR CL 502



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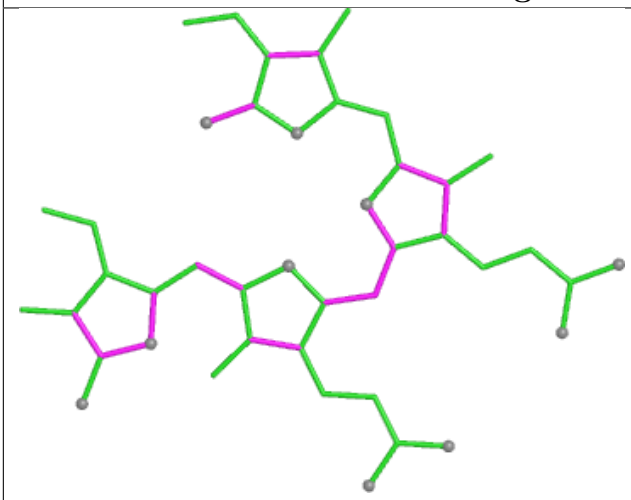
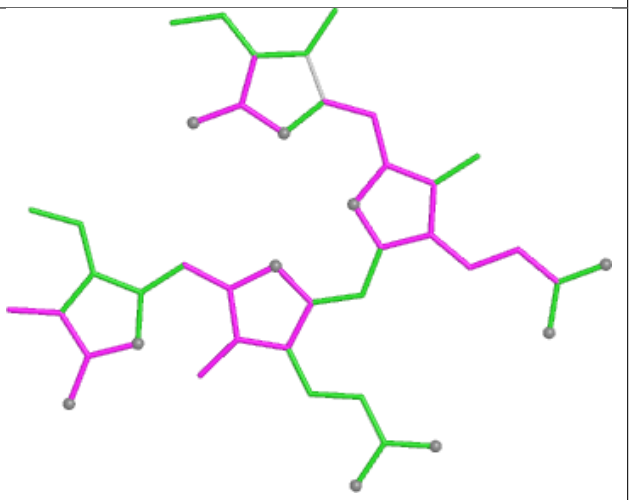
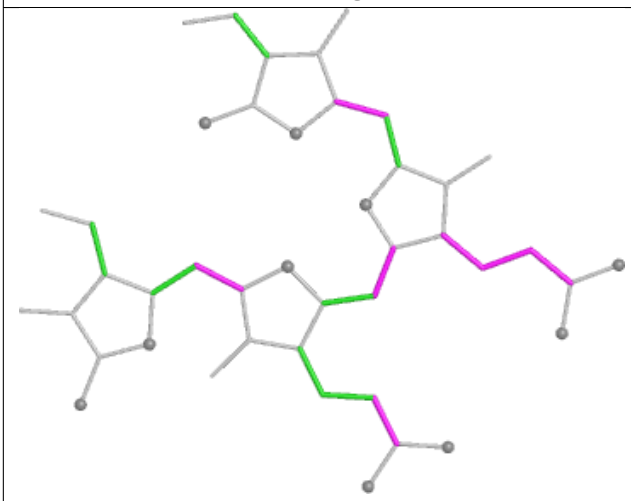


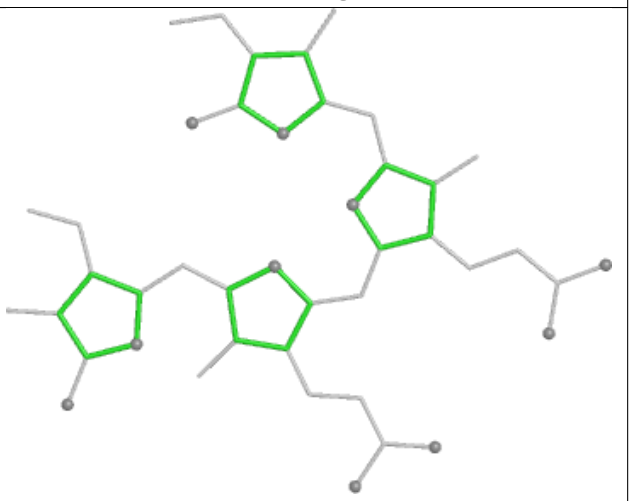
Bond lengths



Bond angles

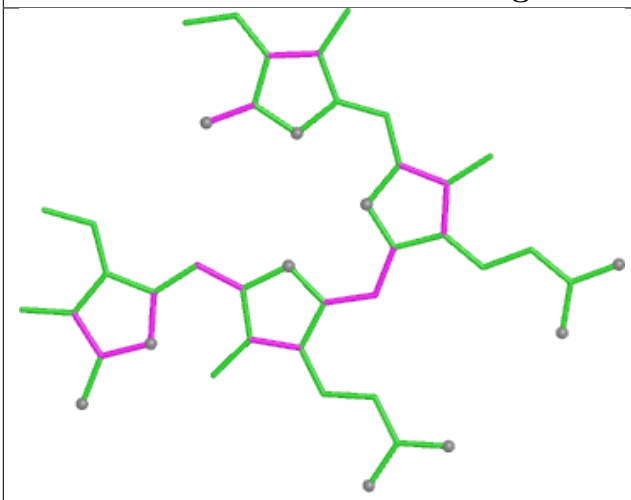


Torsions



Rings

Ligand PEB YP 501



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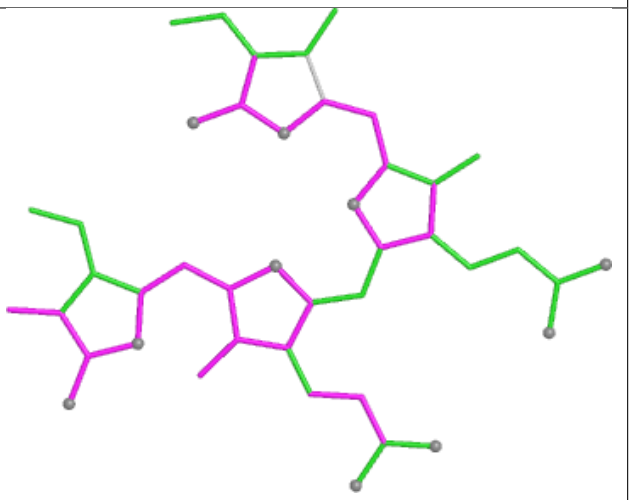
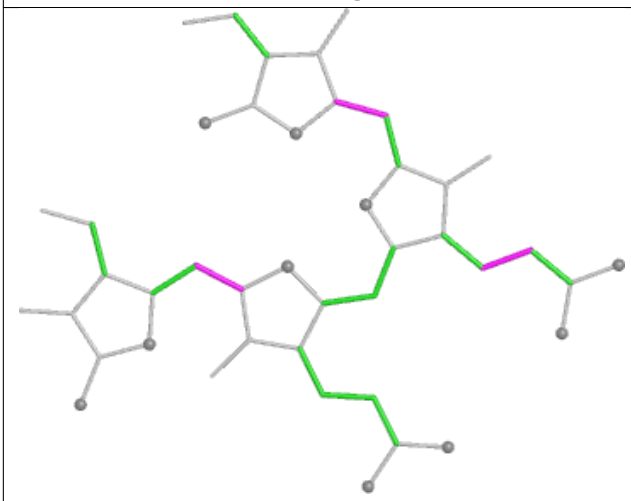


Bond angles



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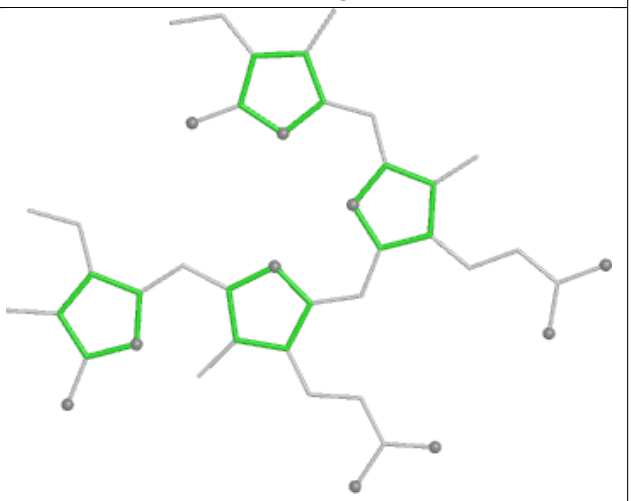
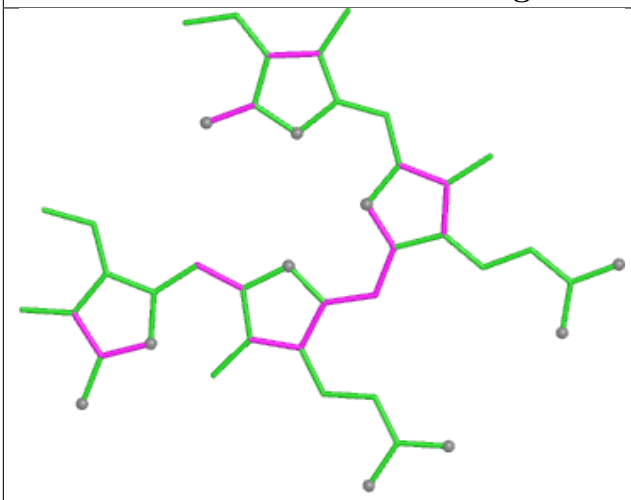


Rings

Ligand PEB LK 201



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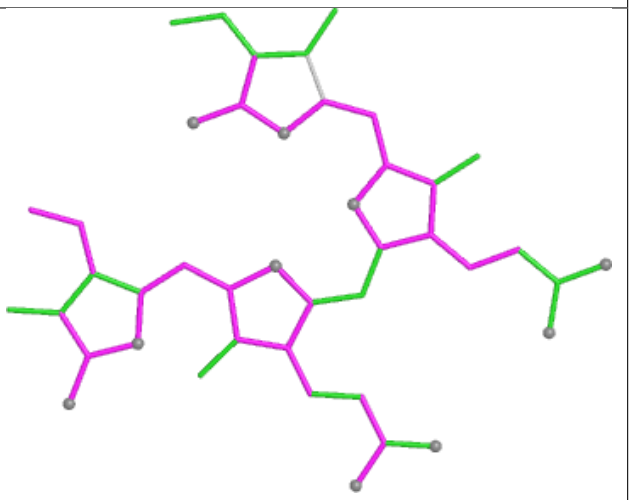

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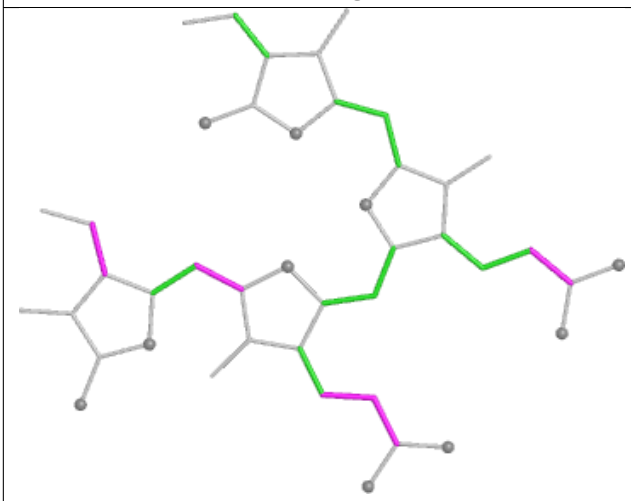

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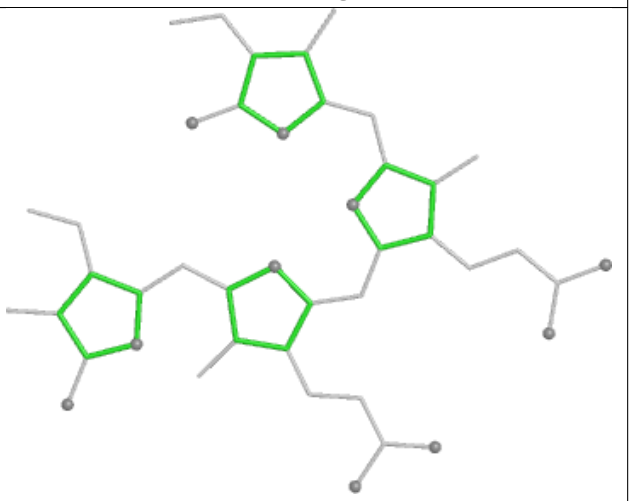
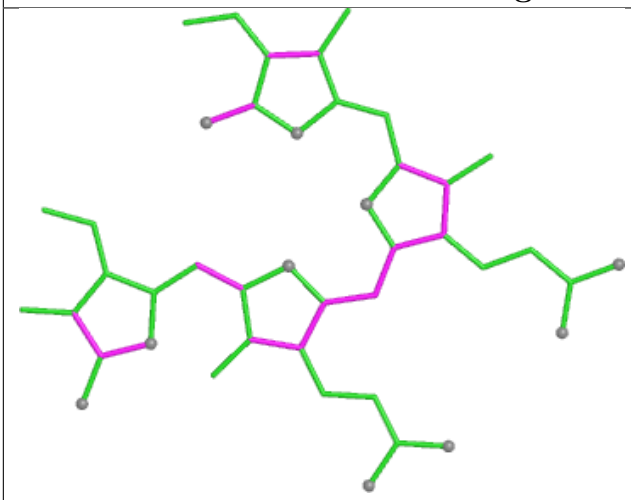


Rings

Ligand PEB H9 202



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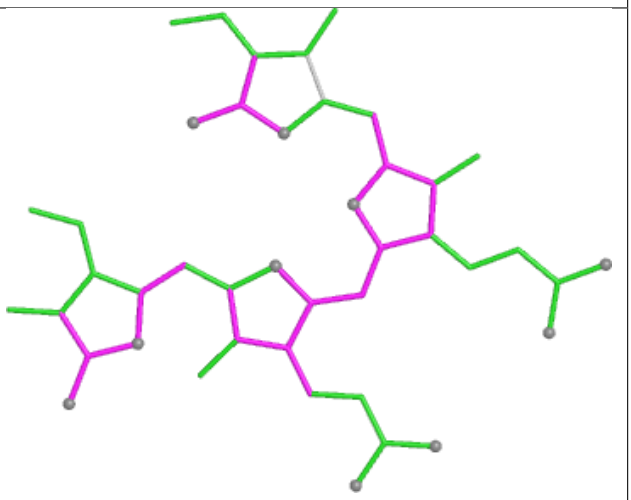

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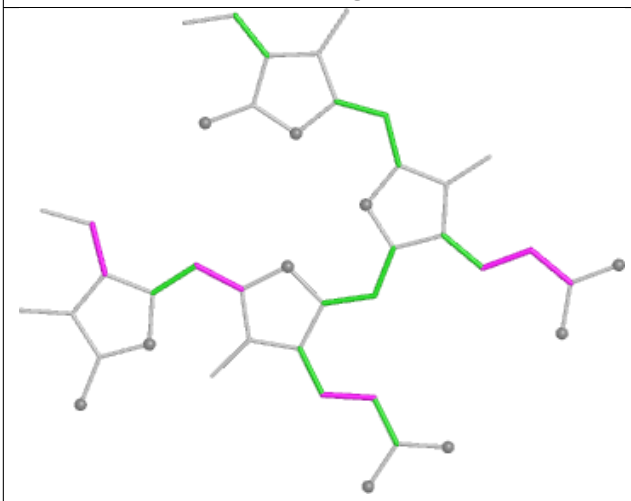

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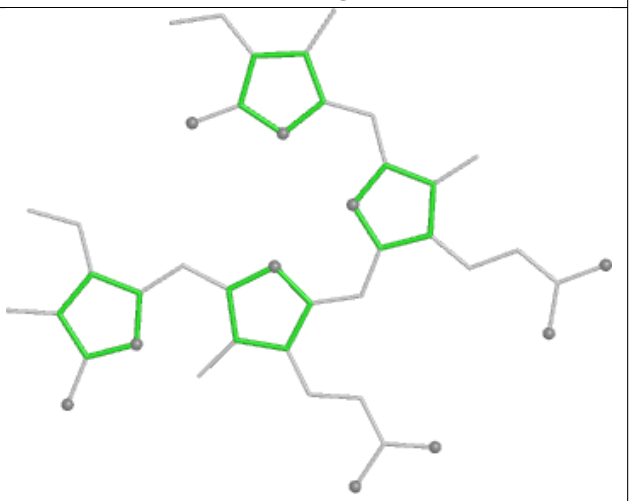
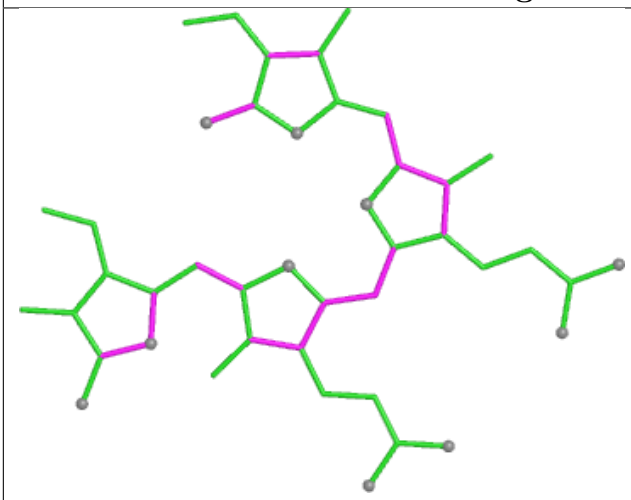


Rings

Ligand PEB cK 201



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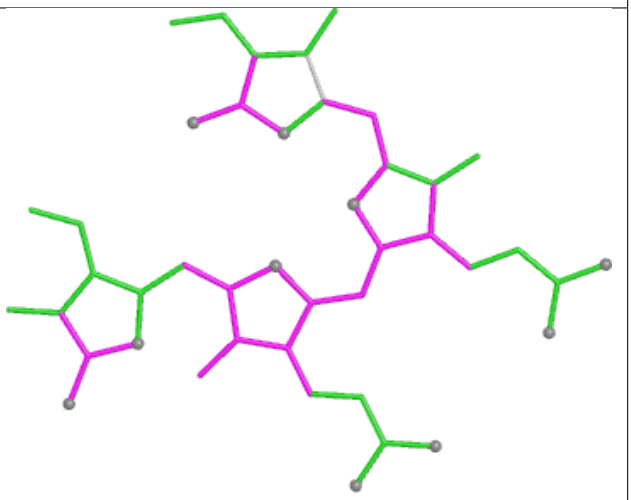

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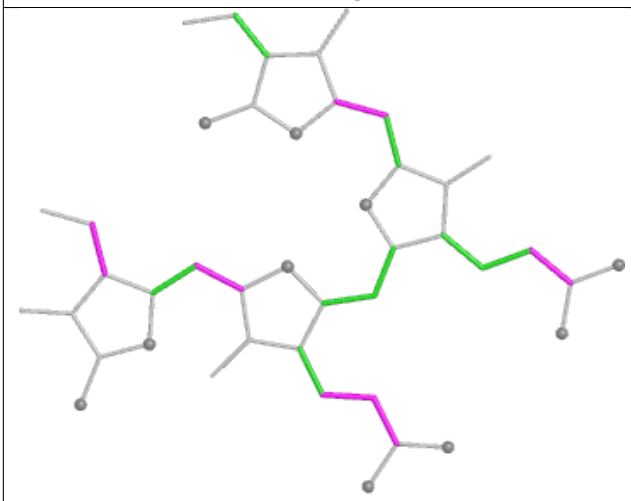

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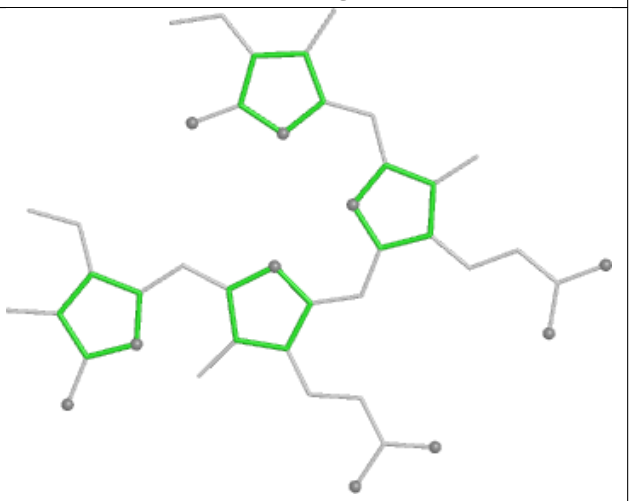
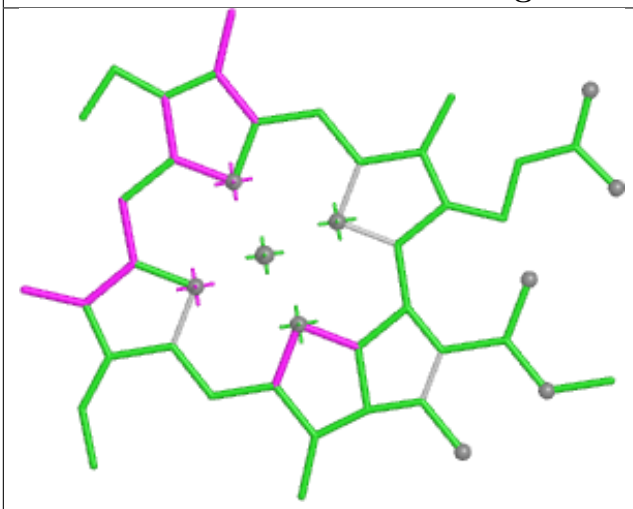


Rings

Ligand CLA O2 203



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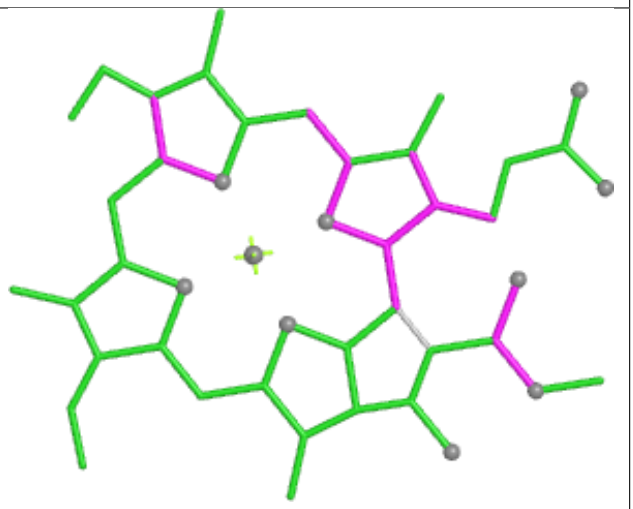

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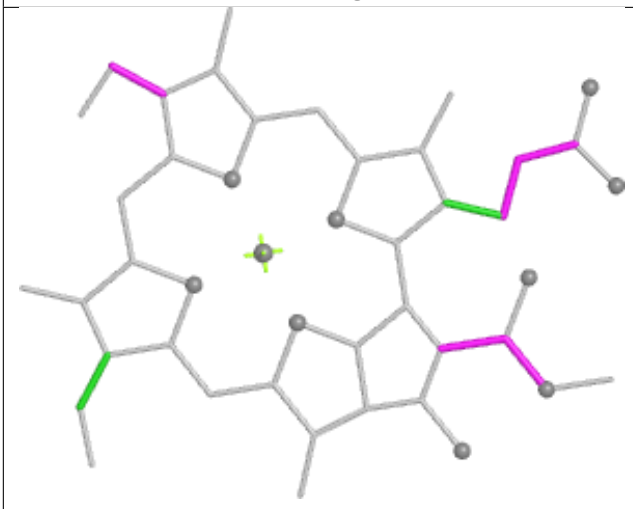
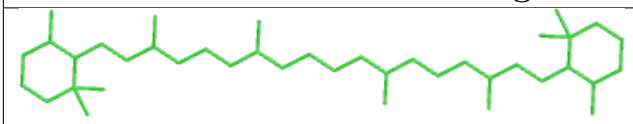


Torsions



Rings

Ligand BCR FL 101



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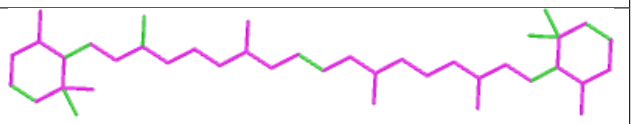

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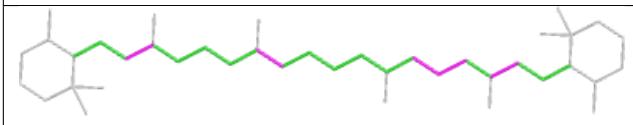

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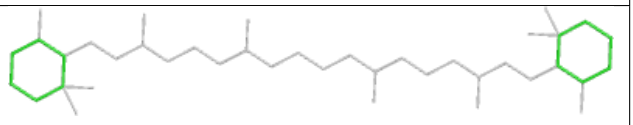
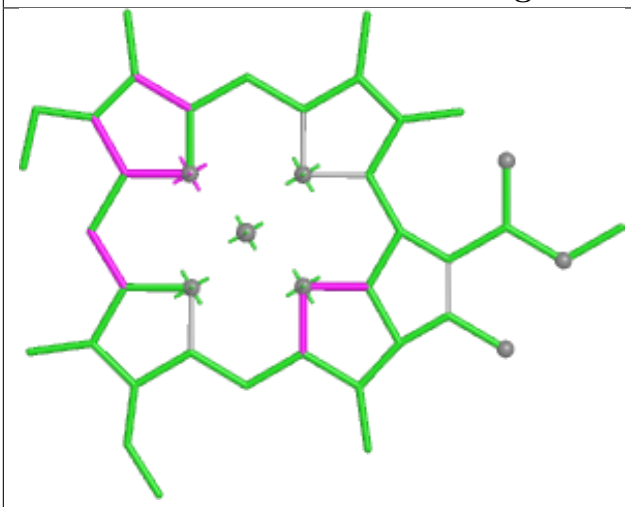


Rings

Ligand CLA 7N 608



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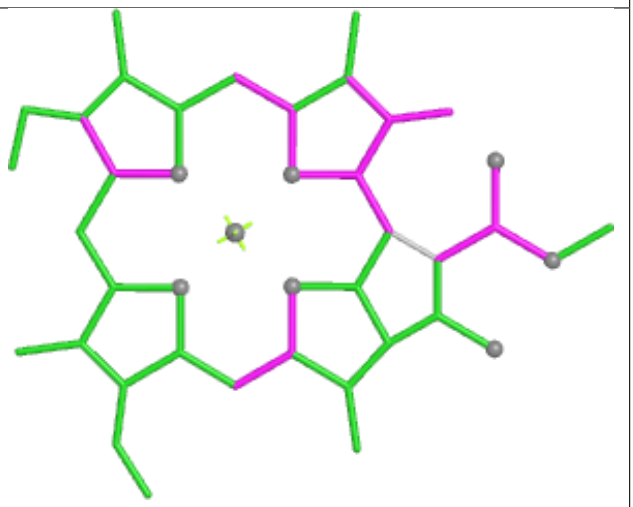
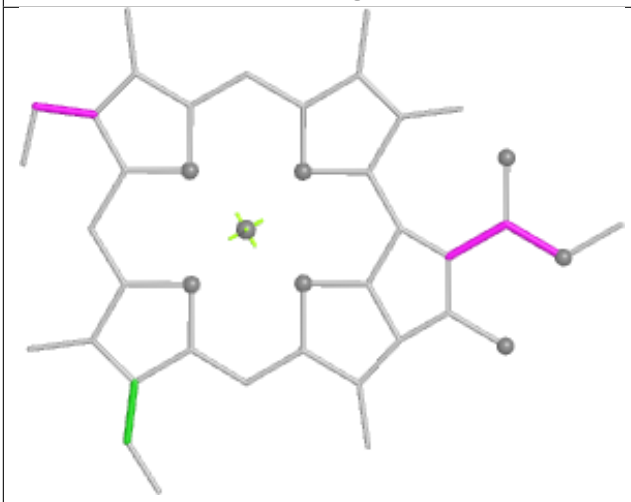


Bond angles



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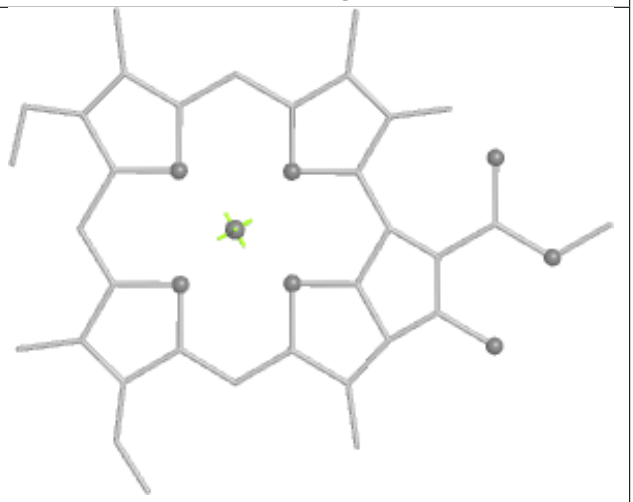
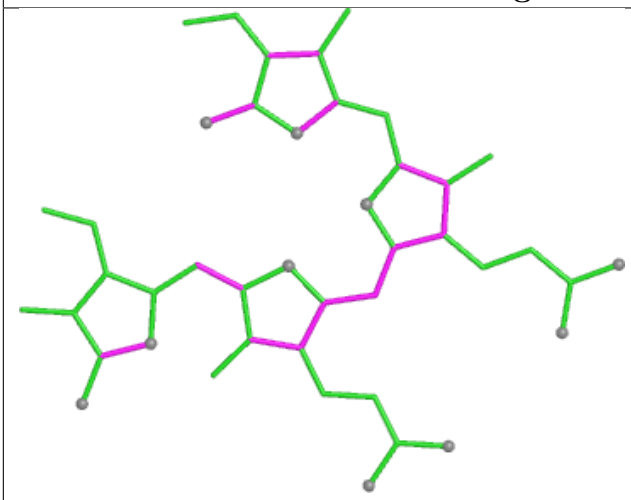


Rings

Ligand PEB dH 201



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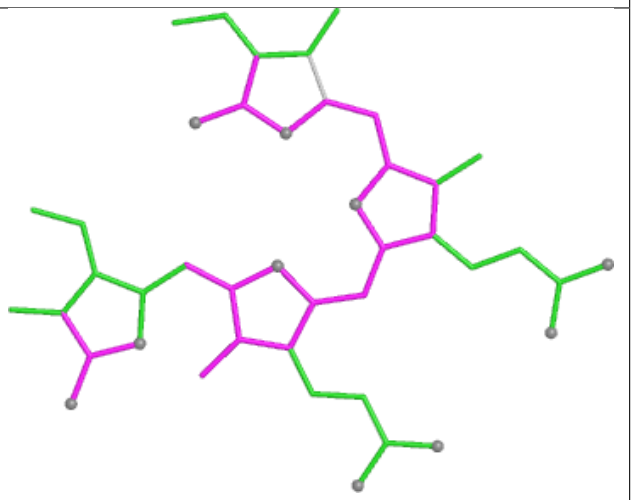

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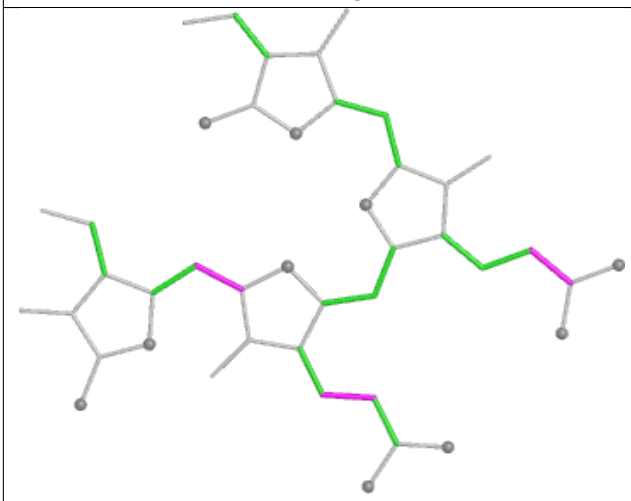

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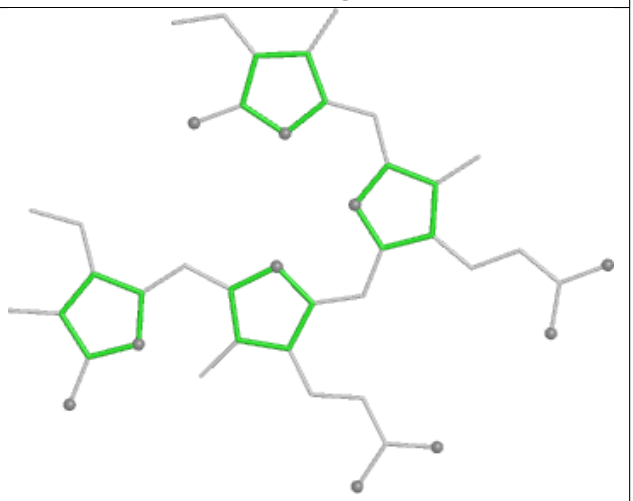
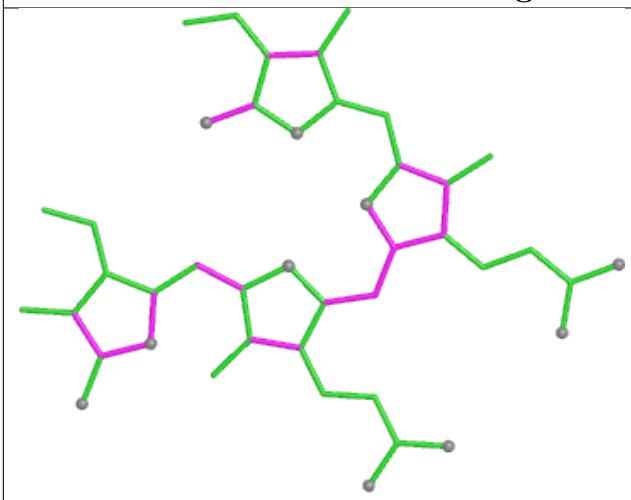


Rings

Ligand PEB bP 501



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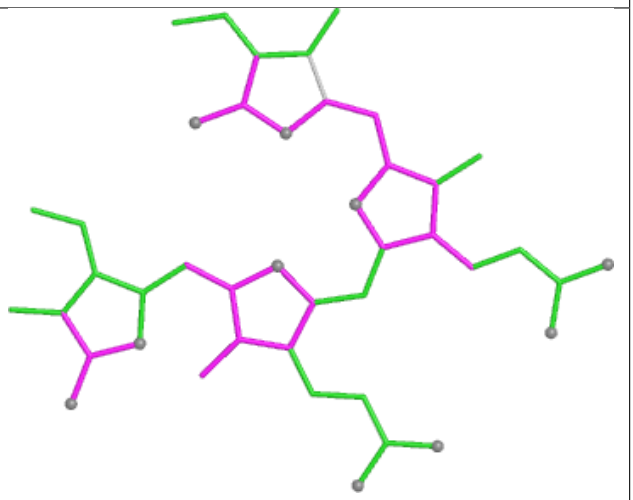

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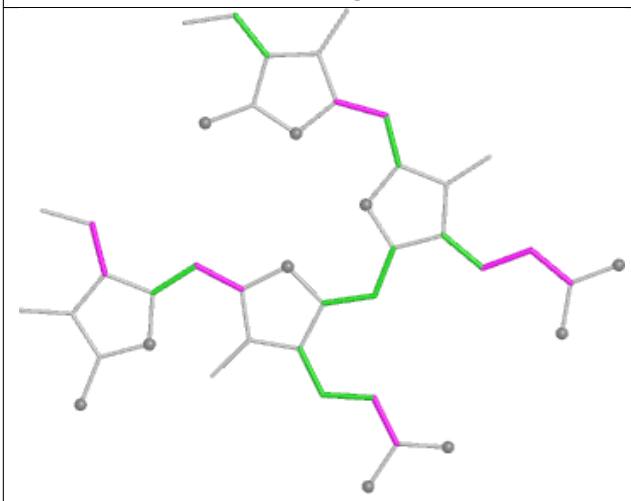

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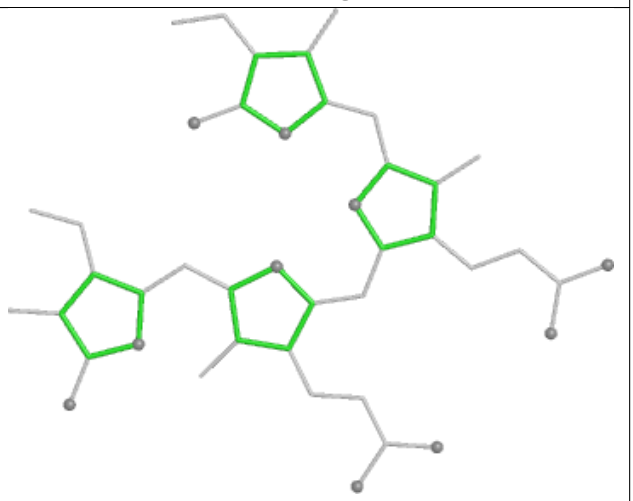
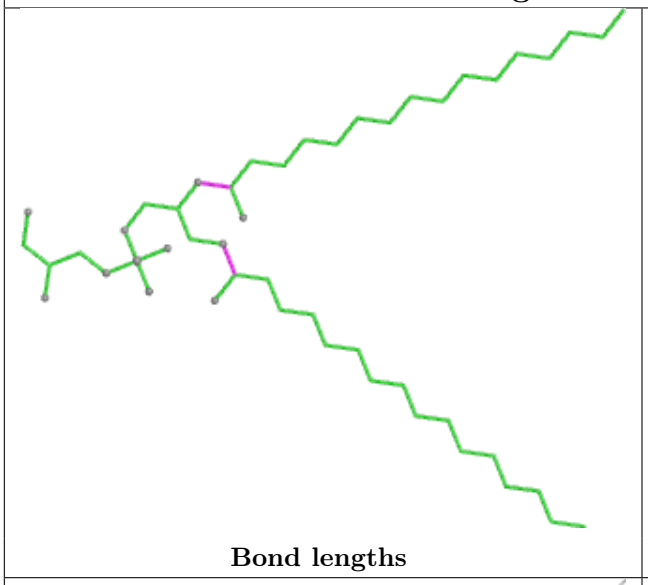


Rings

Ligand LHG AL 406



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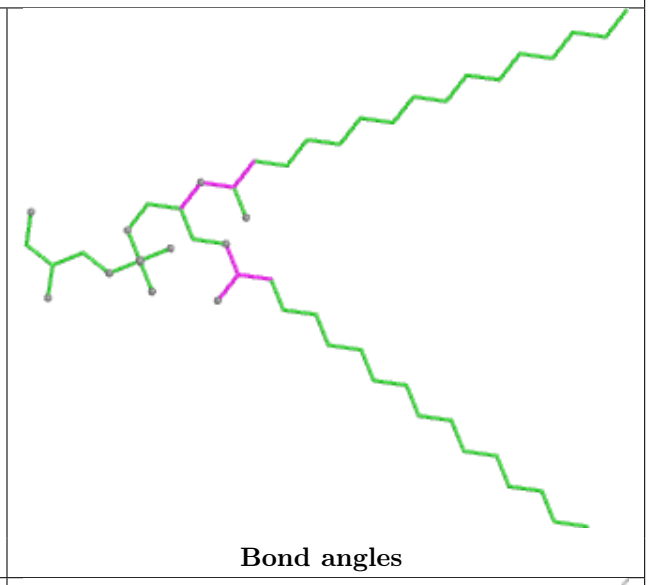
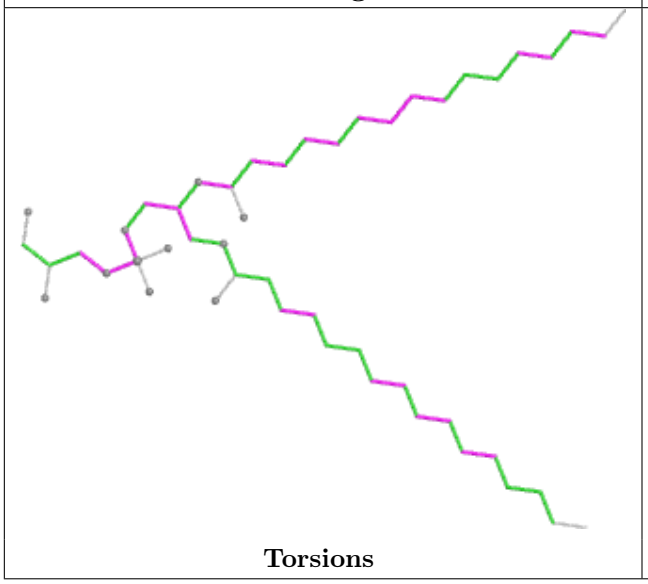


Bond angles



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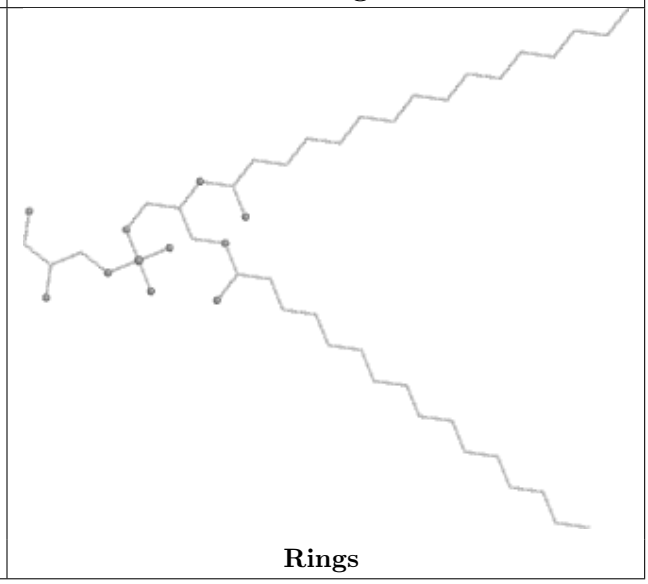
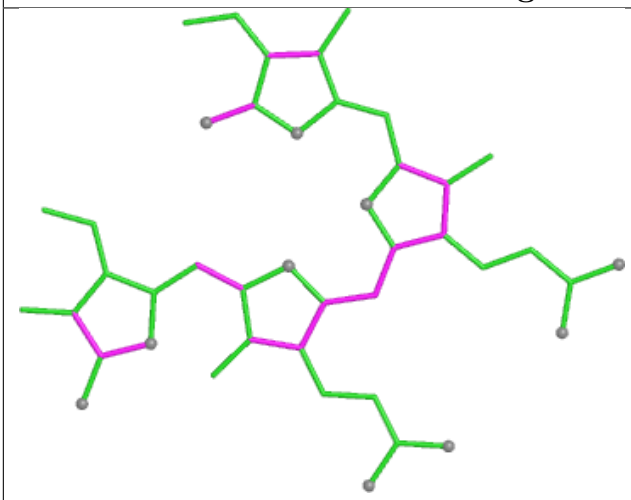


Rings

Ligand PEB F7 202



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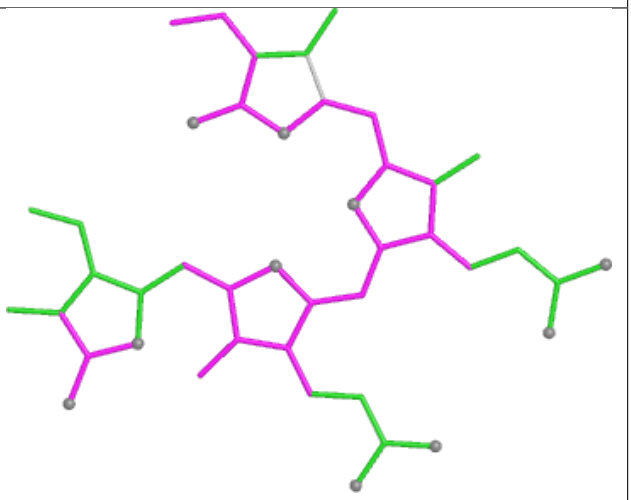
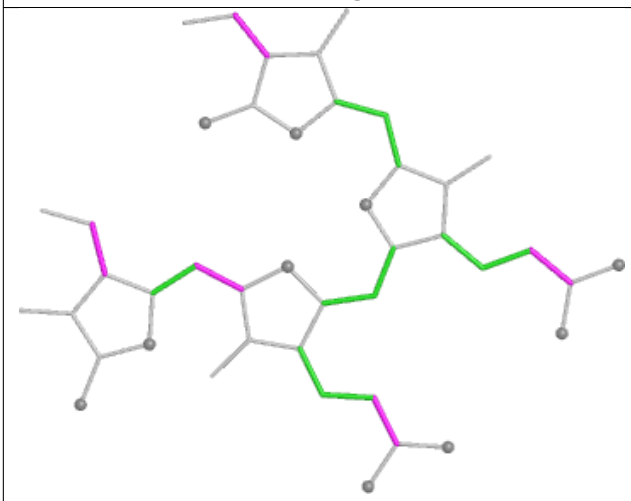


Bond angles



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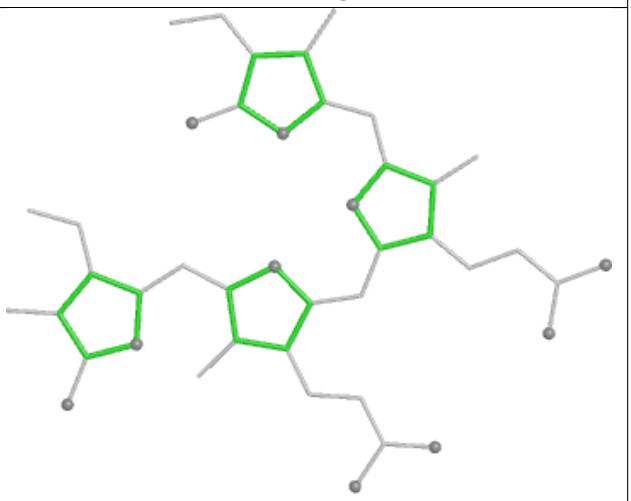
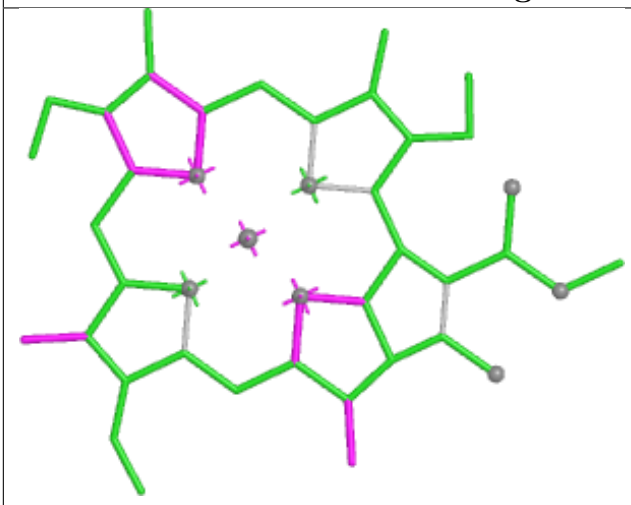


Rings

Ligand CLA K2 104



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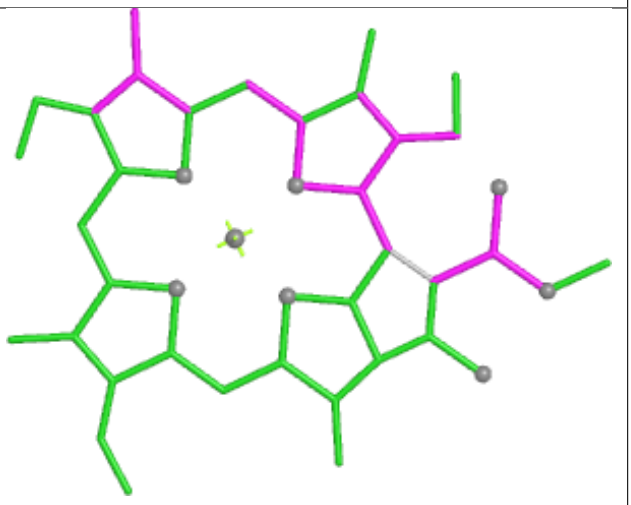
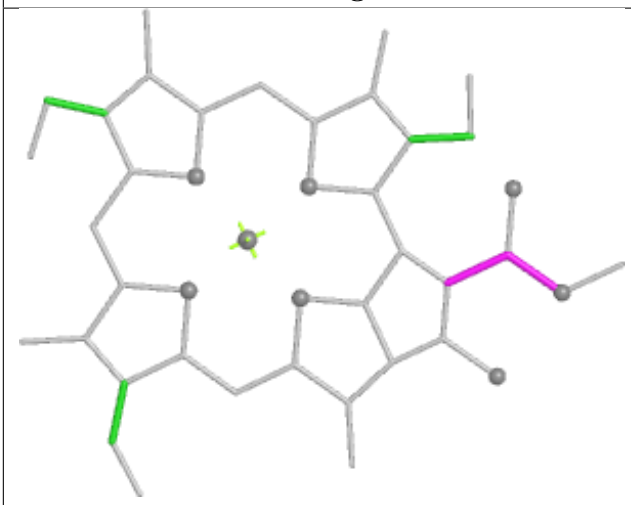


Bond angles

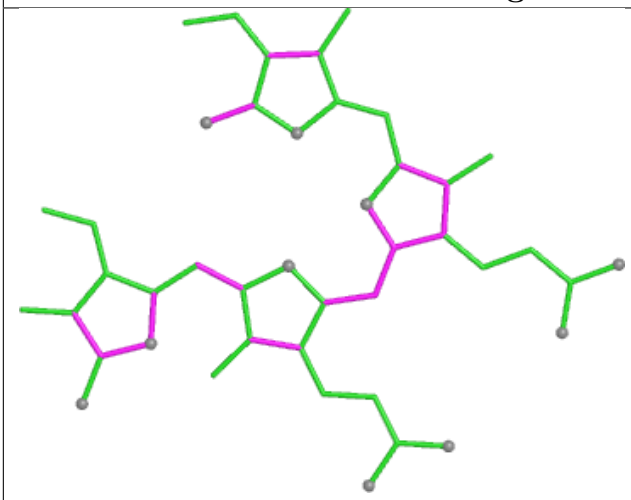


Torsions



Rings

Ligand PEB VM 202



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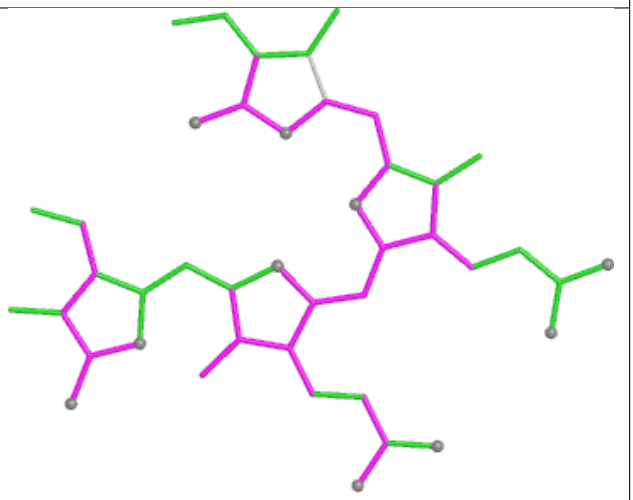
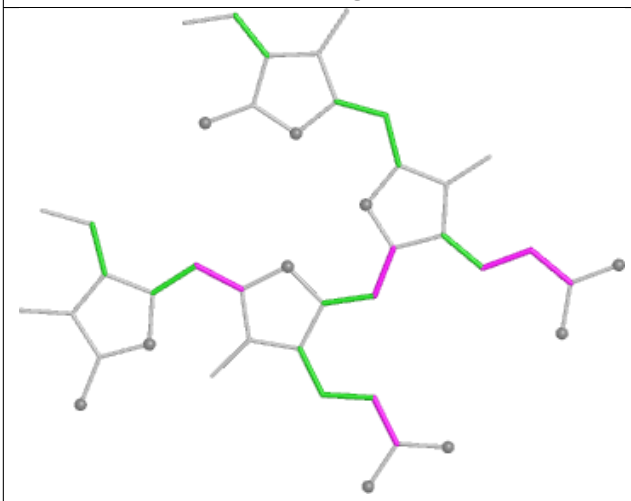


Bond angles



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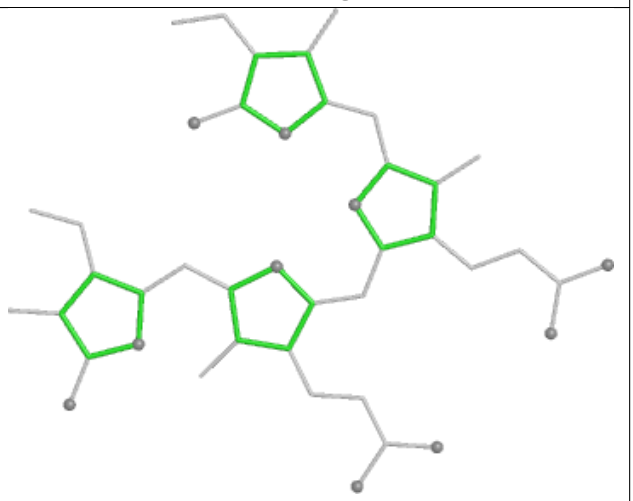

Rings

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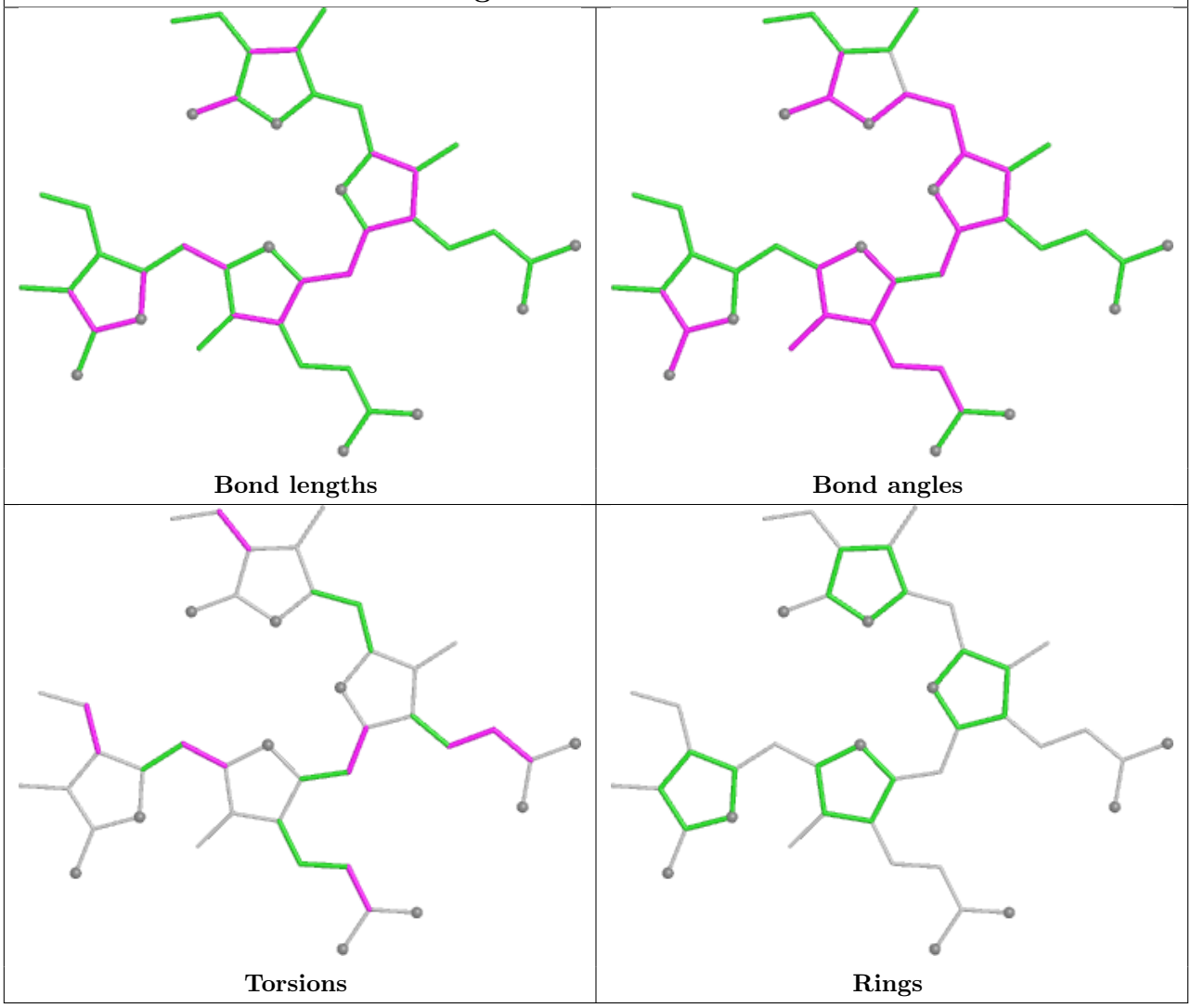
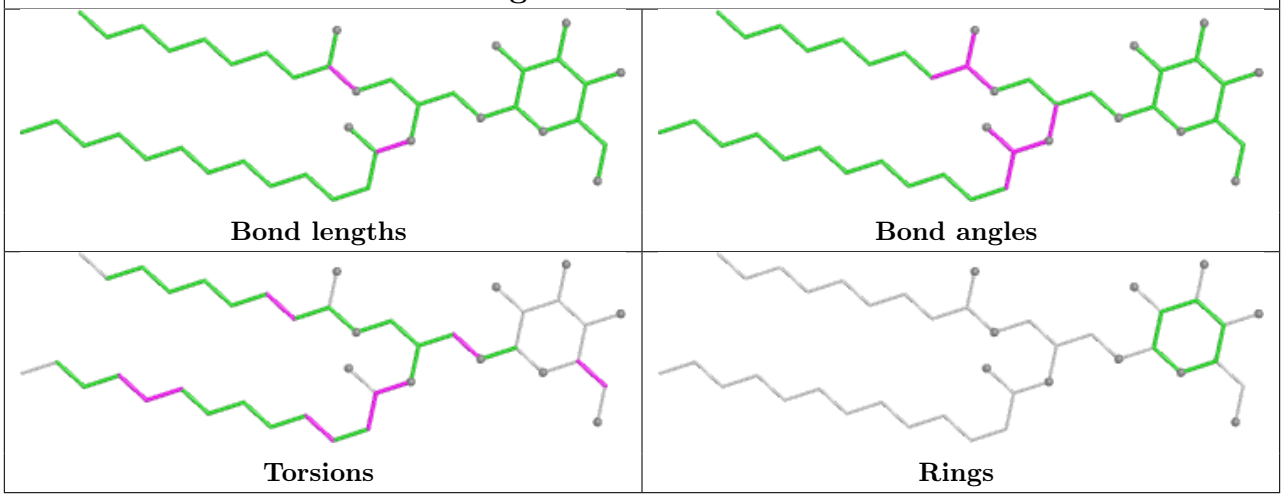
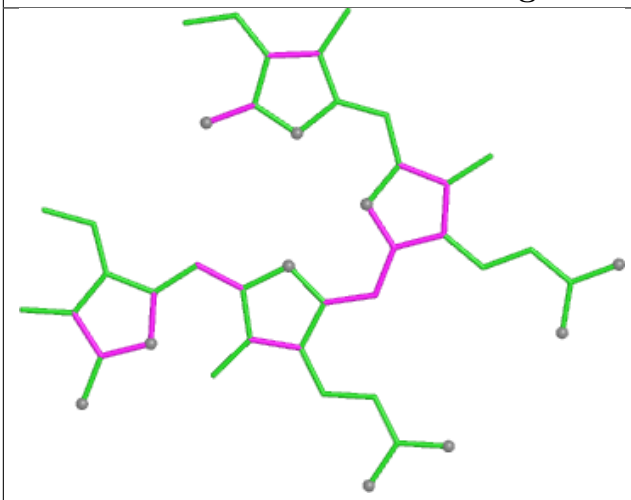


Ligand LMG m6 103



Ligand PEB S5 203



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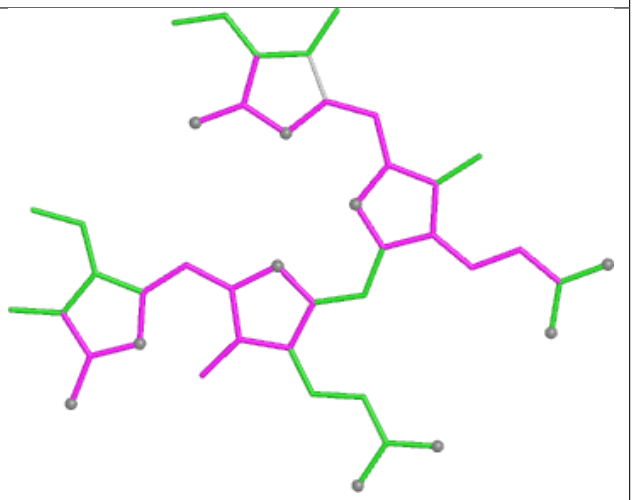
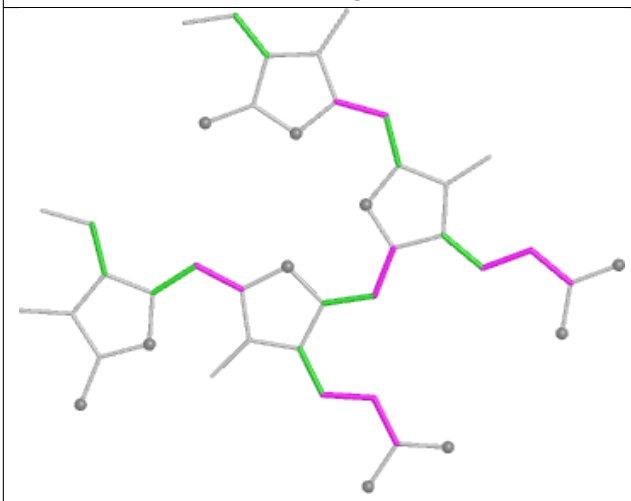


Bond angles



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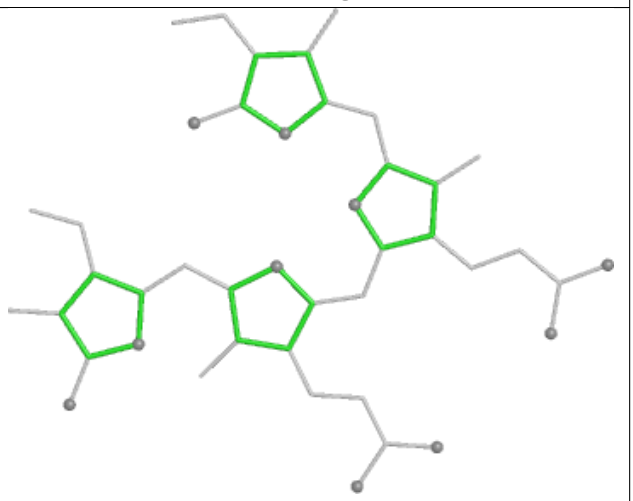

Rings

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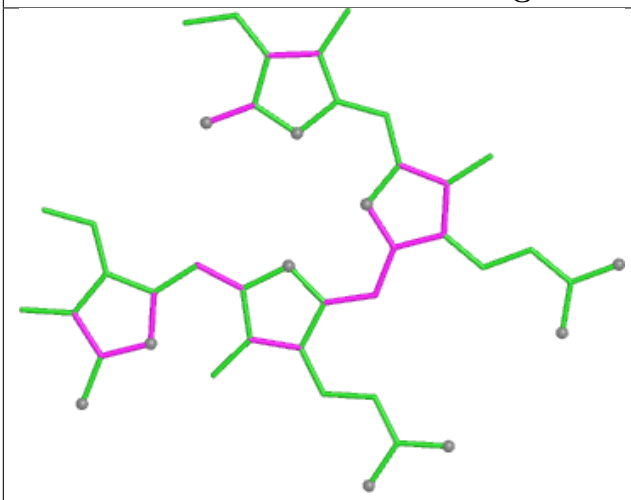
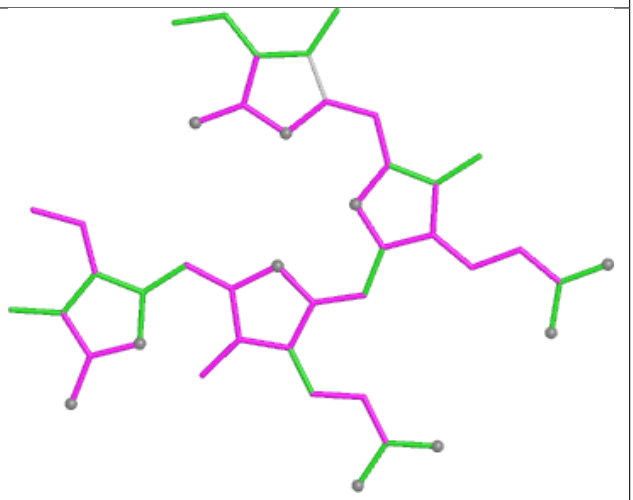
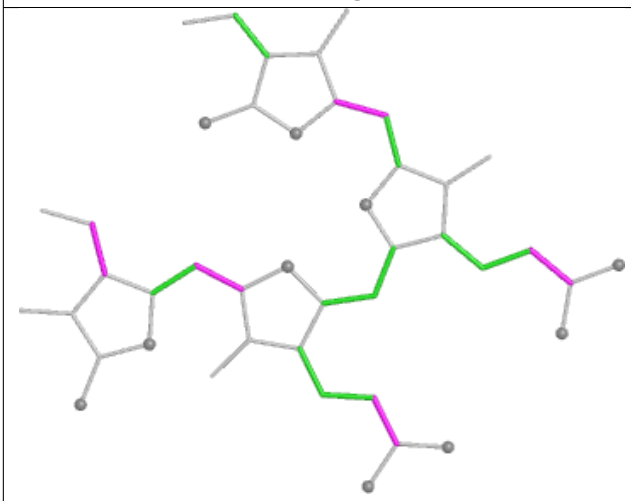


Bond lengths



Bond angles



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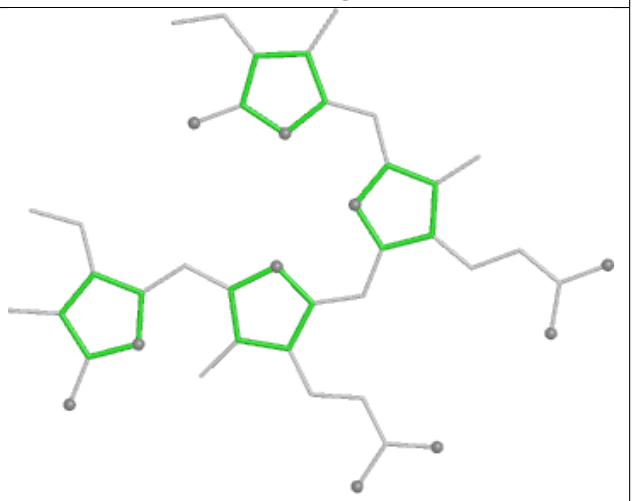
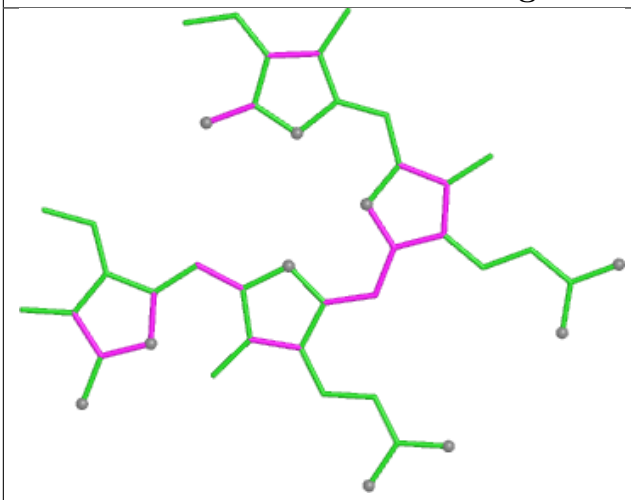


Rings

Ligand PEB PI 201



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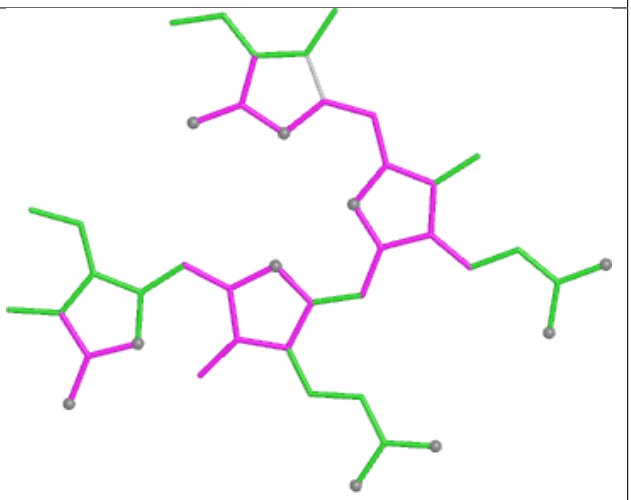

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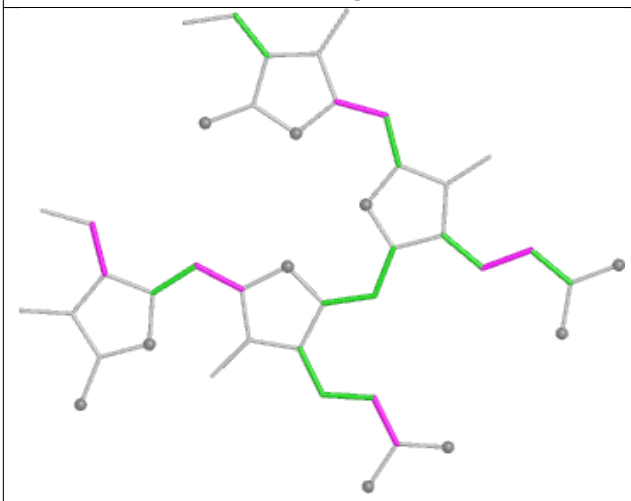

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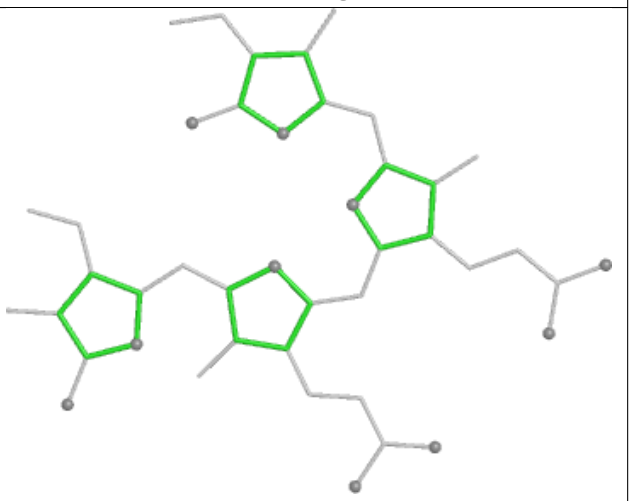
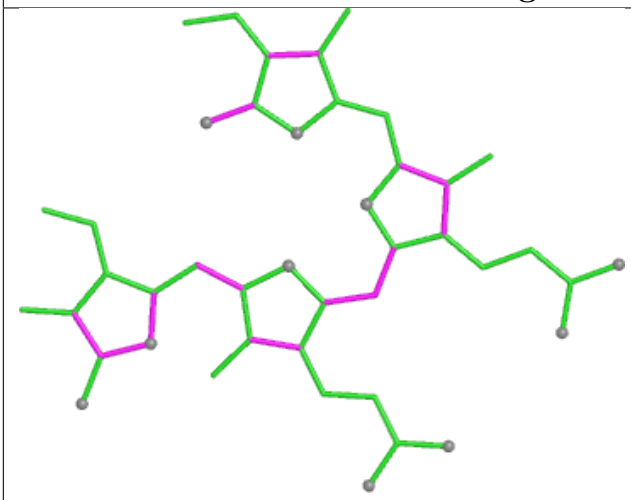


Rings

Ligand PEB fO 201



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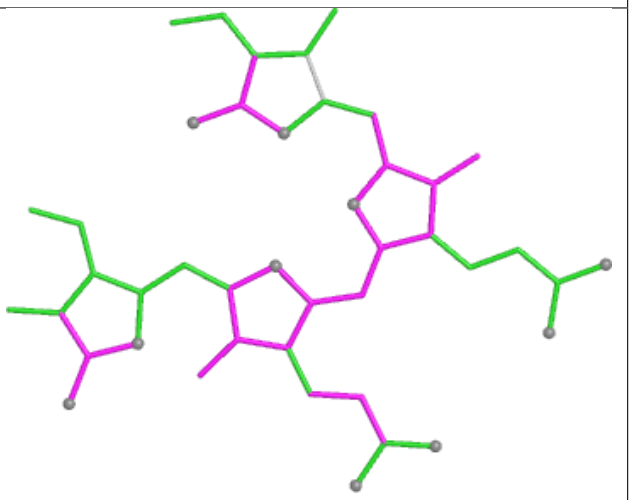

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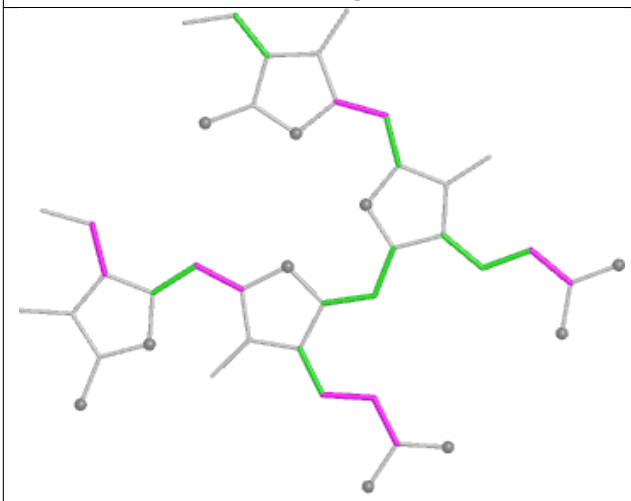

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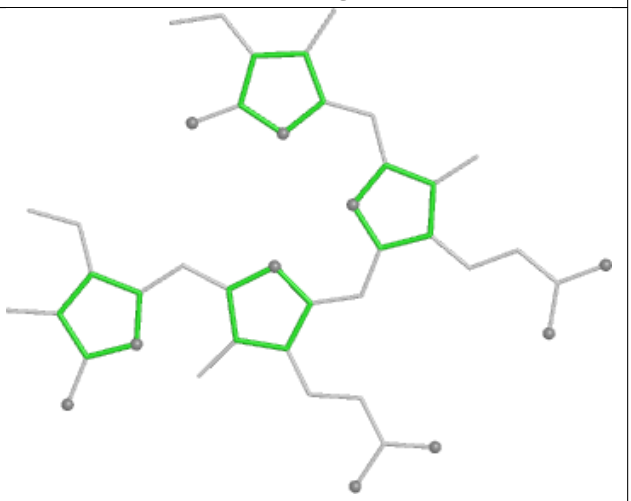

Rings

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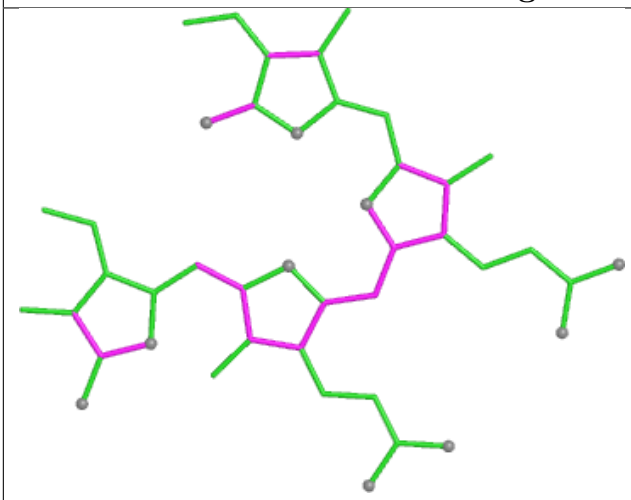

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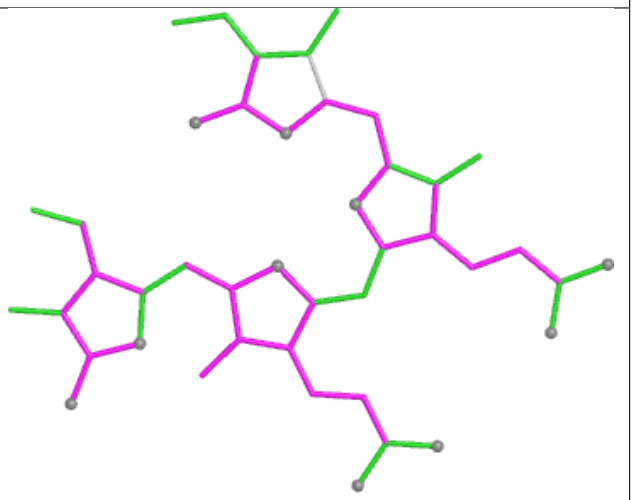

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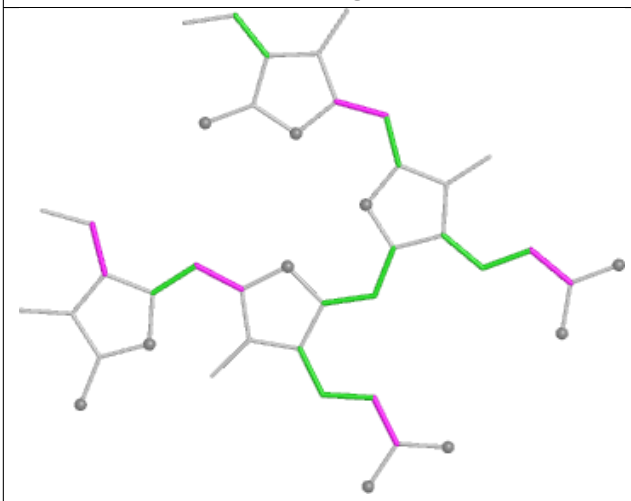

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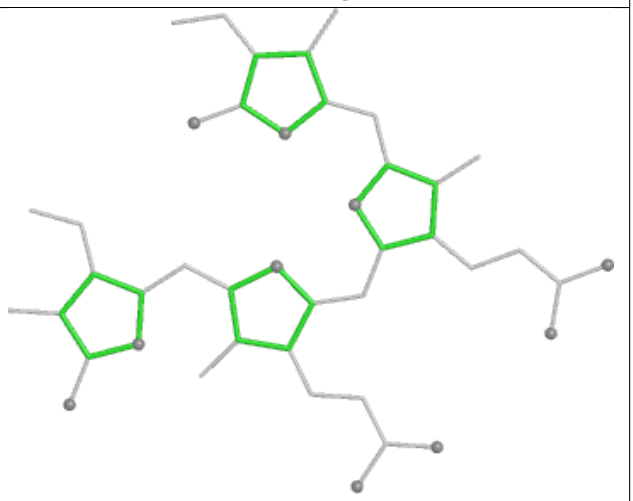
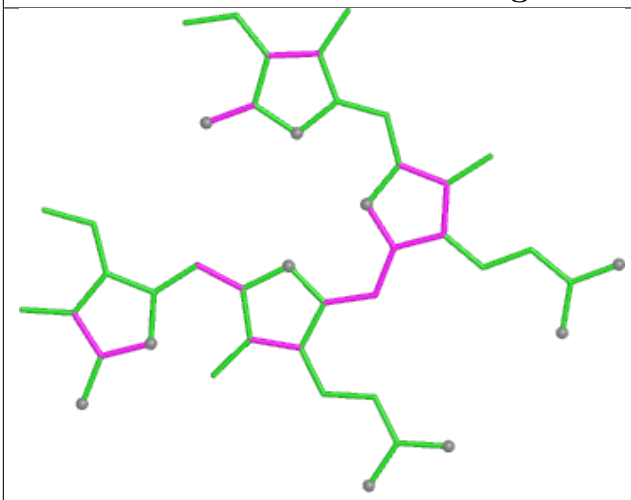


Rings

Ligand PEB hM 203



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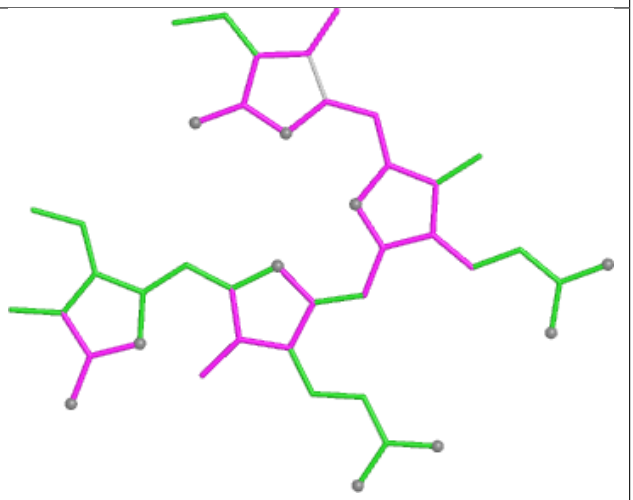

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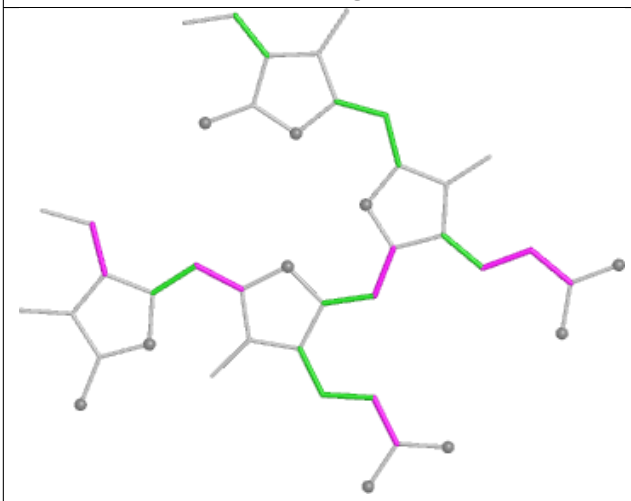

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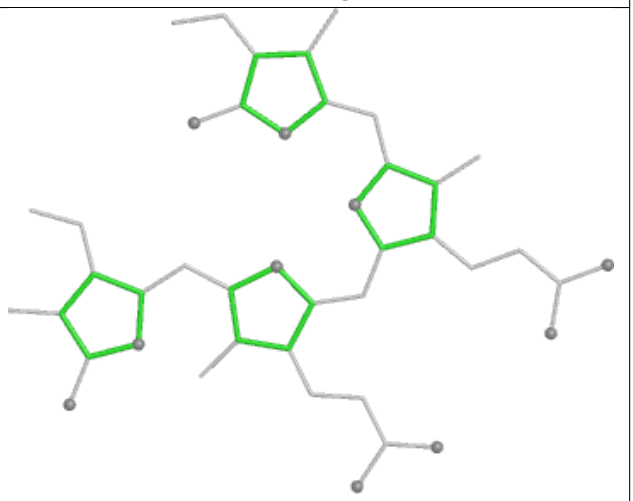
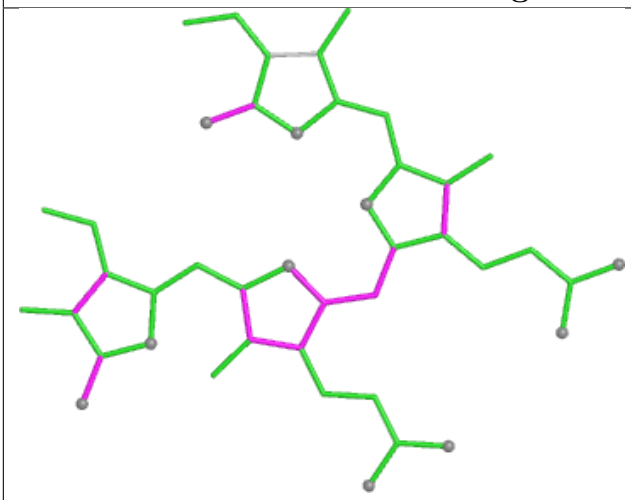


Rings

Ligand PUB wF 304



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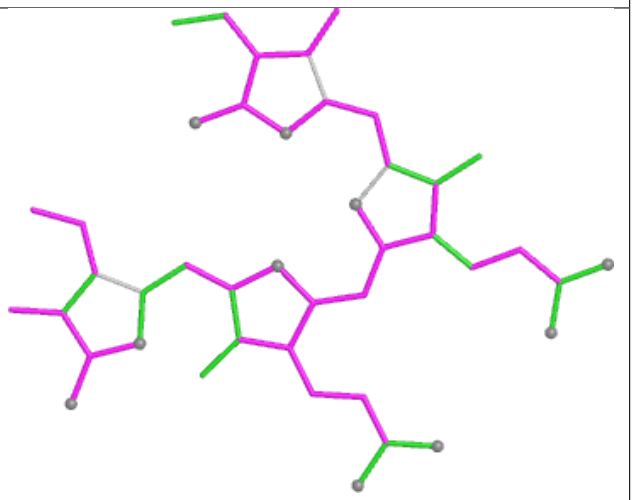

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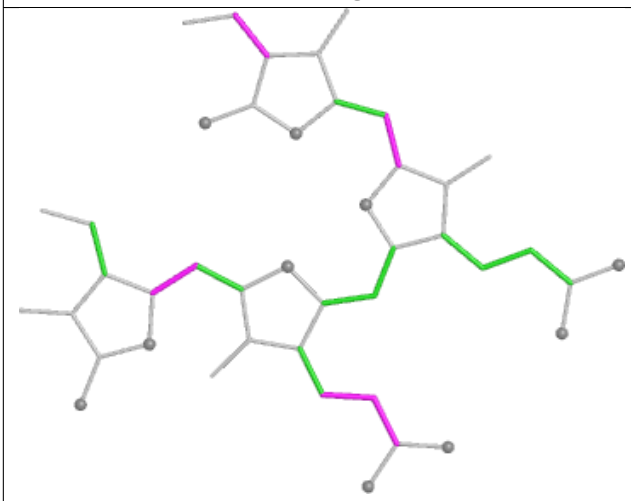

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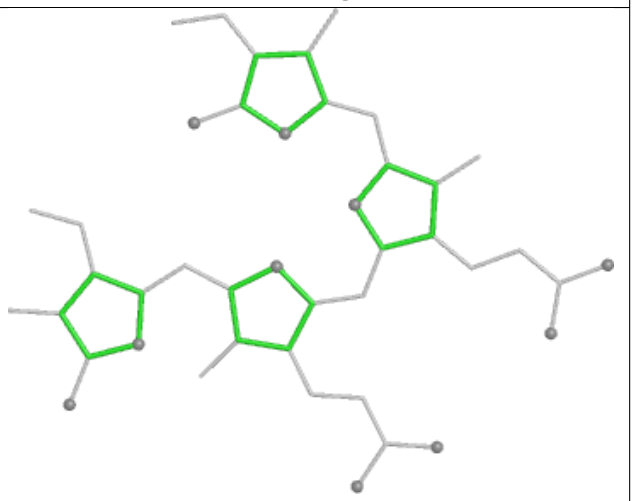
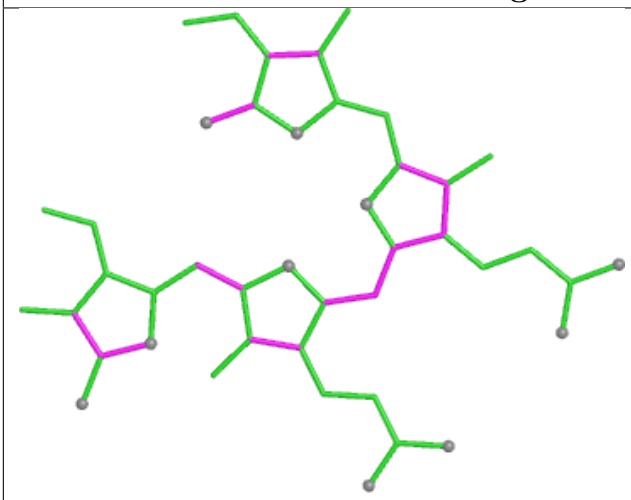


Rings

Ligand PEB UD 202



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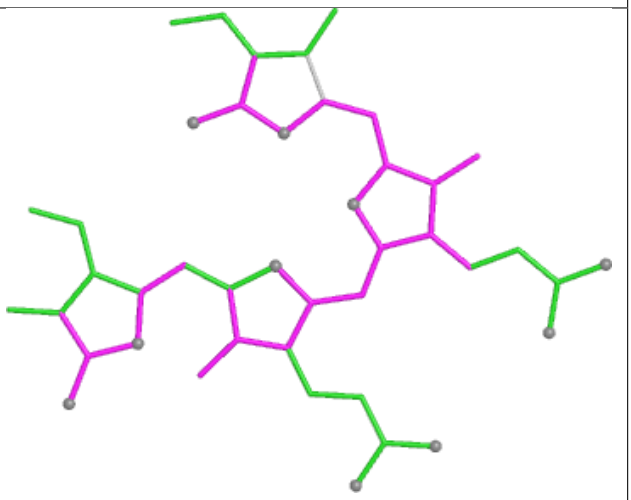
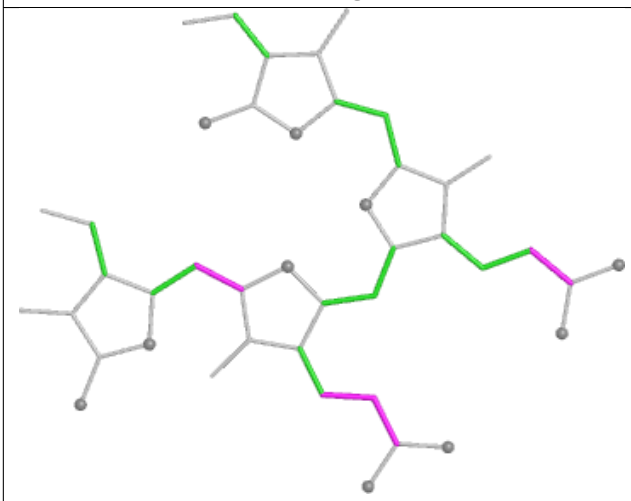


Bond angles



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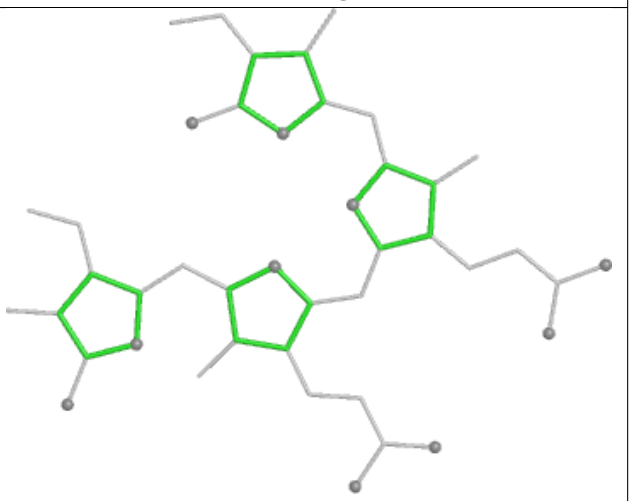
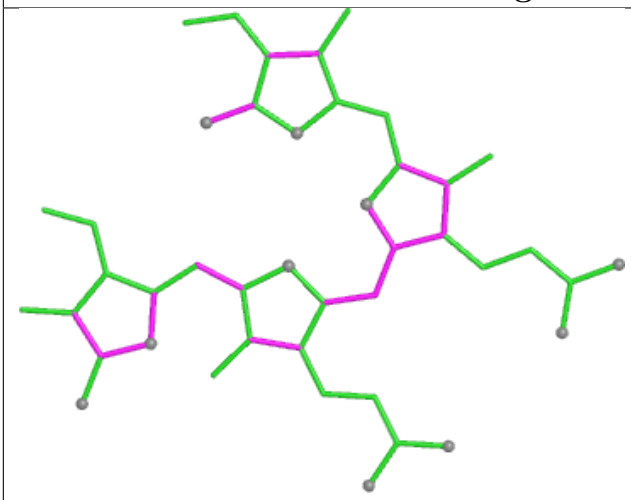


Rings

Ligand PEB K5 202



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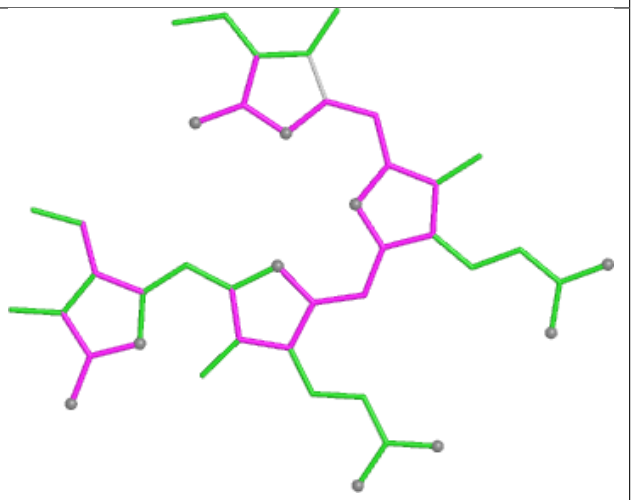

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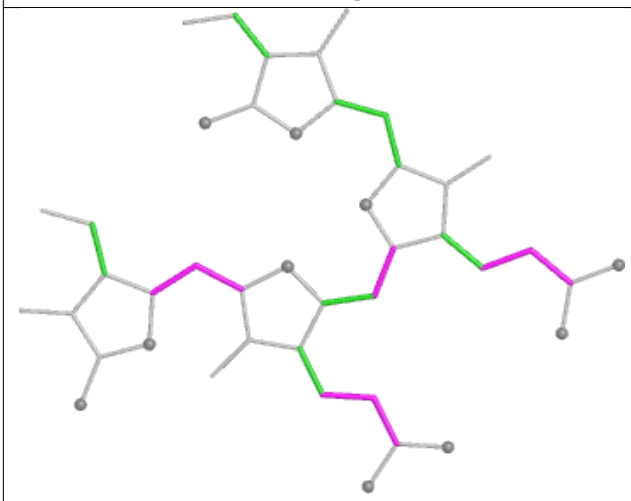

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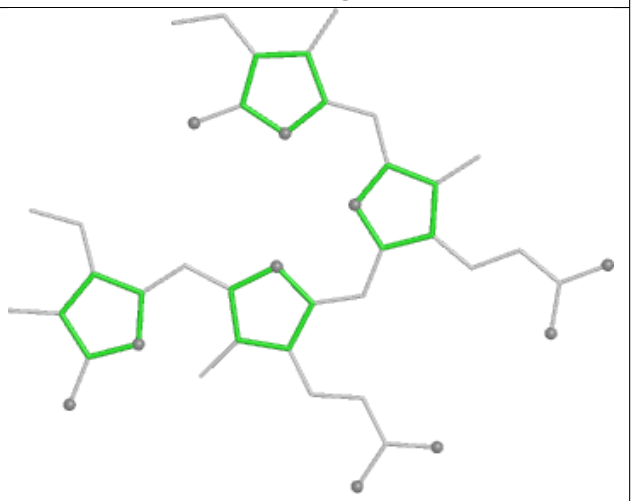
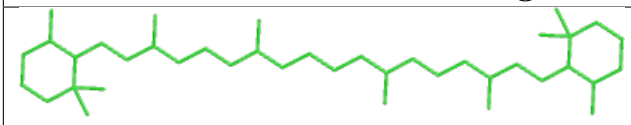


Rings

Ligand BCR cL 503



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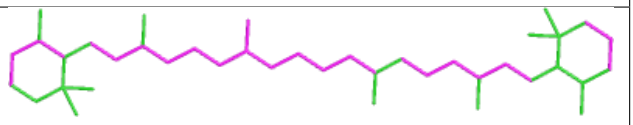

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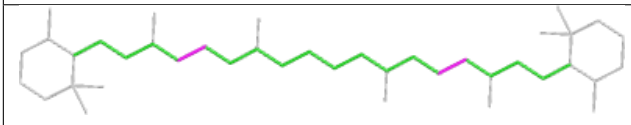

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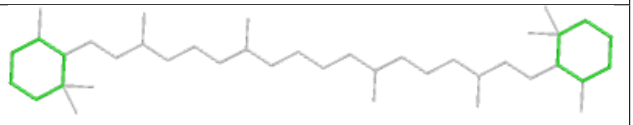
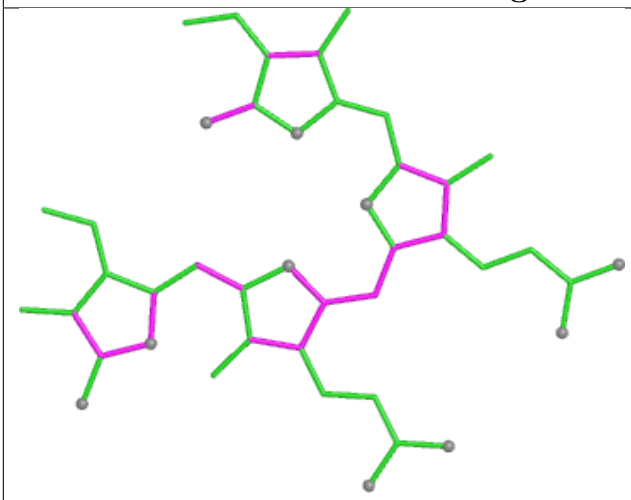


Rings

Ligand PEB QK 203



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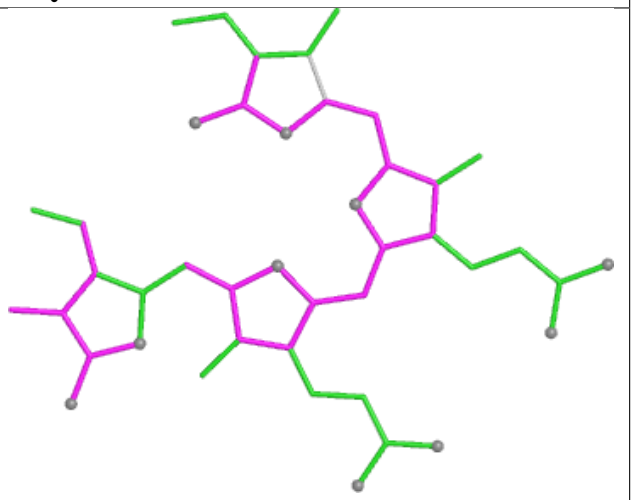

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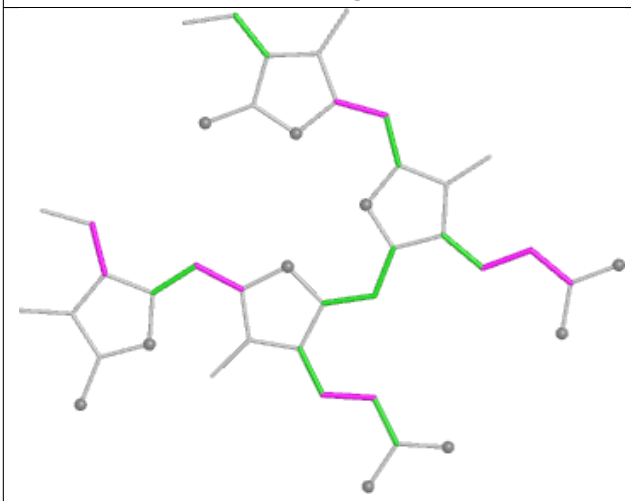

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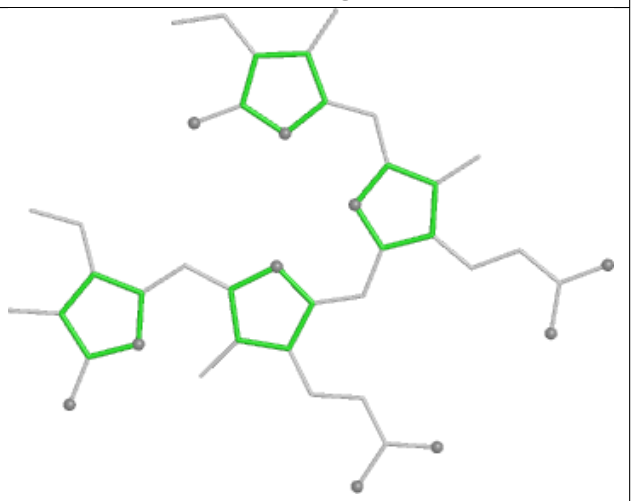
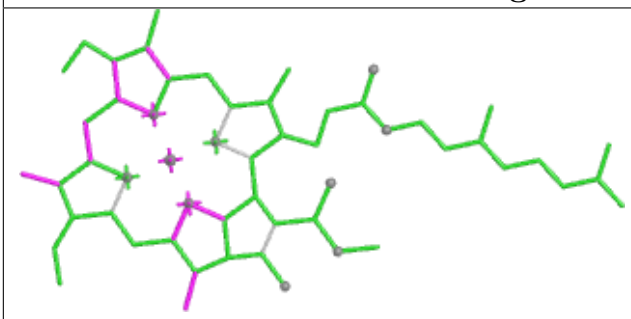


Rings

Ligand CLA AN 827



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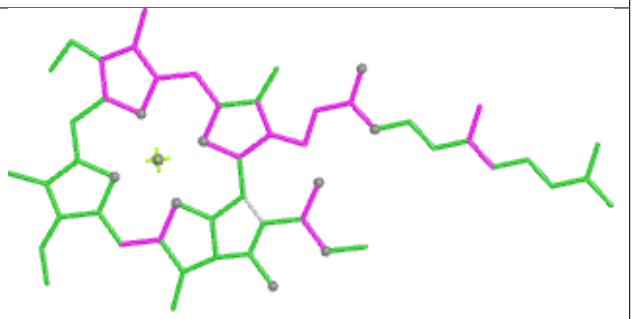
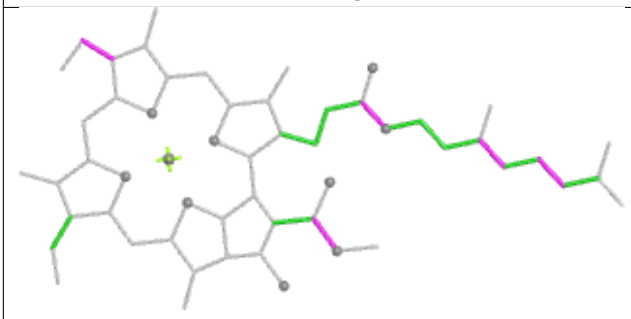


Bond angles



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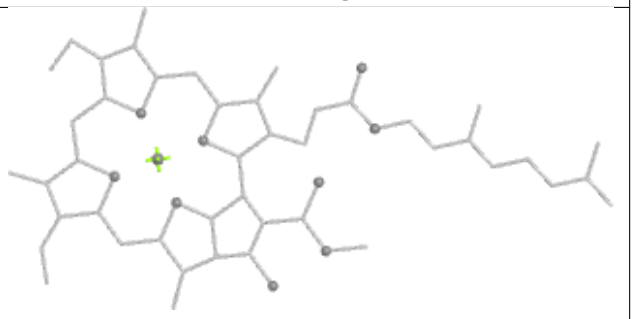
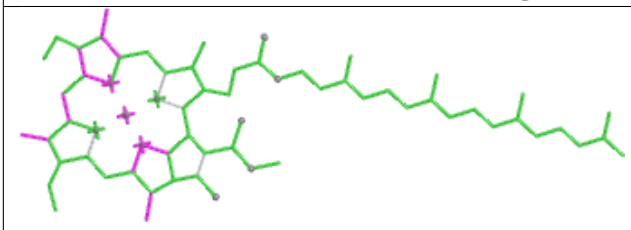


Rings

Ligand CLA bL 622



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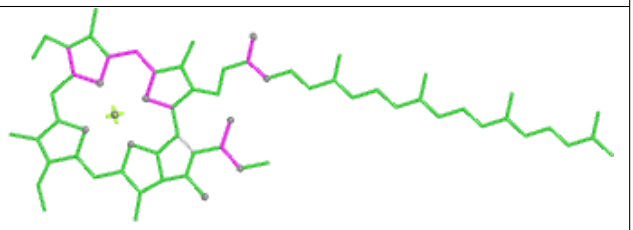
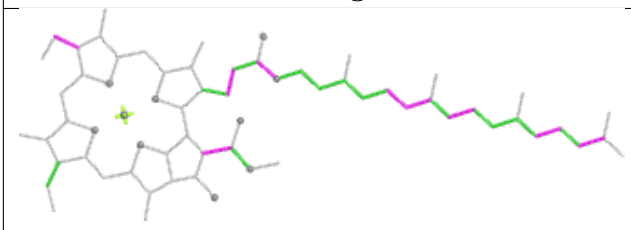


Bond angles



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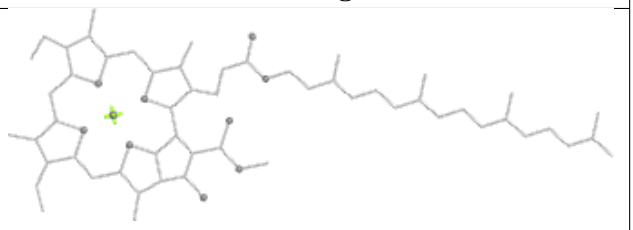
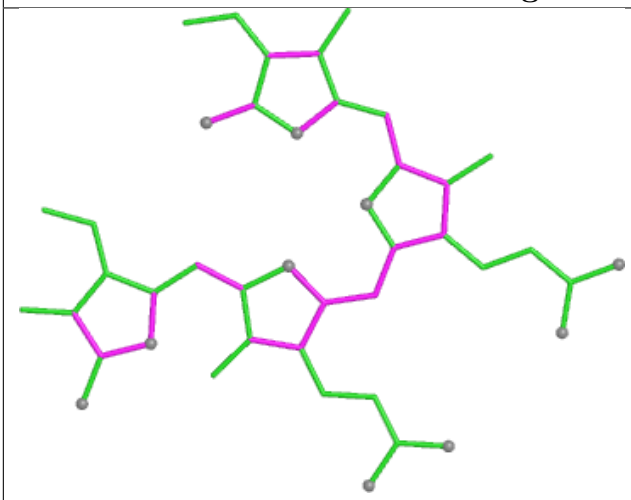


Rings

Ligand PEB lF 203



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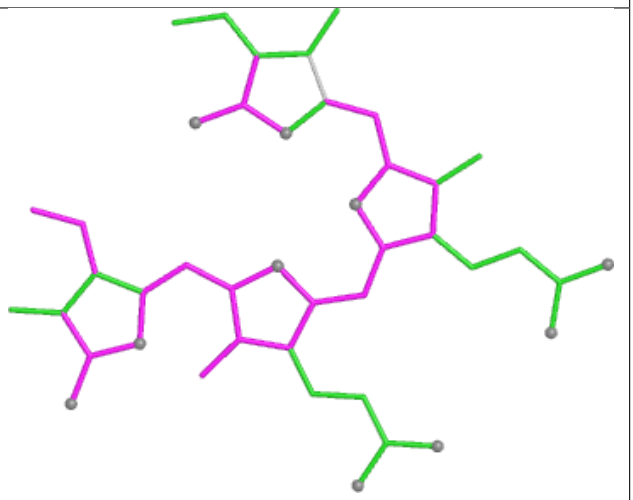
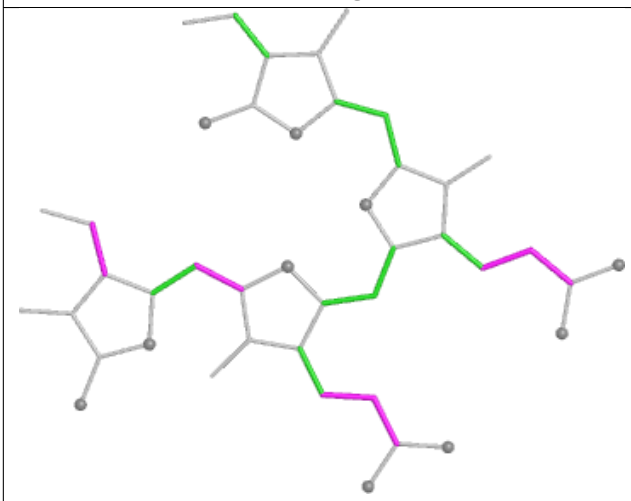


Bond angles



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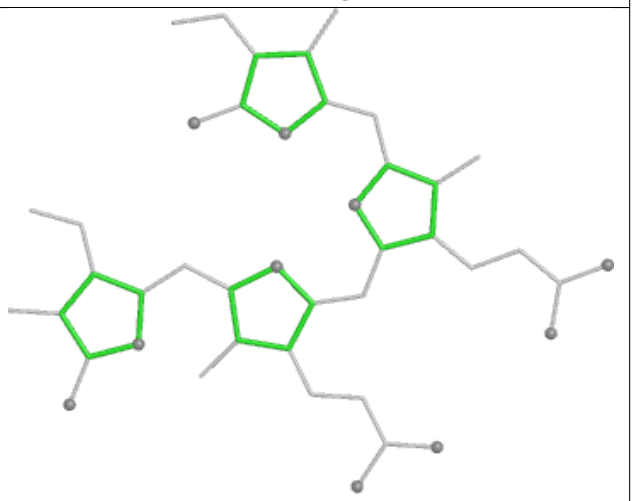
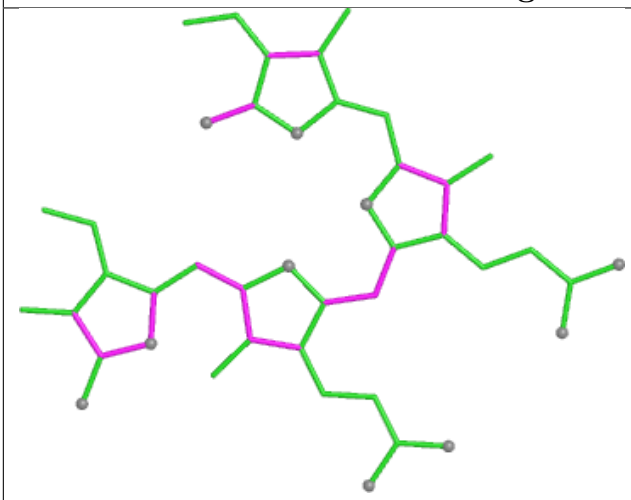


Rings

Ligand PEB aF 202



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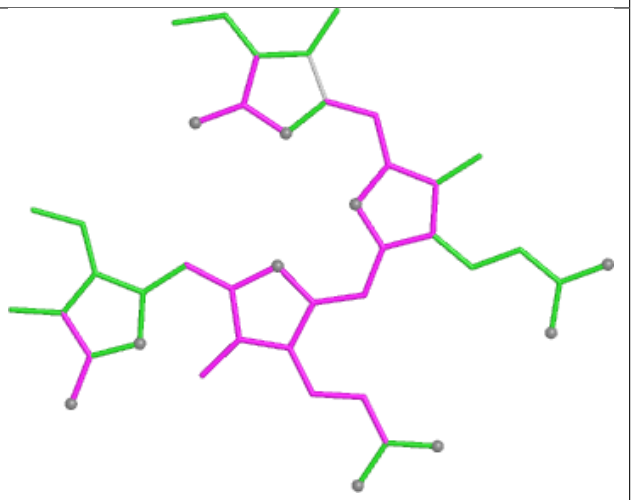

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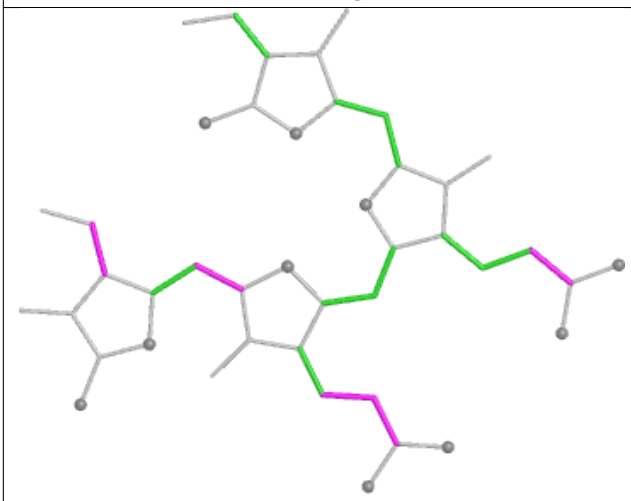

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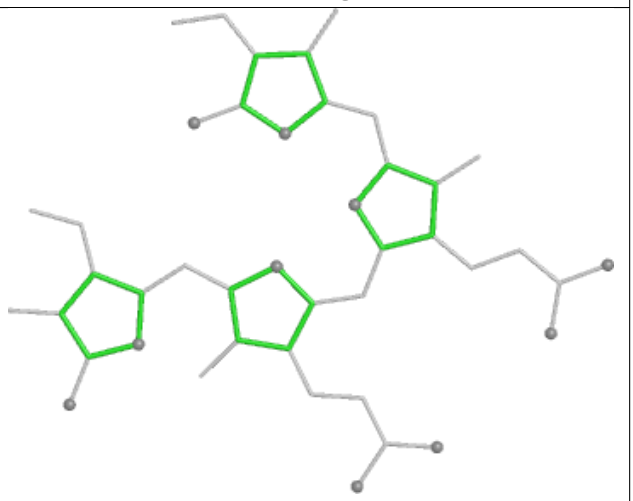
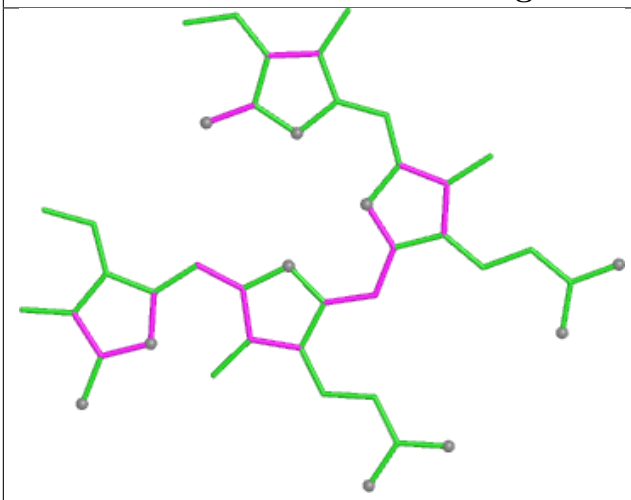


Rings

Ligand PEB R4 201



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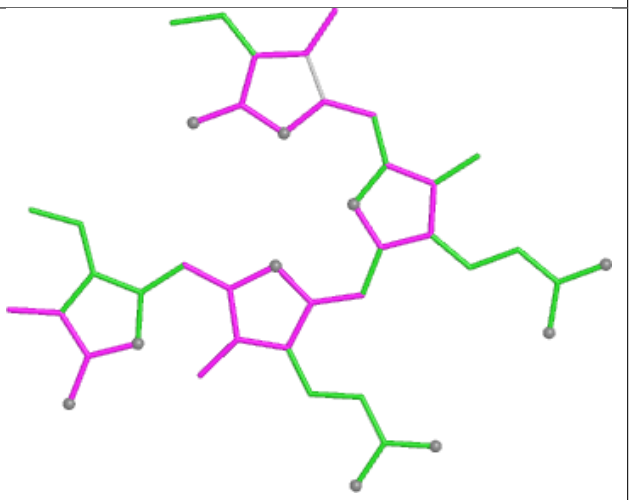
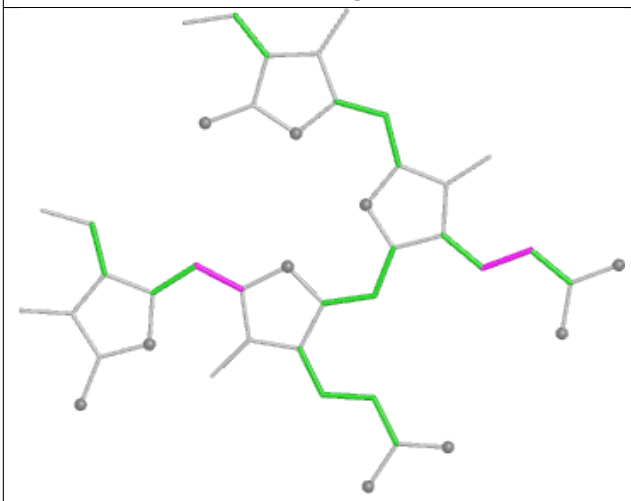
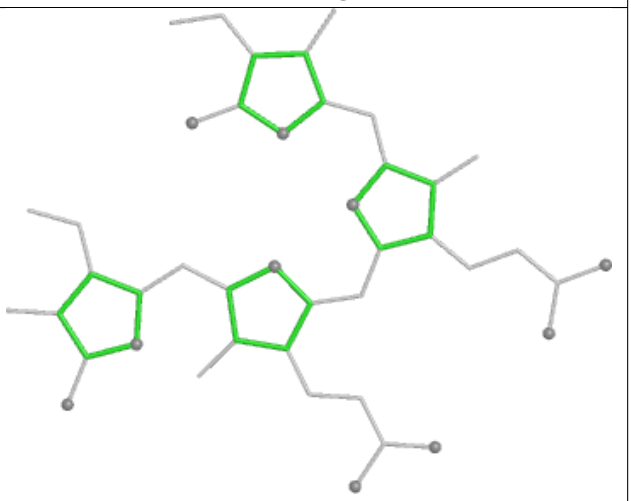


Bond angles

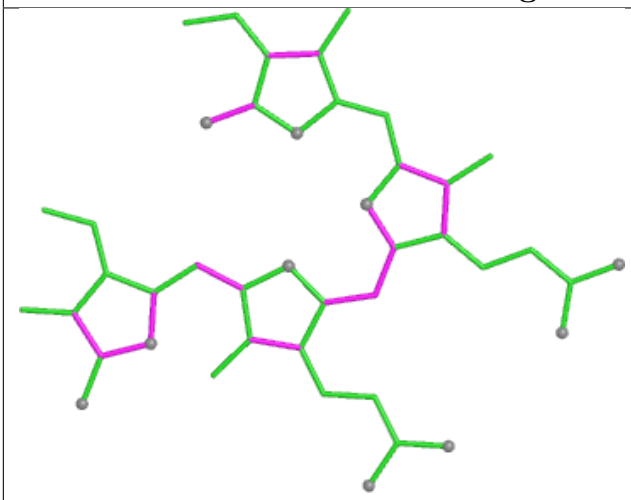


Torsions



Rings

Ligand PEB JJ 202



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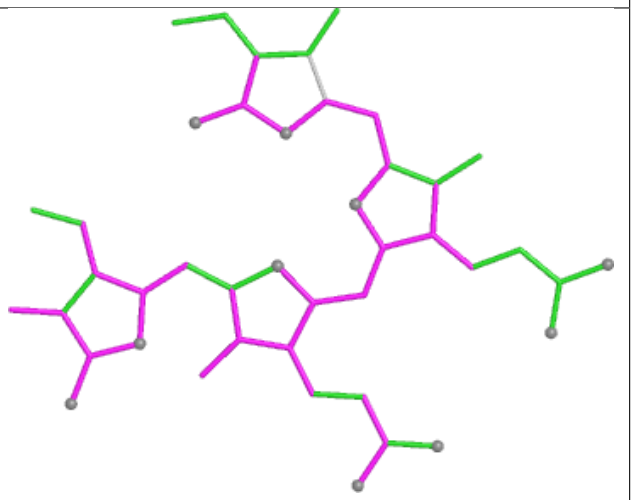
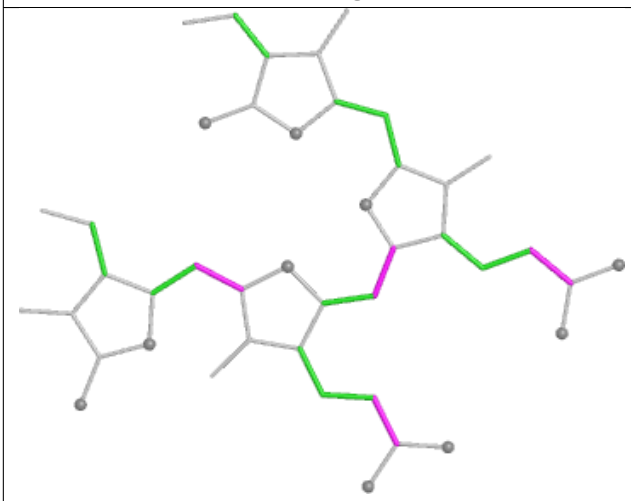


Bond angles



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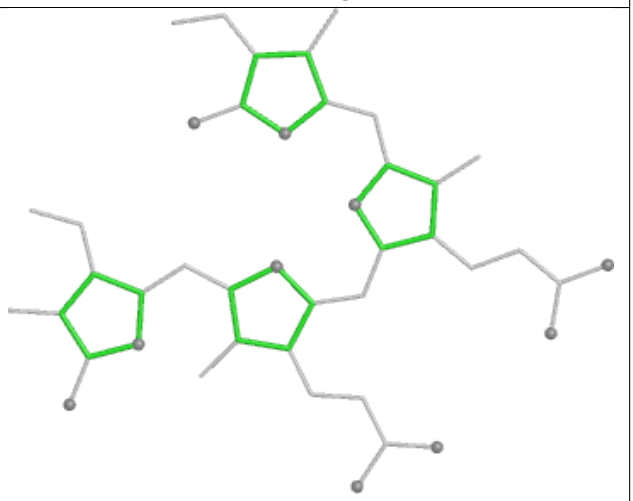
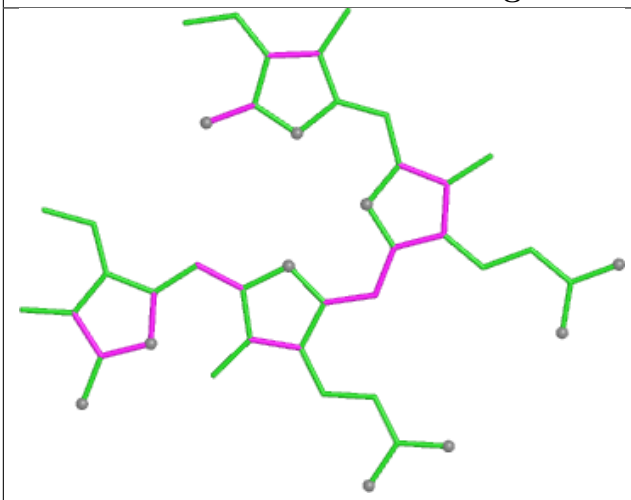


Rings

Ligand PEB MM 201



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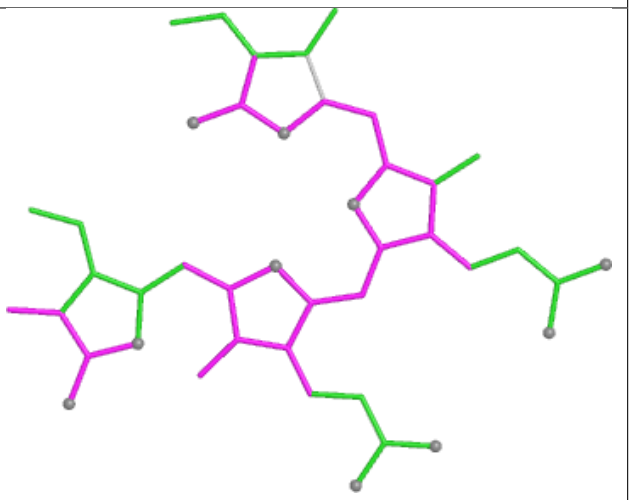

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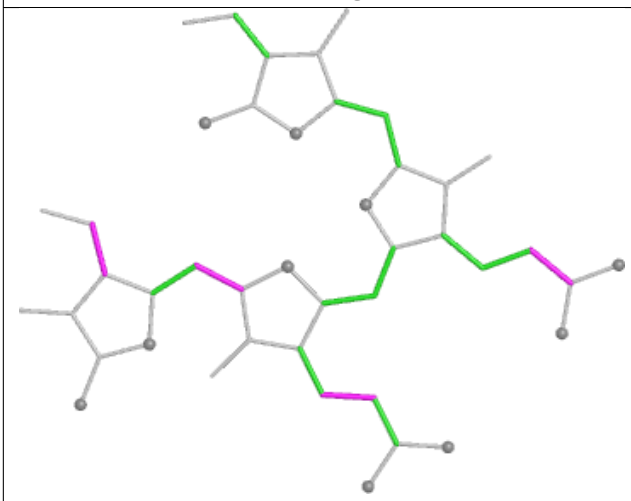

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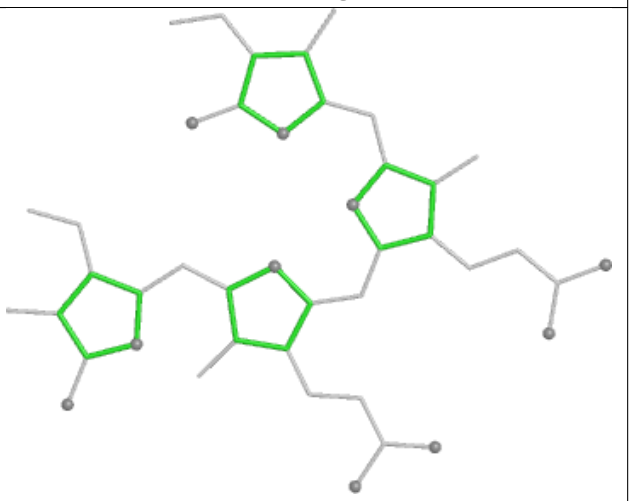
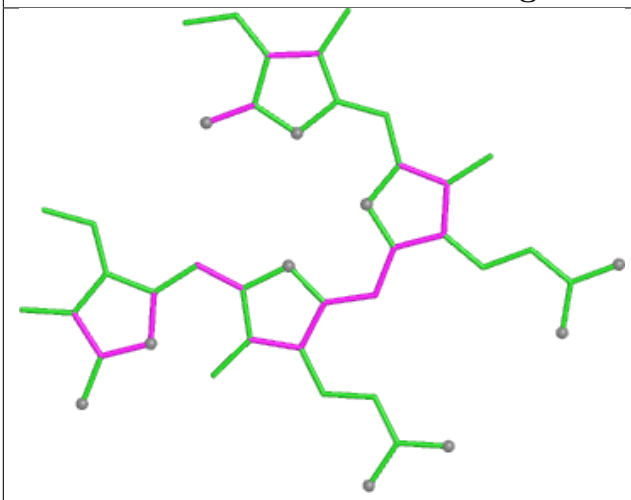


Rings

Ligand PEB y8 203



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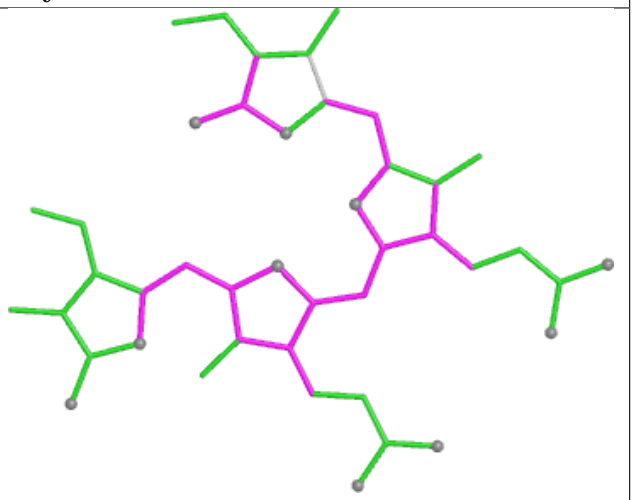

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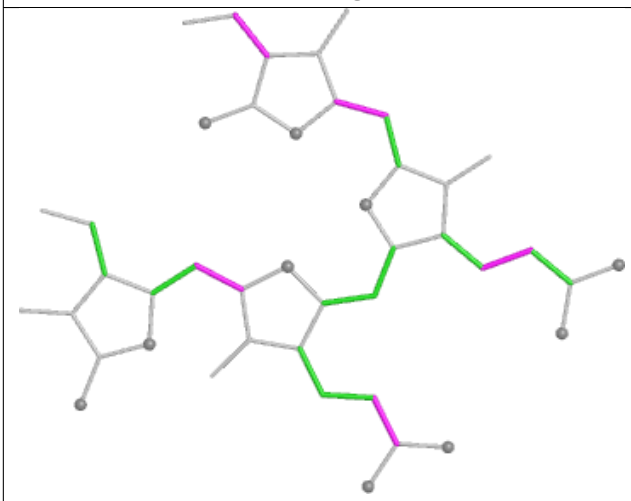

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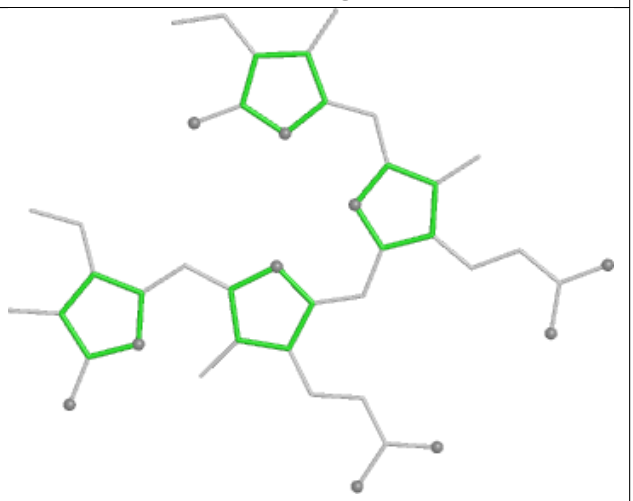
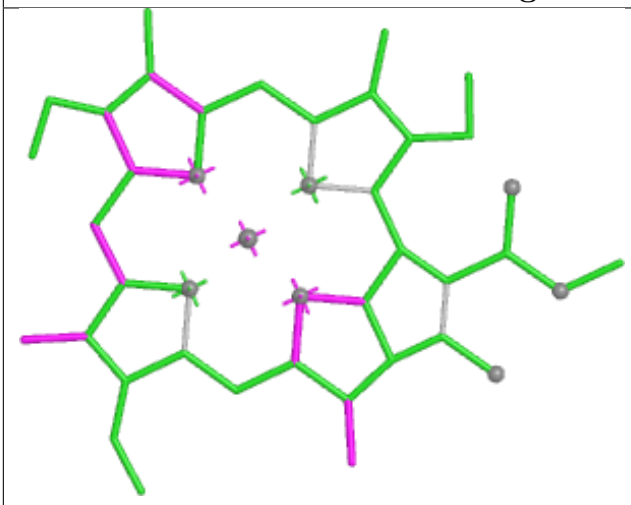


Rings

Ligand CLA 22 604



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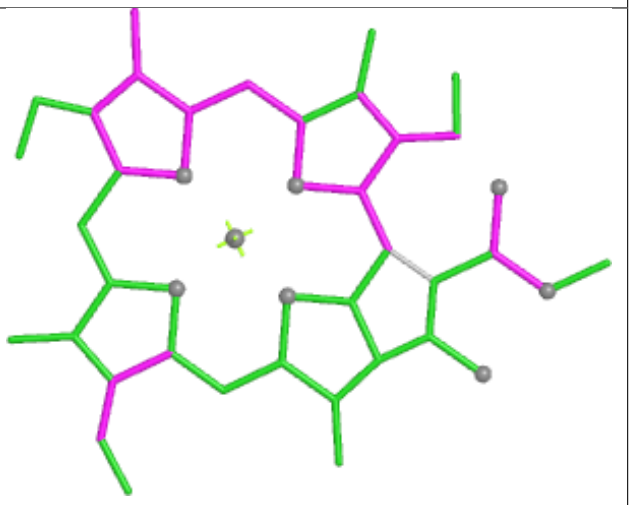

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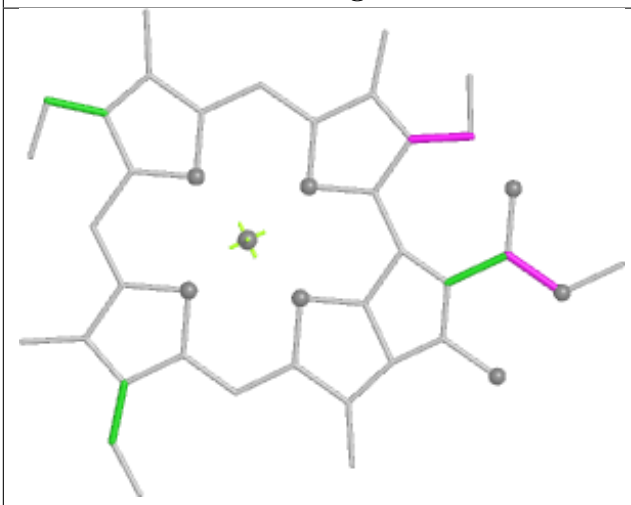
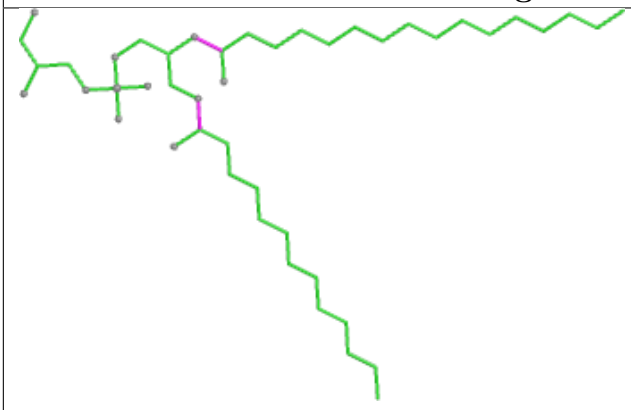


Torsions



Rings

Ligand LHG dL 408



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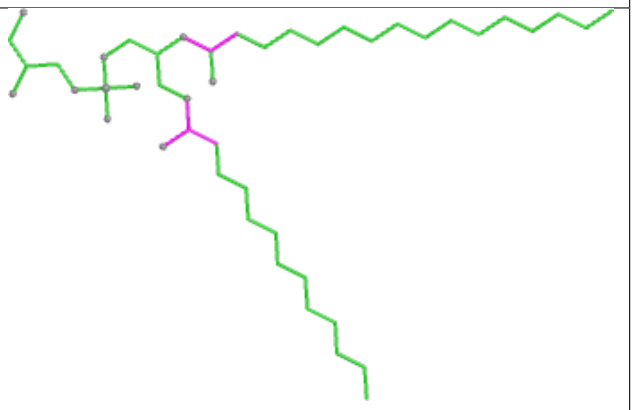

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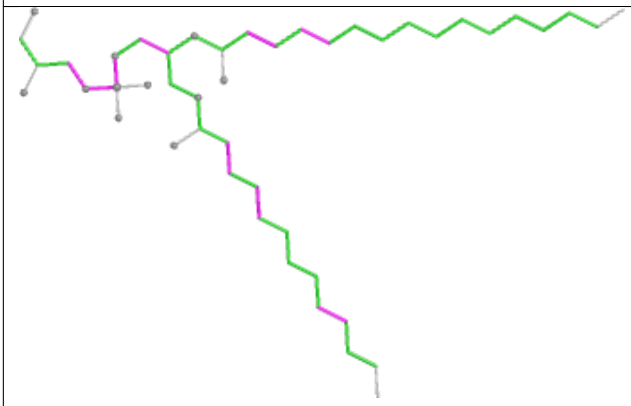

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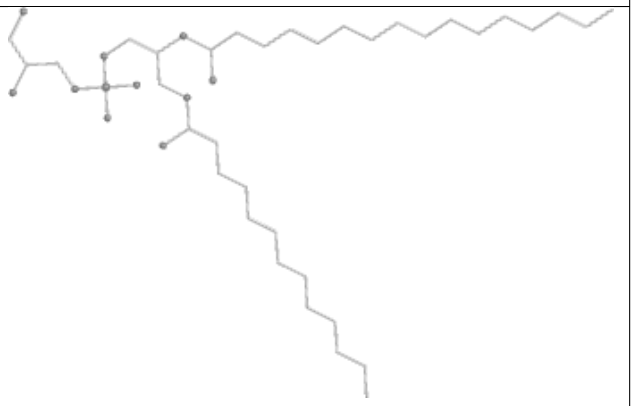
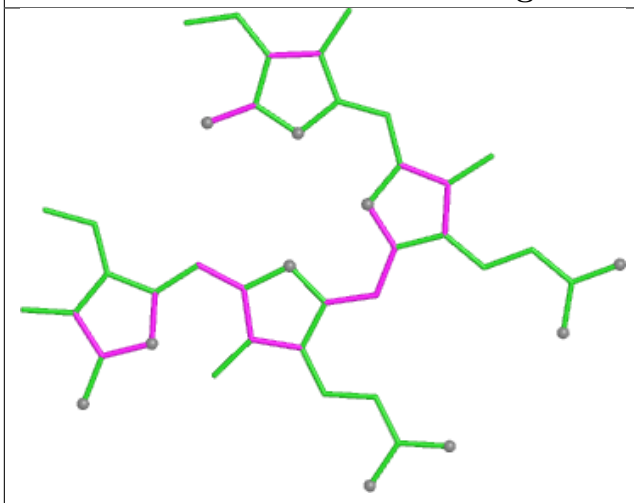


Rings

Ligand PEB X5 201



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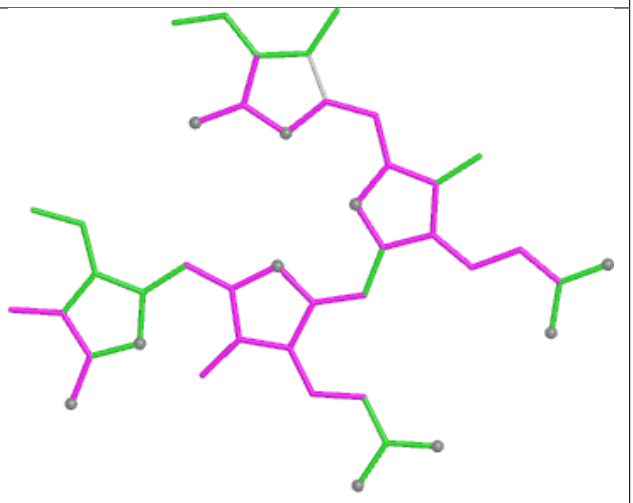
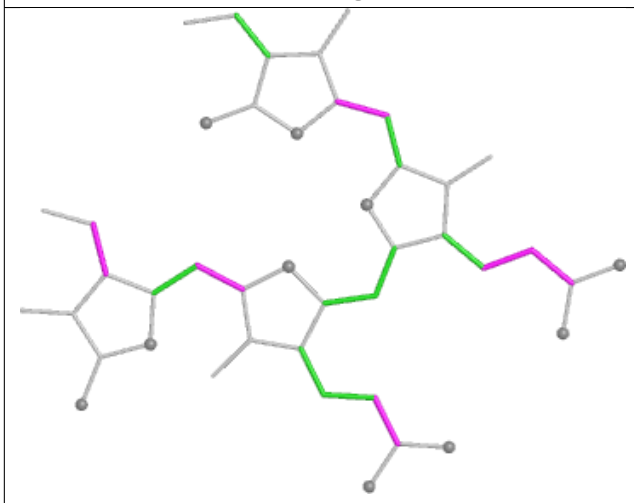


Bond angles



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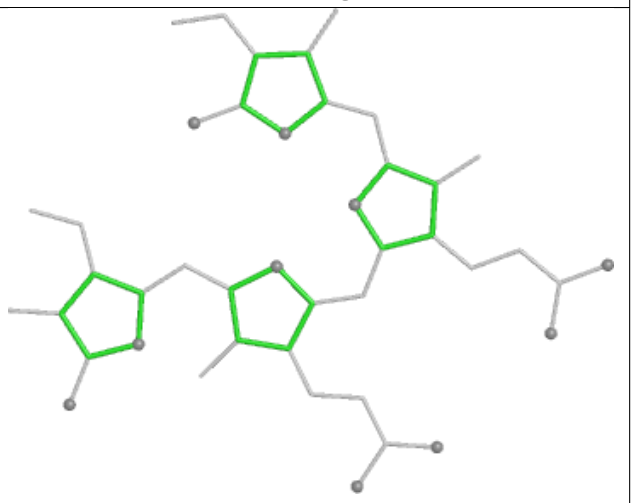
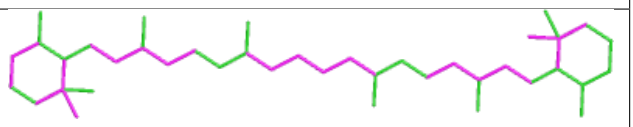


Rings

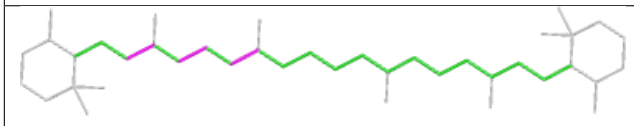
Ligand BCR HL 103



Bond lengths



Bond angles



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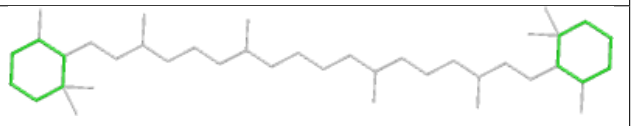
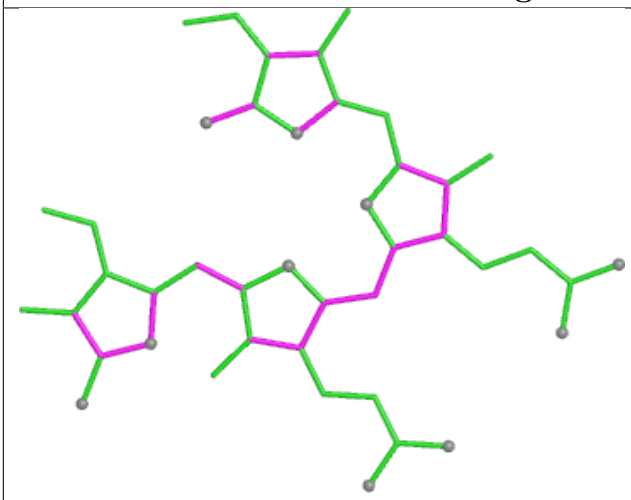


Rings

Ligand PEB JQ 203



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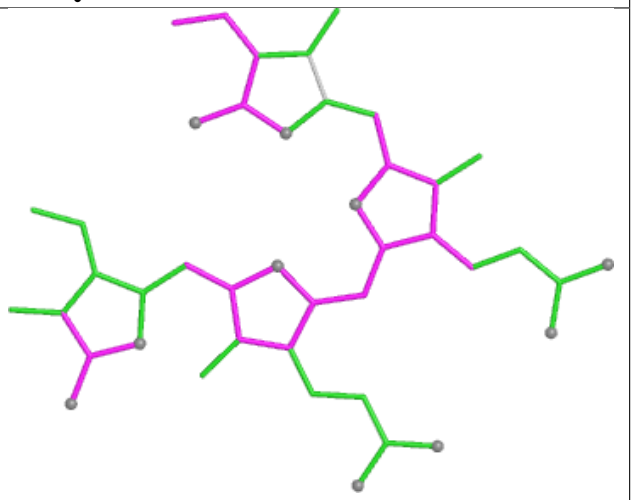

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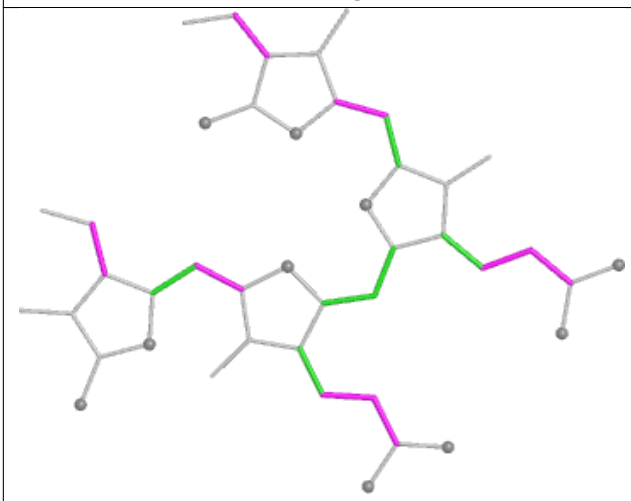

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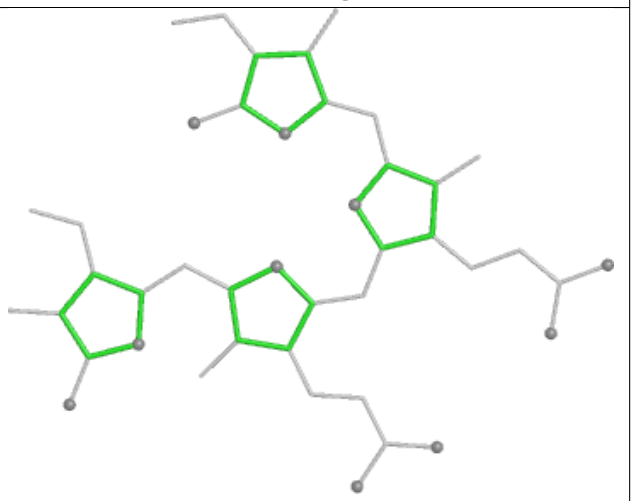
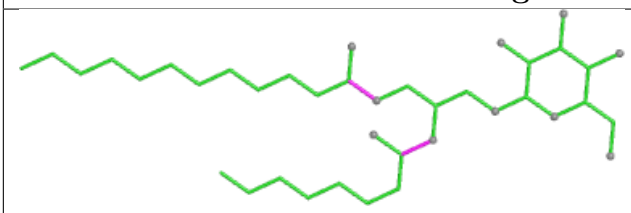


Rings

Ligand LMG bL 624



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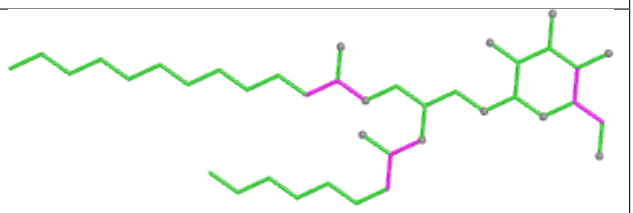
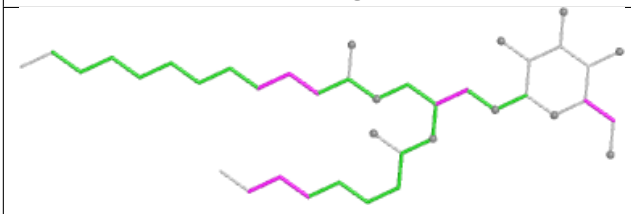


Bond angles



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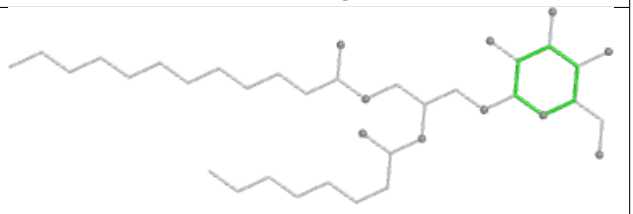
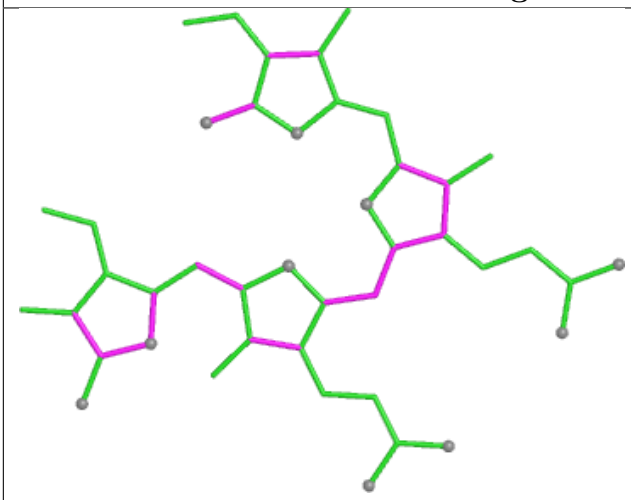


Rings

Ligand PEB KQ 201



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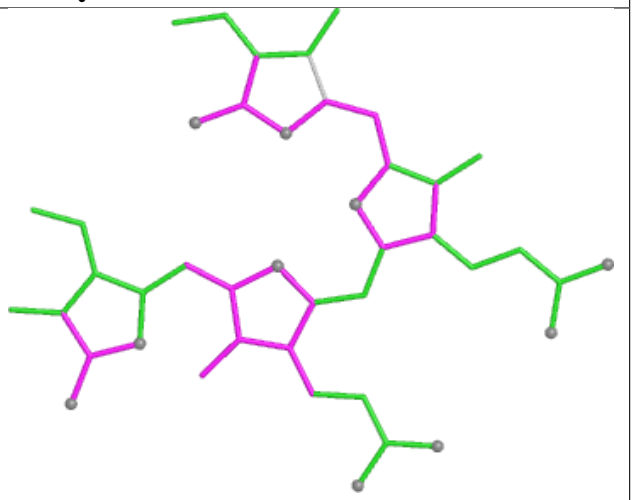

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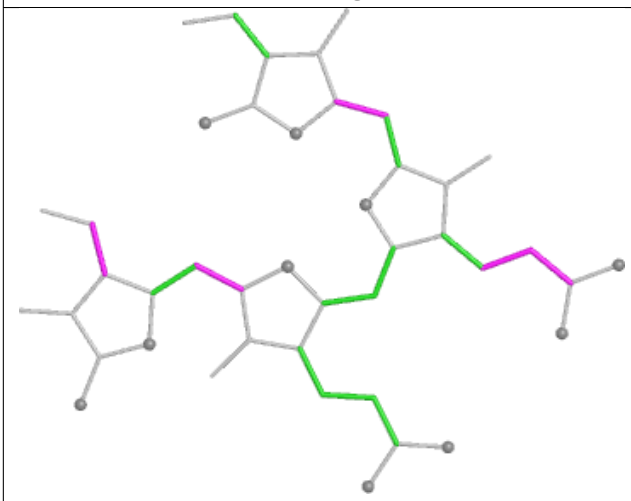

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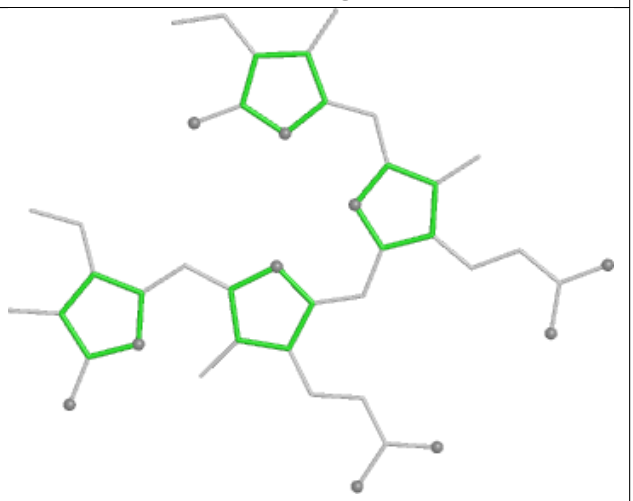
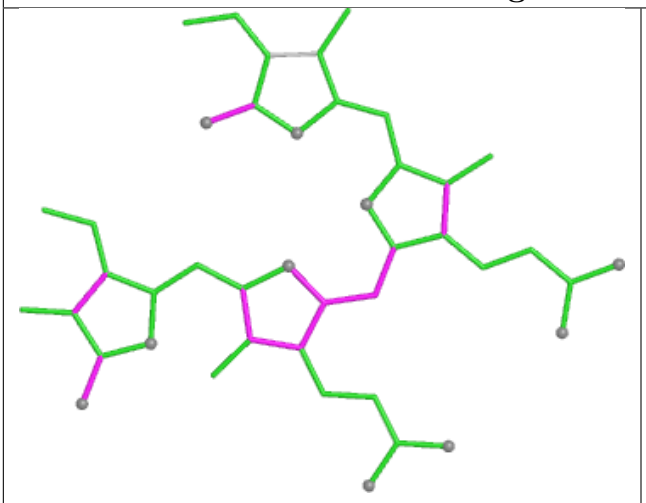


Rings

Ligand PUB AH 303



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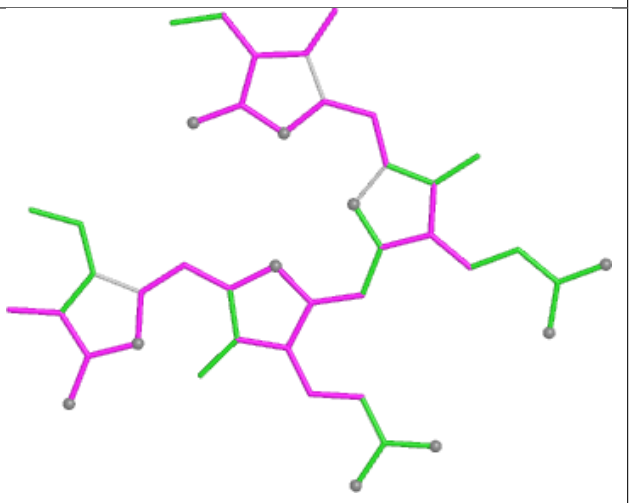
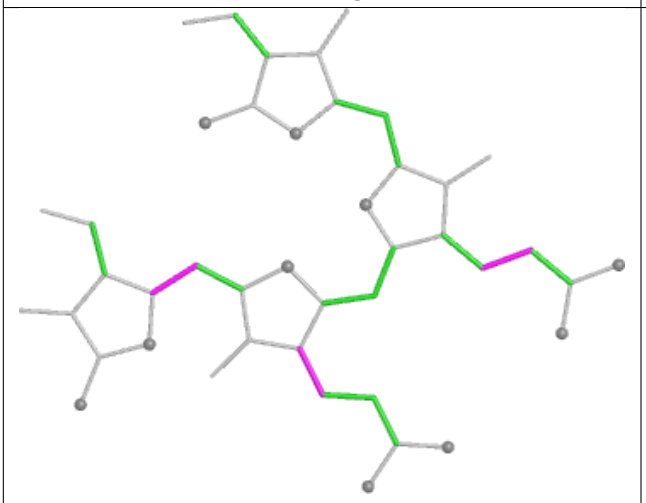


Bond angles



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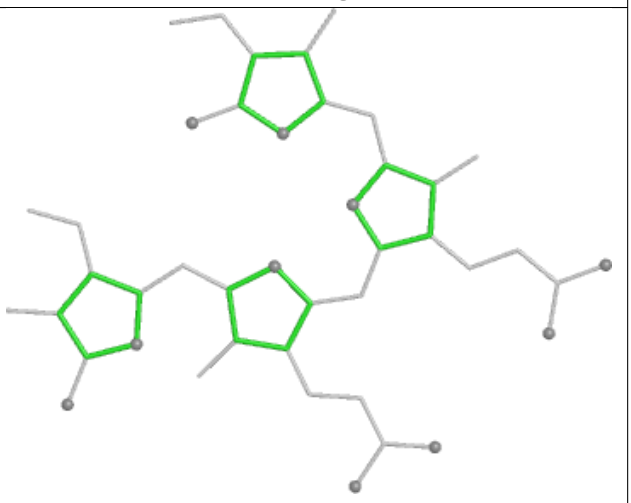
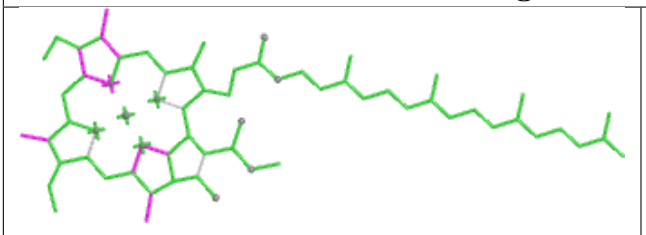


Rings

Ligand CLA B2 809



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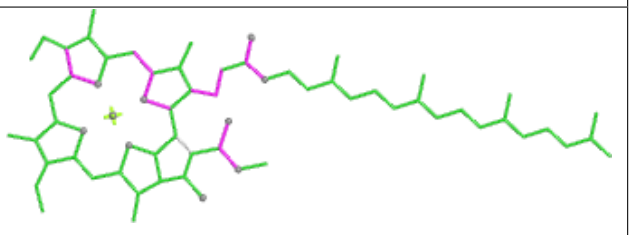

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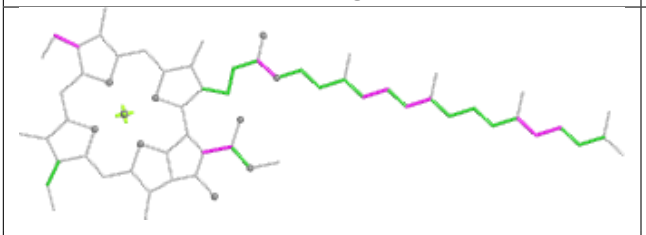

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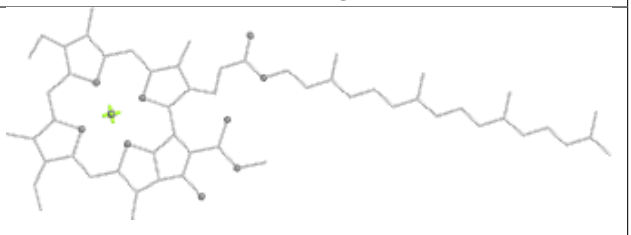
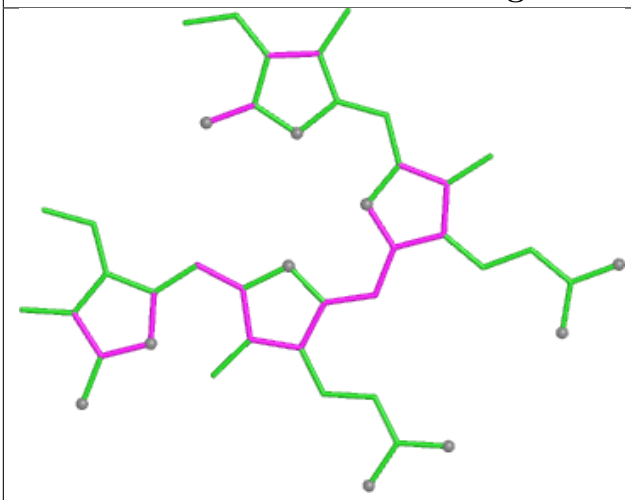


Rings

Ligand PEB XM 202



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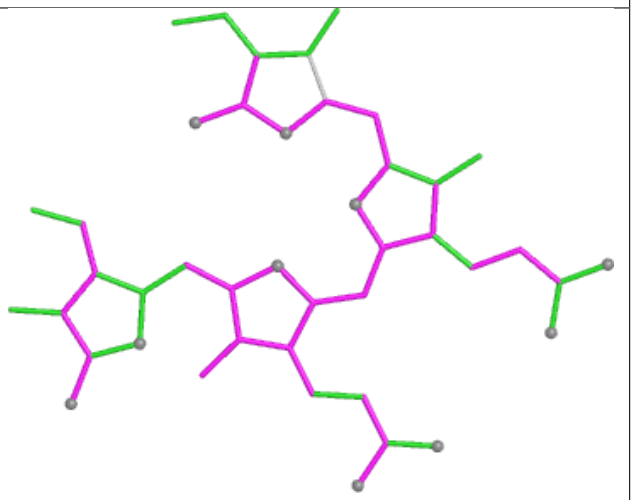
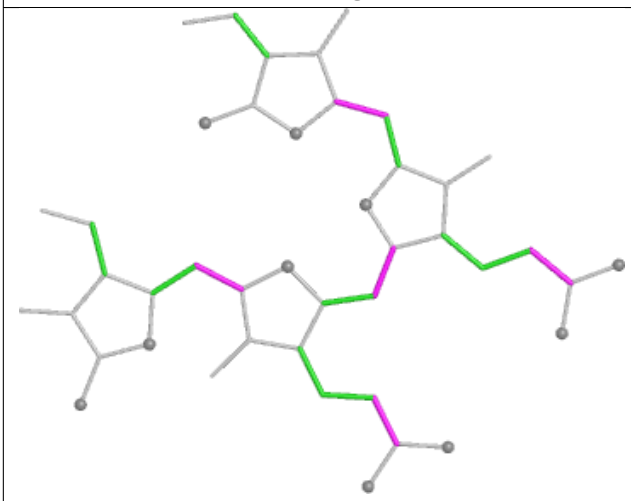


Bond angles



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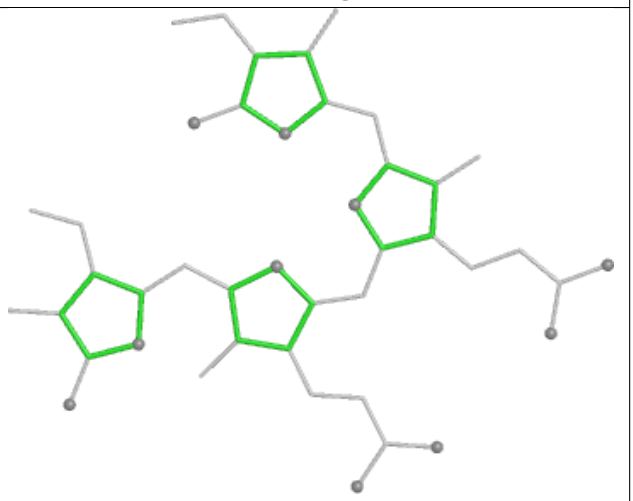
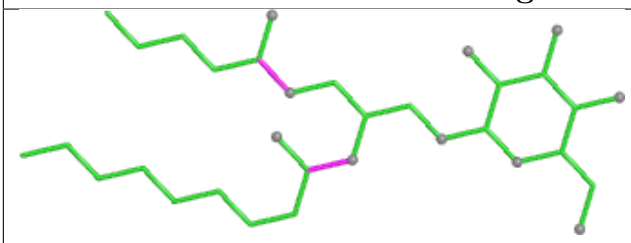


Rings

Ligand LMG jL 101



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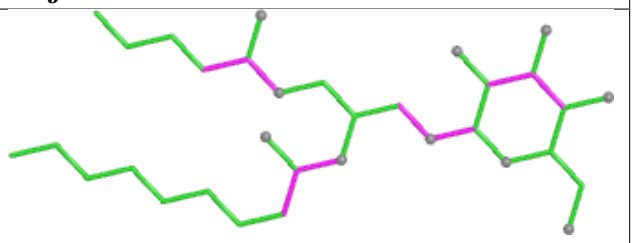
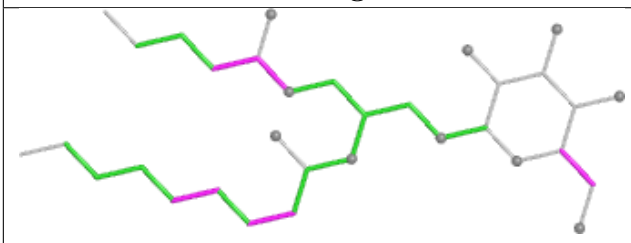


Bond angles



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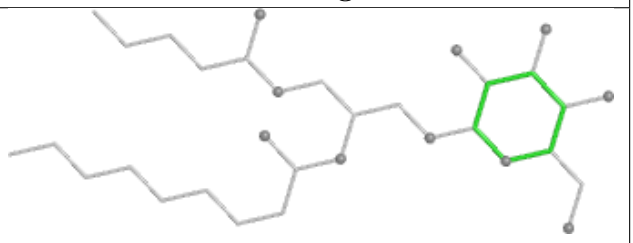
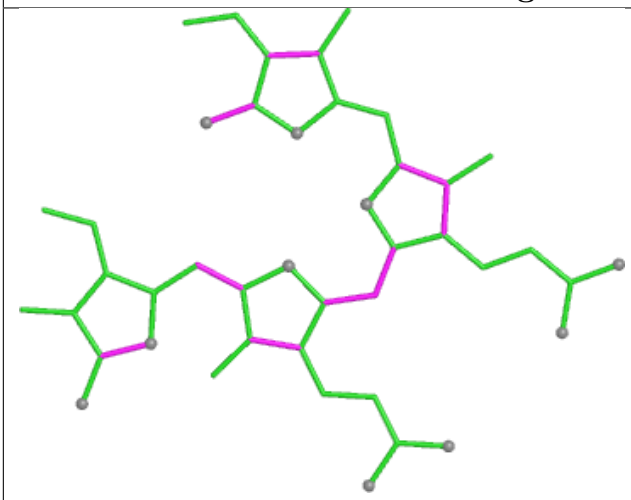


Rings

Ligand PEB F7 201



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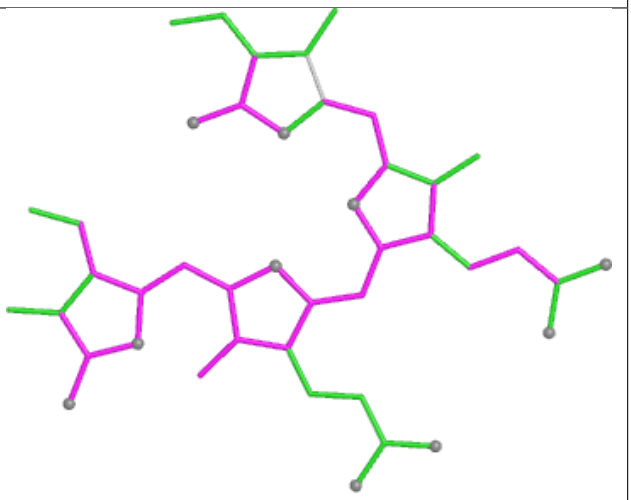
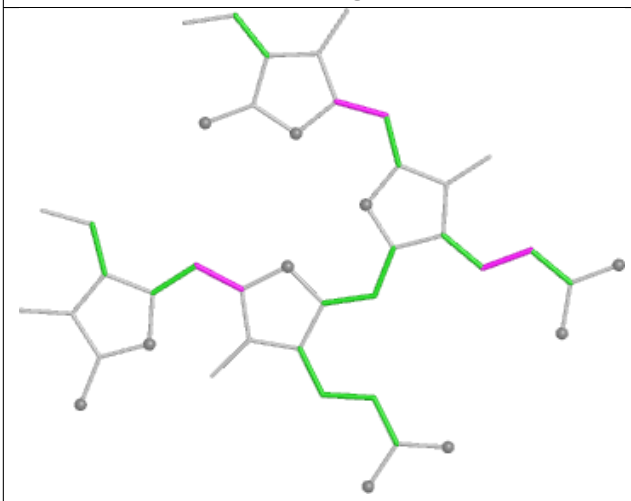
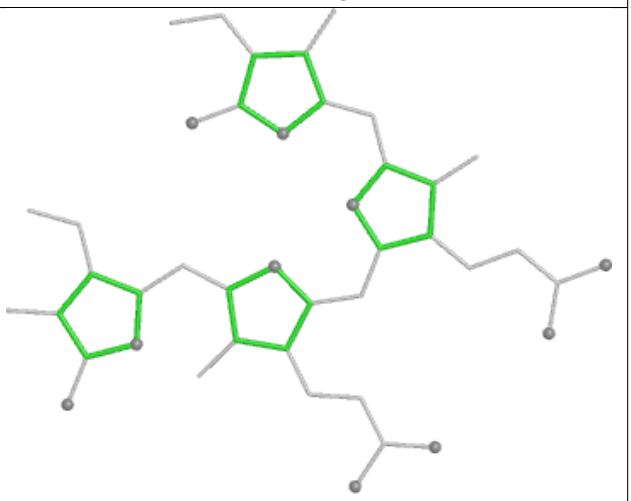


Bond angles

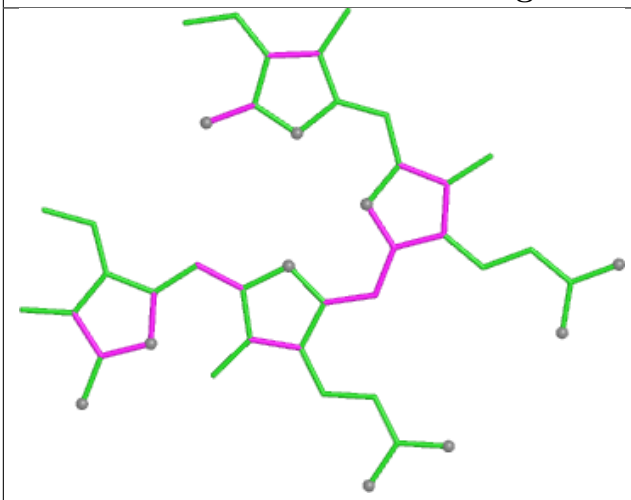


Torsions



Rings

Ligand PEB SE 201



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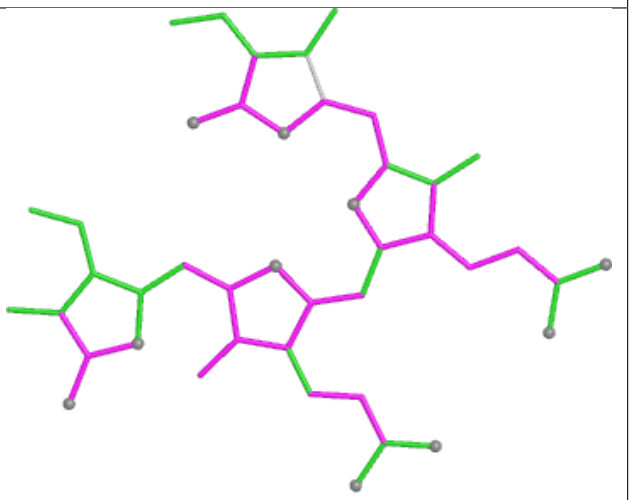

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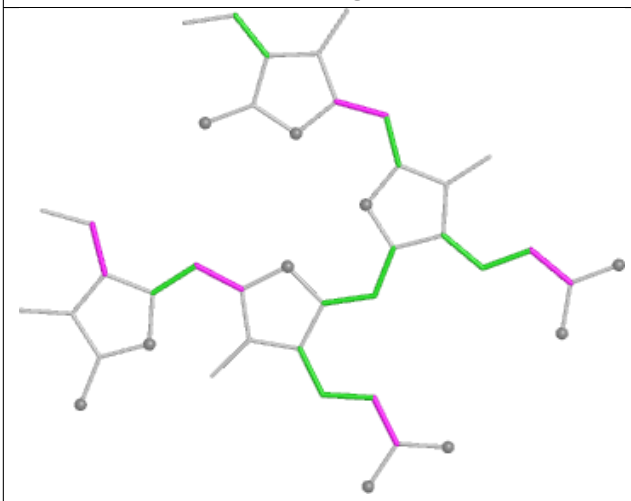

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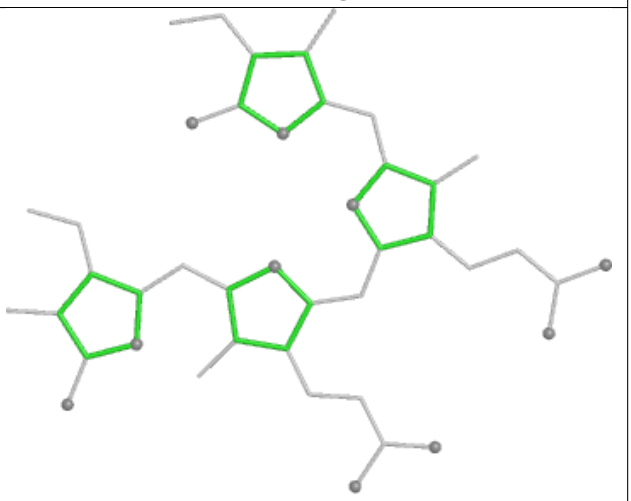

Rings

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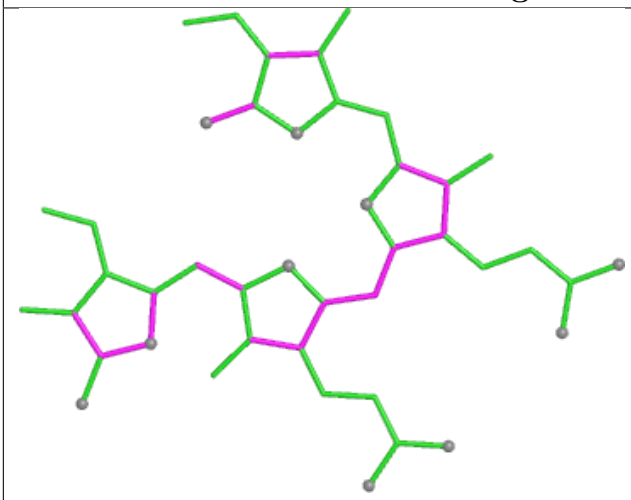

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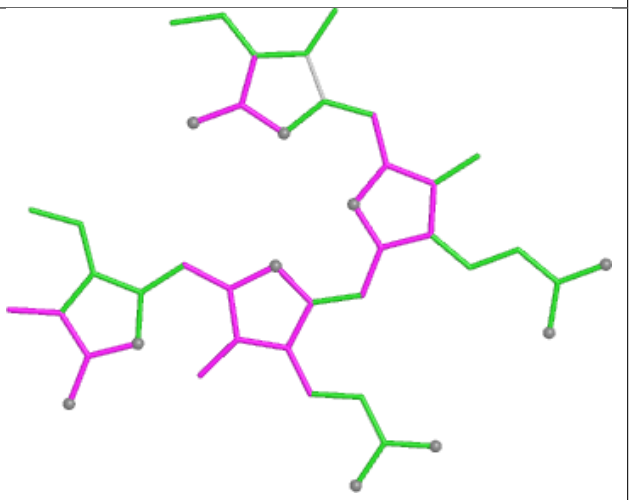

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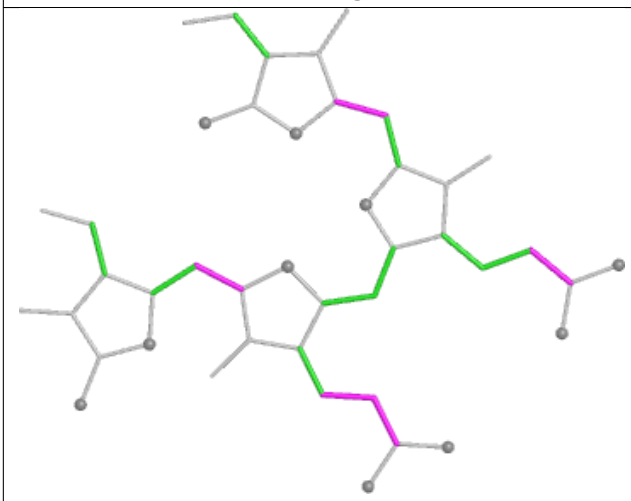

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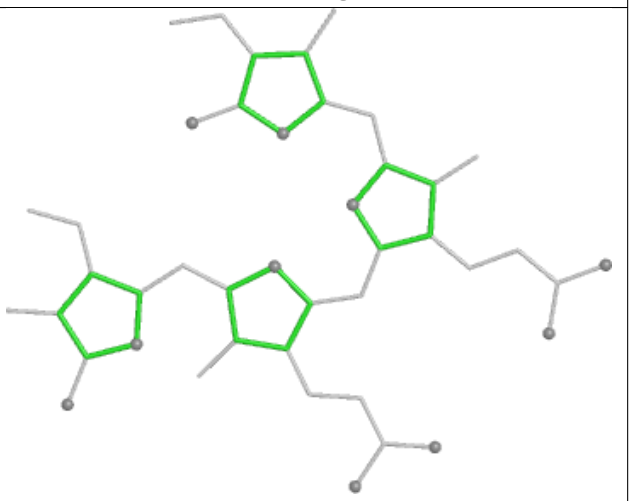
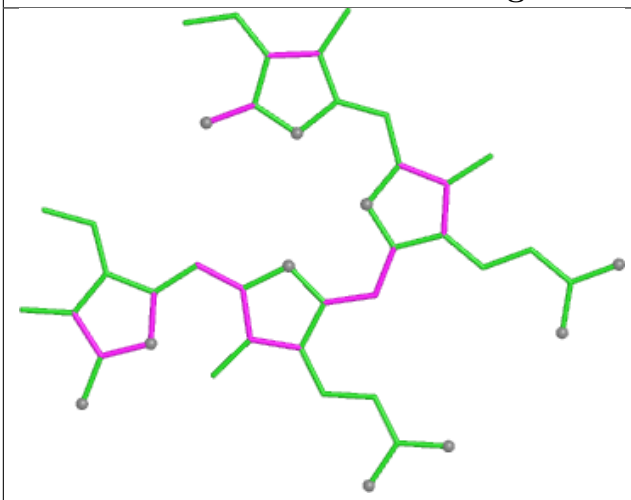


Rings

Ligand PEB OM 201



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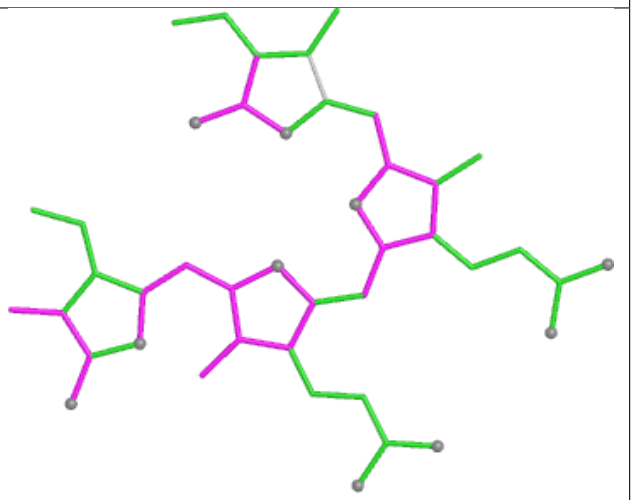

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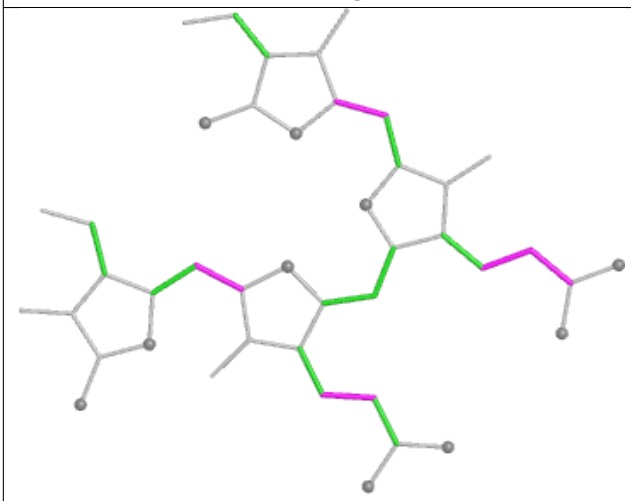

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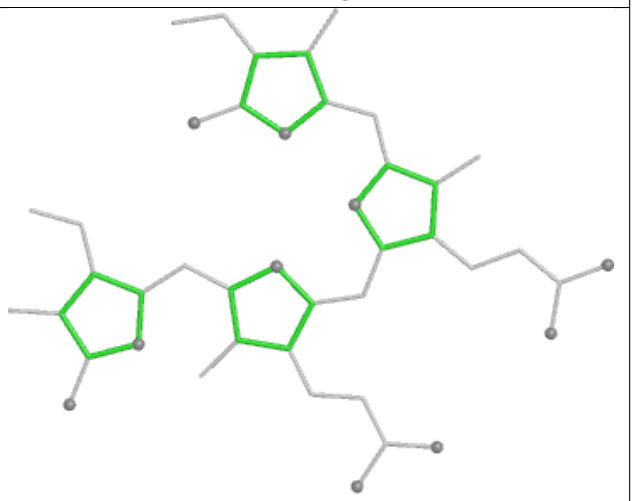
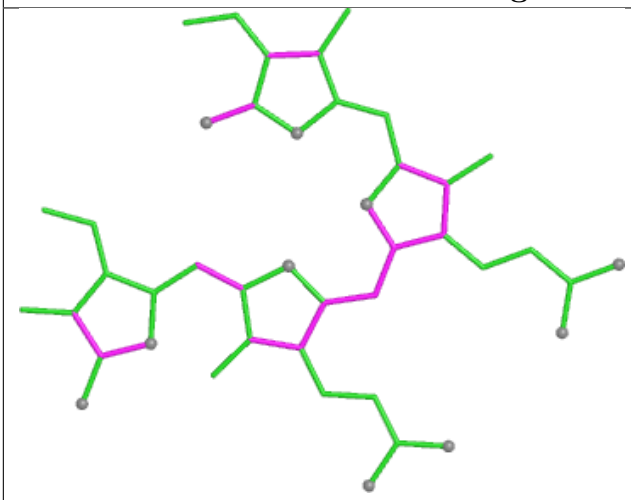


Rings

Ligand PEB AD 304



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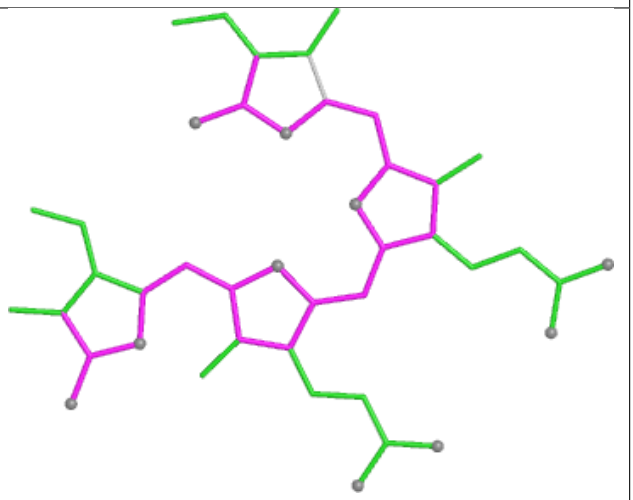

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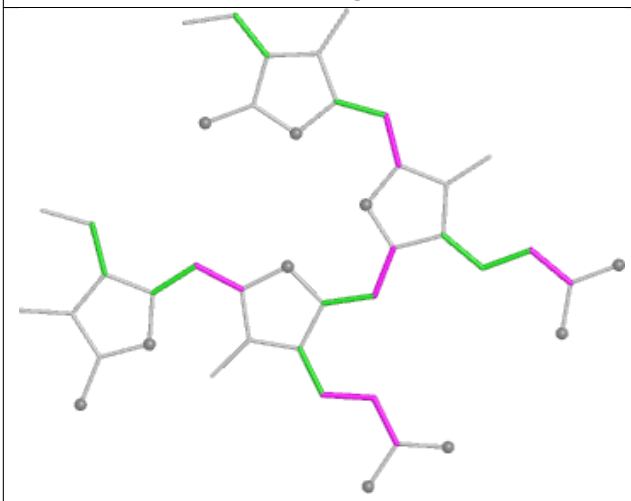

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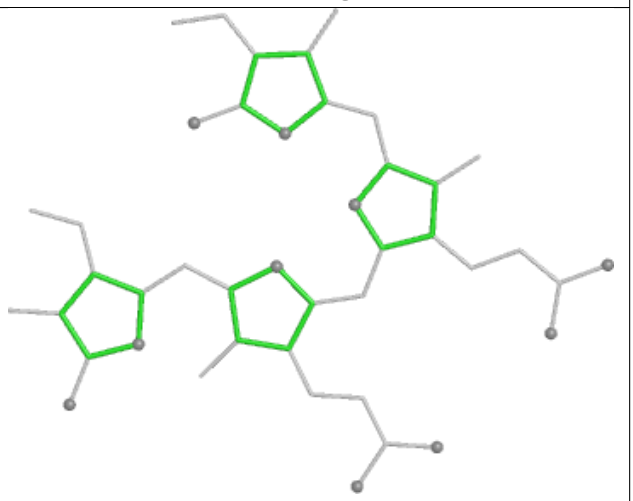

Rings

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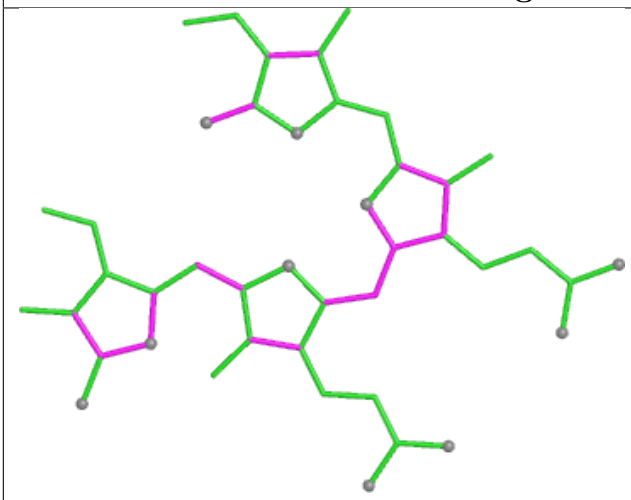

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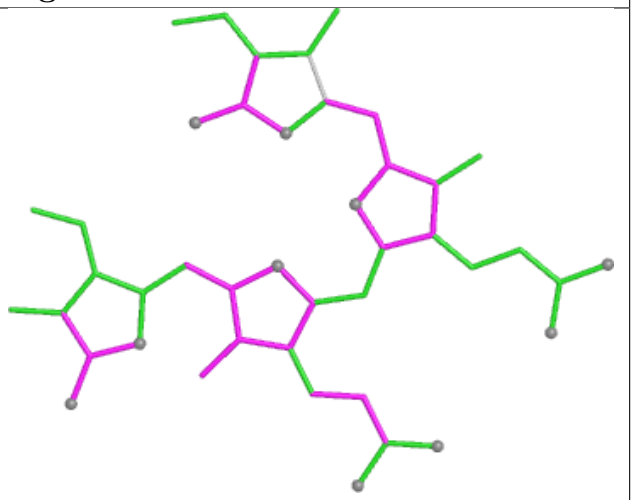

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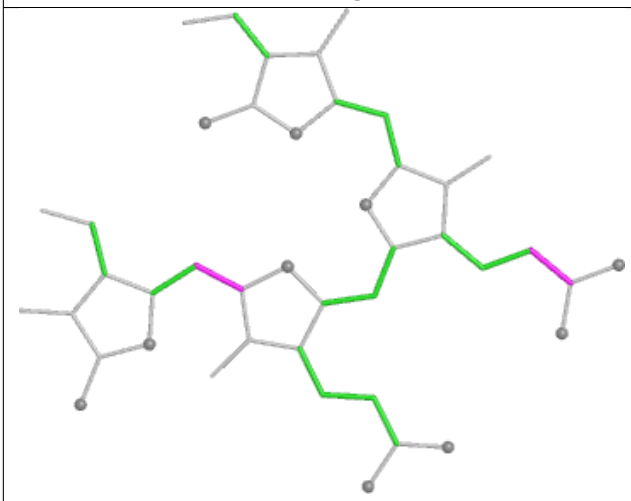

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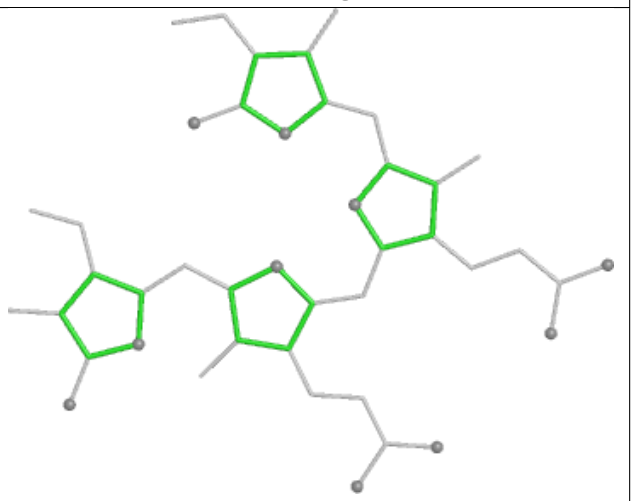

Rings

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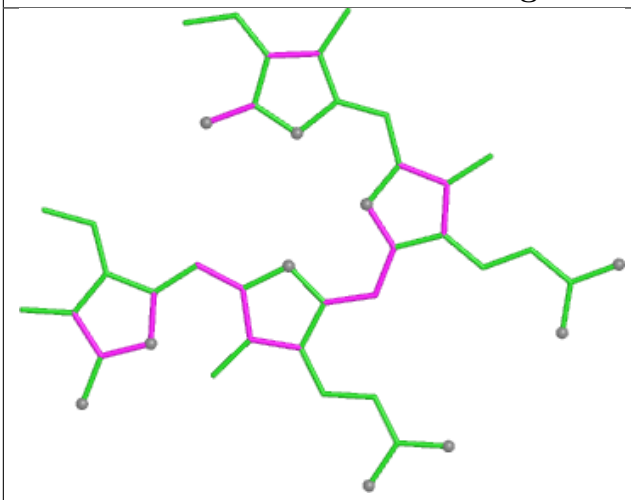

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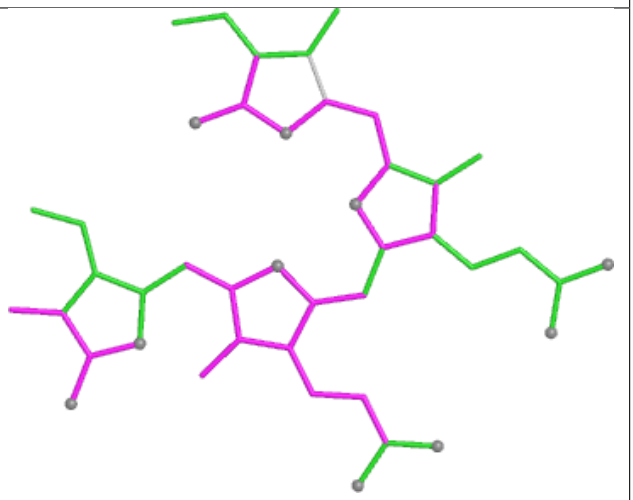

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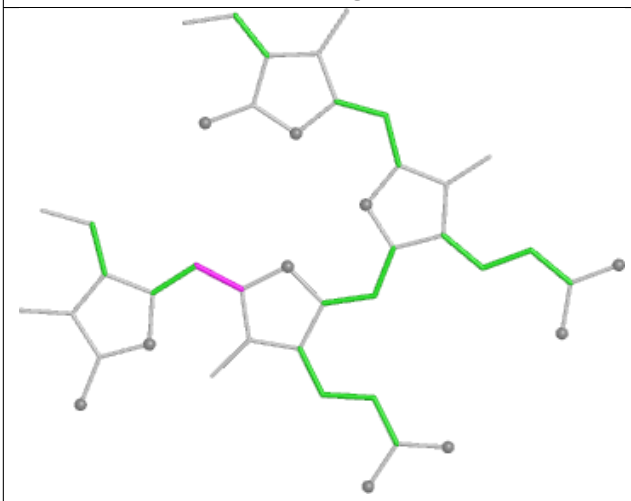

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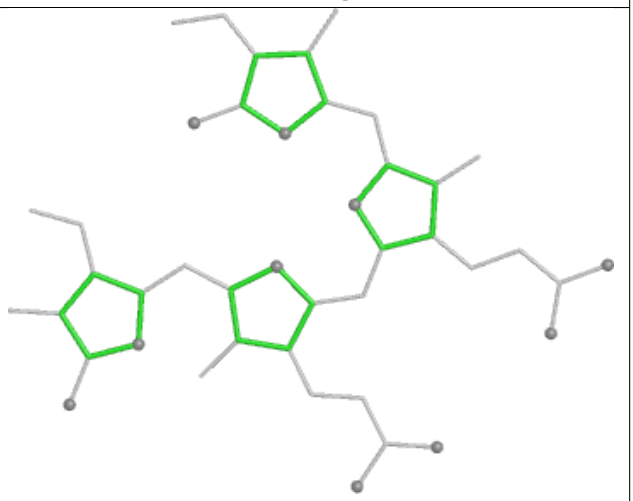

Rings

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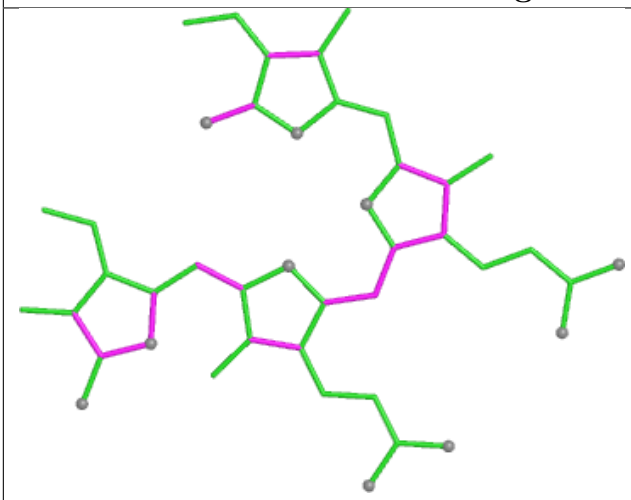

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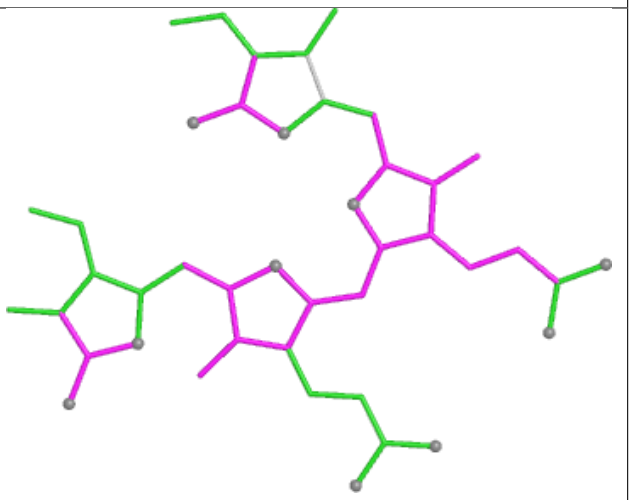

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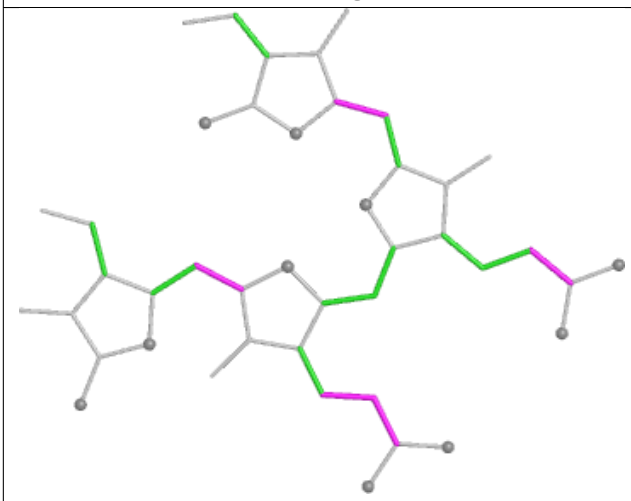

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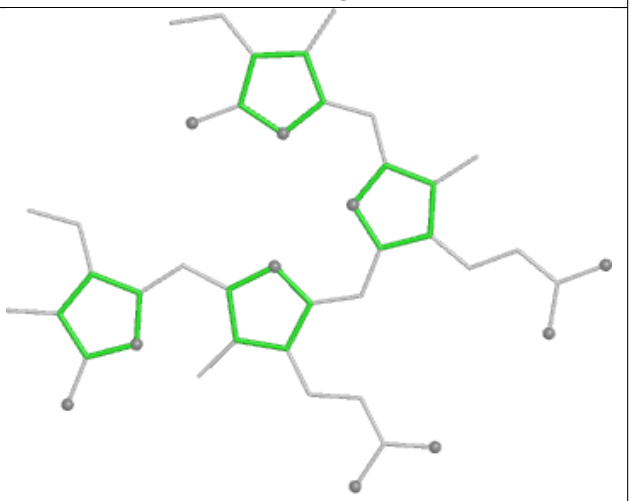

Rings

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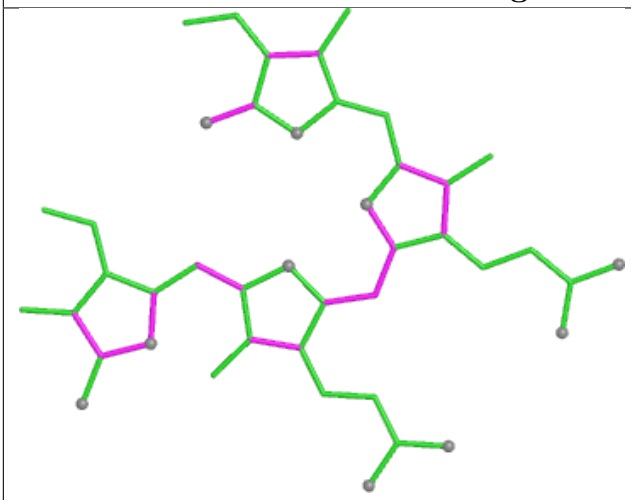

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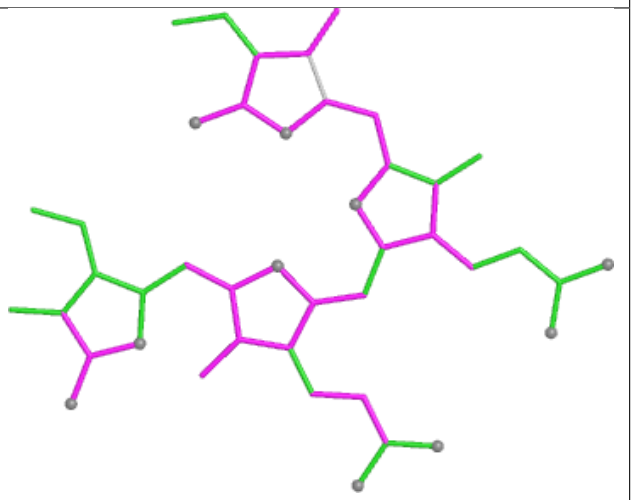

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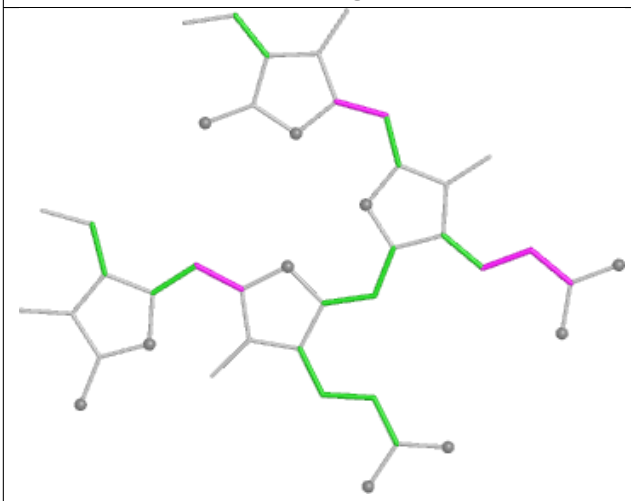

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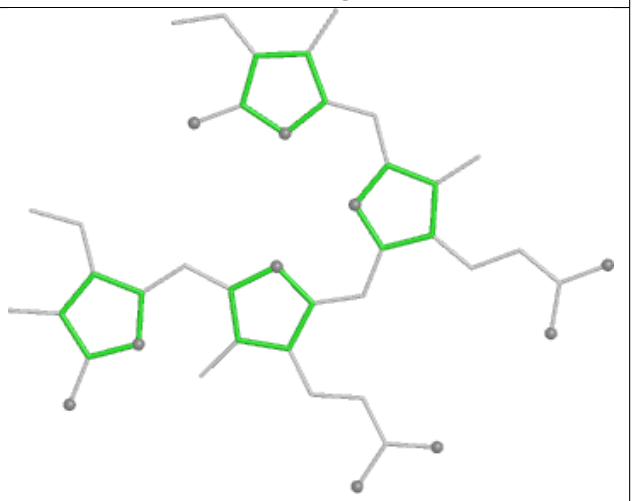
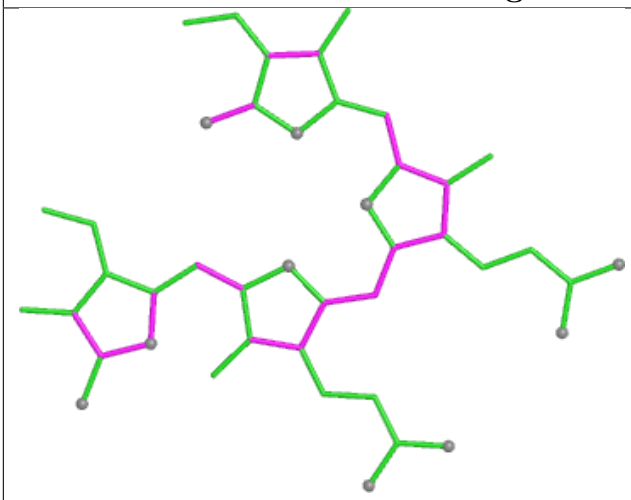


Rings

Ligand PEB H1 1002



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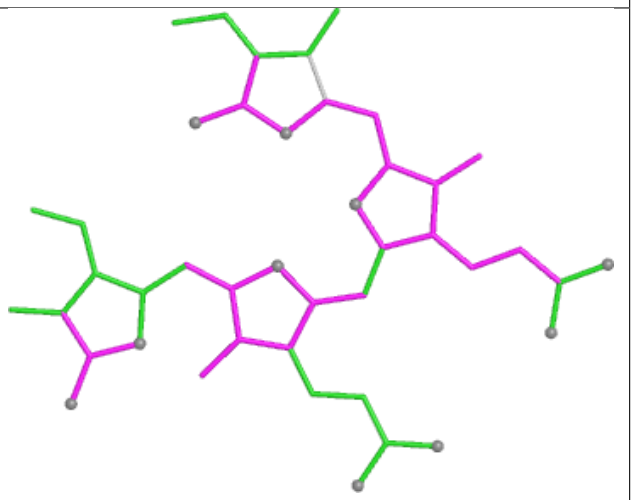

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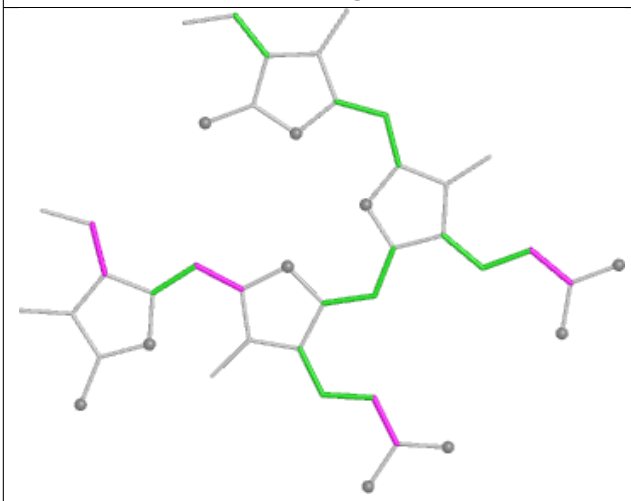

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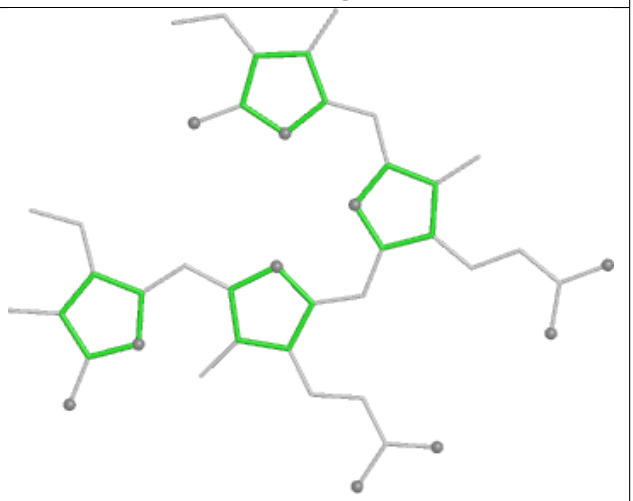
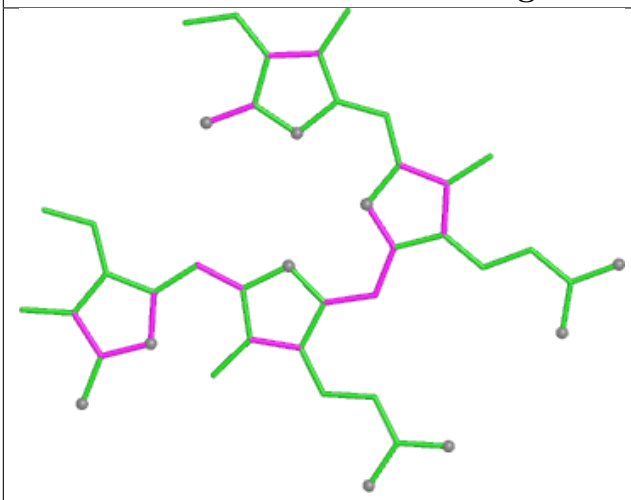


Rings

Ligand PEB Z4 202



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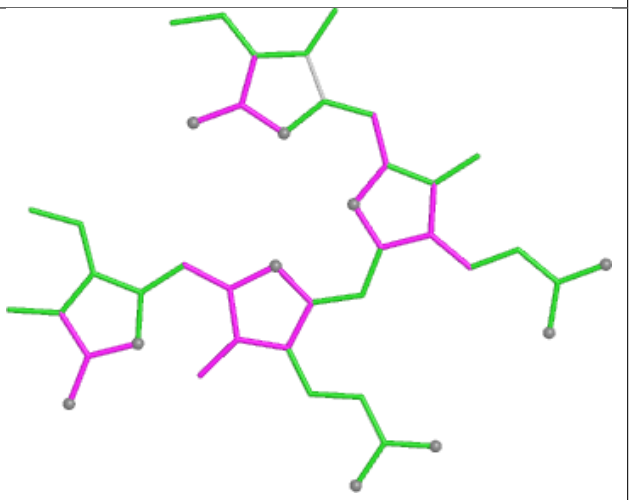

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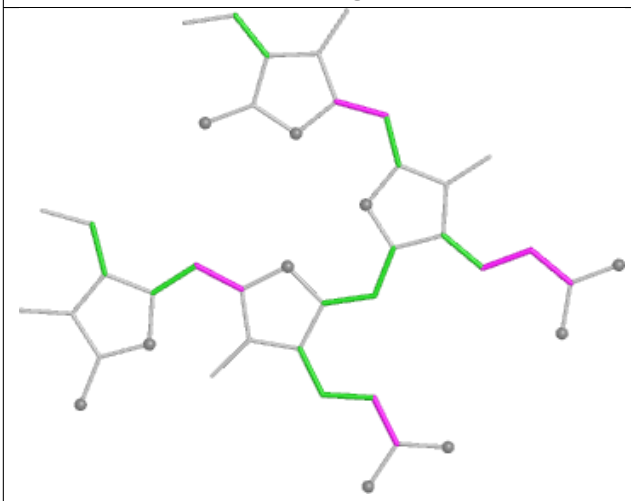

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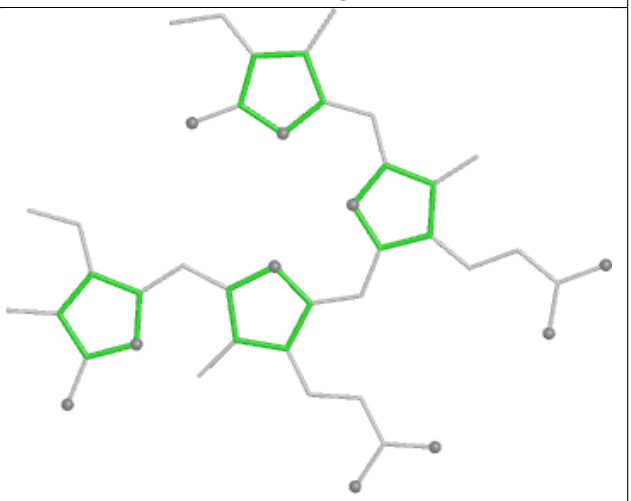
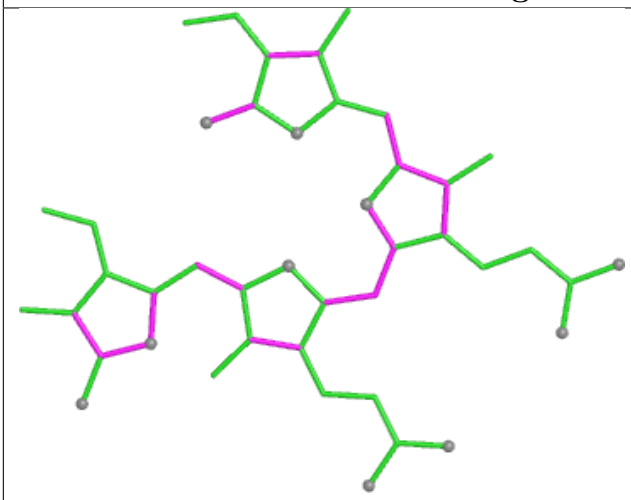


Rings

Ligand PEB gM 201



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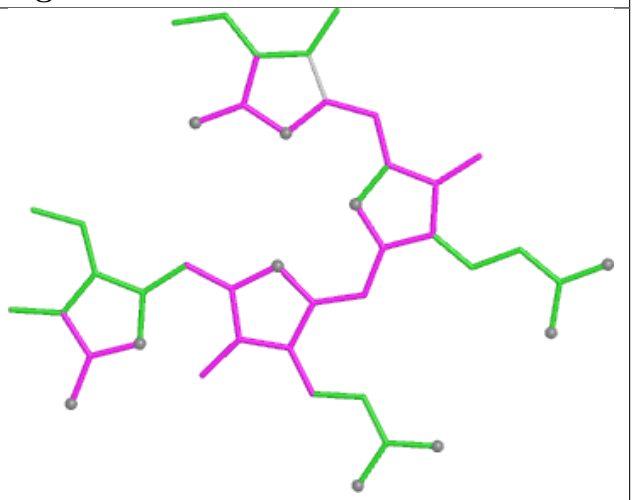

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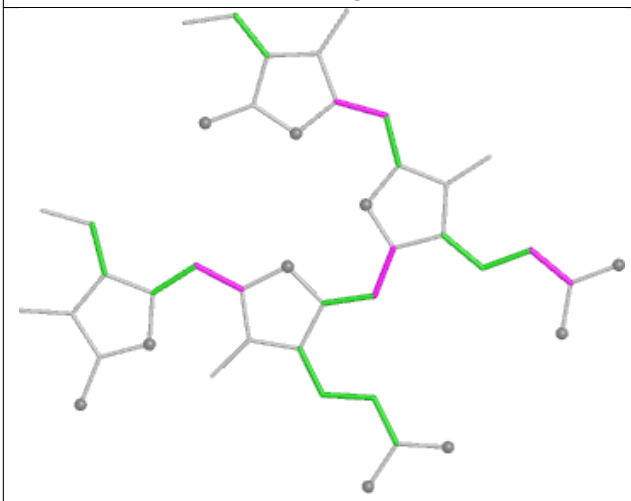

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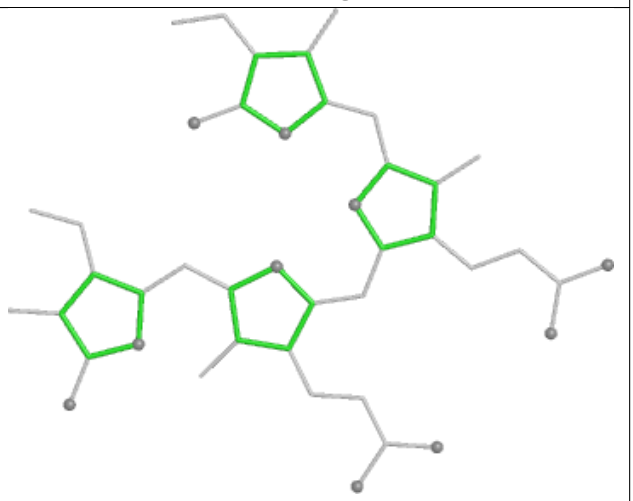
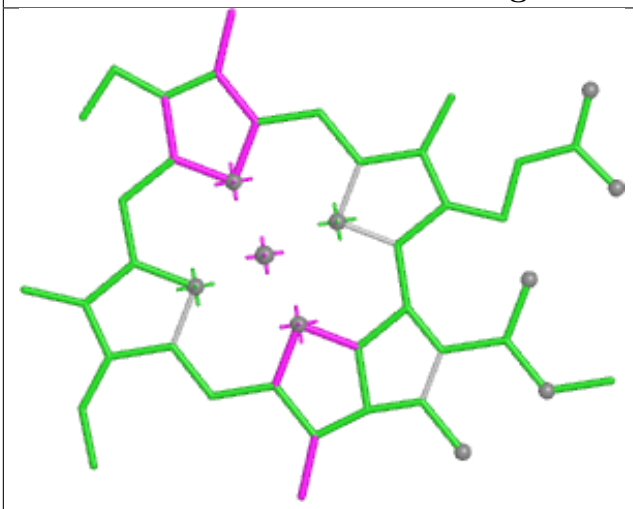


Rings

Ligand CLA AN 822



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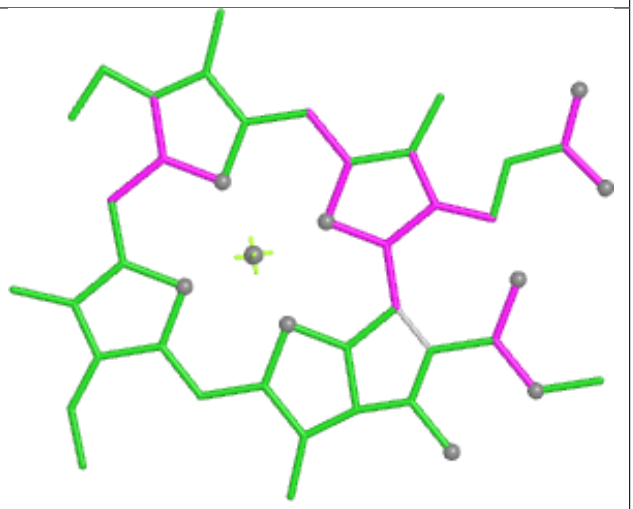

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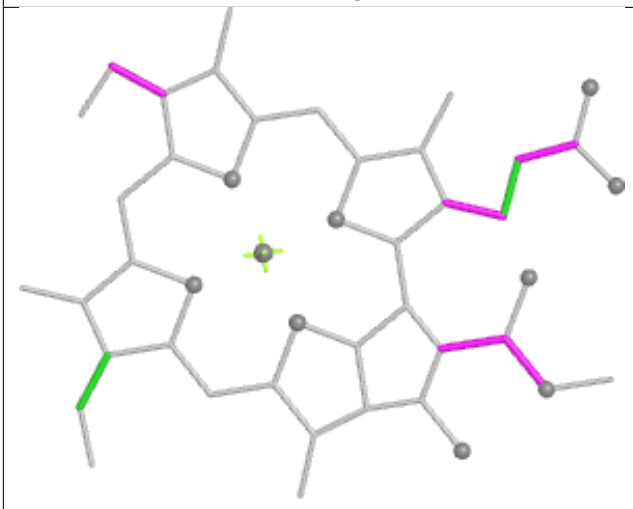
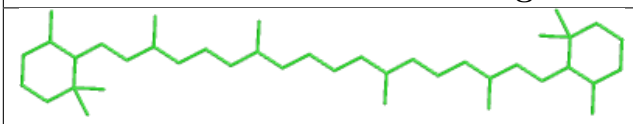


Torsions



Rings

Ligand BCR L2 205



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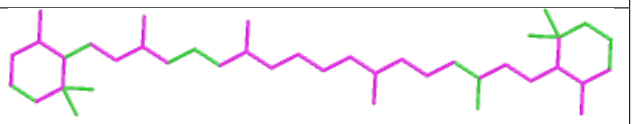
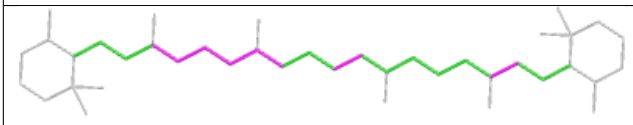


Bond angles



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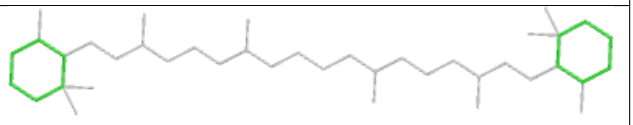
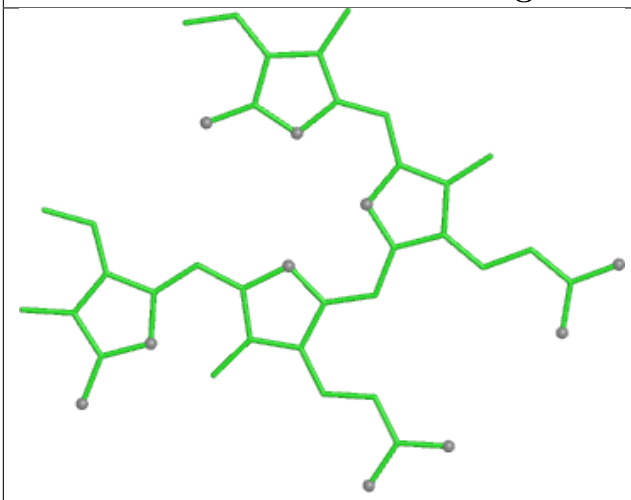


Rings

Ligand PEB yC 201



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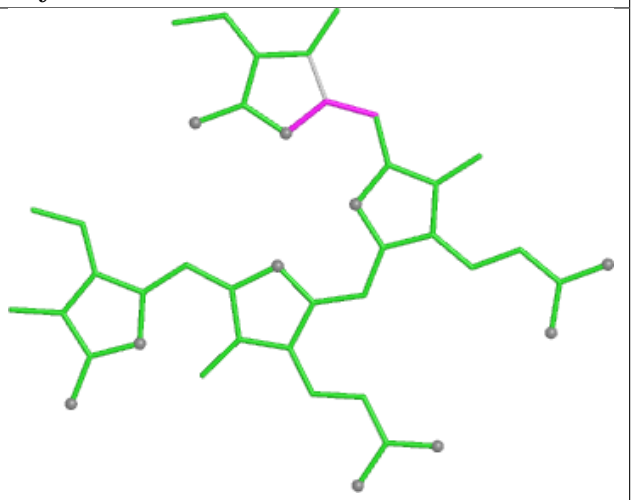
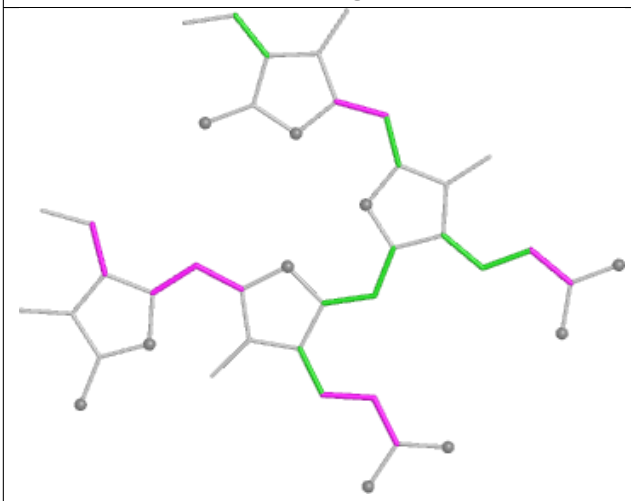


Bond angles



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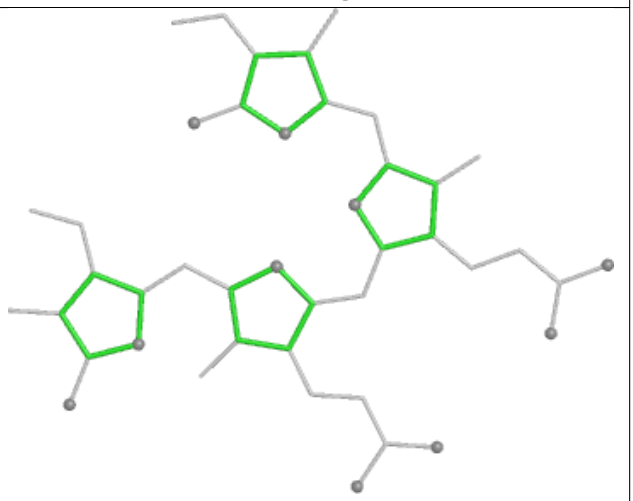
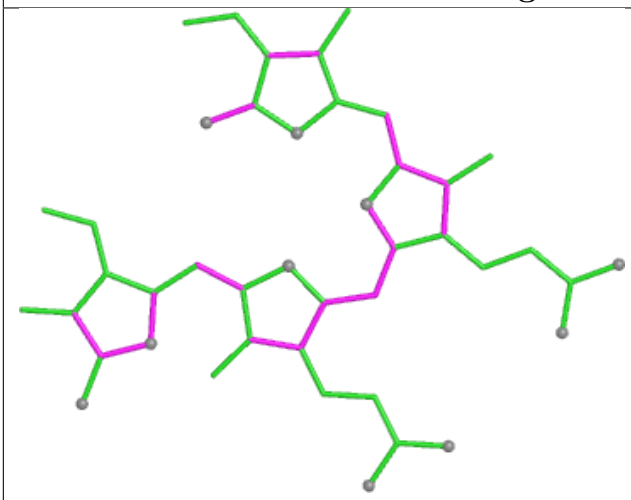


Rings

Ligand PEB fK 202



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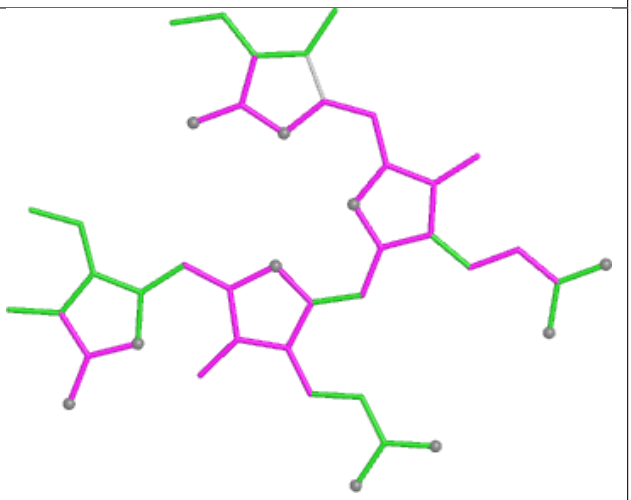
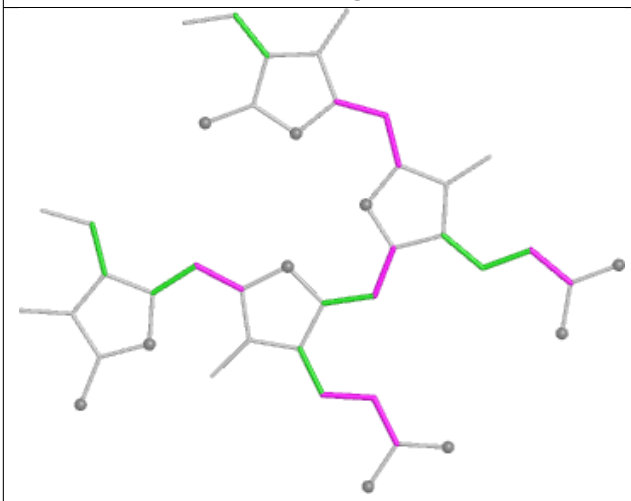
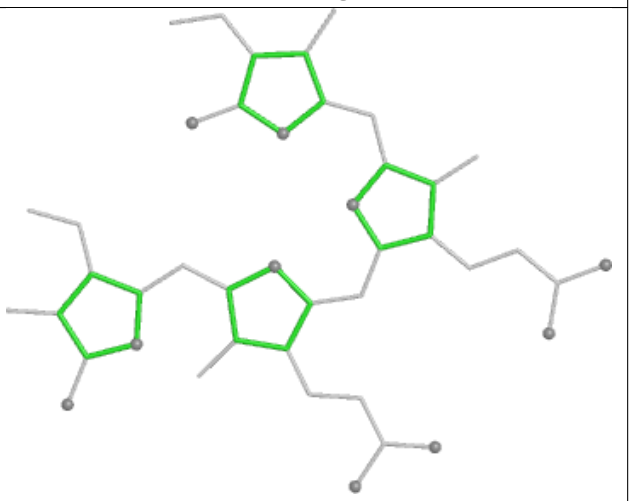


Bond angles

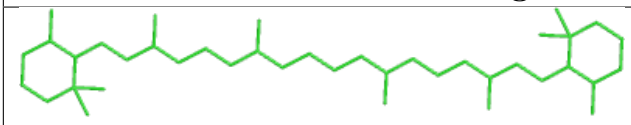


Torsions



Rings

Ligand BCR AL 401



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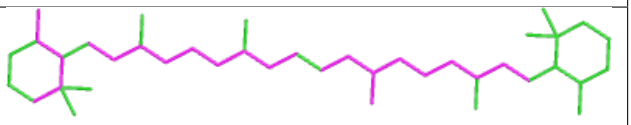

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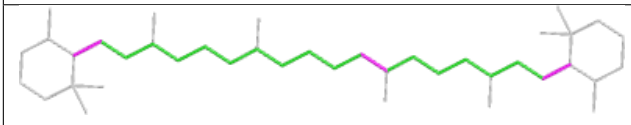

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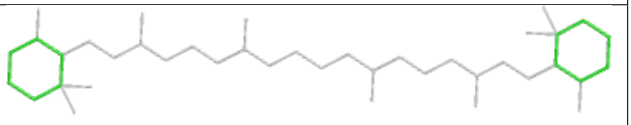
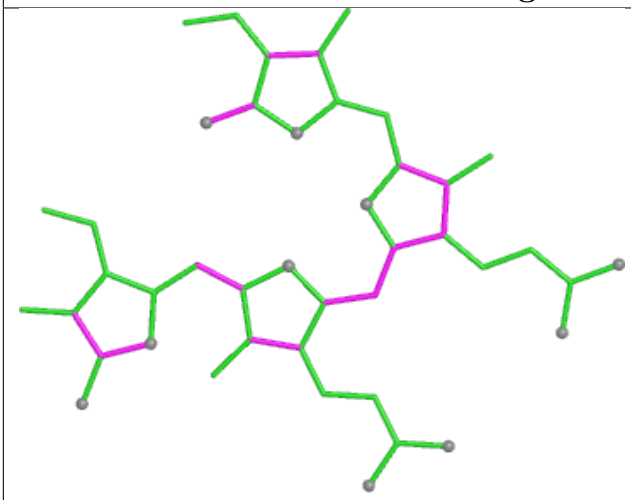


Rings

Ligand PEB BI 203



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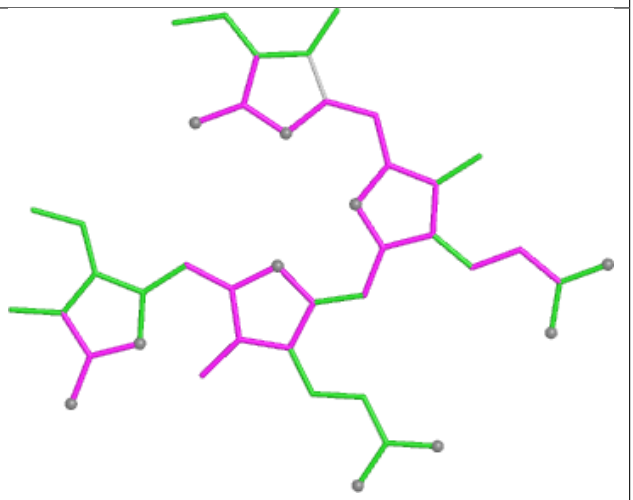

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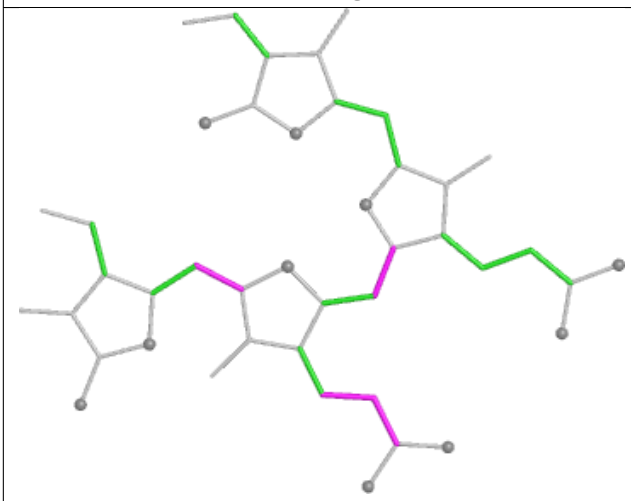

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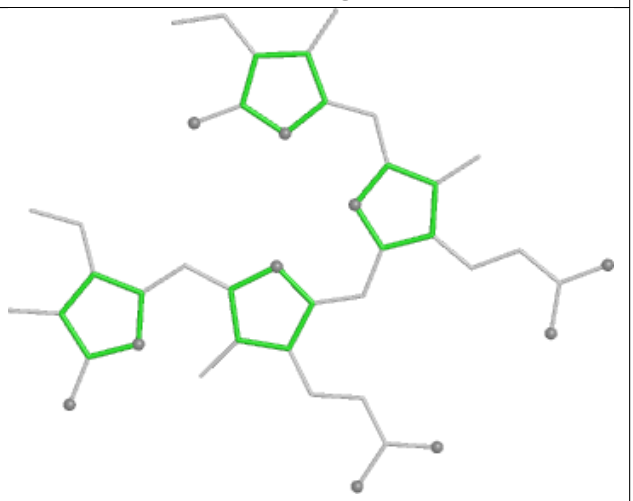
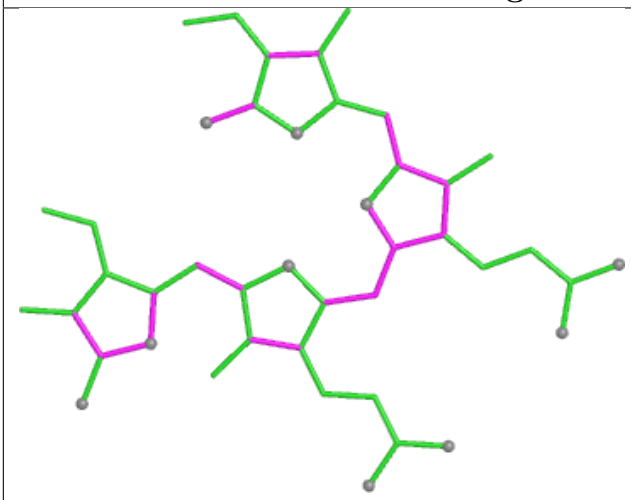


Rings

Ligand PEB LE 1002



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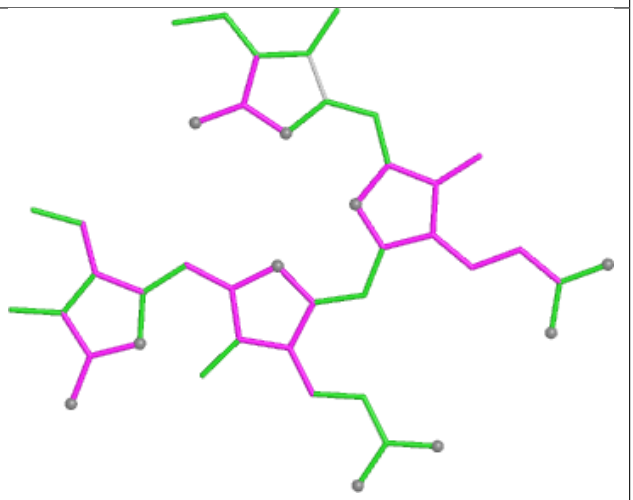

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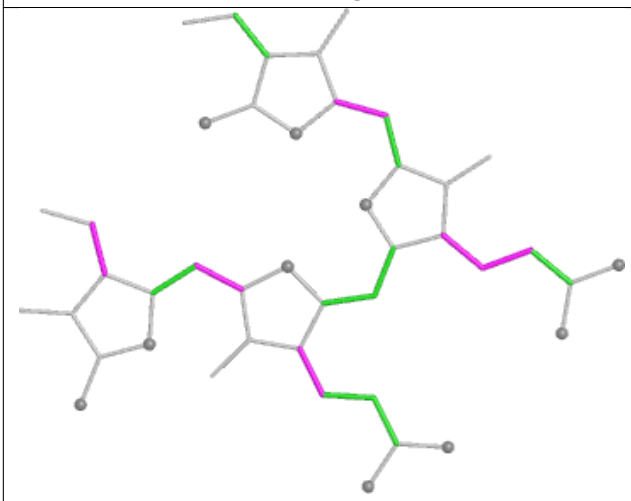

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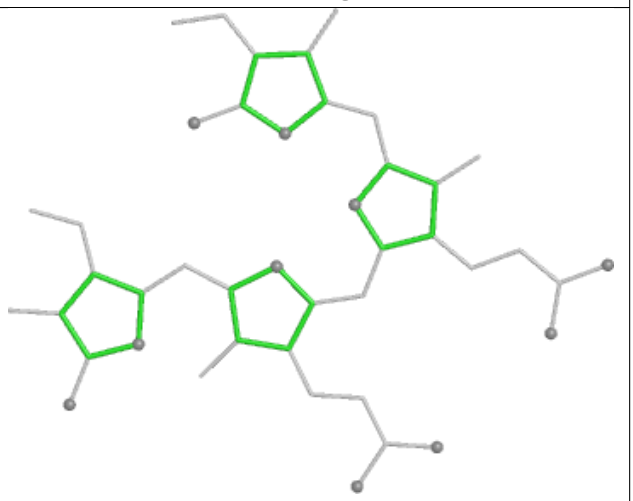
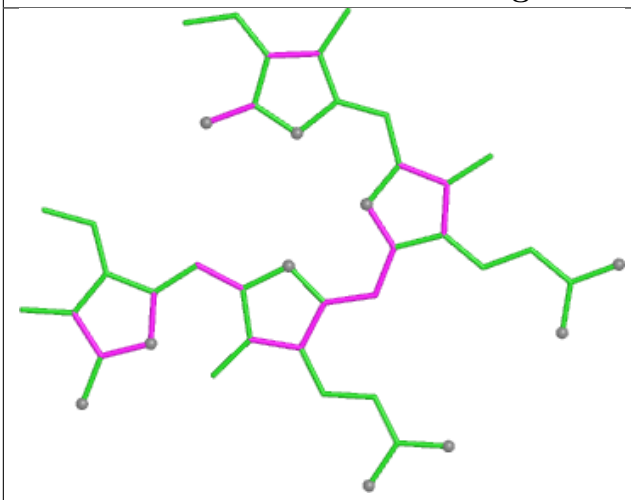


Rings

Ligand PEB EK 202



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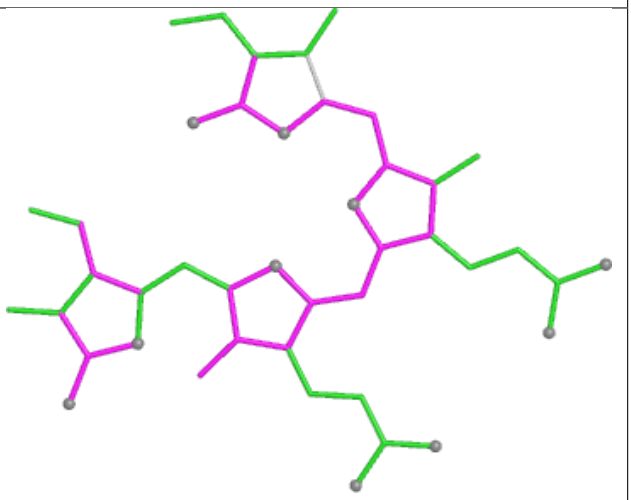
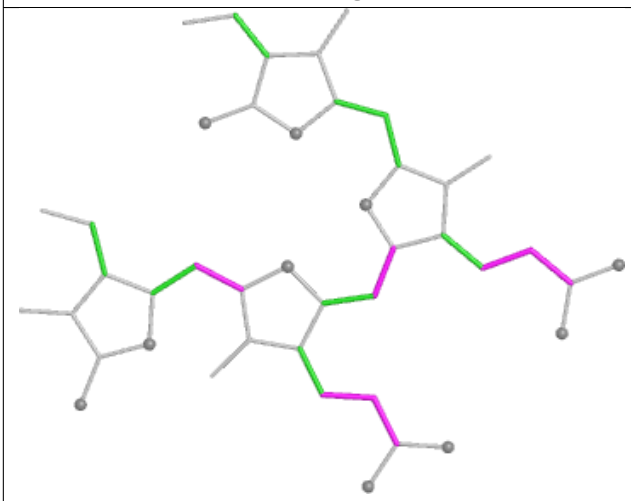


Bond angles



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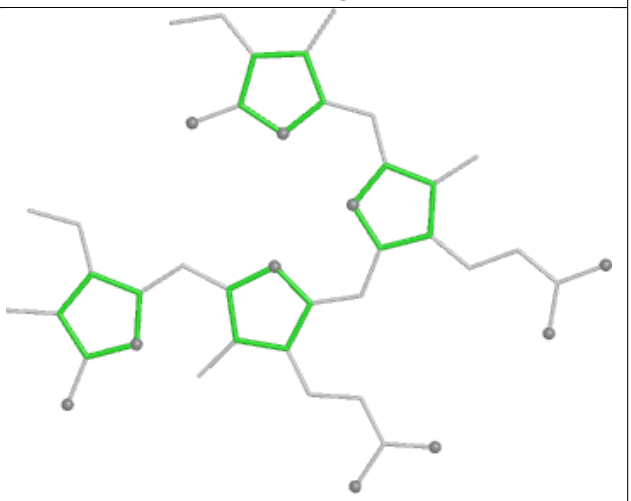
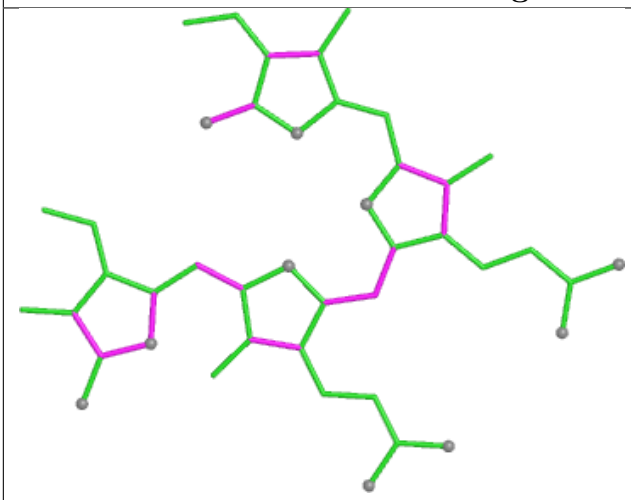


Rings

Ligand PEB mF 201



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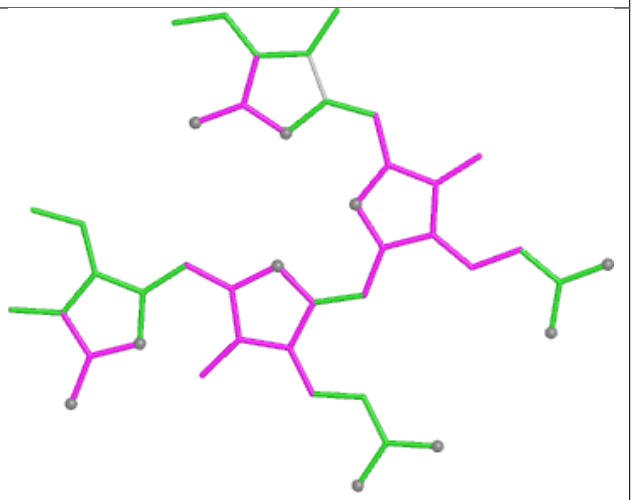

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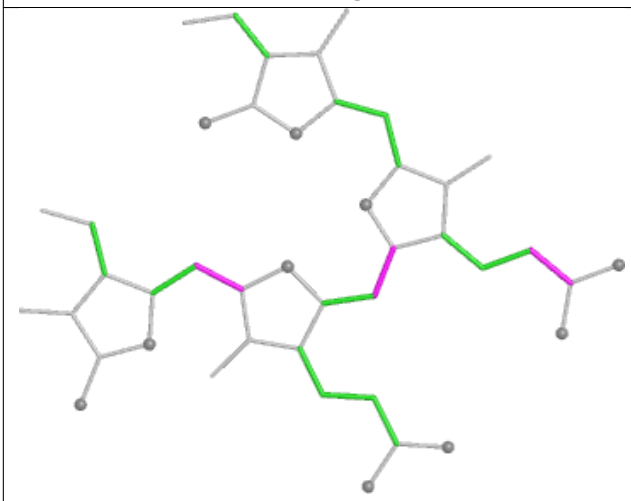

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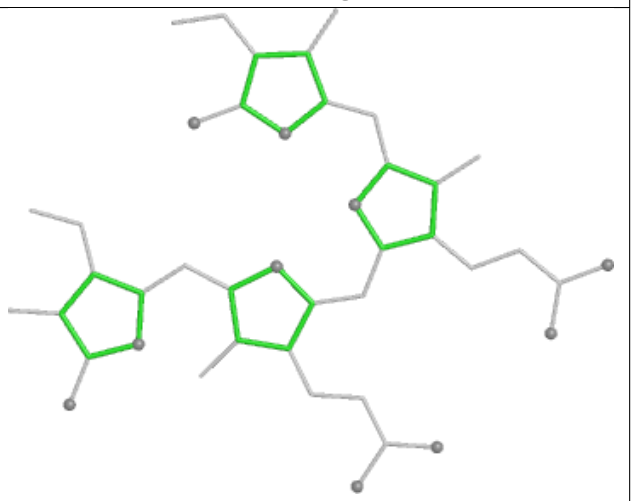

Rings

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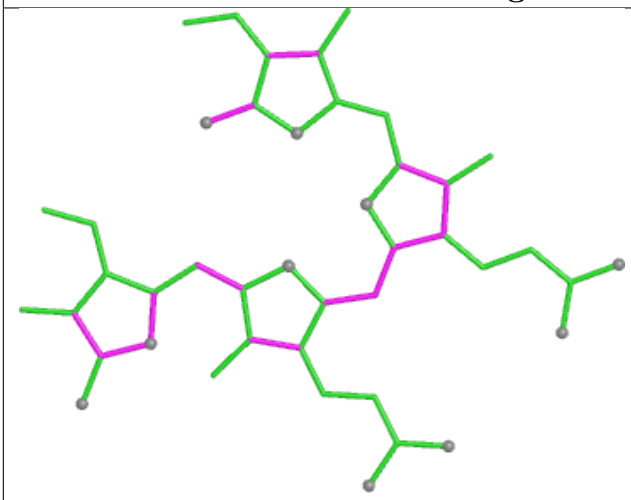

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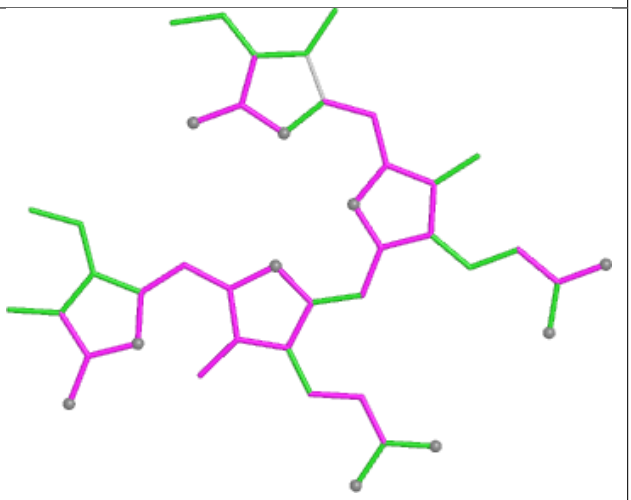

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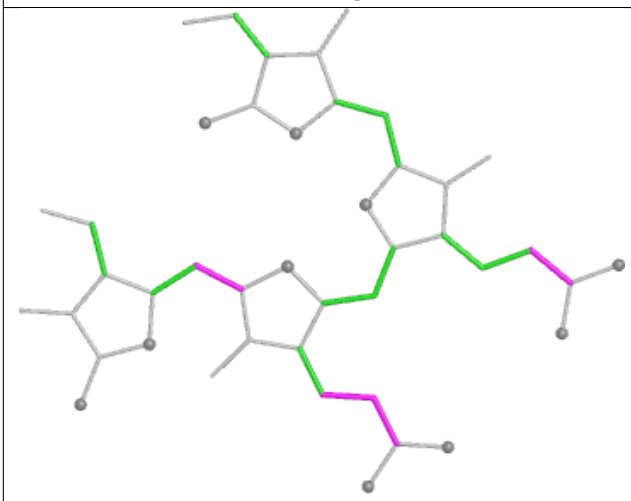

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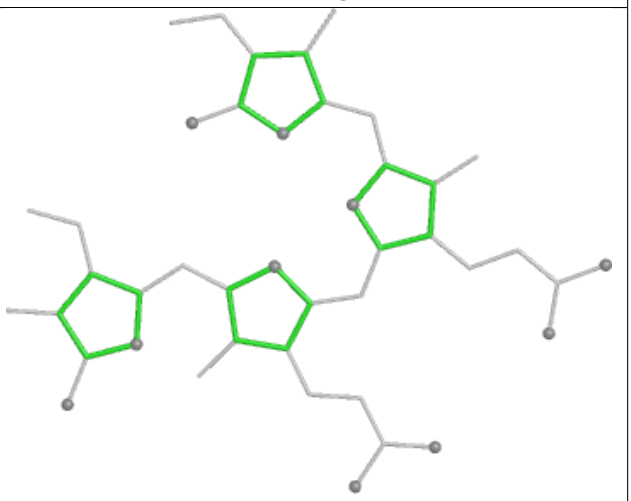
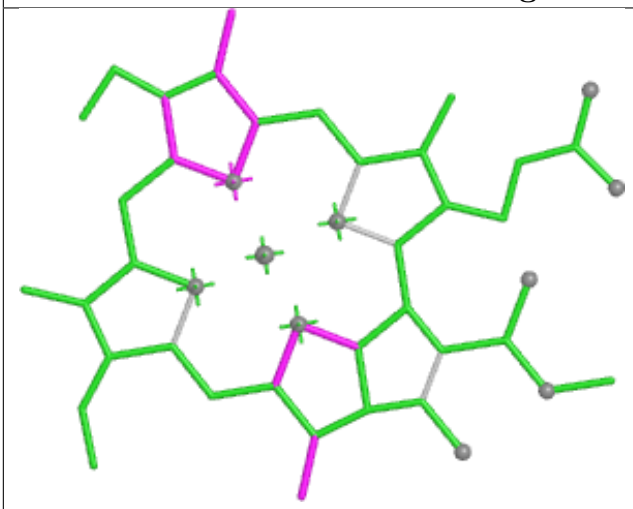


Rings

Ligand CLA 42 605



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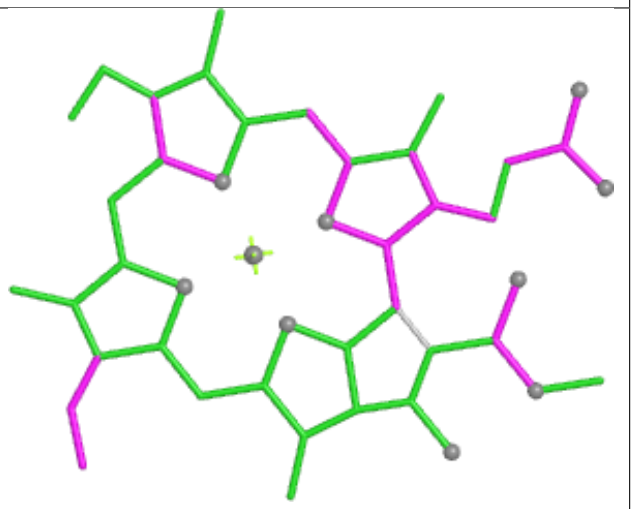

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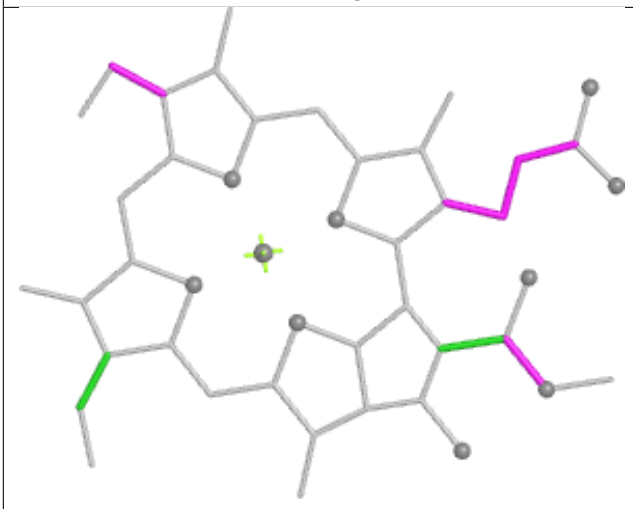
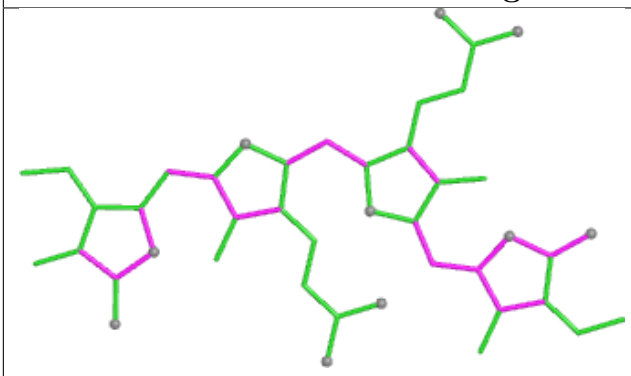


Torsions



Rings

Ligand CYC K4 1001



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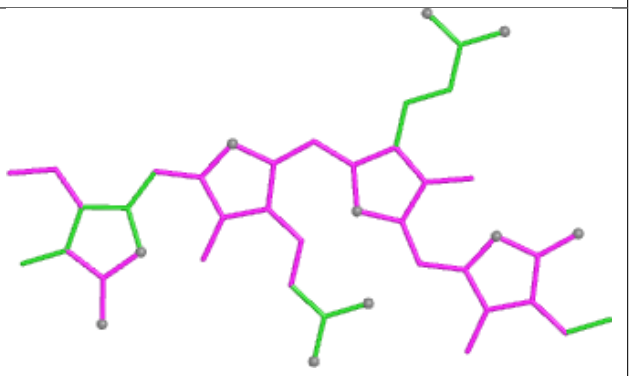

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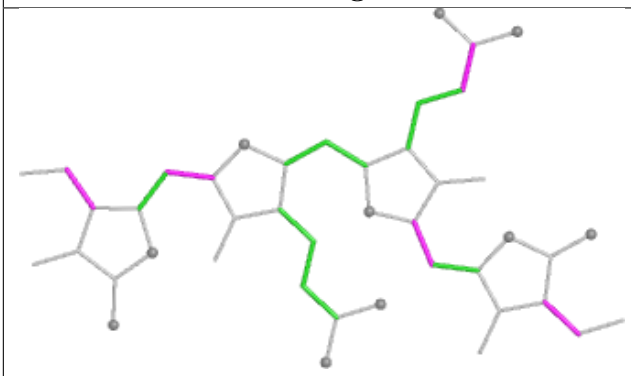

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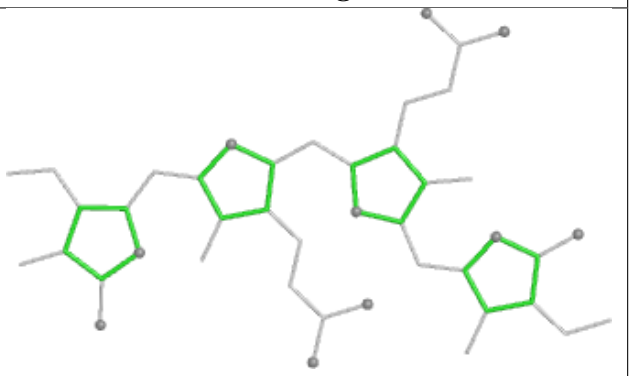
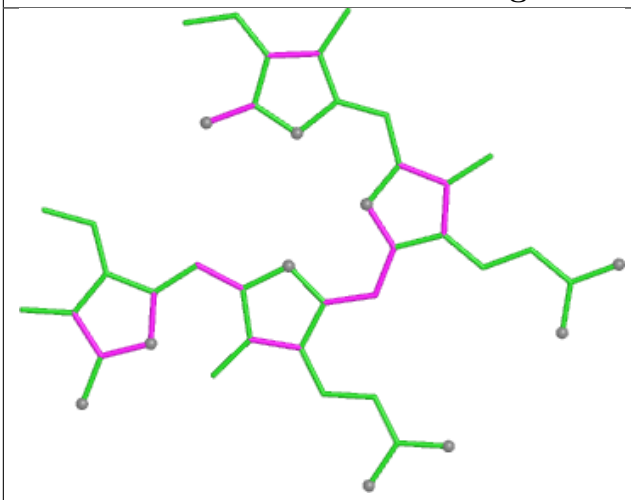


Rings

Ligand PEB HK 202



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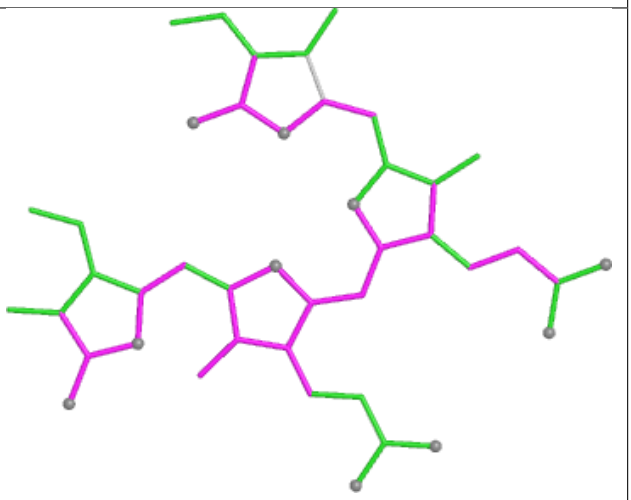
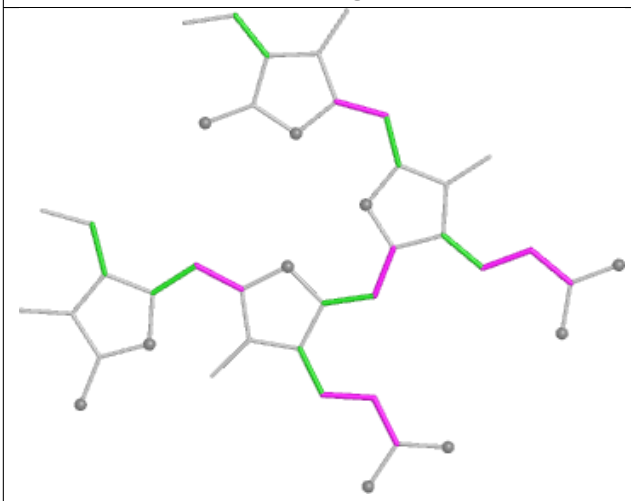


Bond angles



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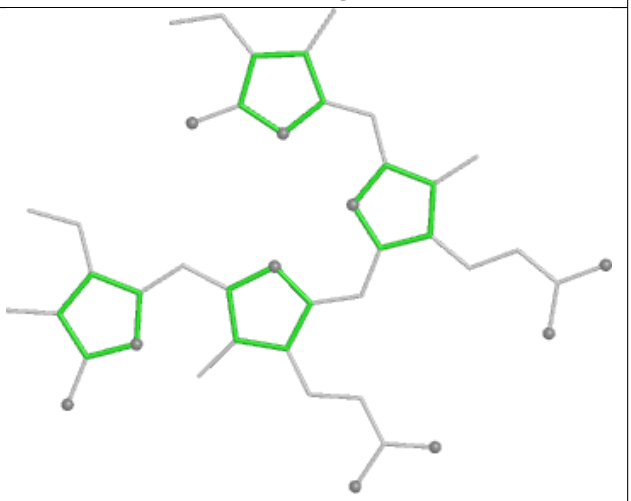
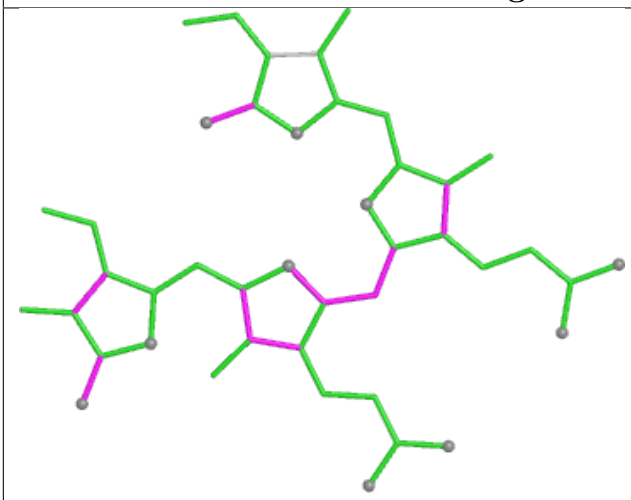


Rings

Ligand PUB KA 203



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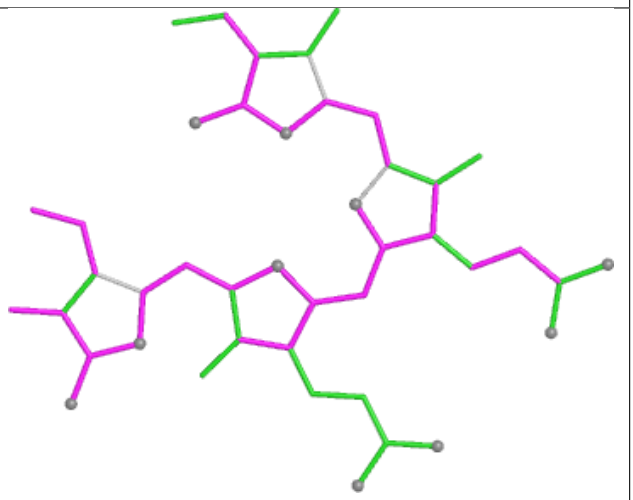
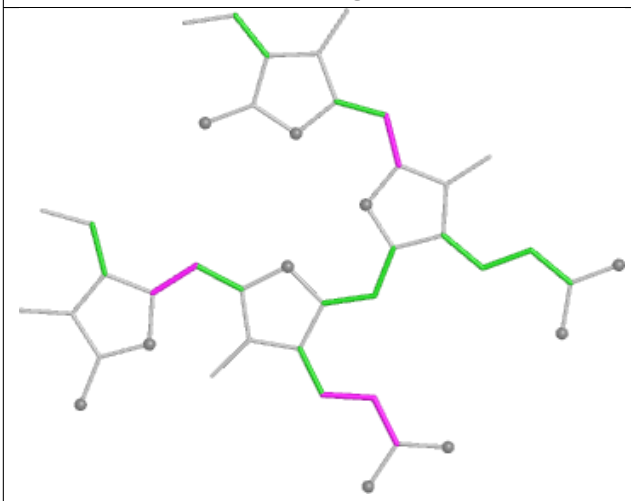


Bond angles



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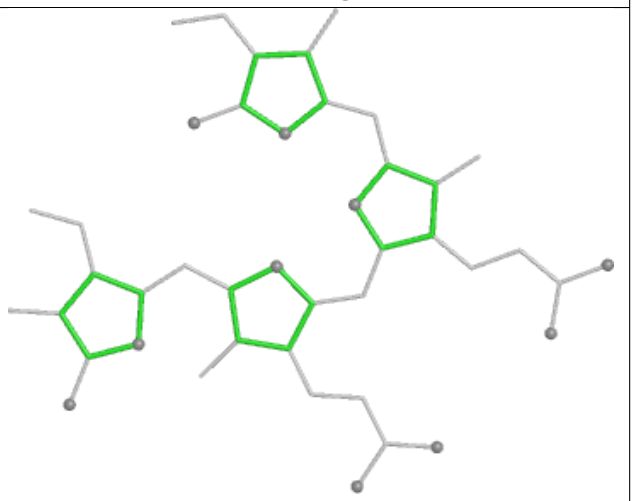
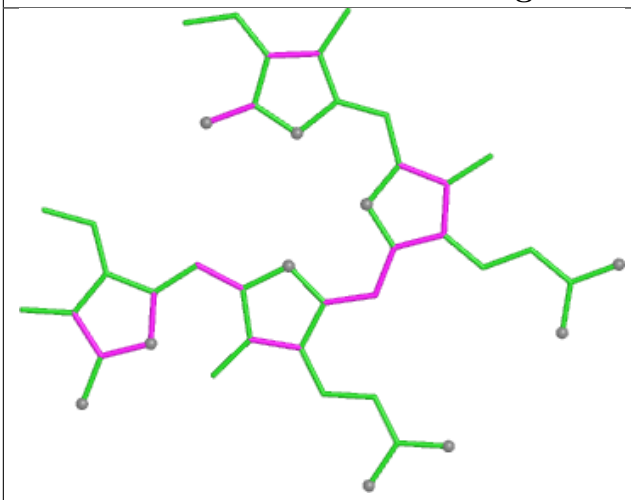


Rings

Ligand PEB jM 201



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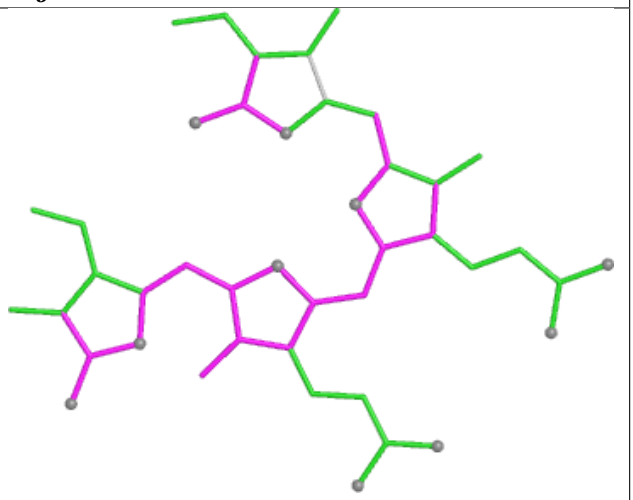
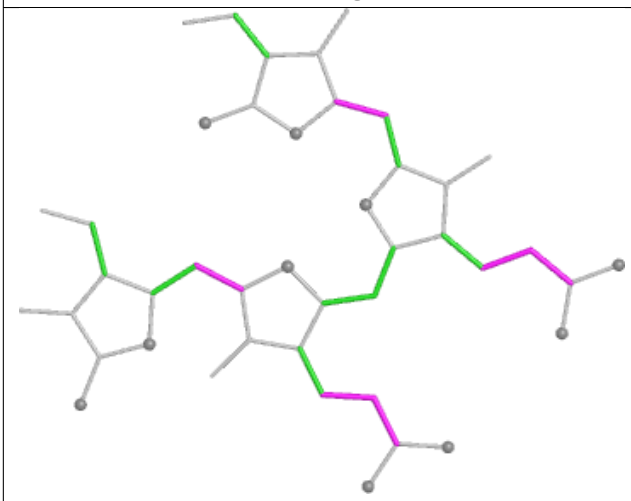


Bond angles



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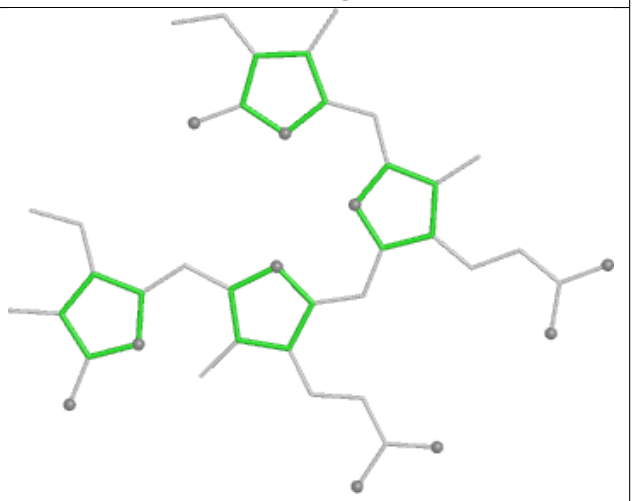
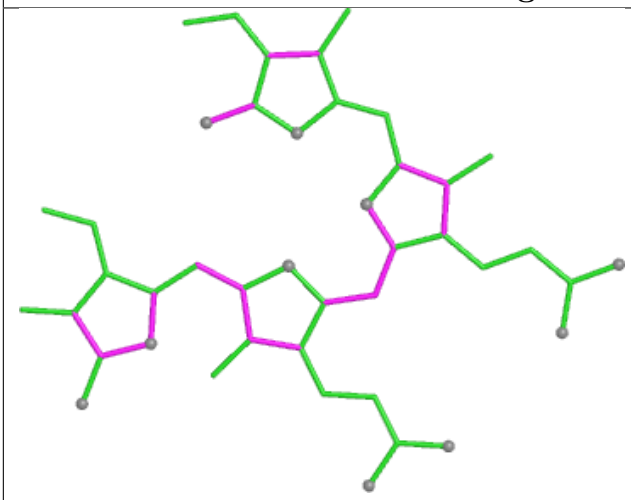


Rings

Ligand PEB Z5 304



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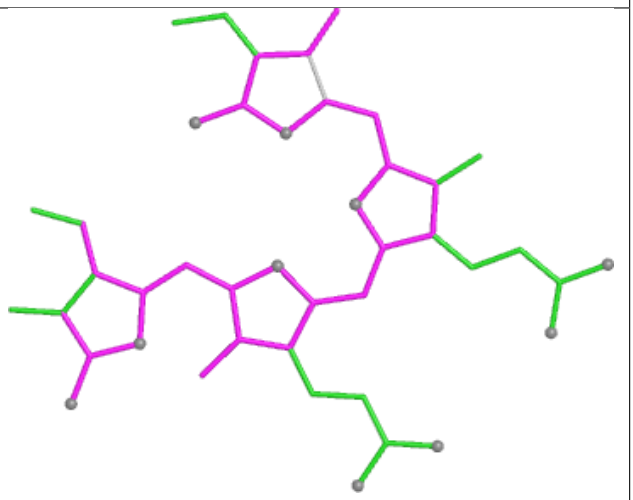
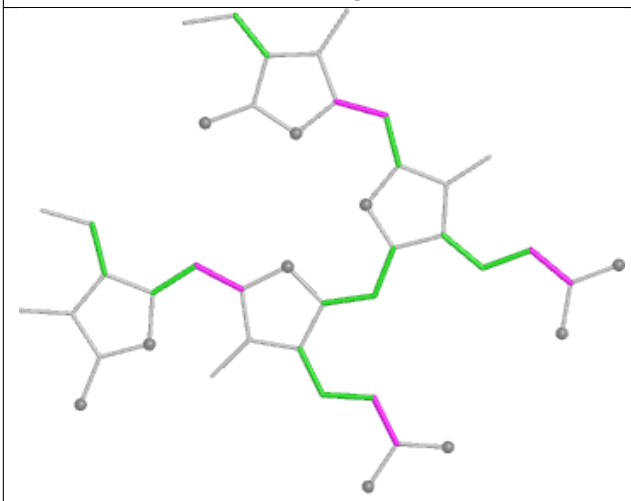


Bond angles



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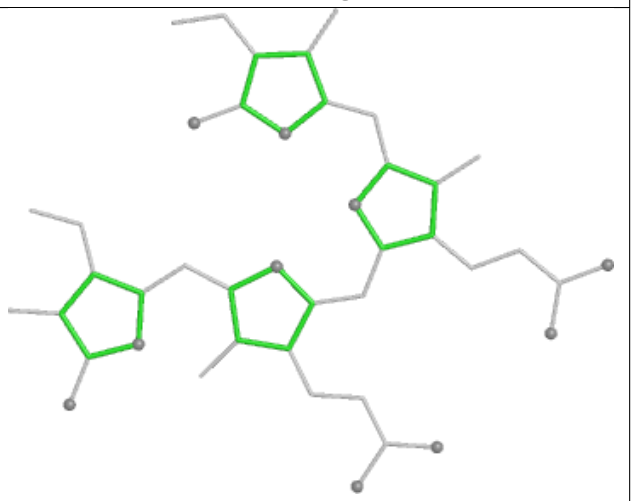
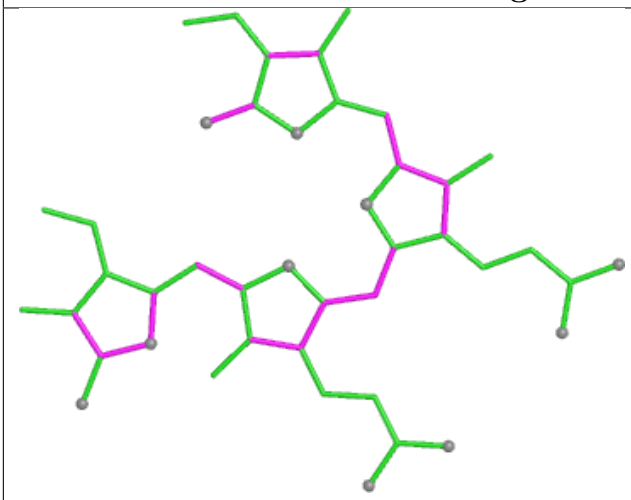
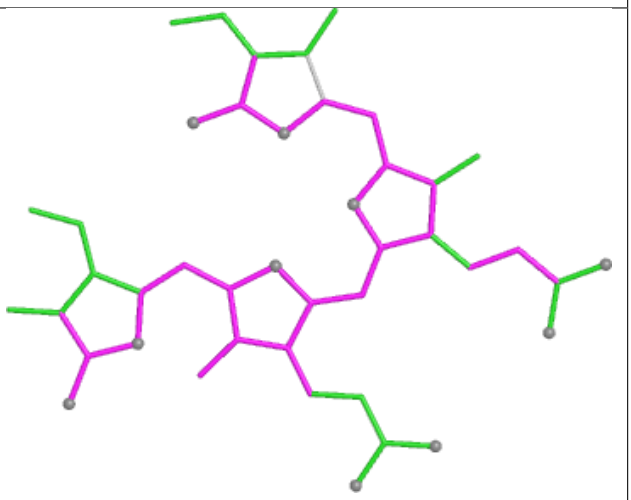


Rings

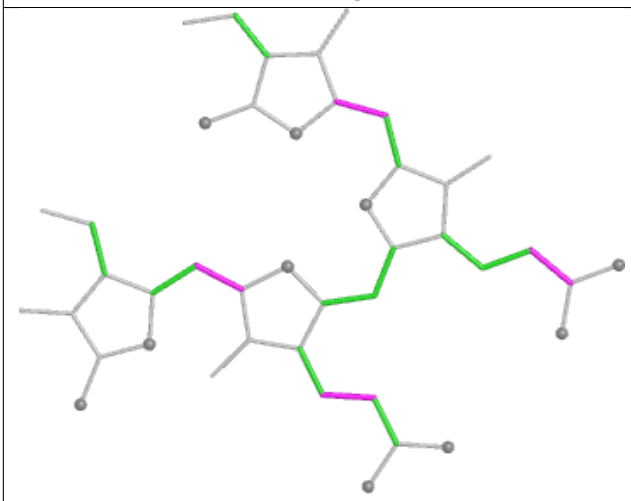
Ligand PEB OK 201



Bond lengths



Bond angles



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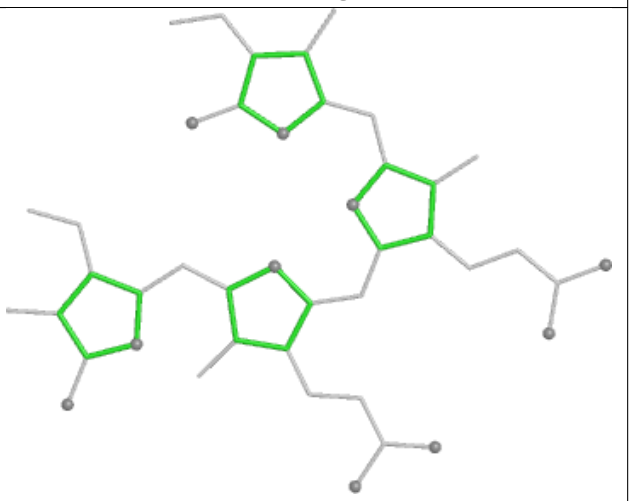
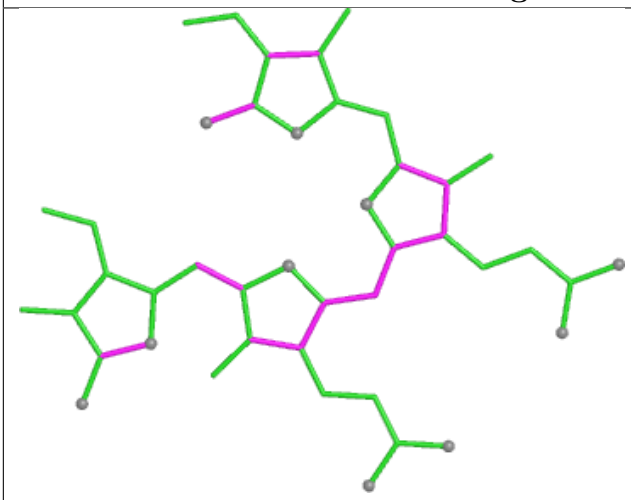


Rings

Ligand PEB XD 201



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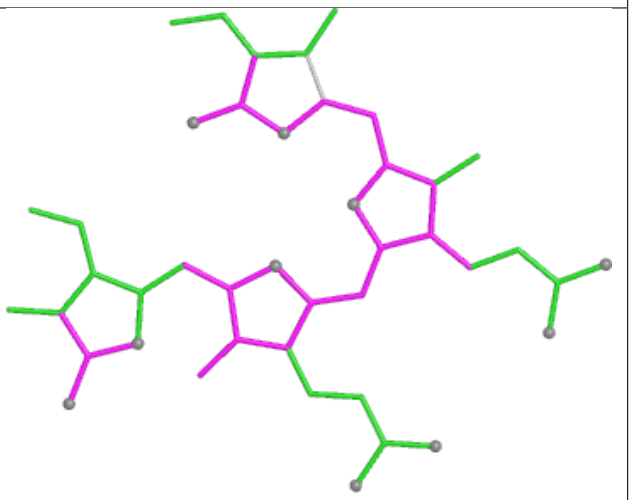
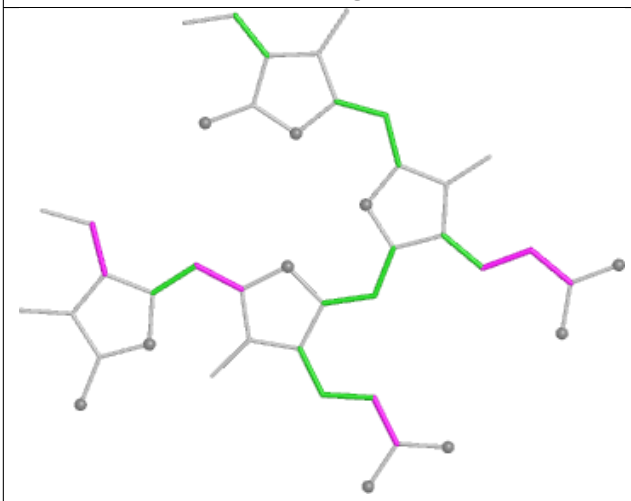


Bond angles



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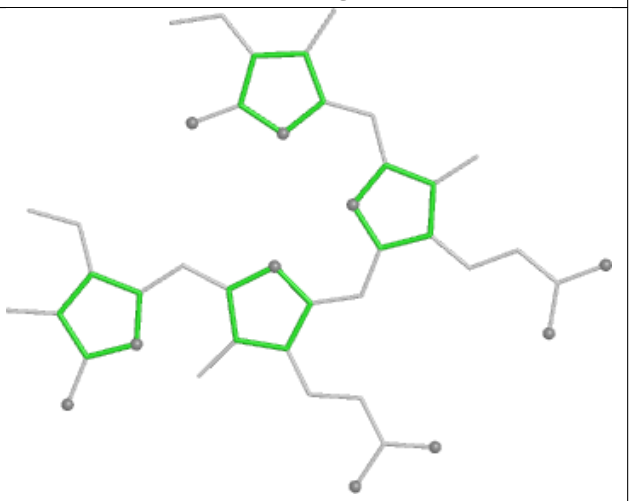
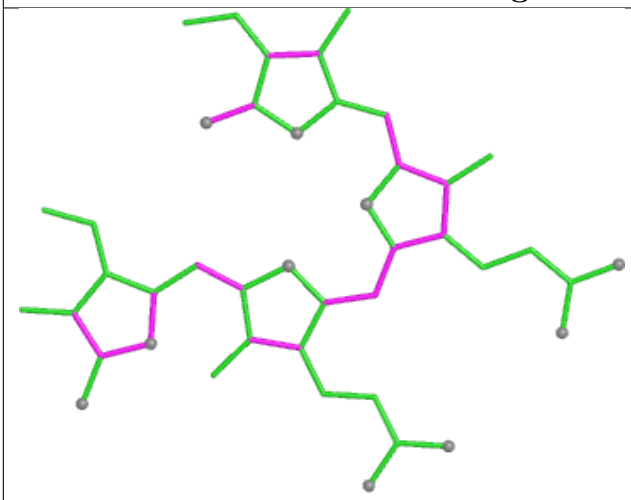
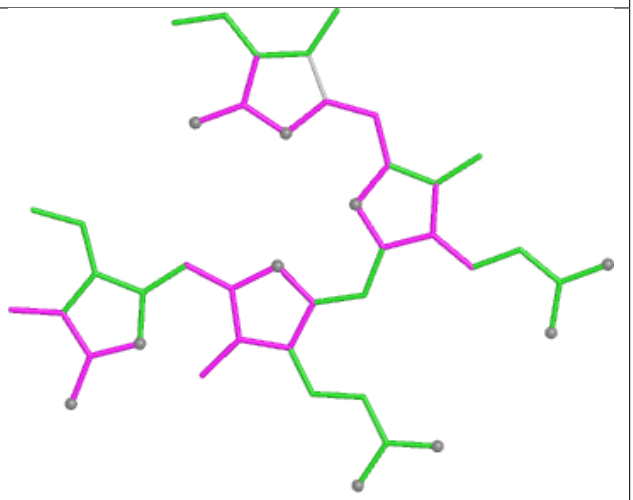


Rings

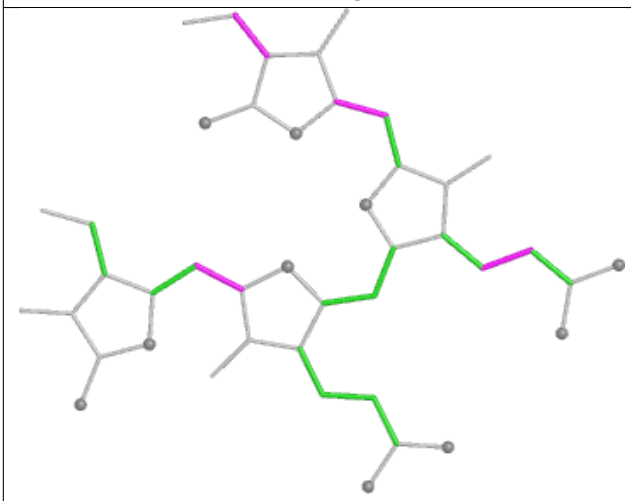
Ligand PEB KB 302



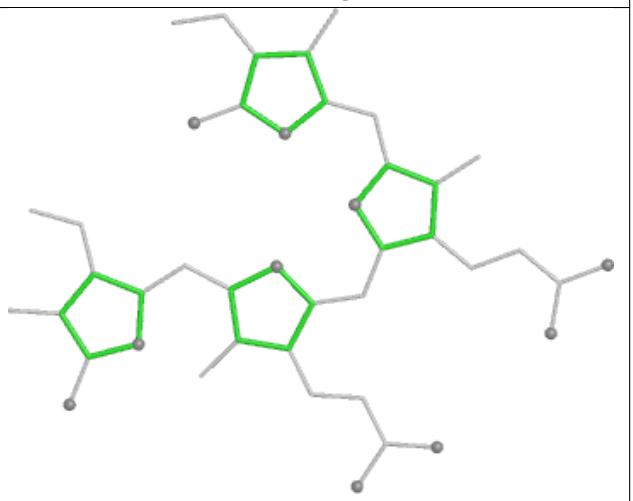
Bond lengths



Bond angles

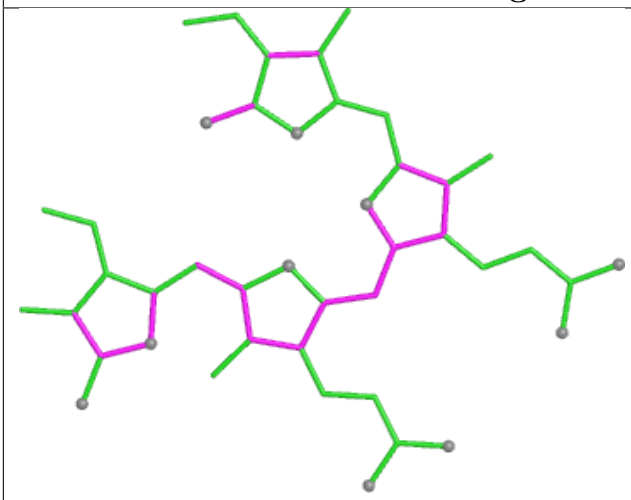


Torsions



Rings

Ligand PEB ZM 202



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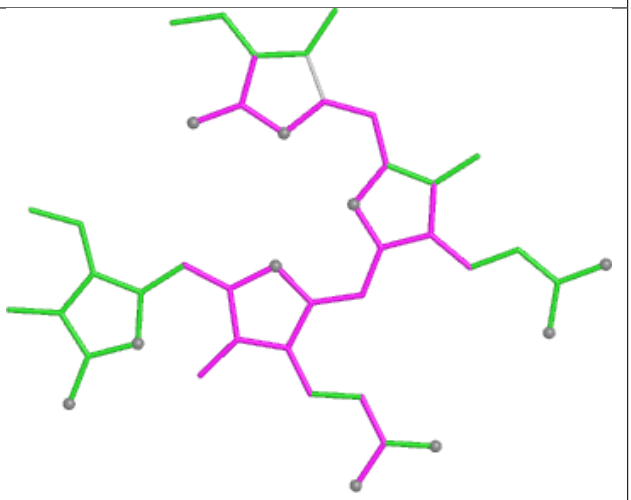

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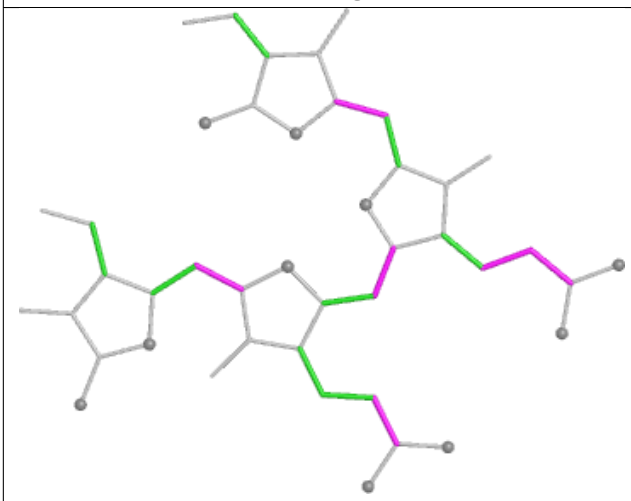

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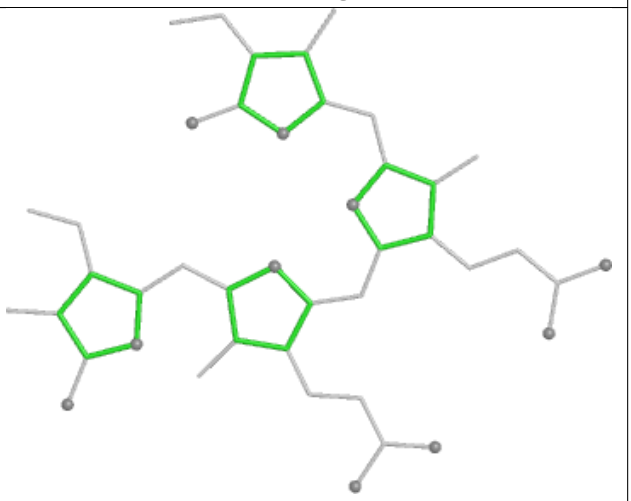
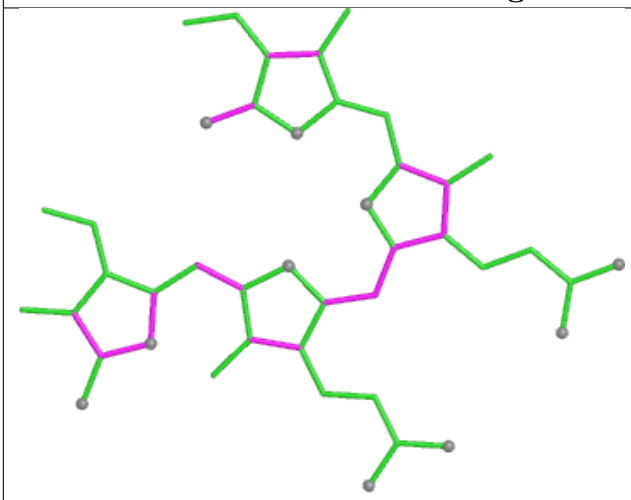


Rings

Ligand PEB QM 203



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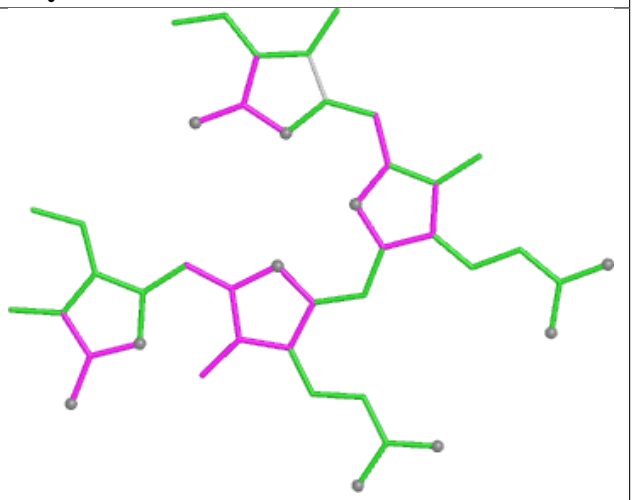

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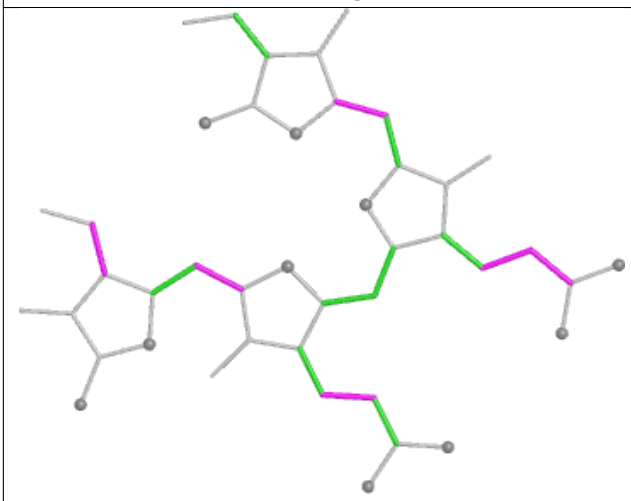

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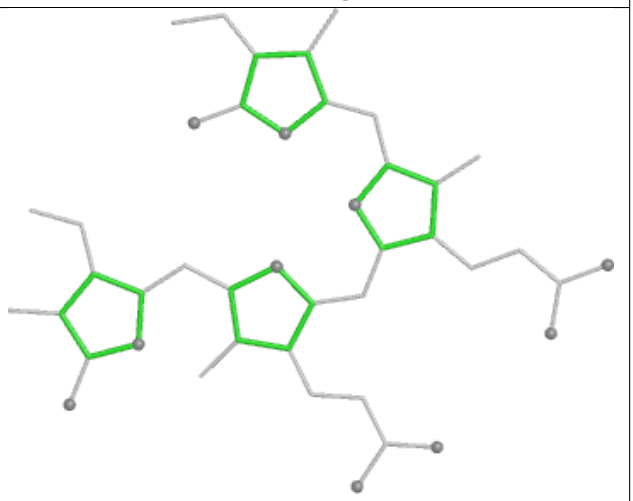
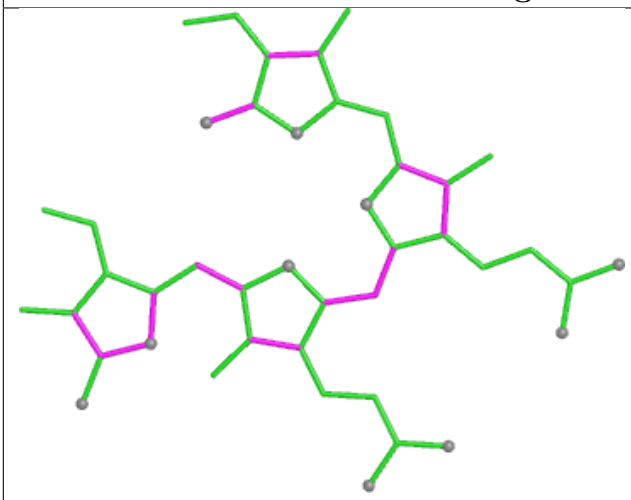


Rings

Ligand PEB SA 202



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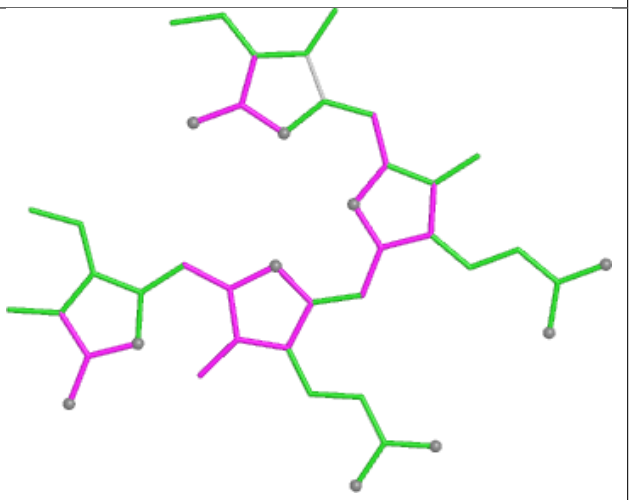

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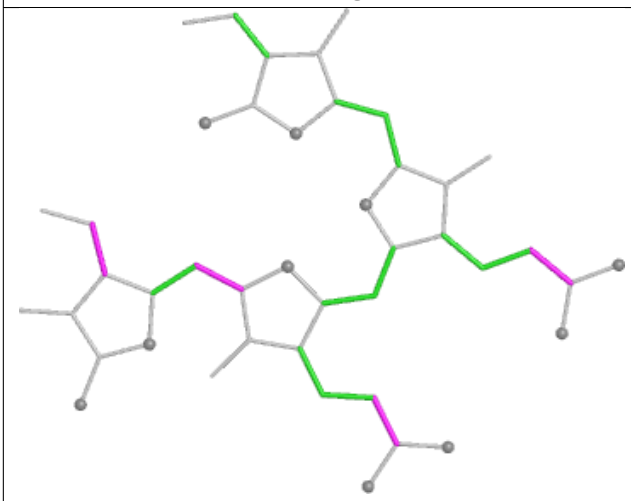

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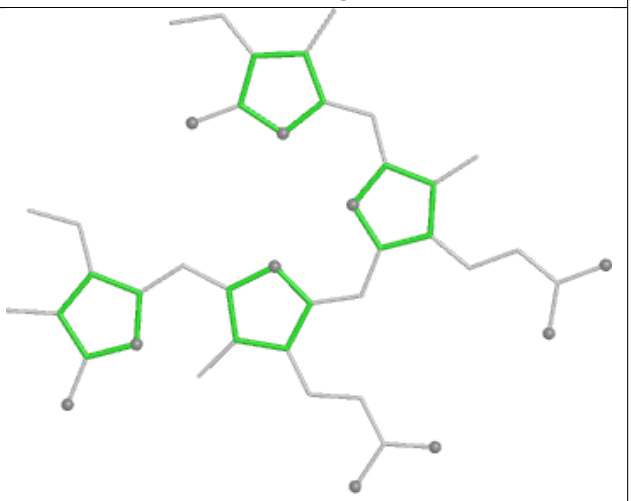
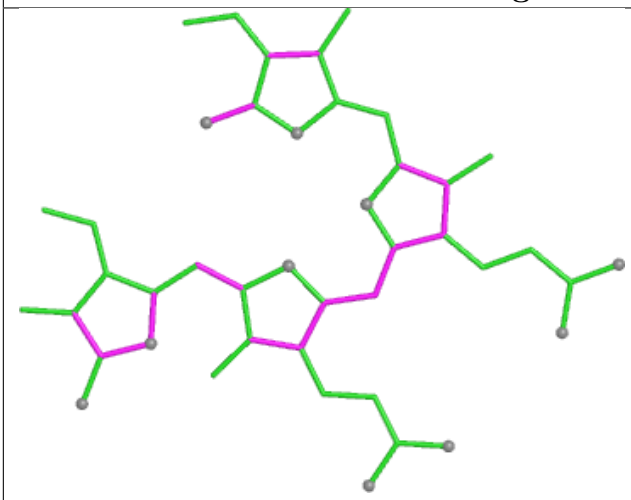


Rings

Ligand PEB AE 301



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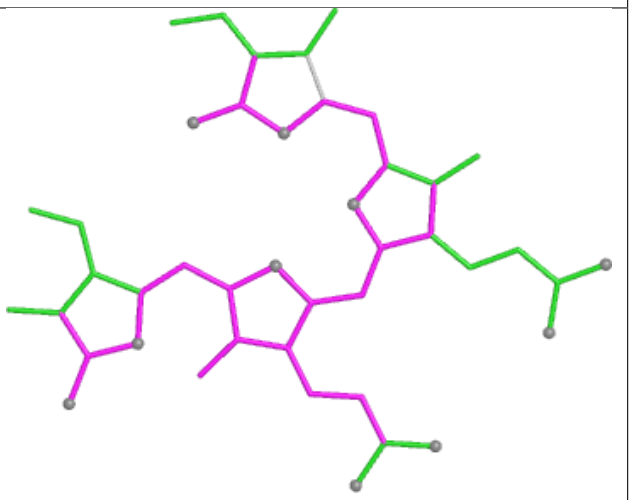

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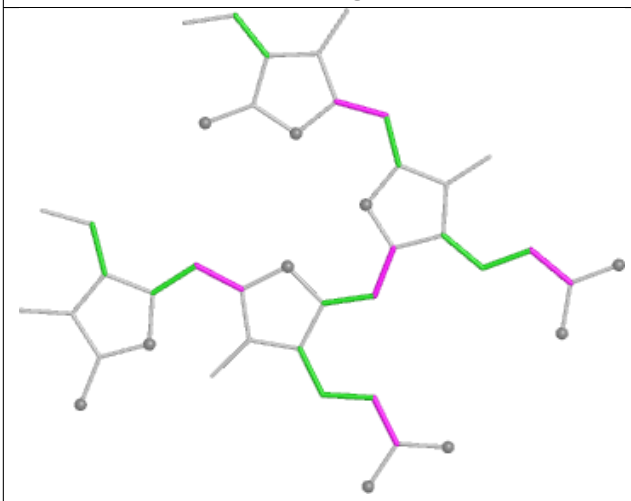

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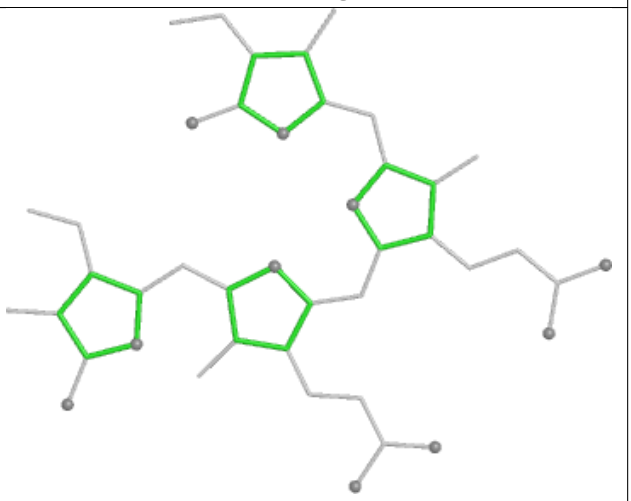
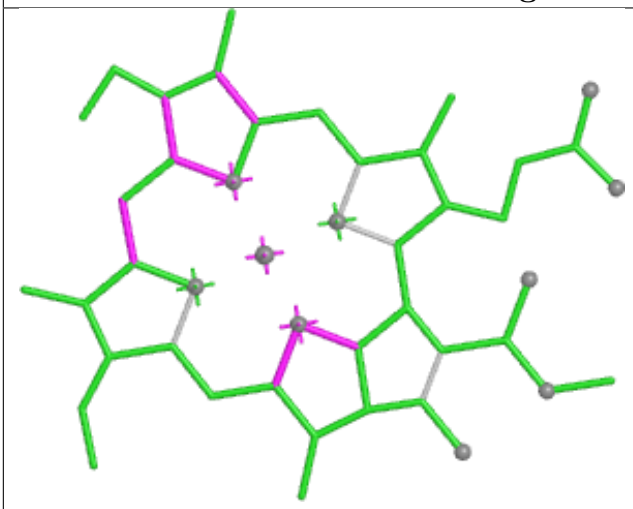


Rings

Ligand CLA 12 610



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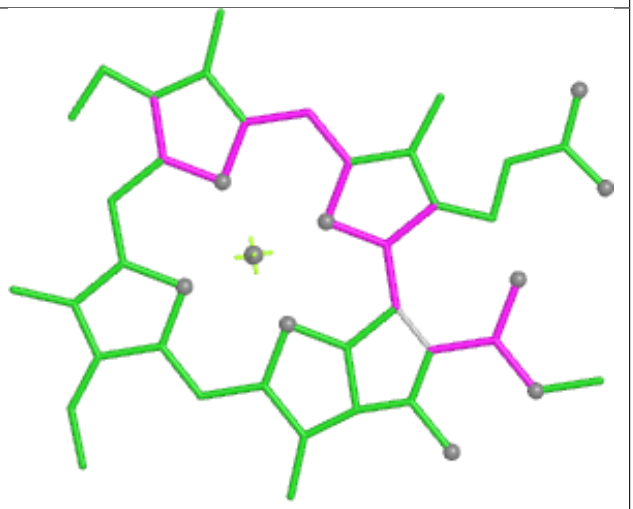

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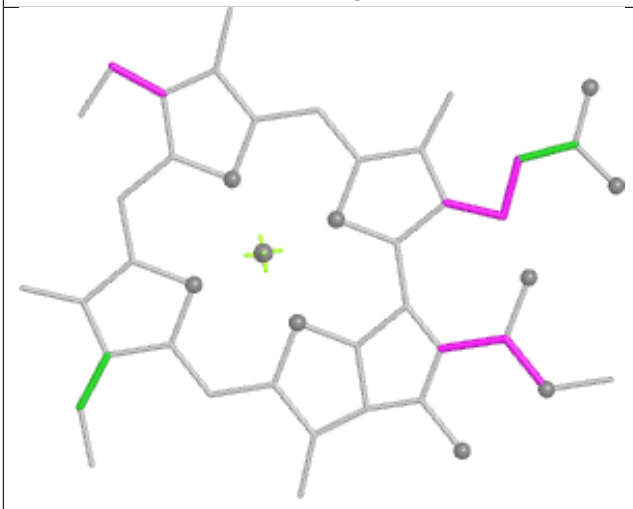
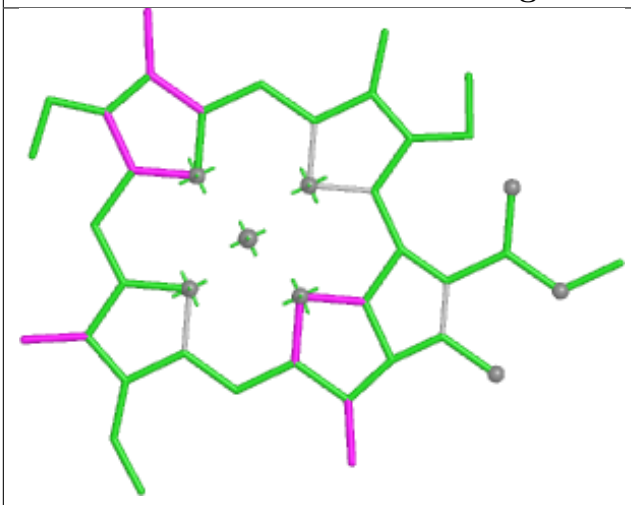


Torsions



Rings

Ligand CLA 52 609



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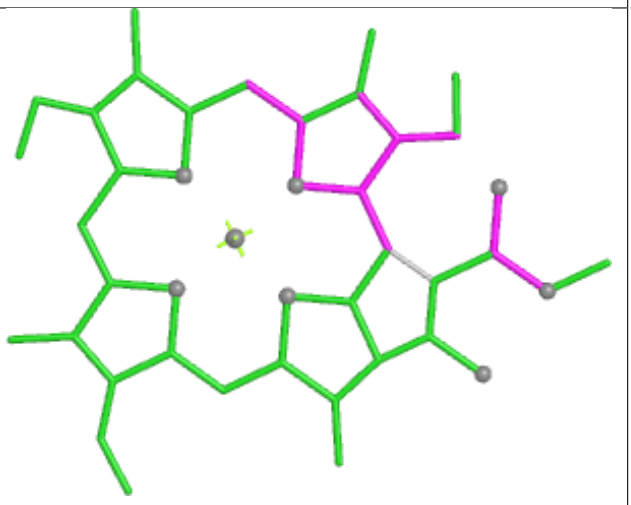

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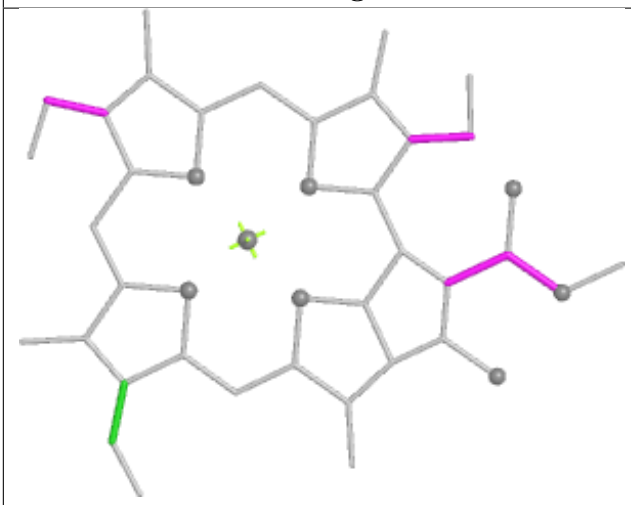
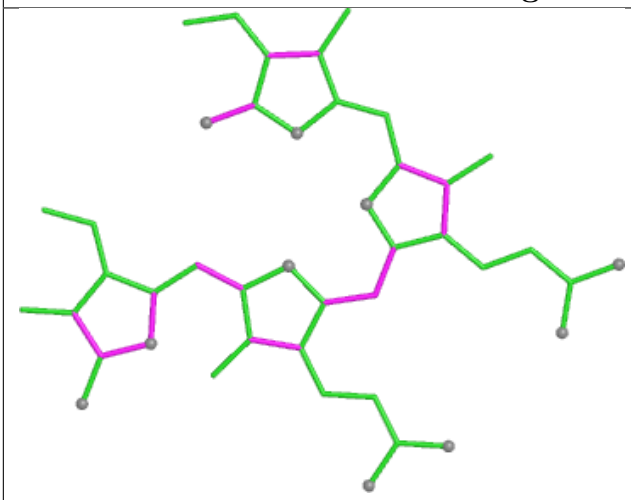


Torsions



Rings

Ligand PEB IJ 201



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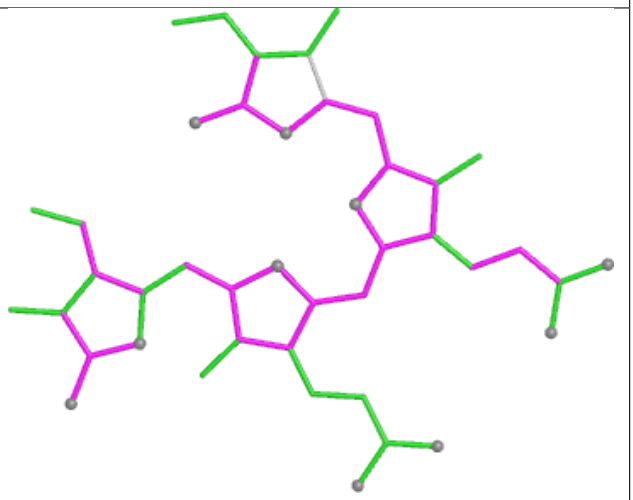

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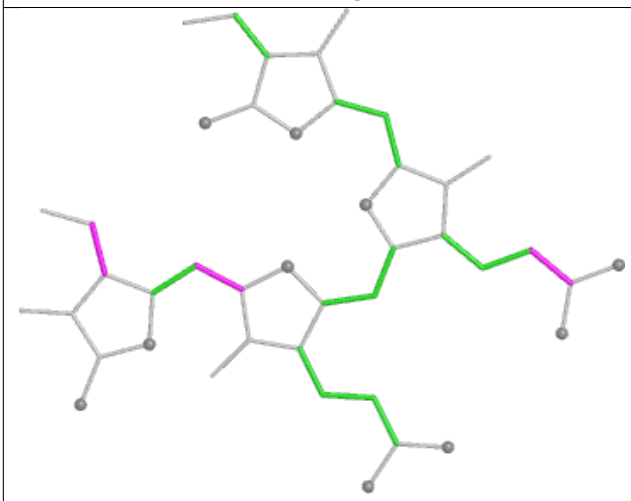

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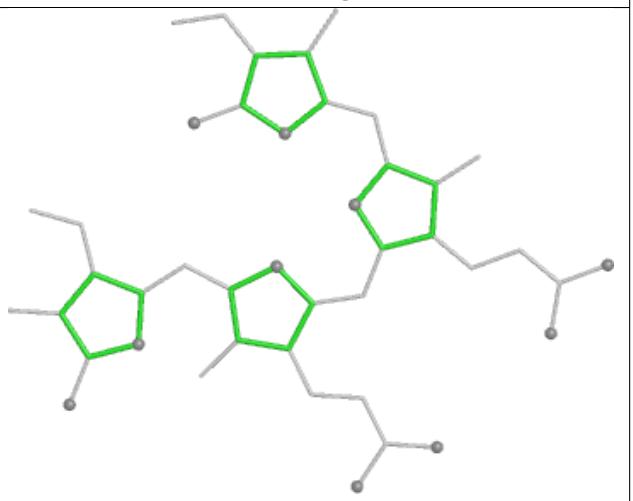
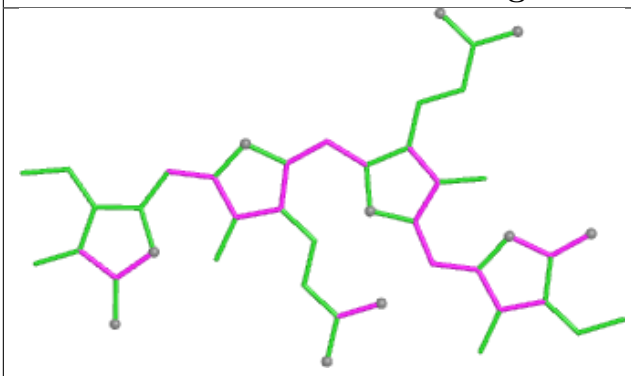


Rings

Ligand CYC 73 1001



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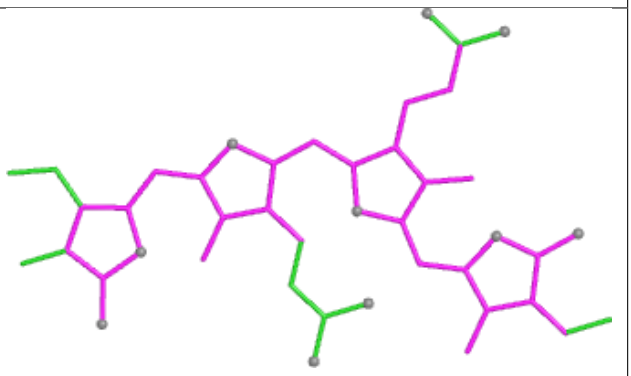

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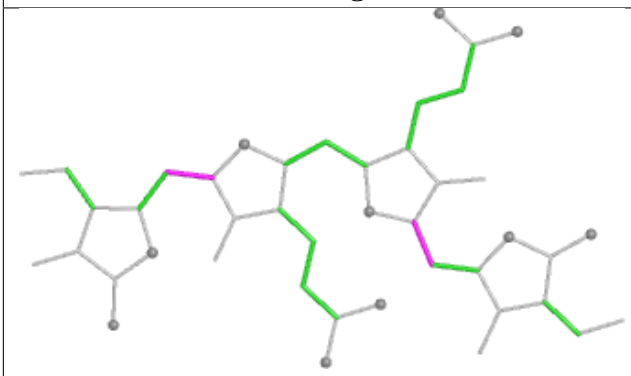

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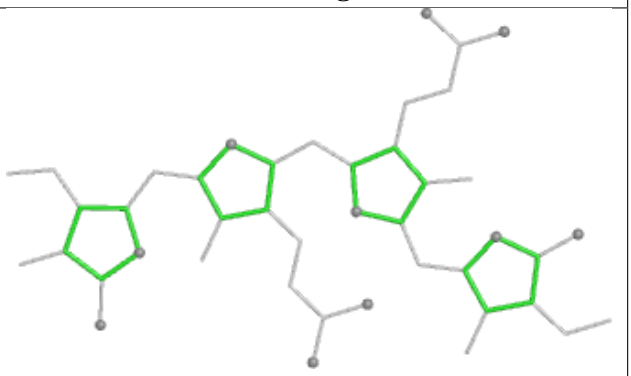
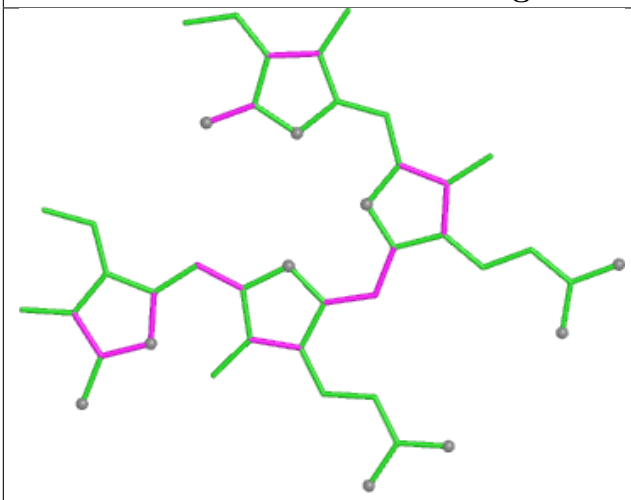


Rings

Ligand PEB DF 202



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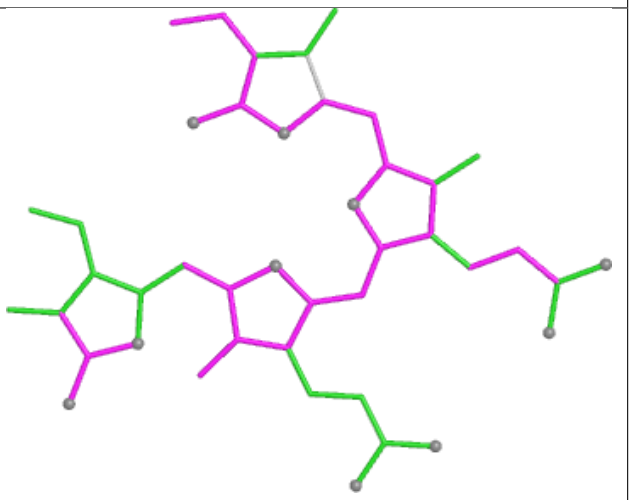

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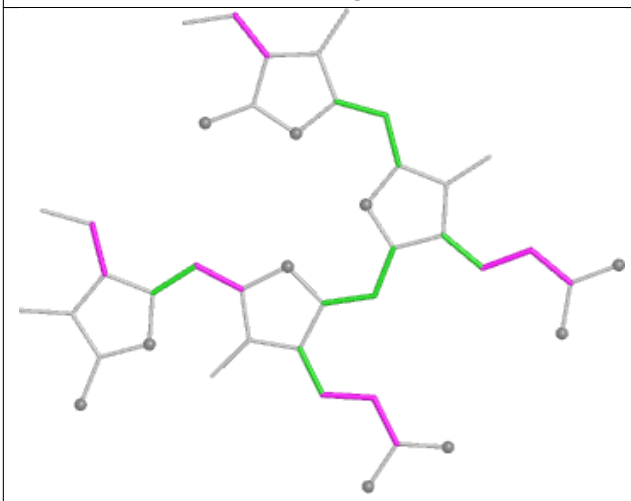

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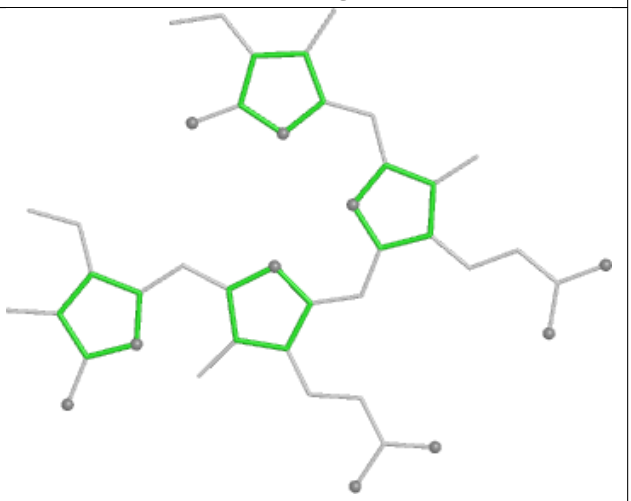

Rings

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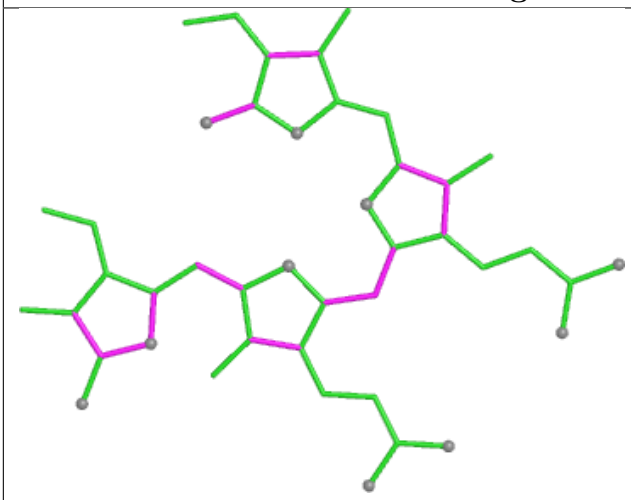

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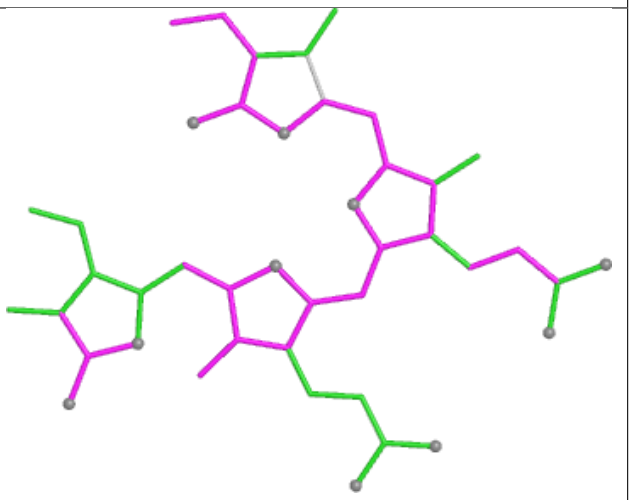
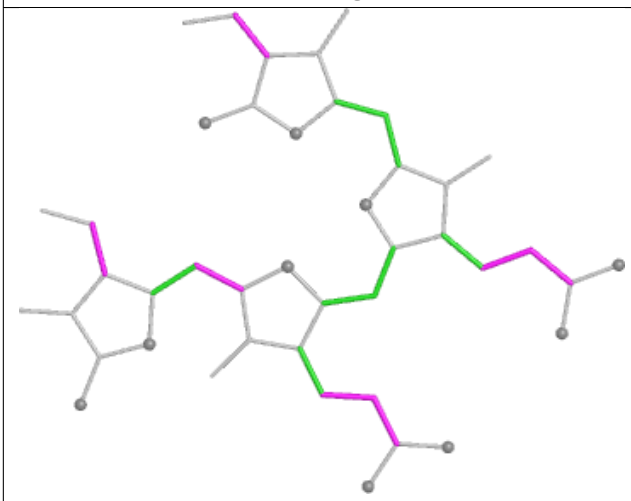


Bond angles



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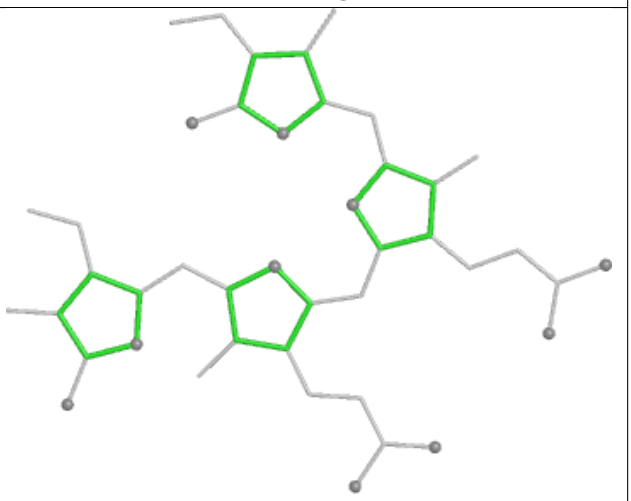
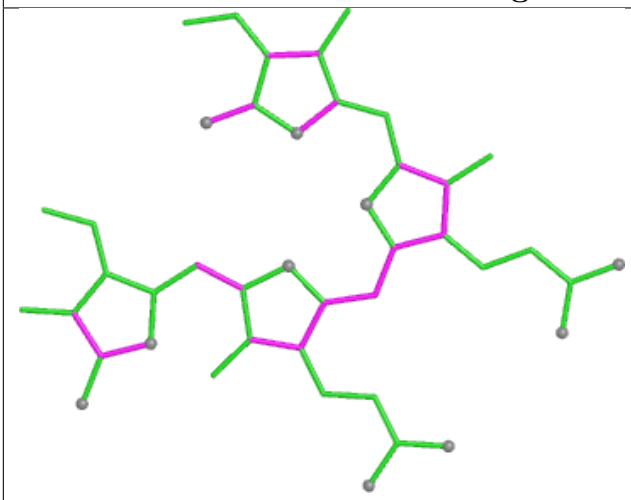


Rings

Ligand PEB RQ 201



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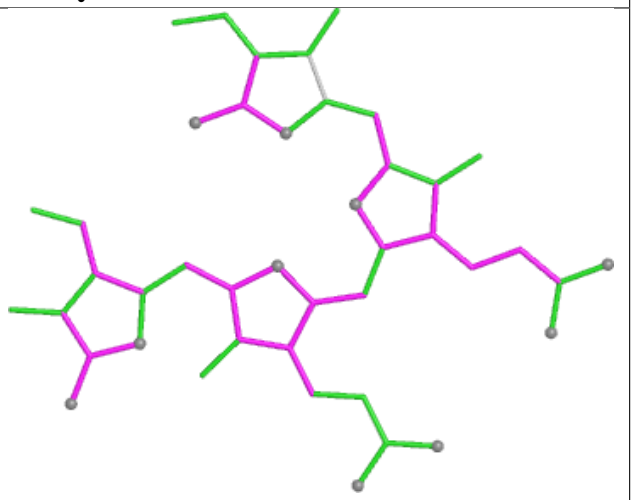
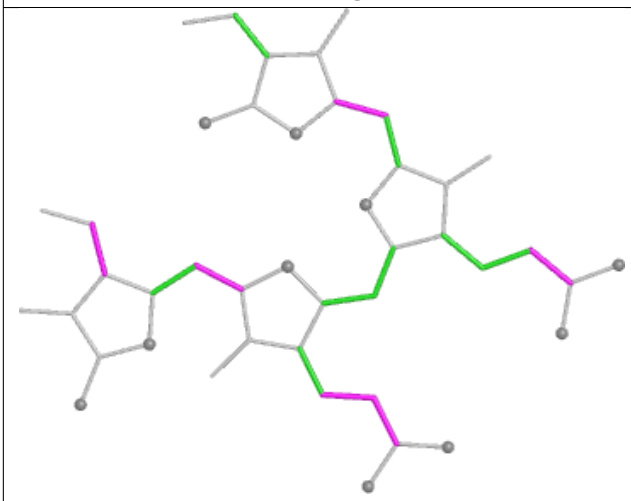


Bond angles



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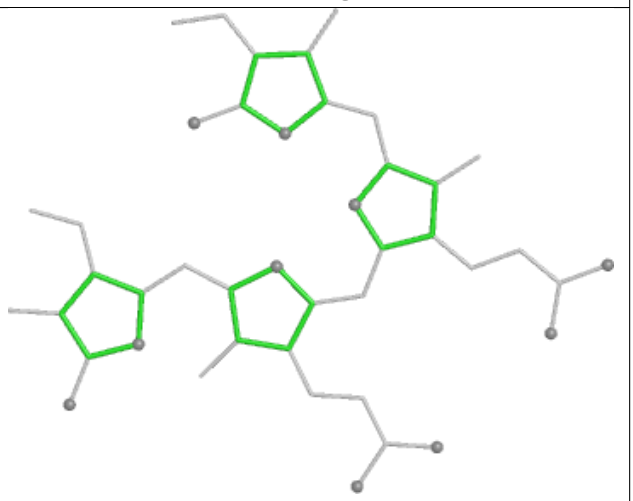
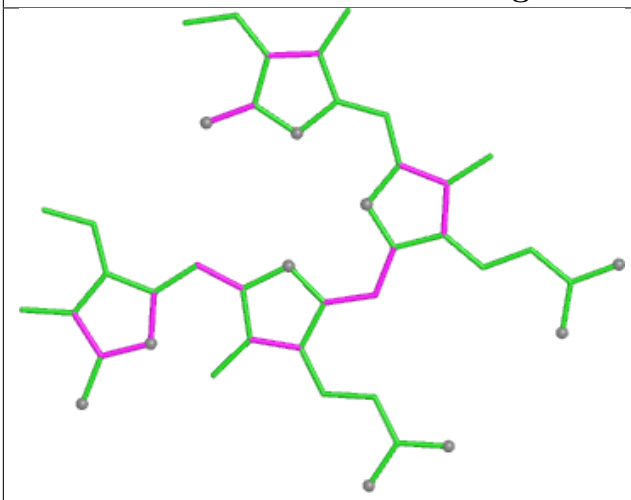


Rings

Ligand PEB UE 201



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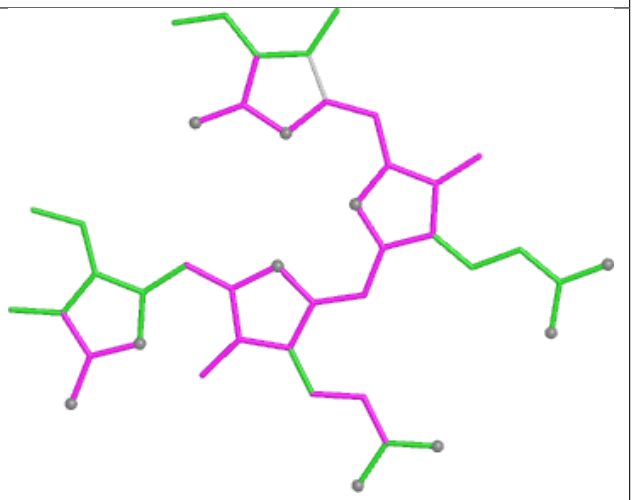
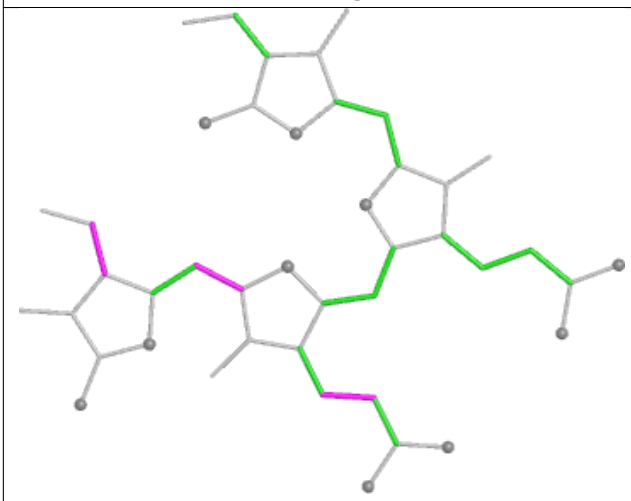


Bond angles



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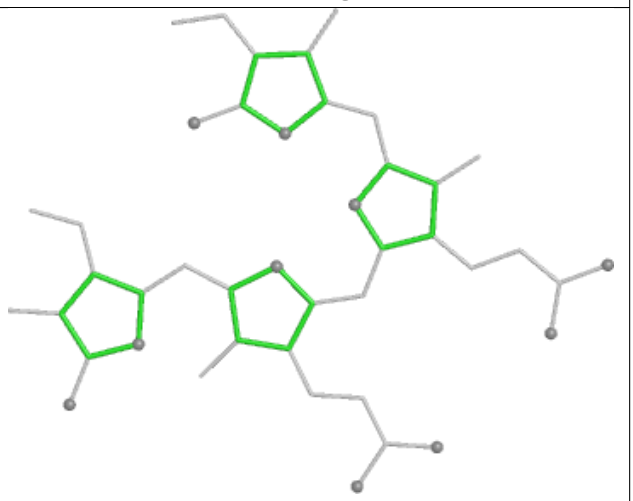
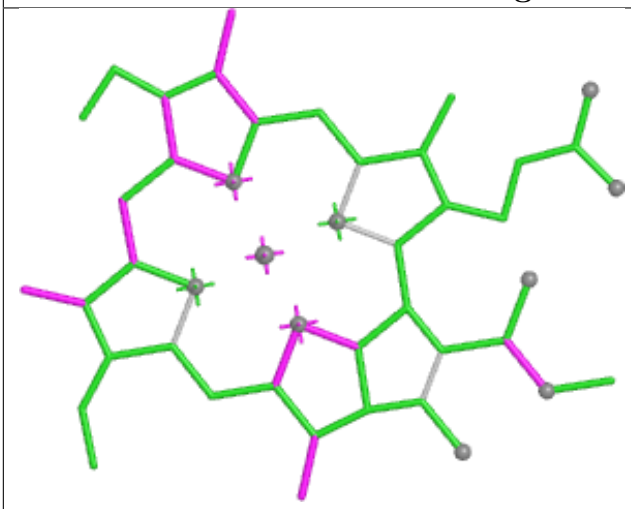


Rings

Ligand CLA 8N 306



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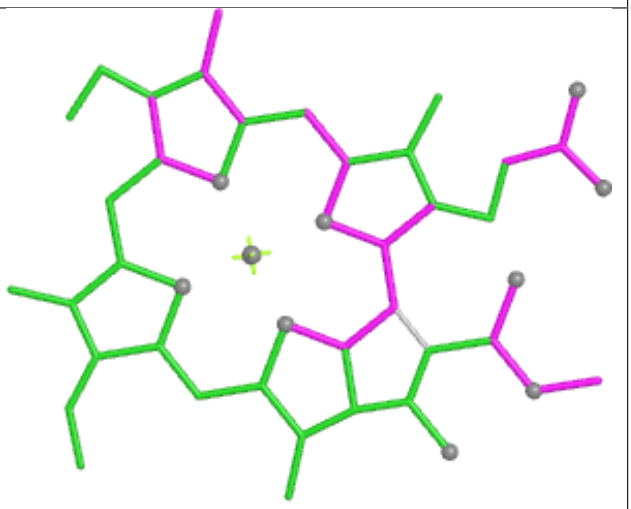
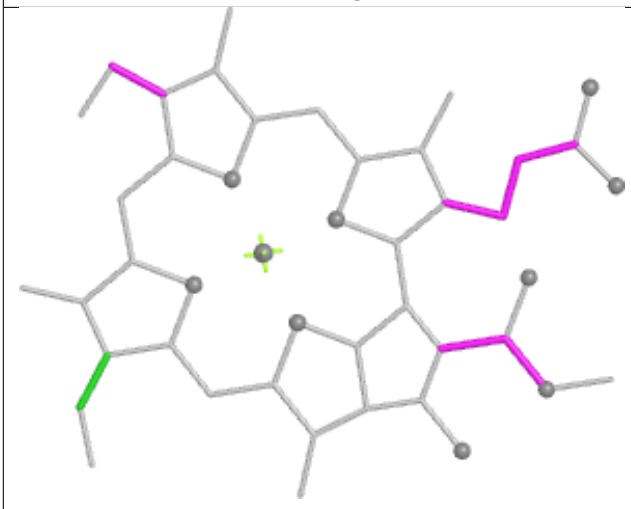


Bond angles

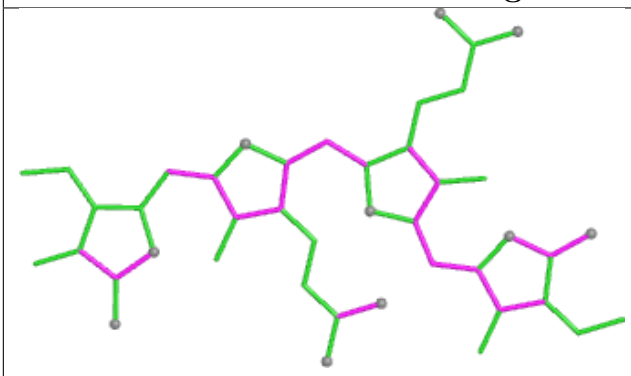


Torsions



Rings

Ligand CYC B3 1001



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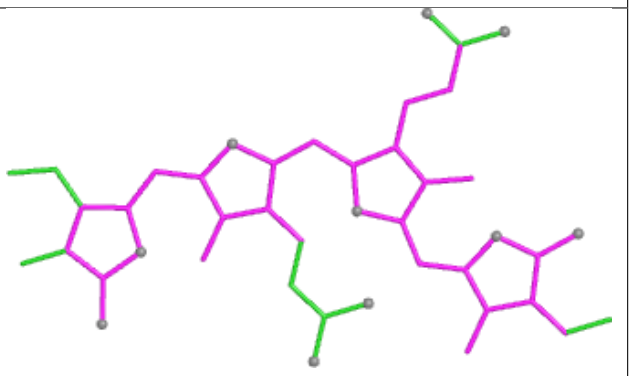
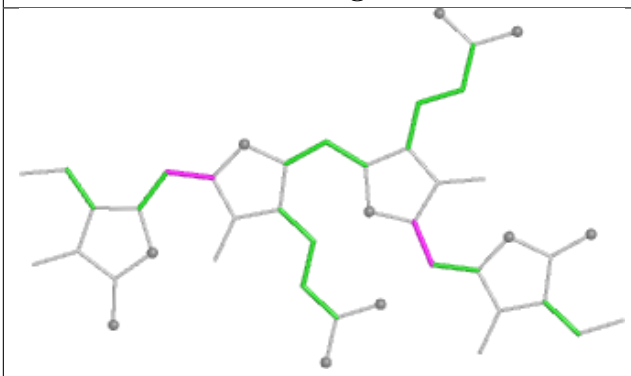


Bond angles



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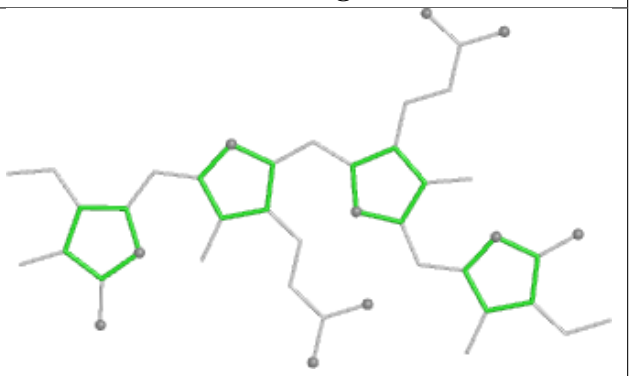
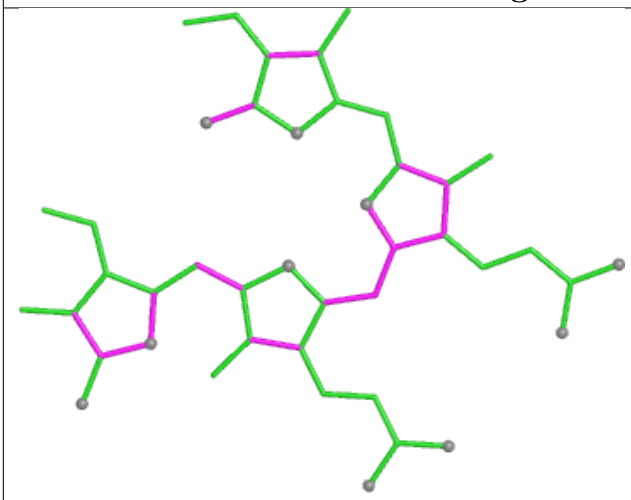


Rings

Ligand PEB RA 201



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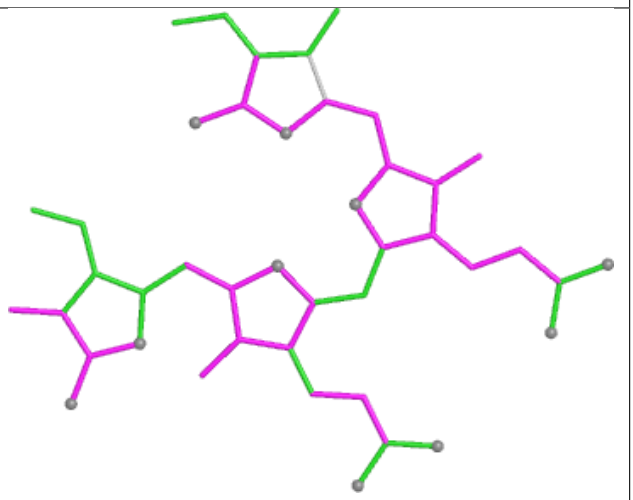
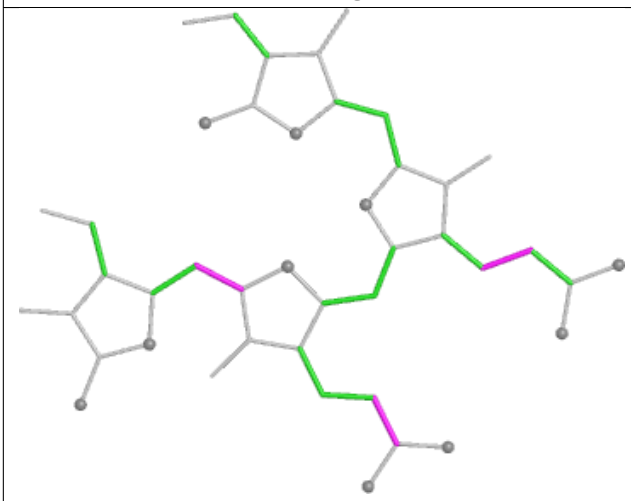
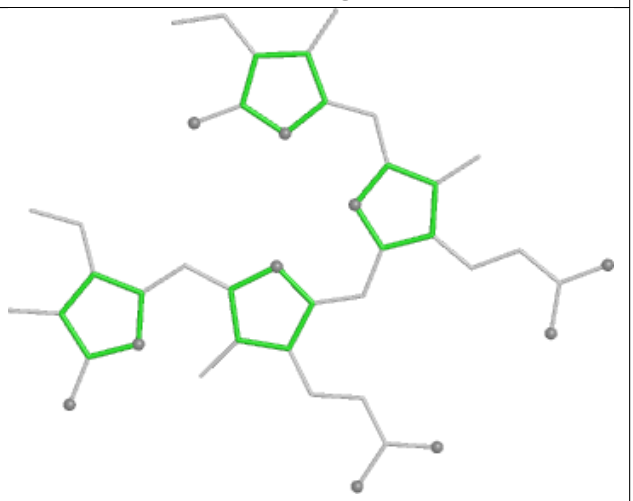


Bond angles

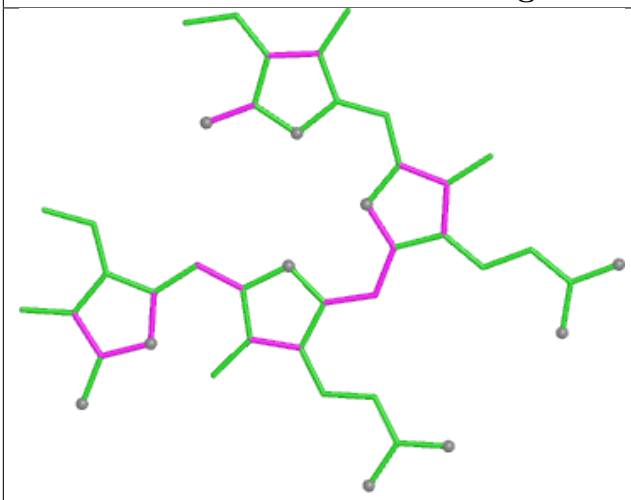


Torsions

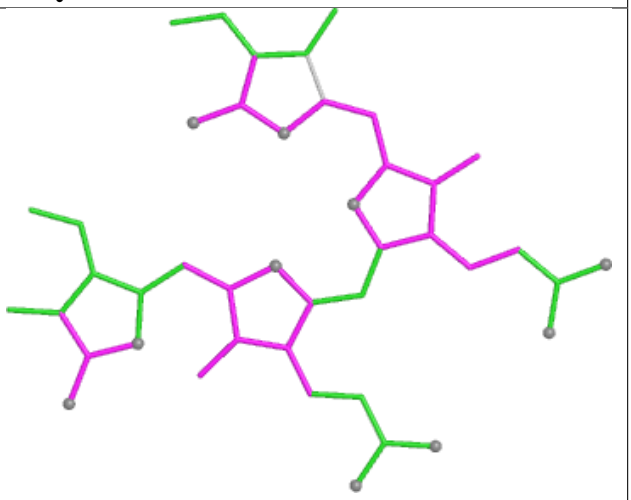


Rings

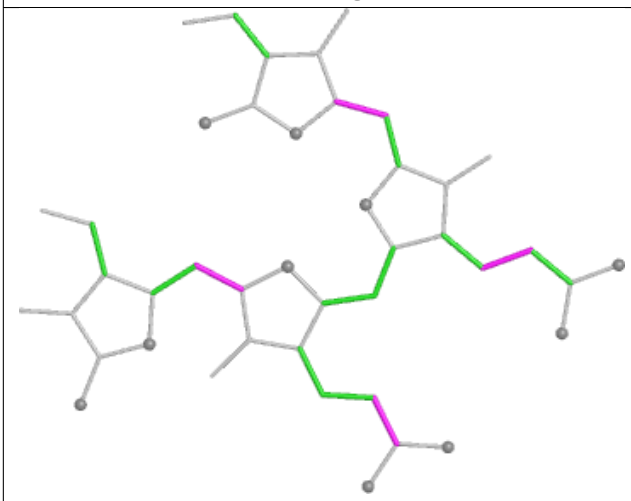
Ligand PEB QI 201



Bond lengths



Bond angles



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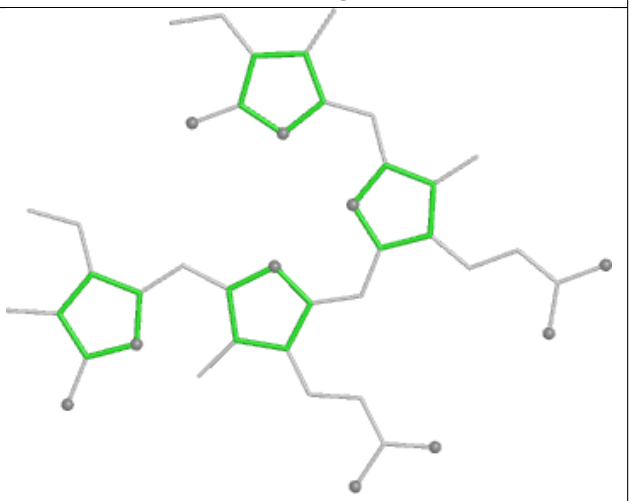
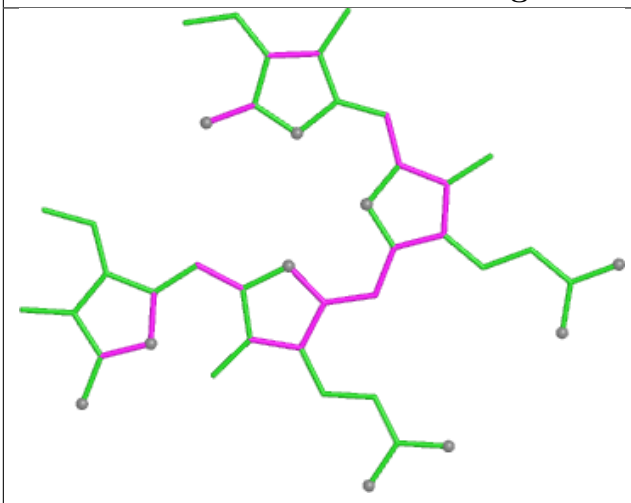


Rings

Ligand PEB RD 203



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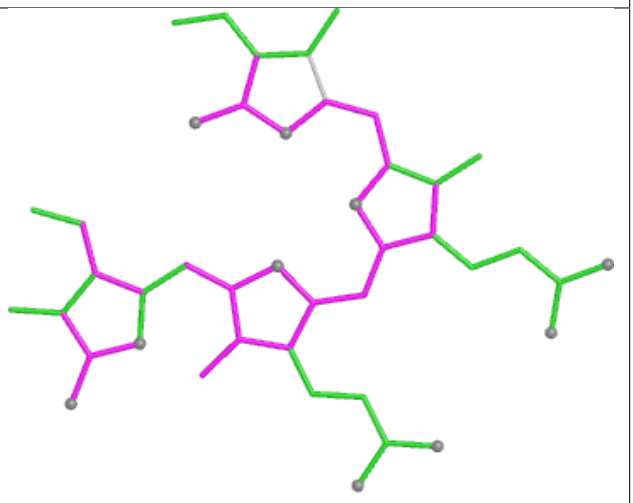
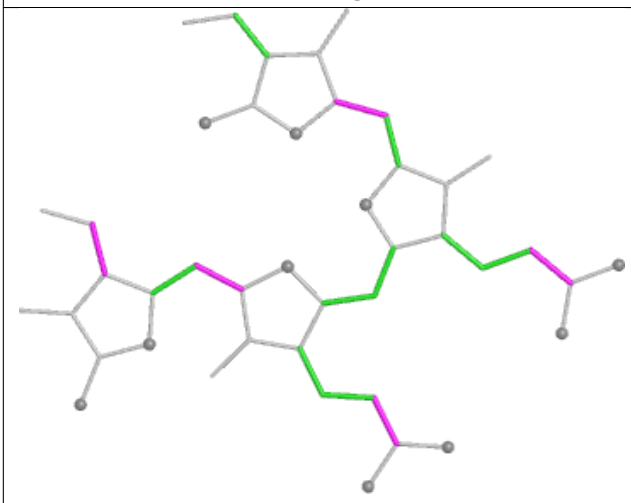


Bond angles



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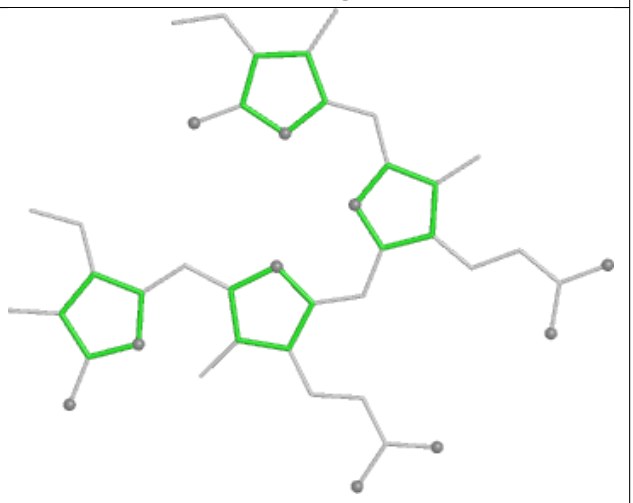
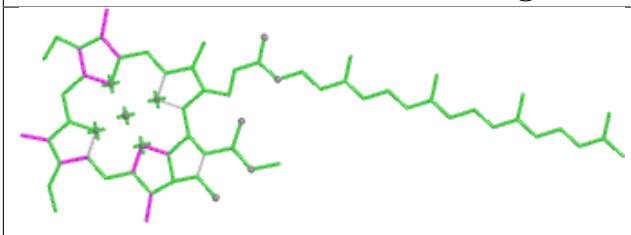


Rings

Ligand CLA F2 205



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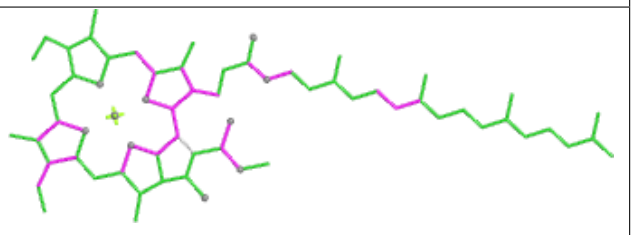
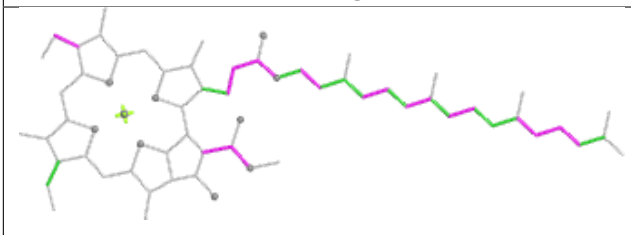


Bond angles



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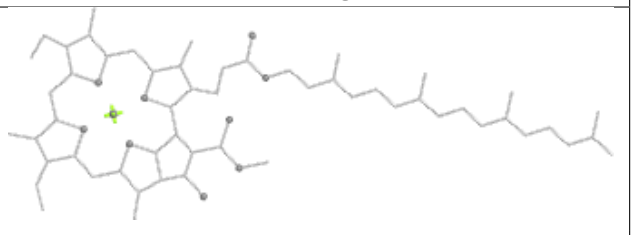
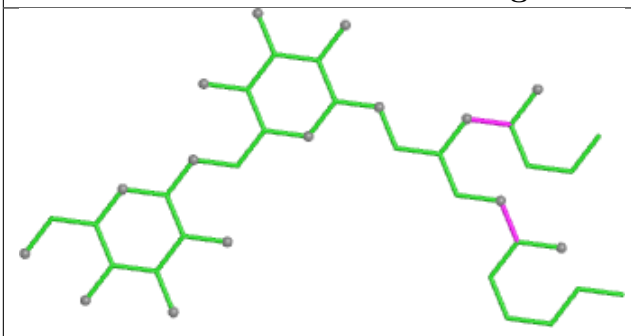


Rings

Ligand DGD O6 301



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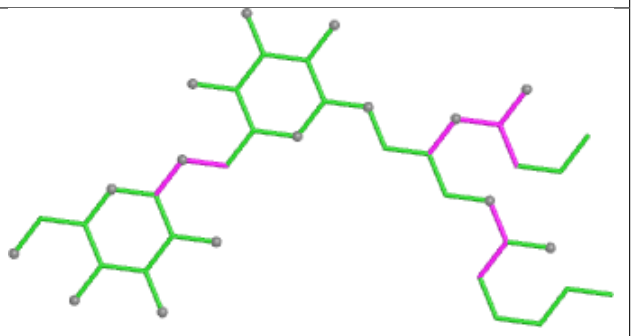
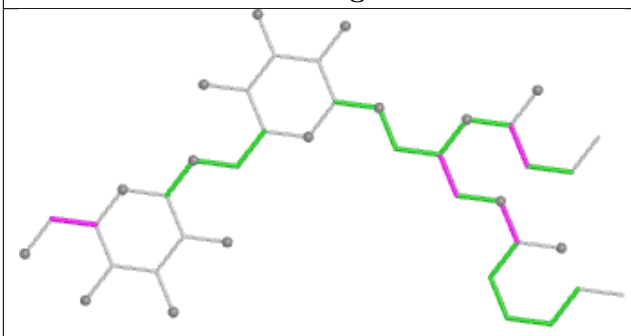


Bond angles



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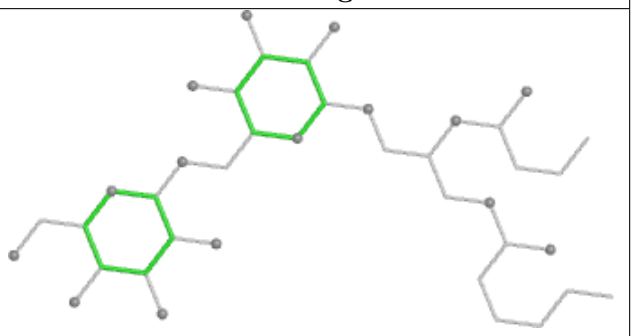
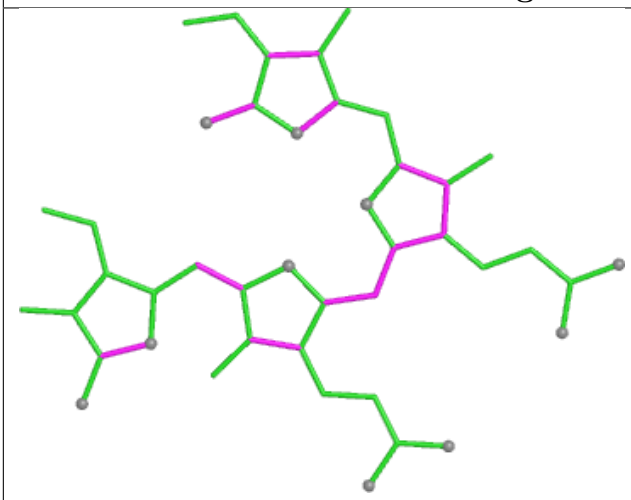


Rings

Ligand PEB T1 202



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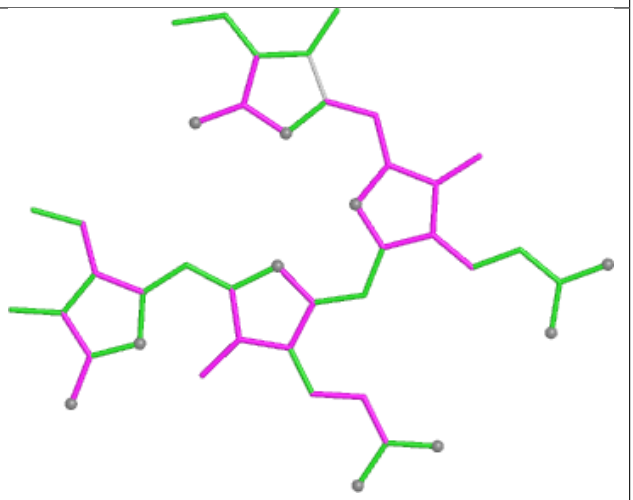

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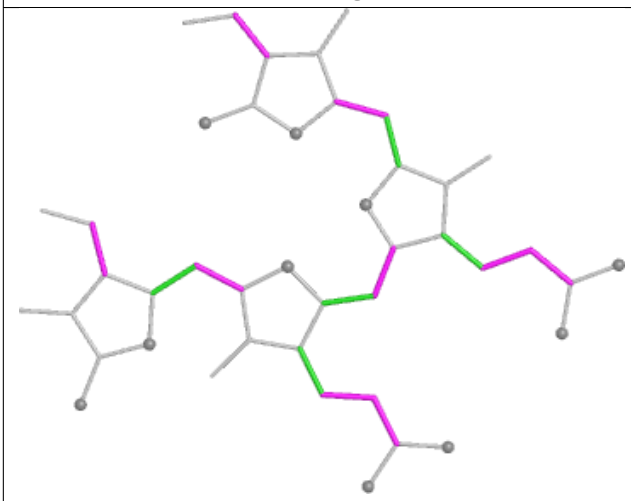

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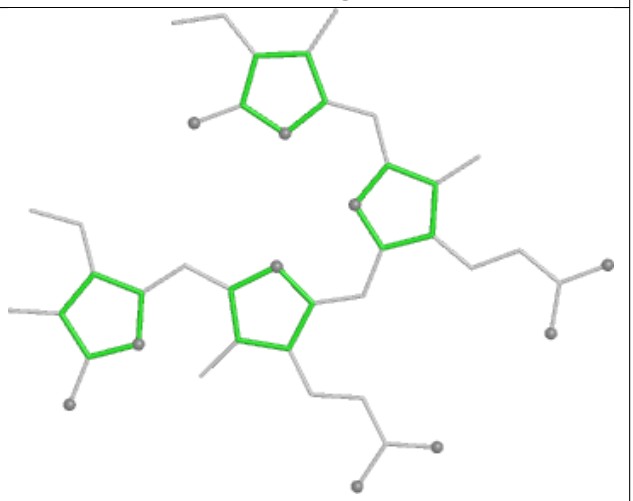
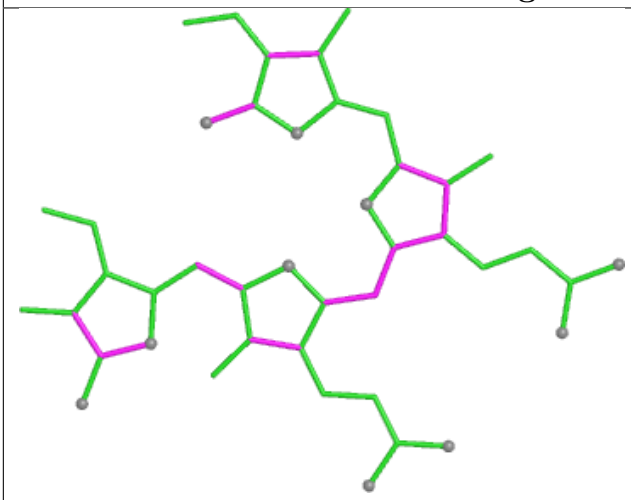


Rings

Ligand PEB fK 201



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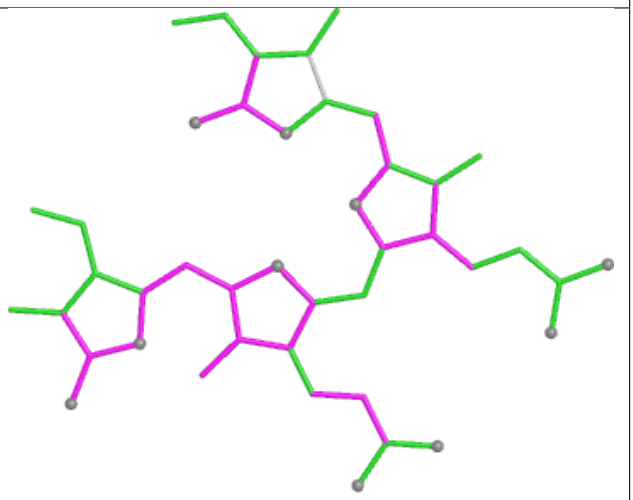
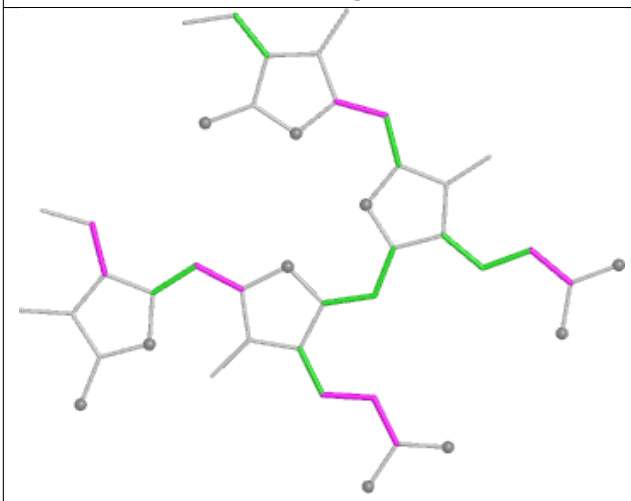


Bond angles



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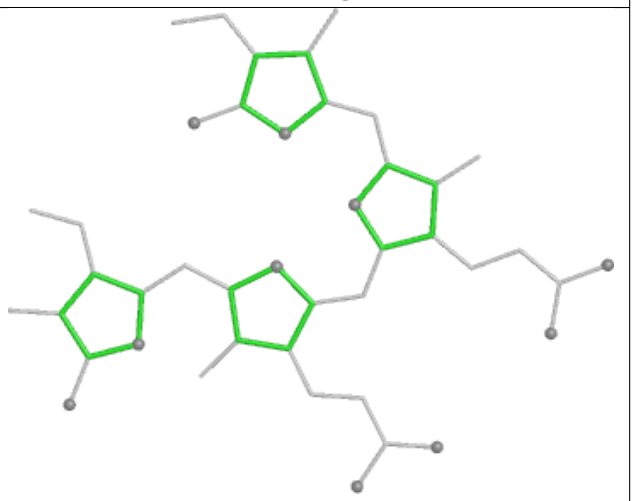
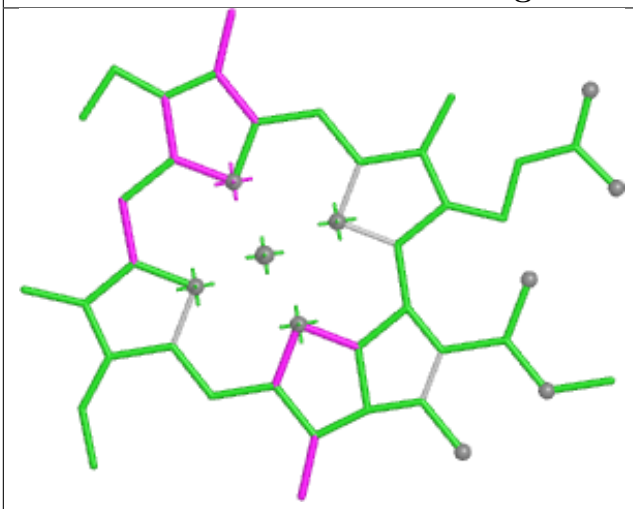


Rings

Ligand CLA 1N 603



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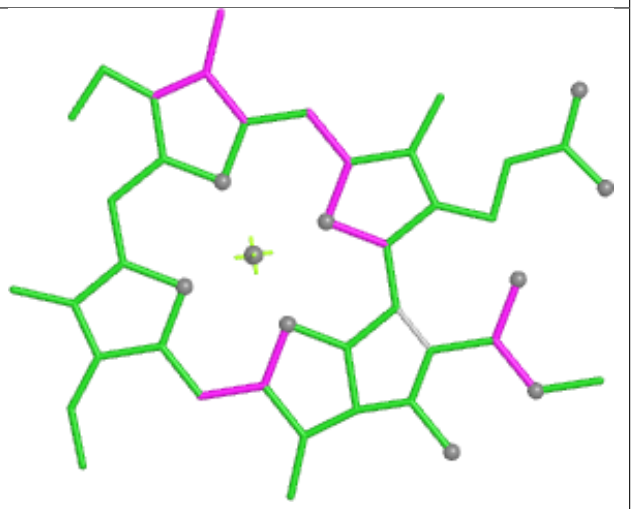

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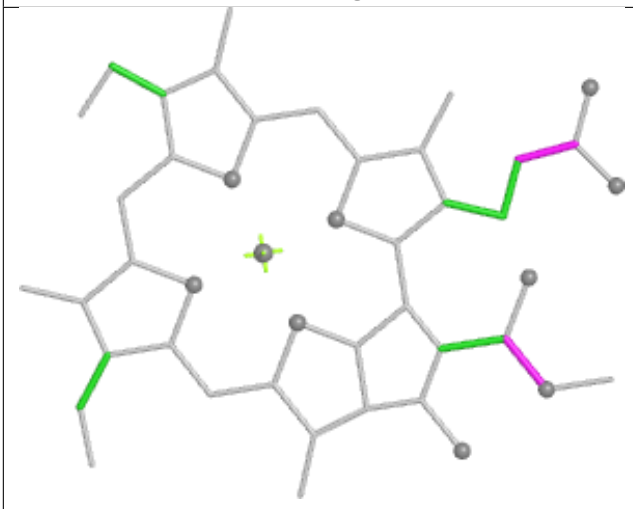
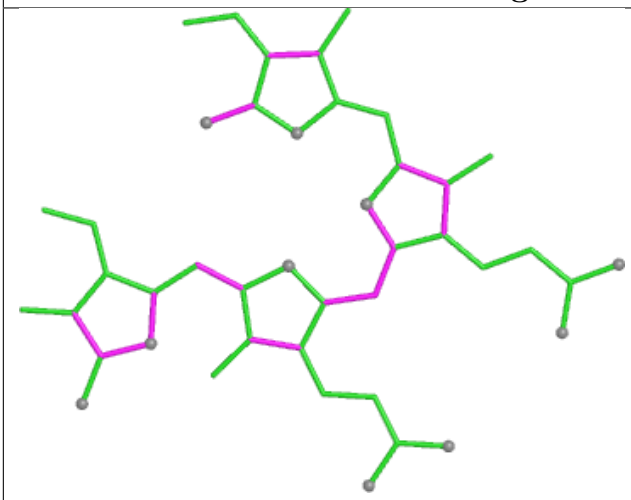


Torsions



Rings

Ligand PEB TG 201



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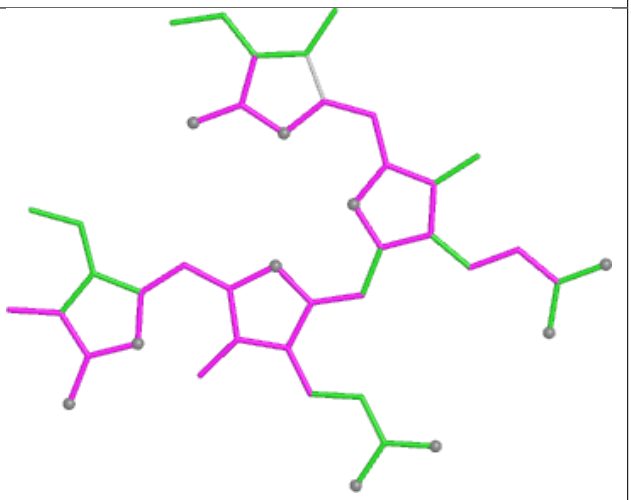
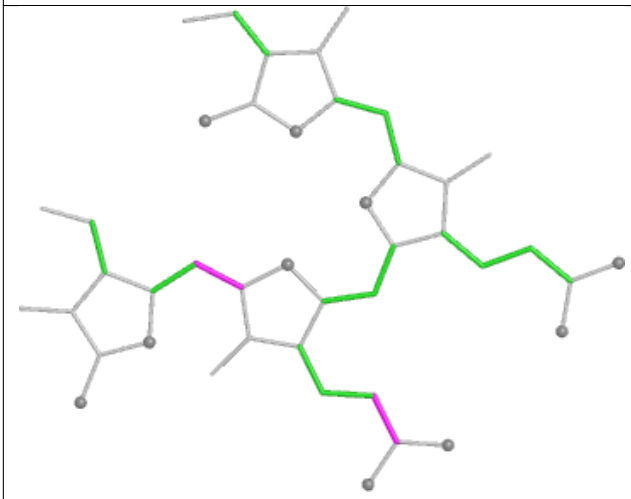


Bond angles



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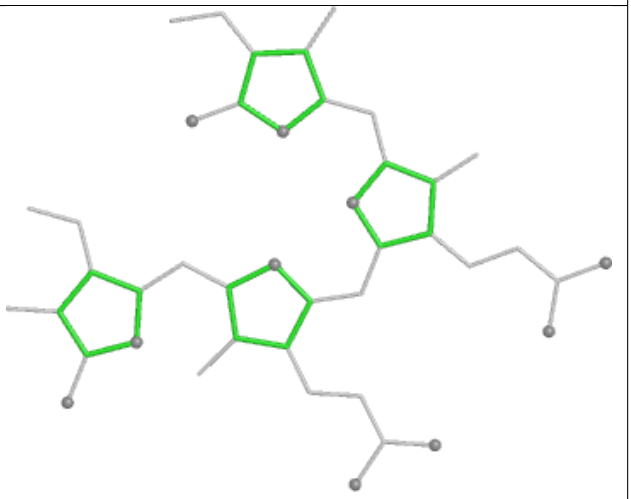
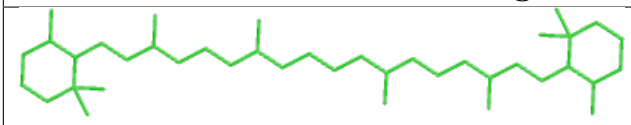


Rings

Ligand BCR B2 841



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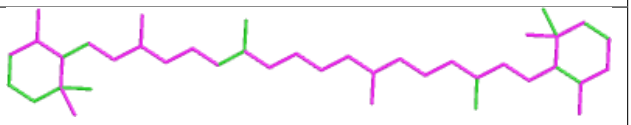

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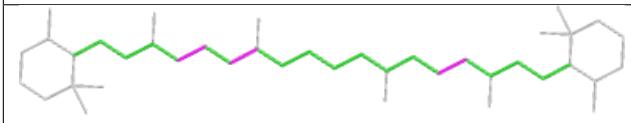

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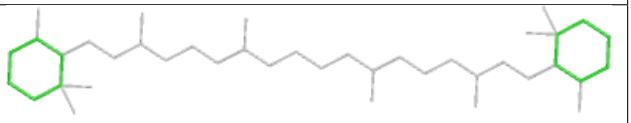
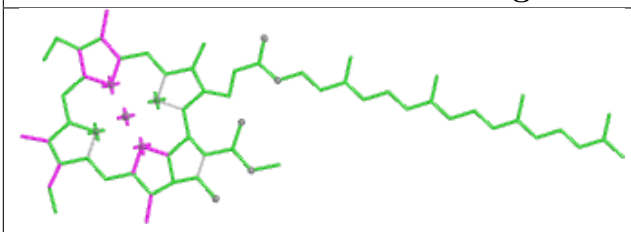


Rings

Ligand CLA DL 403



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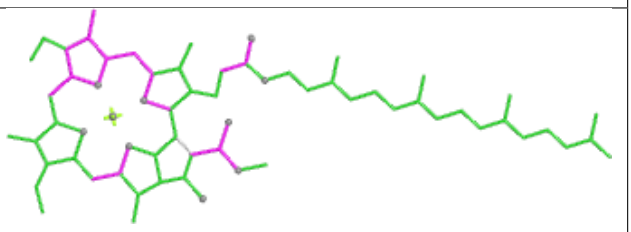
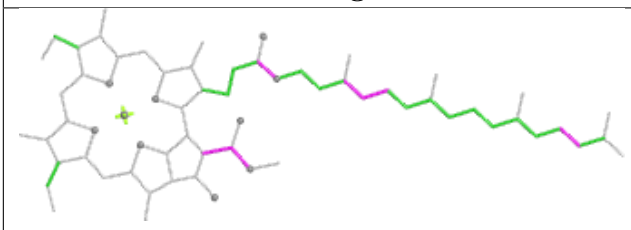


Bond angles



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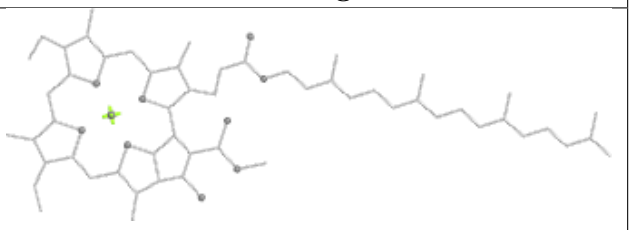
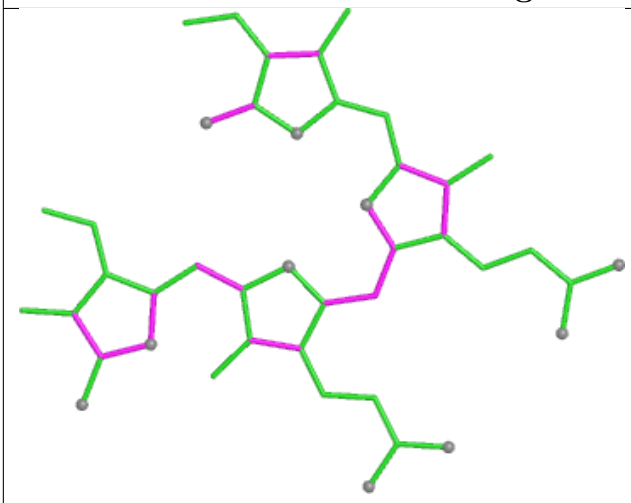


Rings

Ligand PEB eK 203



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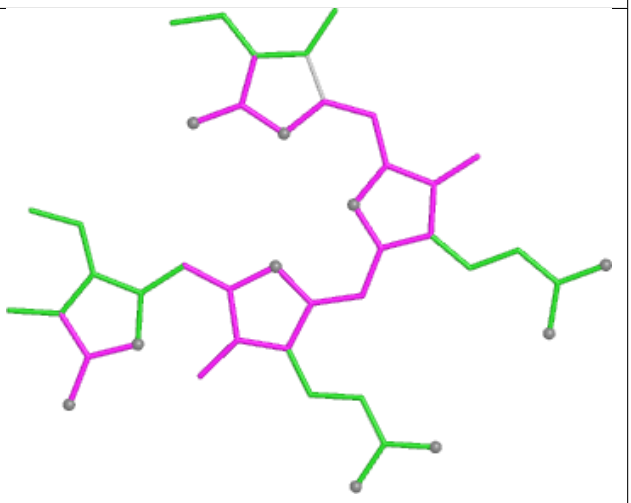

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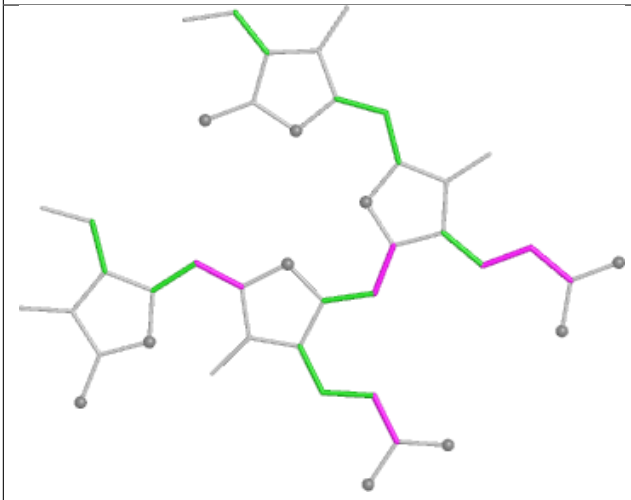

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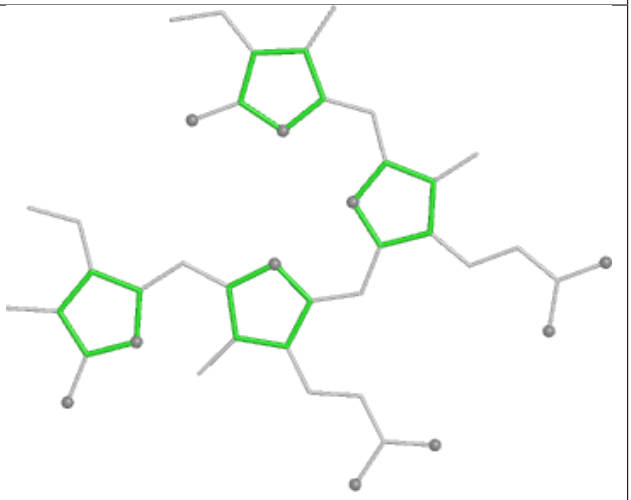
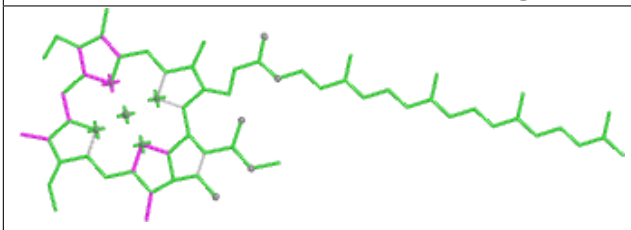
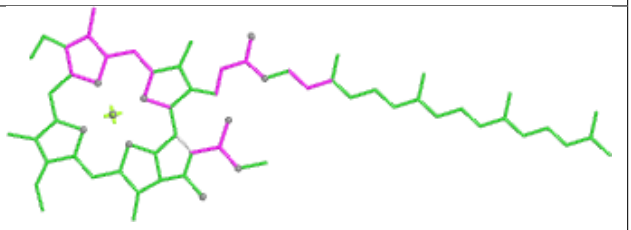
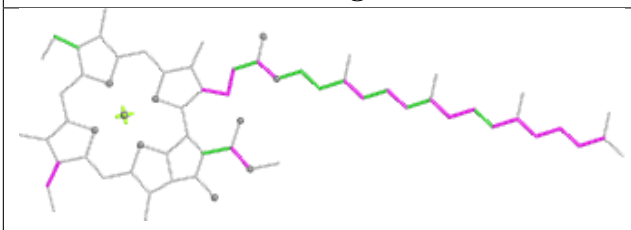
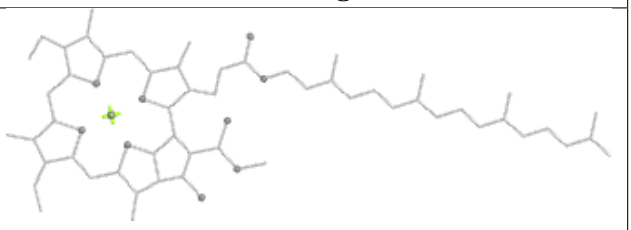


Rings

Ligand CLA A6 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

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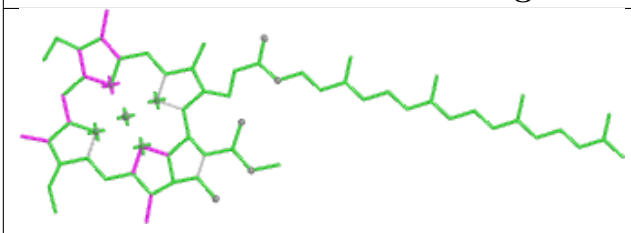
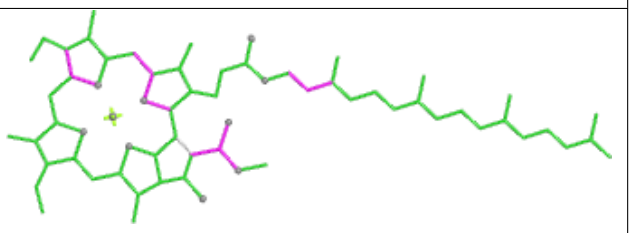
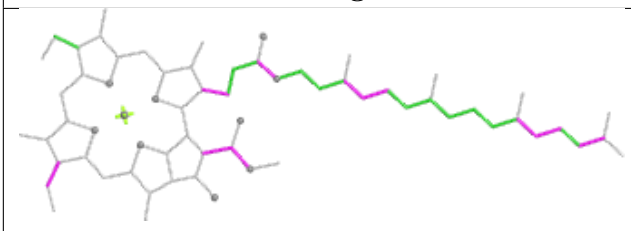
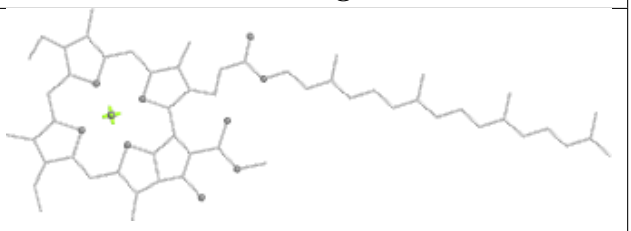
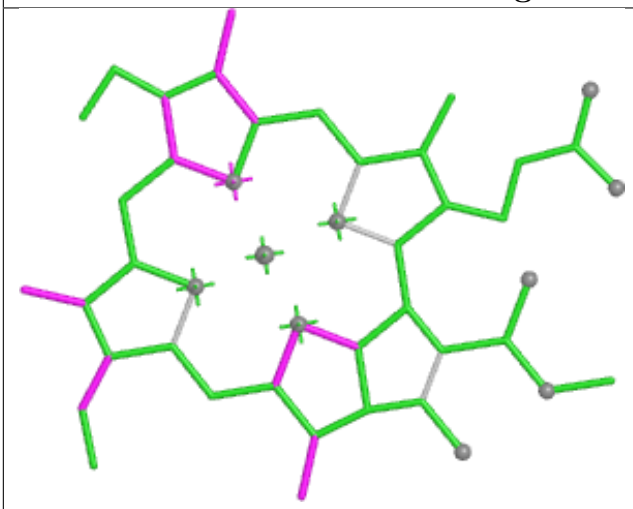
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 8N 304



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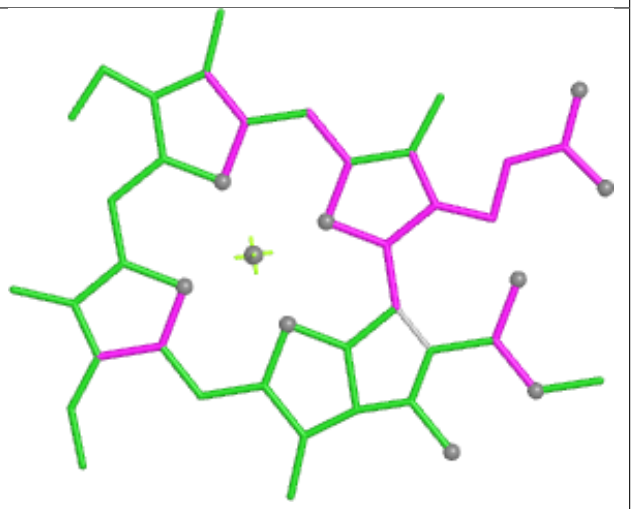
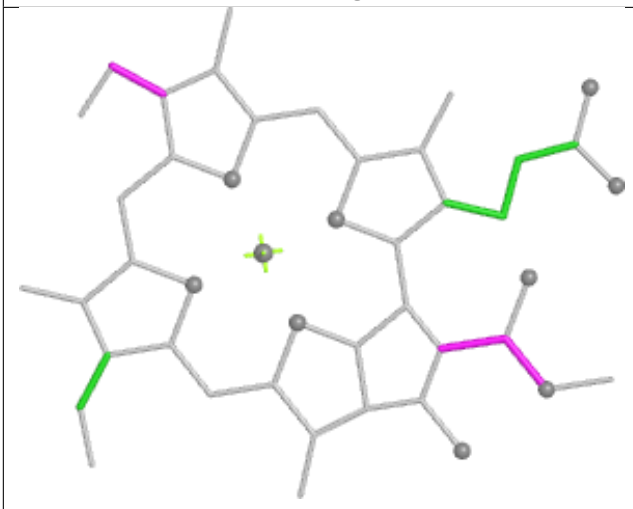


Bond angles

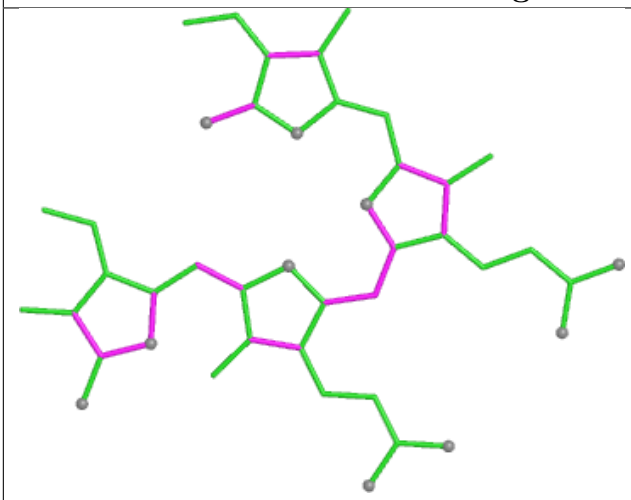


Torsions



Rings

Ligand PEB ED 202



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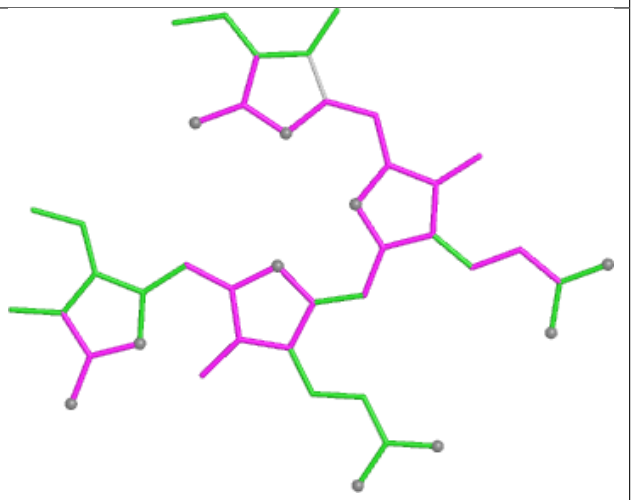
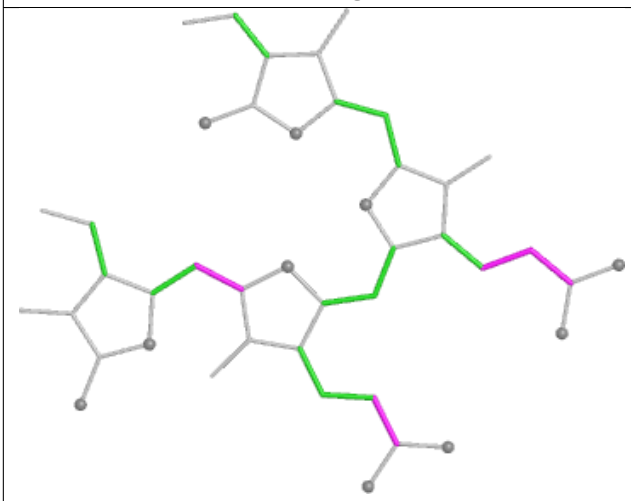


Bond angles



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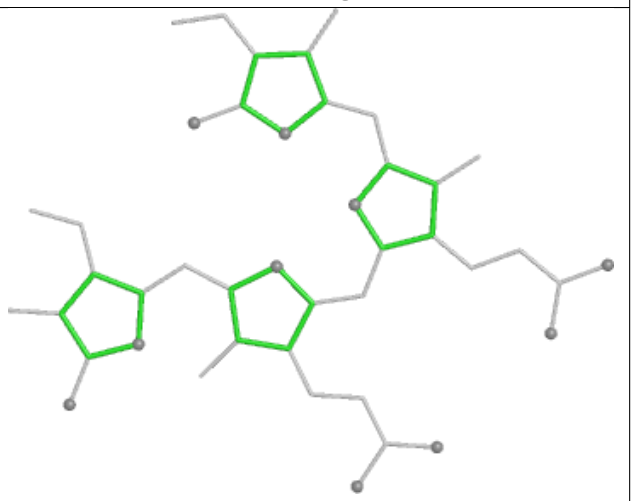
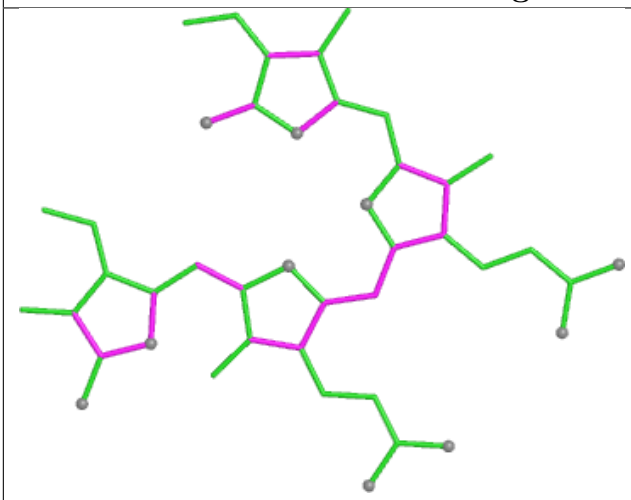


Rings

Ligand PEB PQ 201



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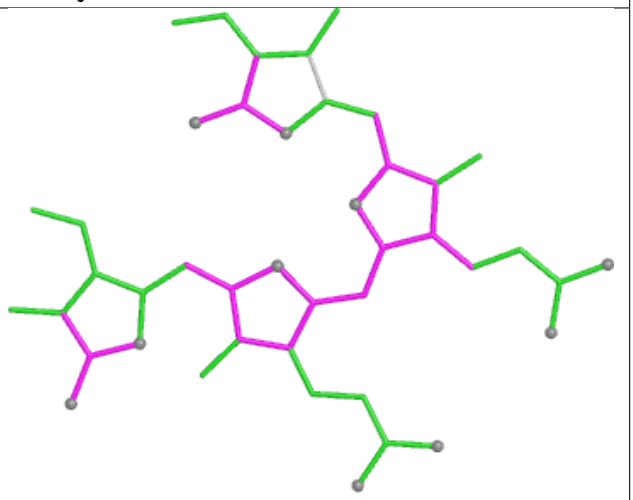

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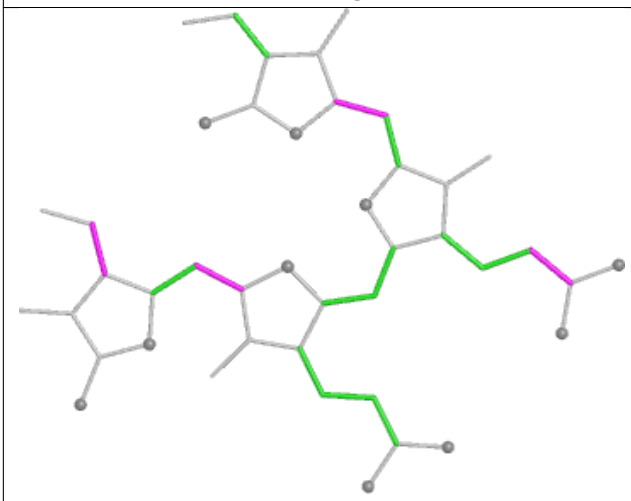

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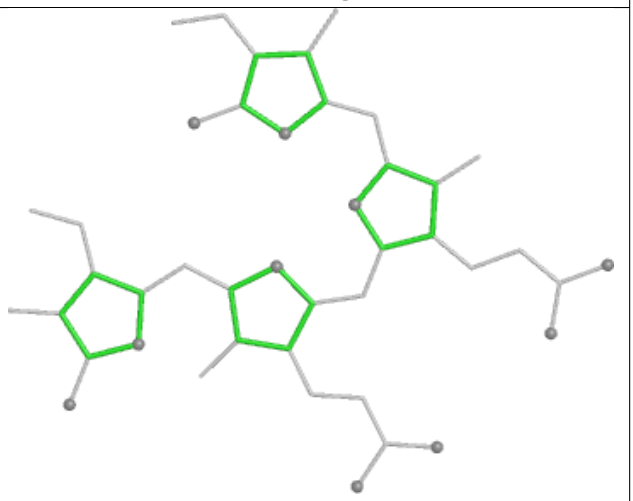
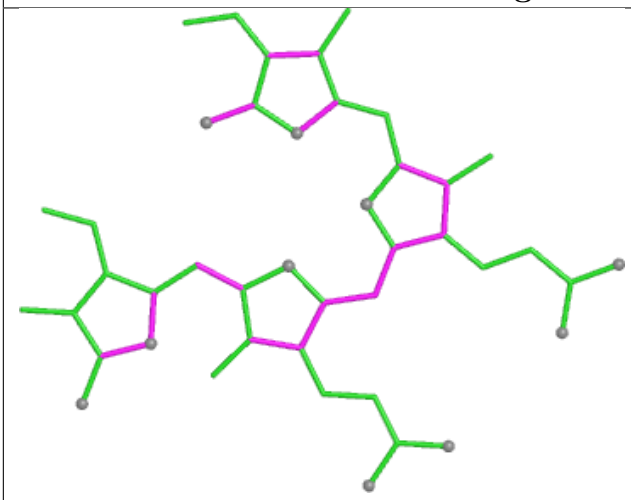


Rings

Ligand PEB kK 203



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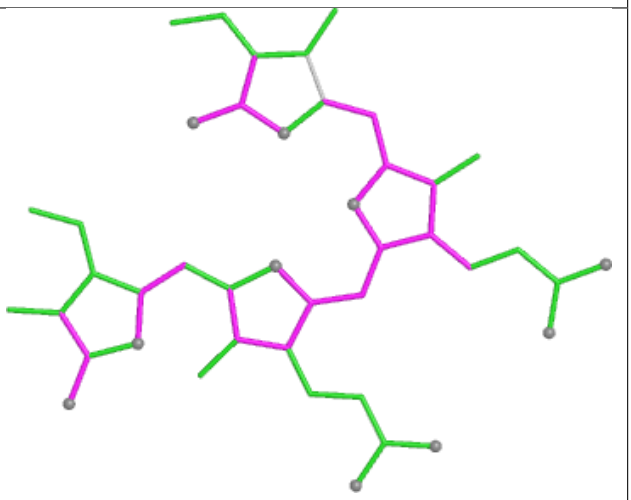

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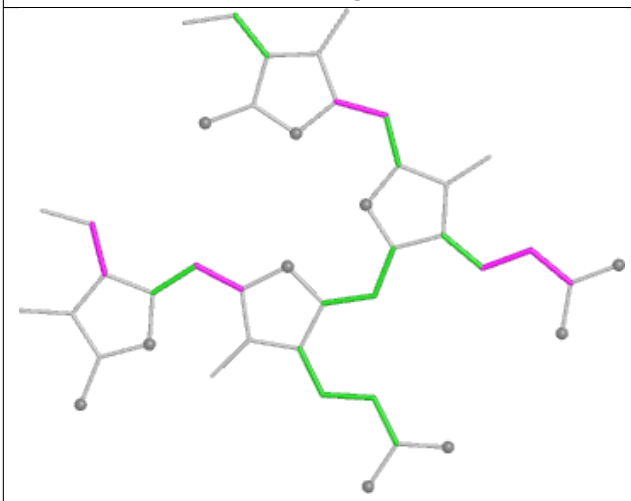

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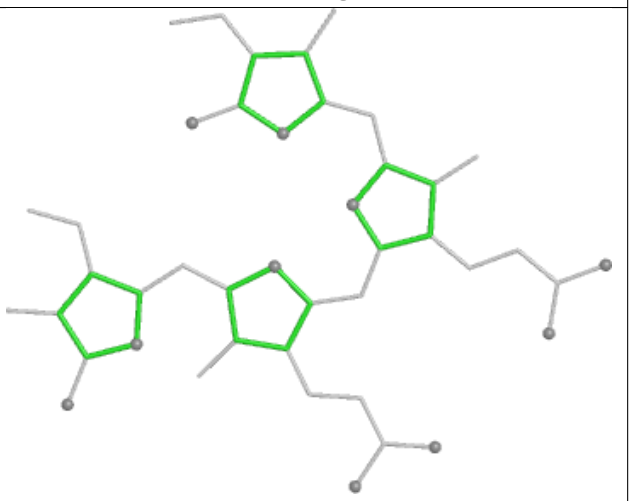

Rings

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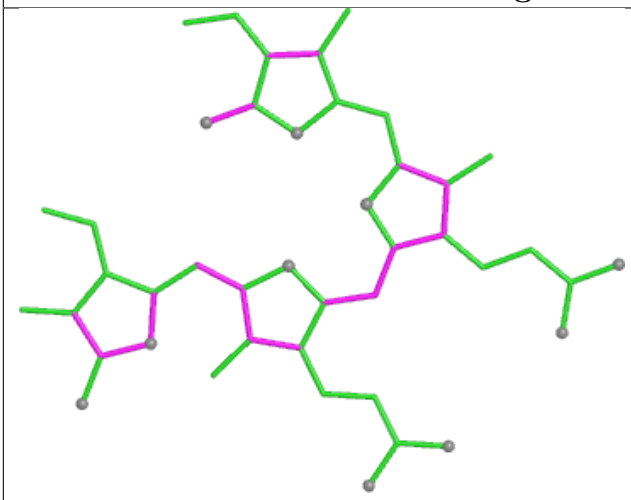

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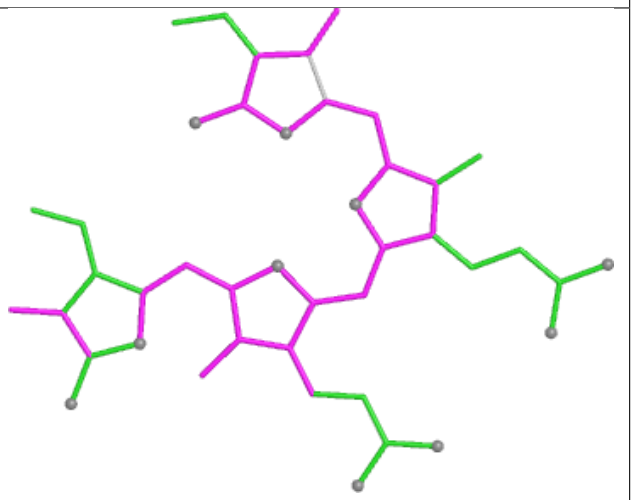

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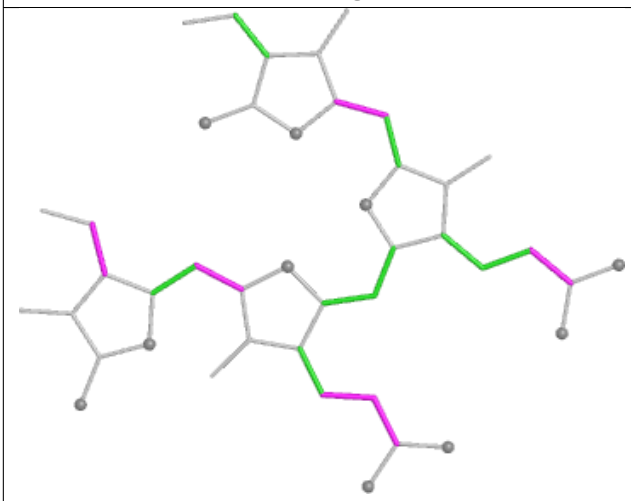

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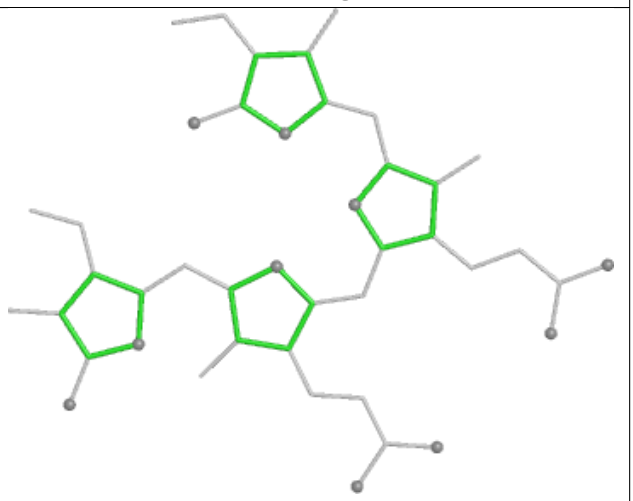
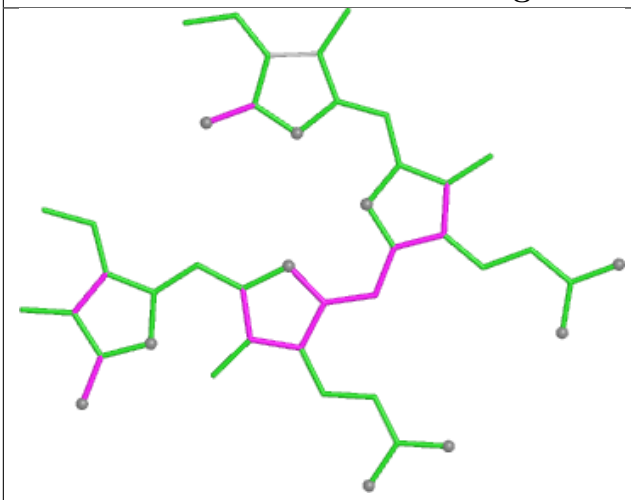


Rings

Ligand PUB A1 304



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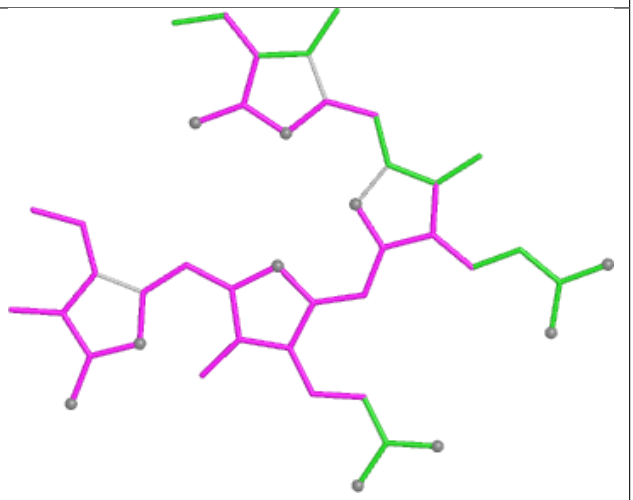

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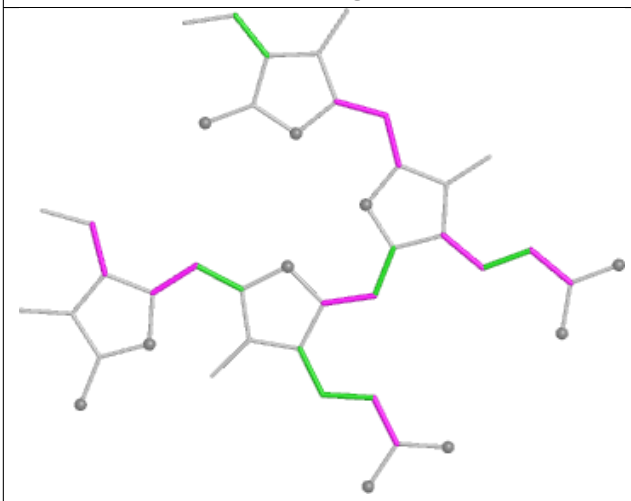

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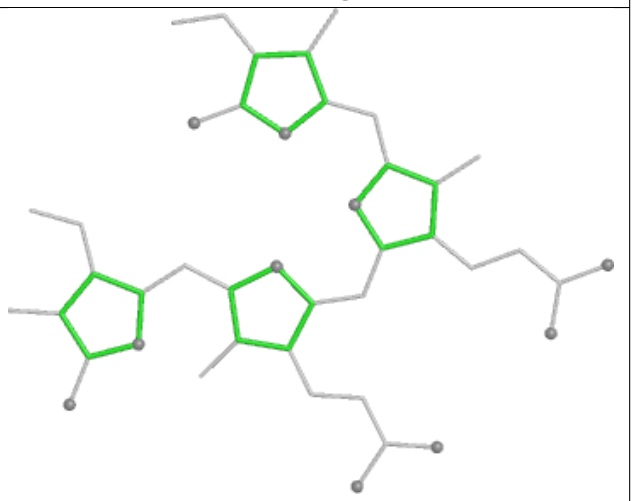

Rings

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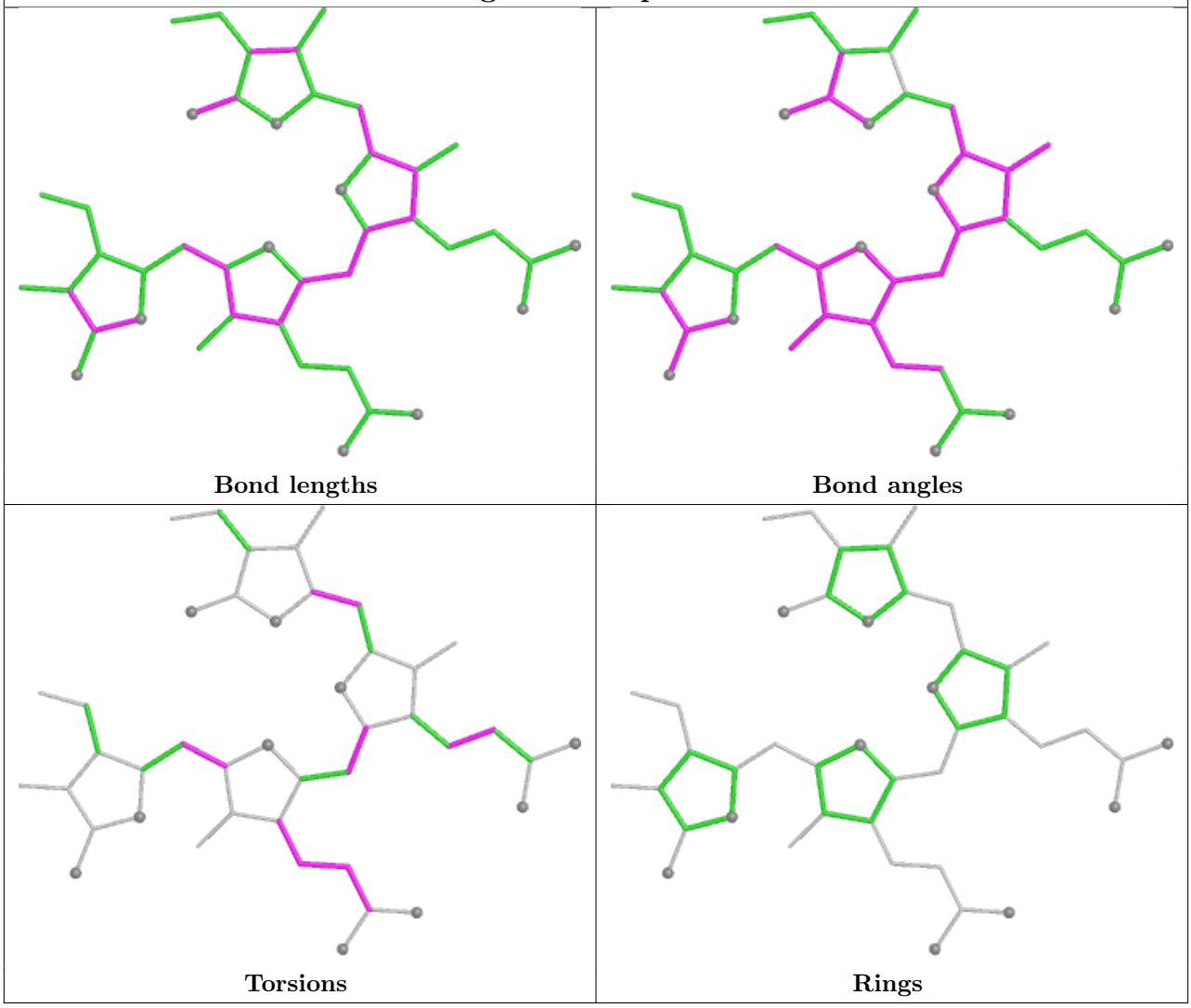

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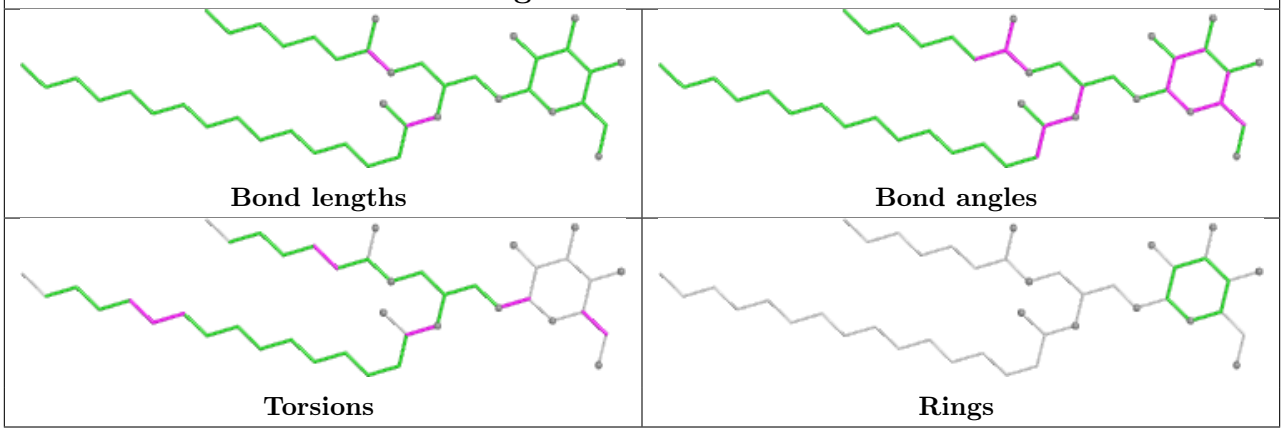

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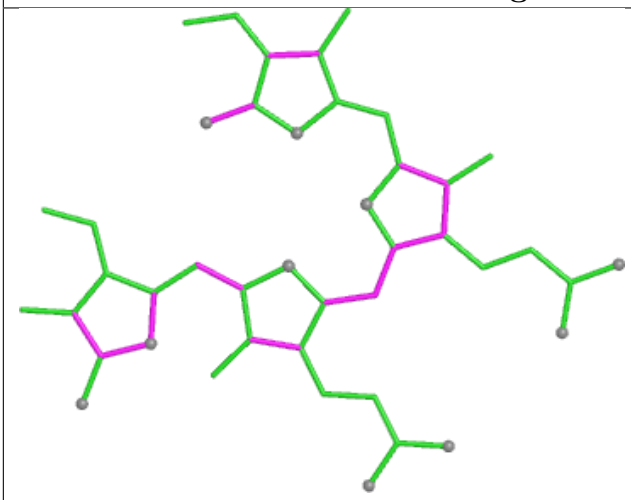

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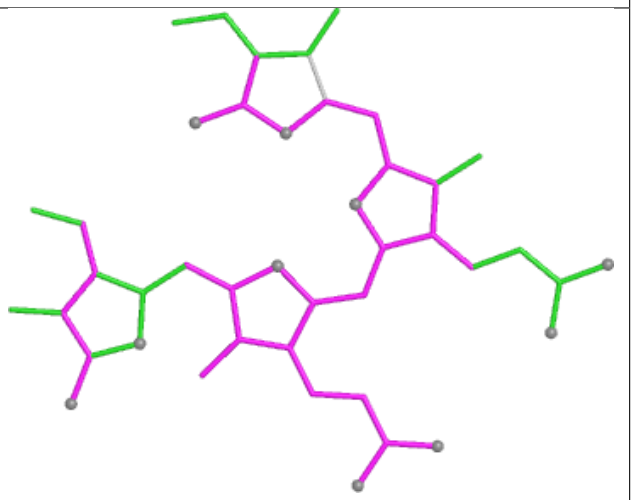

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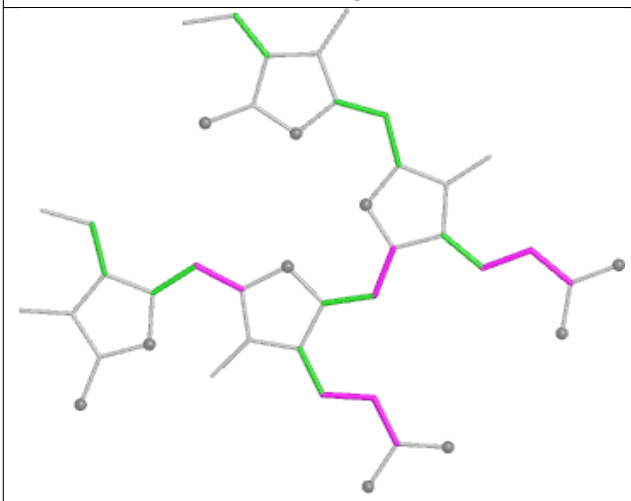

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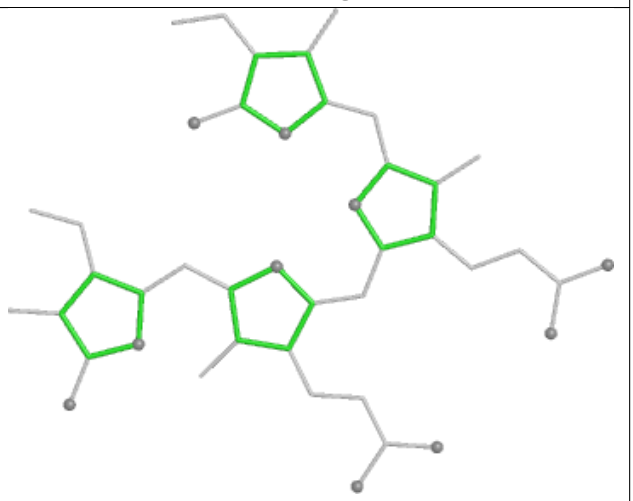

Rings

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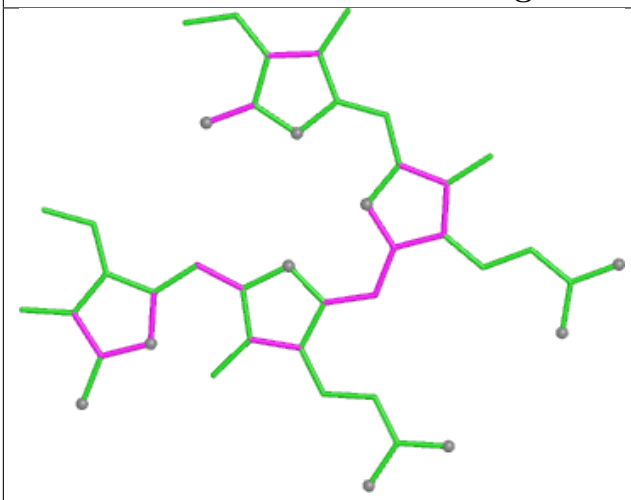

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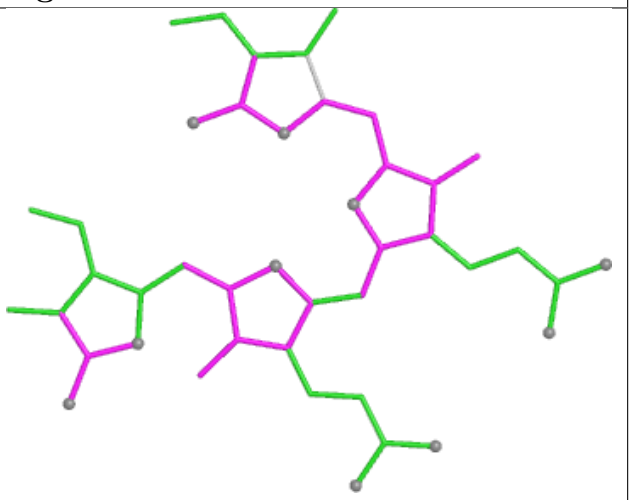

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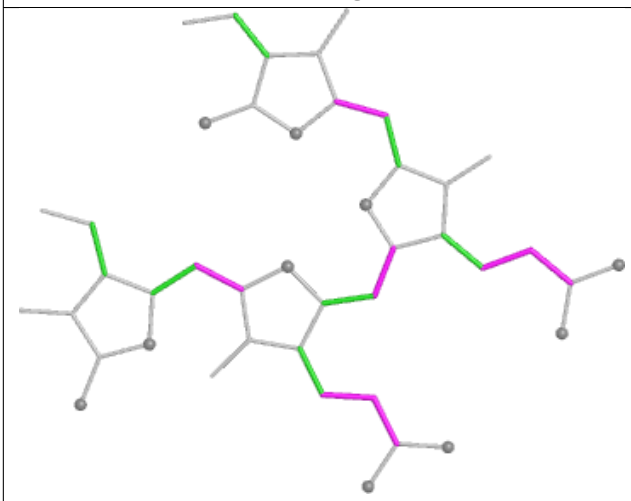

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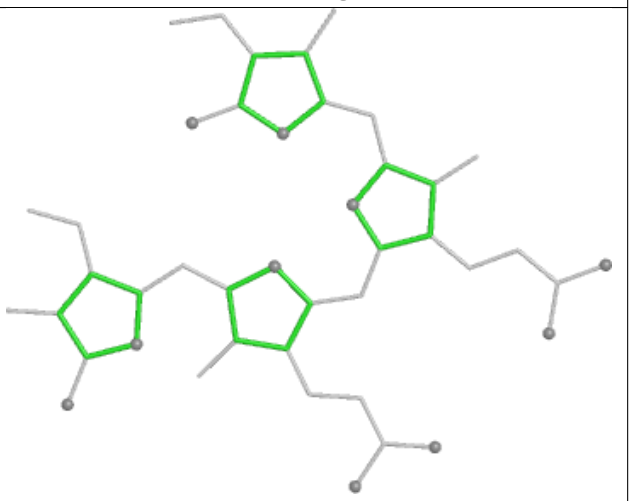
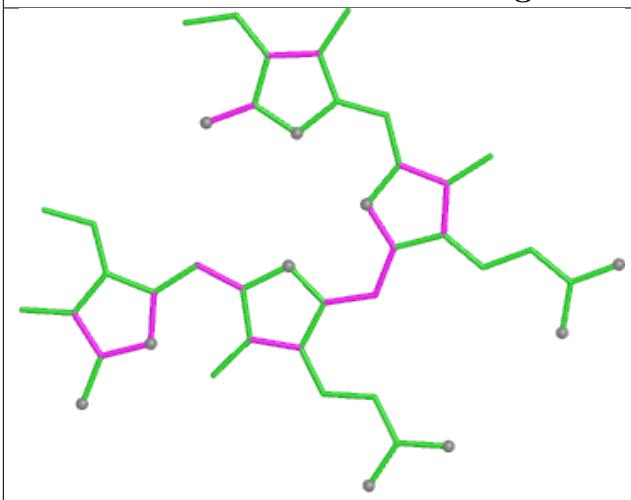


Rings

Ligand PEB HJ 201



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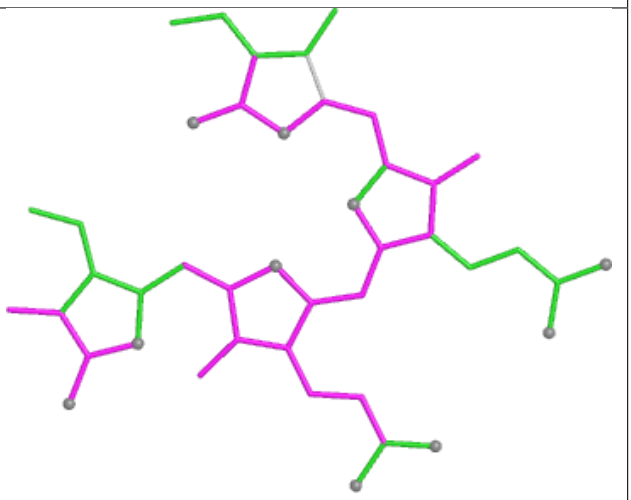

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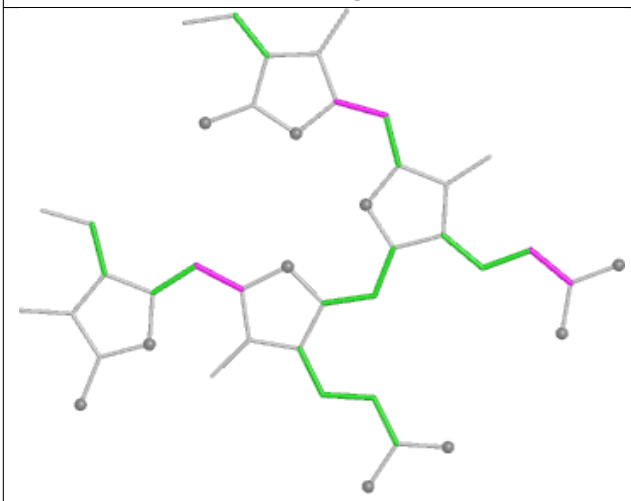

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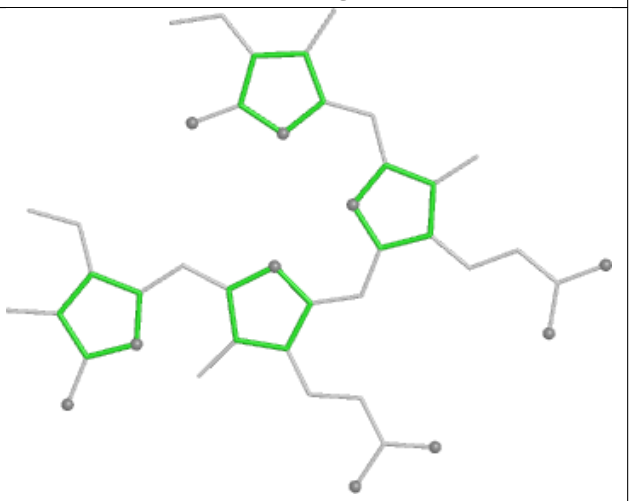

Rings

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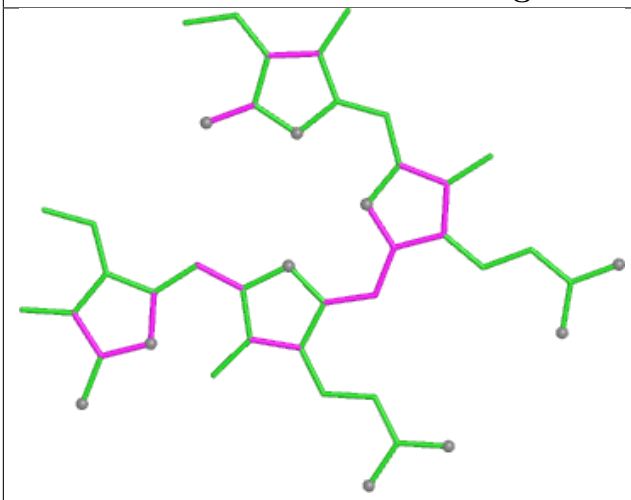

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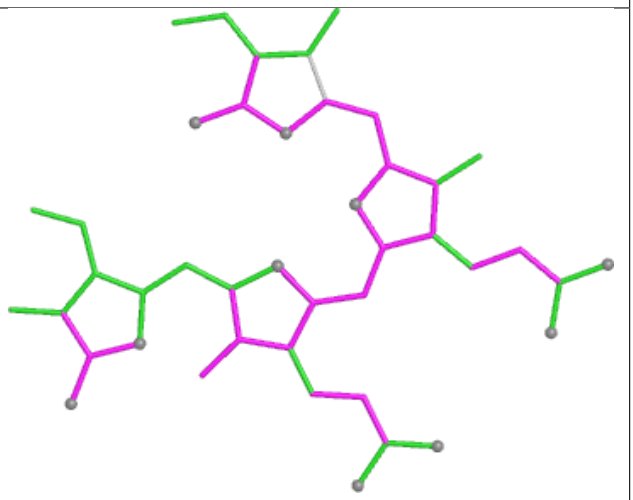

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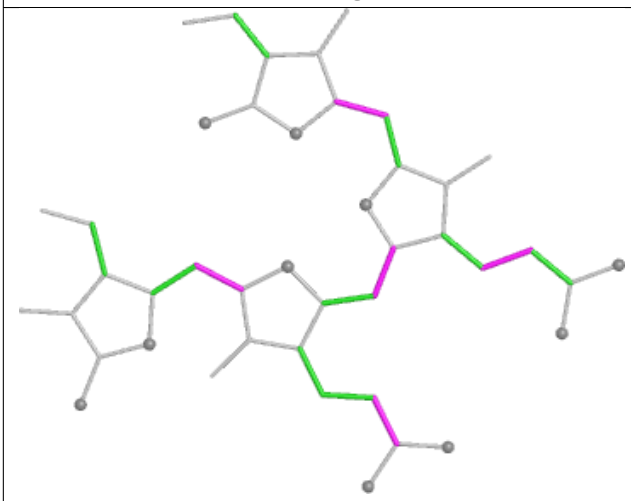

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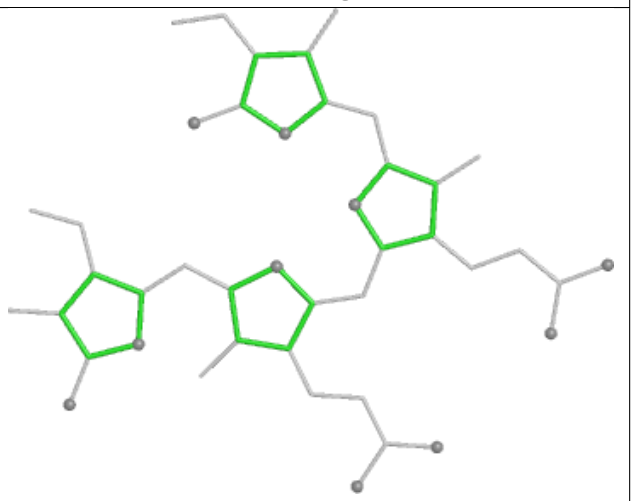

Rings

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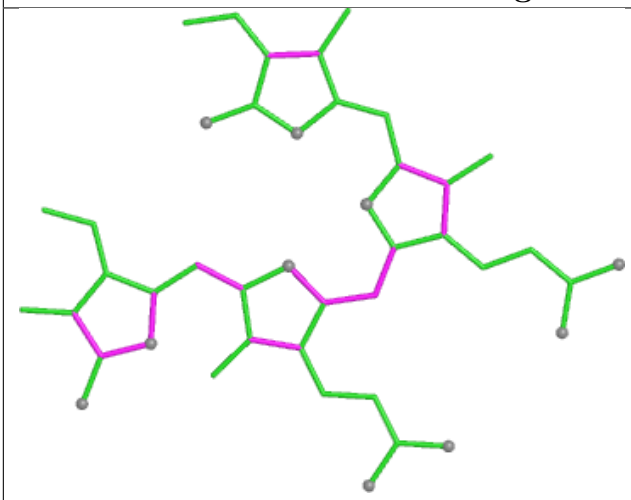

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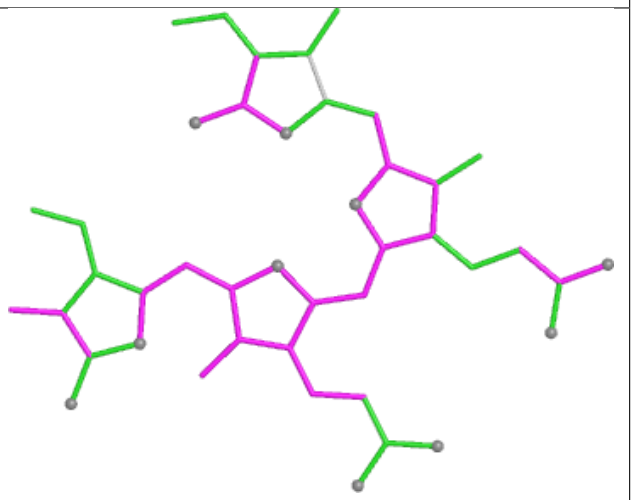

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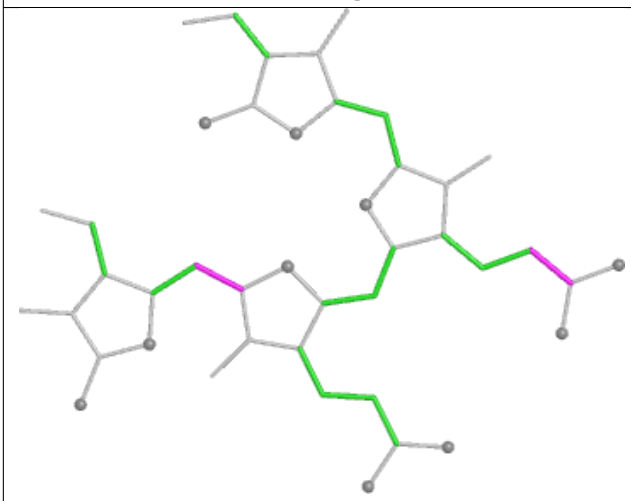

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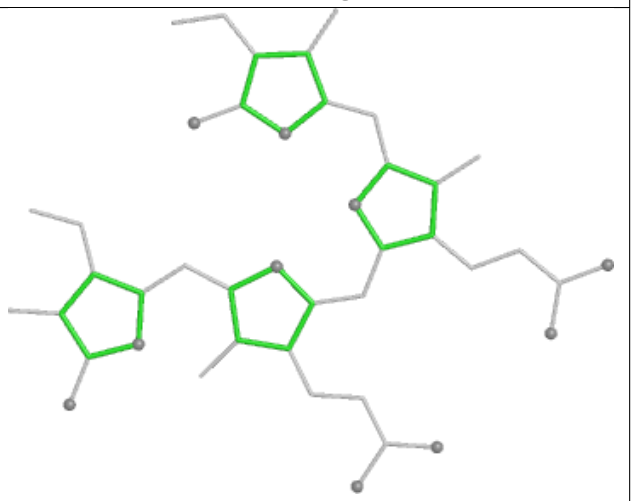
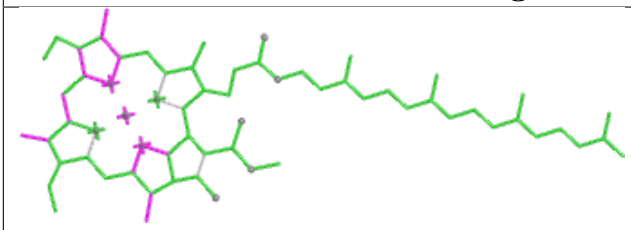


Rings

Ligand CLA AN 830



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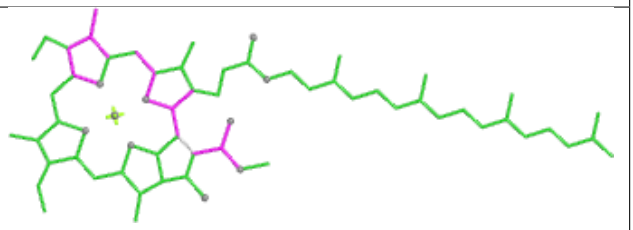

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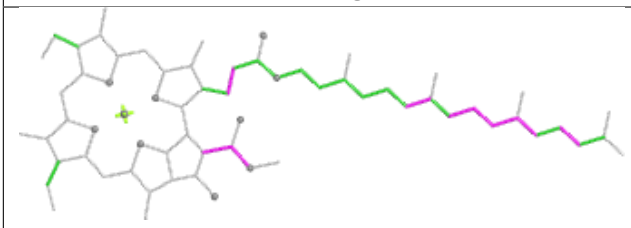

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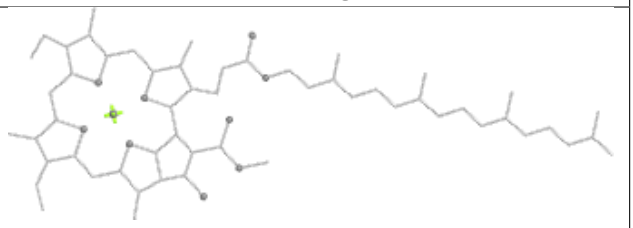
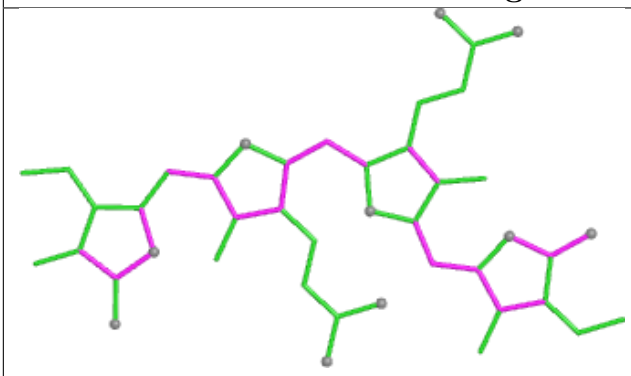


Rings

Ligand CYC E3 1001



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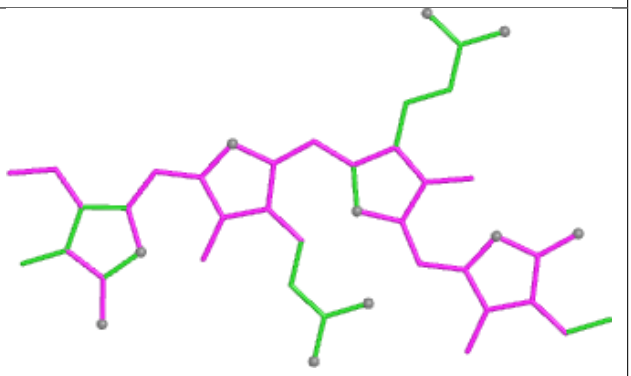

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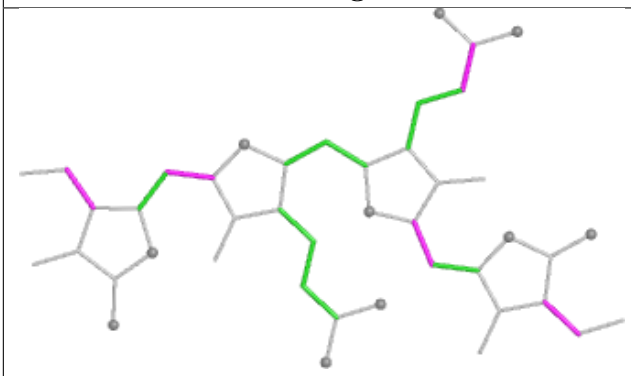

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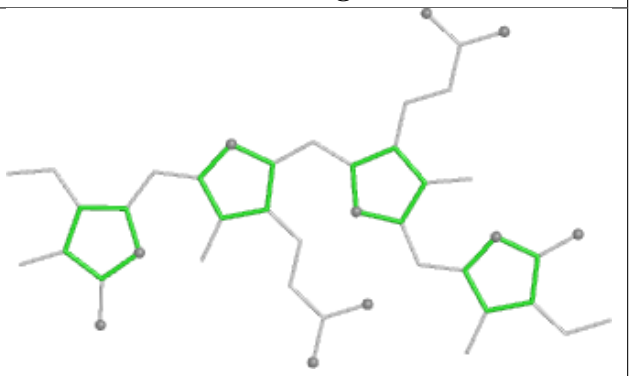
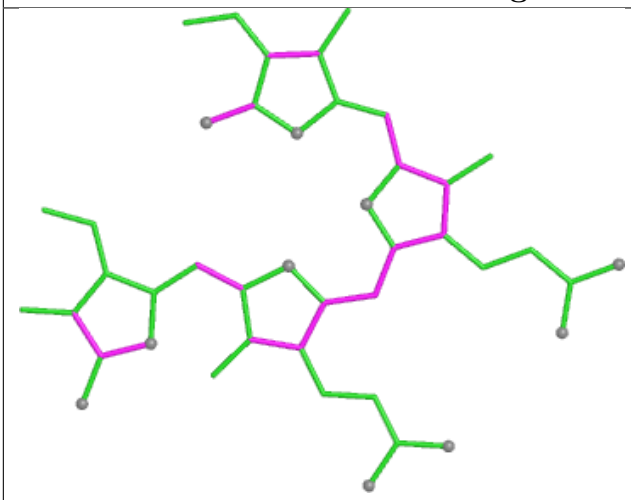


Rings

Ligand PEB HA 202



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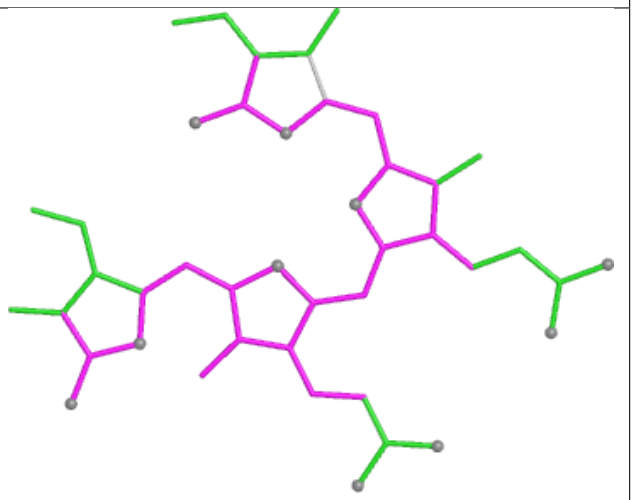
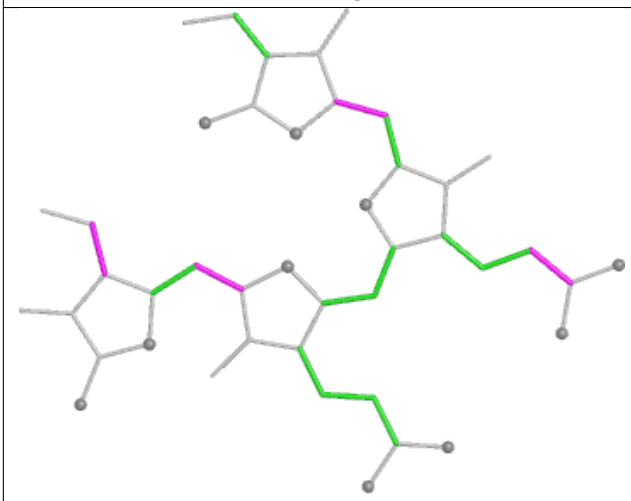


Bond angles



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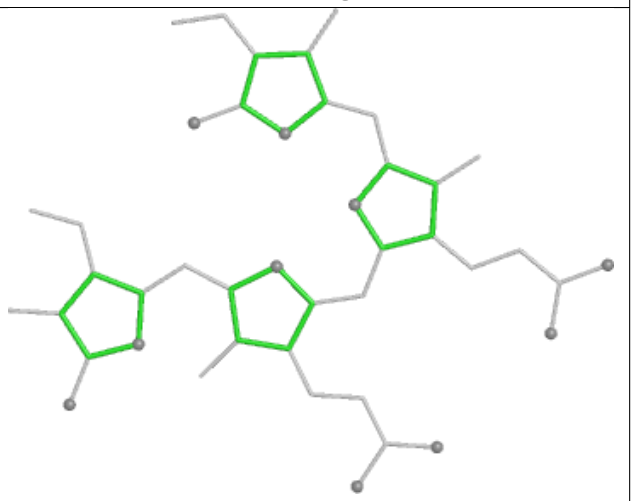
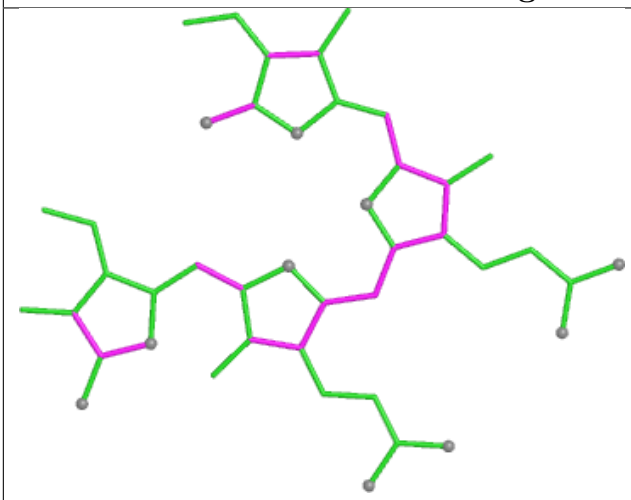


Rings

Ligand PEB fH 203



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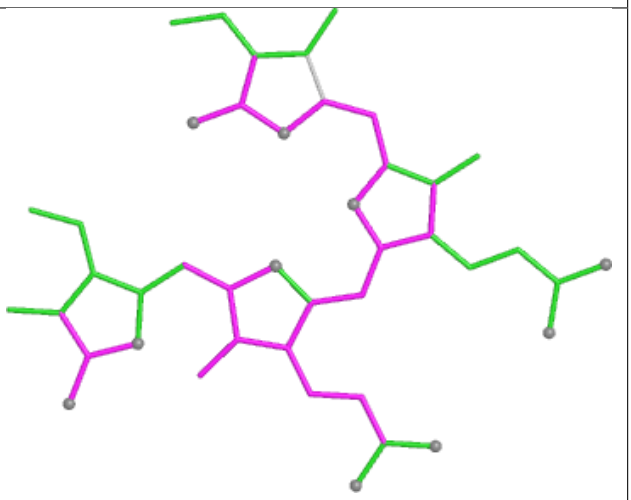
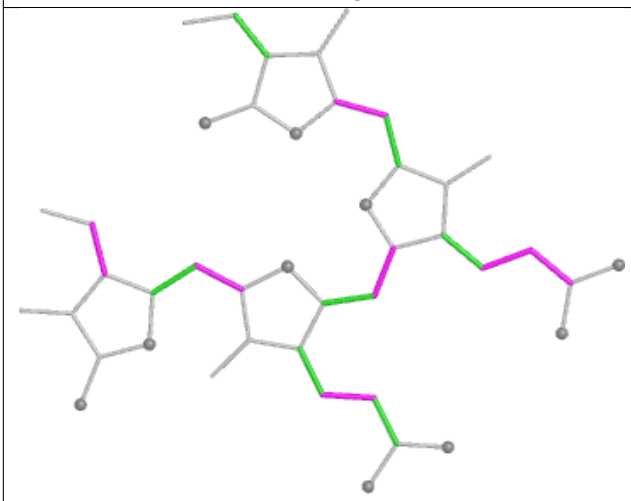


Bond angles



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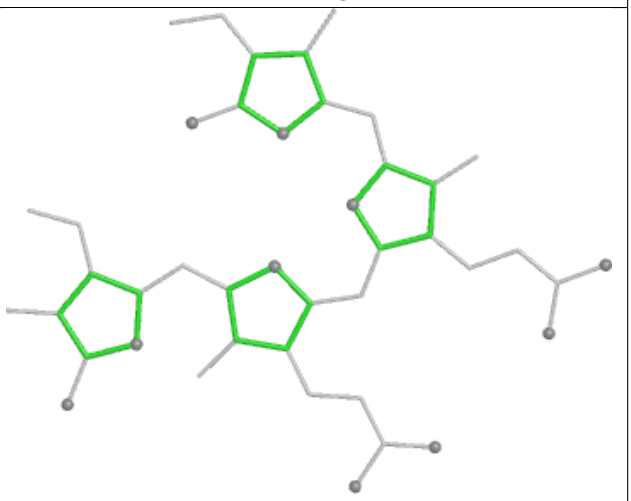

Rings

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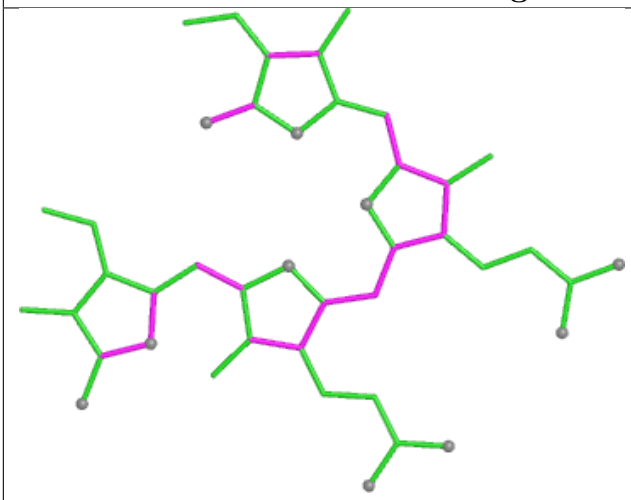

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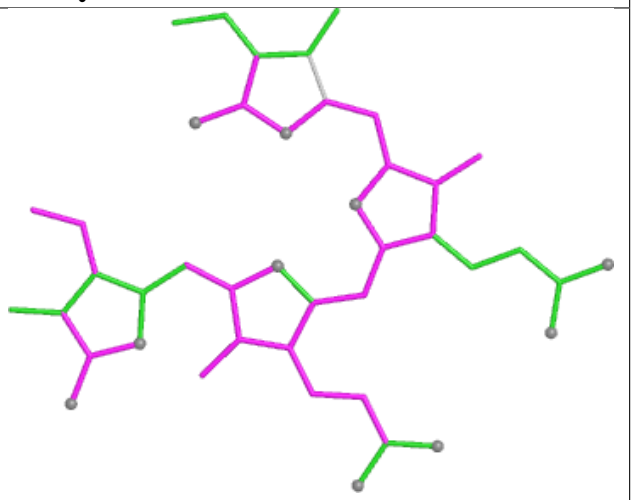
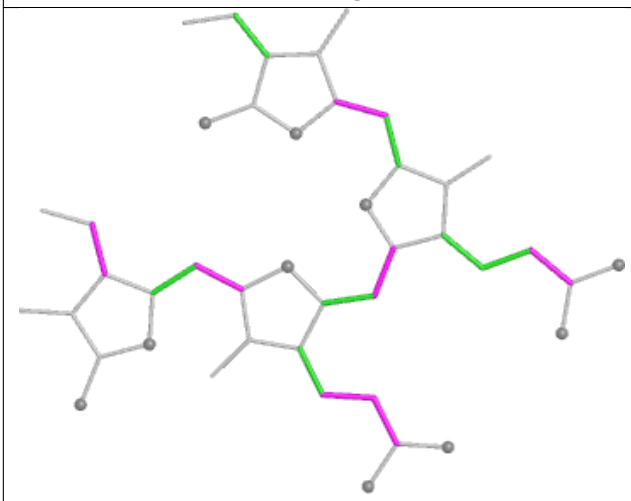
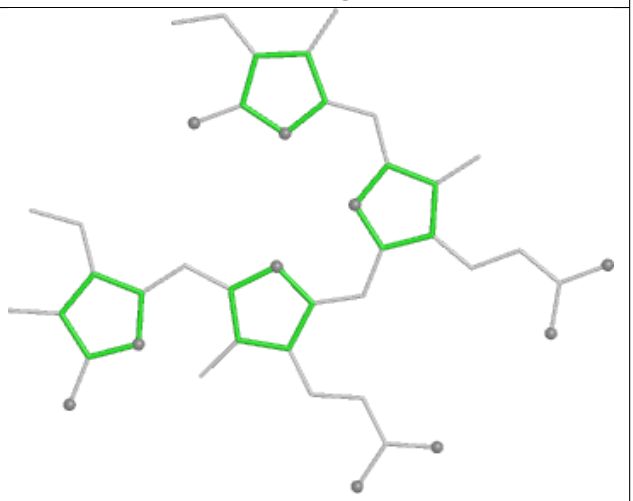


Bond angles

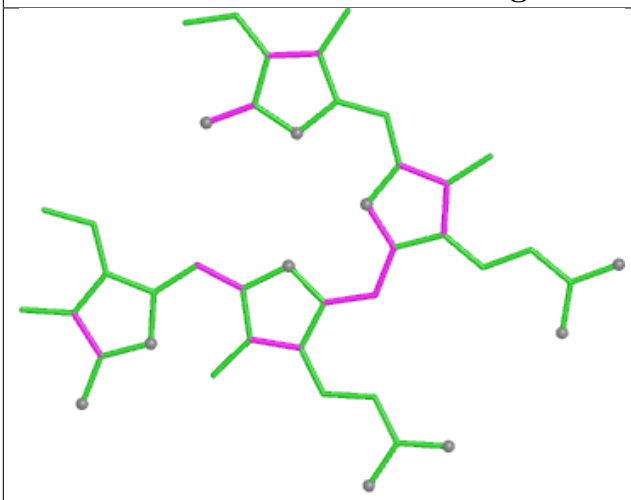


Torsions



Rings

Ligand PEB DK 201



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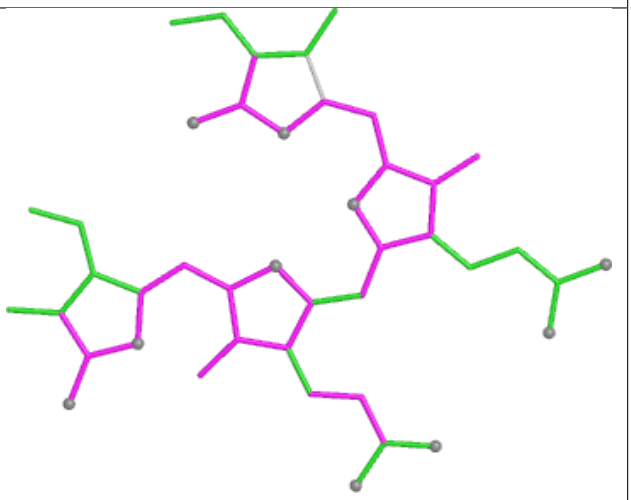
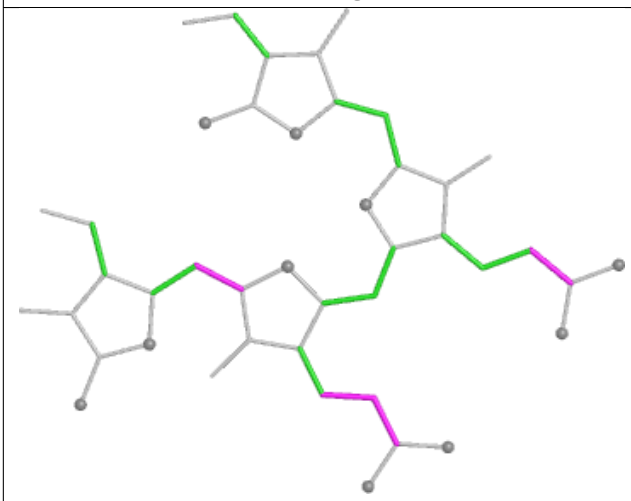


Bond angles



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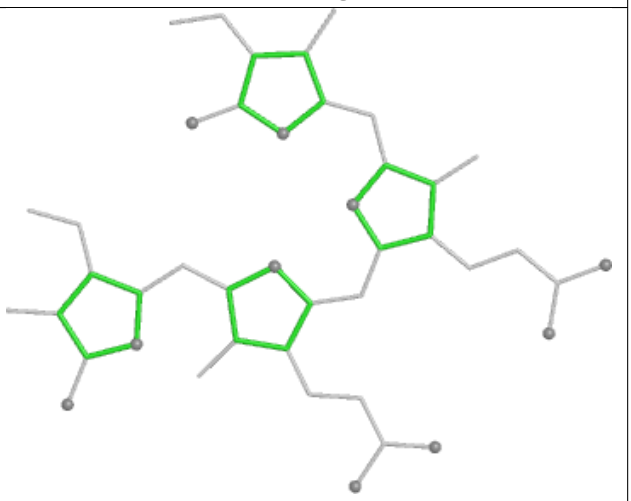
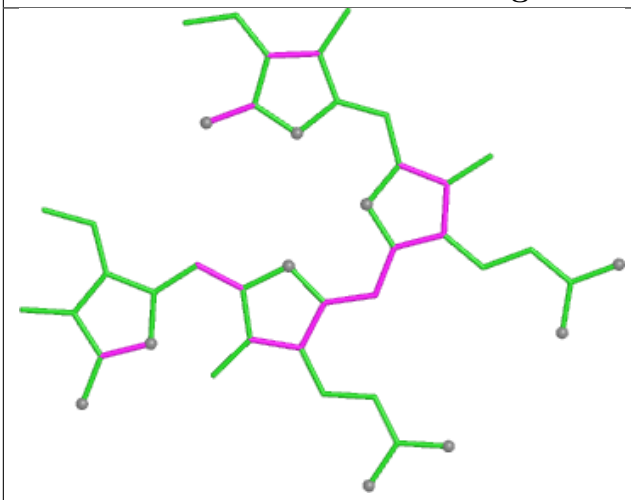


Rings

Ligand PEB RO 203



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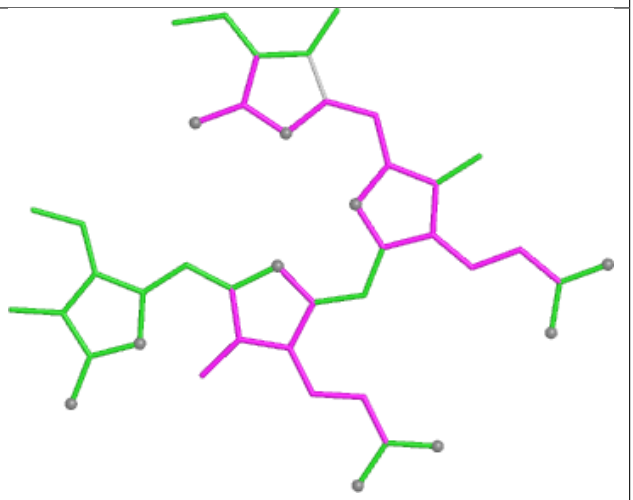

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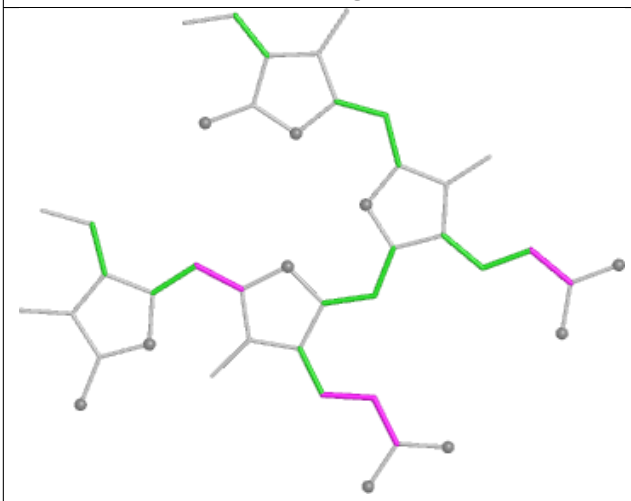

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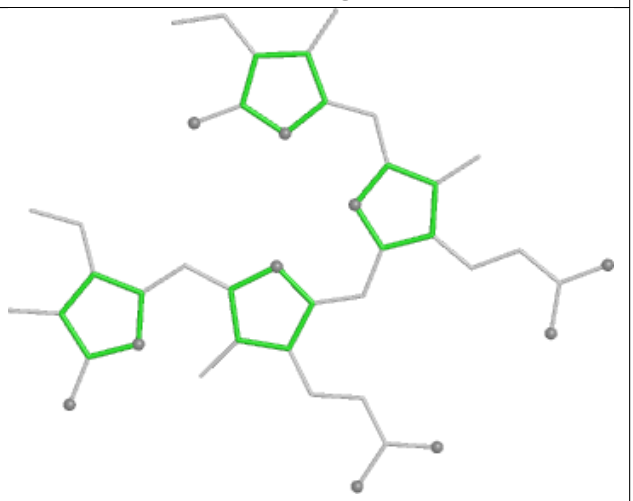
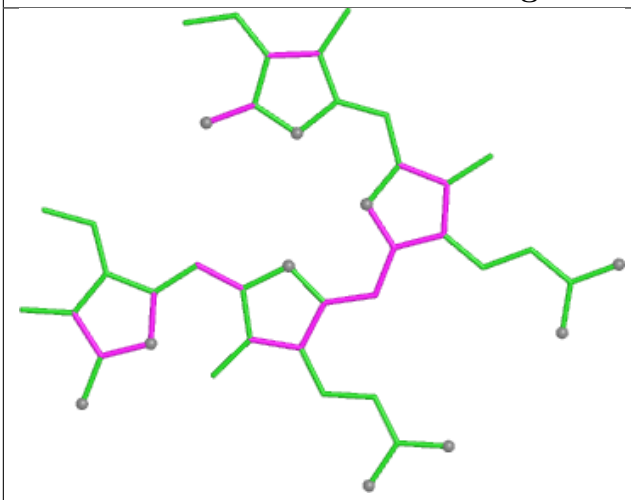


Rings

Ligand PEB z8 202



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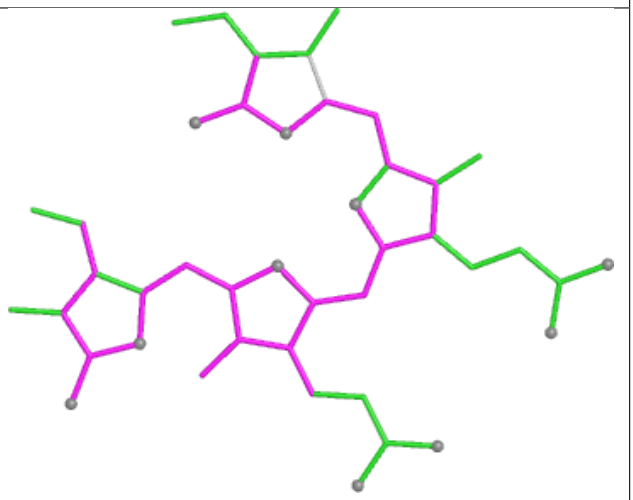

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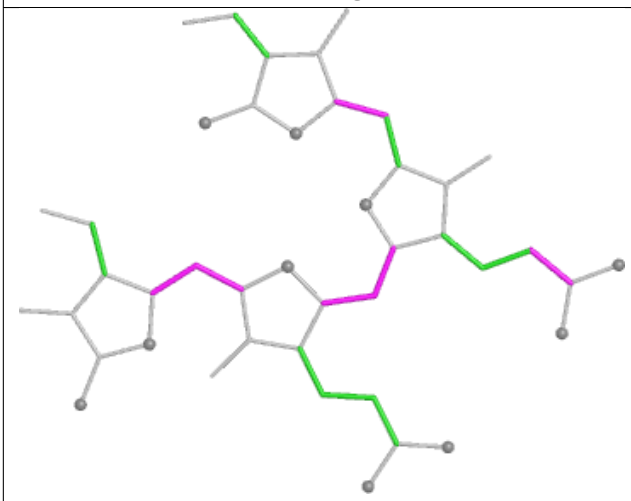

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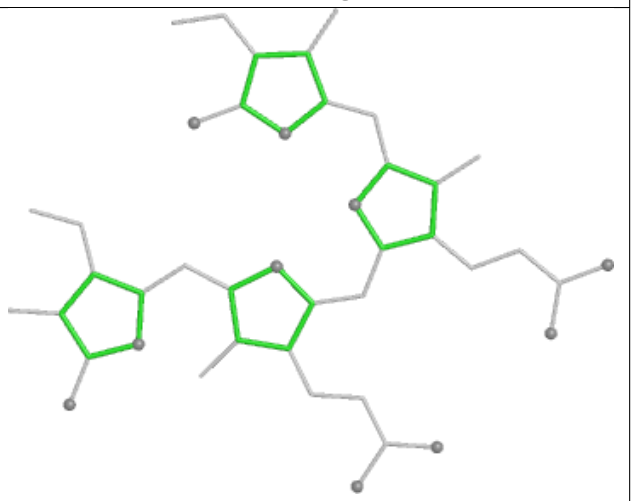
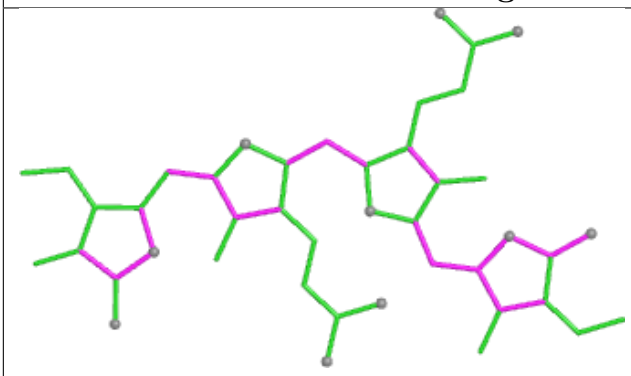


Rings

Ligand CYC ME 1001



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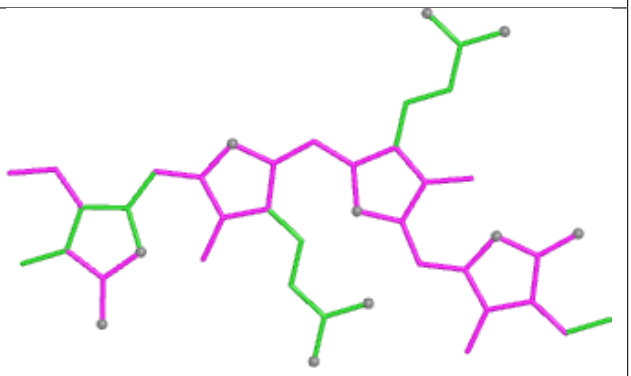
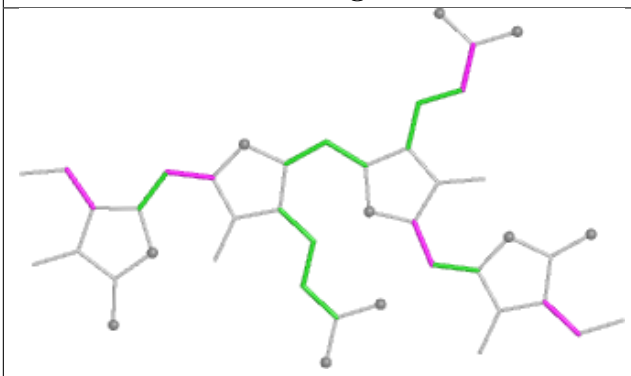


Bond angles



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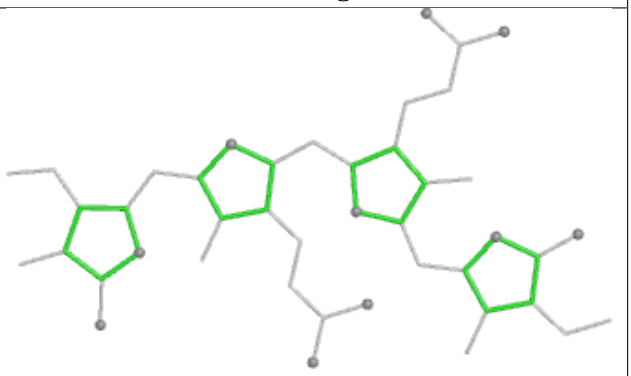
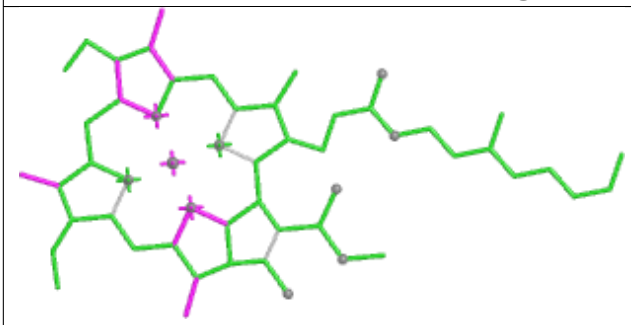


Rings

Ligand CLA A2 814



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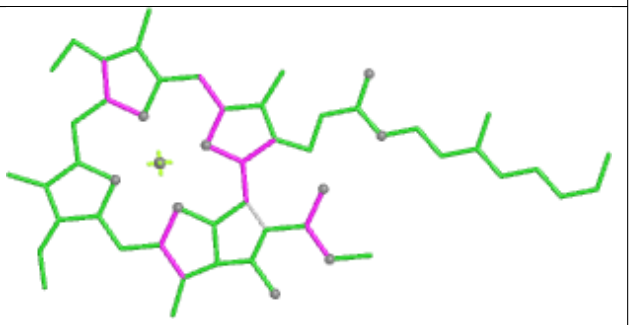

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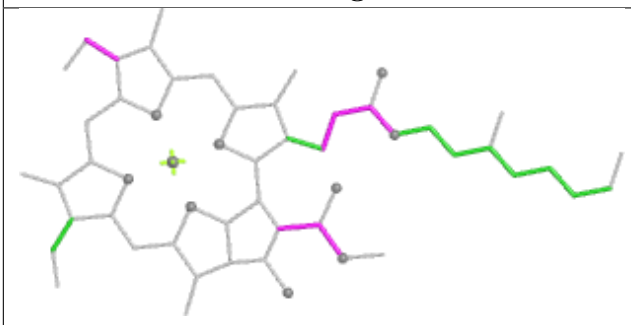

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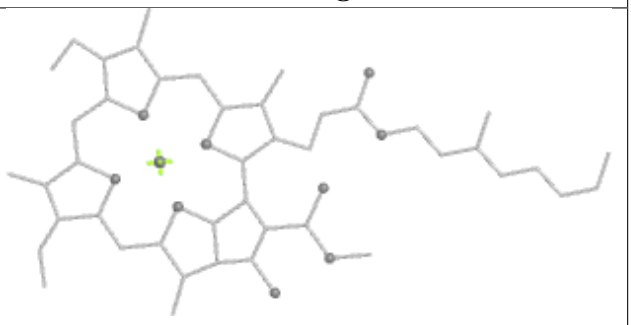
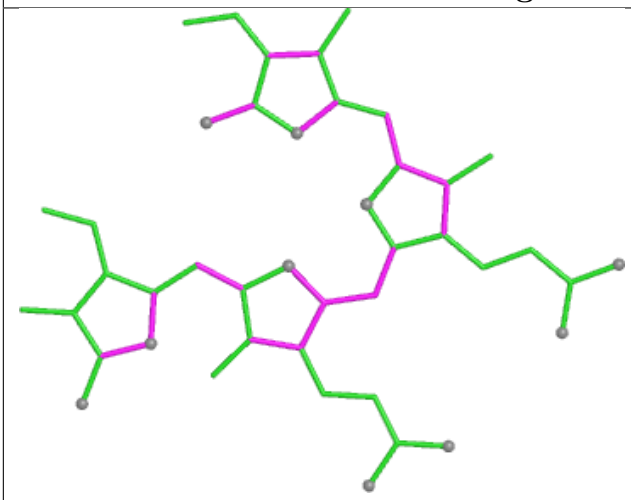


Rings

Ligand PEB B9 202



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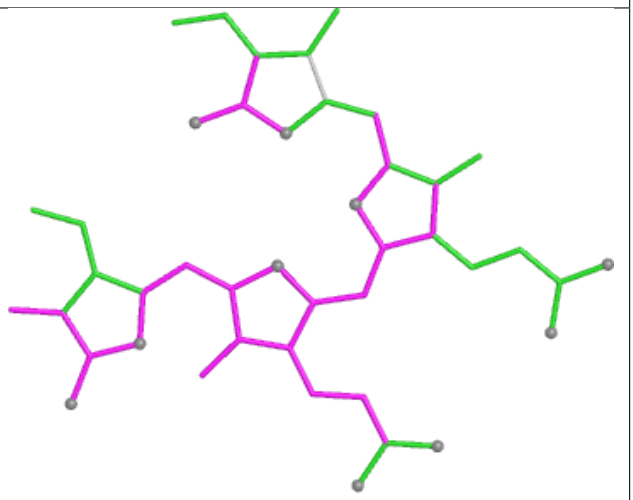

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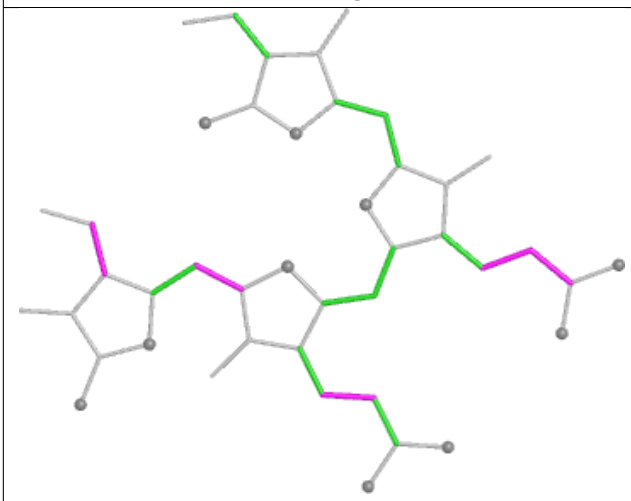

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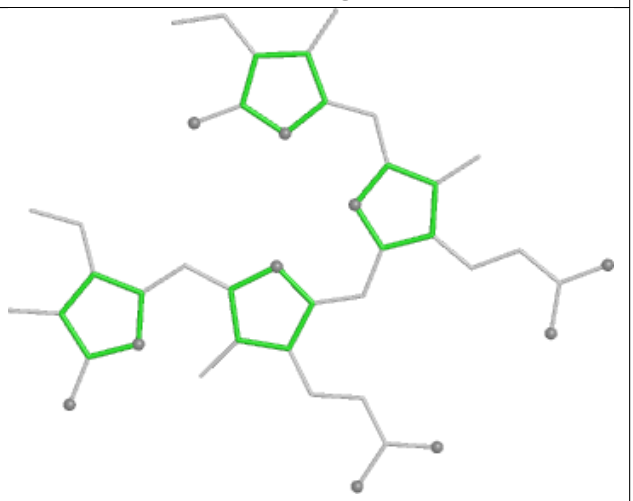
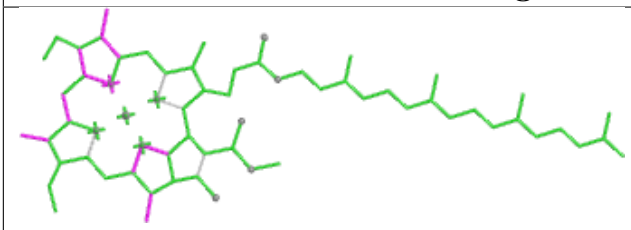


Rings

Ligand CLA D6 405



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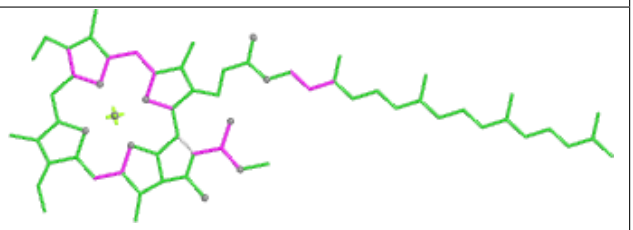

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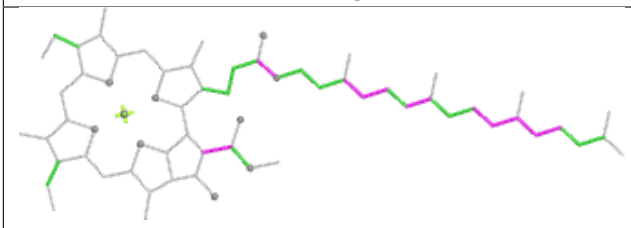

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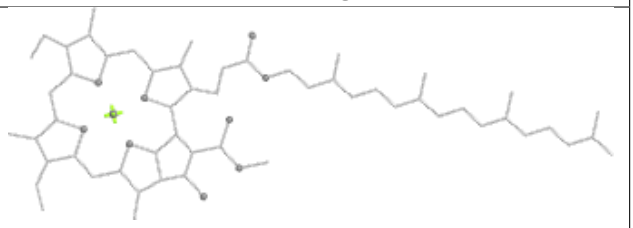
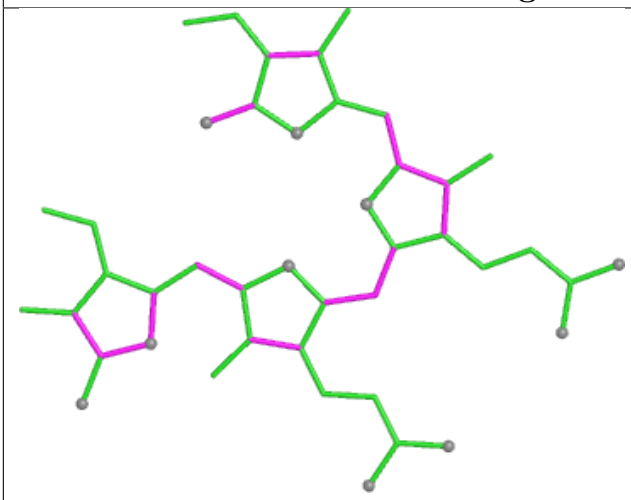


Rings

Ligand PEB iK 202



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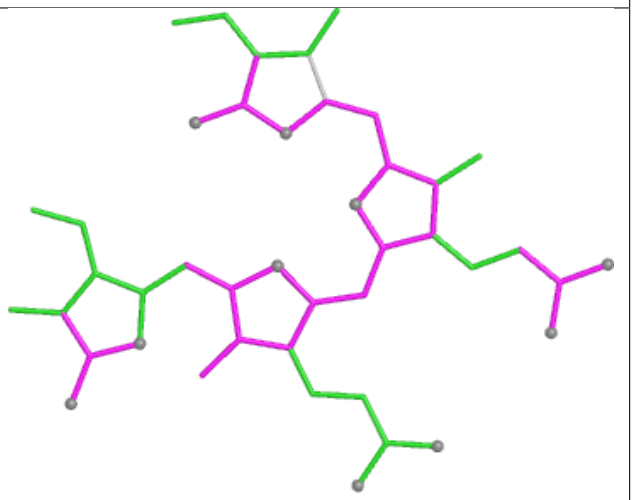

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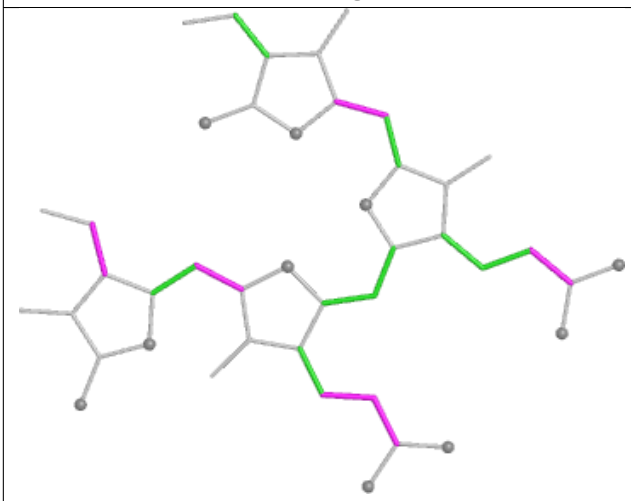

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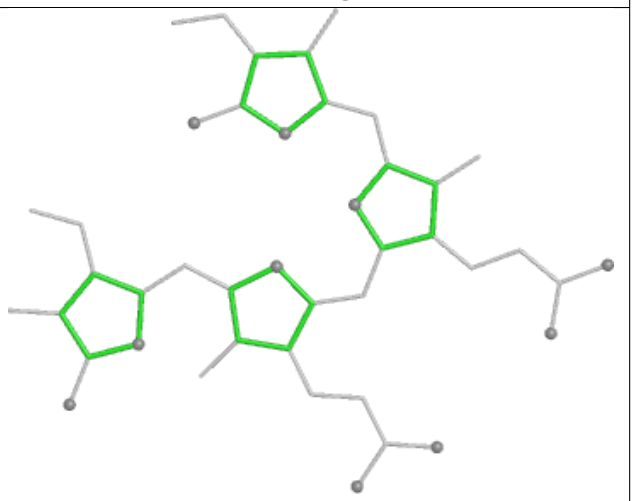
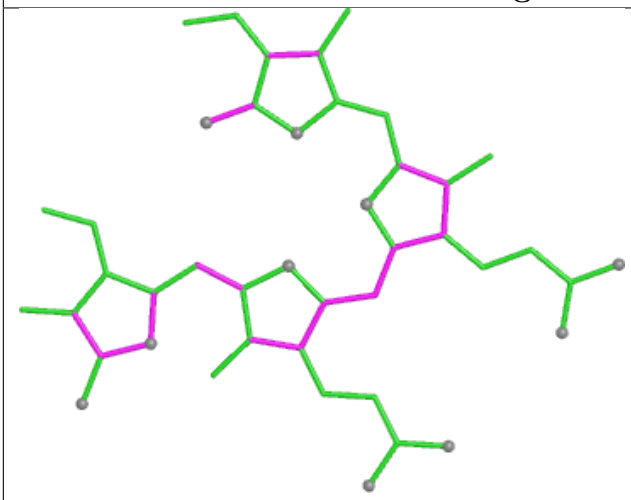


Rings

Ligand PEB dH 203



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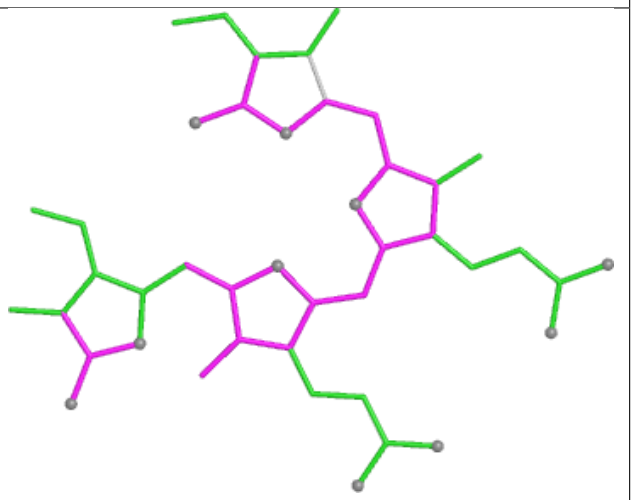
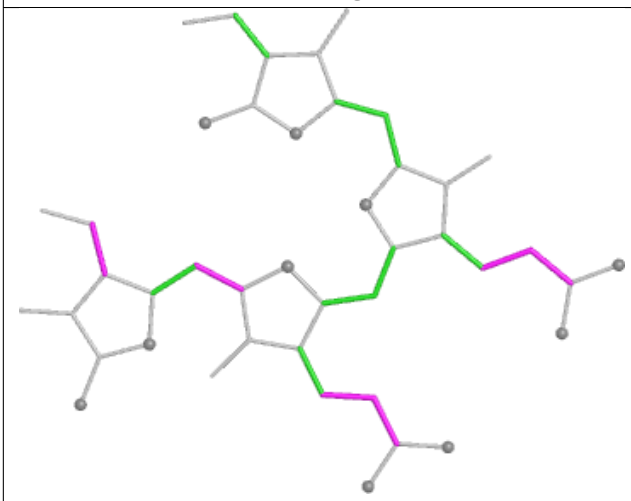


Bond angles



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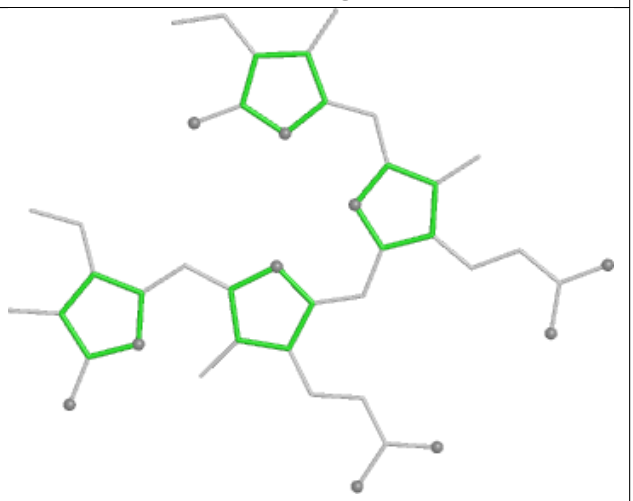
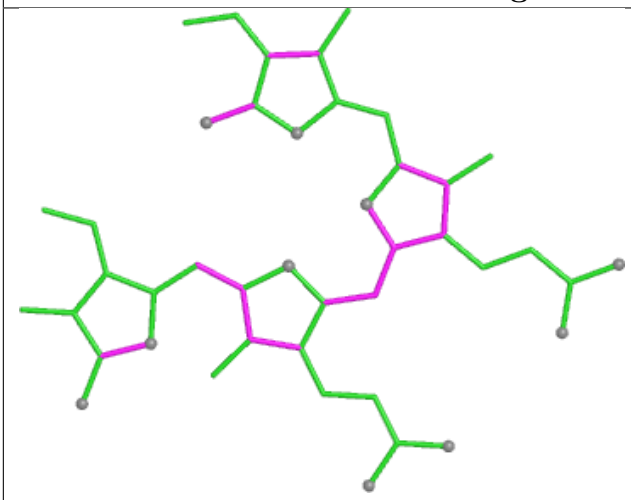


Rings

Ligand PEB W1 202



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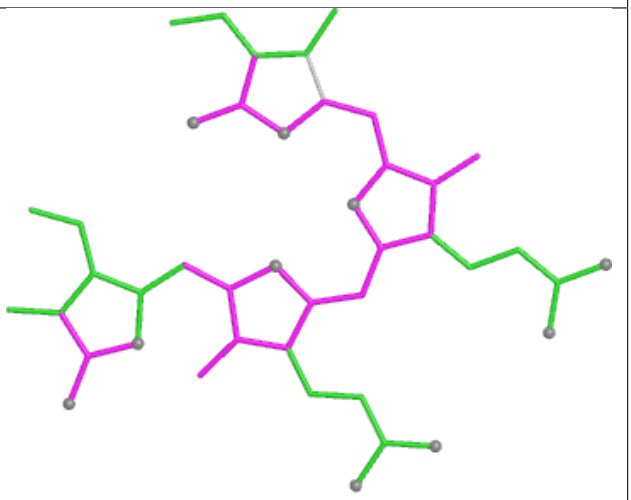

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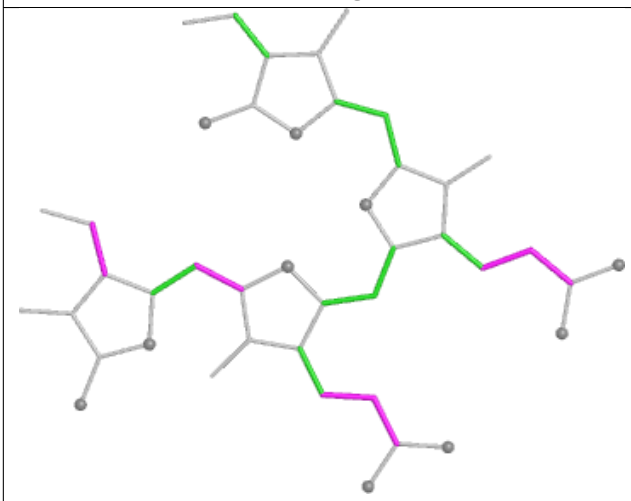

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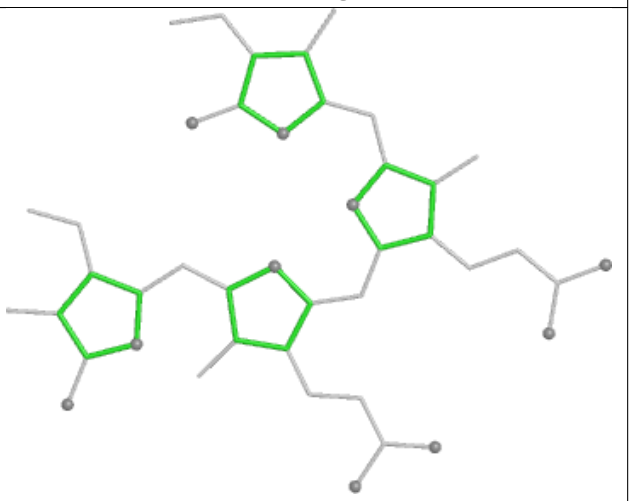
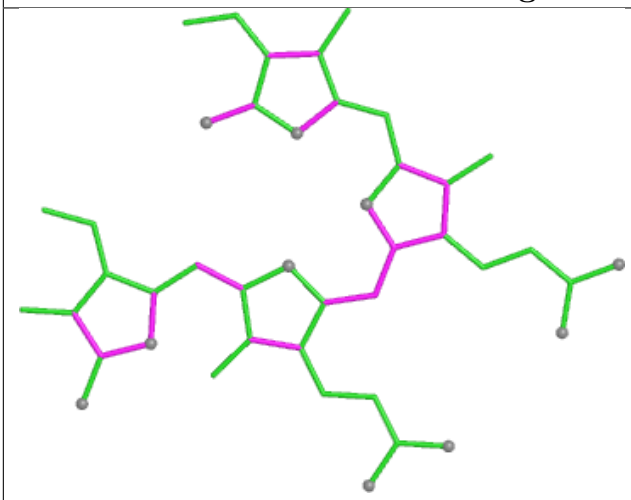


Rings

Ligand PEB d4 202



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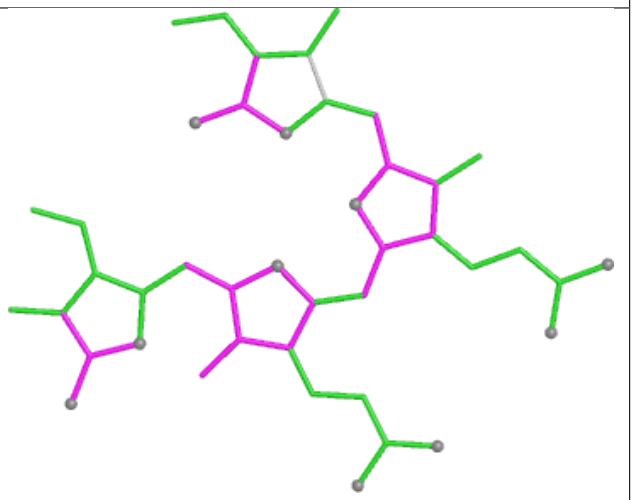
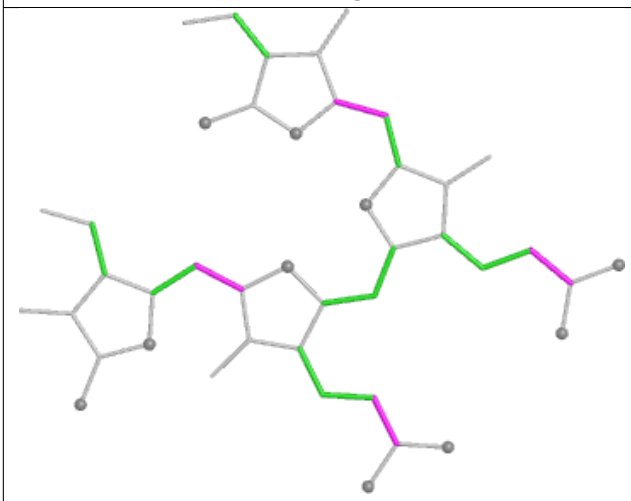


Bond angles



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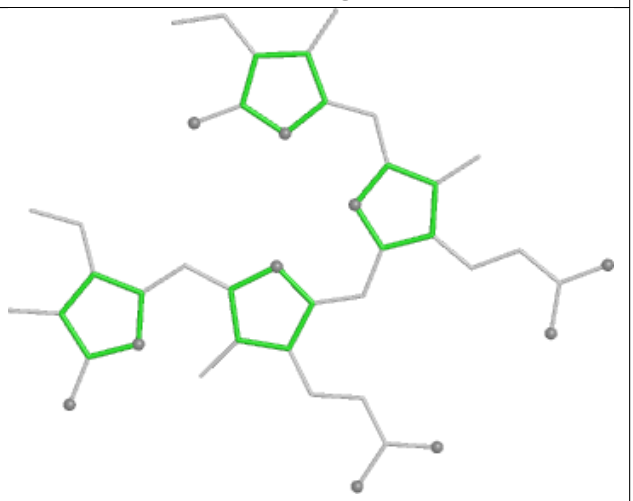
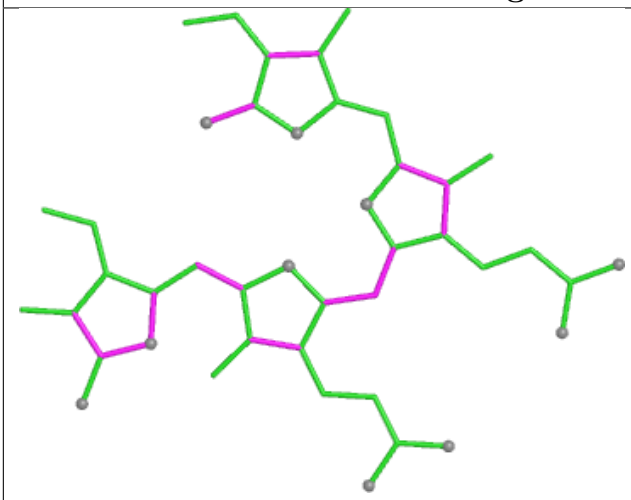


Rings

Ligand PEB YM 202



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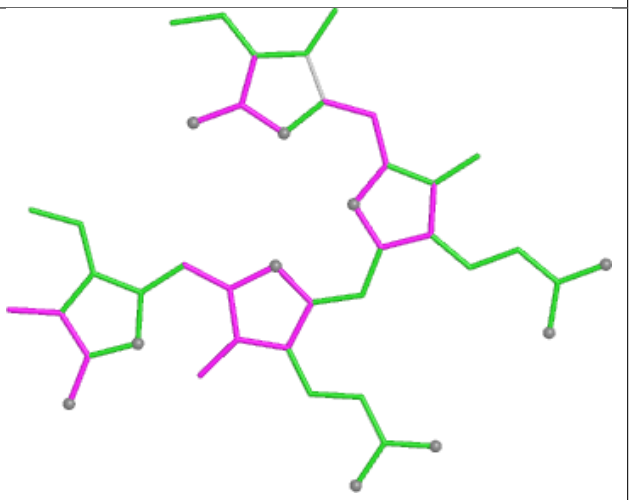
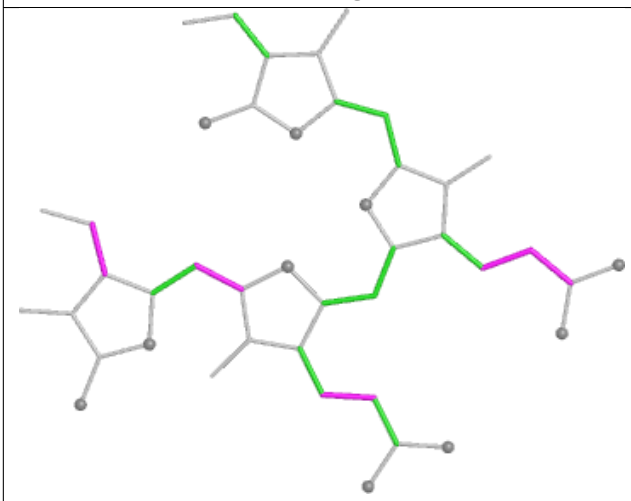


Bond angles



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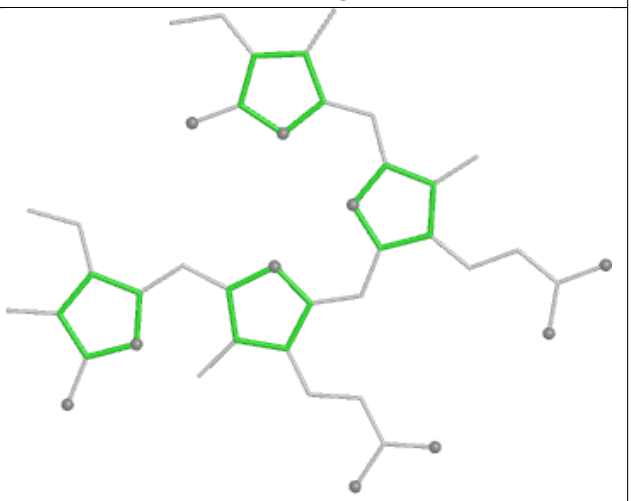
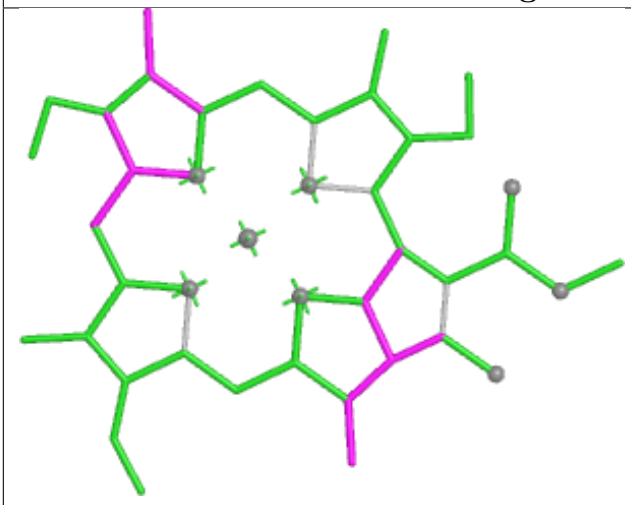


Rings

Ligand CLA 42 604



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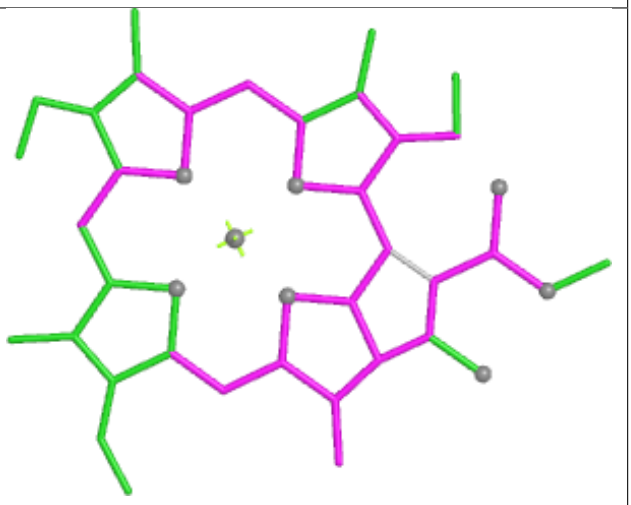
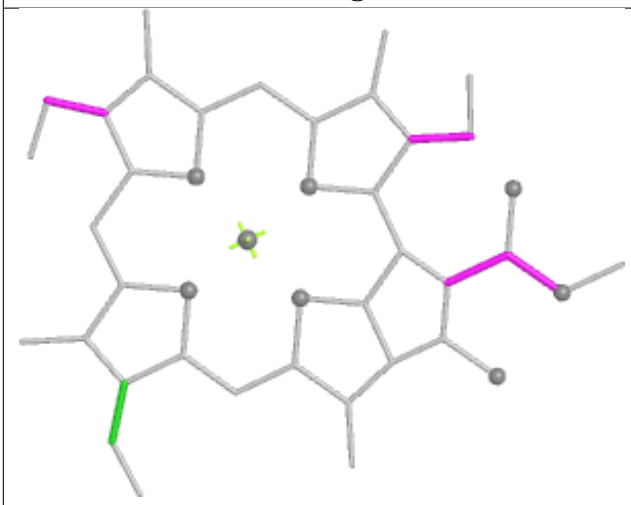


Bond angles

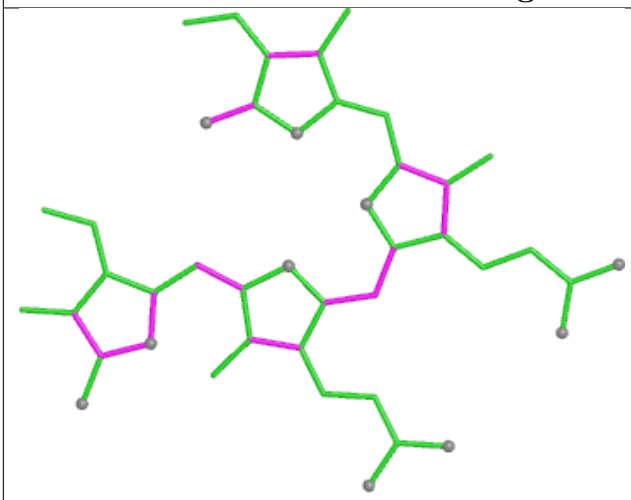


Torsions



Rings

Ligand PEB cB 401



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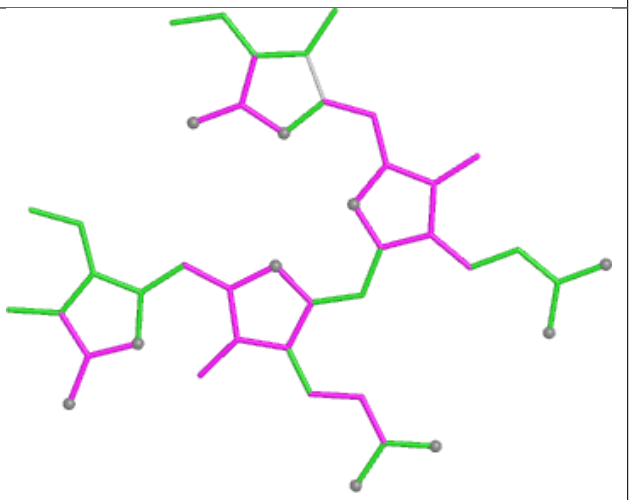
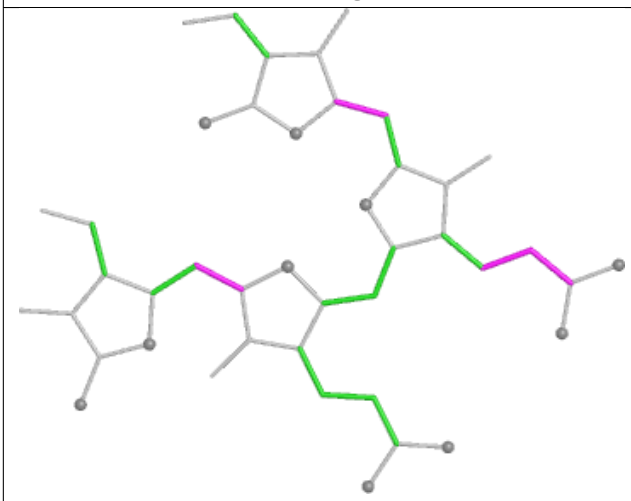


Bond angles



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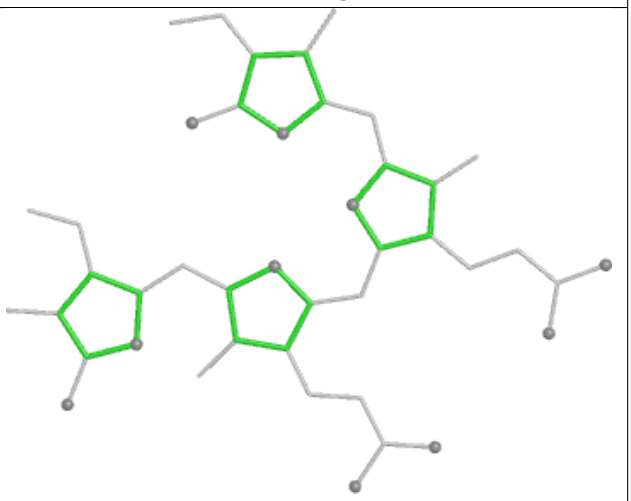
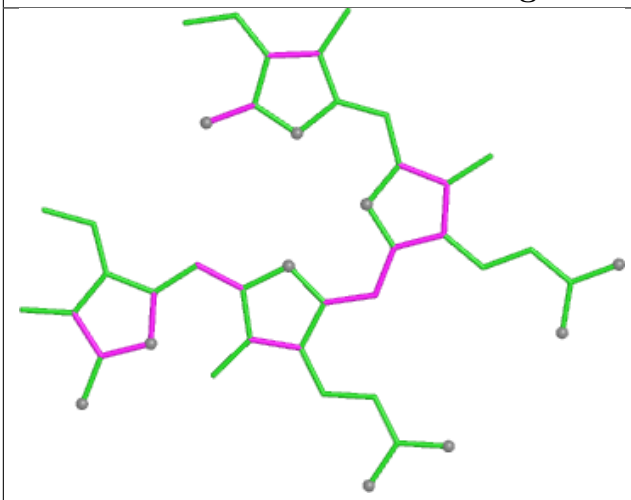
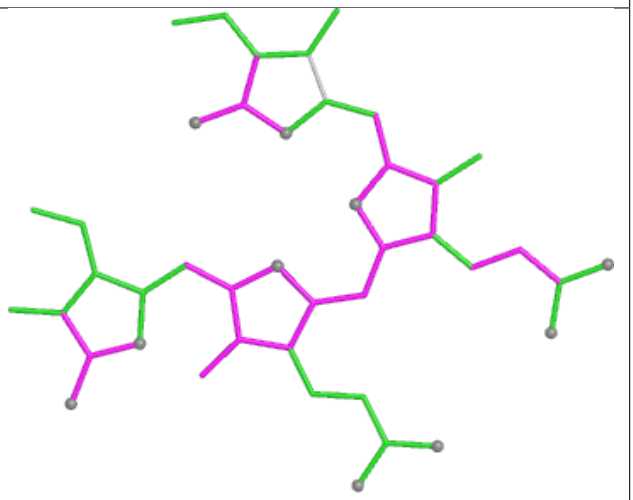


Rings

Ligand PEB iO 202



Bond lengths



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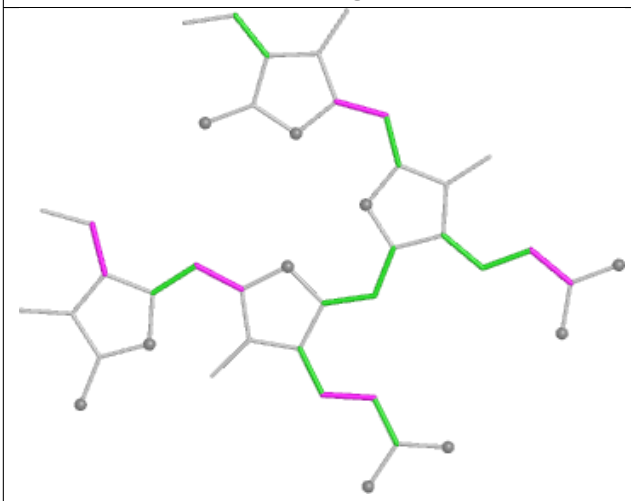
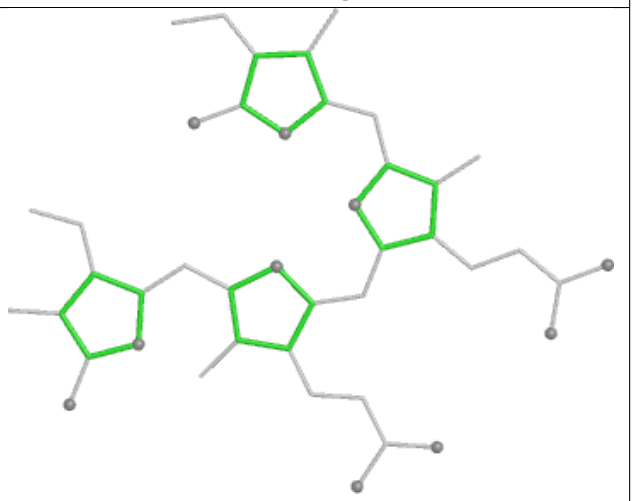
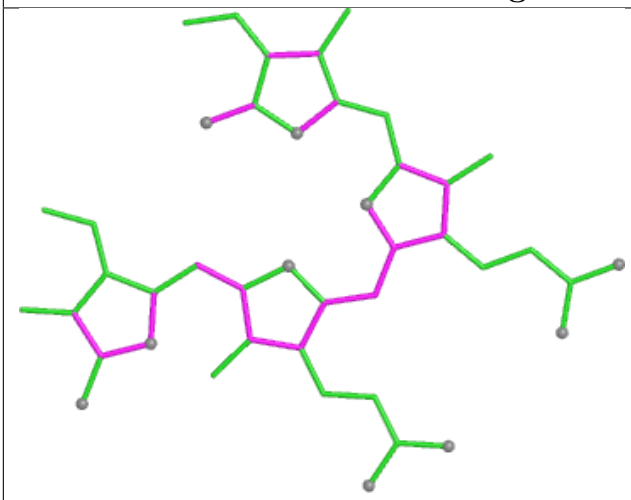


Torsions



Rings

Ligand PEB mG 201



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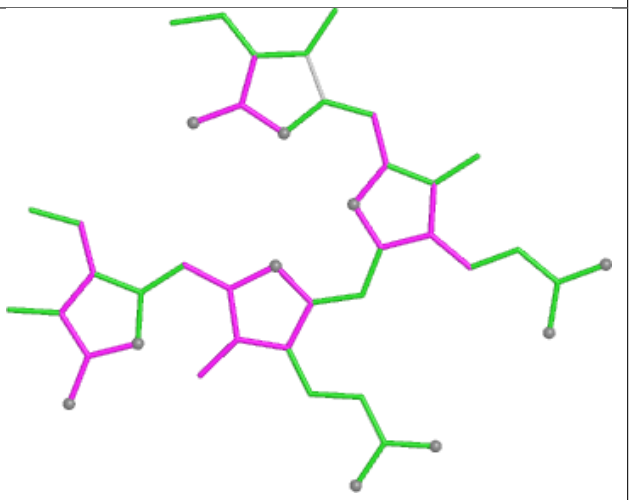

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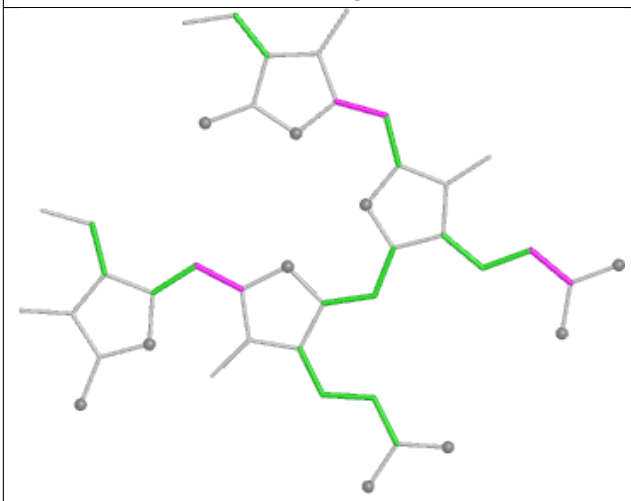

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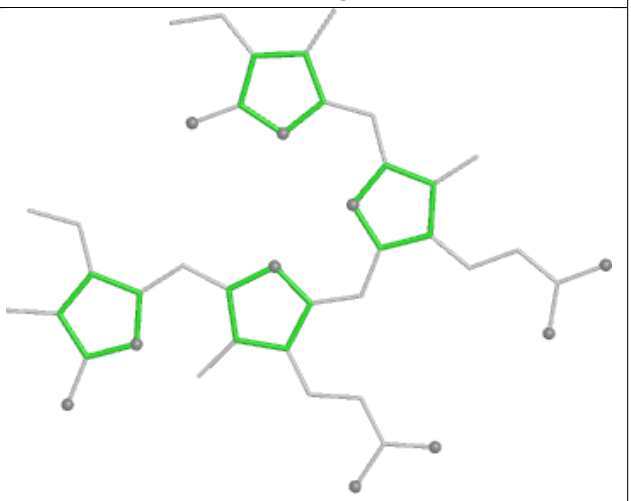
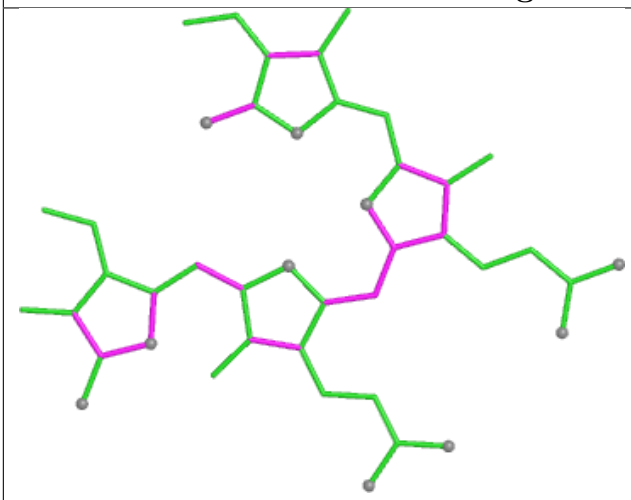


Rings

Ligand PEB T5 202



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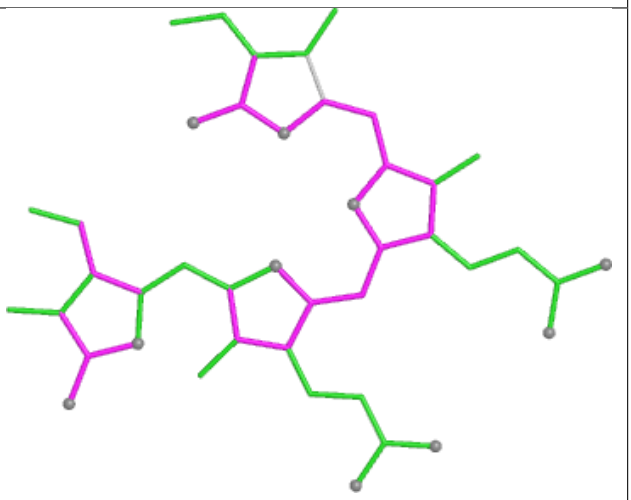

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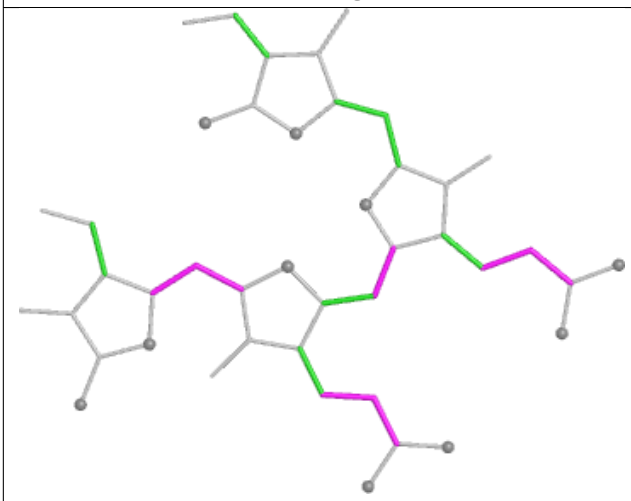

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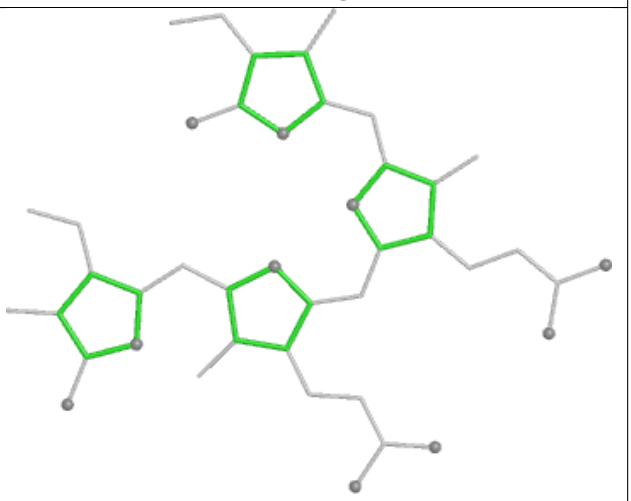
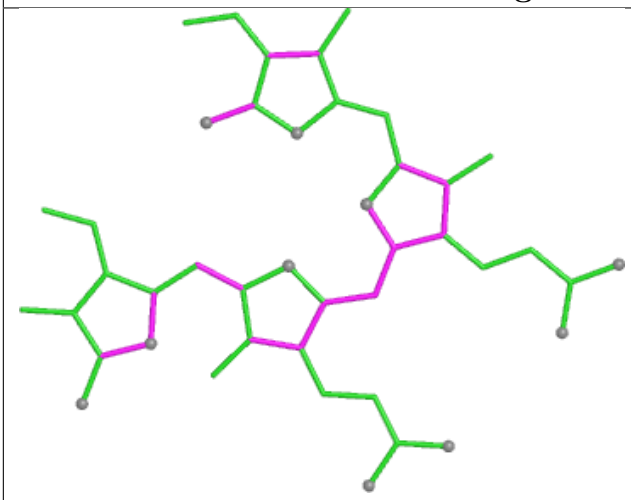


Rings

Ligand PEB gH 201



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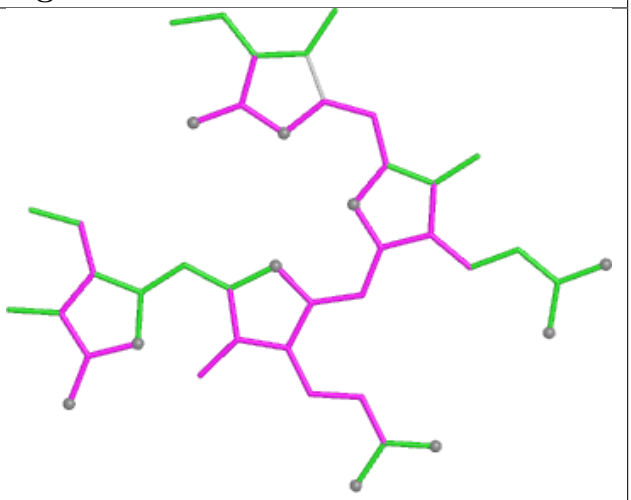

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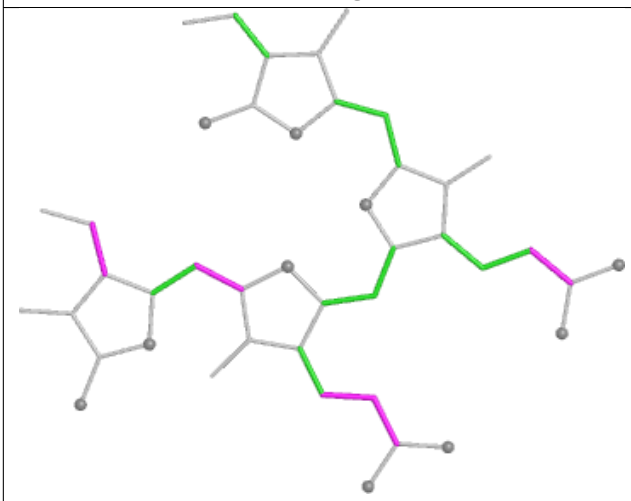

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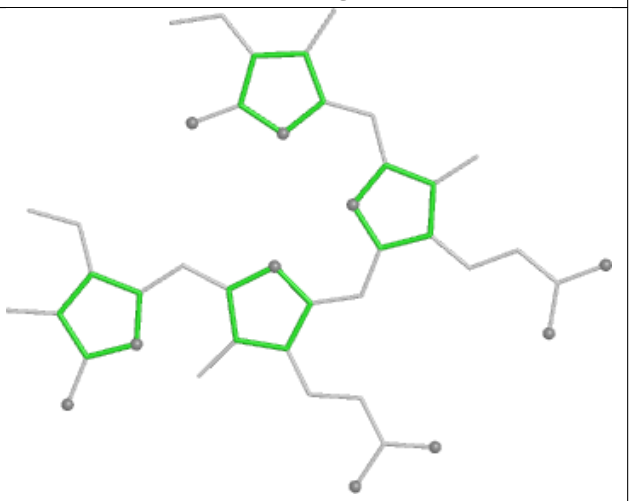
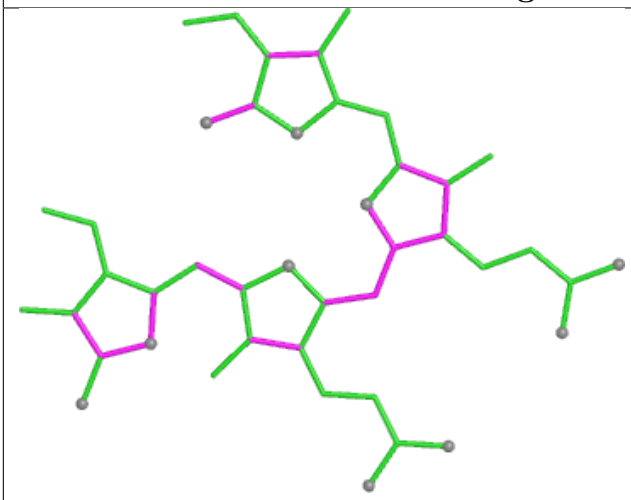


Rings

Ligand PEB ZJ 202



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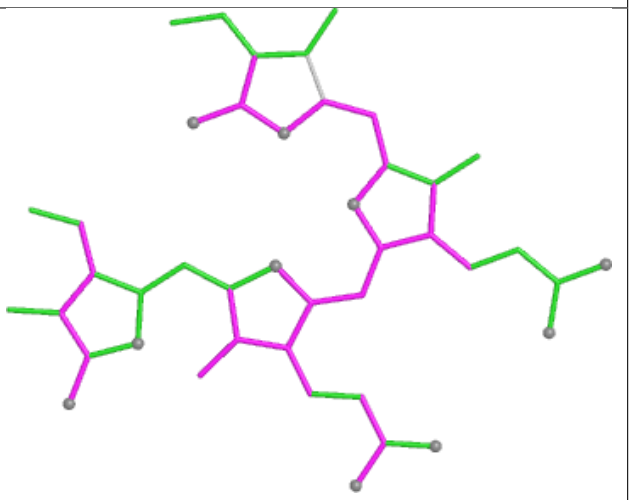

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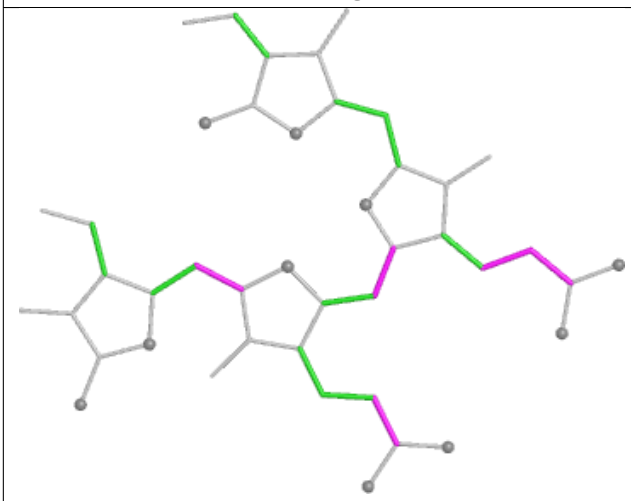

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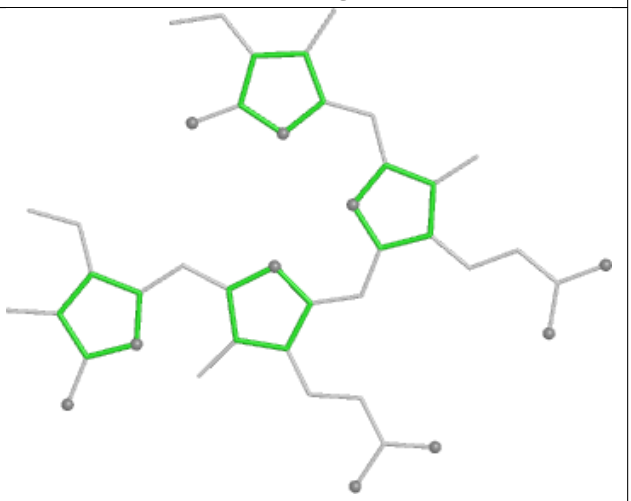
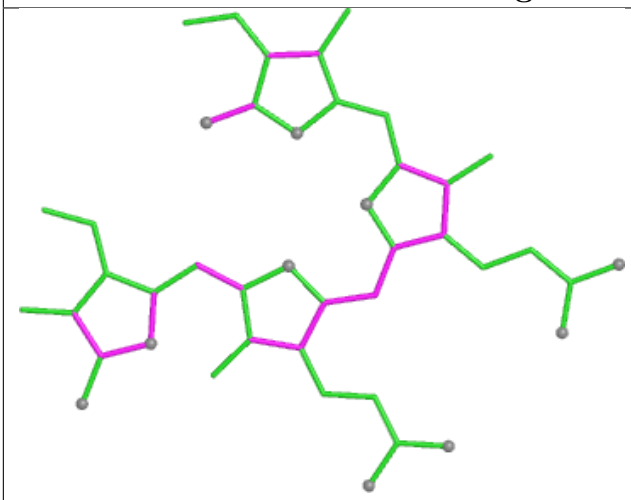


Rings

Ligand PEB Y4 202



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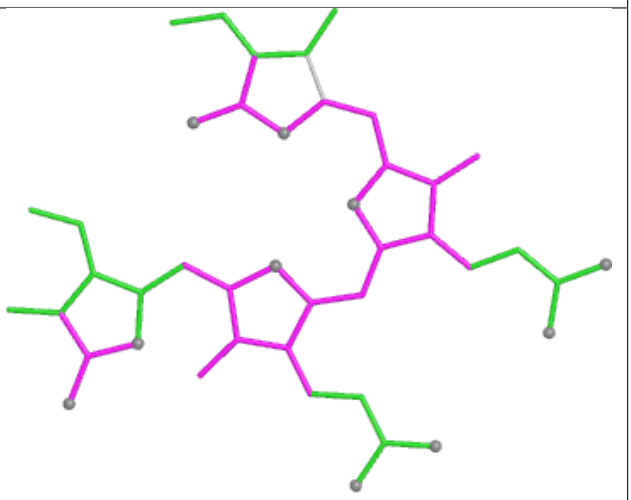

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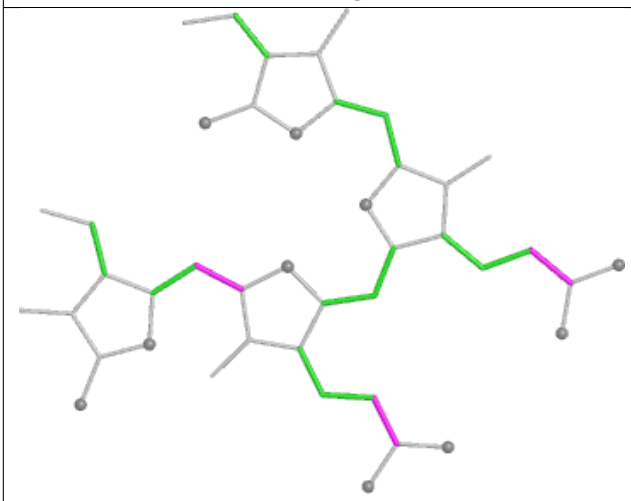

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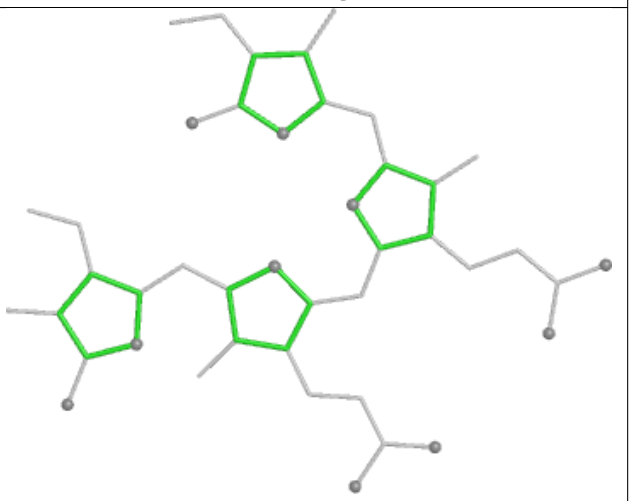
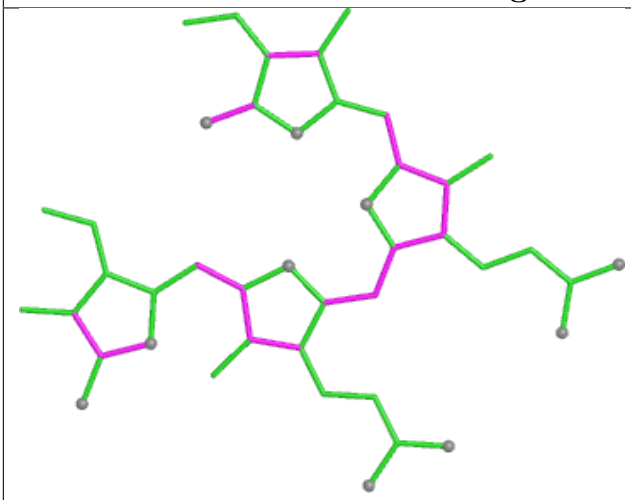


Rings

Ligand PEB VH 202



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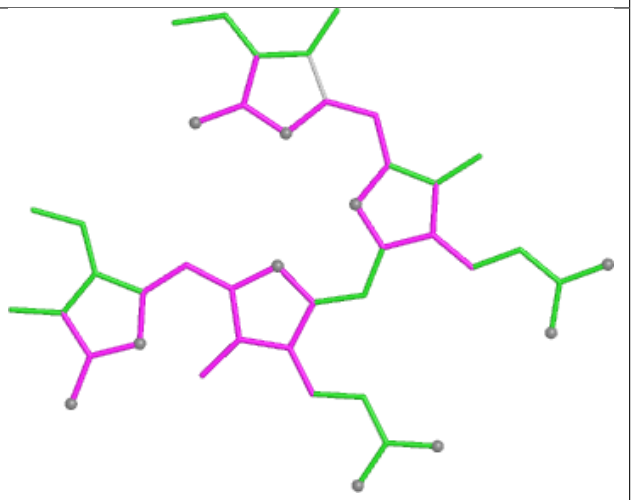
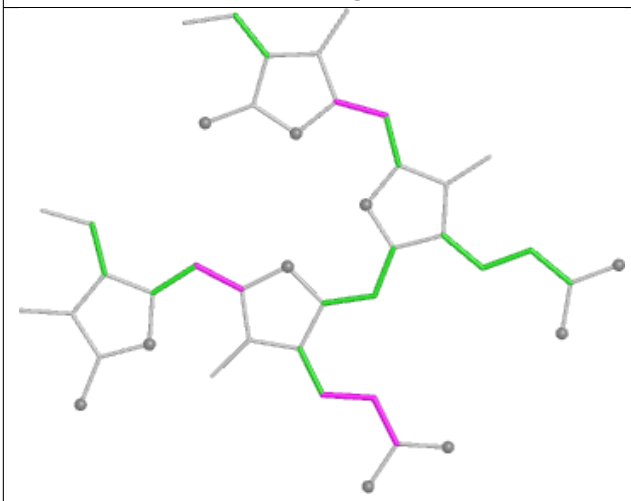


Bond angles



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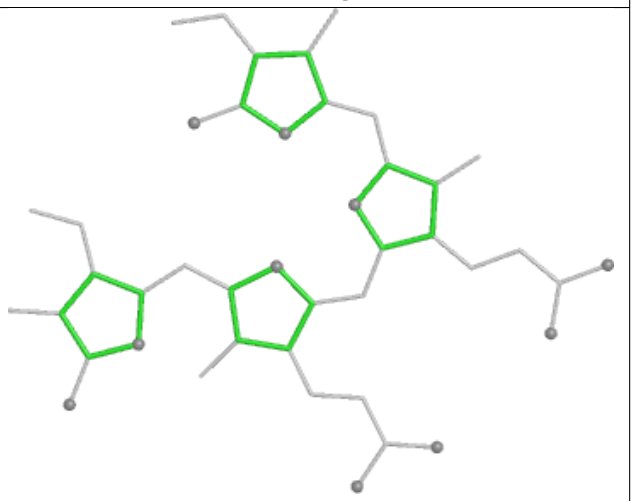
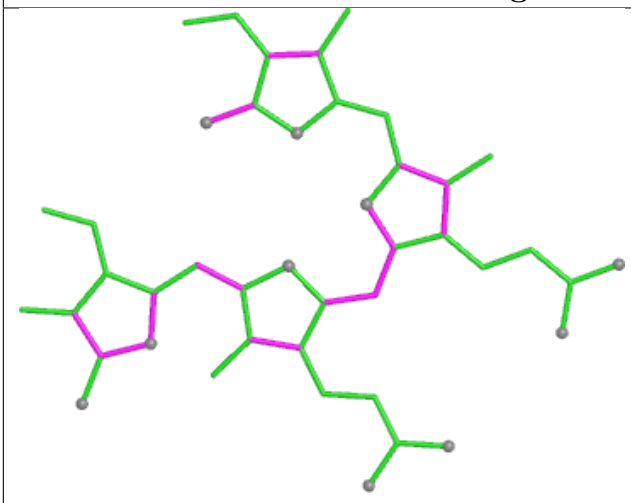


Rings

Ligand PEB AK 201



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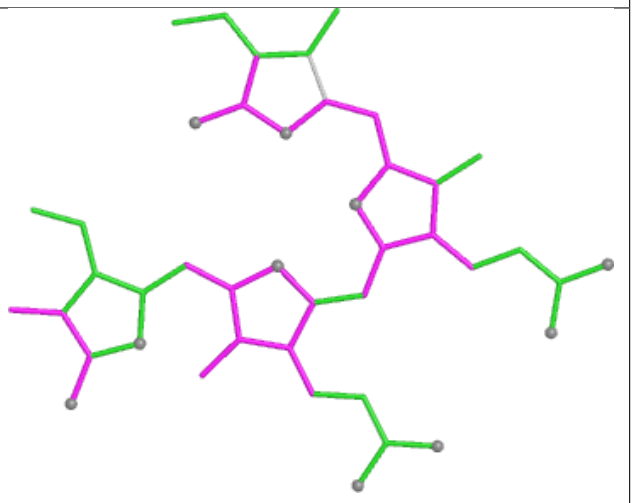

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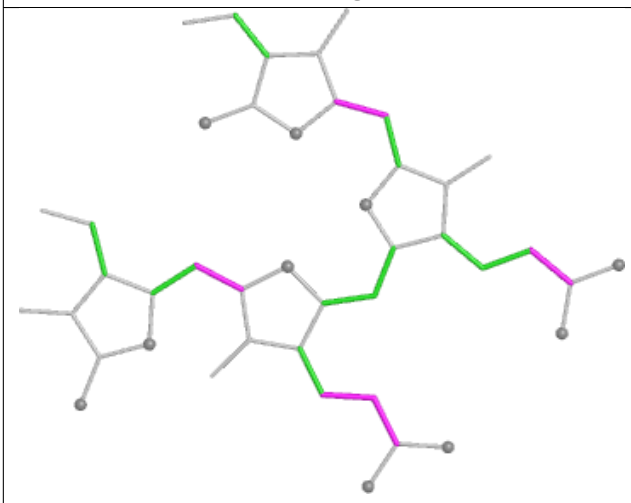

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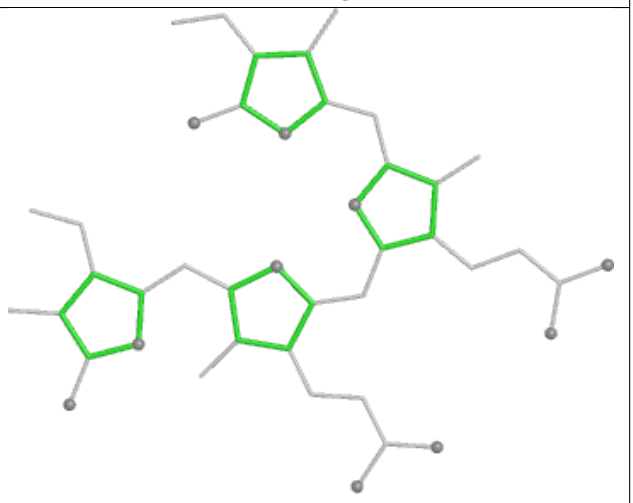
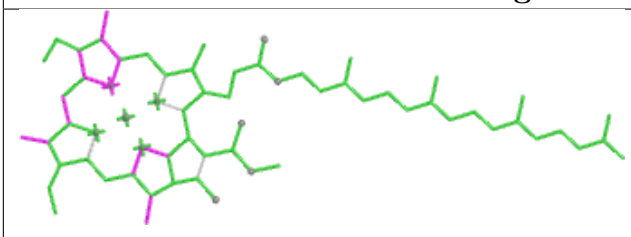


Rings

Ligand CLA BL 623



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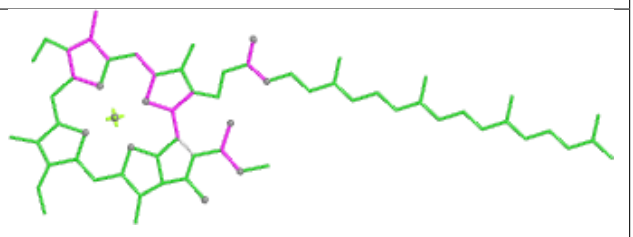

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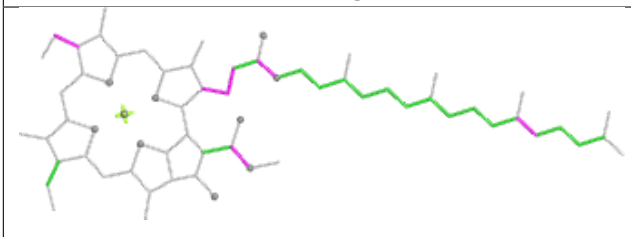

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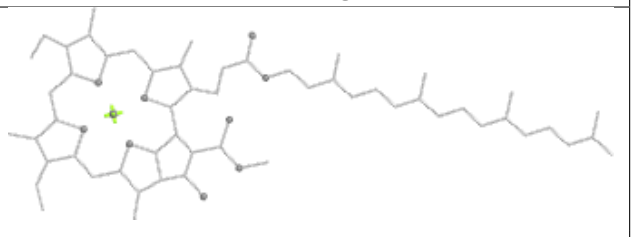
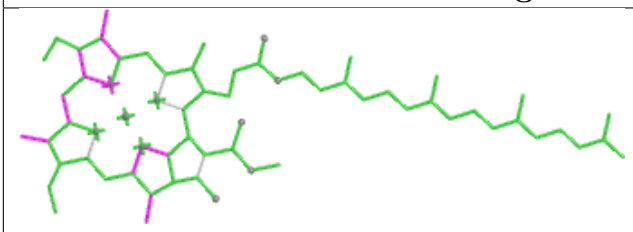


Rings

Ligand CLA C6 513



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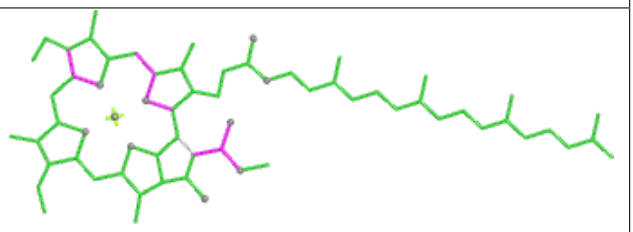

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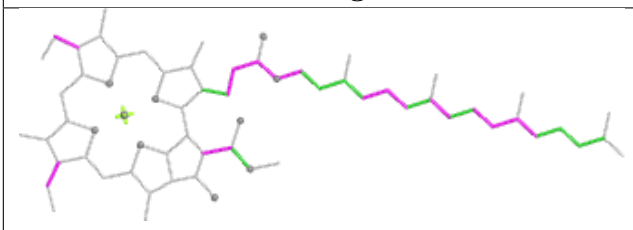

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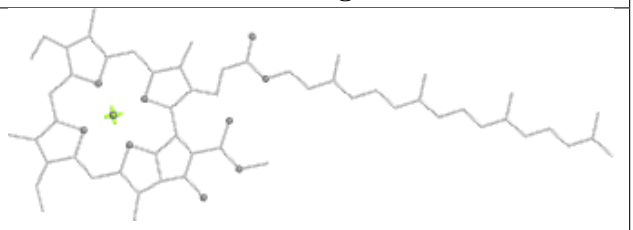
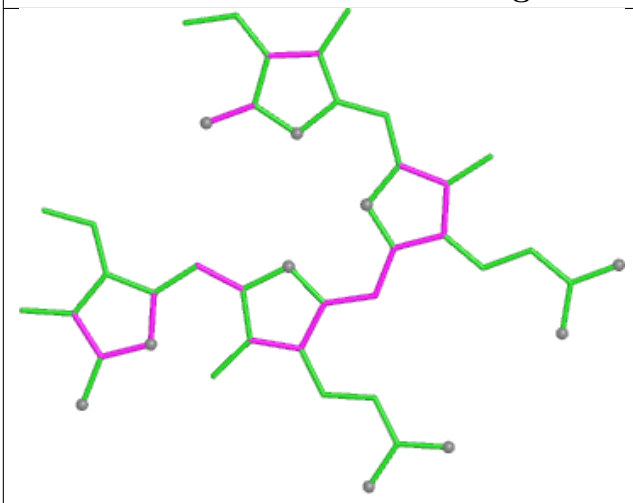


Rings

Ligand PEB VA 203



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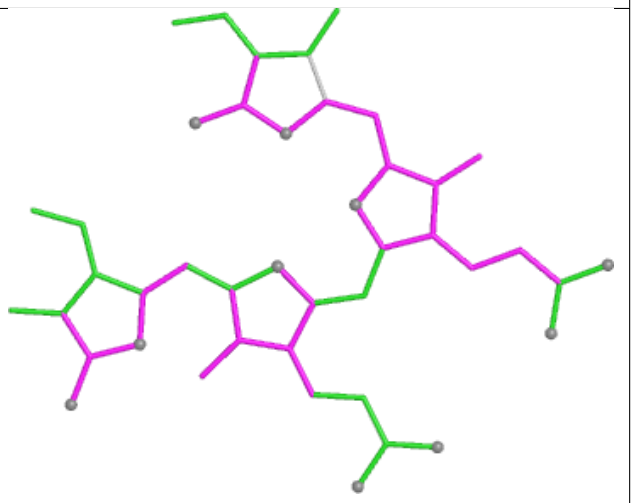

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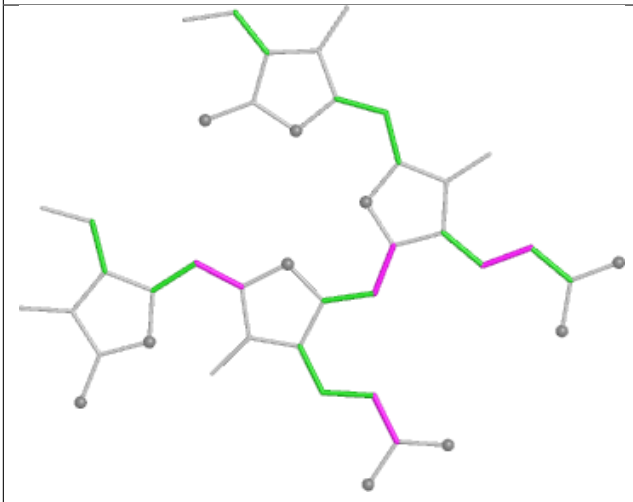

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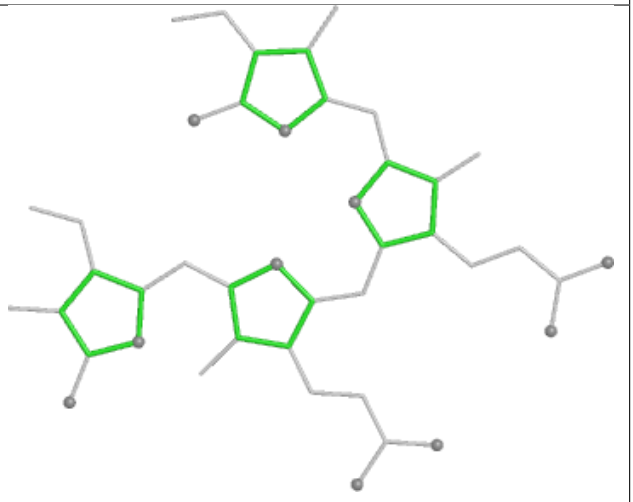
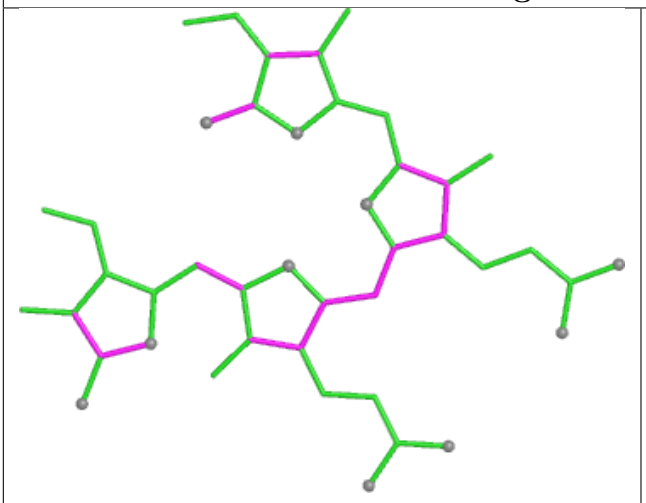


Rings

Ligand PEB hG 203



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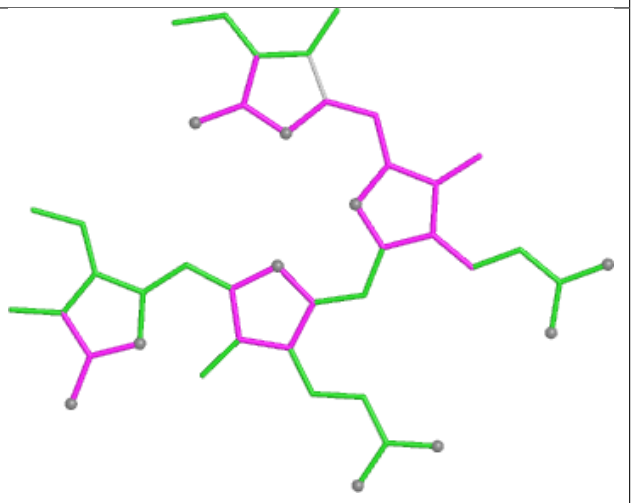

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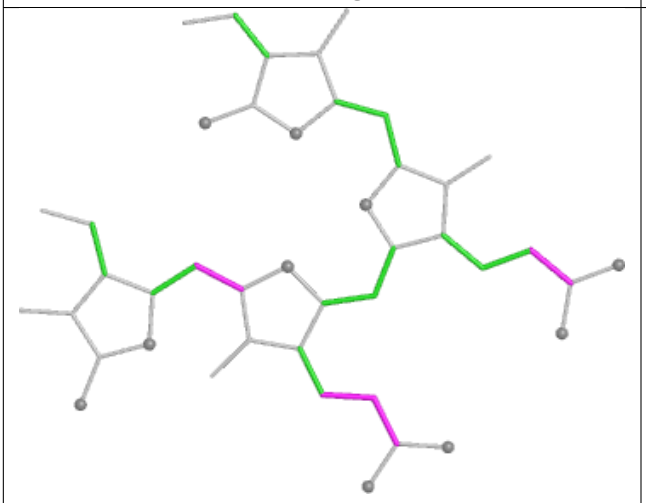

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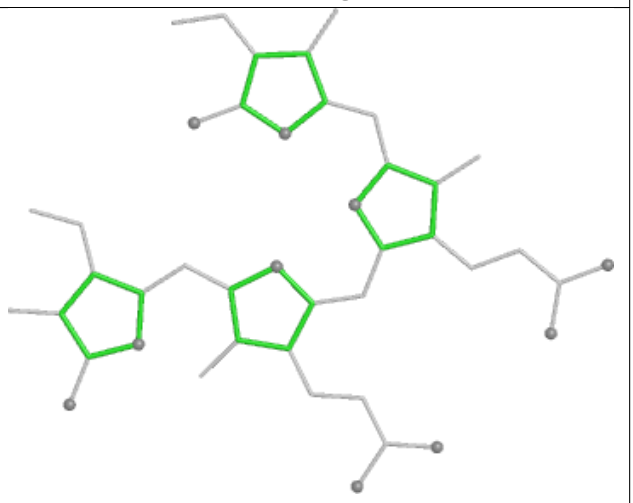
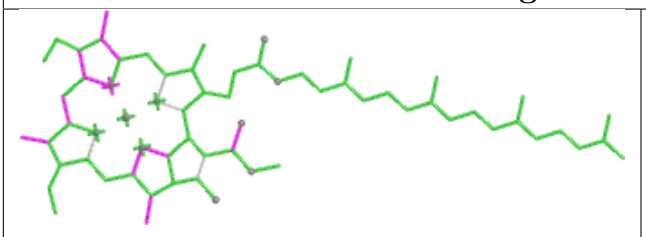


Rings

Ligand CLA 42 602



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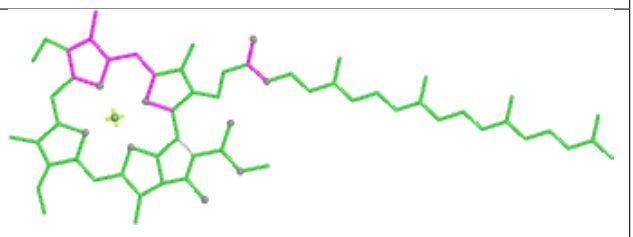
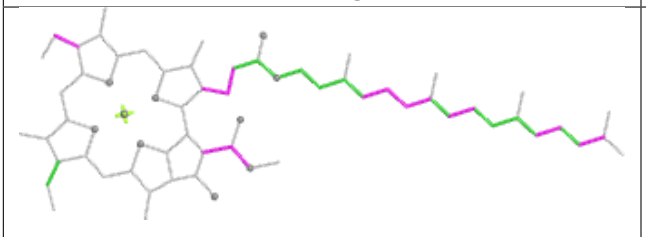


Bond angles



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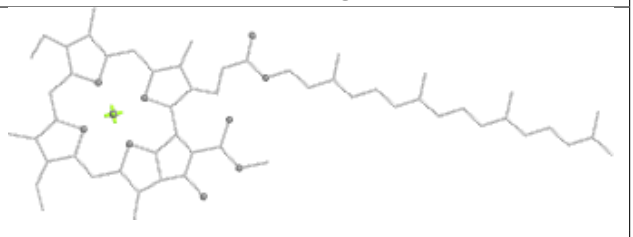
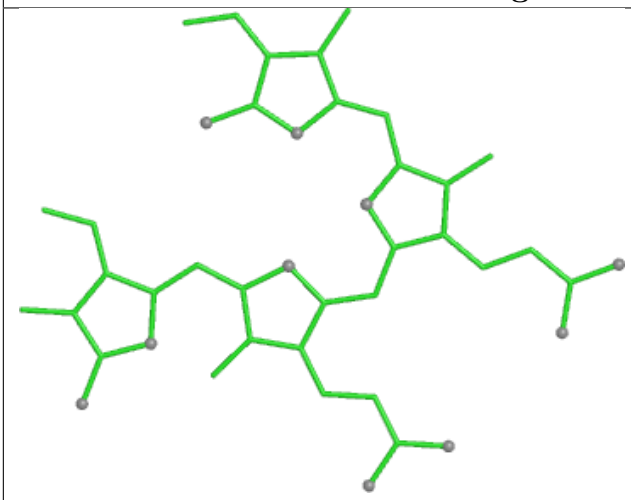


Rings

Ligand PEB CA 202



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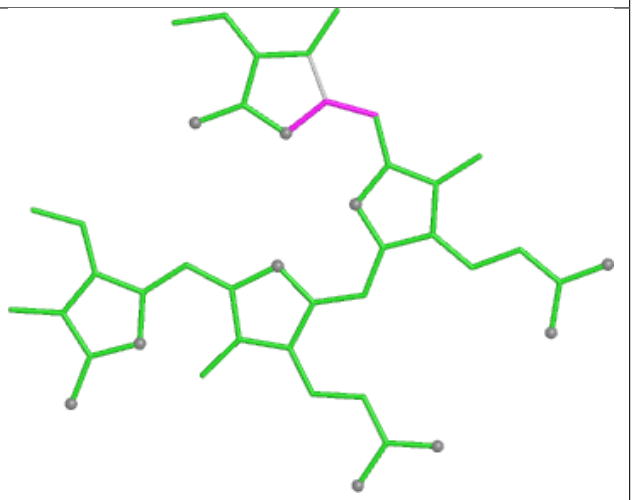
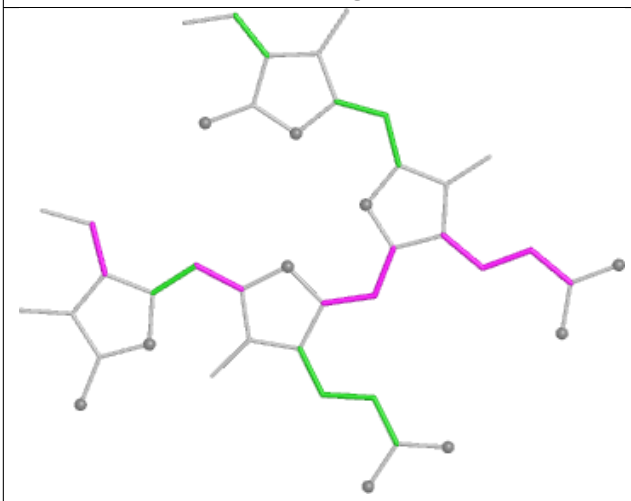


Bond angles



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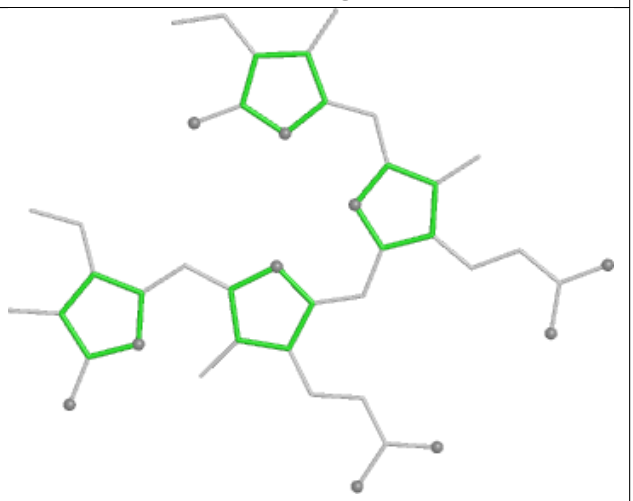
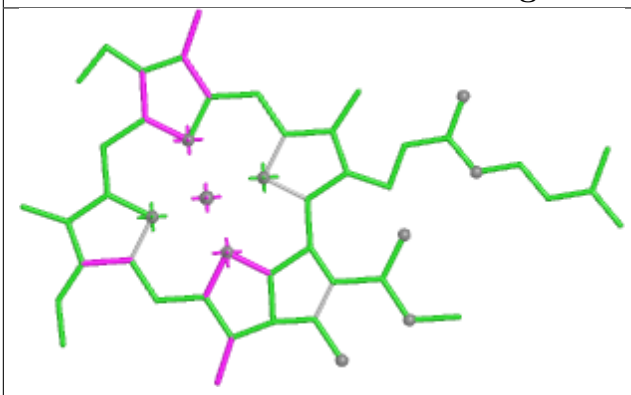
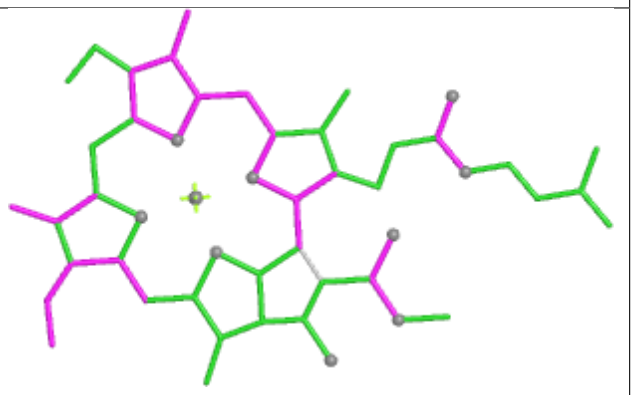


Rings

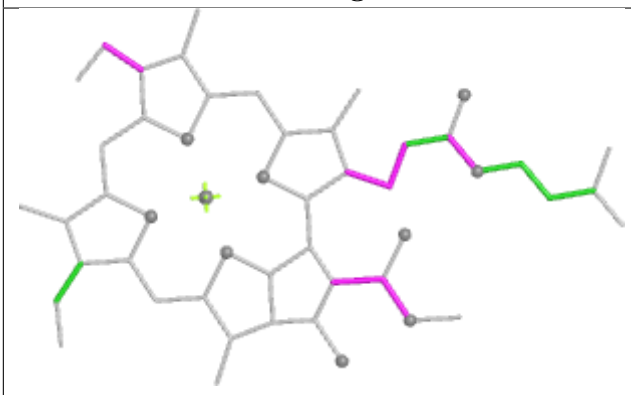
Ligand CLA 22 609



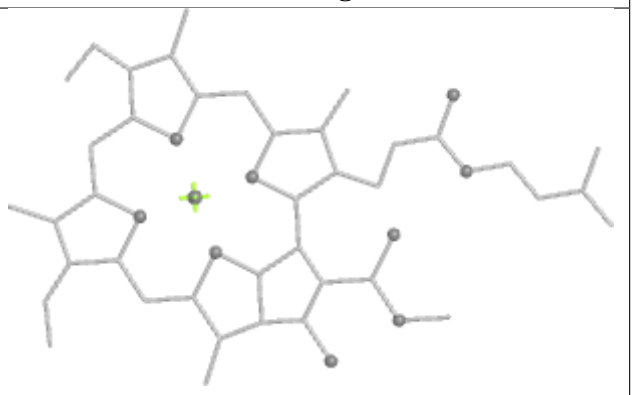
Bond lengths



Bond angles

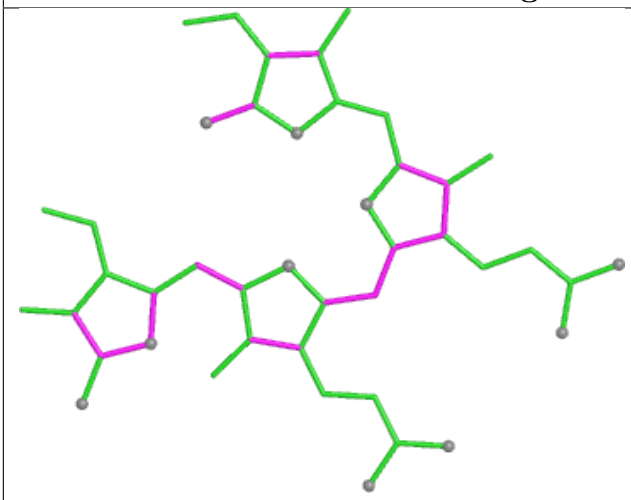


Torsions



Rings

Ligand PEB e4 202



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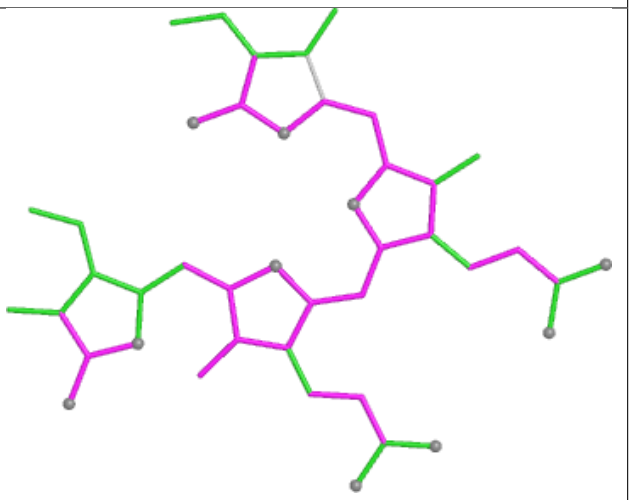

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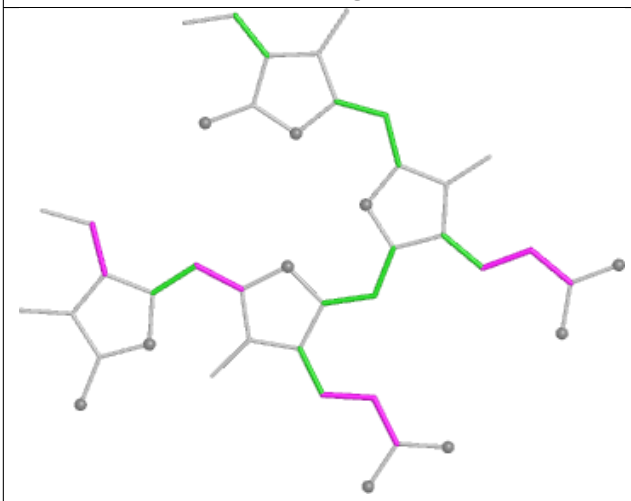

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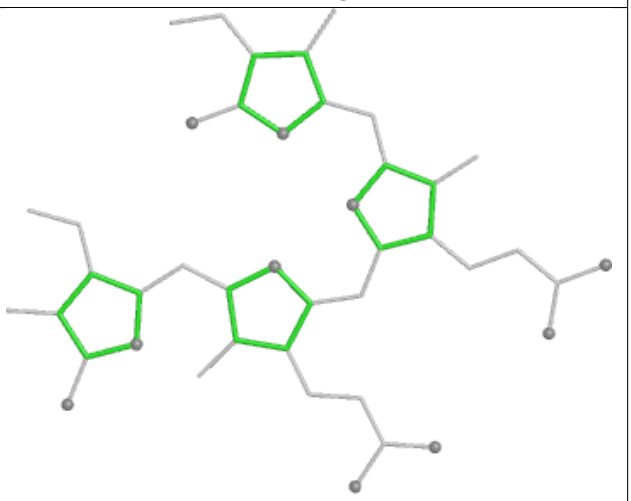
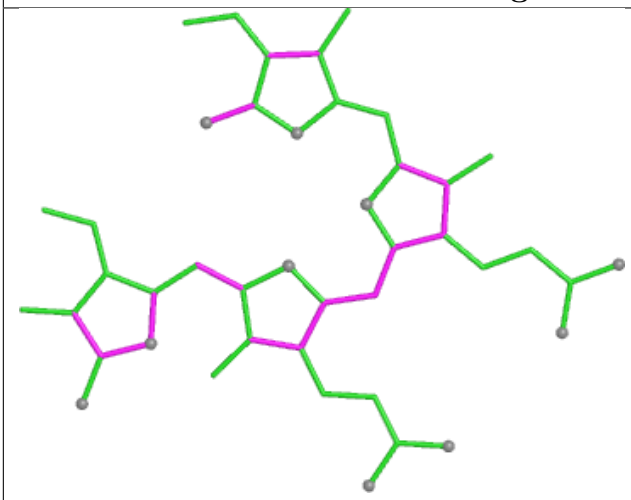


Rings

Ligand PEB hM 202



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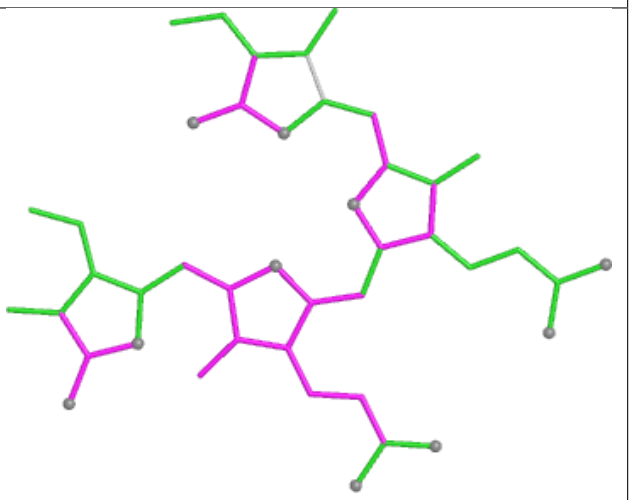

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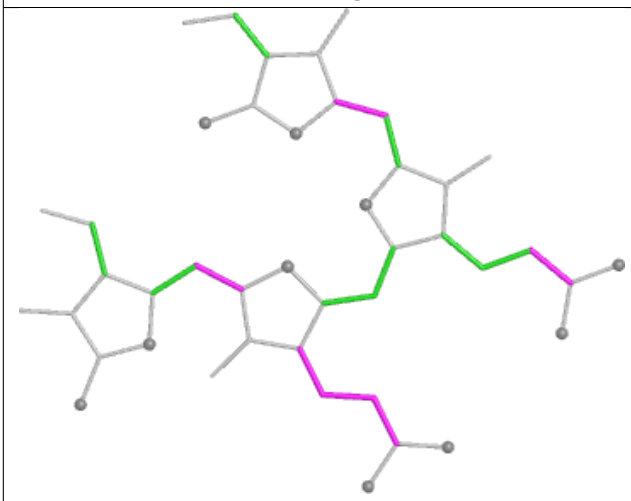

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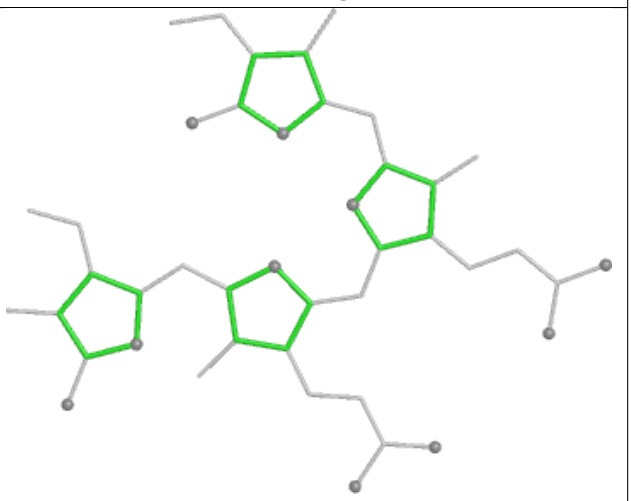
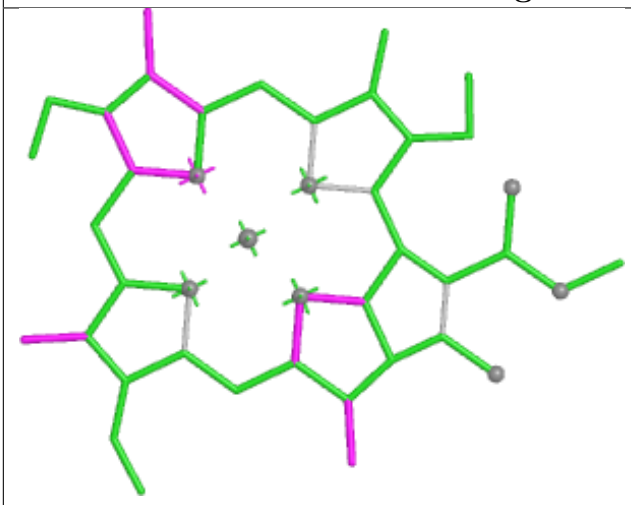


Rings

Ligand CLA A2 817



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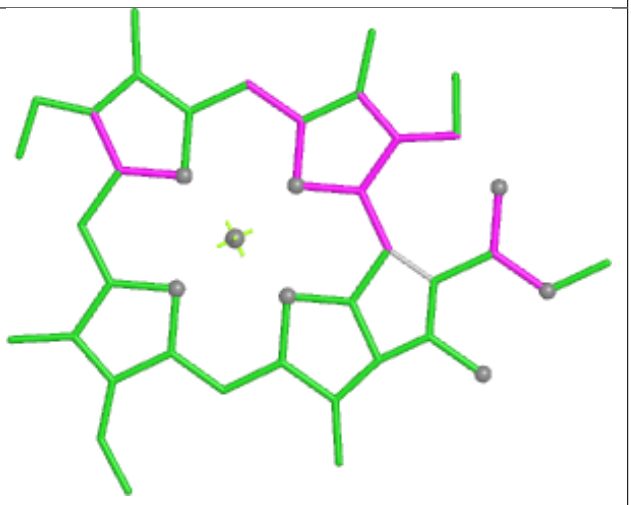

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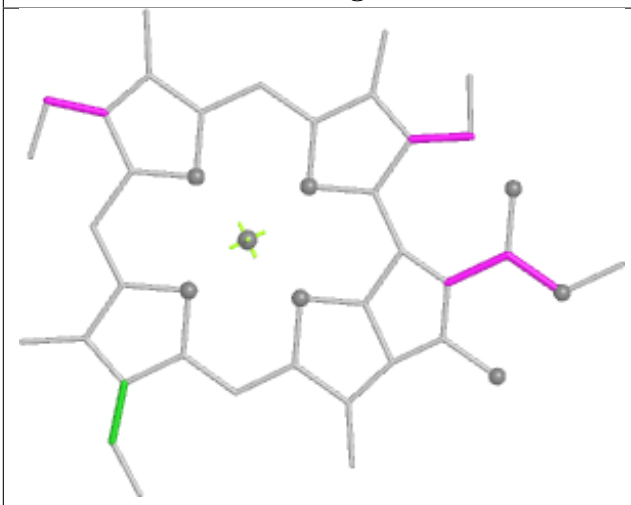
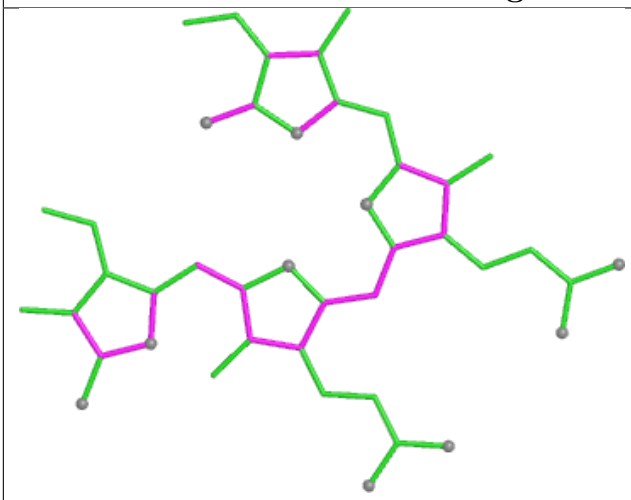


Torsions



Rings

Ligand PEB WQ 202



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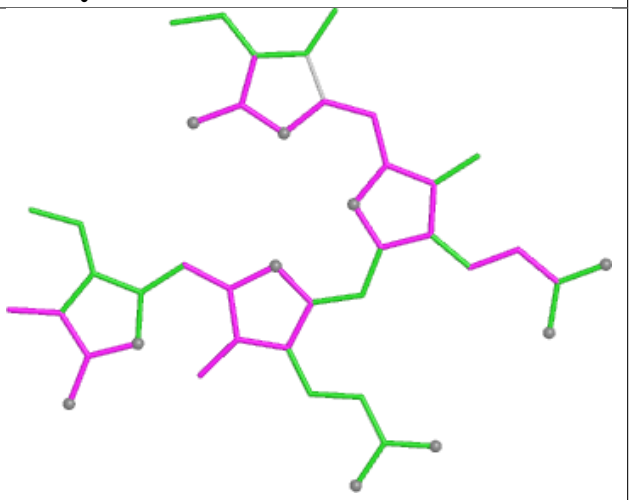

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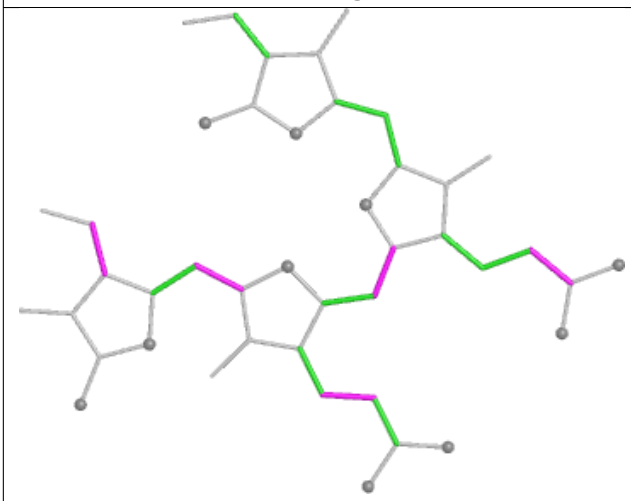

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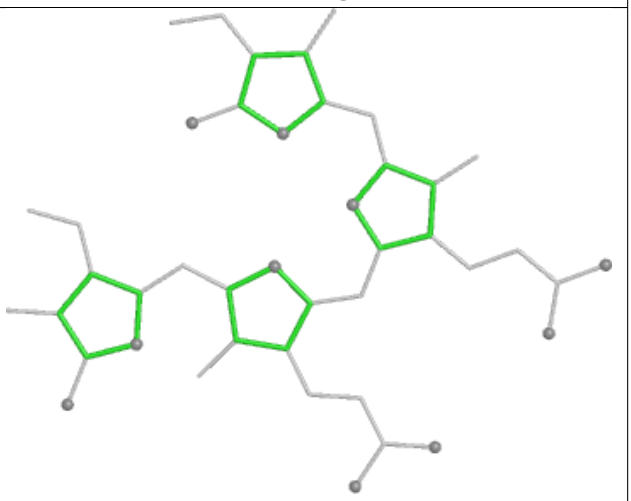
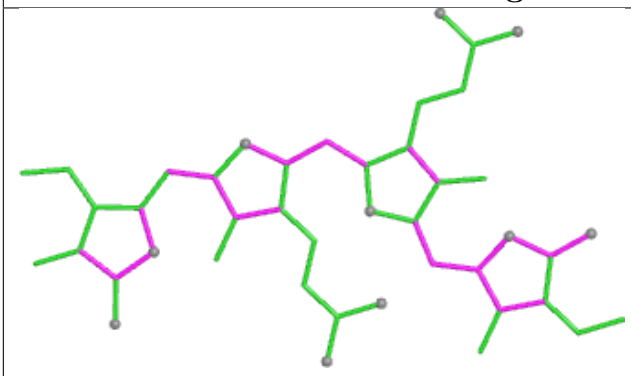


Rings

Ligand CYC IO 1001



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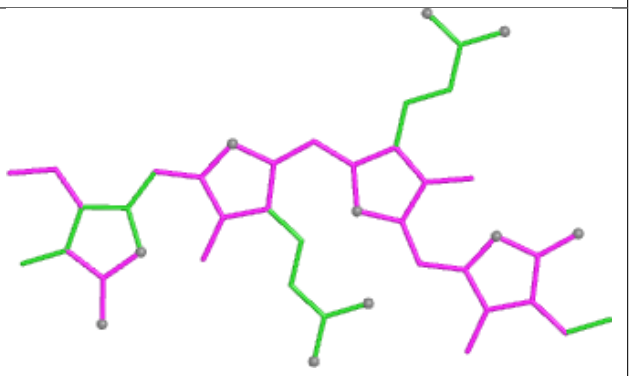

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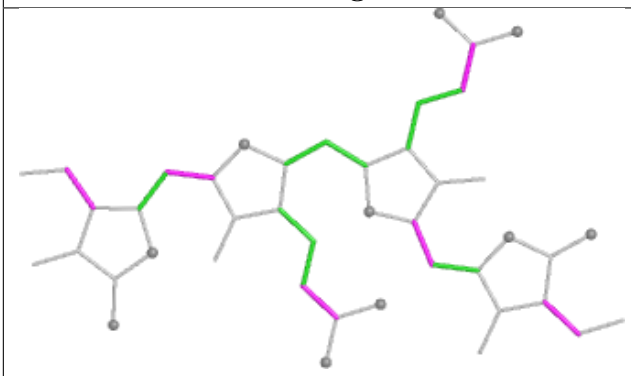

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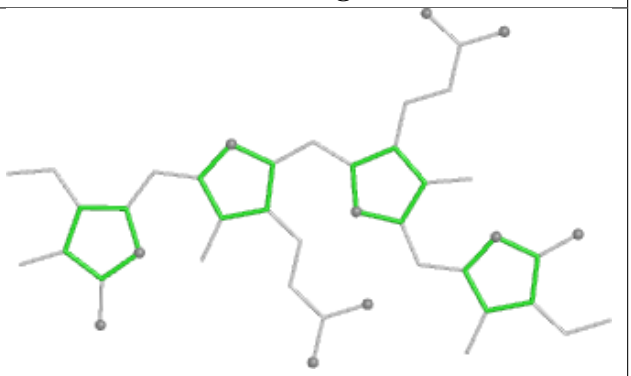
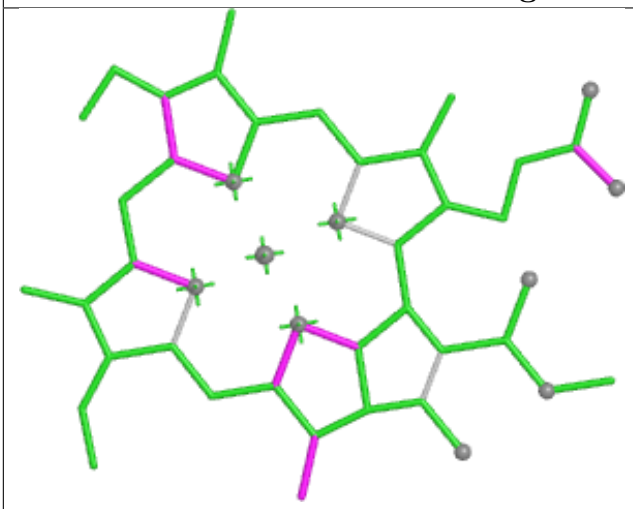


Rings

Ligand CLA 32 307



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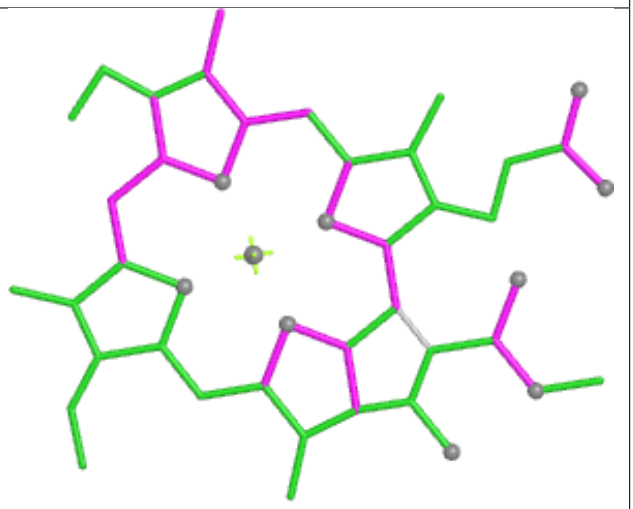

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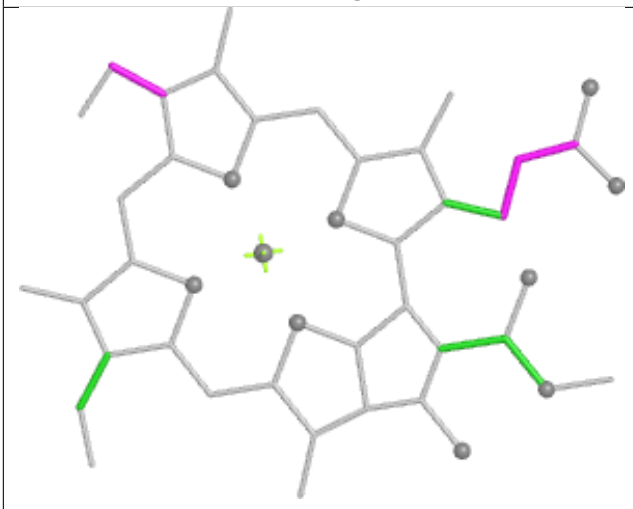

Torsions



Rings

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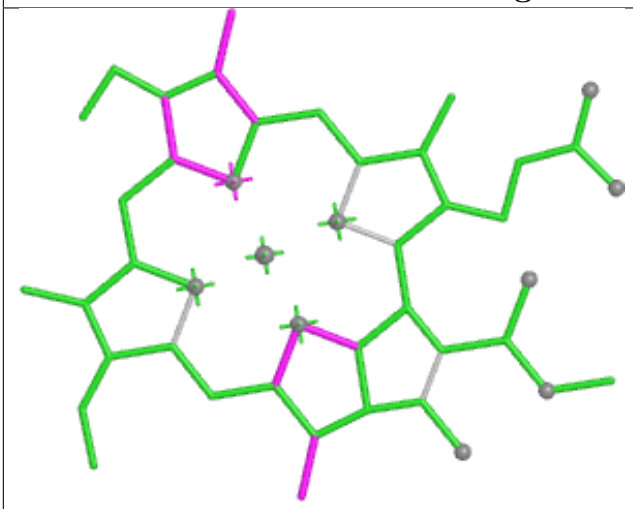

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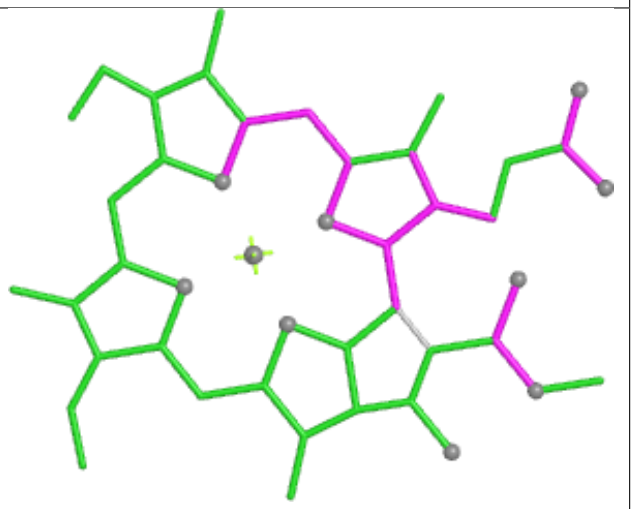

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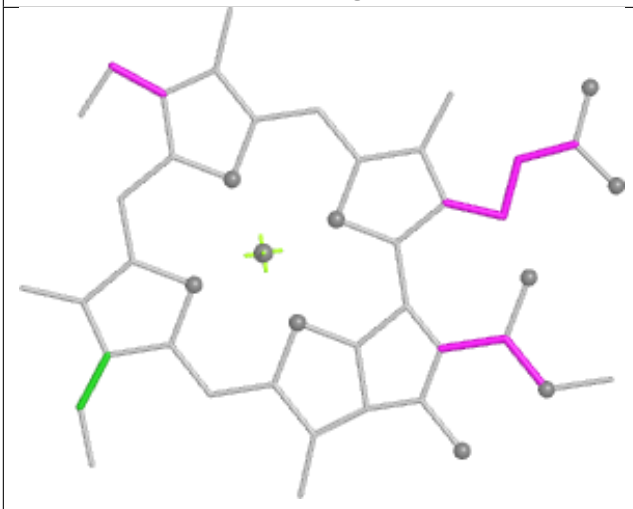
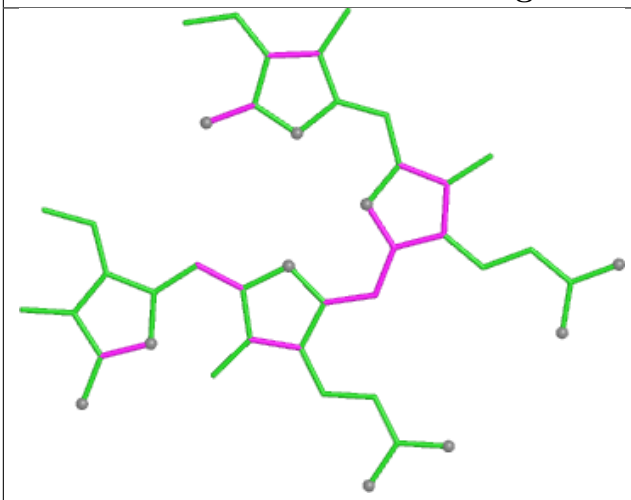


Torsions



Rings

Ligand PEB cK 202



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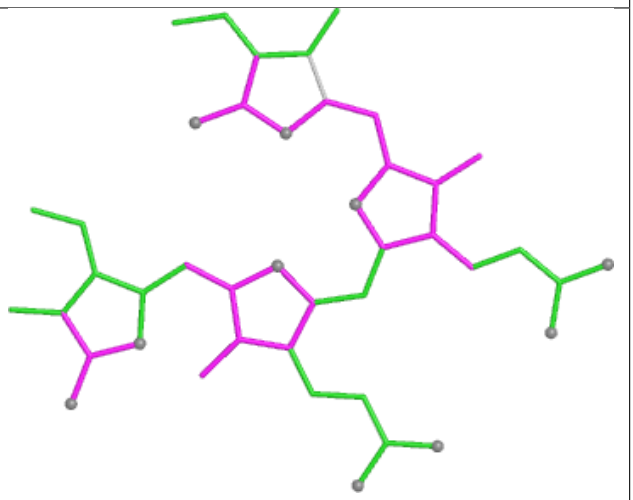

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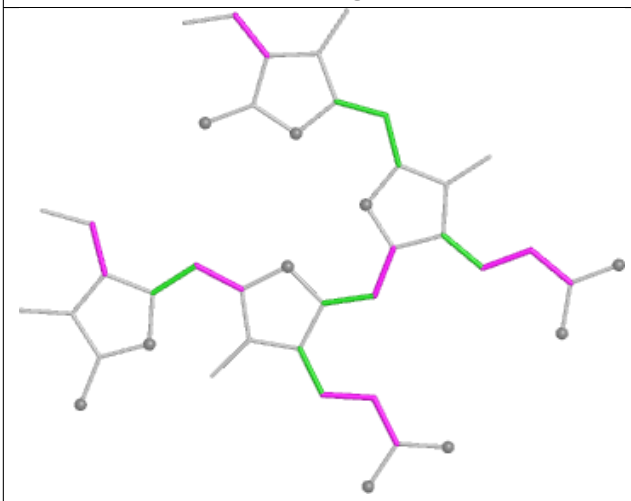

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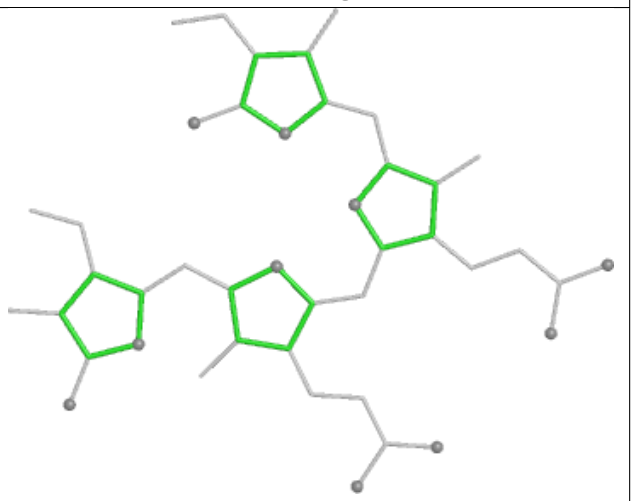
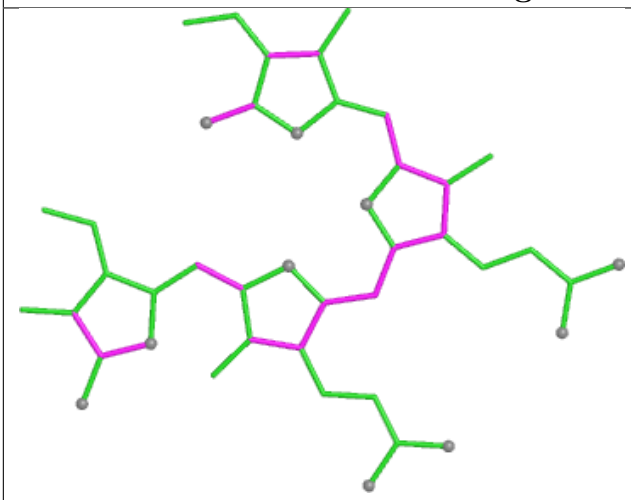


Rings

Ligand PEB gH 202



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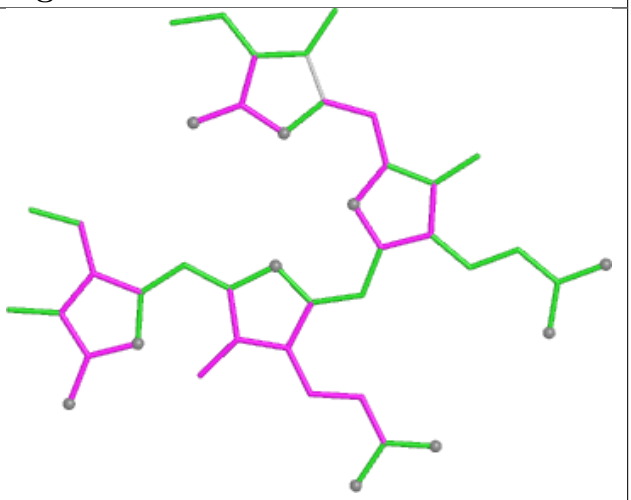

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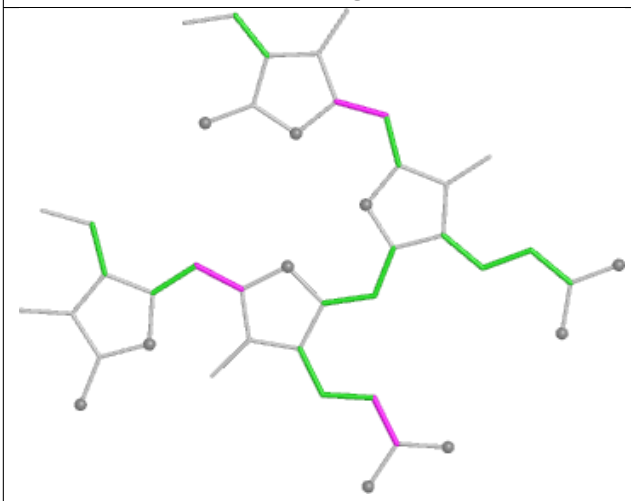

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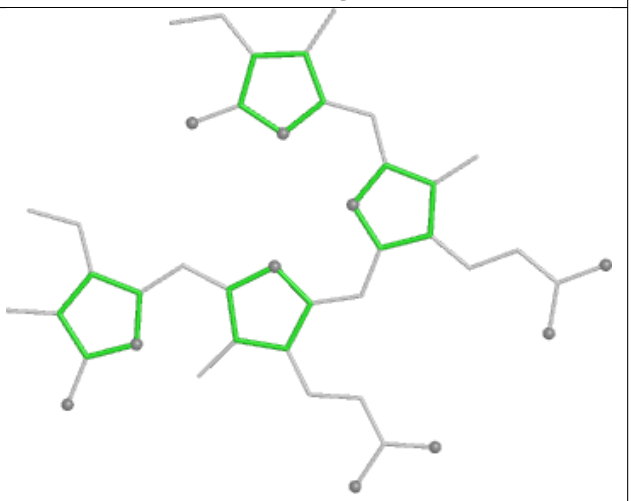
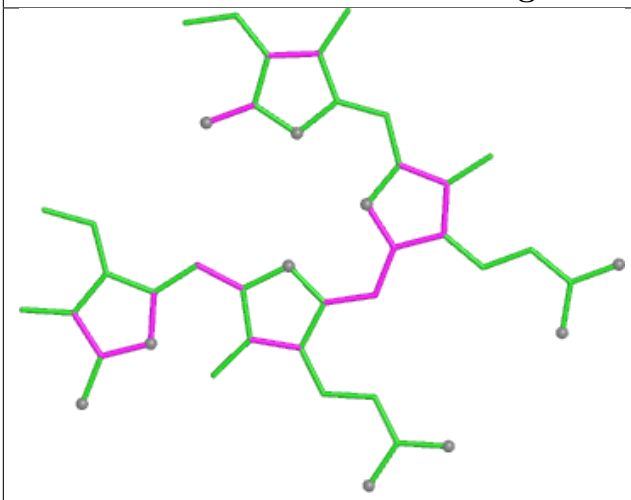


Rings

Ligand PEB L7 201



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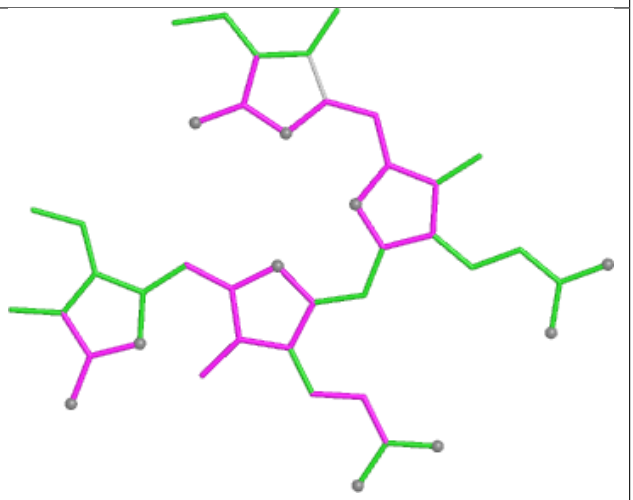

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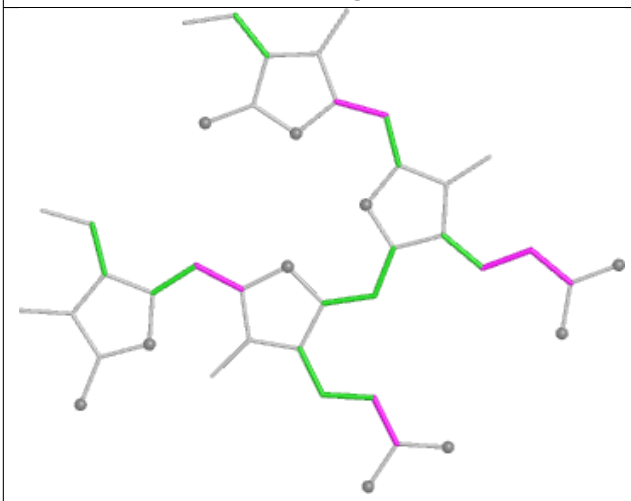

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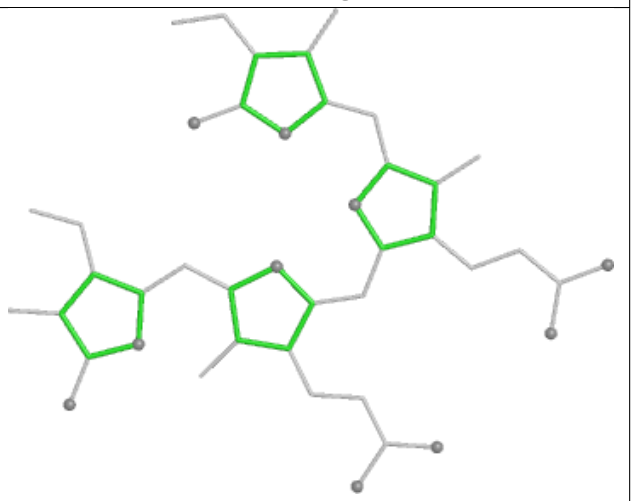
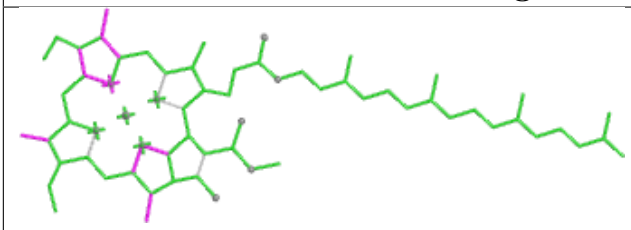


Rings

Ligand CLA BL 608



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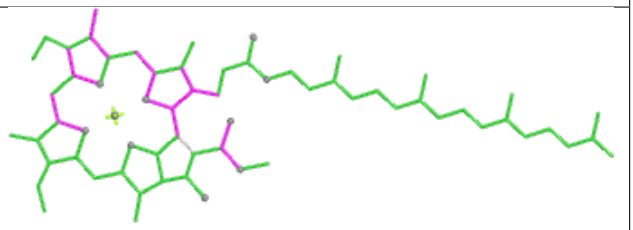

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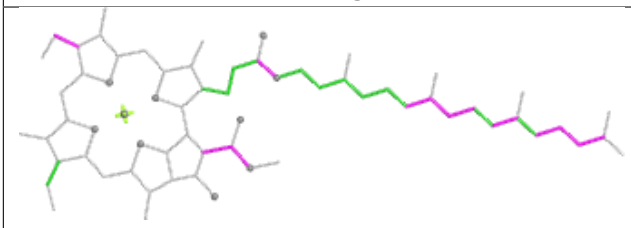

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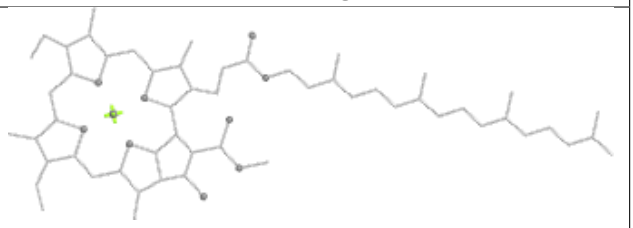
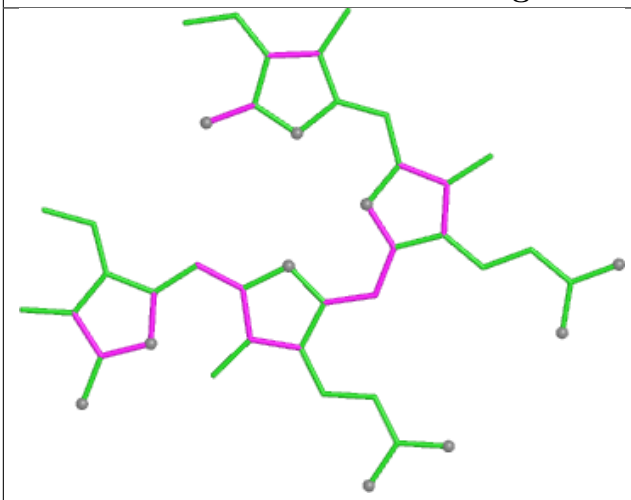


Rings

Ligand PEB YE 201



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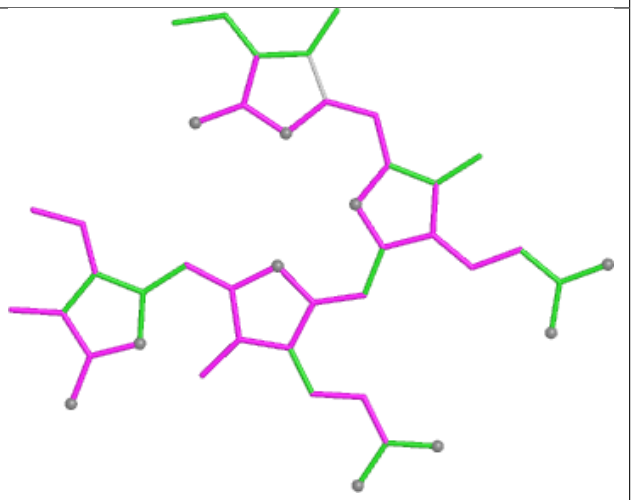

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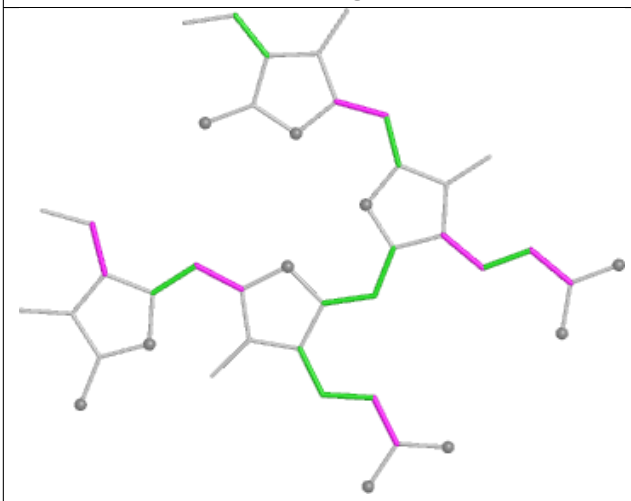

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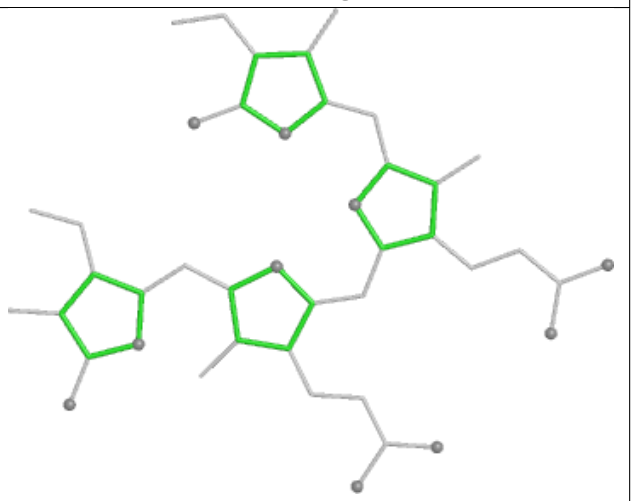
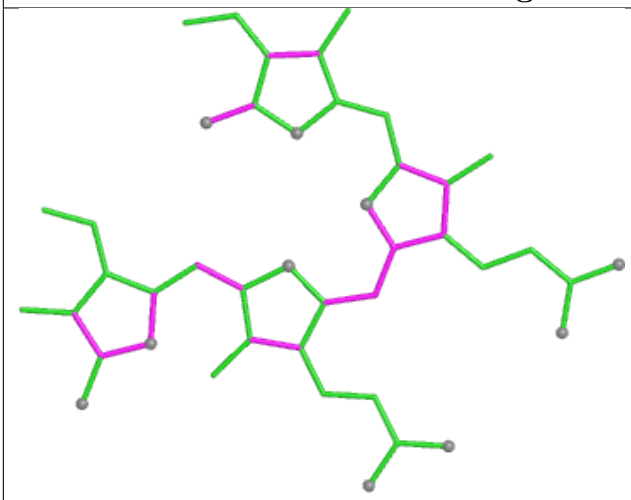


Rings

Ligand PEB dE 201



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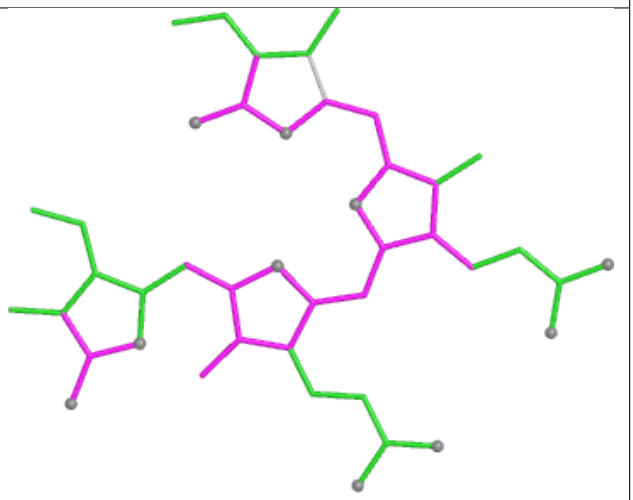

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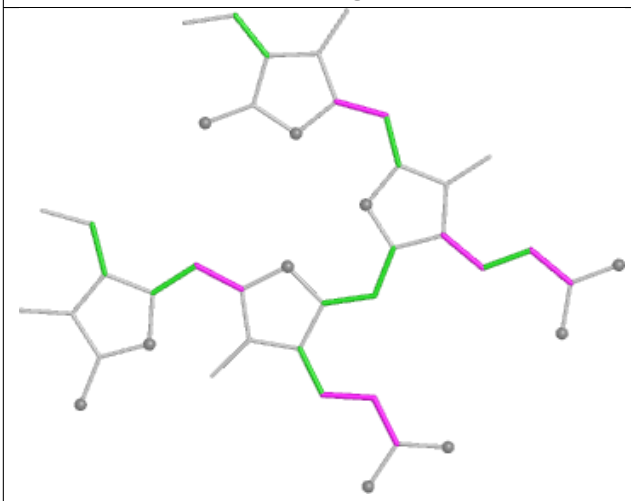

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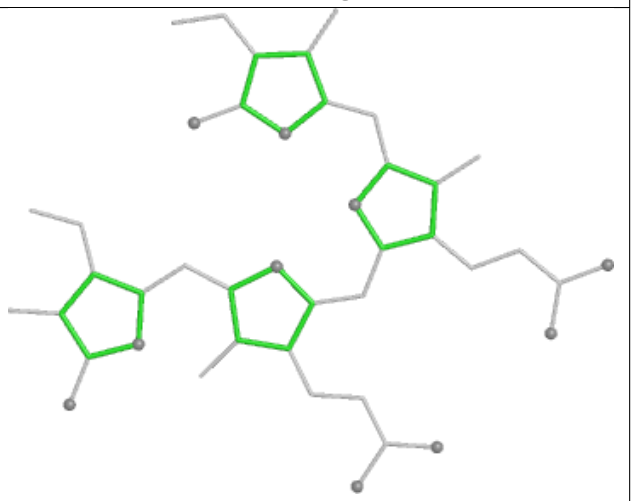
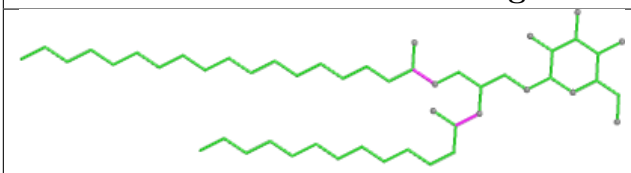


Rings

Ligand LMG XL 601



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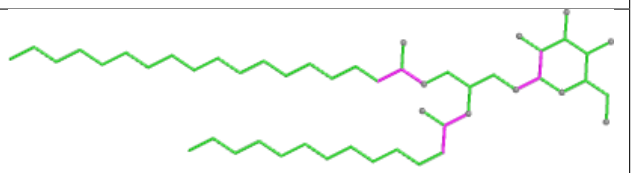

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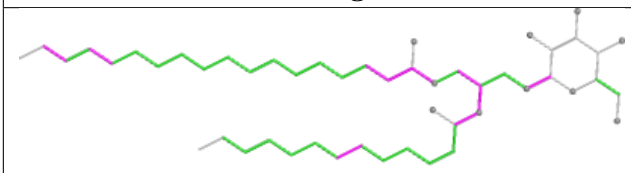

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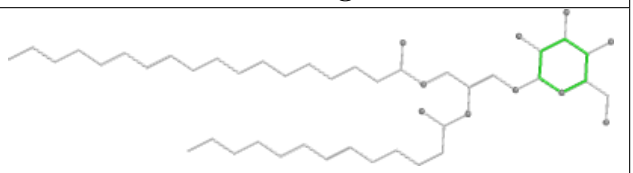
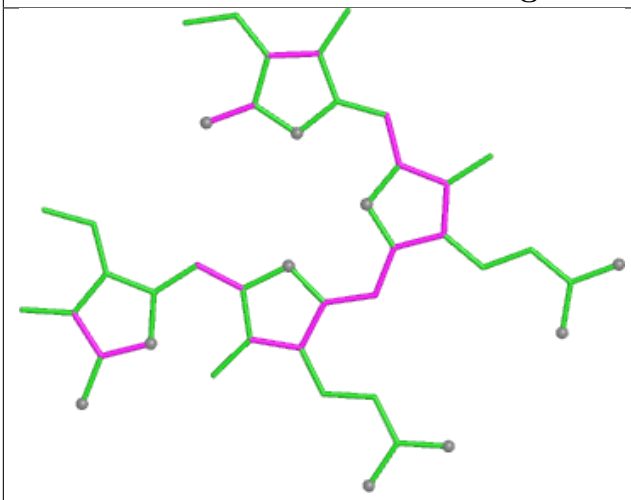


Rings

Ligand PEB fE 203



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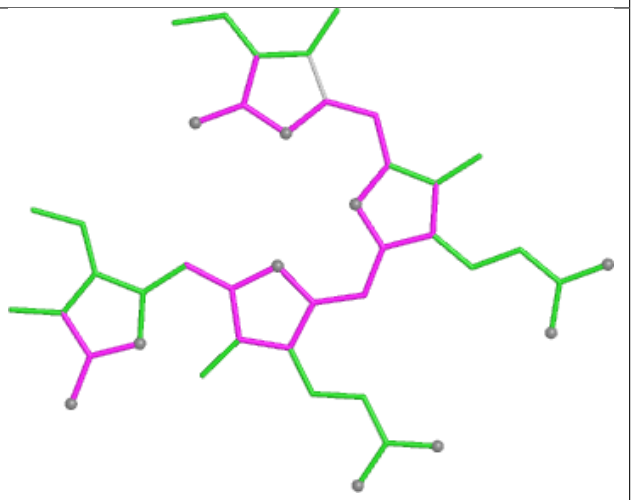

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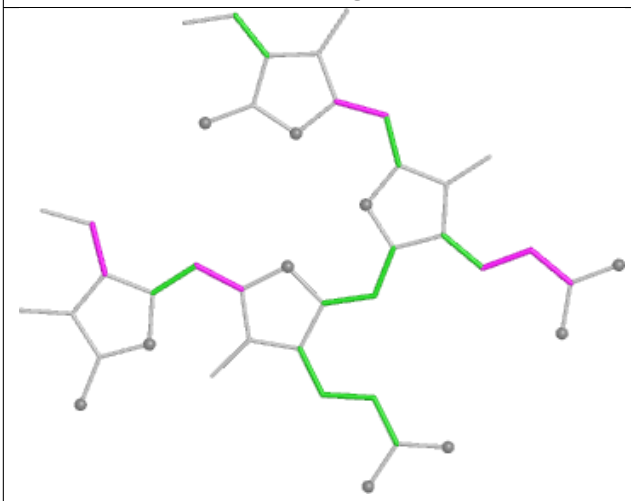

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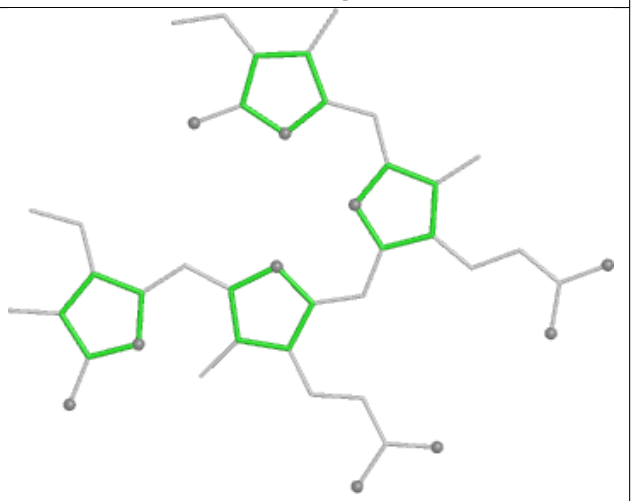
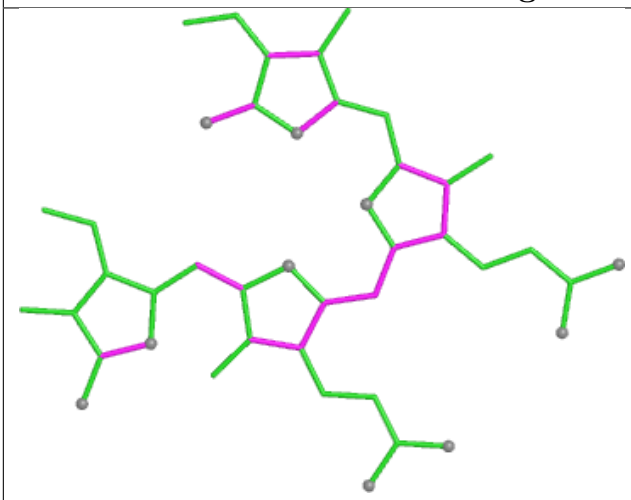


Rings

Ligand PEB b1 201



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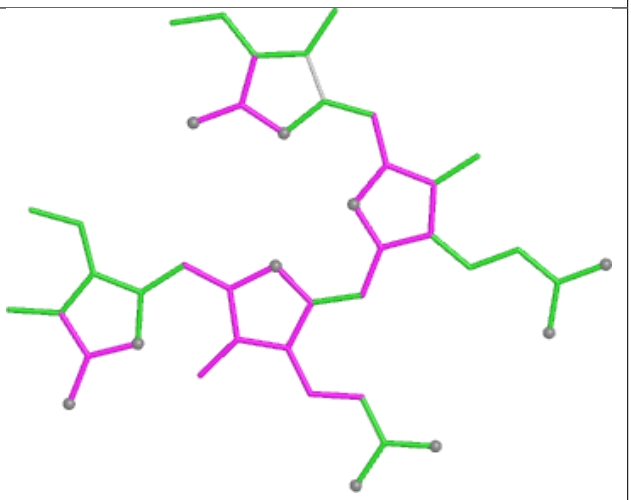
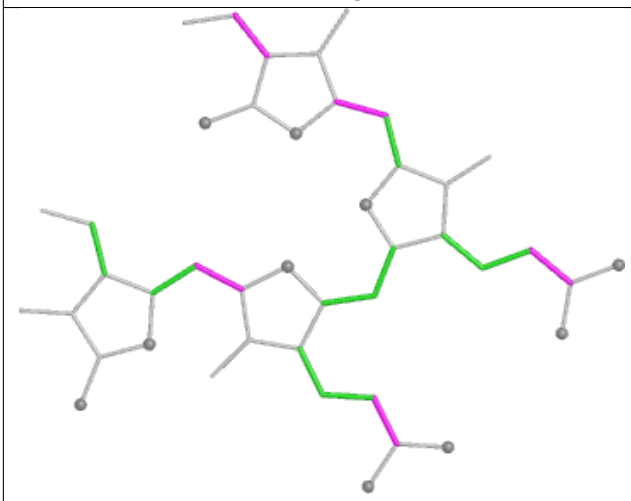
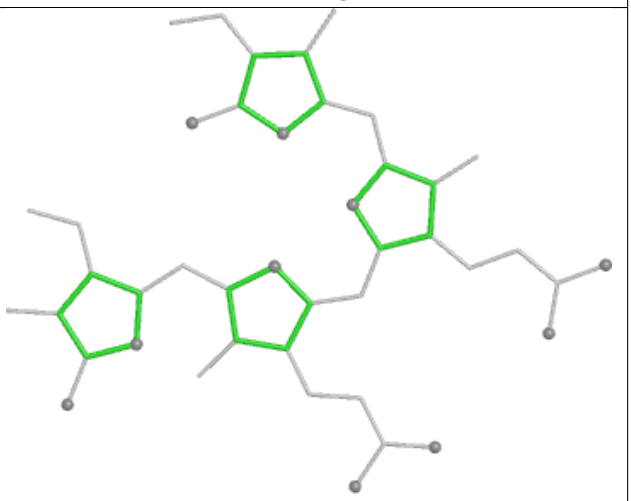


Bond angles

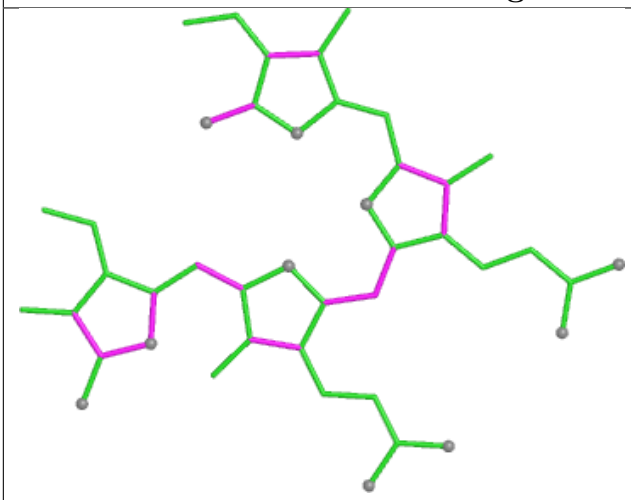


Torsions



Rings

Ligand PEB MA 201



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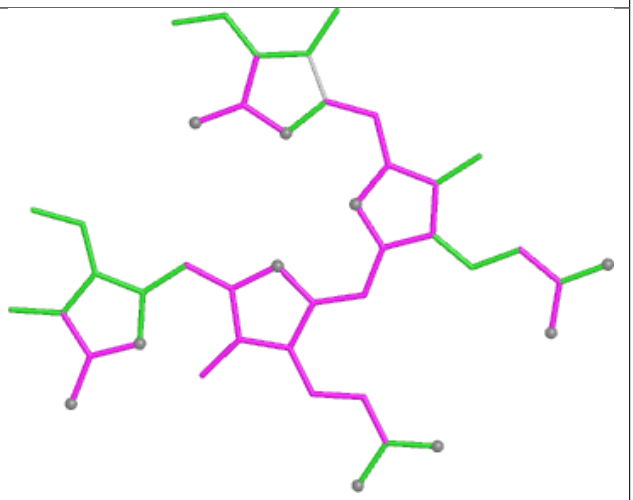

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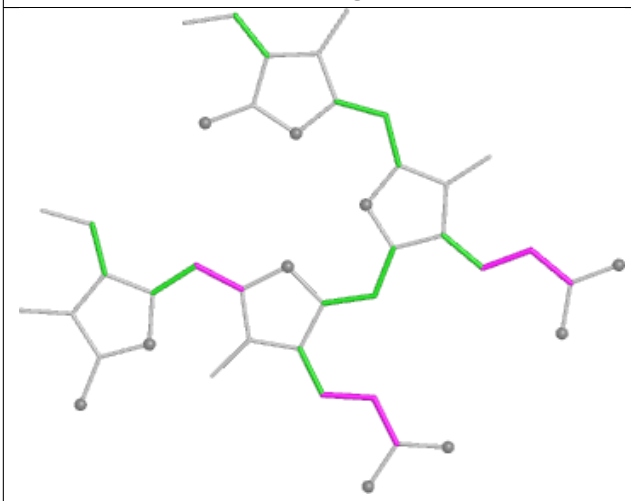

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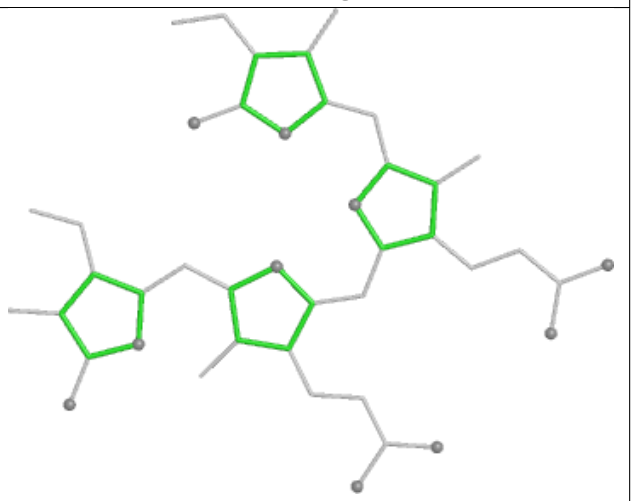
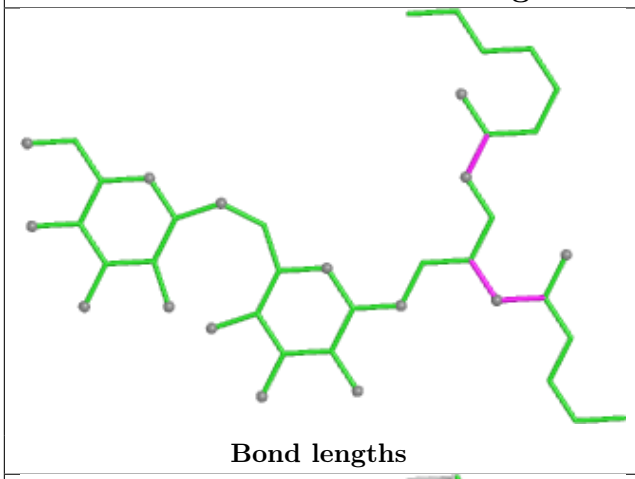


Rings

Ligand DGD C6 503



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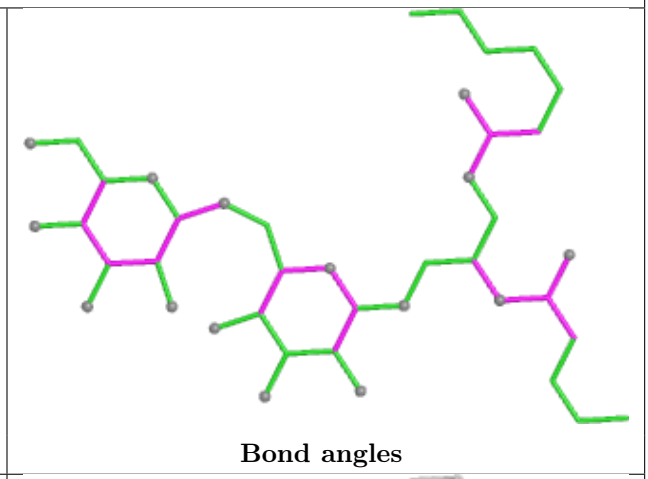

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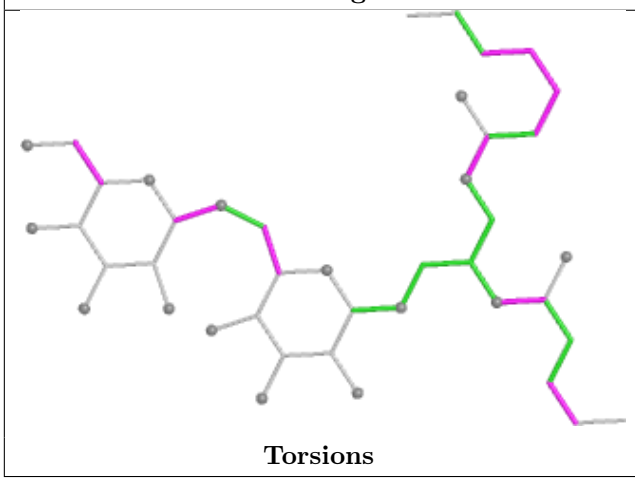

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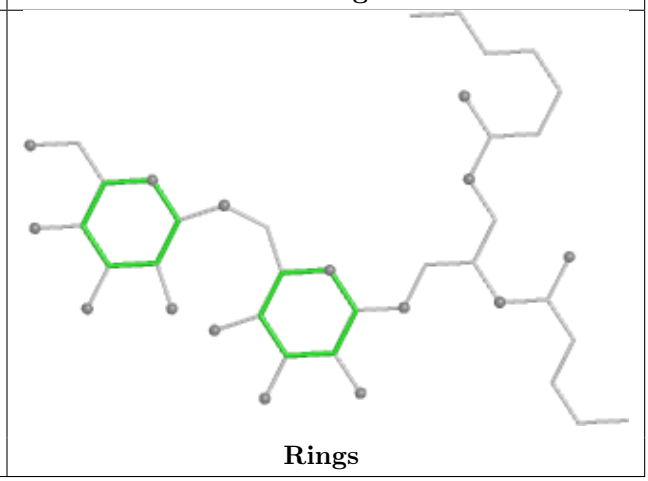
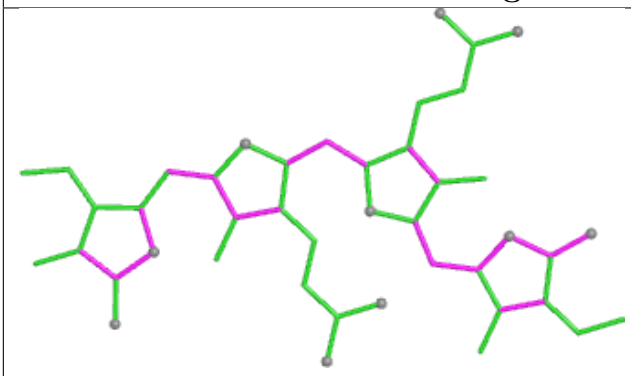


Rings

Ligand CYC D4 1001



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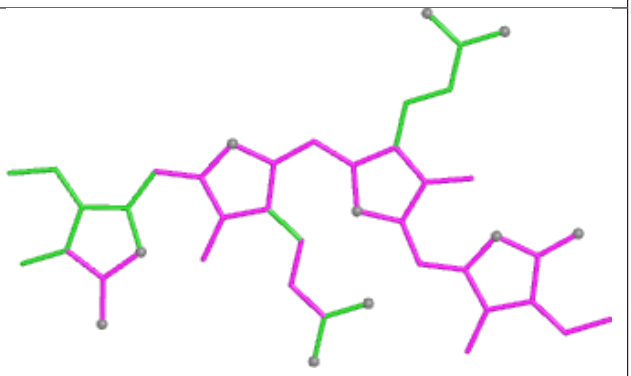

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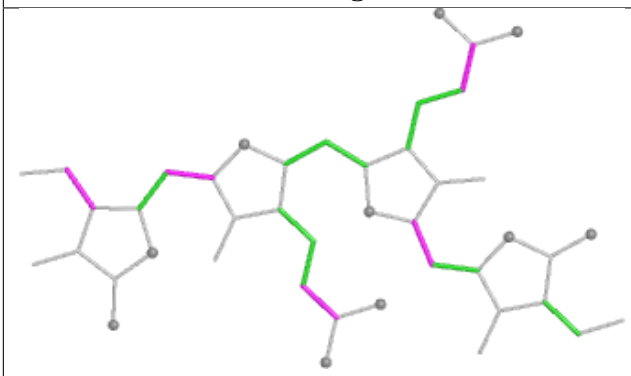

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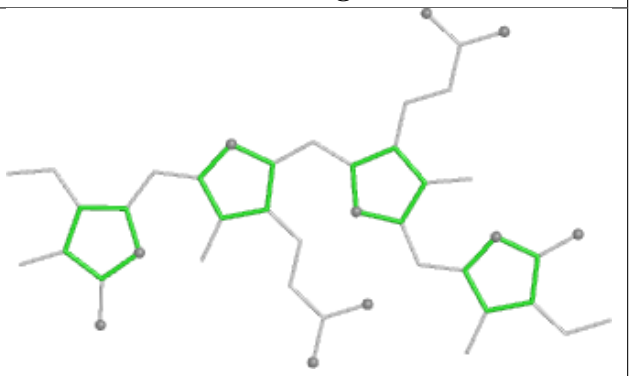
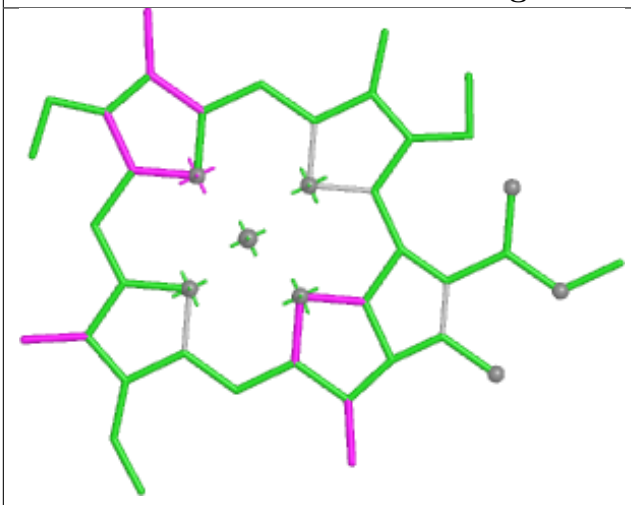


Rings

Ligand CLA AN 817



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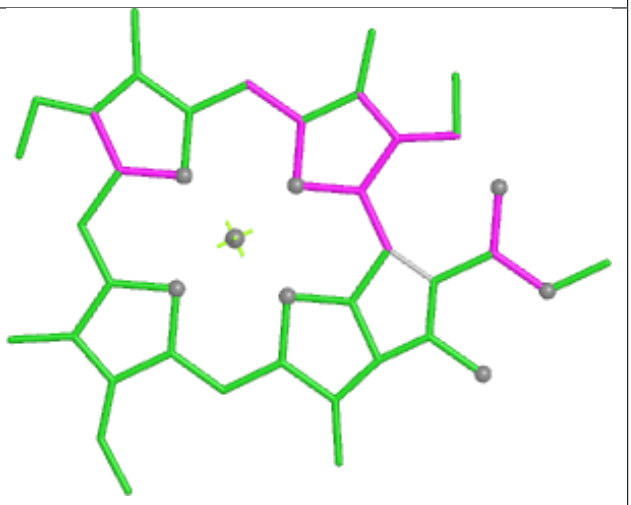

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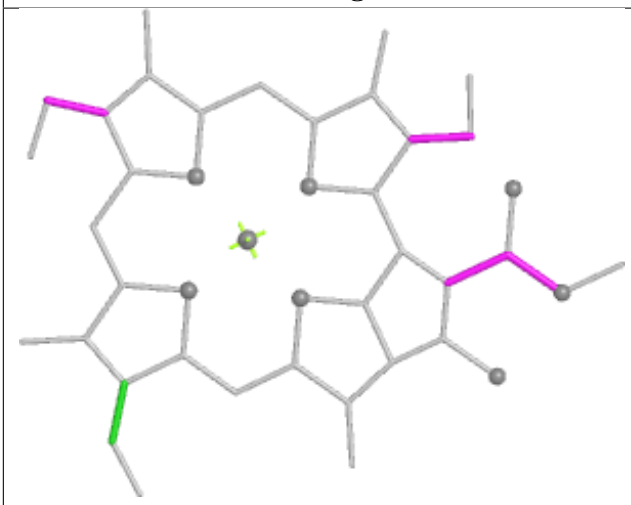
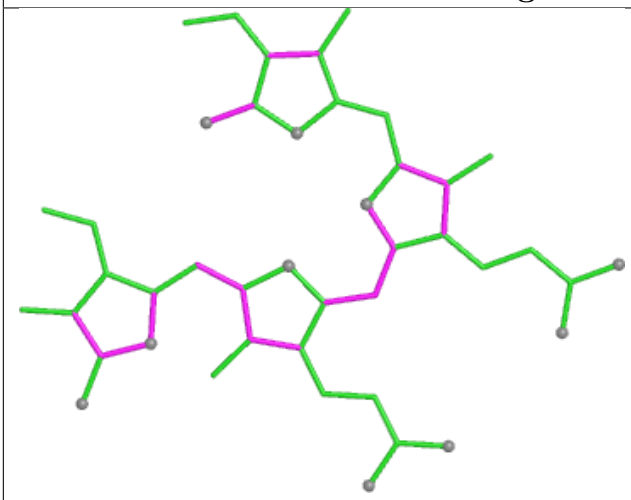


Torsions



Rings

Ligand PEB Z5 301



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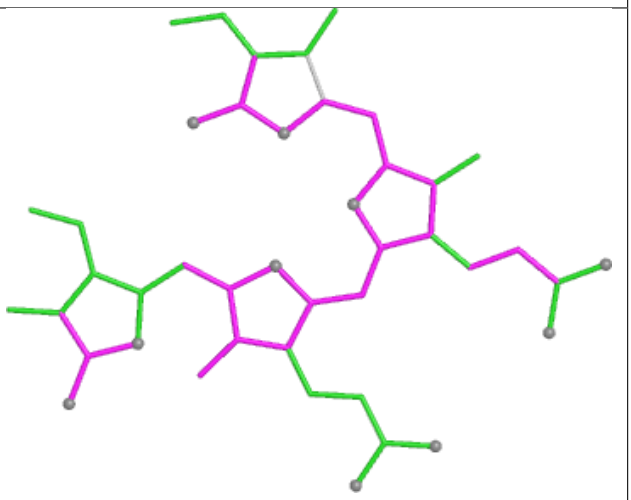

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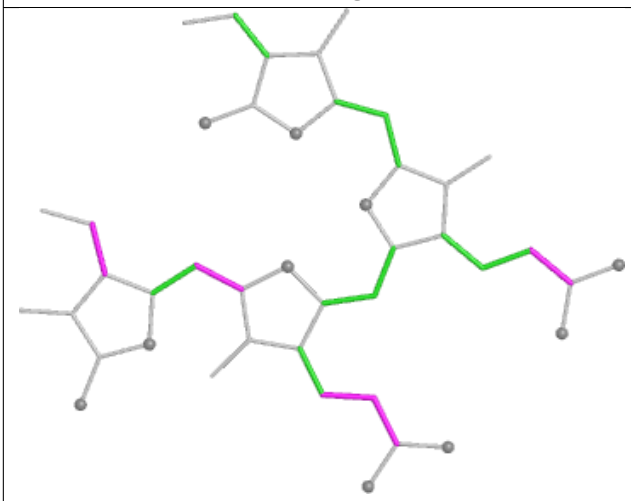

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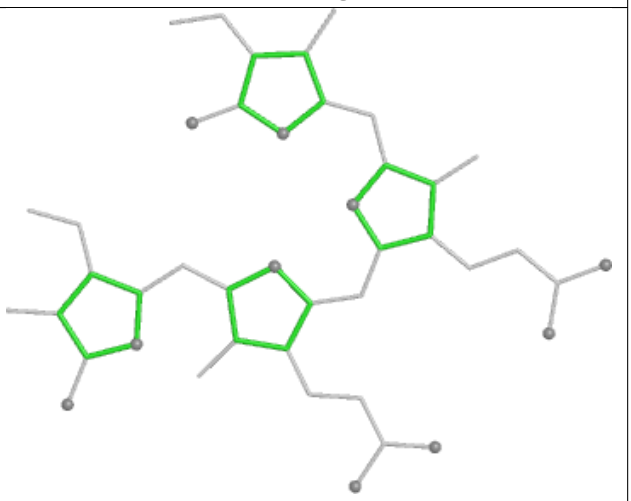
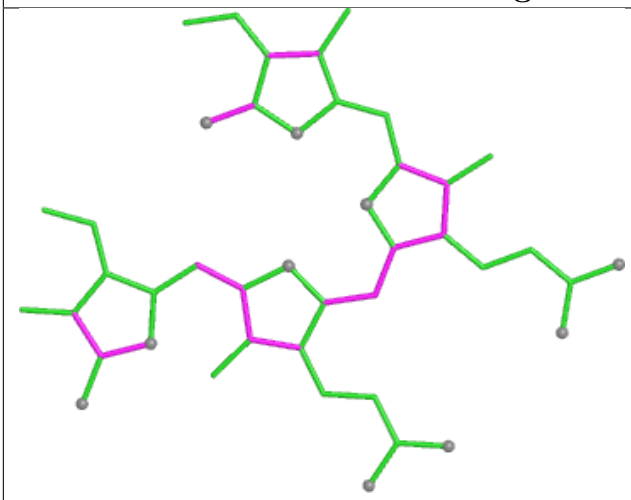


Rings

Ligand PEB SD 202



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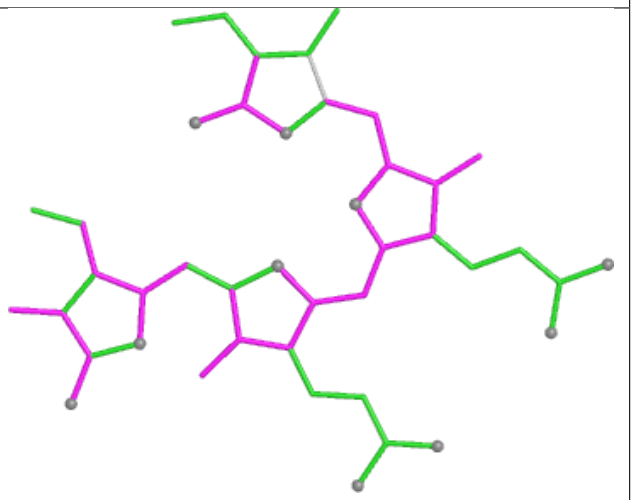

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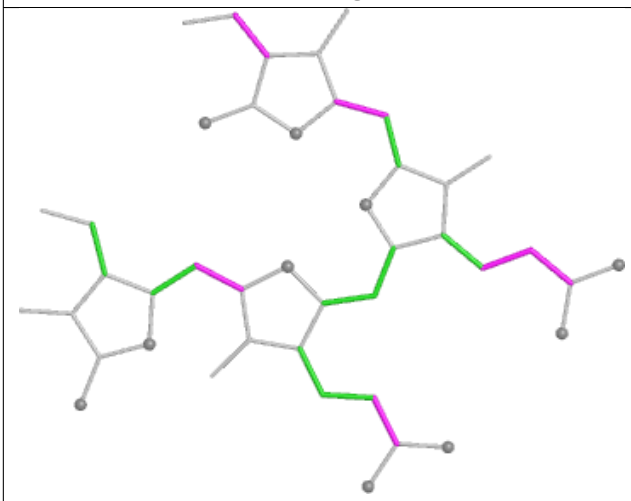

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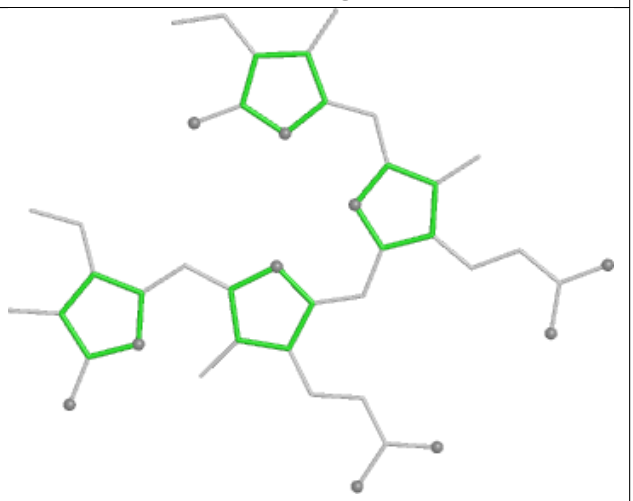

Rings

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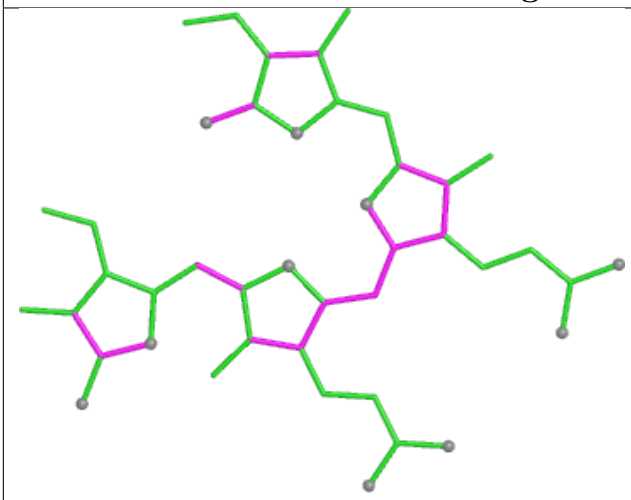

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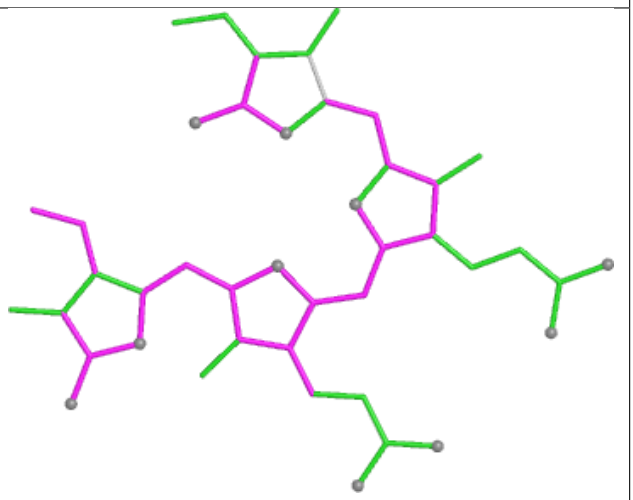

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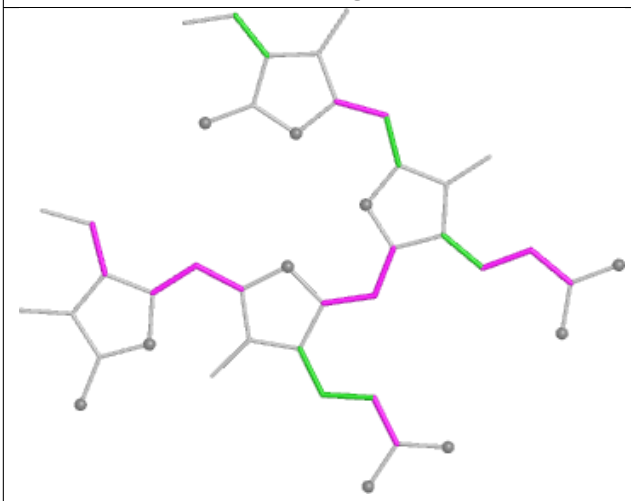

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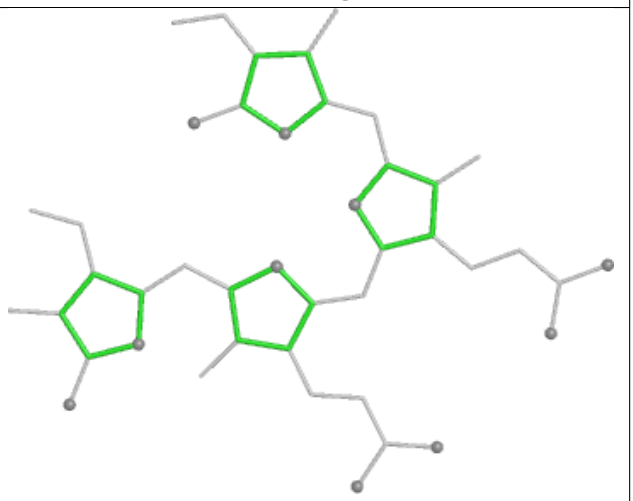
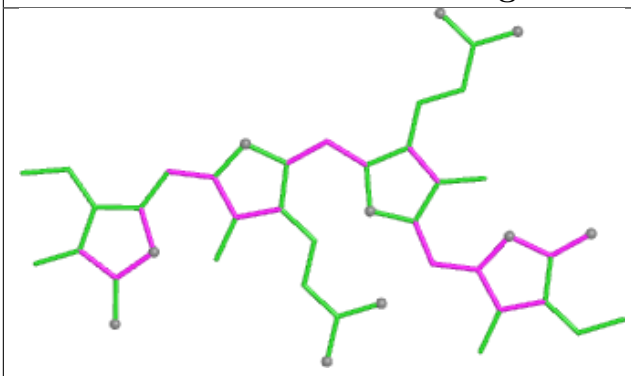


Rings

Ligand CYC HO 1001



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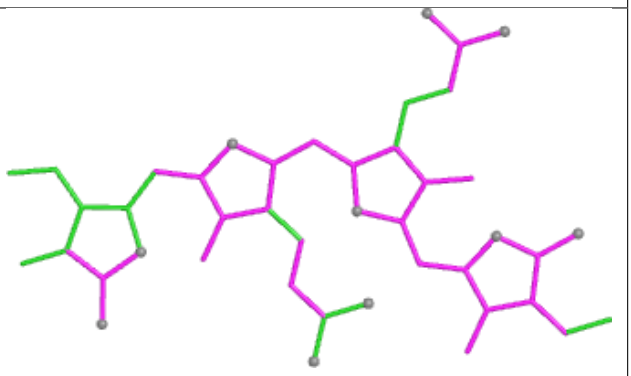

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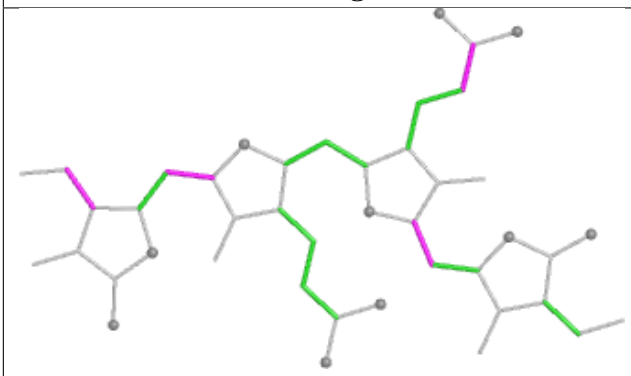

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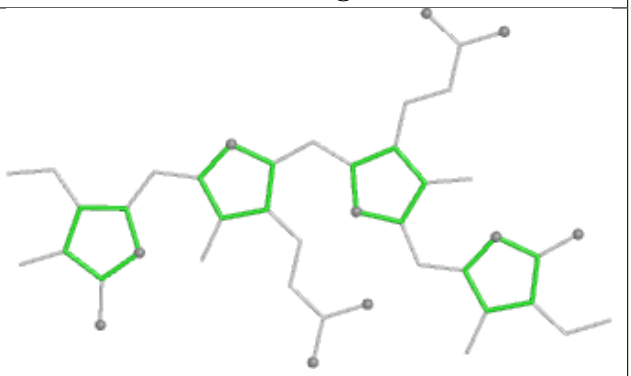
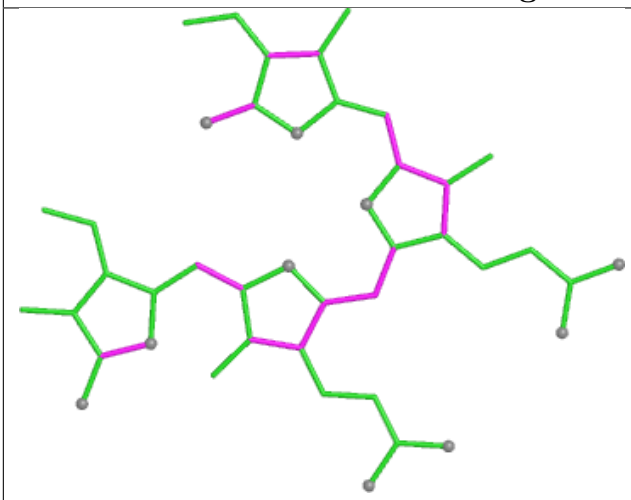


Rings

Ligand PEB y8 202



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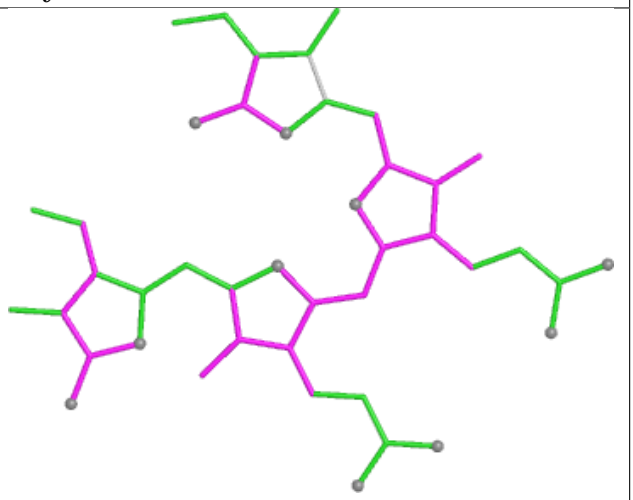

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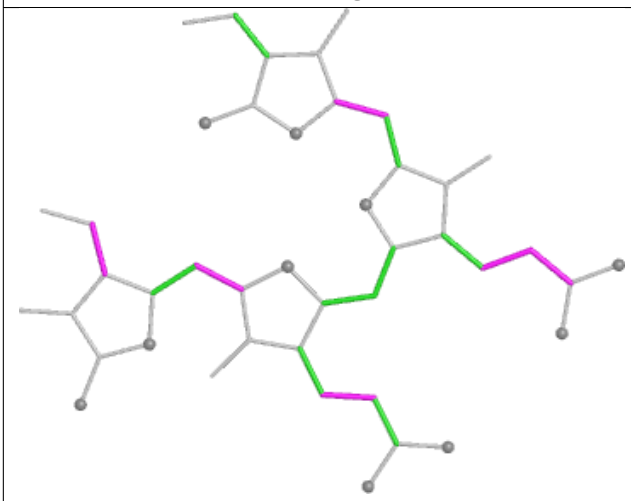

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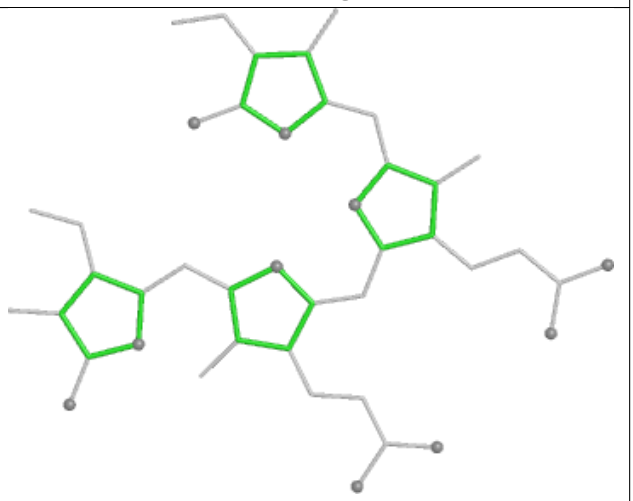
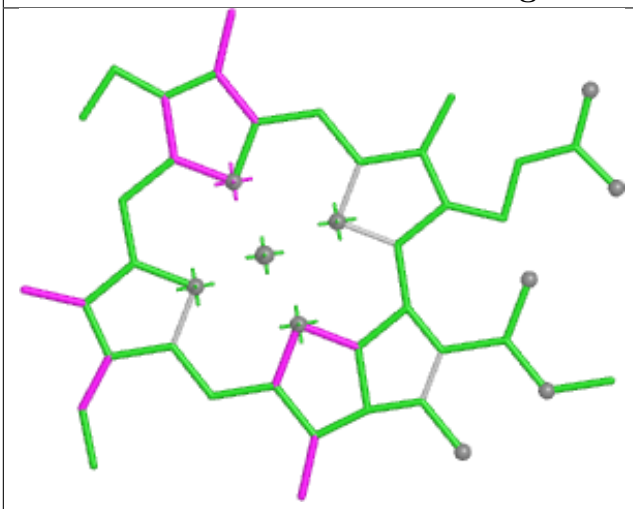


Rings

Ligand CLA 82 303



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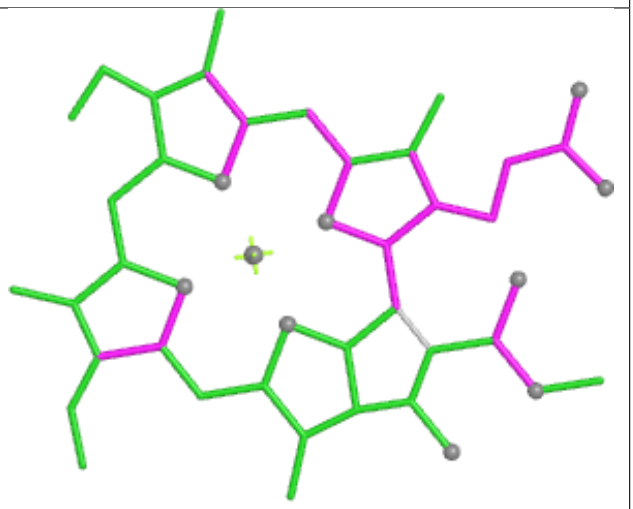

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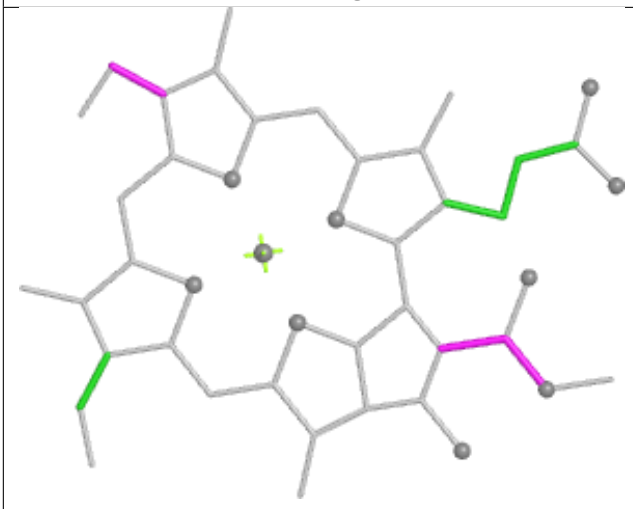
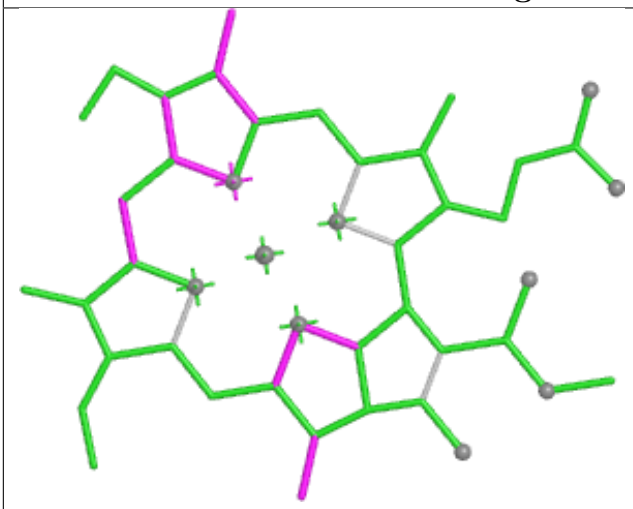


Torsions



Rings

Ligand CLA 7N 603



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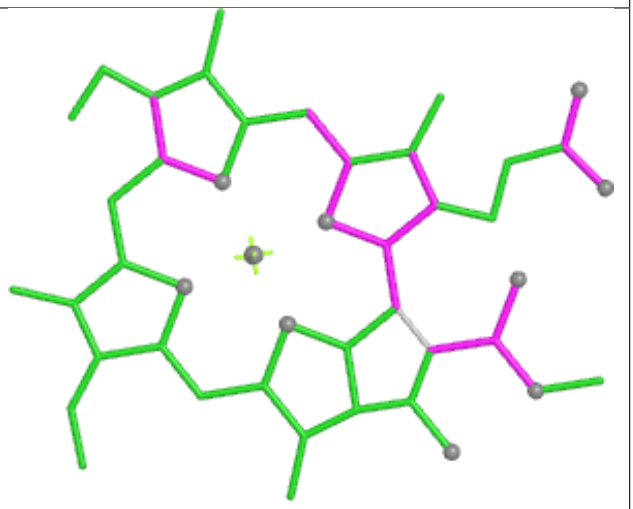

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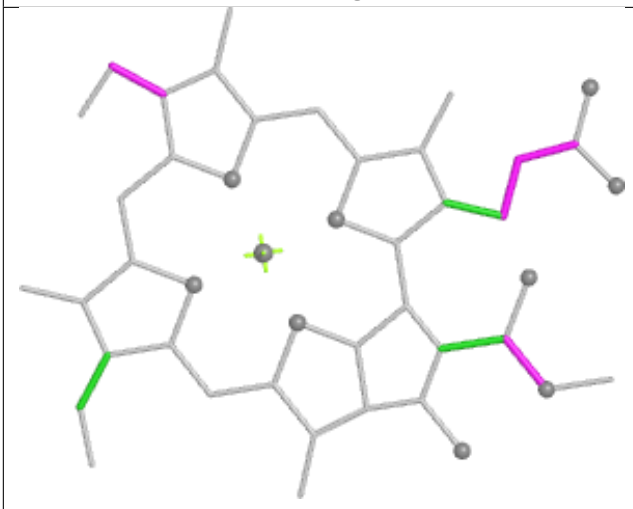
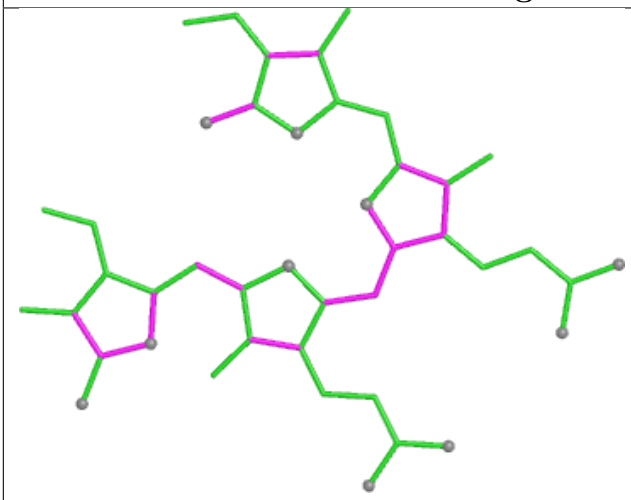


Torsions



Rings

Ligand PEB X7 201



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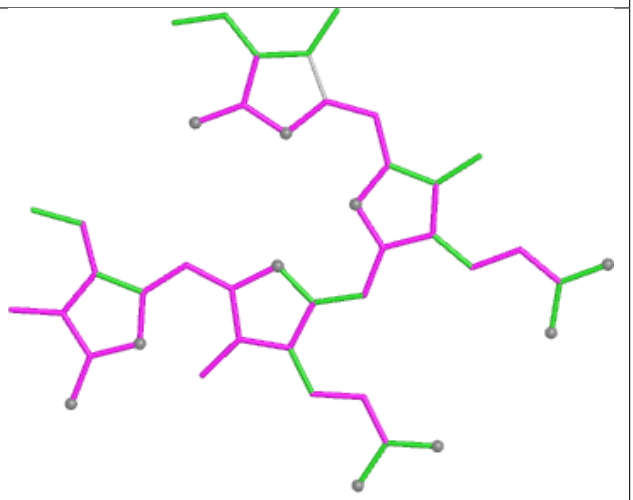

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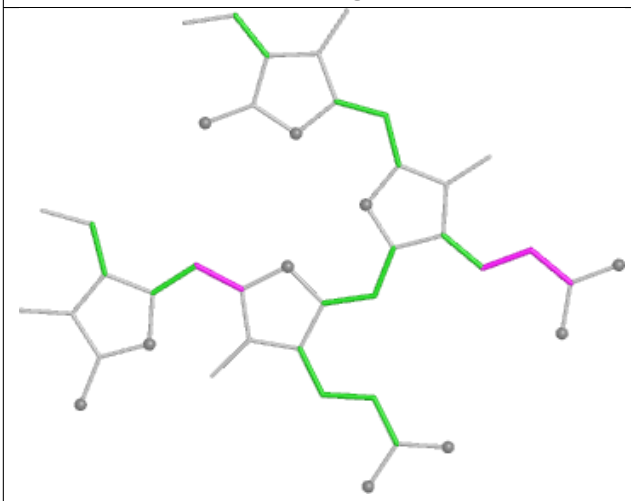

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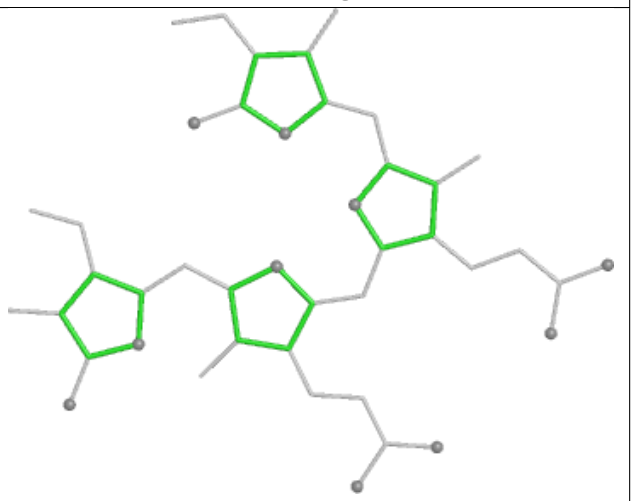
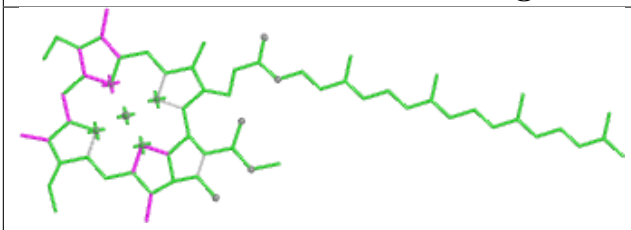


Rings

Ligand CLA B6 604



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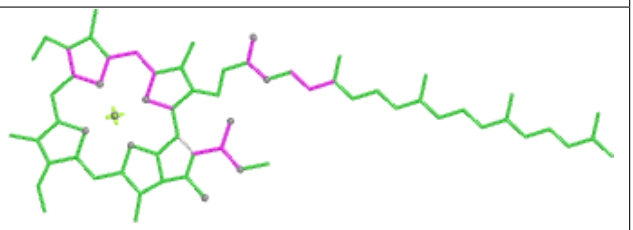

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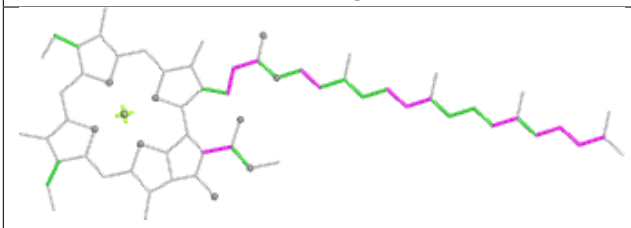

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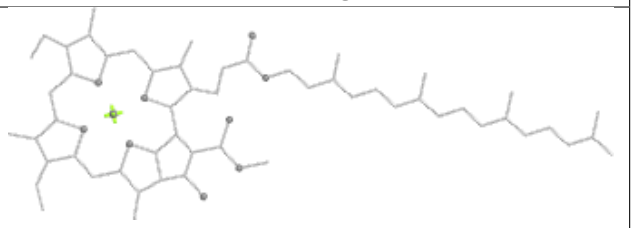
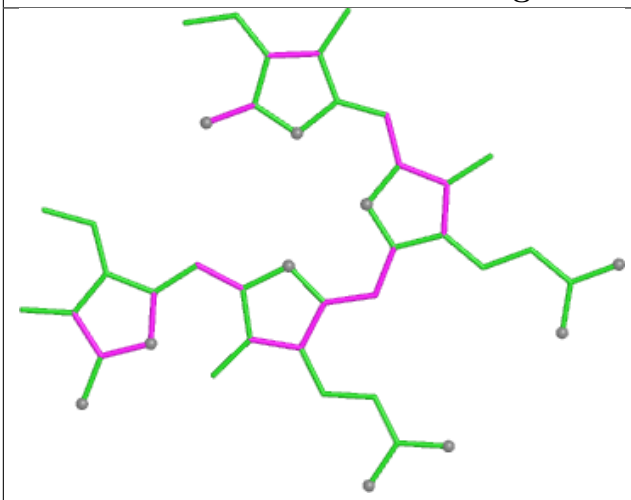


Rings

Ligand PEB OF 201



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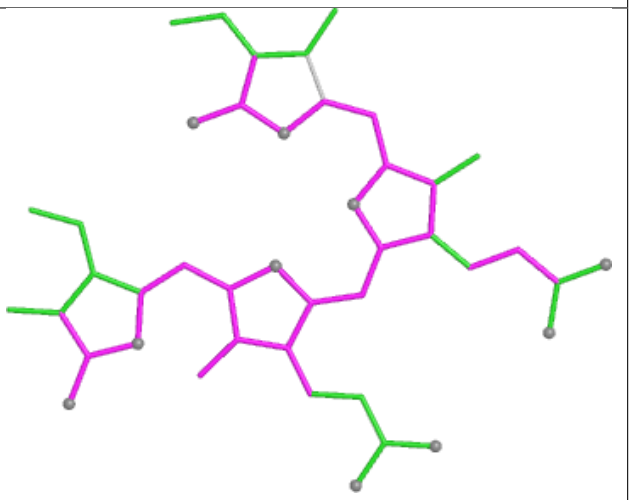

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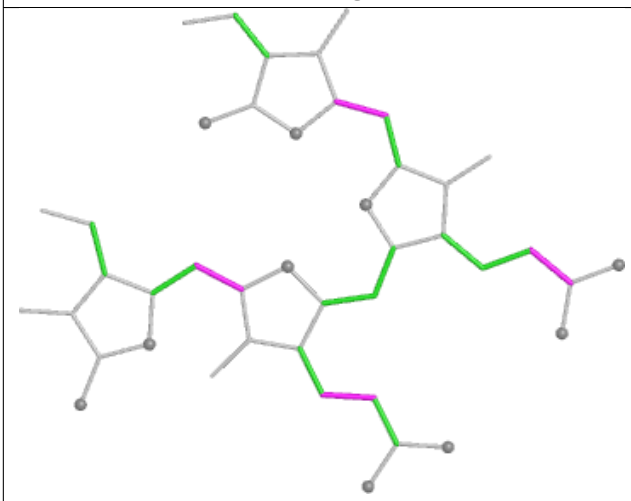

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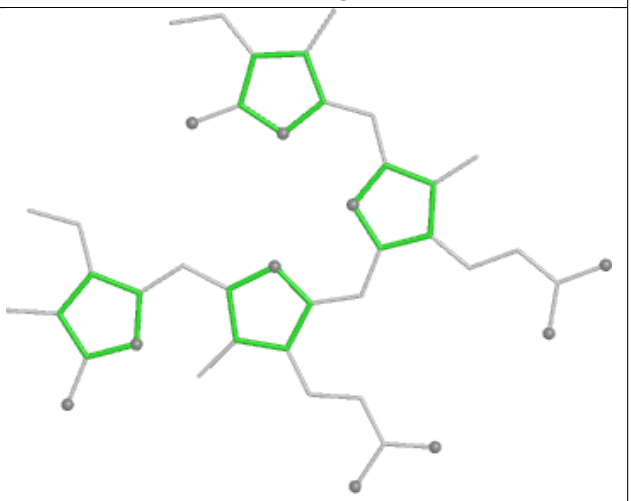
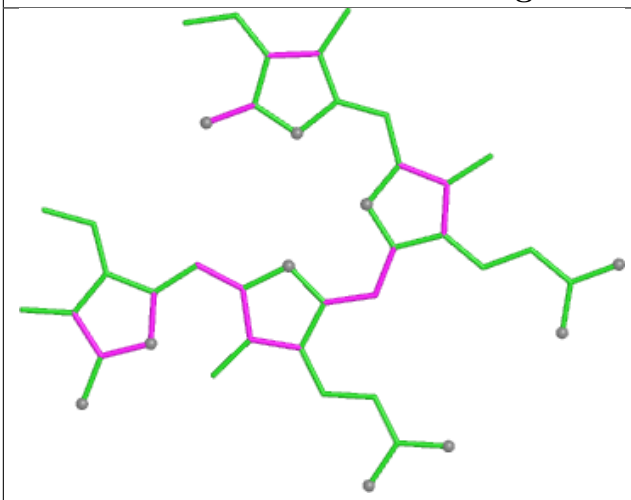


Rings

Ligand PEB Q1 202



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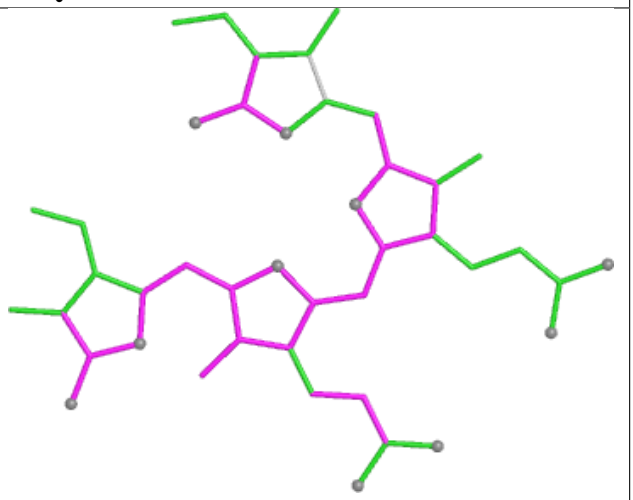
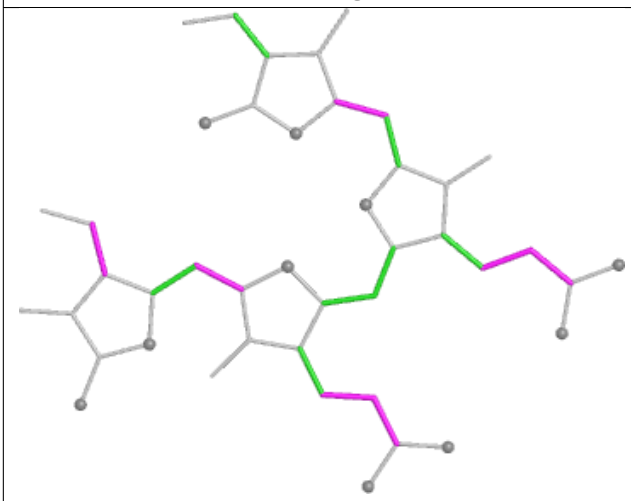
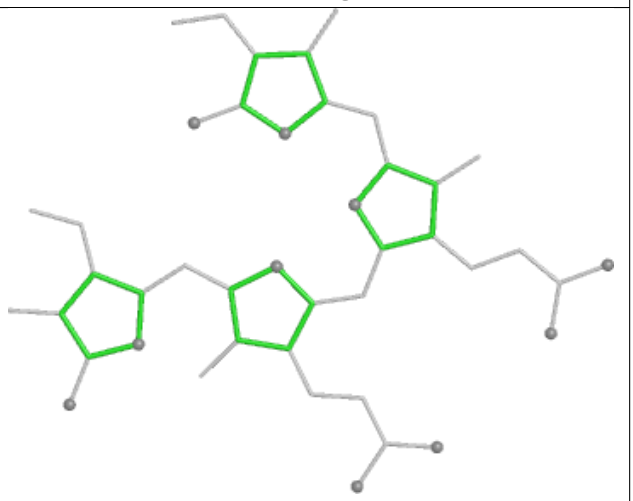


Bond angles

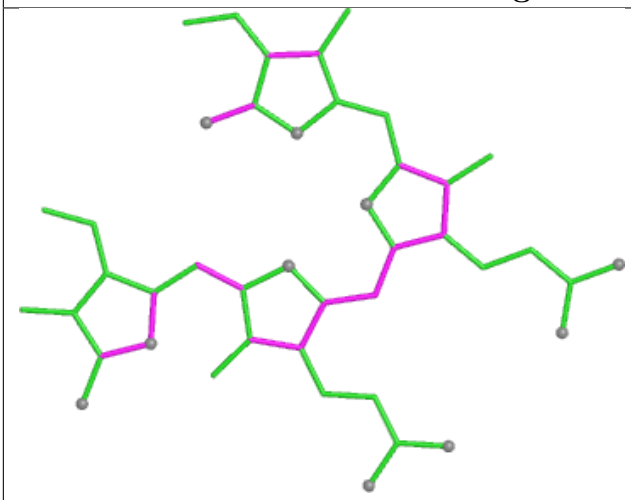


Torsions



Rings

Ligand PEB YF 202



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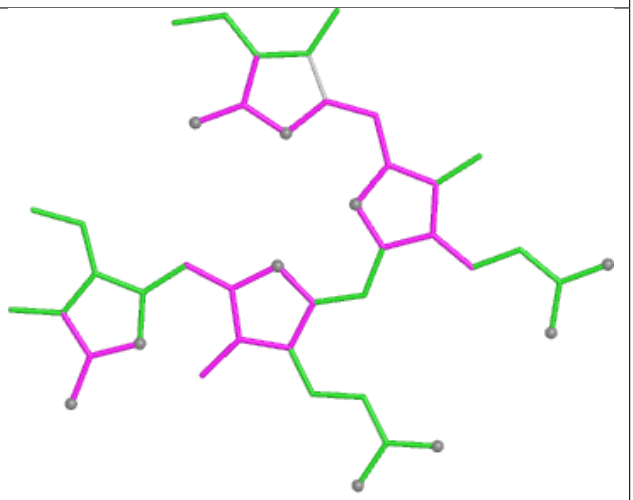

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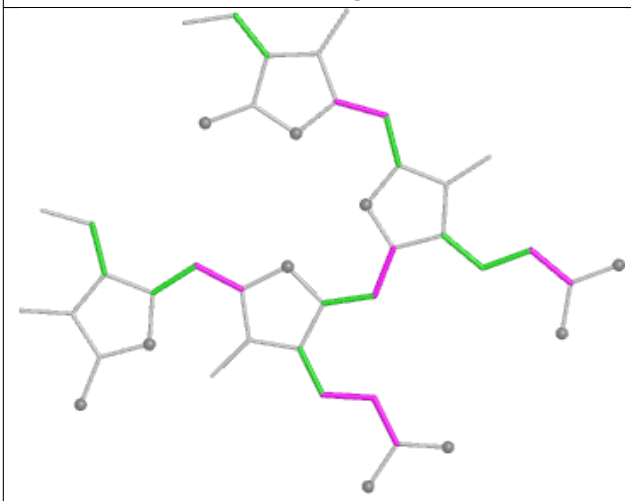

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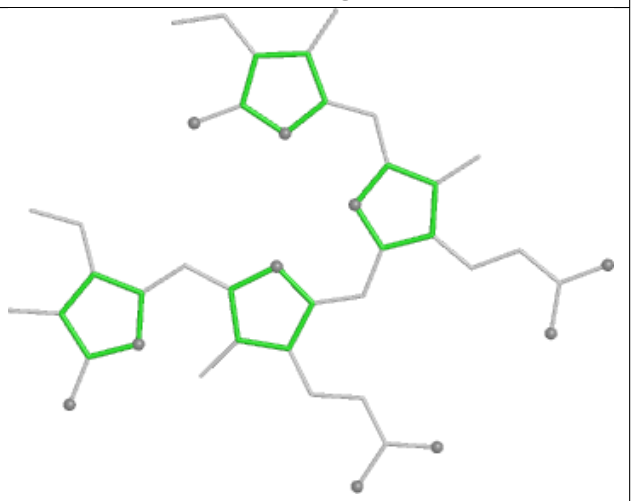
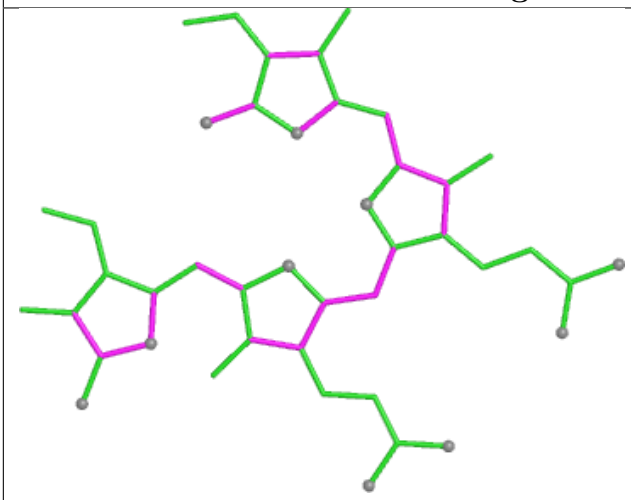


Rings

Ligand PEB DA 201



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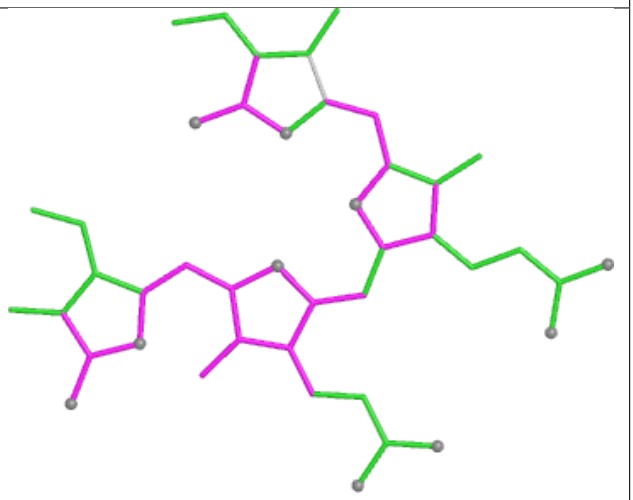

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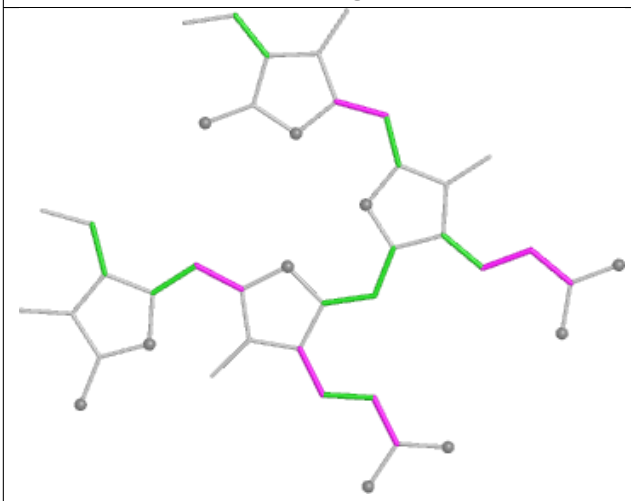

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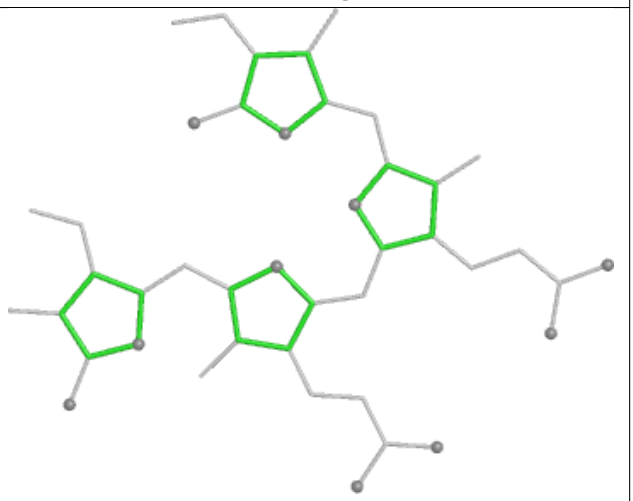
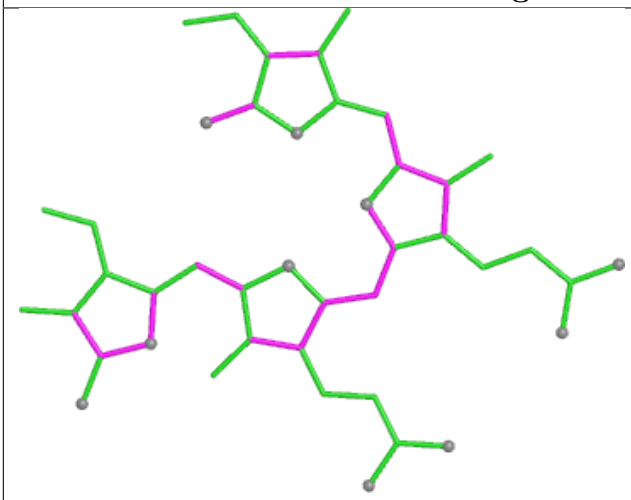


Rings

Ligand PEB QP 203



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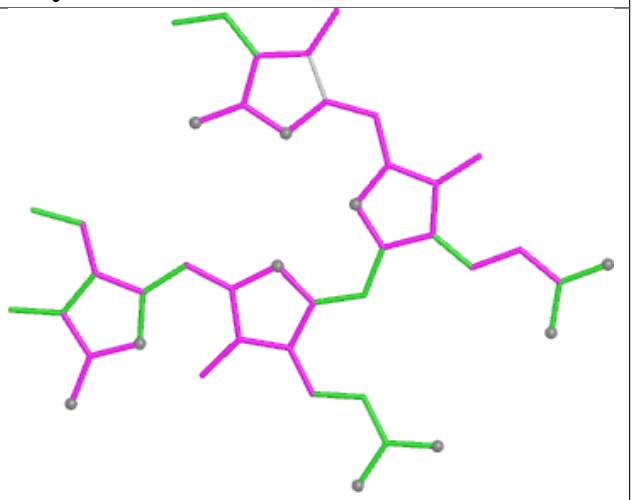

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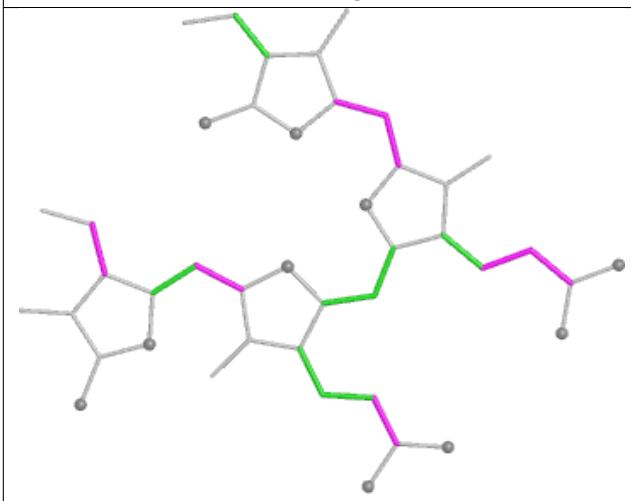

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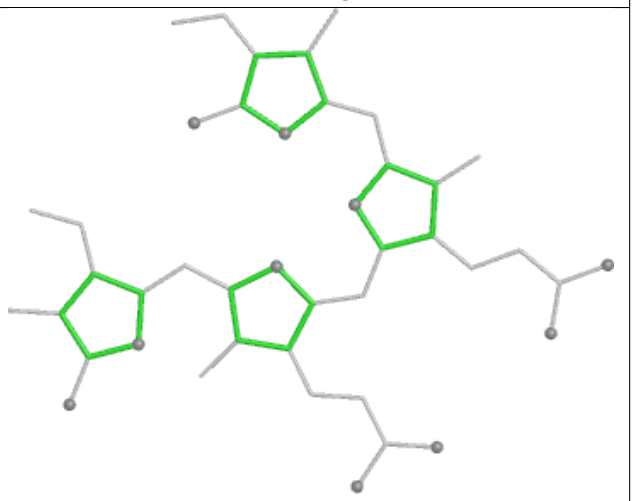
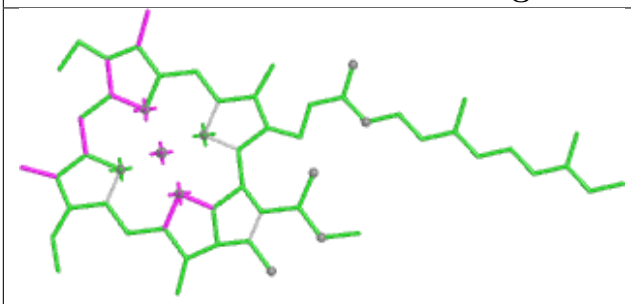


Rings

Ligand CLA LN 206



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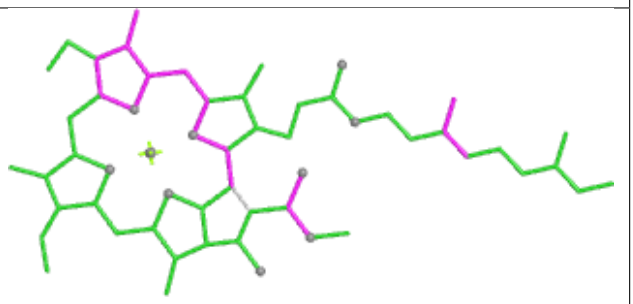

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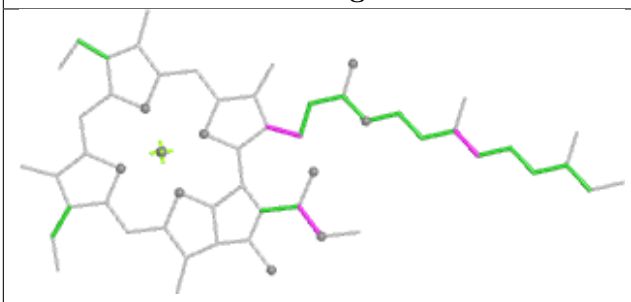

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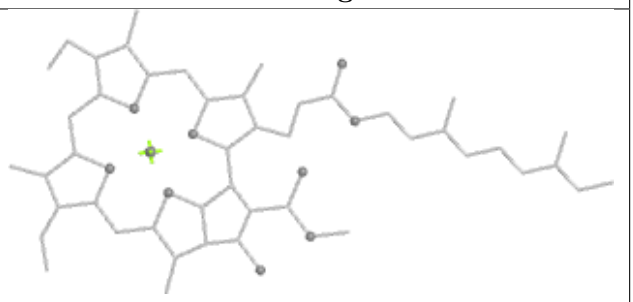
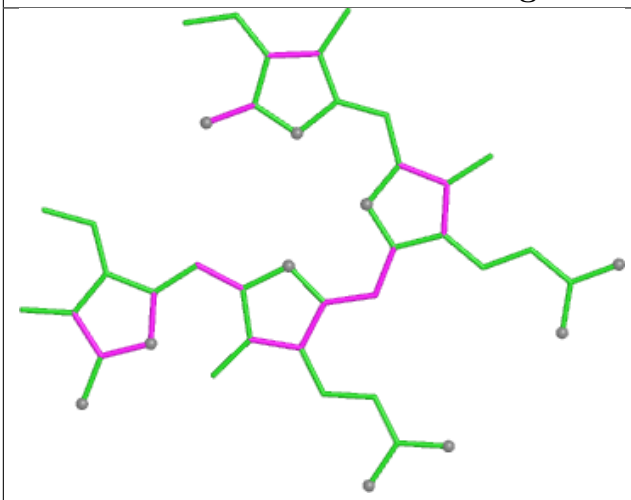


Rings

Ligand PEB J5 202



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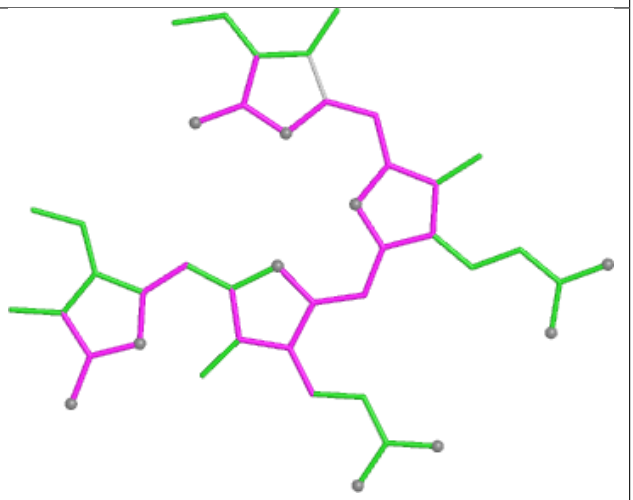

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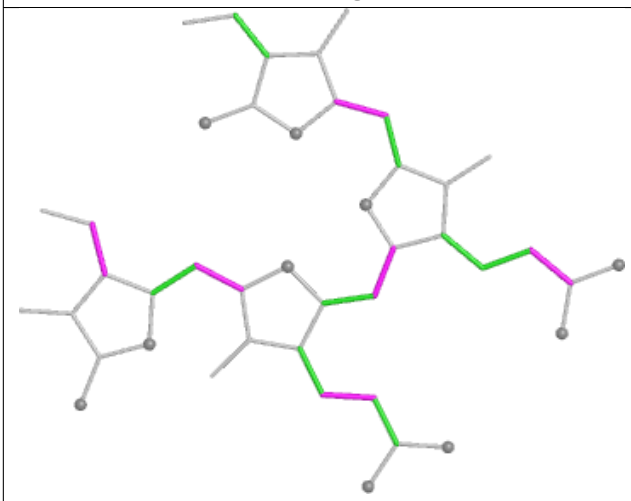

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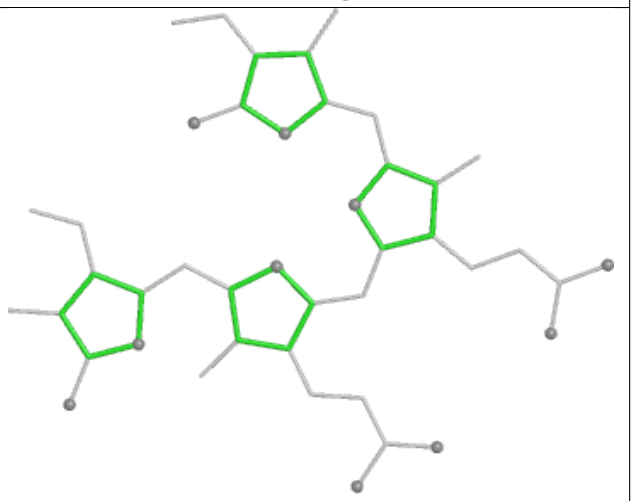
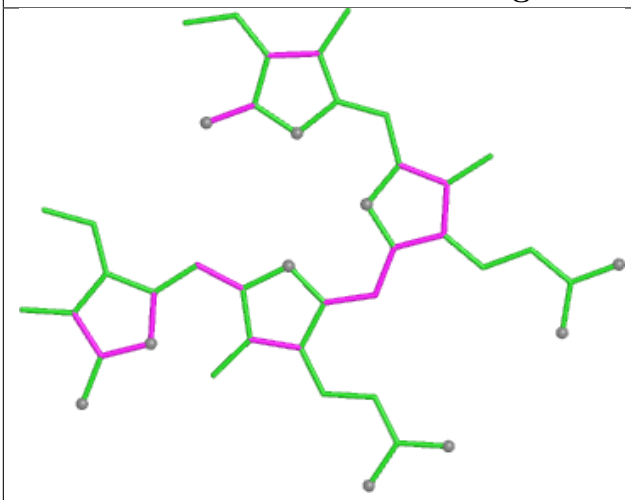


Rings

Ligand PEB RE 202



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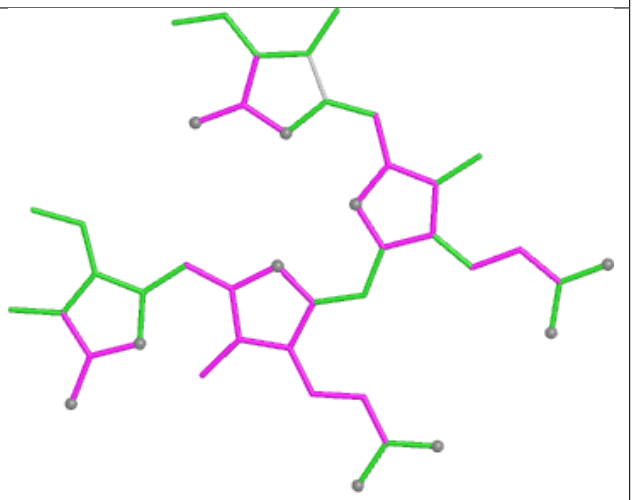
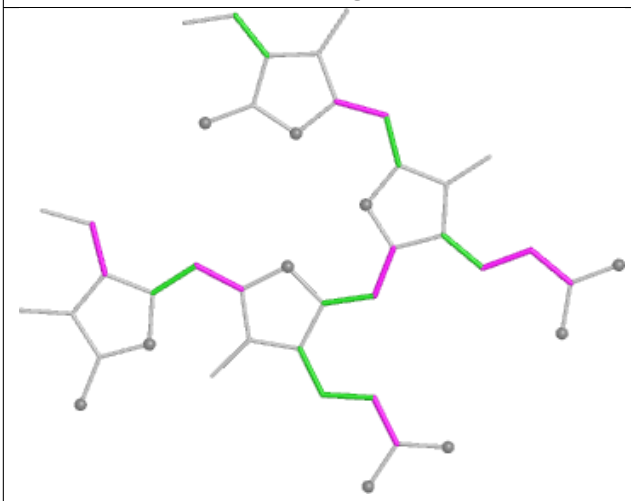


Bond angles



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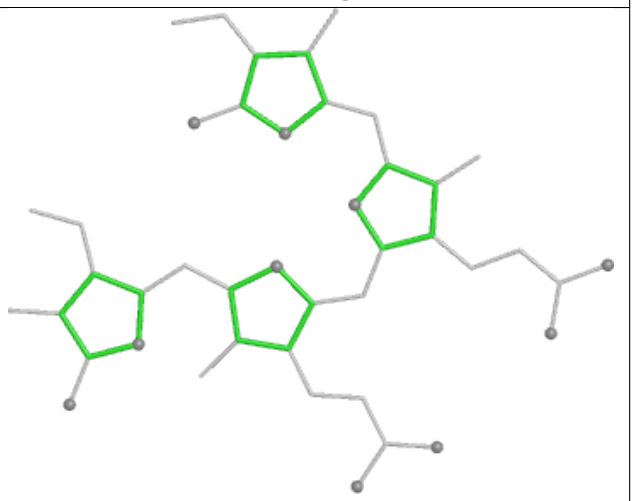
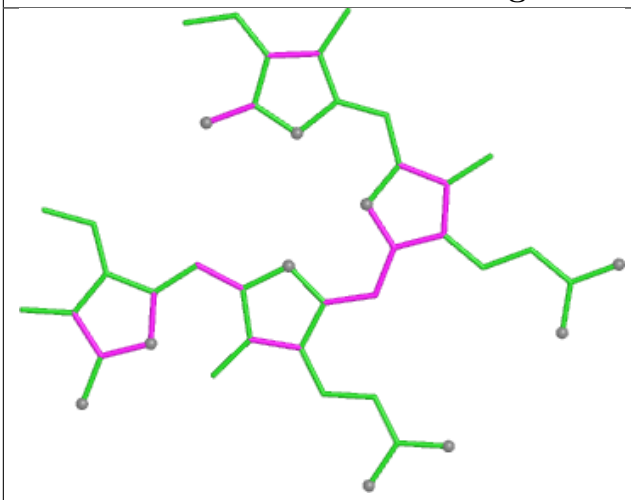


Rings

Ligand PEB F1 1002



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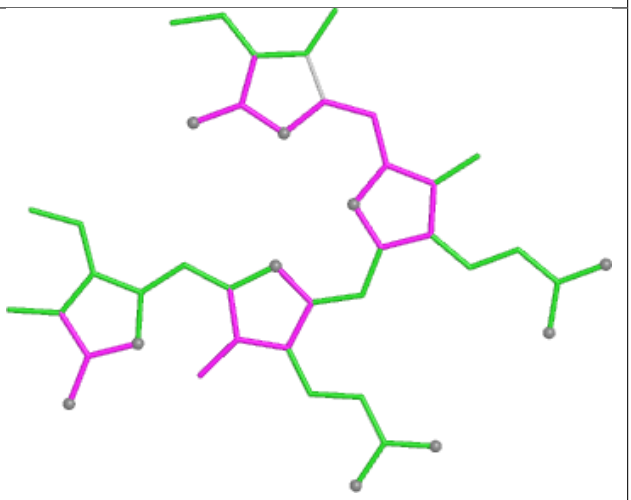

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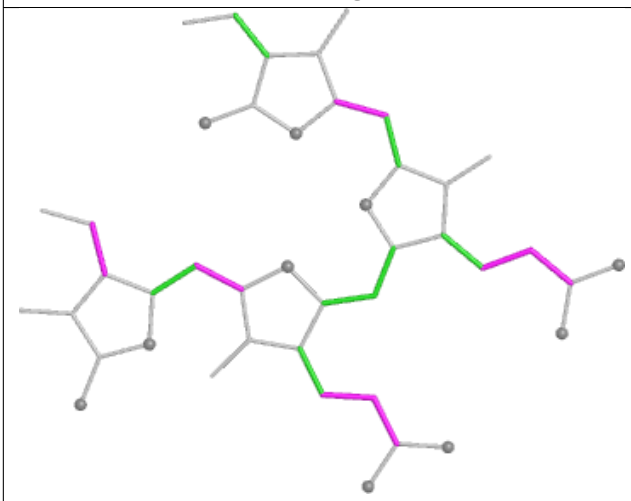

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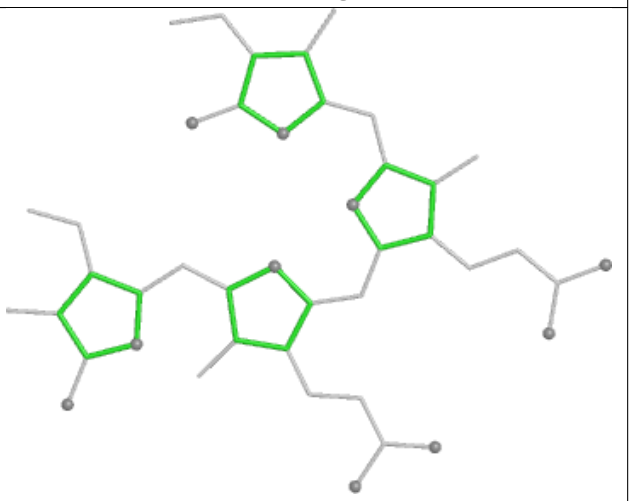
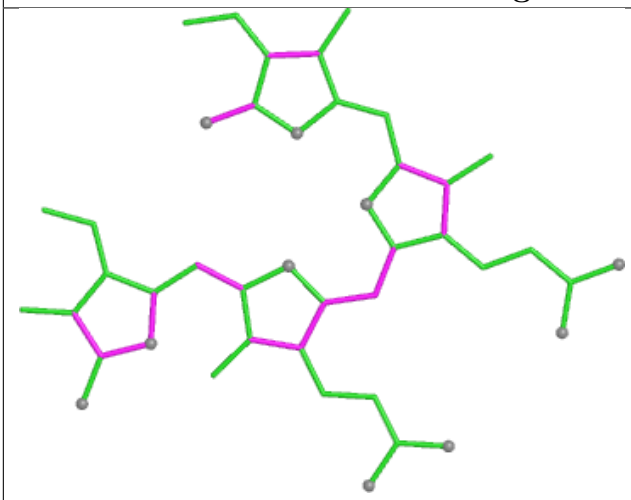


Rings

Ligand PEB XF 202



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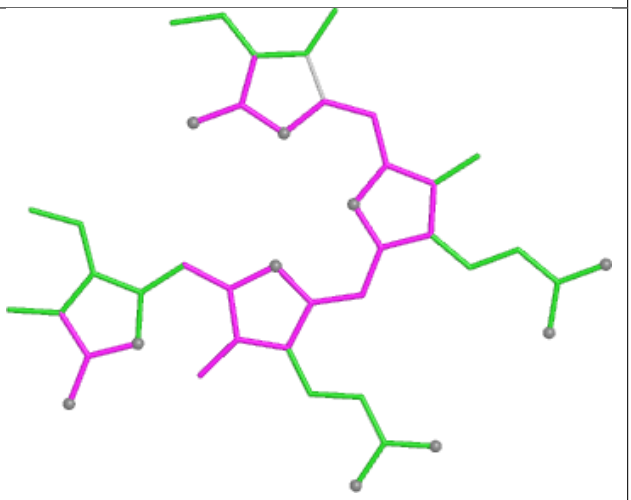

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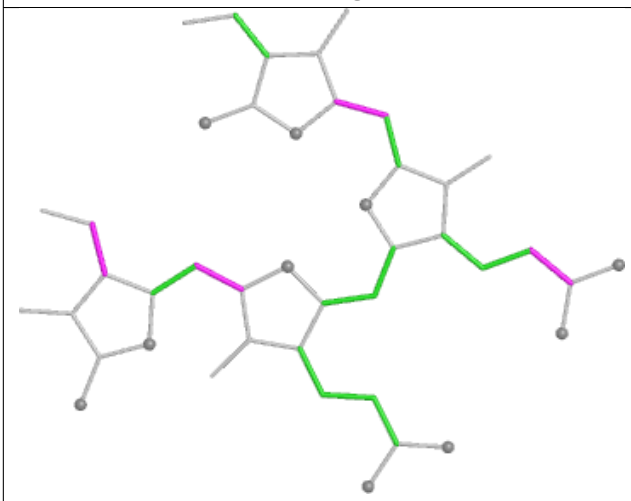

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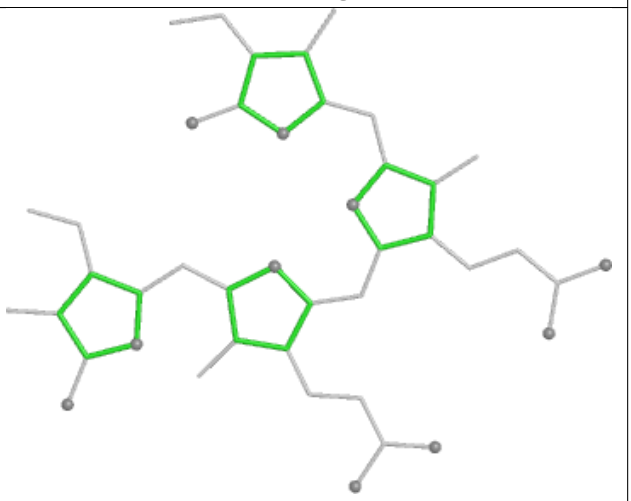
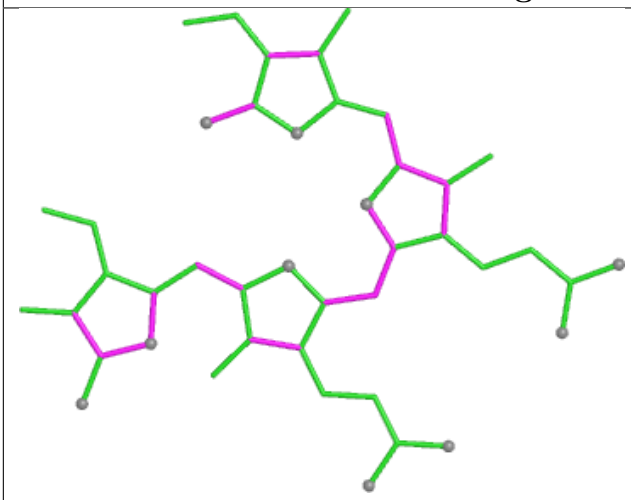


Rings

Ligand PEB XJ 201



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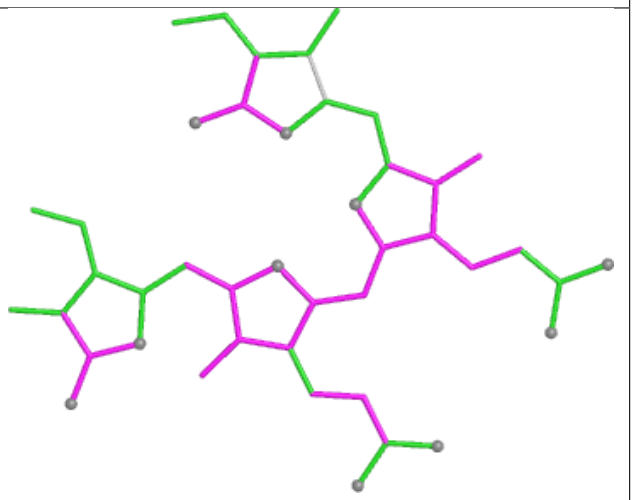

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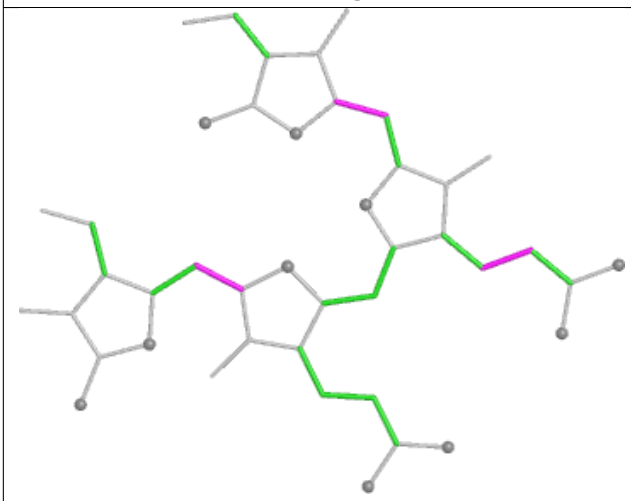

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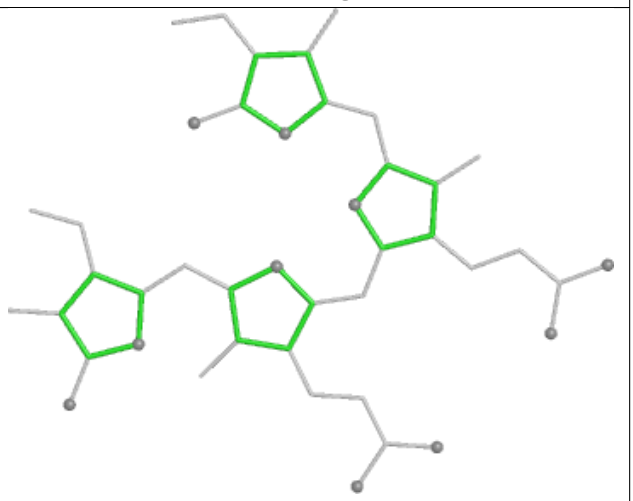
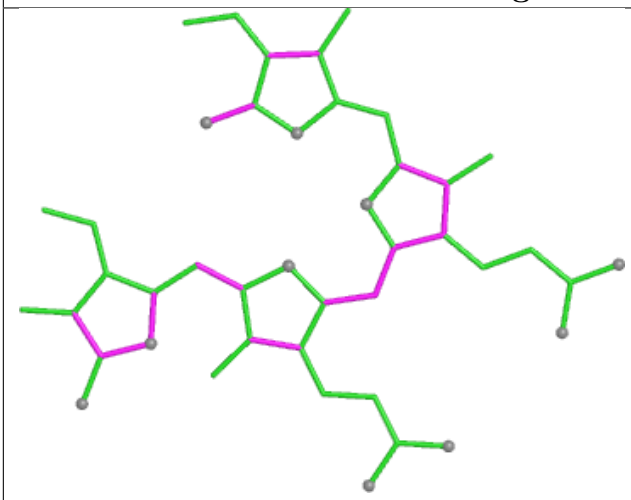


Rings

Ligand PEB BB 201



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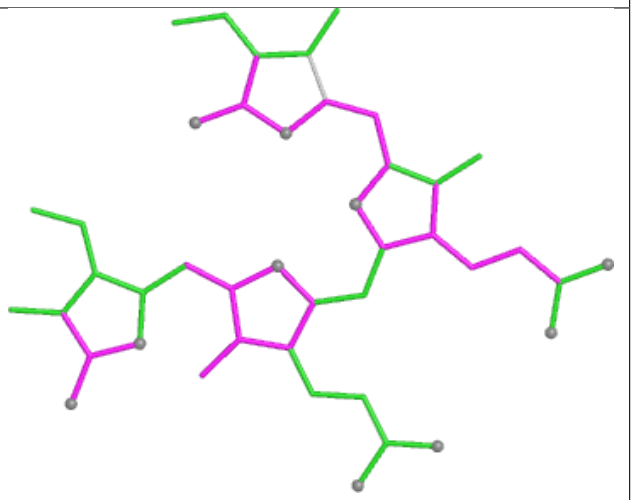

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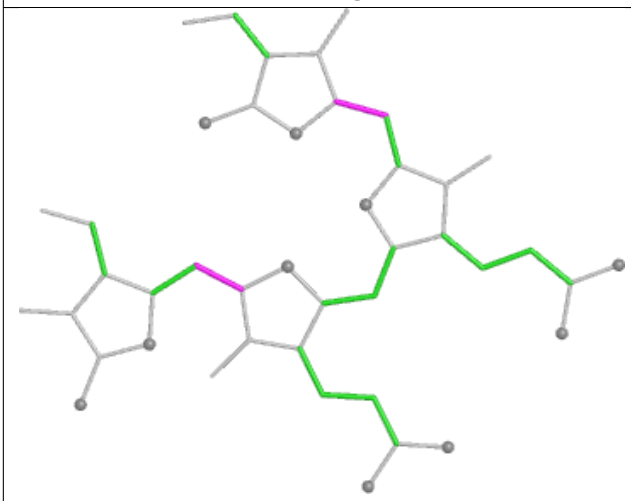

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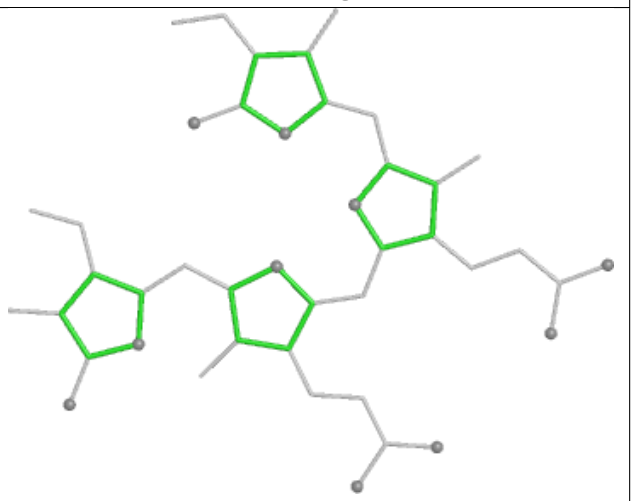
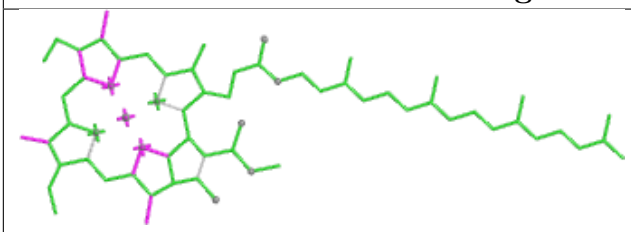


Rings

Ligand CLA A2 820



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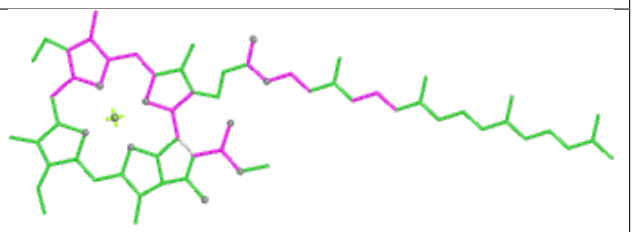

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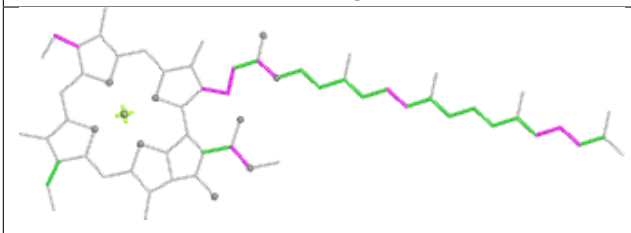

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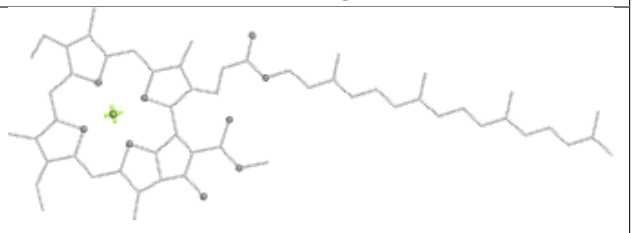
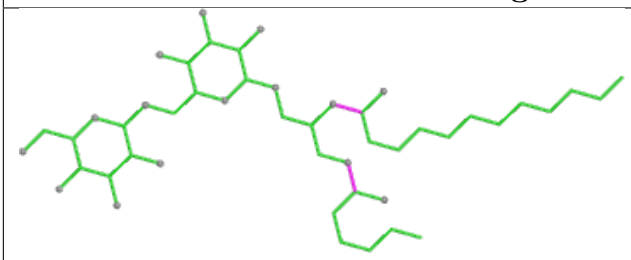


Rings

Ligand DGD C6 523



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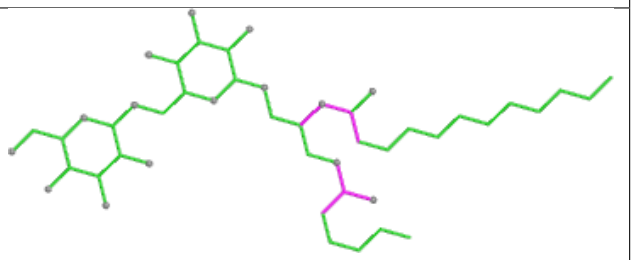

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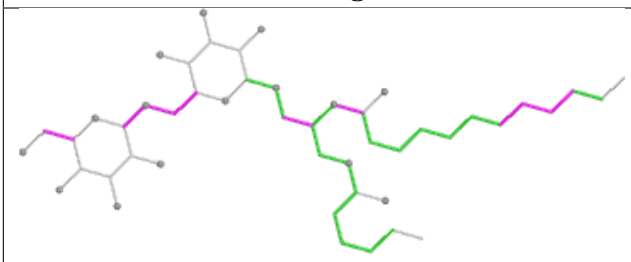

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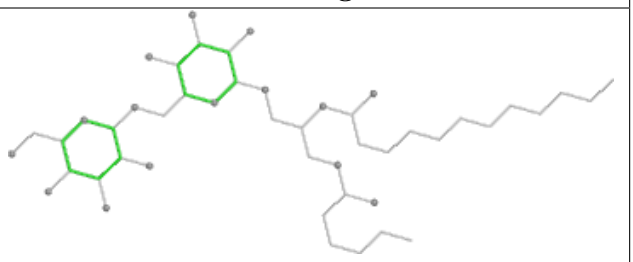
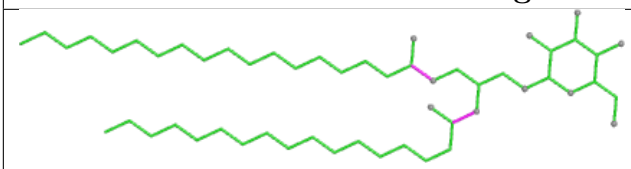


Rings

Ligand LMG d6 409



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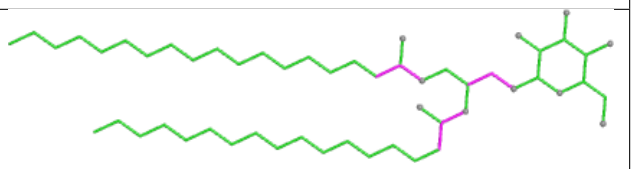
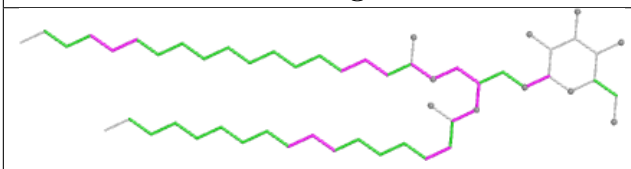


Bond angles



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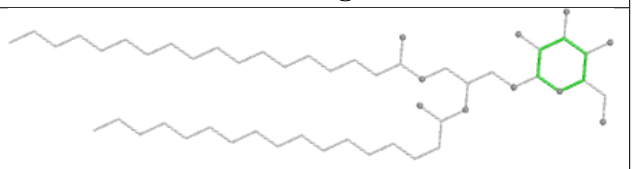
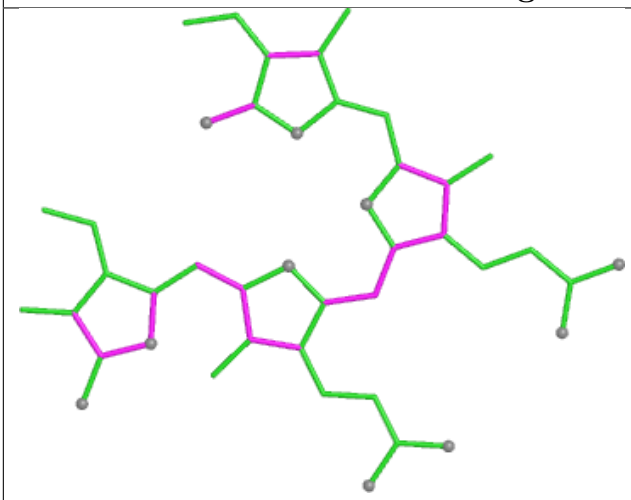


Rings

Ligand PEB Z1 203



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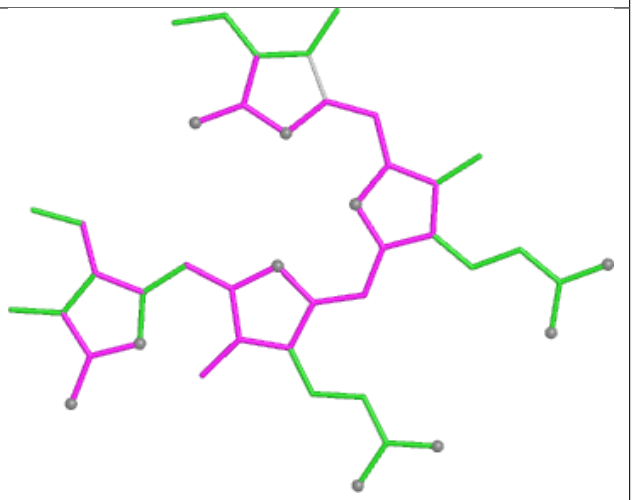
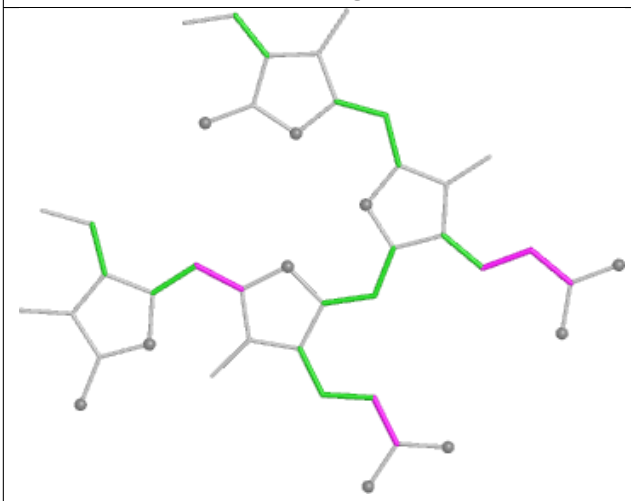


Bond angles



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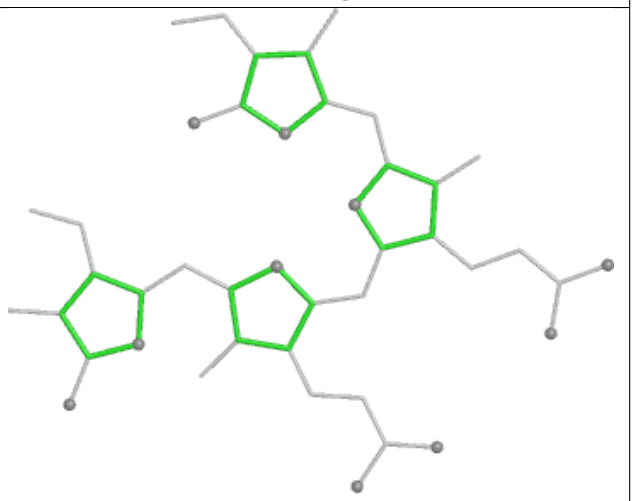
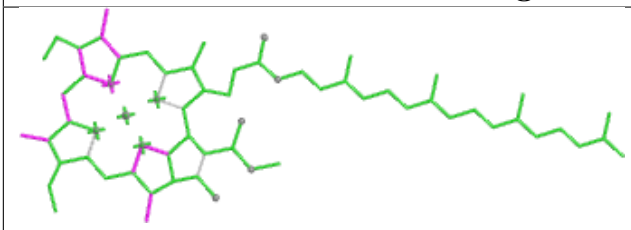


Rings

Ligand CLA C6 514



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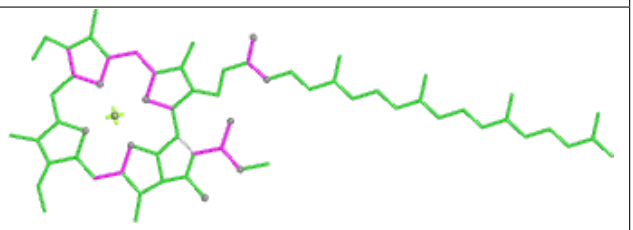

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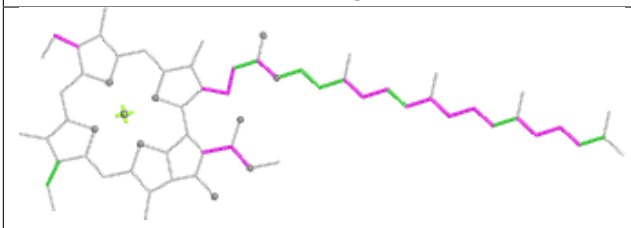

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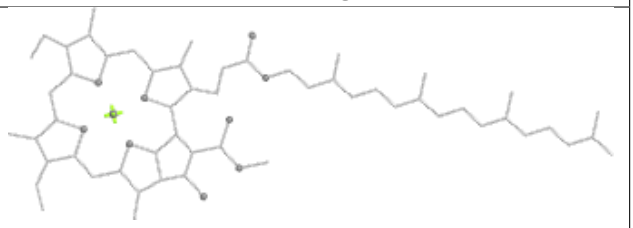
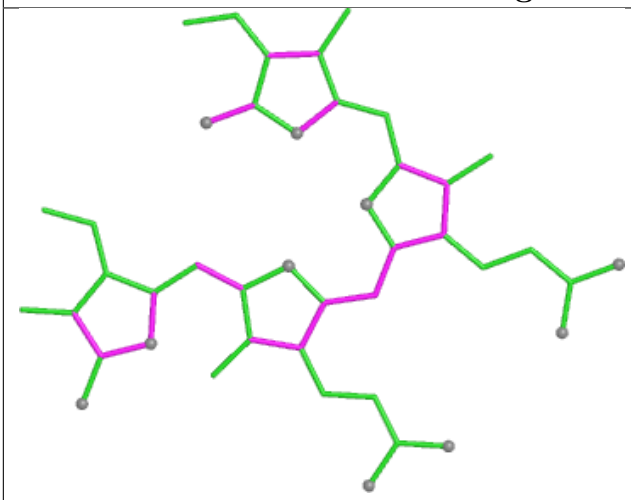


Rings

Ligand PEB O1 201



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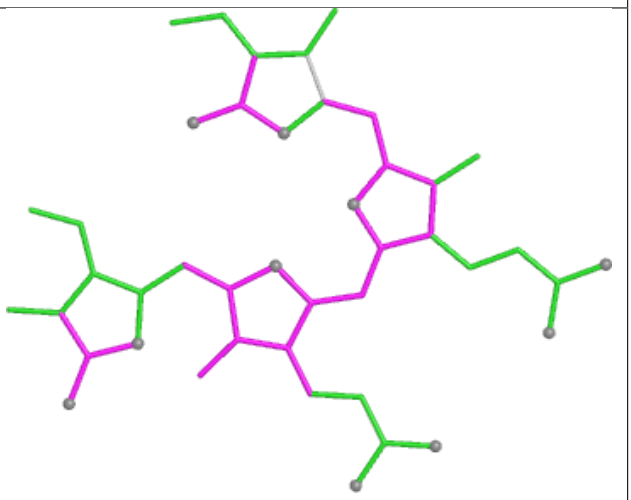

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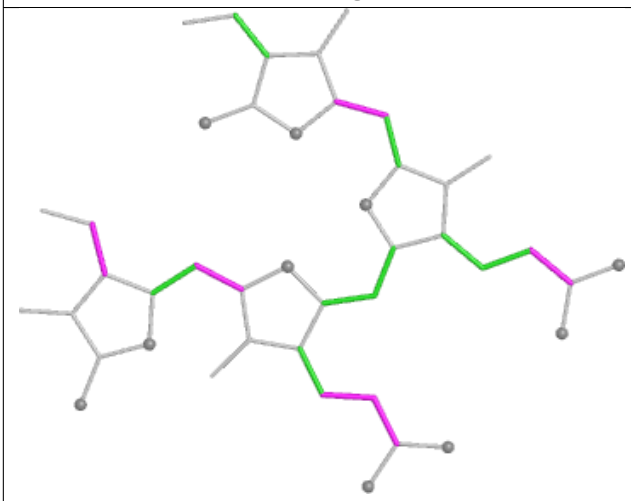

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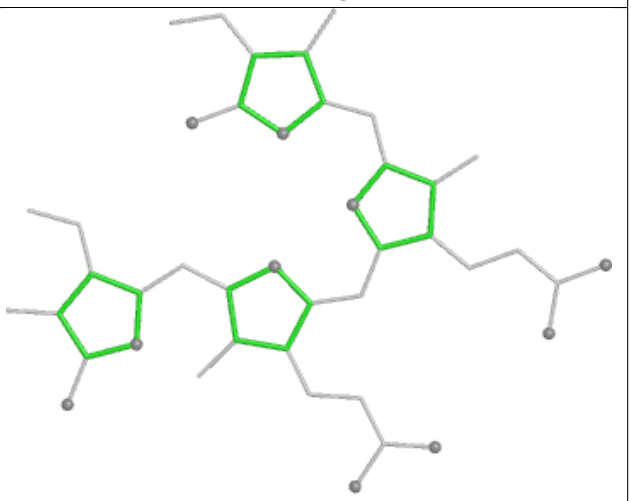
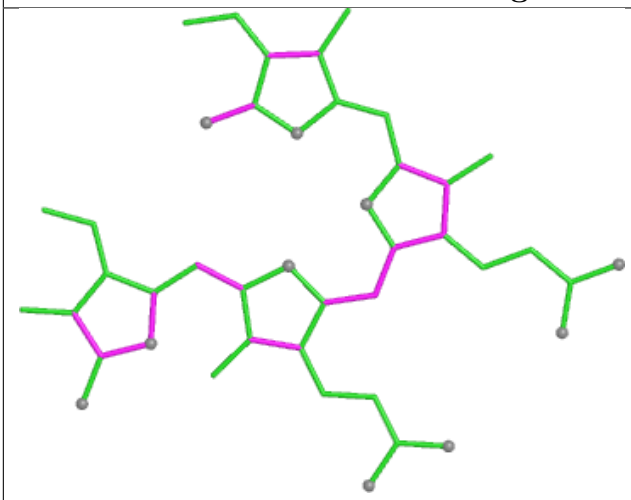


Rings

Ligand PEB YO 202



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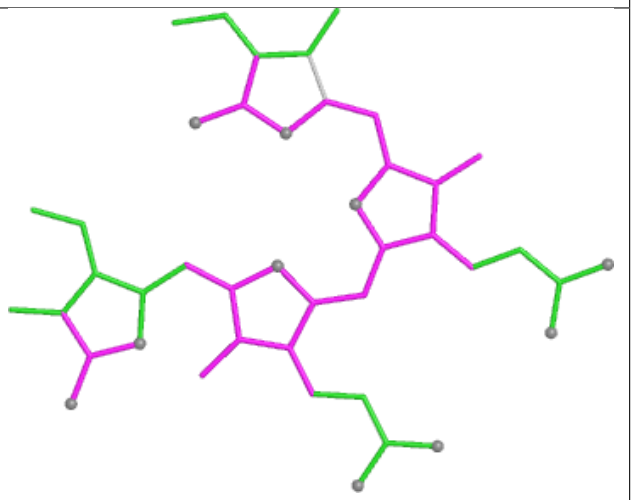

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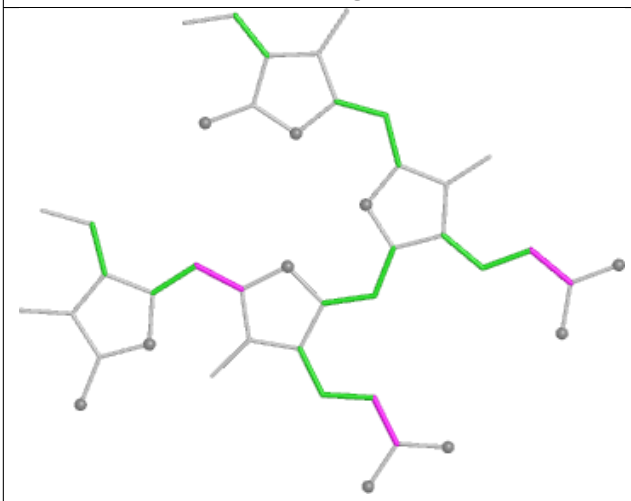

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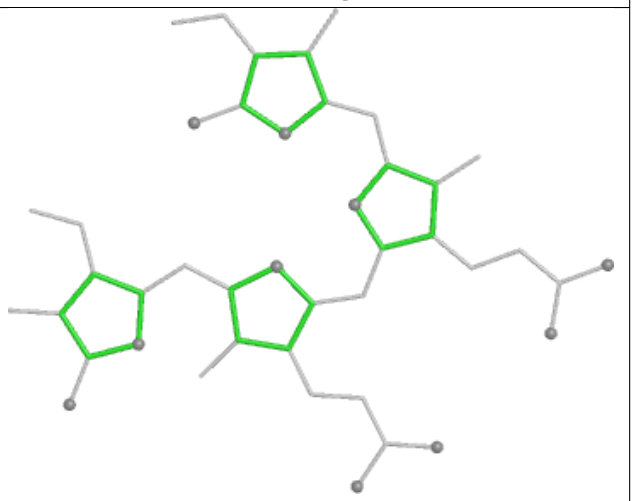
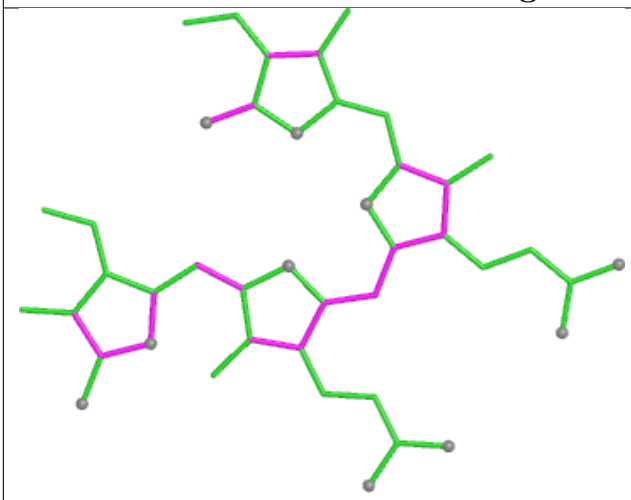


Rings

Ligand PEB q8 202



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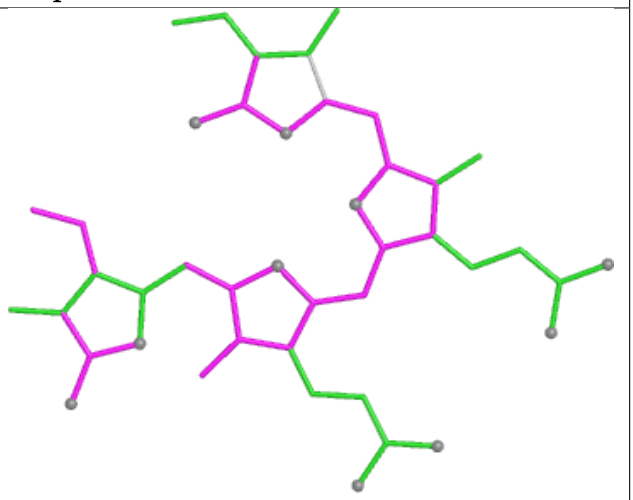

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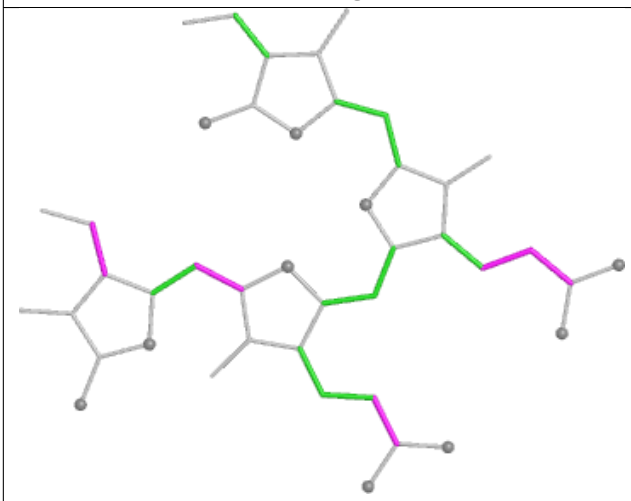

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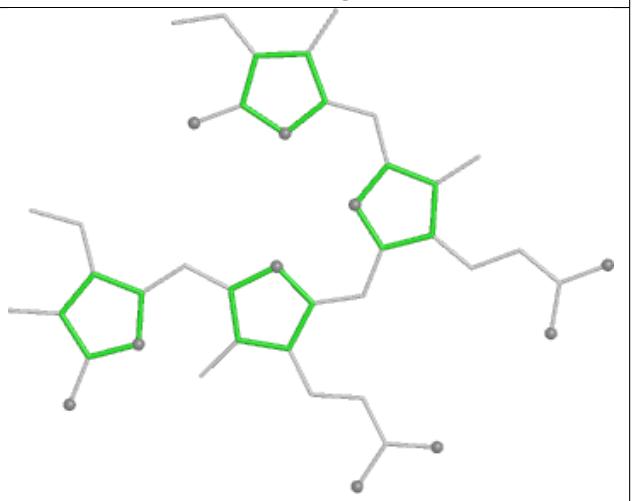

Rings

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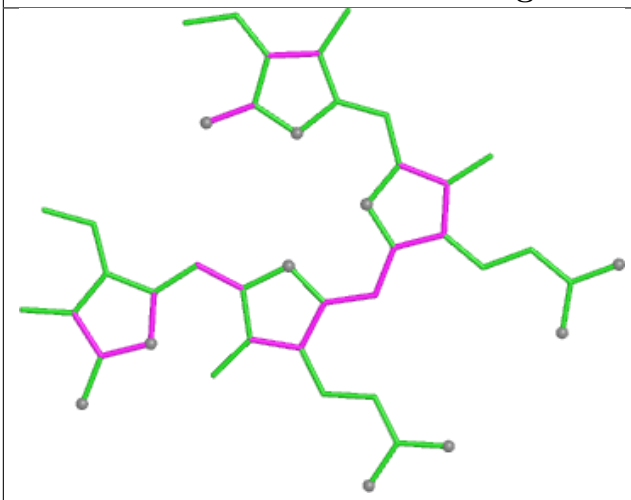

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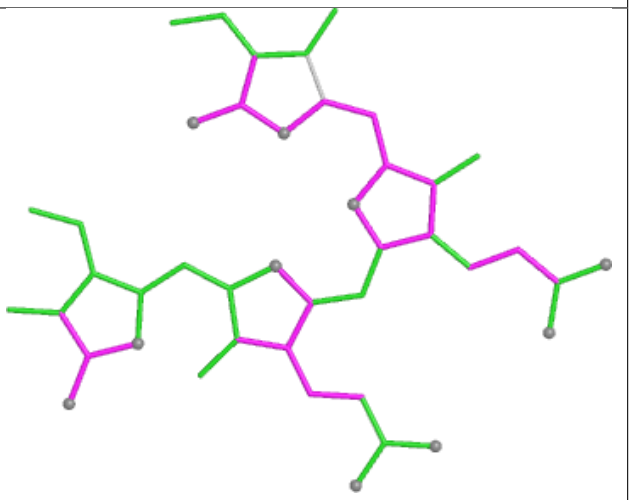

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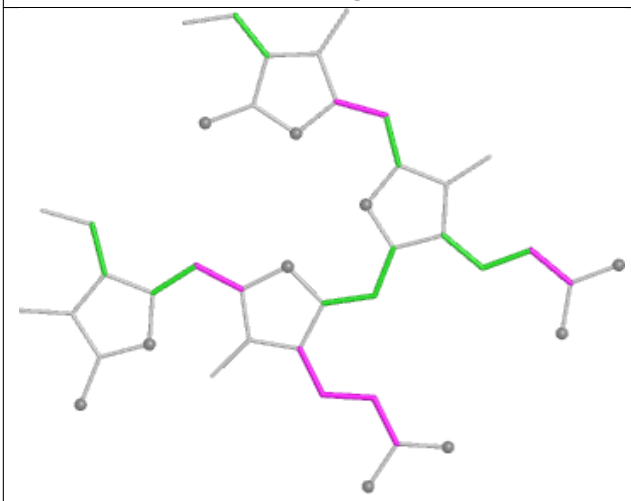

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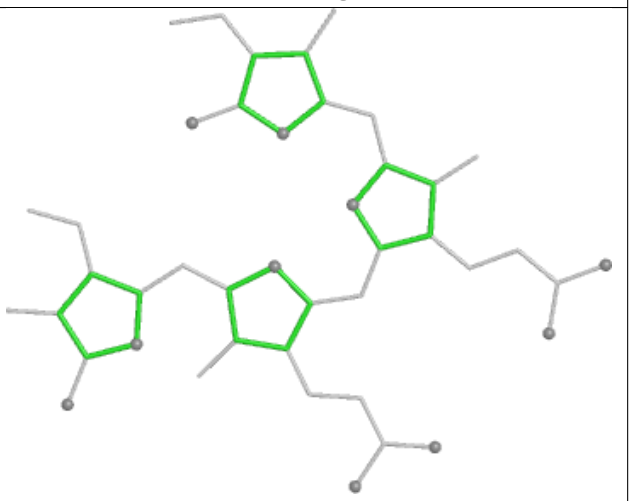
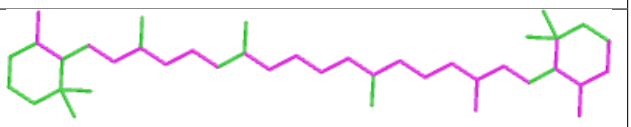


Rings

Ligand BCR J2 102



Bond lengths



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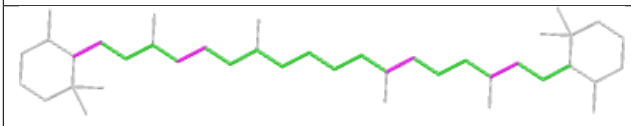

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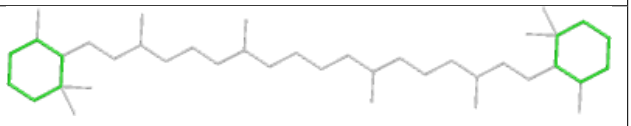
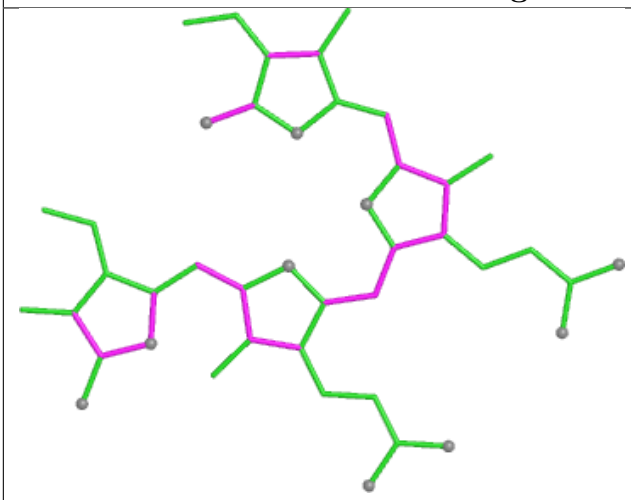


Rings

Ligand PEB HQ 202



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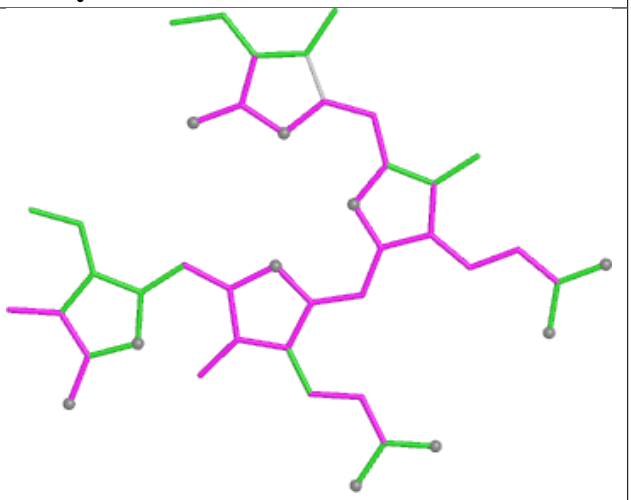

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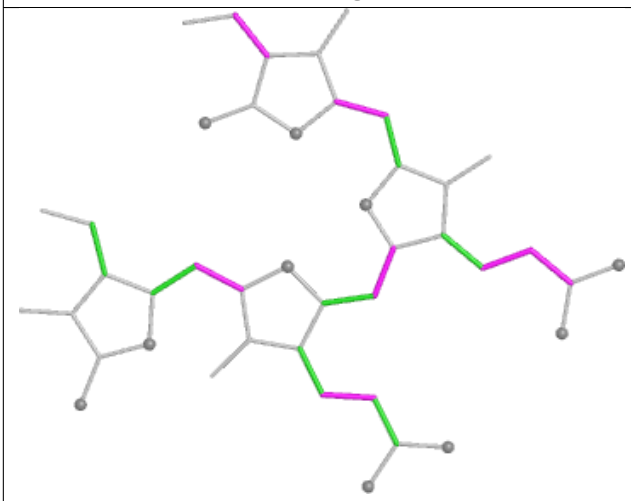

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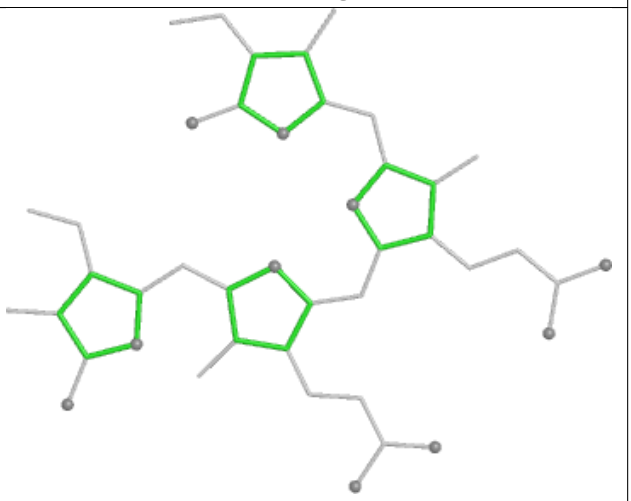
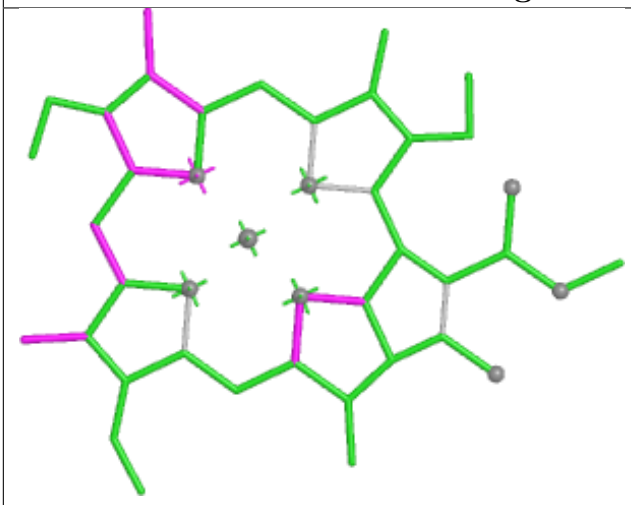


Rings

Ligand CLA 6N 610



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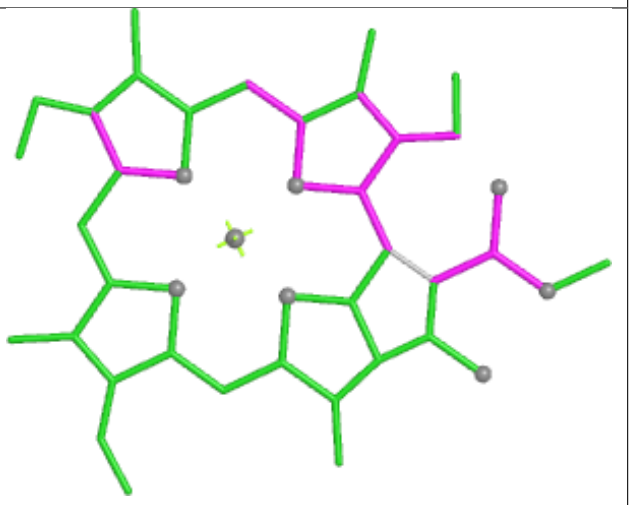

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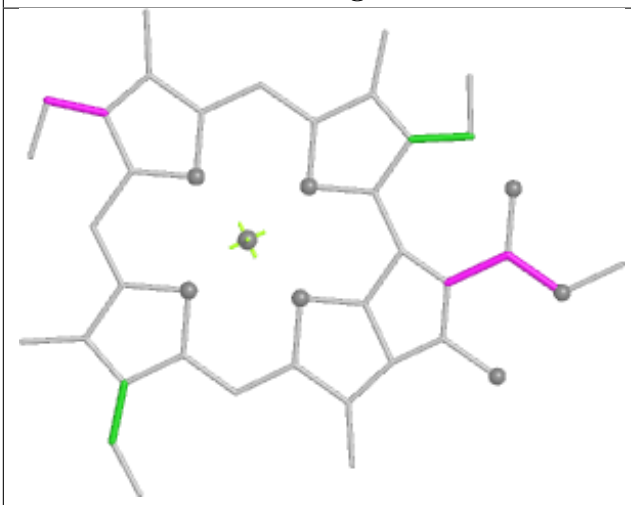
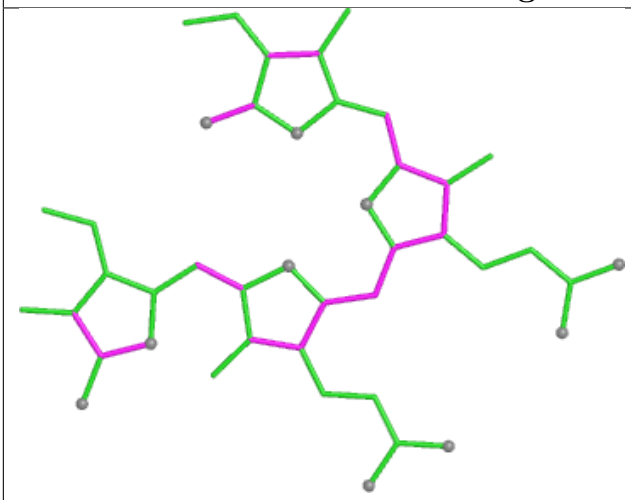


Torsions



Rings

Ligand PEB fG 203



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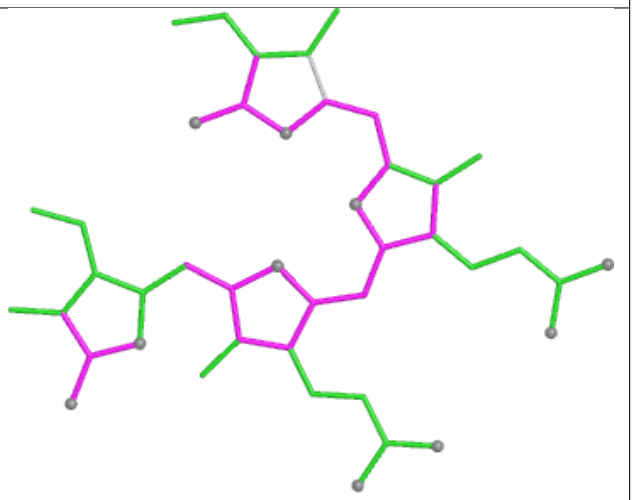

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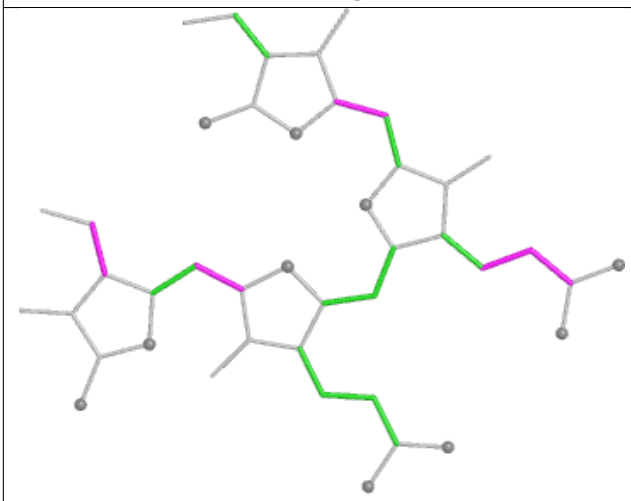

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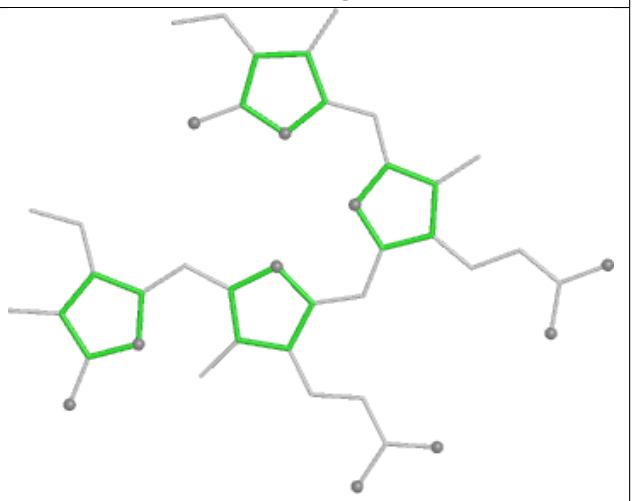
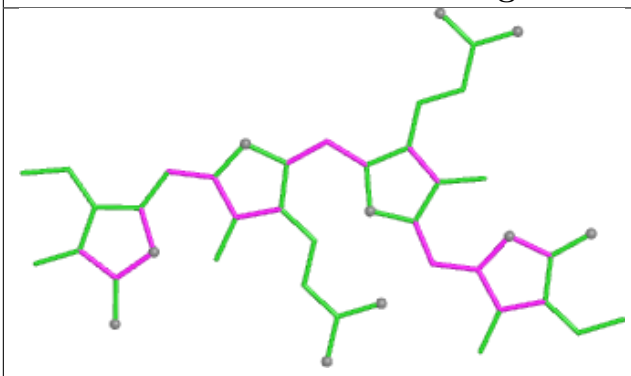


Rings

Ligand CYC HG 1001



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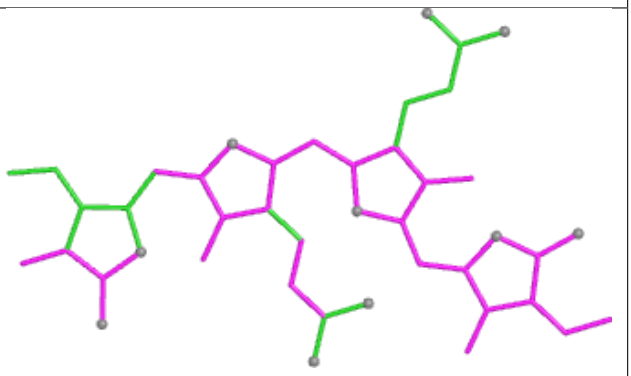

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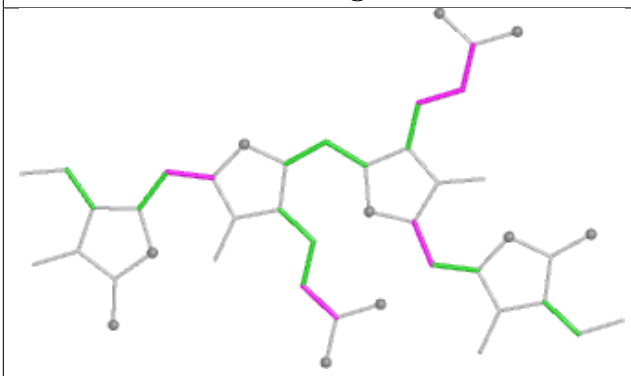

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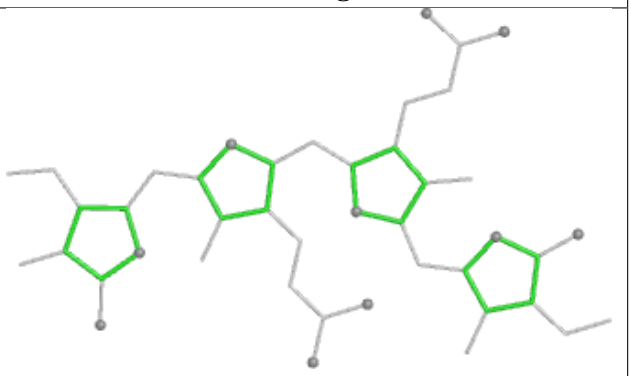
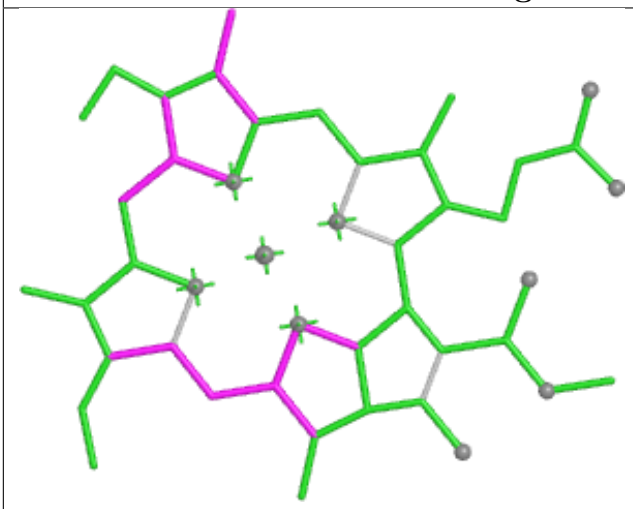


Rings

Ligand CLA A2 852



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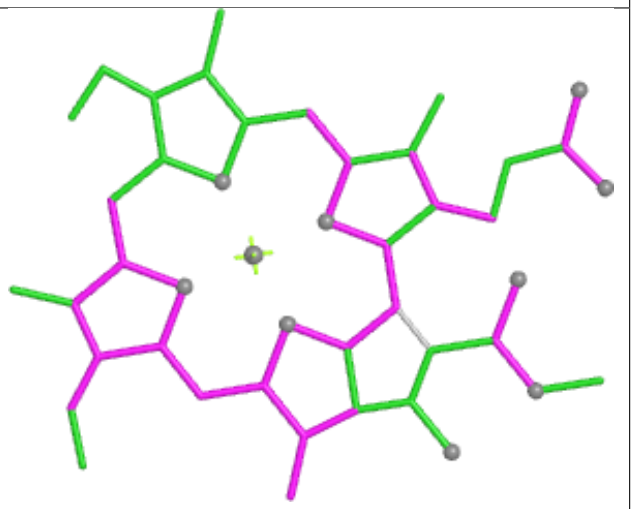

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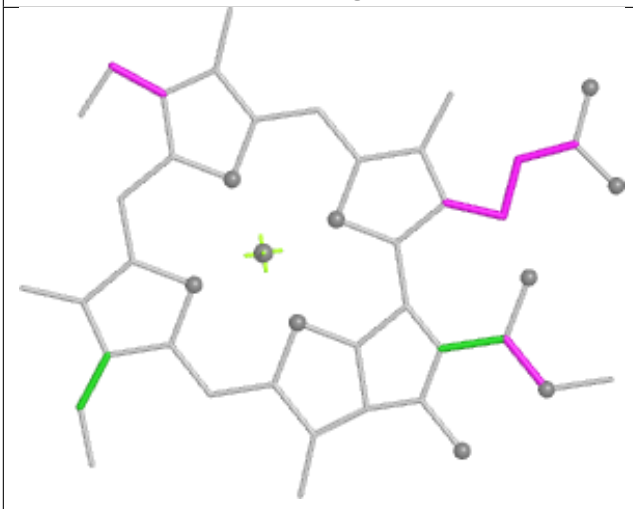
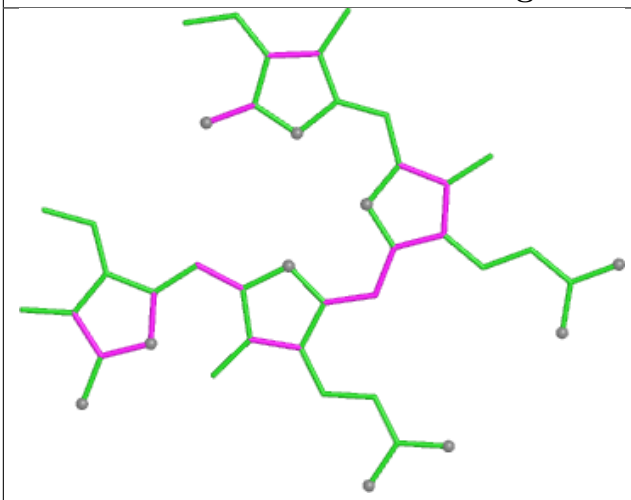


Torsions



Rings

Ligand PEB PJ 202



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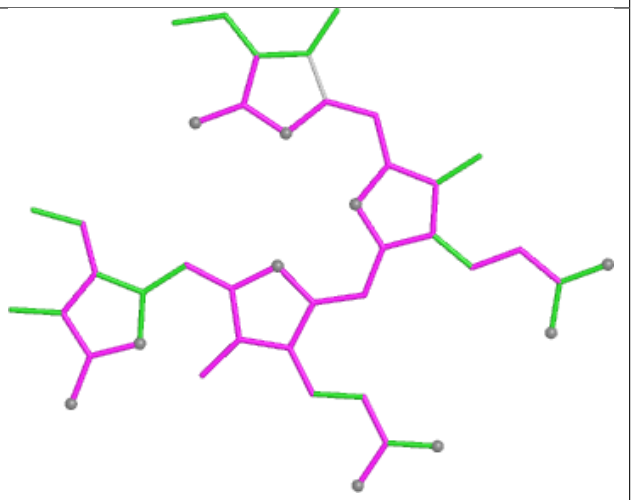

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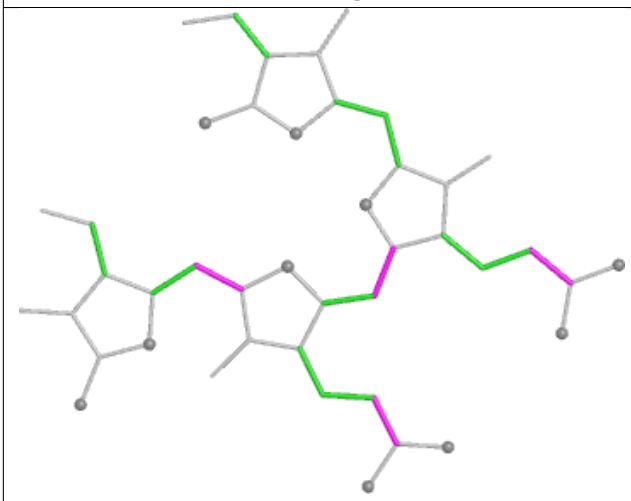

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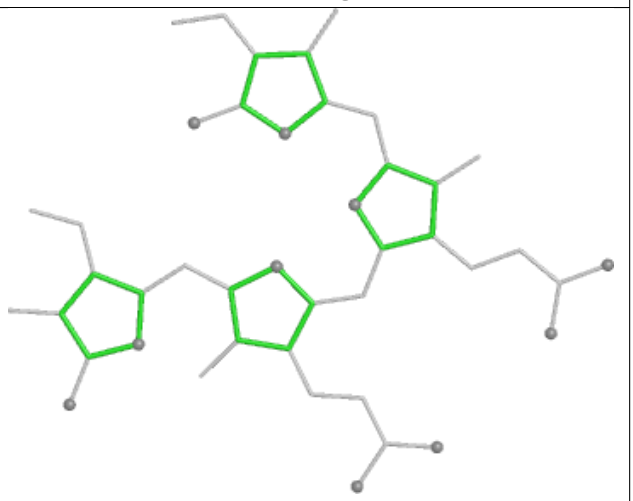
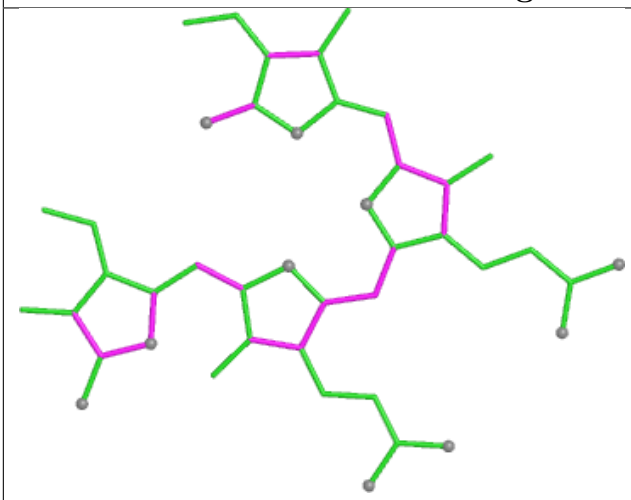


Rings

Ligand PEB B5 202



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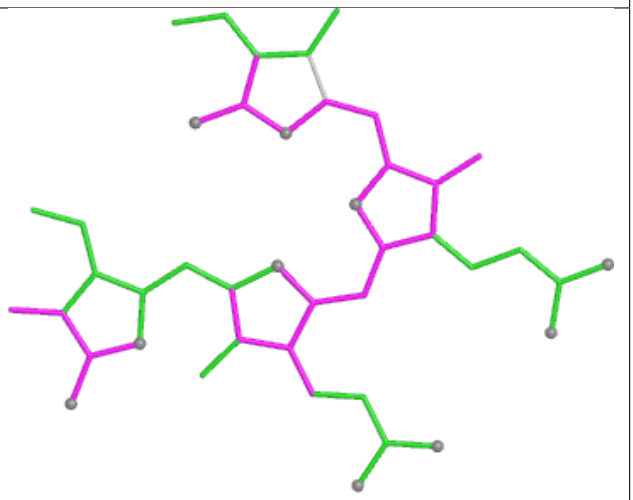

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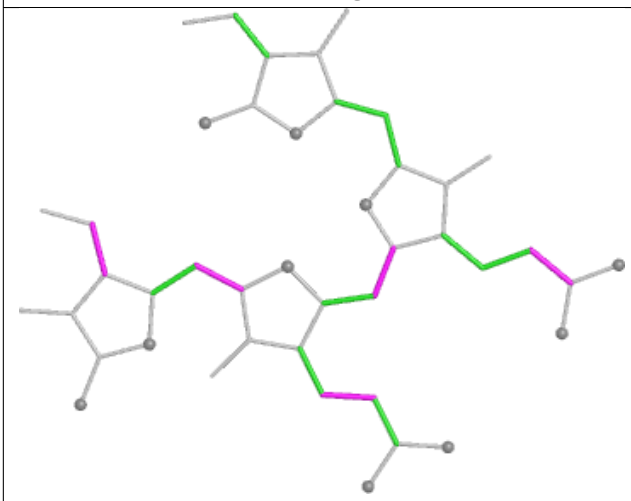

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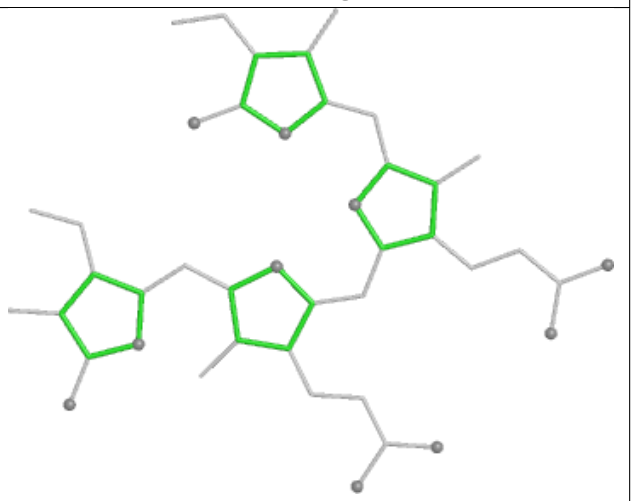
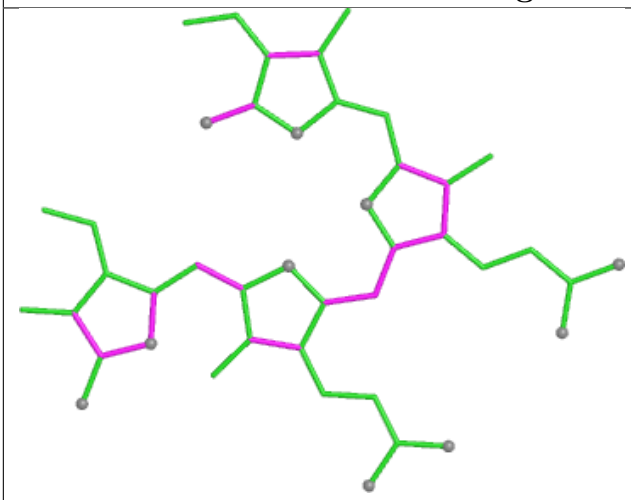


Rings

Ligand PEB gB 202



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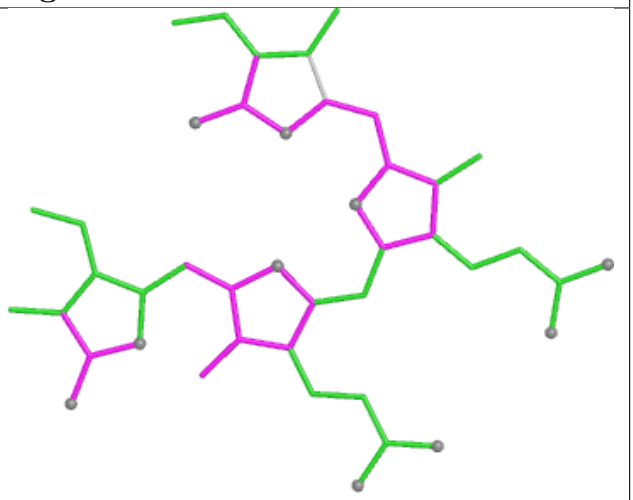

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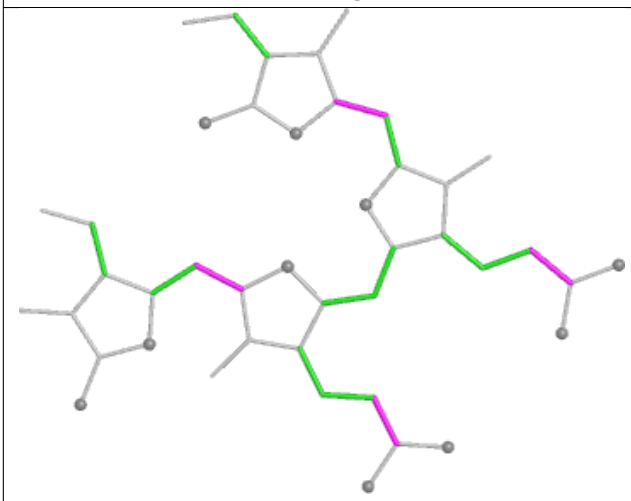

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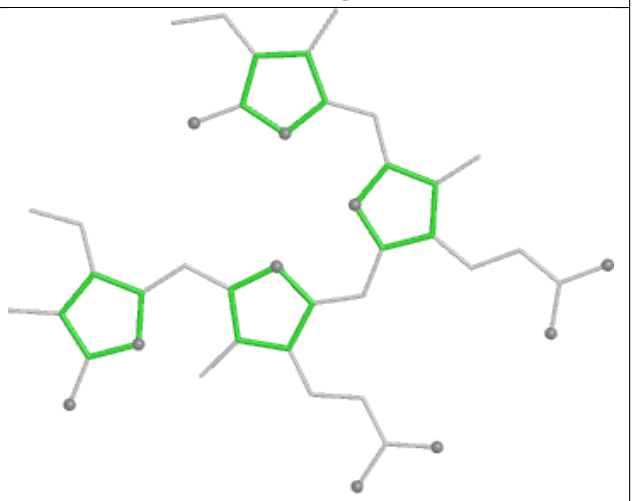
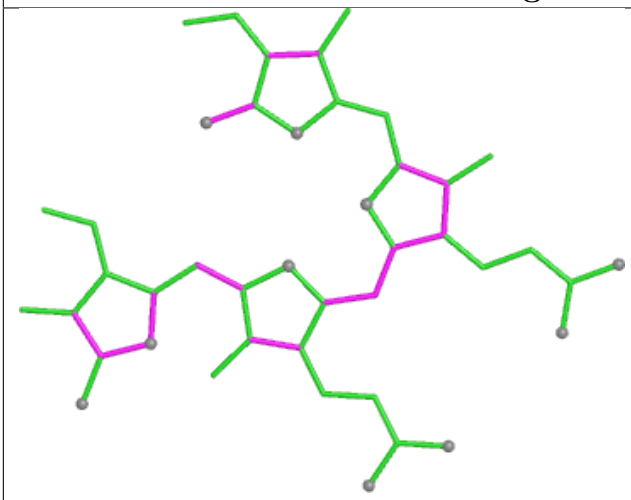


Rings

Ligand PEB iJ 202



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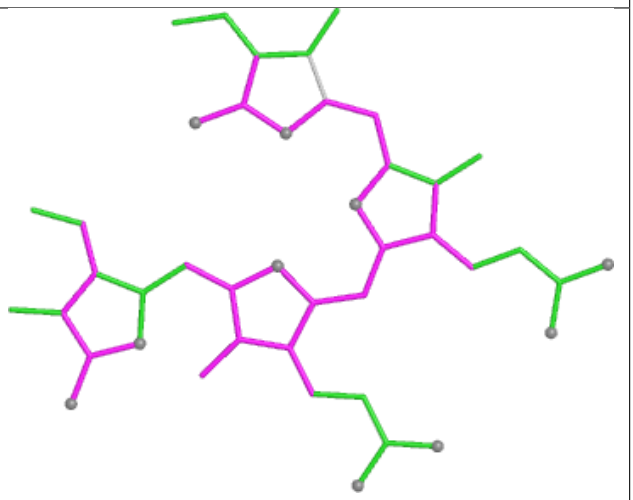

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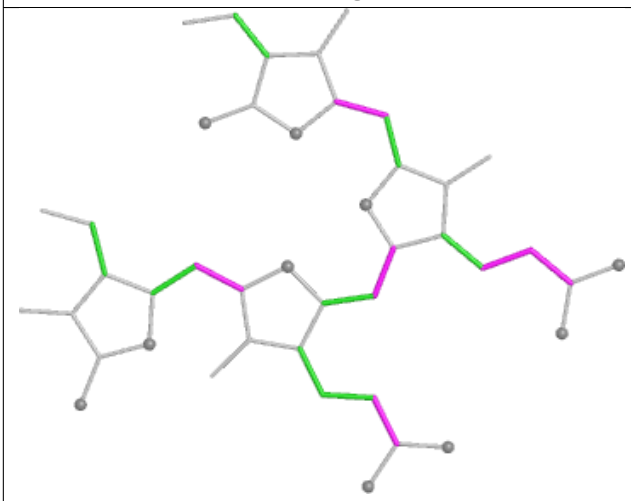

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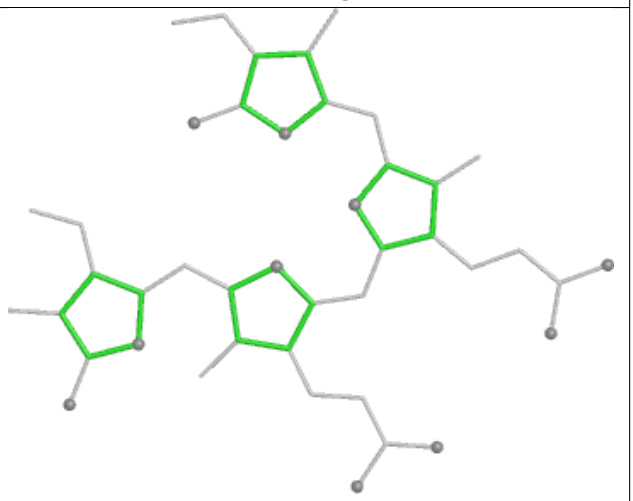
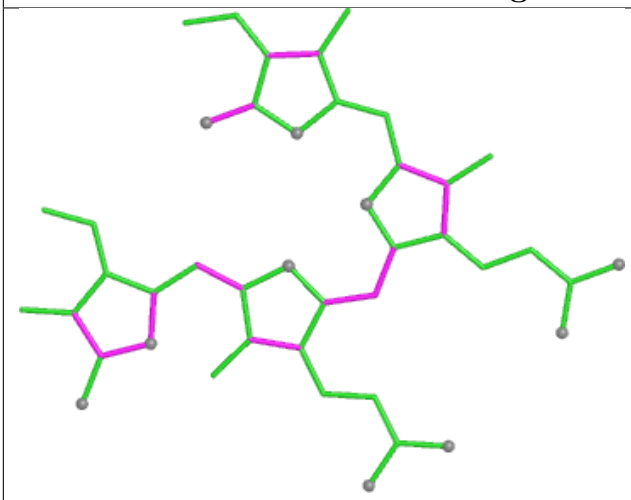


Rings

Ligand PEB WJ 203



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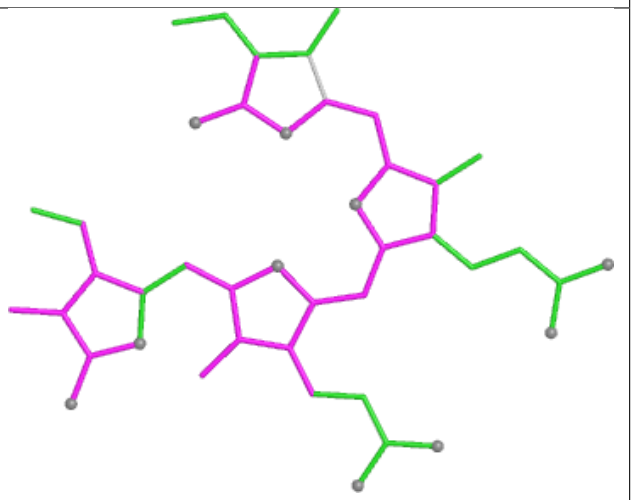
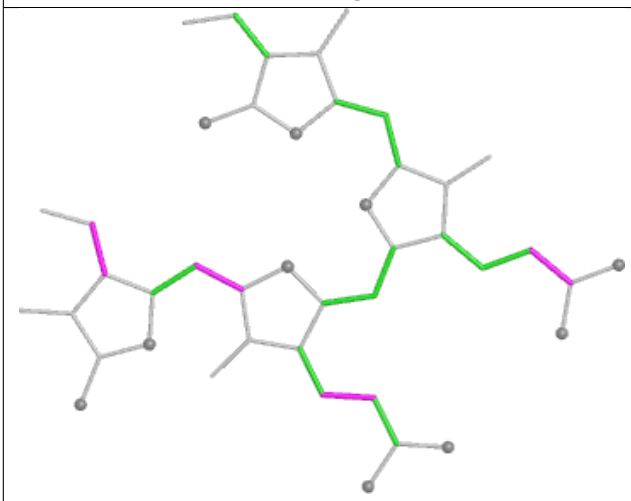
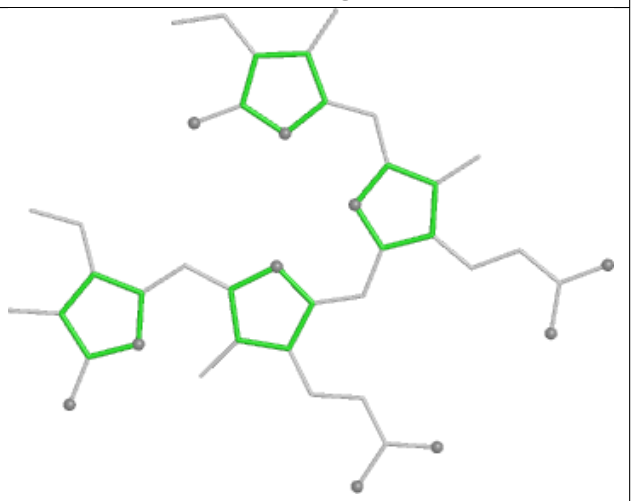


Bond angles

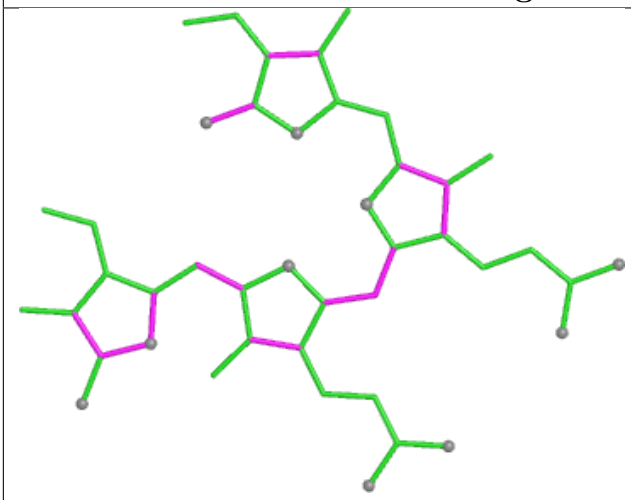


Torsions



Rings

Ligand PEB eG 202



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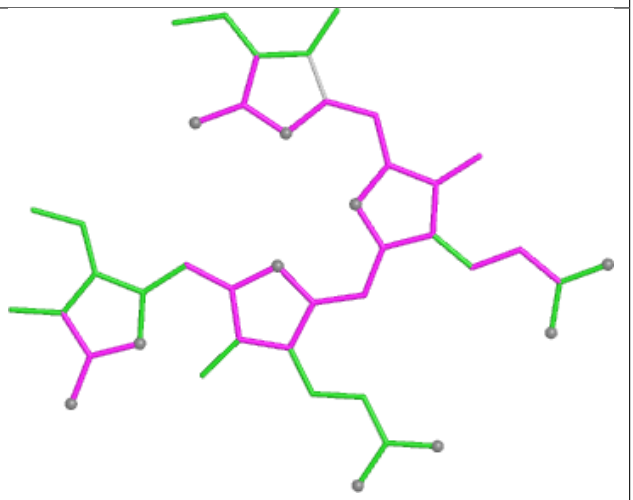

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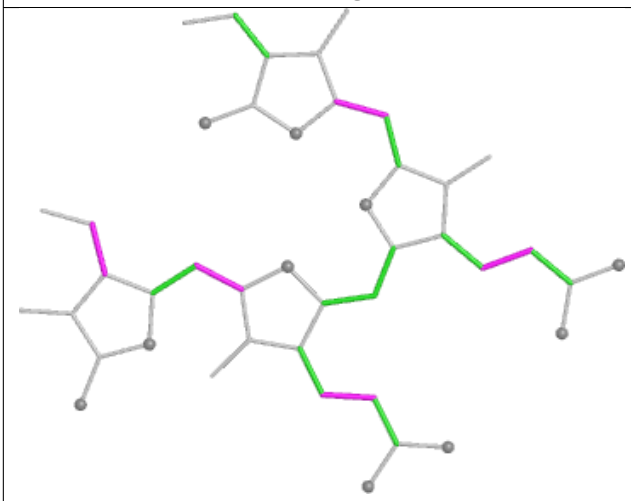

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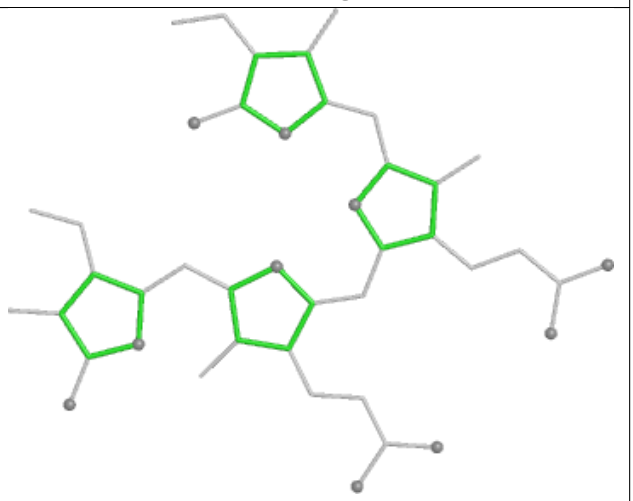
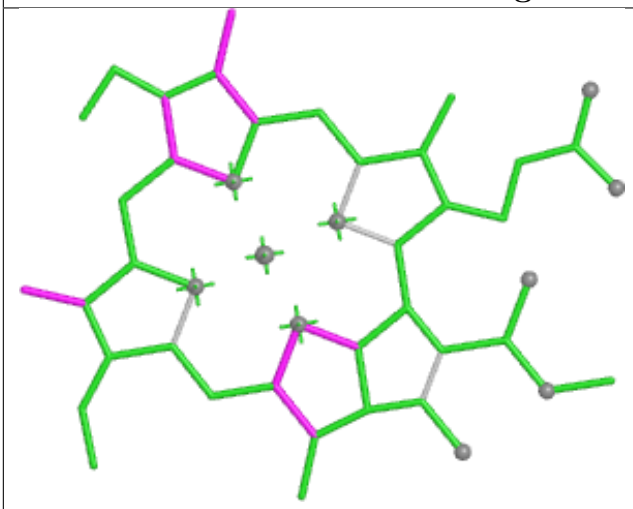


Rings

Ligand CLA 3N 303



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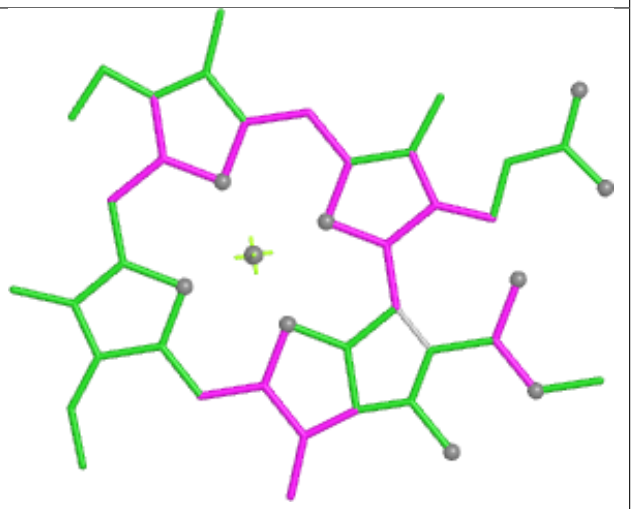

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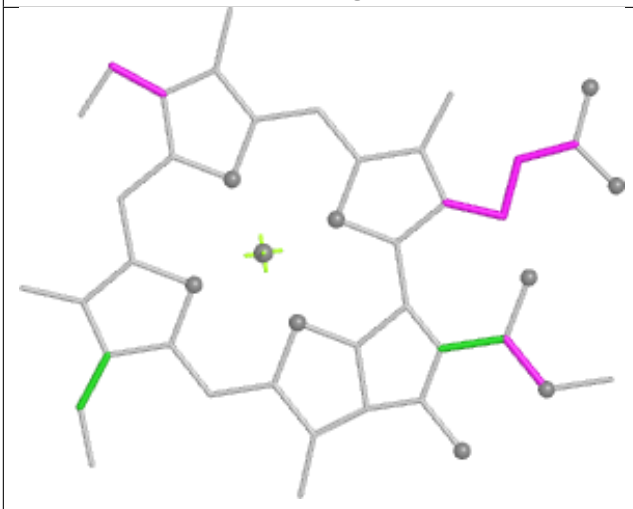
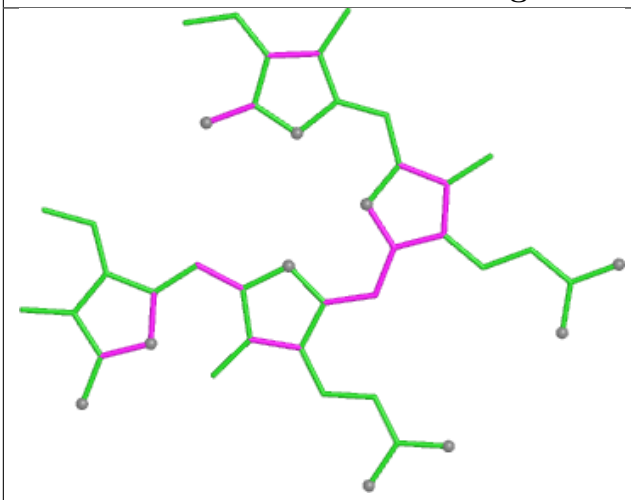


Torsions



Rings

Ligand PEB AH 305



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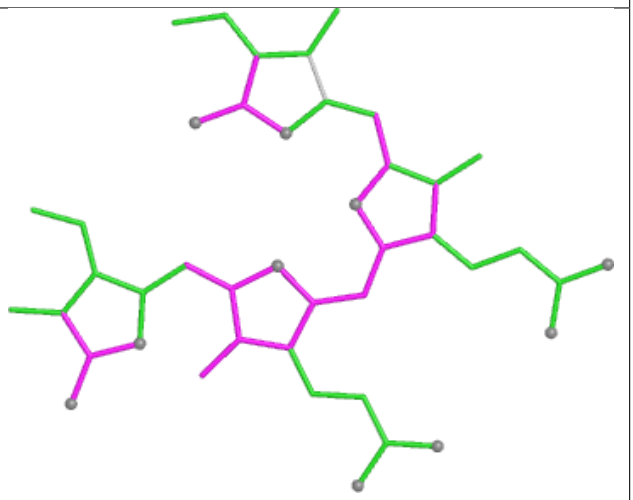

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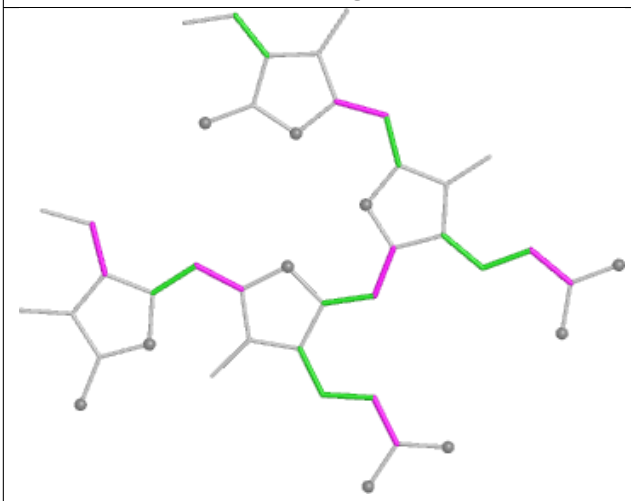

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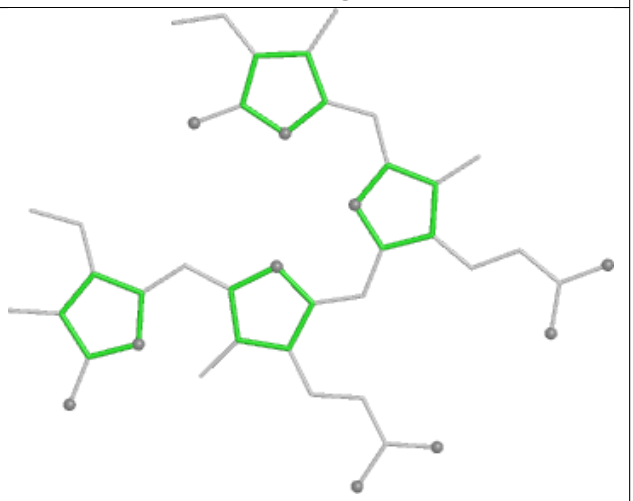
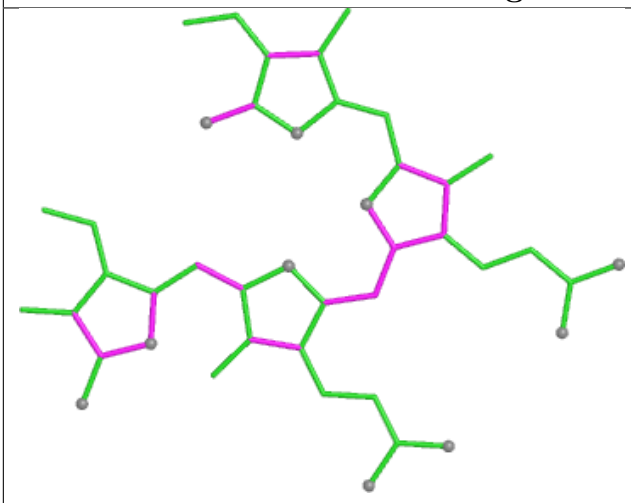


Rings

Ligand PEB H4 1002



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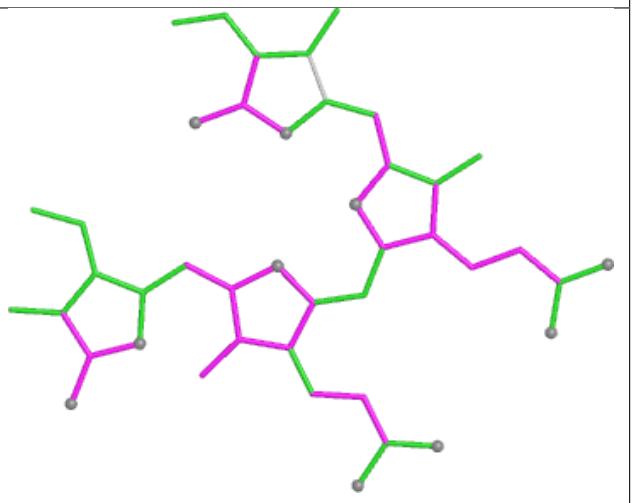

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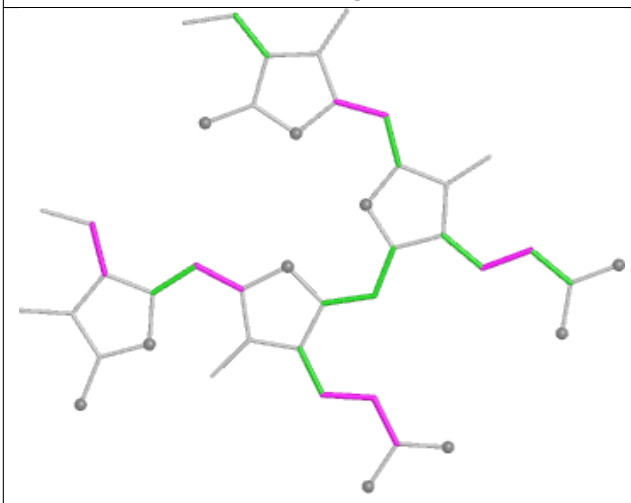

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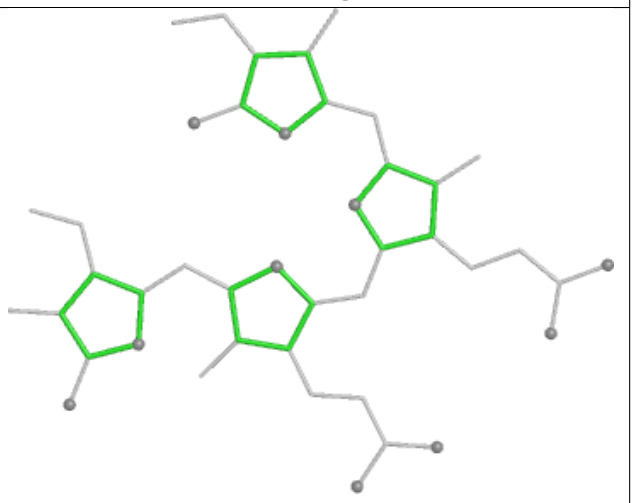
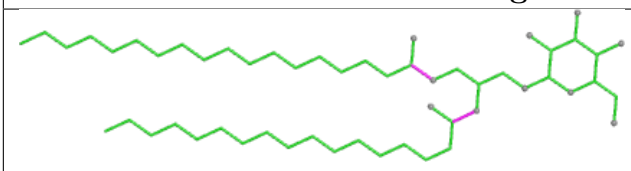


Rings

Ligand LMG D6 409



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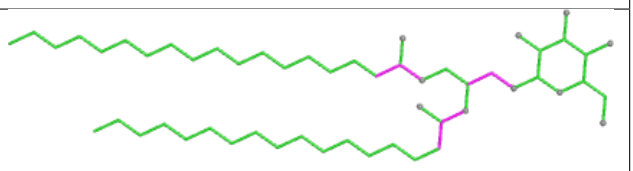
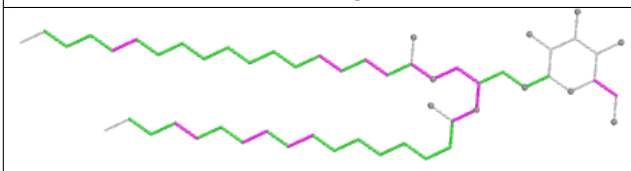


Bond angles



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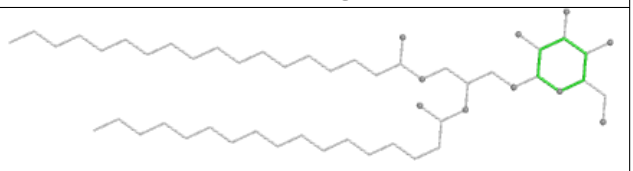
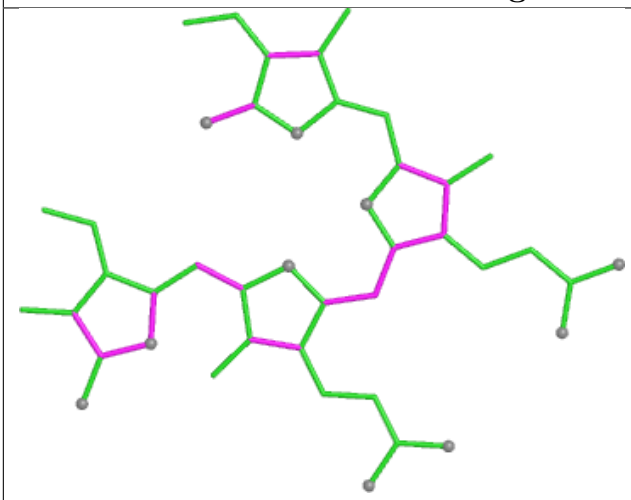


Rings

Ligand PEB mK 202



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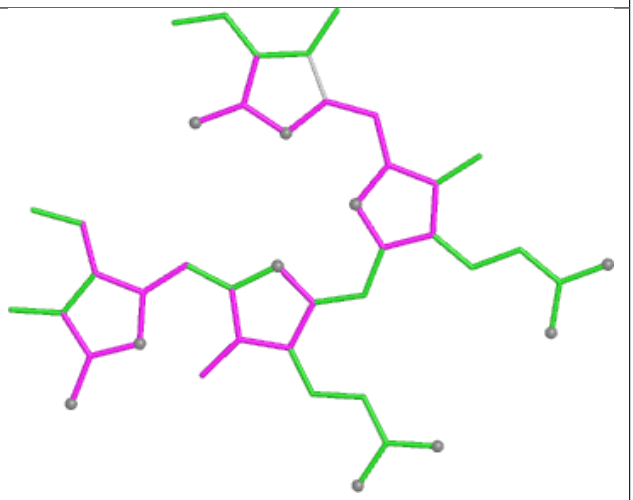
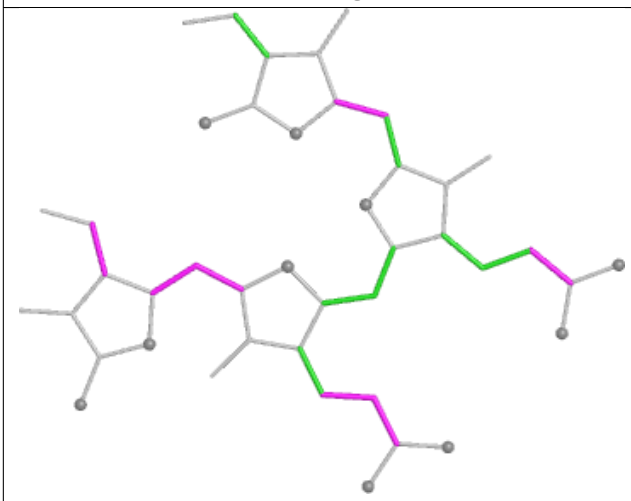


Bond angles



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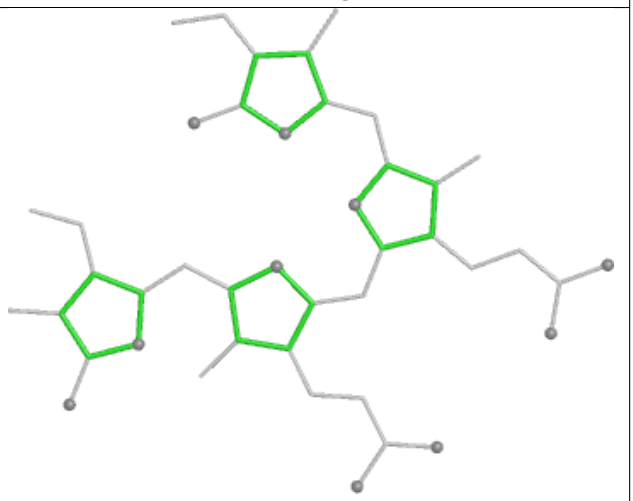
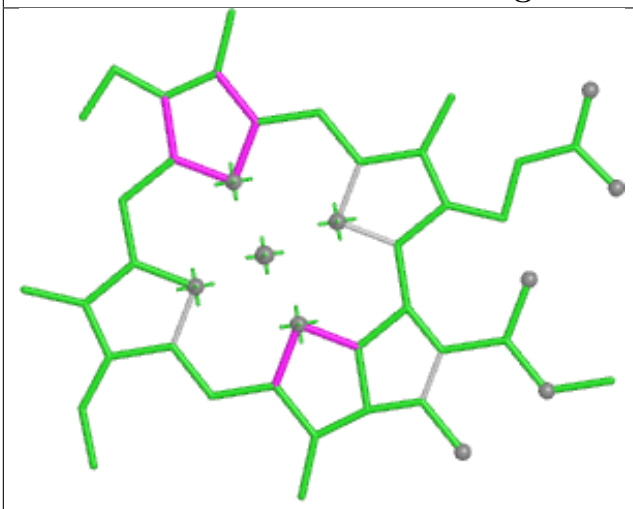


Rings

Ligand CLA 3N 304



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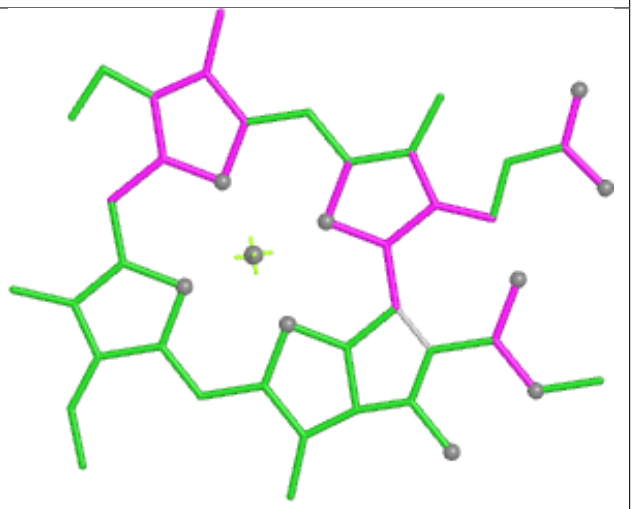
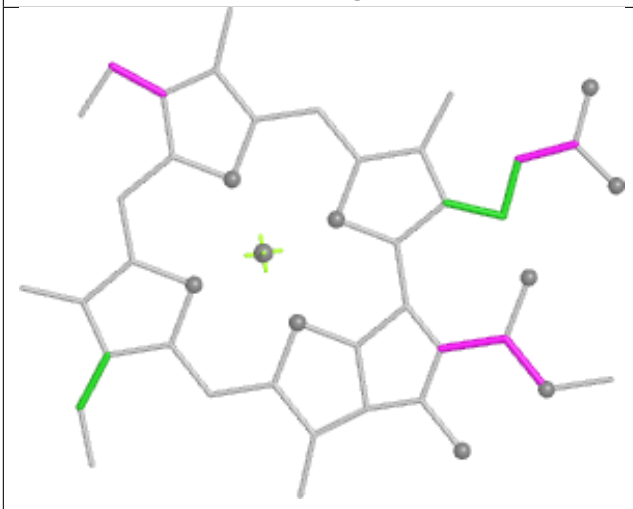


Bond angles

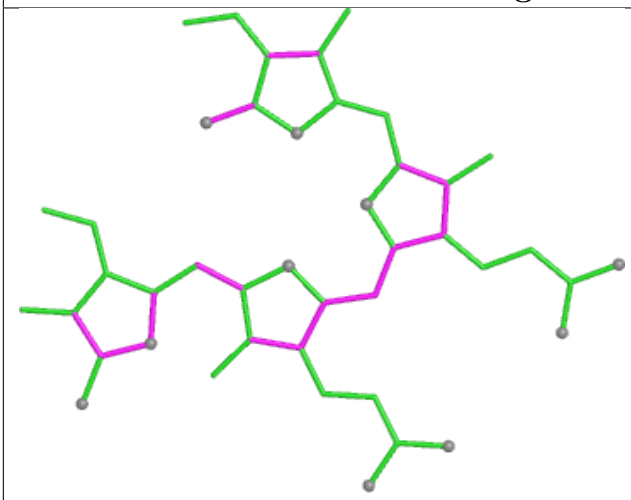


Torsions



Rings

Ligand PEB H7 203



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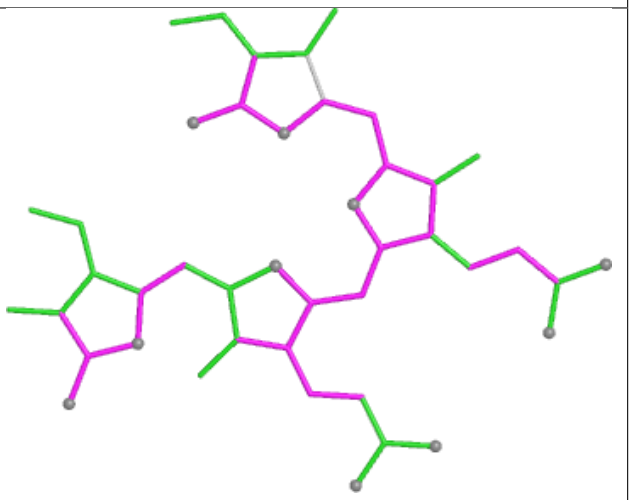

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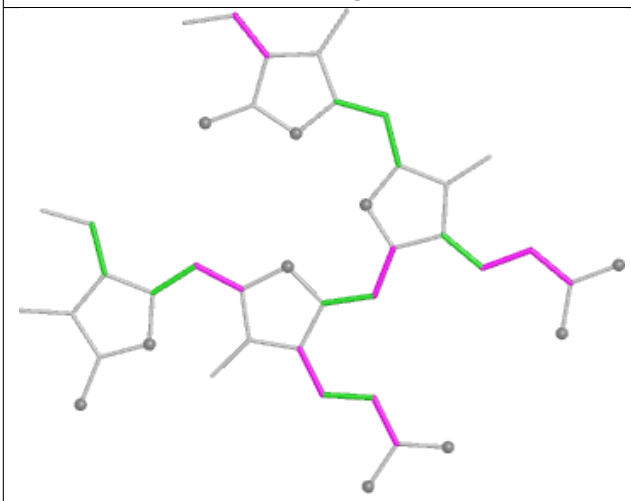

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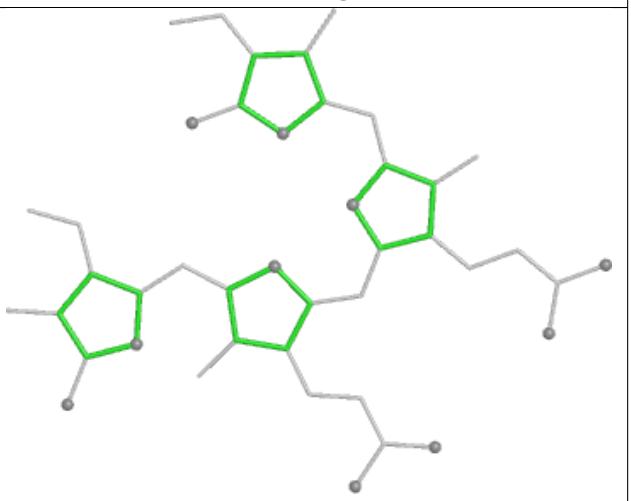
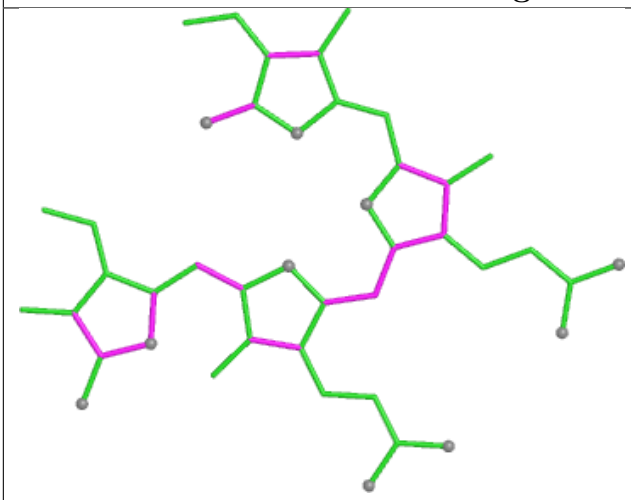


Rings

Ligand PEB TP 202



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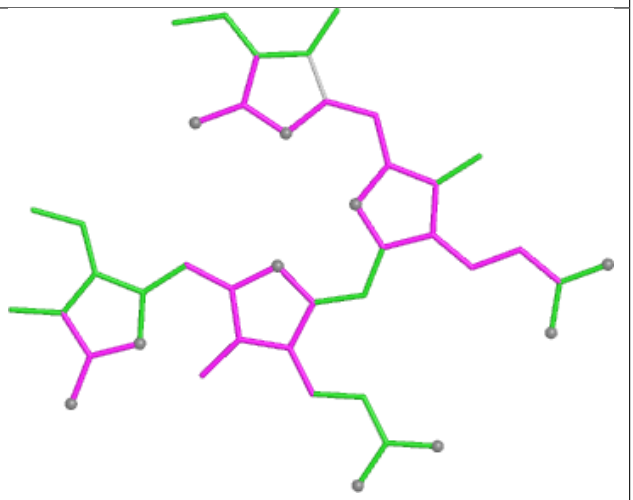
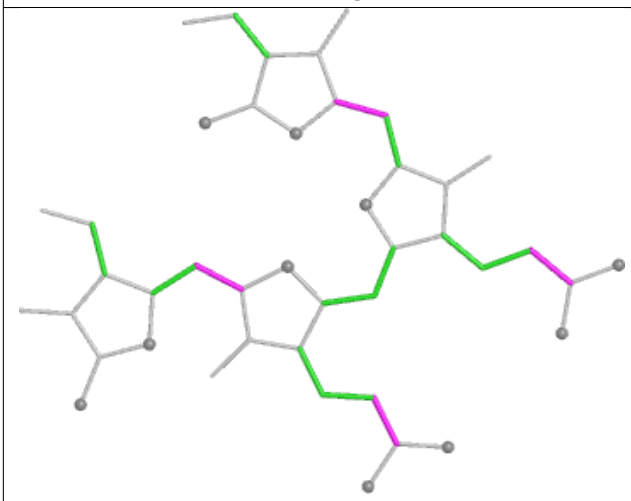


Bond angles



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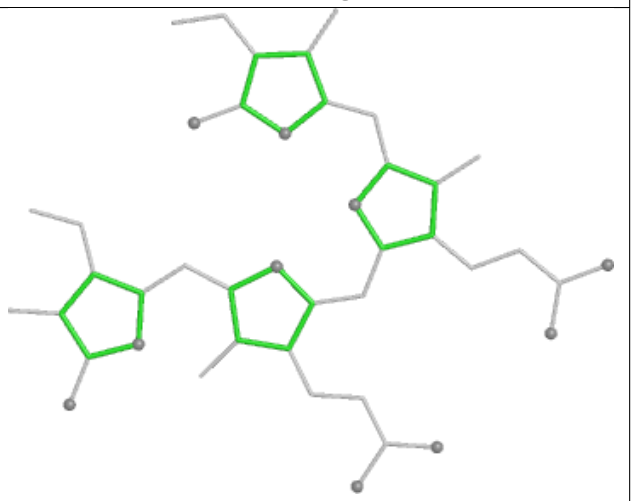
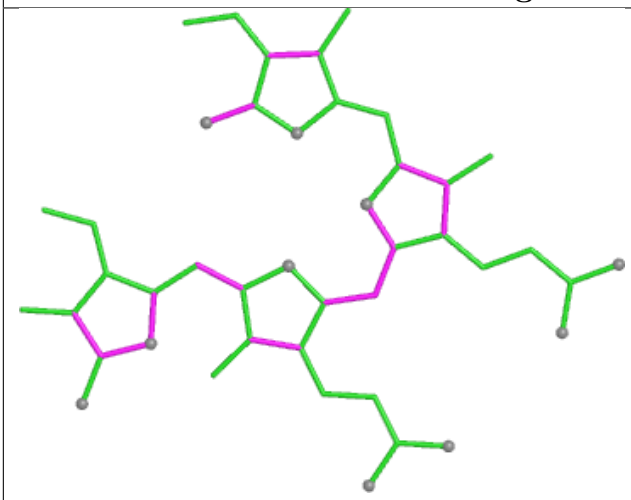


Rings

Ligand PEB O5 203



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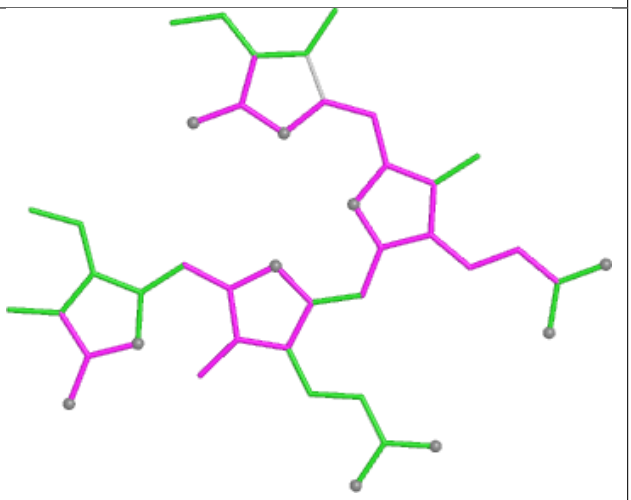
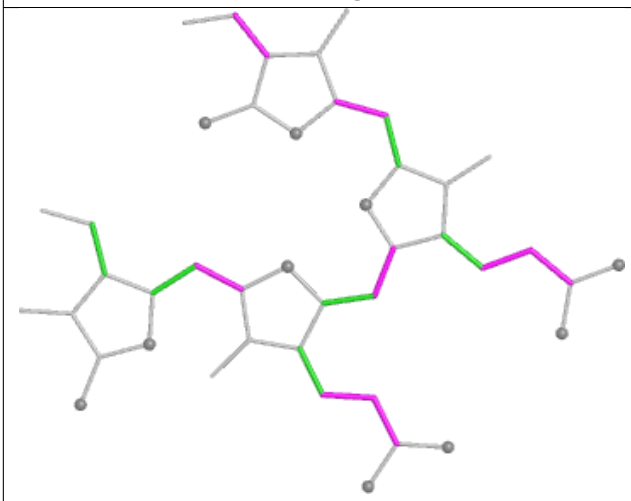


Bond angles



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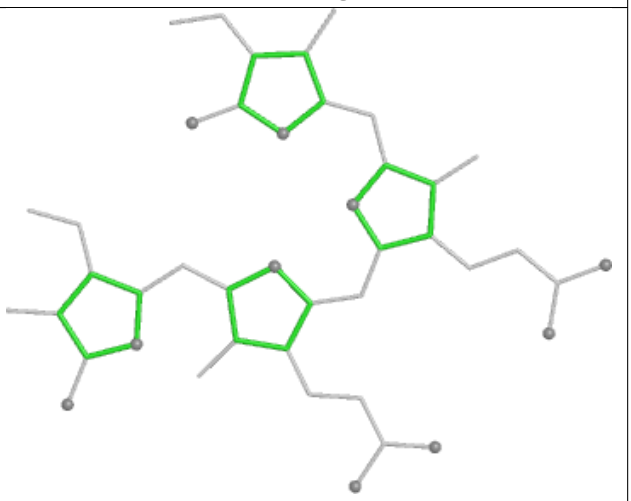
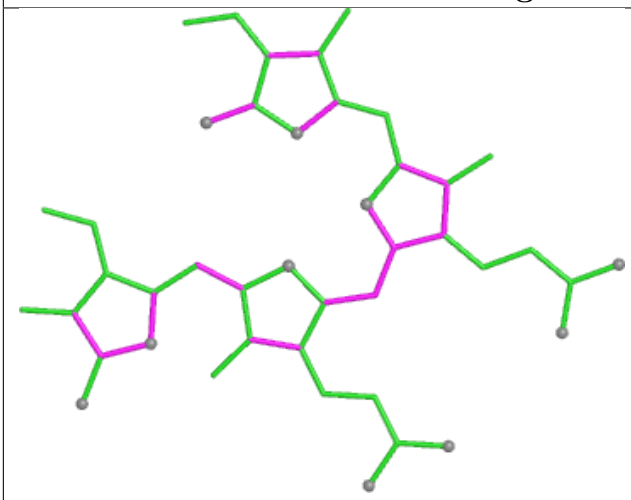


Rings

Ligand PEB hE 202



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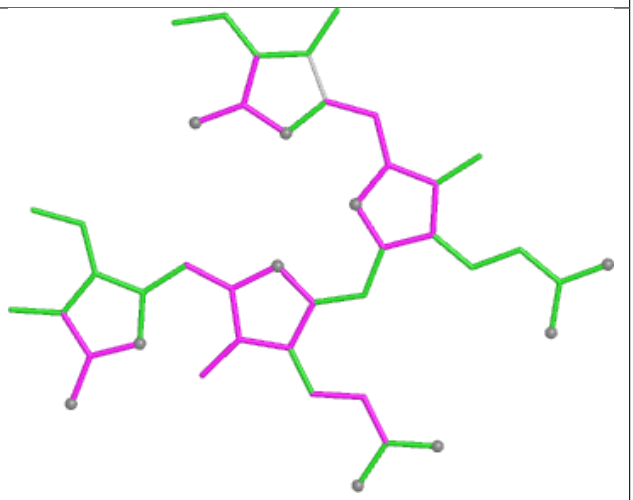
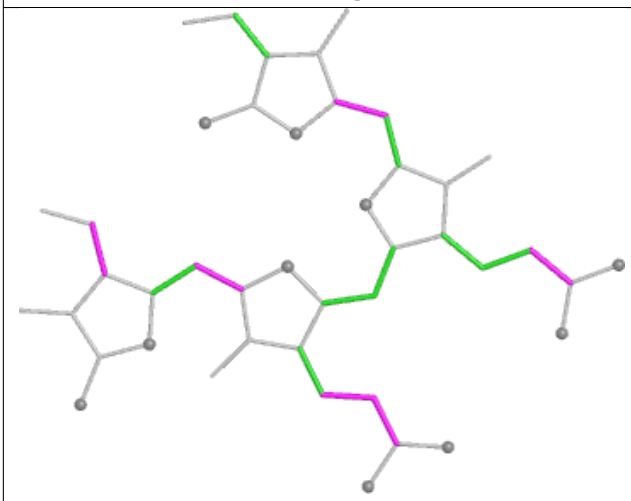


Bond angles



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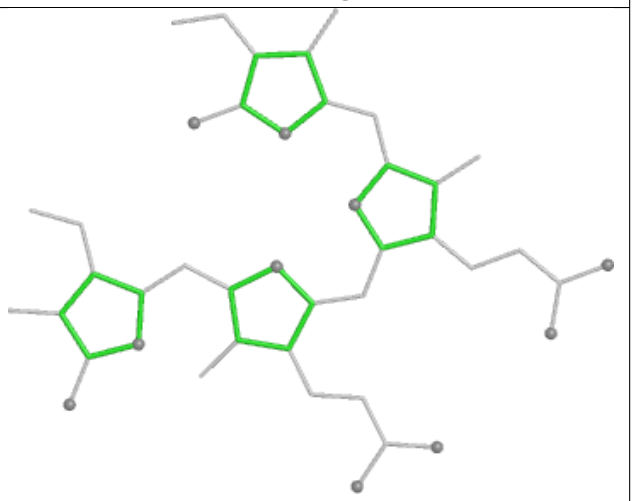
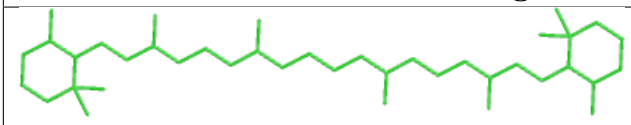


Rings

Ligand BCR JN 103



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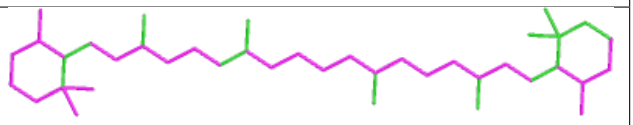
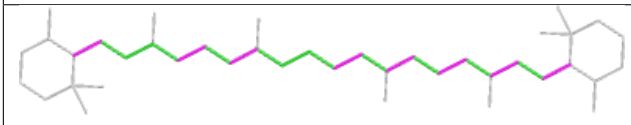


Bond angles



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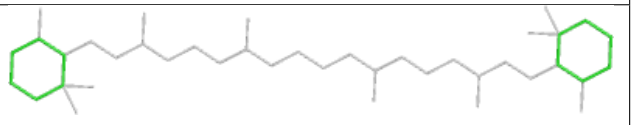
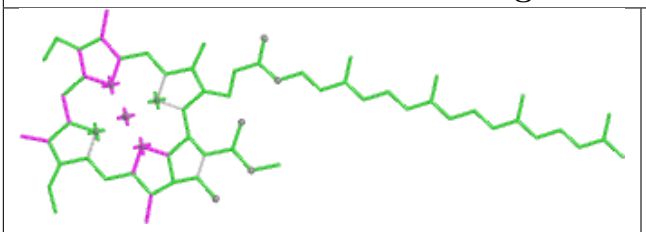


Rings

Ligand CLA A2 830



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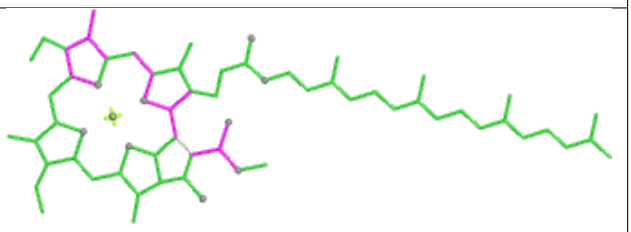
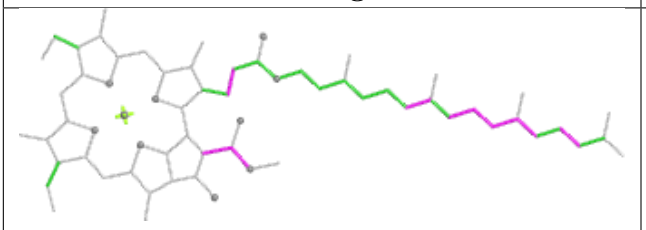


Bond angles



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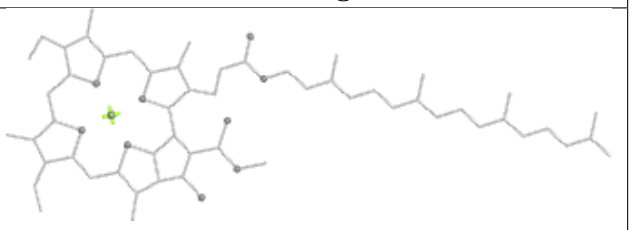
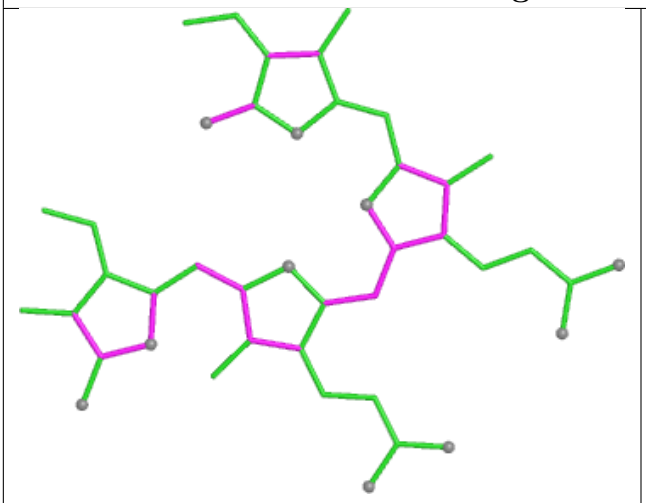


Rings

Ligand PEB CB 202



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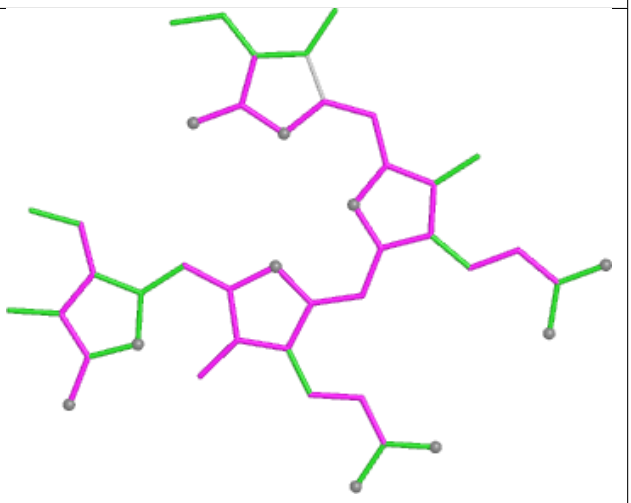
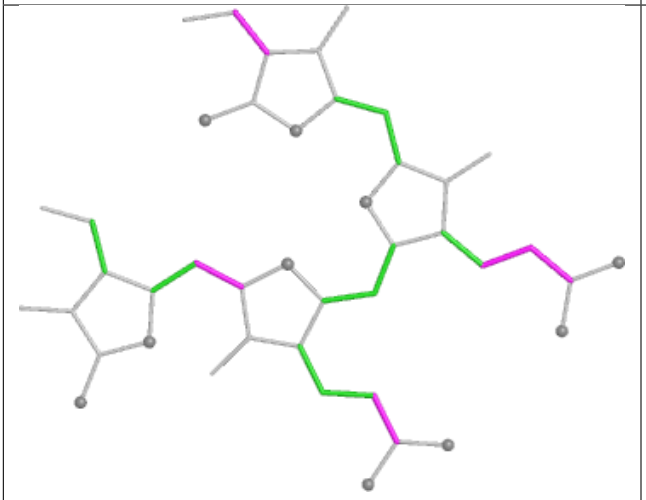


Bond angles



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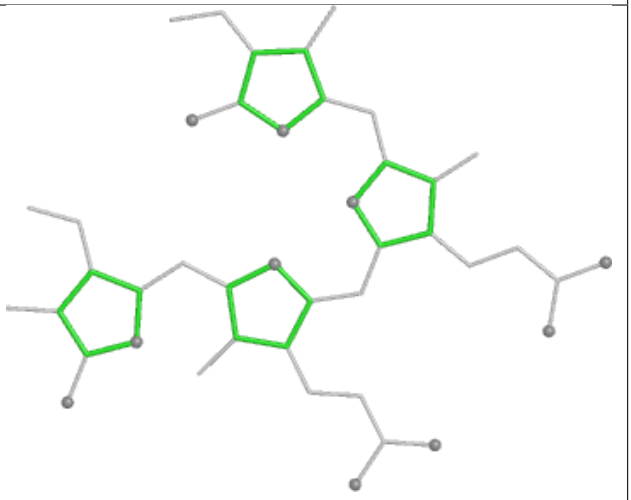
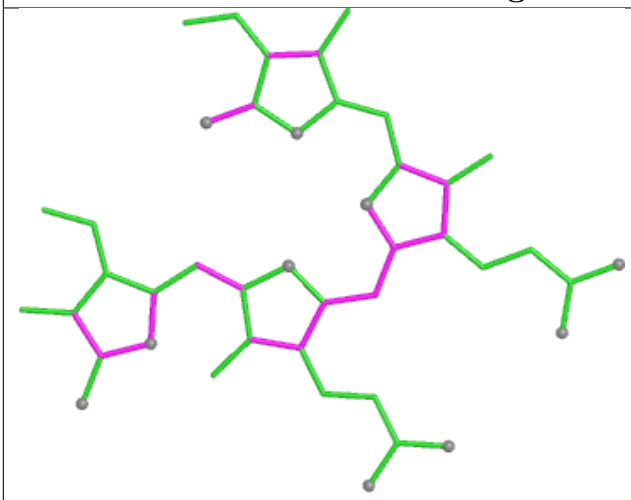


Rings

Ligand PEB CM 202



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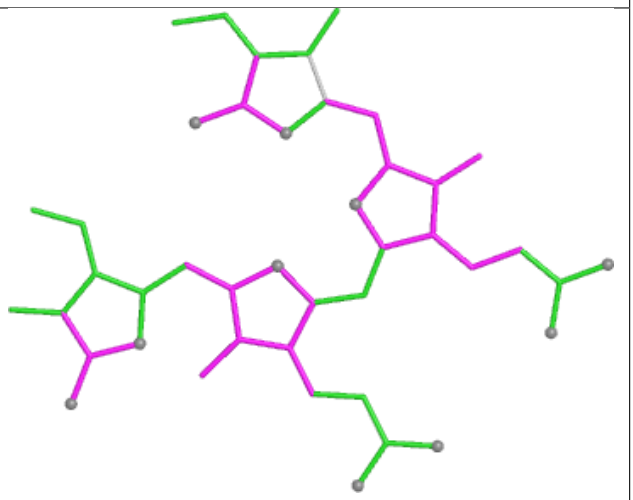
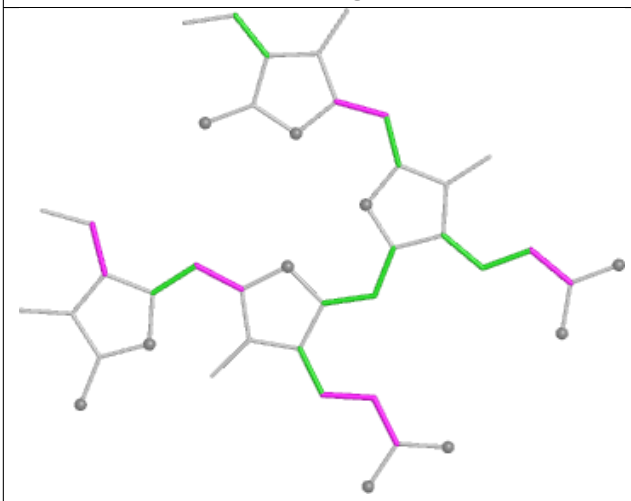
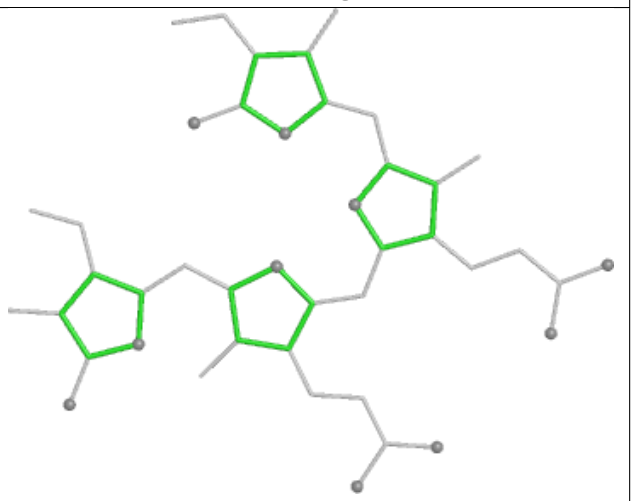


Bond angles

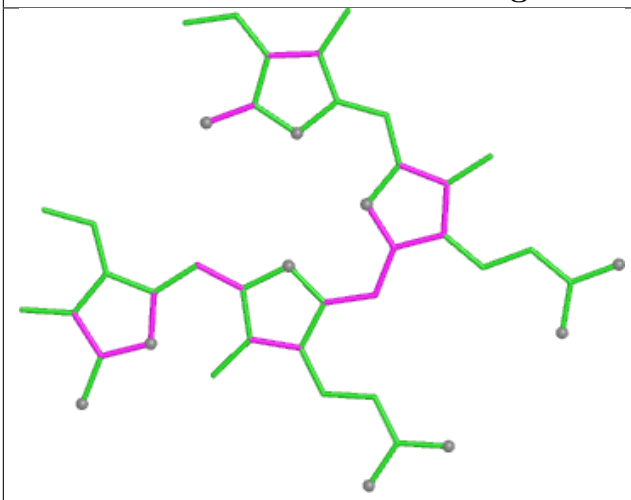


Torsions



Rings

Ligand PEB UA 202



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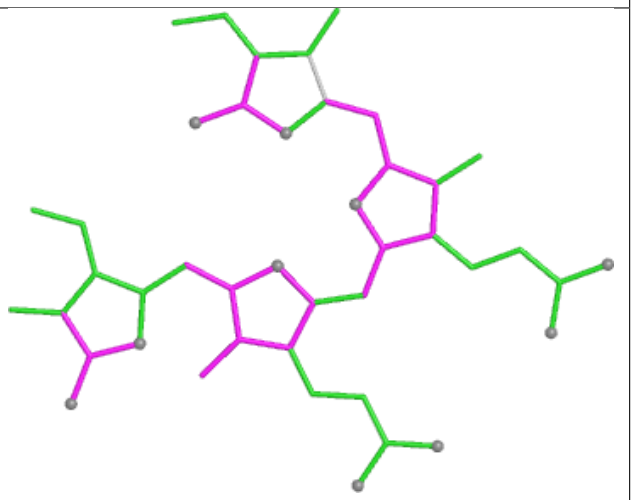

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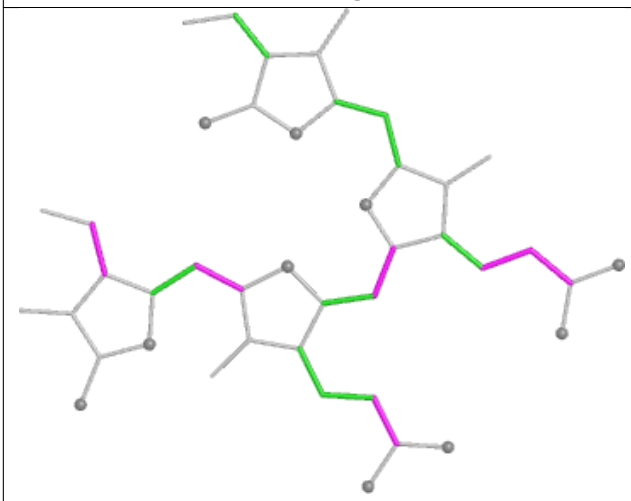

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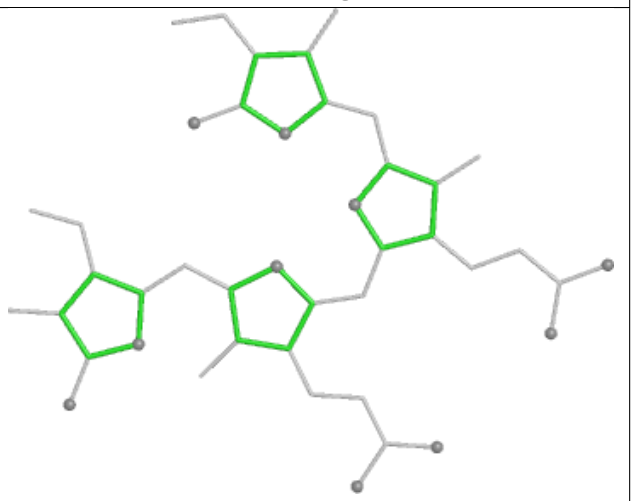
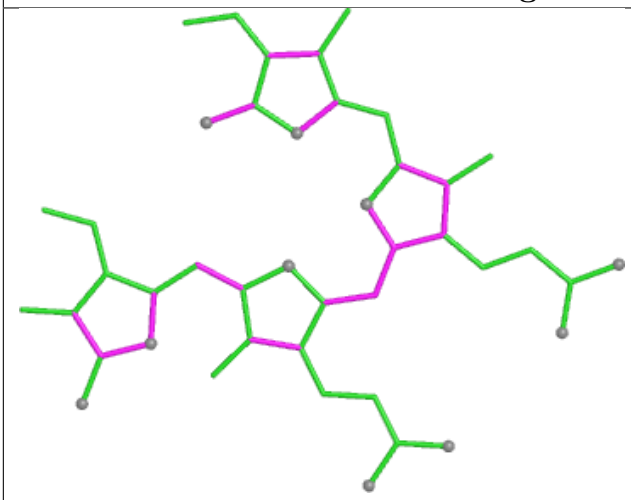


Rings

Ligand PEB gJ 201



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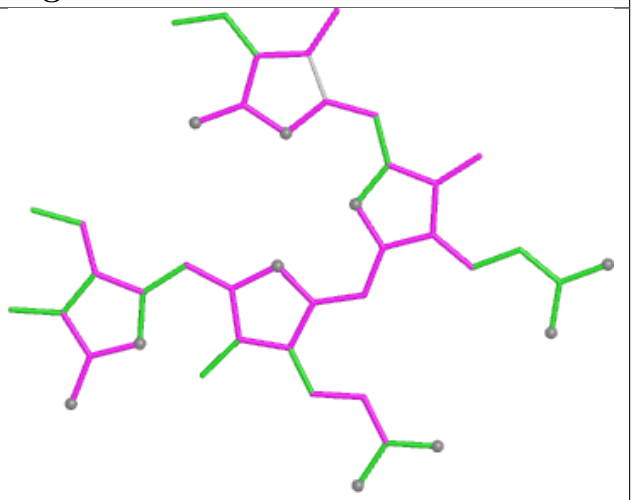

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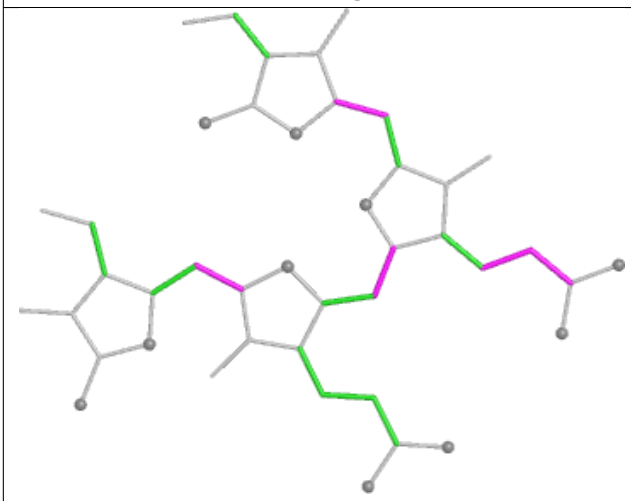

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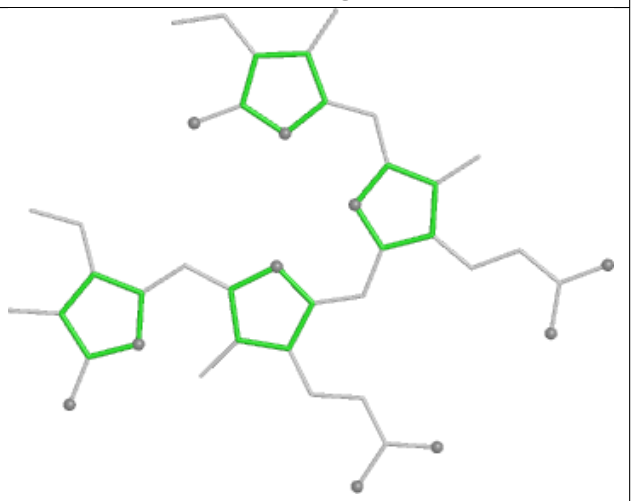
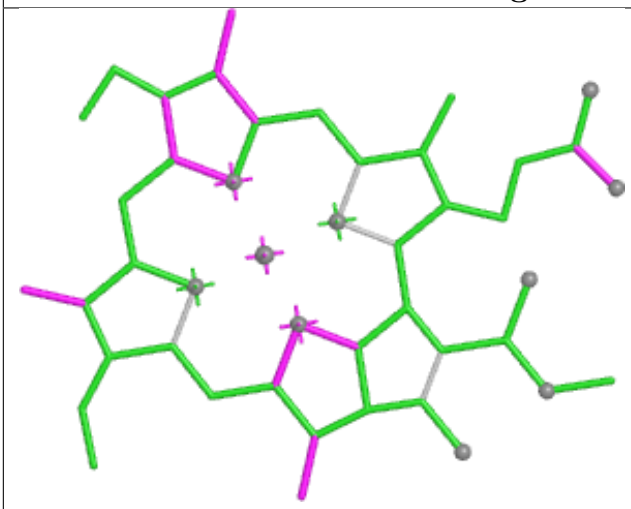


Rings

Ligand CLA BN 820



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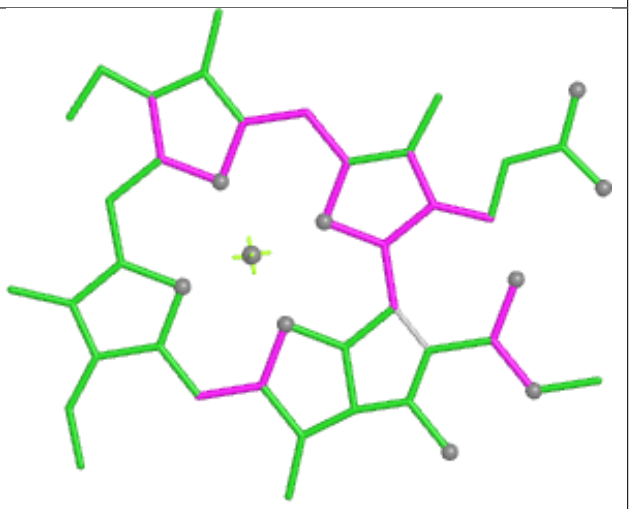

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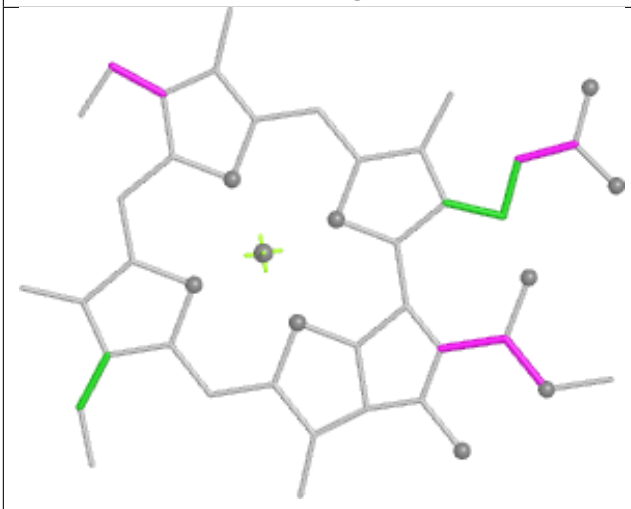
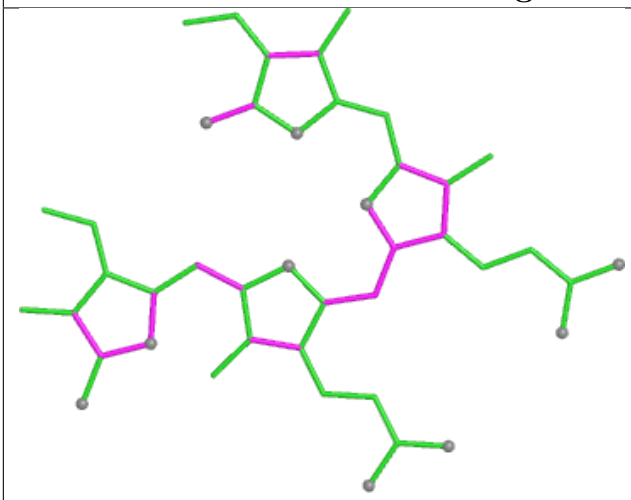


Torsions



Rings

Ligand PEB Y4 201



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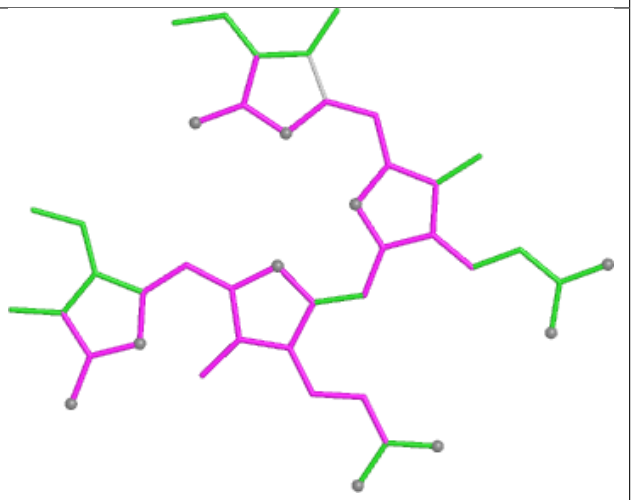

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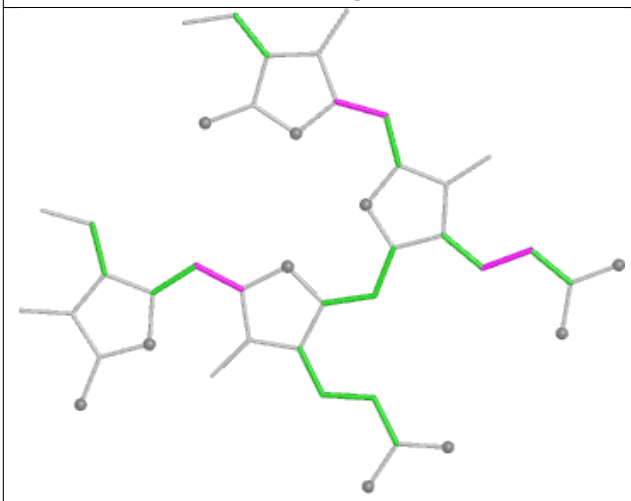

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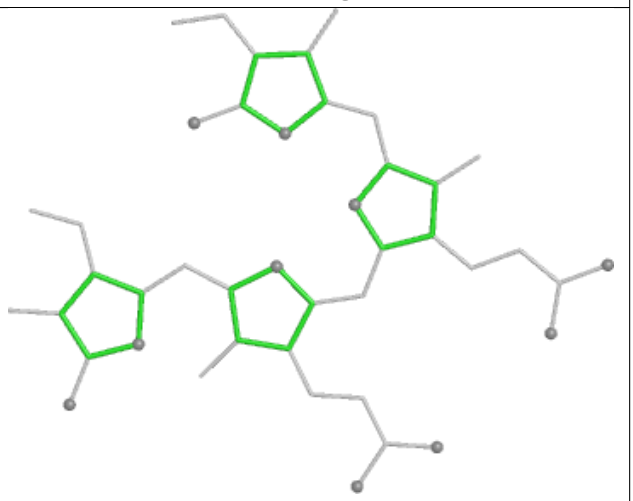
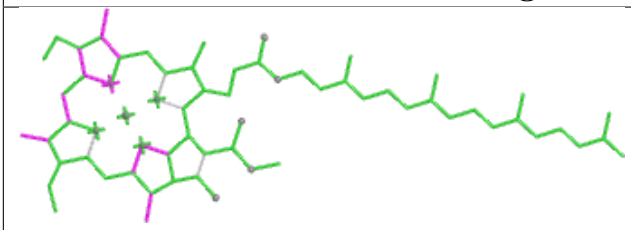


Rings

Ligand CLA b6 607



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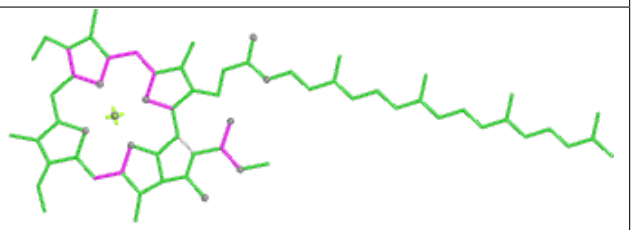

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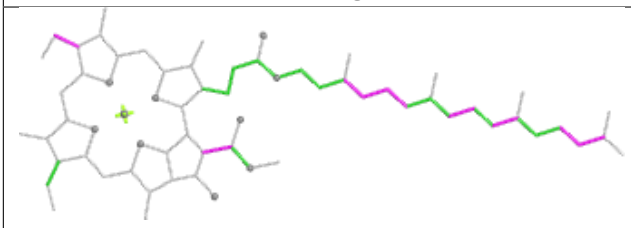

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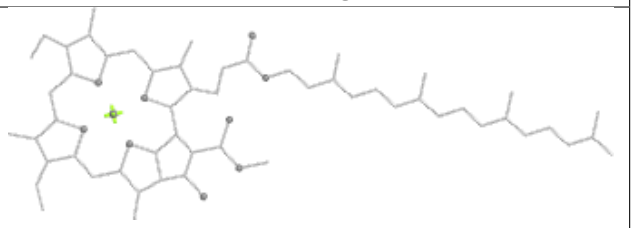
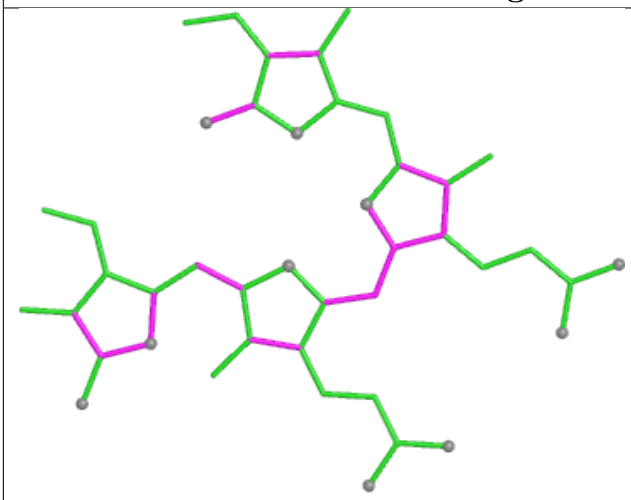


Rings

Ligand PEB MD 201



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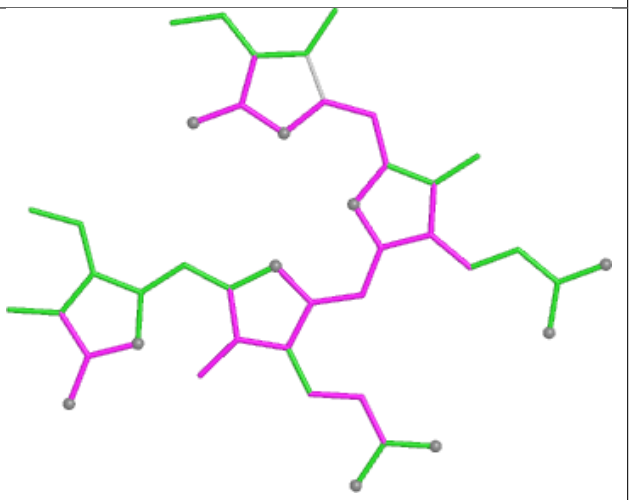

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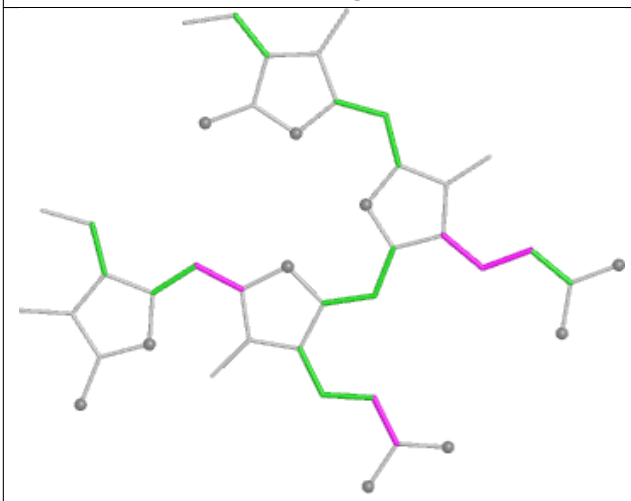

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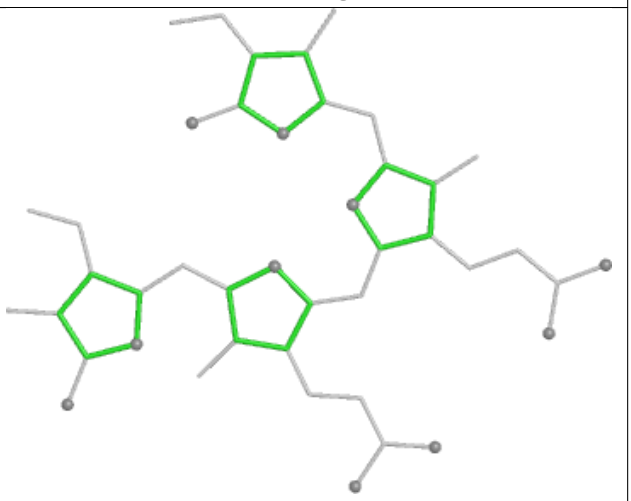
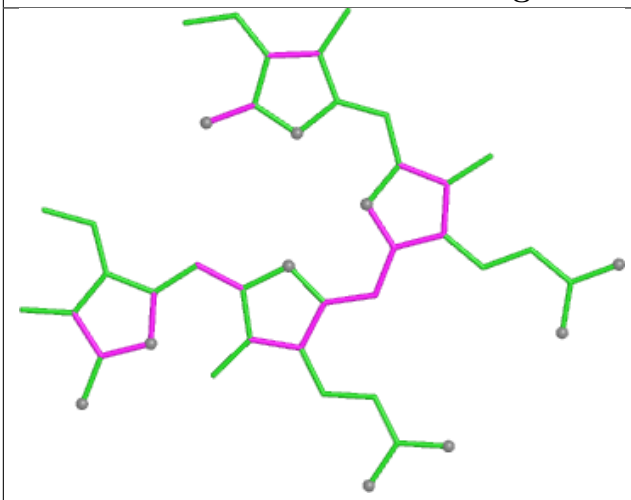


Rings

Ligand PEB AF 202



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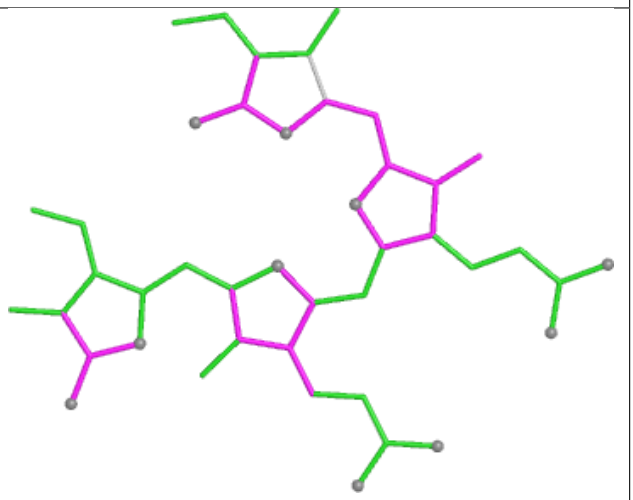

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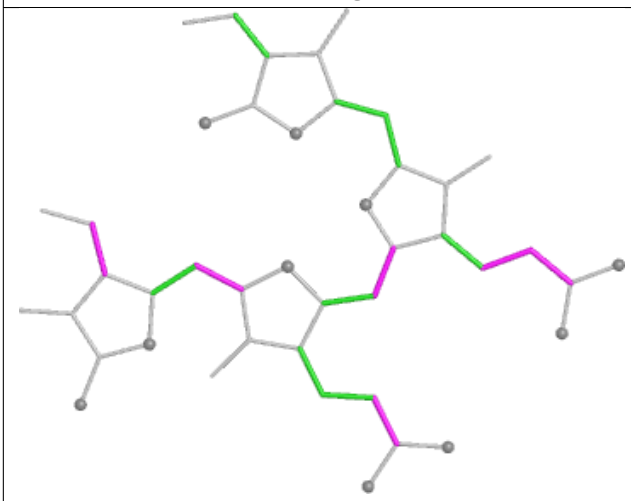

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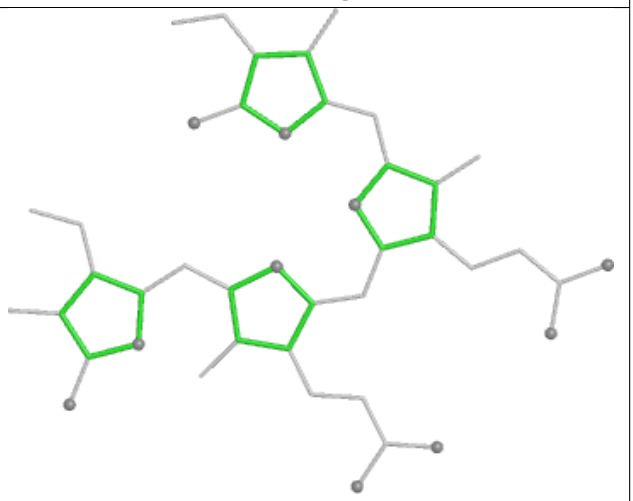

Rings

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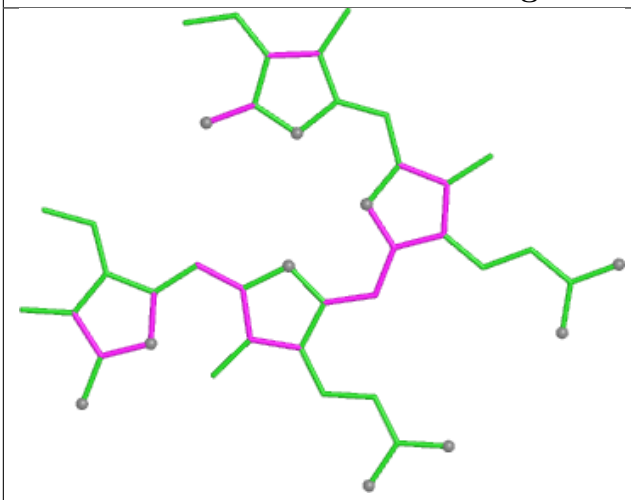

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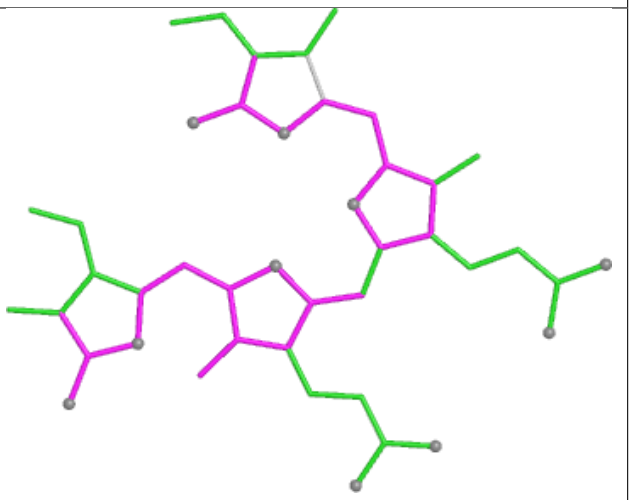

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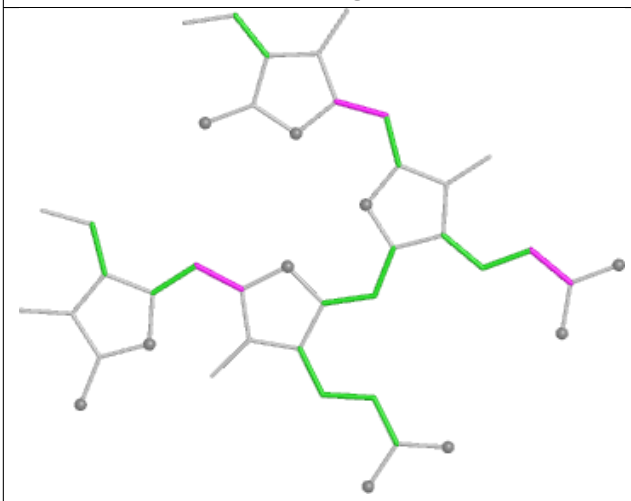

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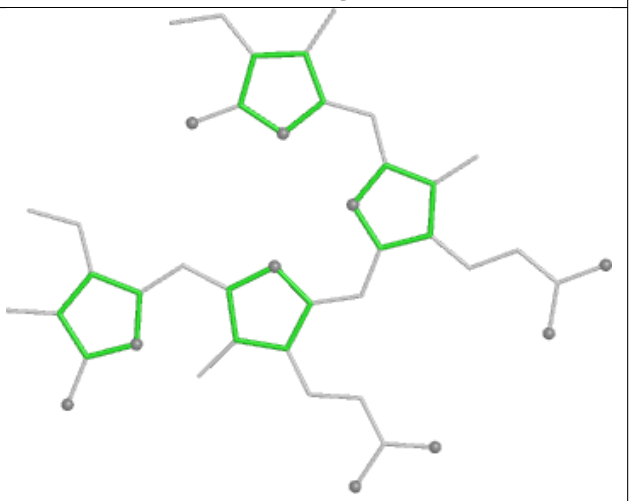
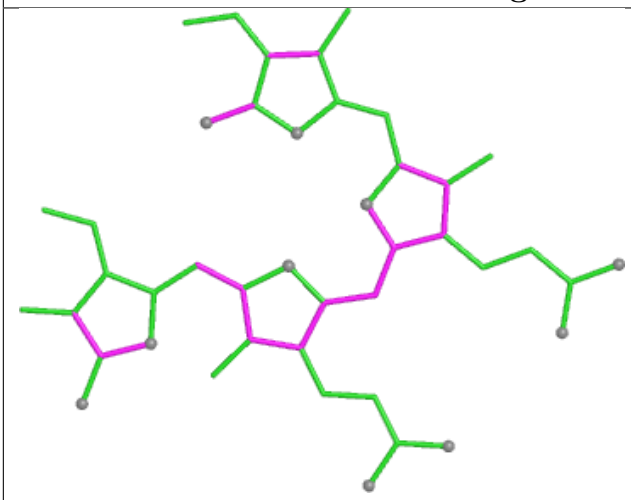


Rings

Ligand PEB VH 201



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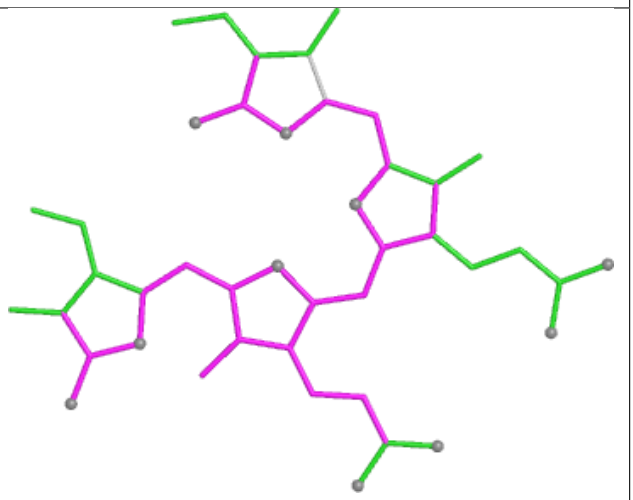

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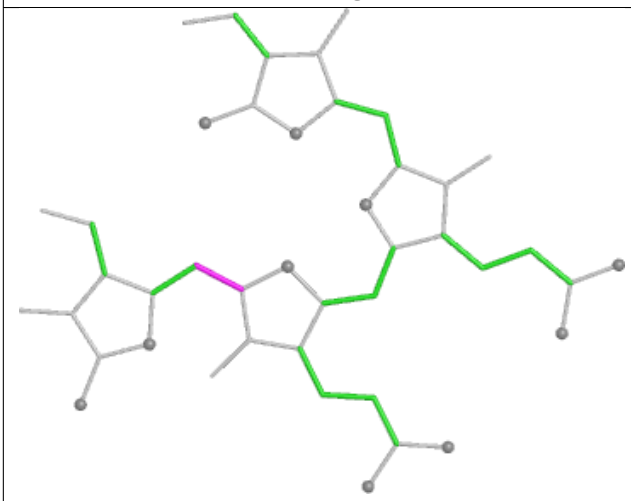

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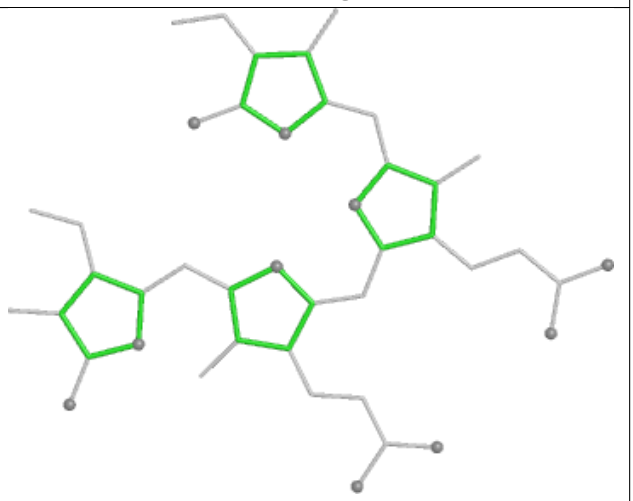
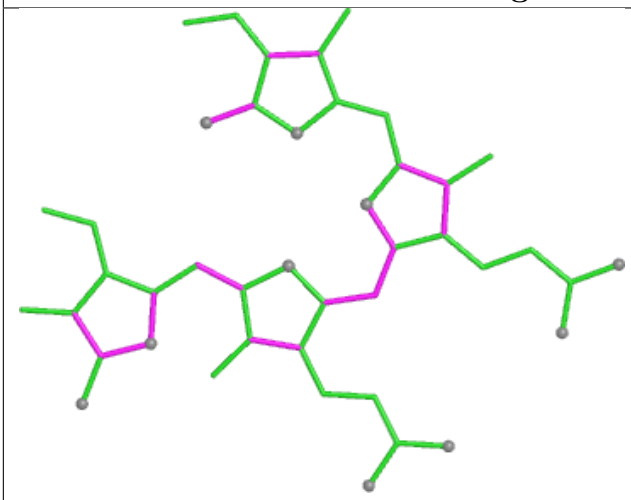


Rings

Ligand PEB KB 301



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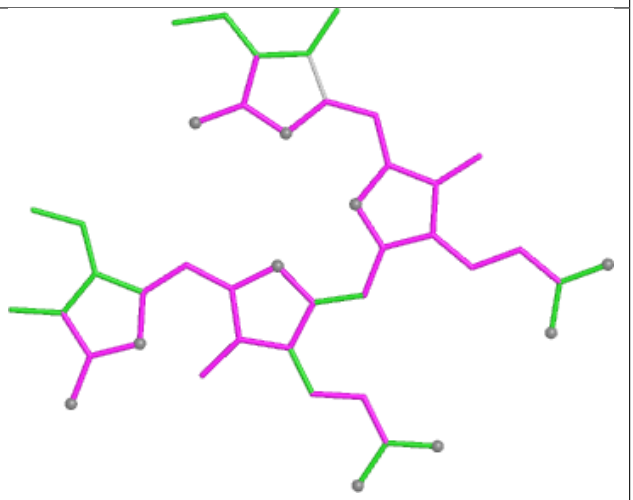

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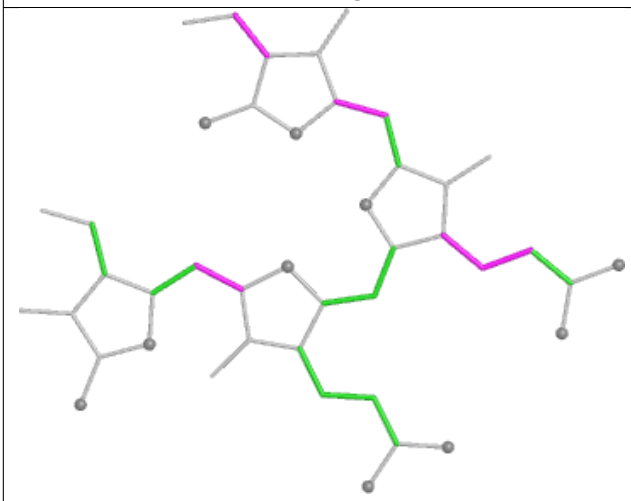

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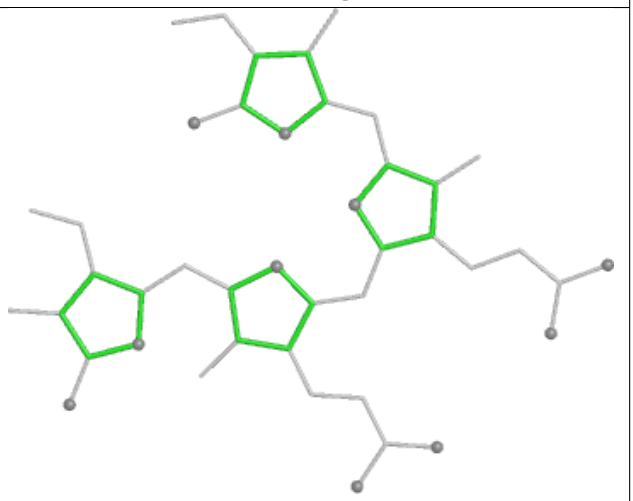
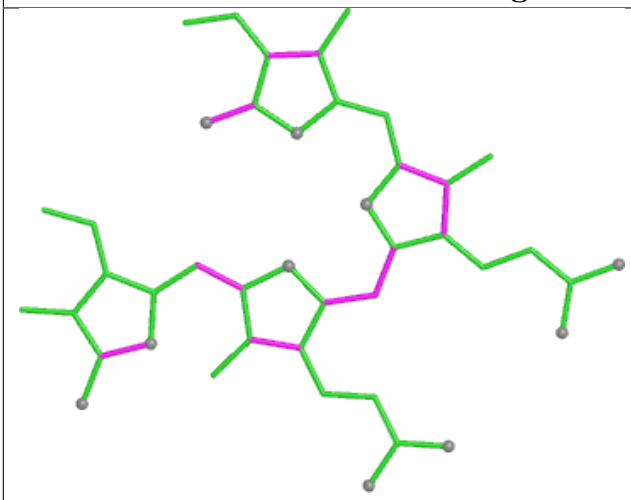


Rings

Ligand PEB CK 202



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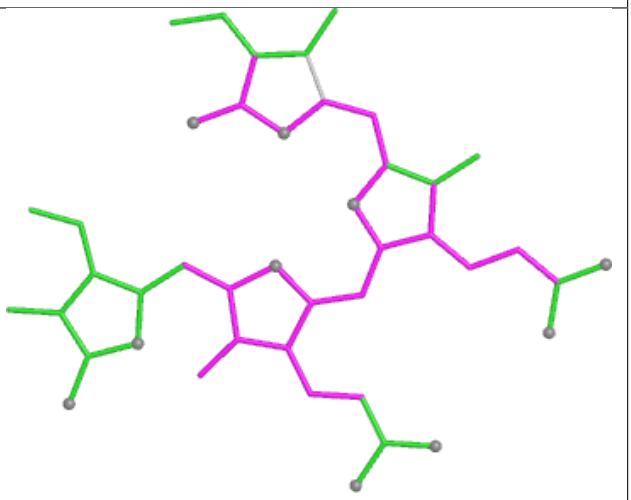

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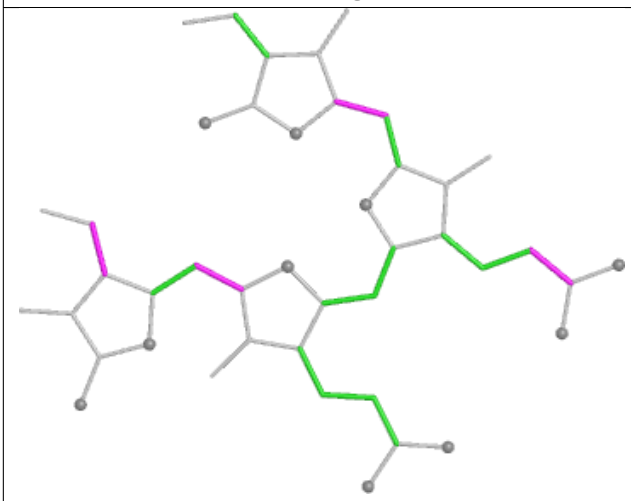

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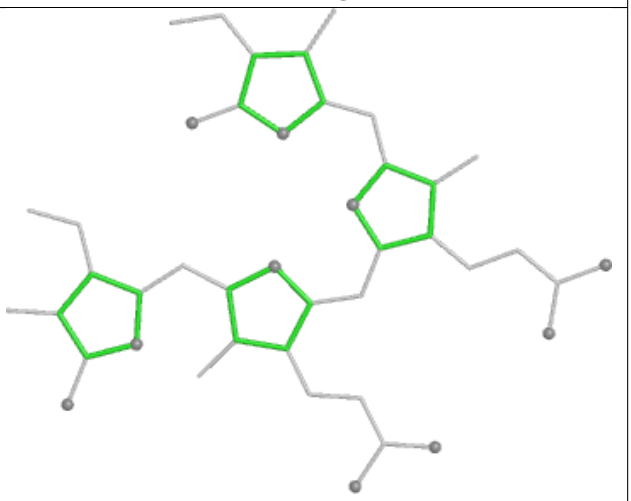
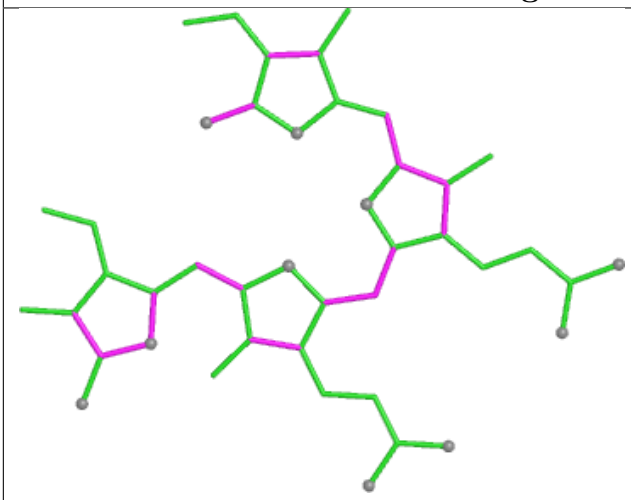


Rings

Ligand PEB iF 202



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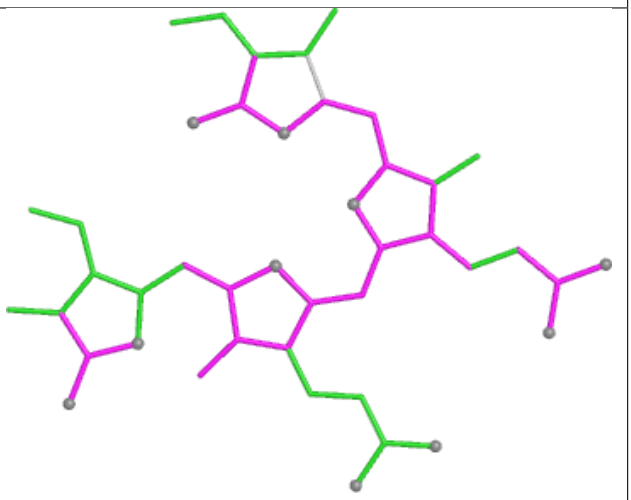
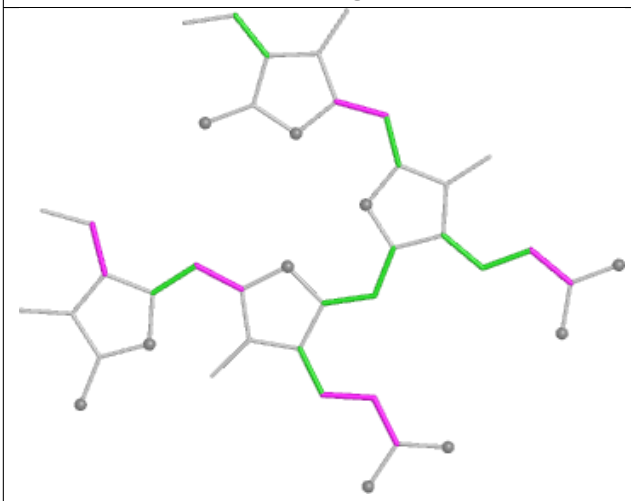


Bond angles



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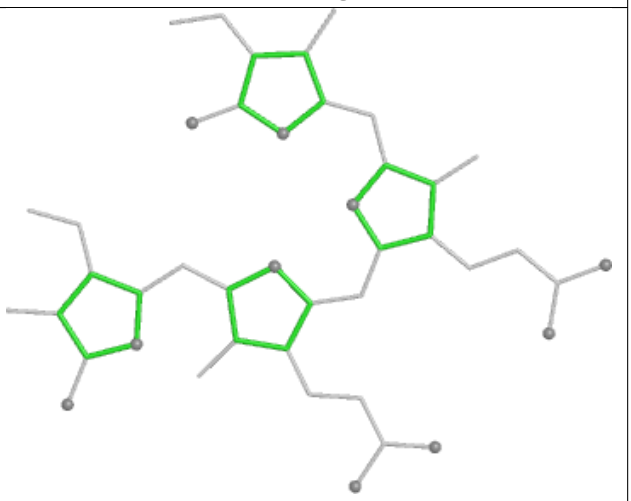
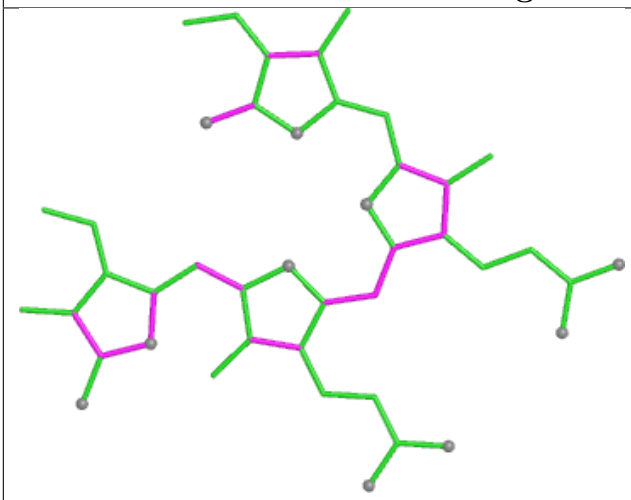


Rings

Ligand PEB eA 301



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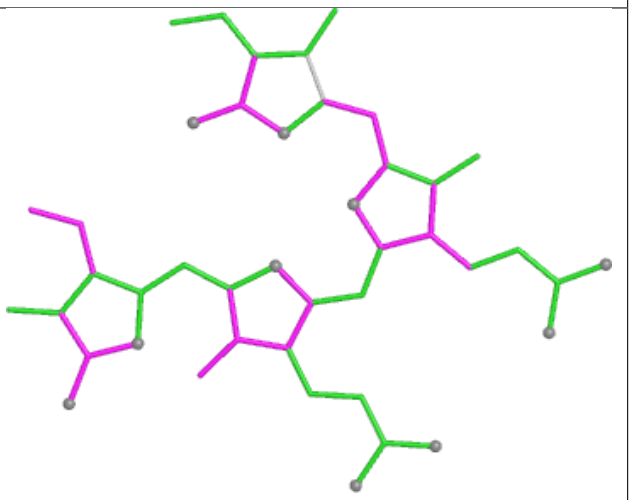

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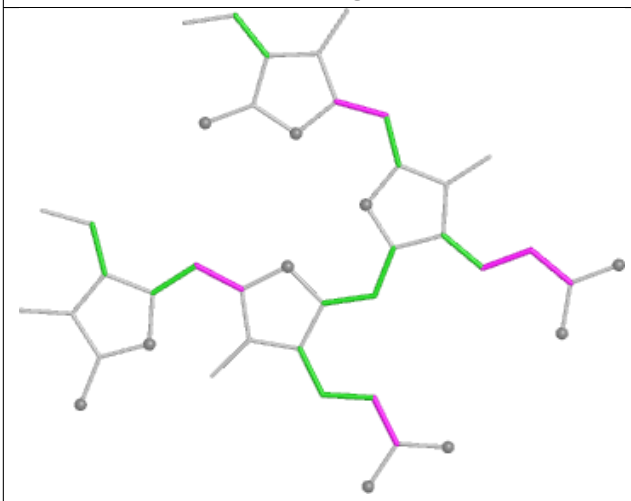

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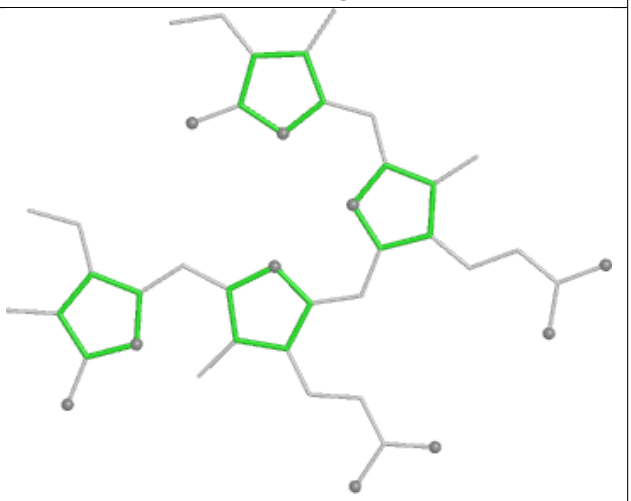
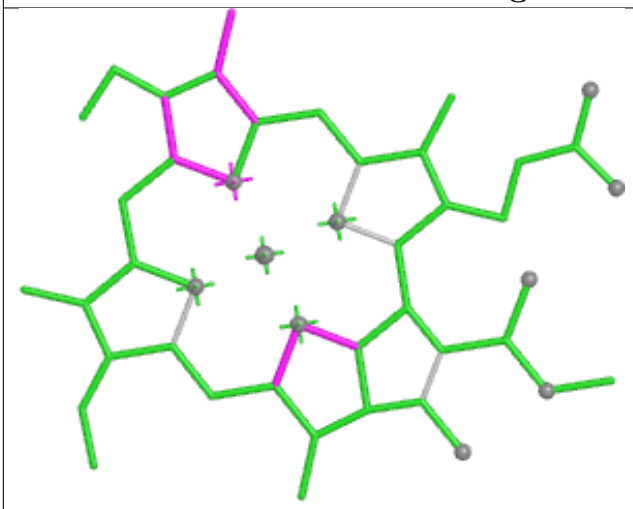


Rings

Ligand CLA RN 201



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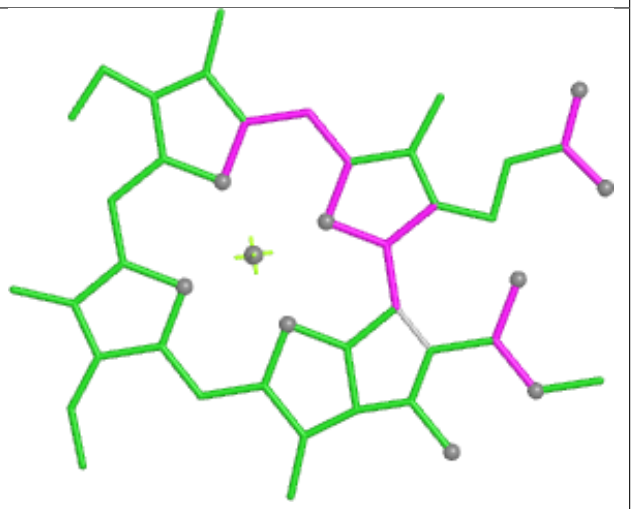
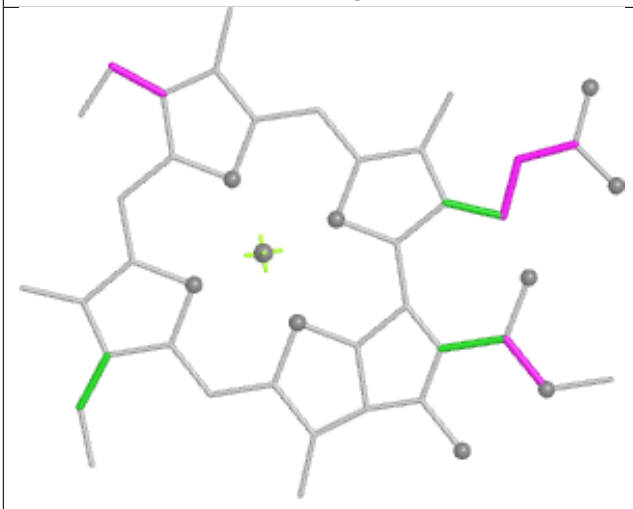


Bond angles

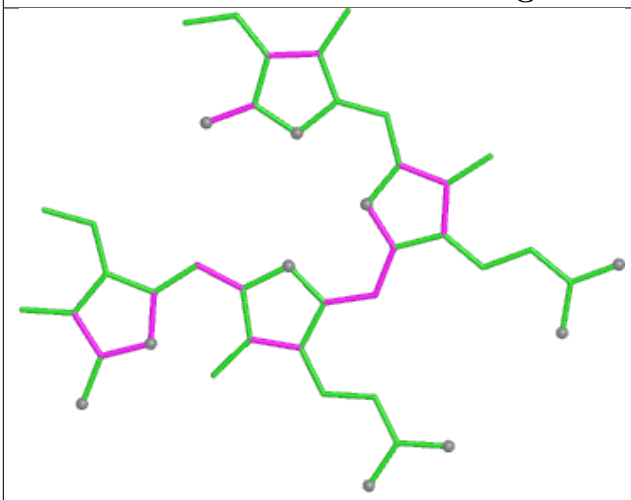


Torsions



Rings

Ligand PEB cB 403



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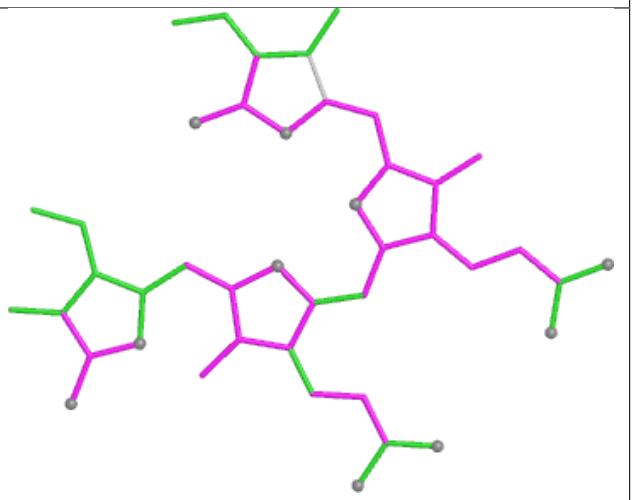
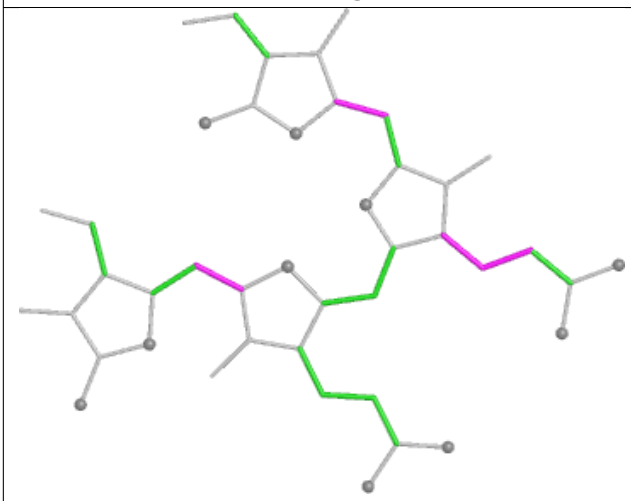


Bond angles



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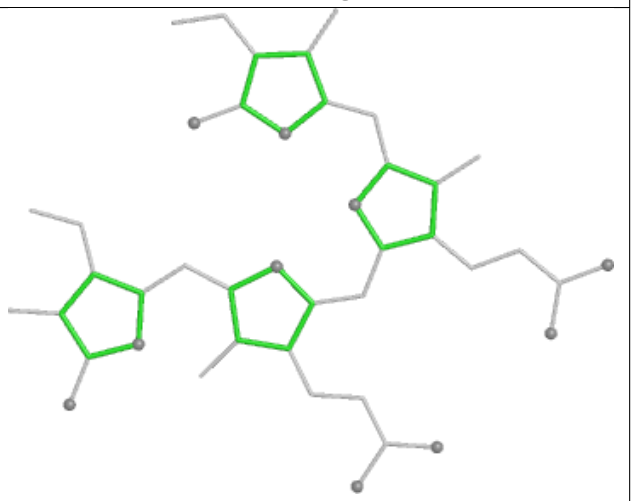
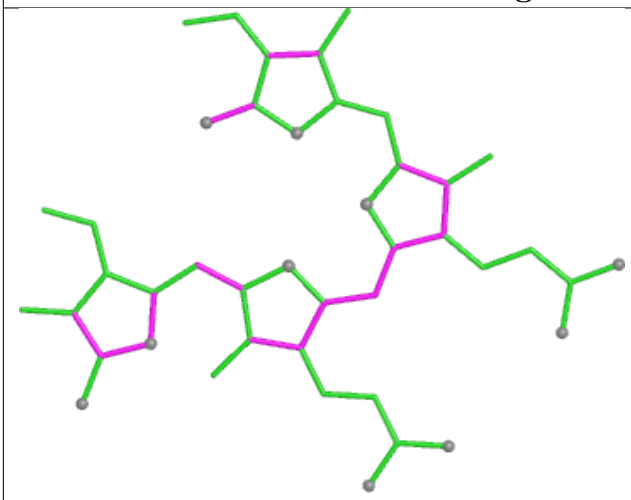


Rings

Ligand PEB dB 201



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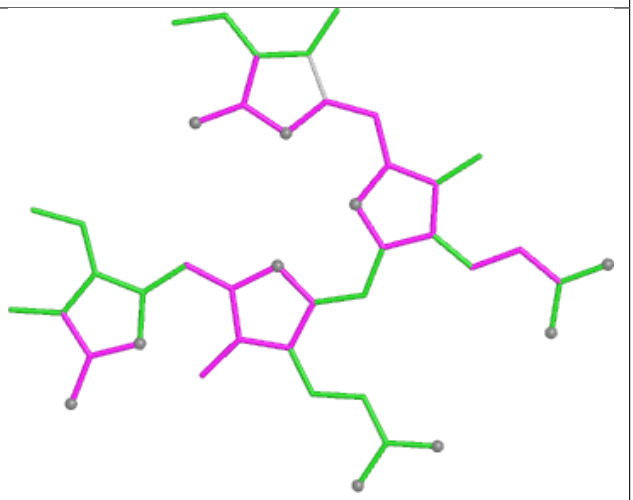

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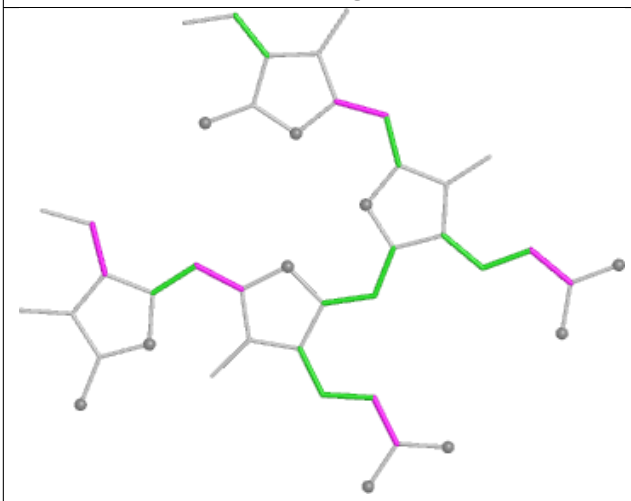

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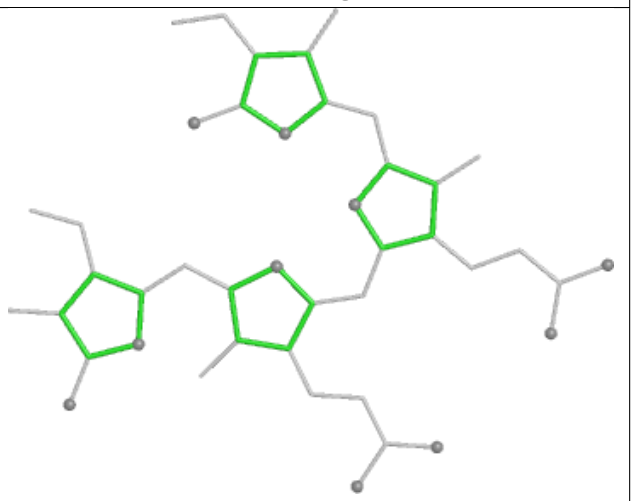
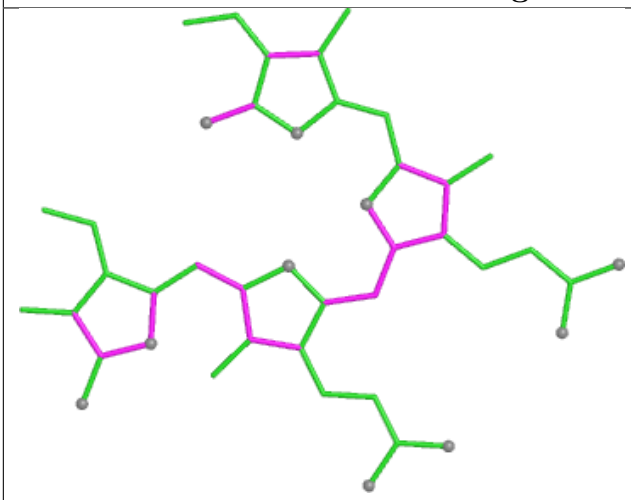


Rings

Ligand PEB CQ 201



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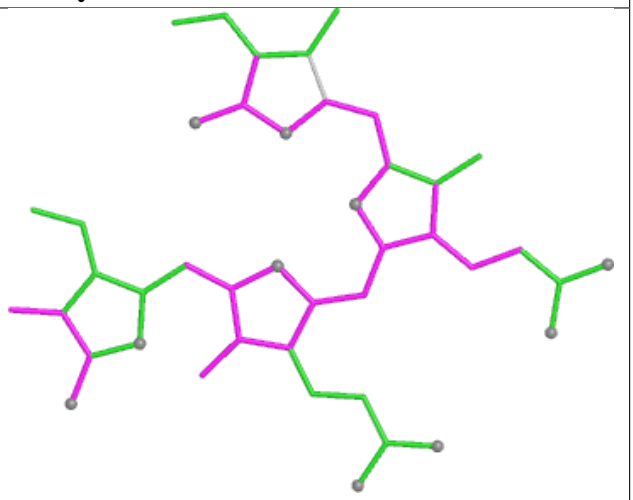

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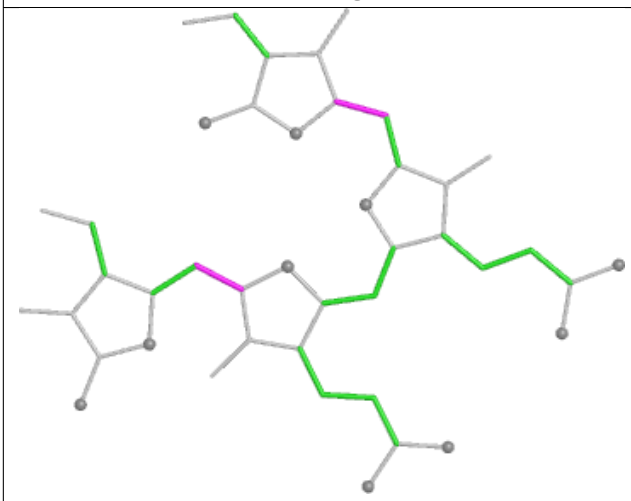

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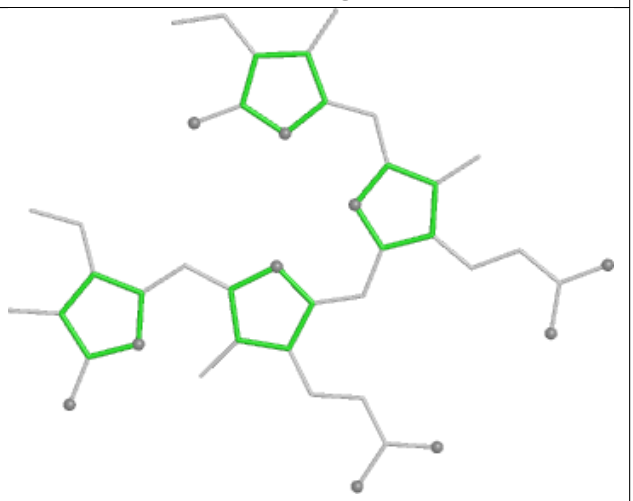
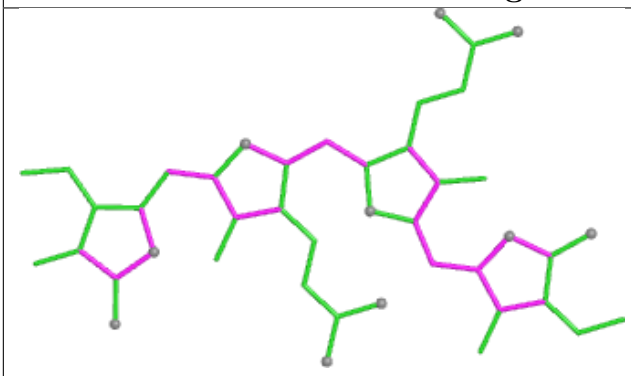


Rings

Ligand CYC E1 1001



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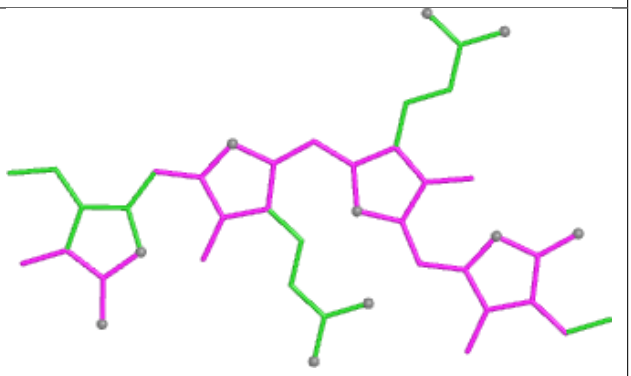

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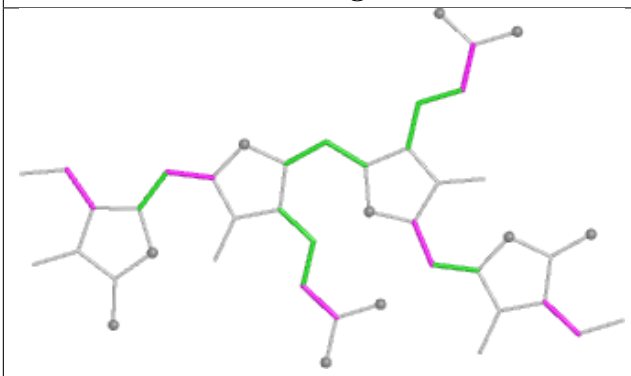

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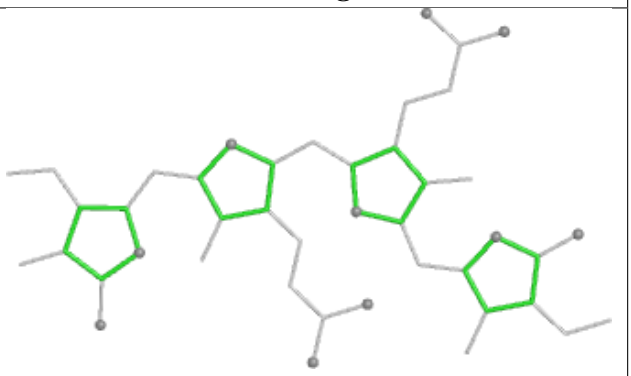
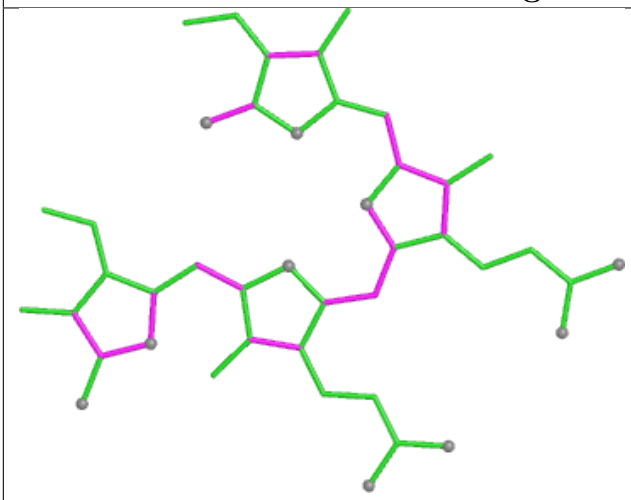


Rings

Ligand PEB iJ 201



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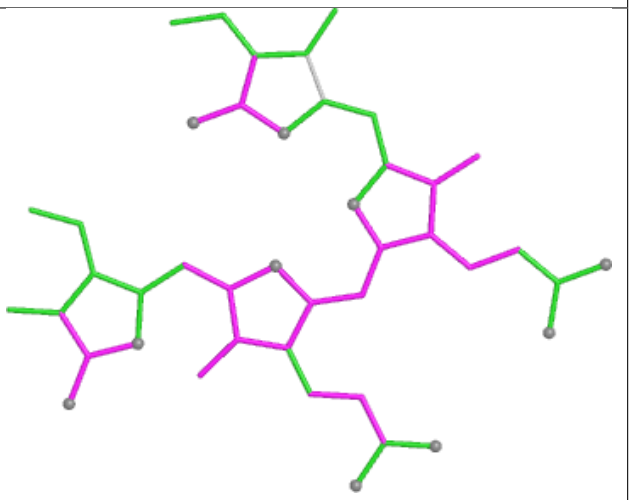

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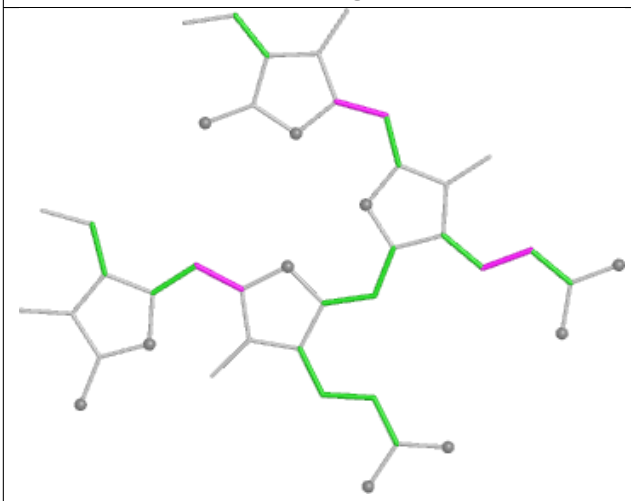

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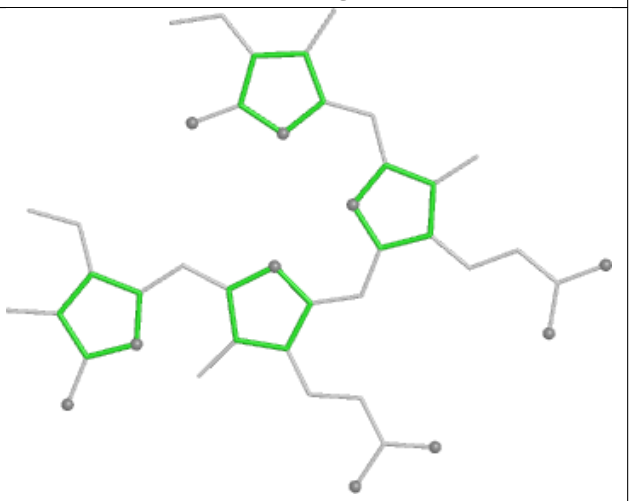
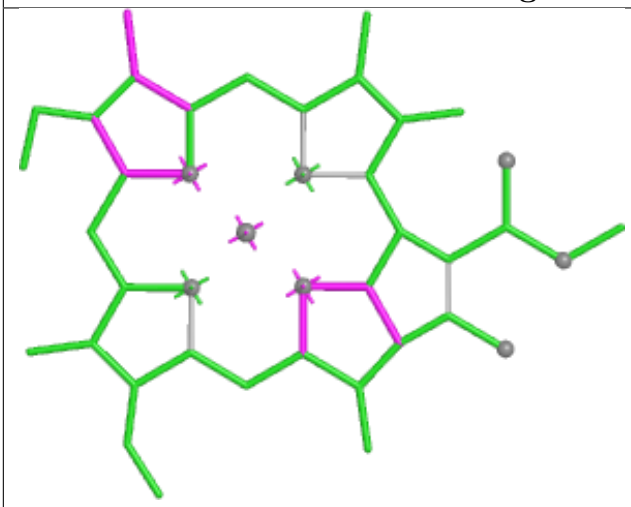


Rings

Ligand CLA 22 610



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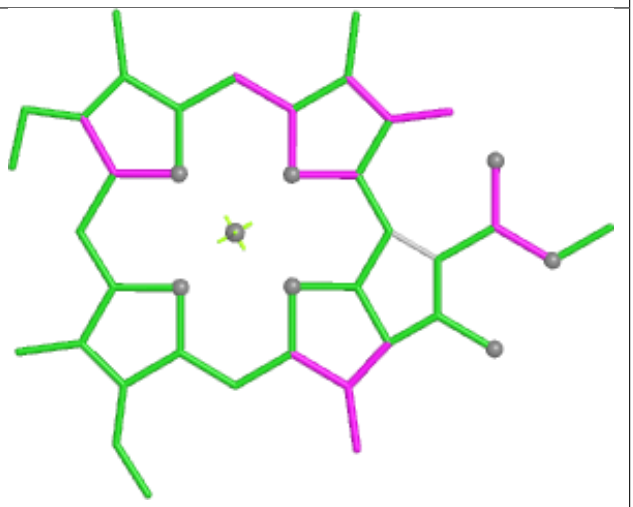

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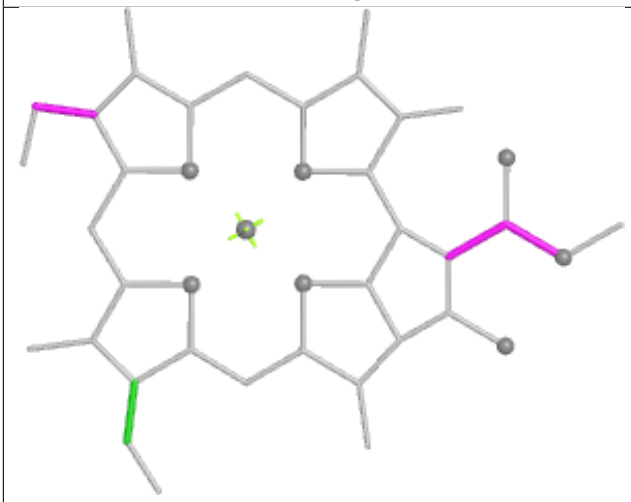

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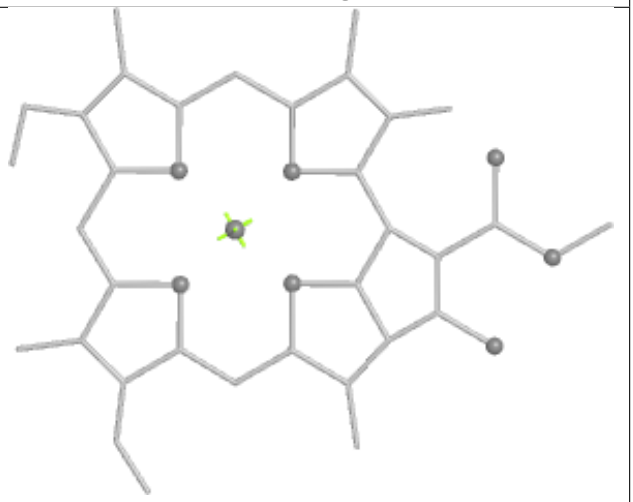
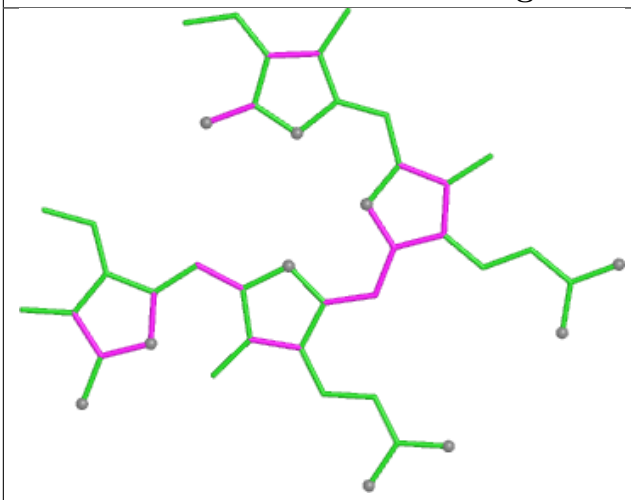


Rings

Ligand PEB P7 203



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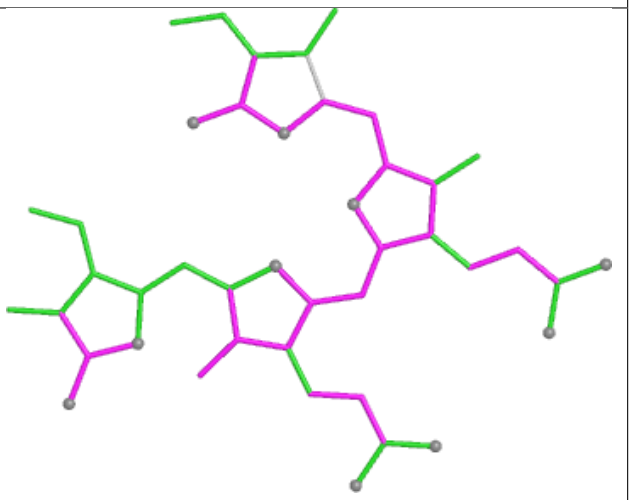

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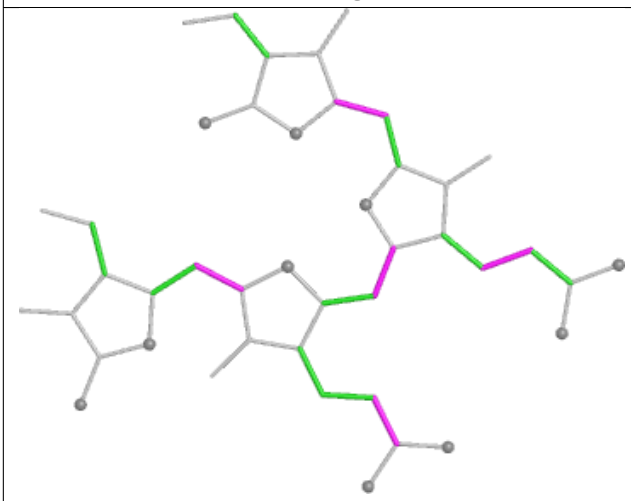

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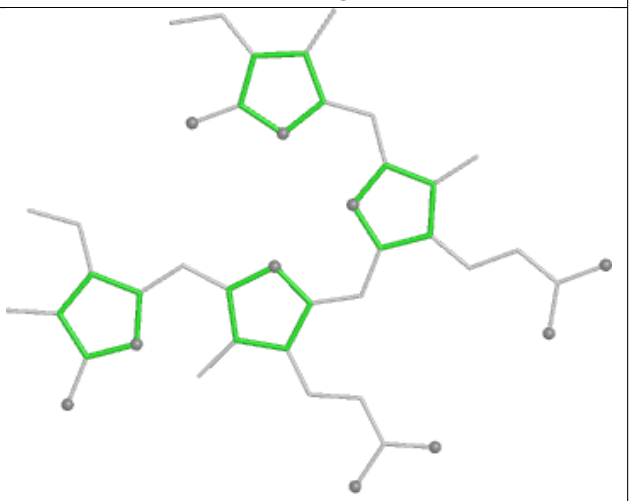
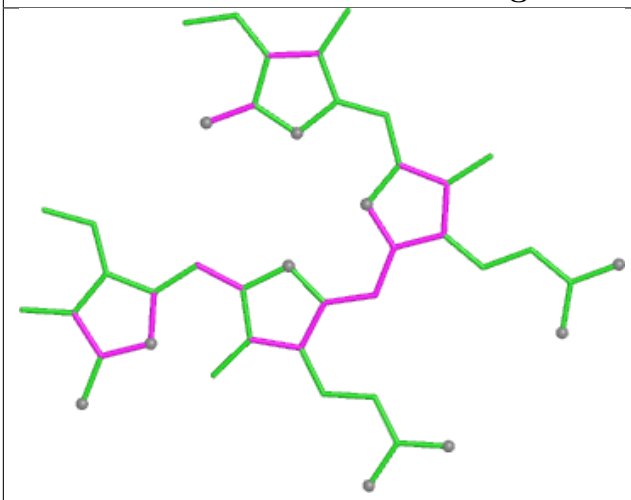


Rings

Ligand PEB GQ 201



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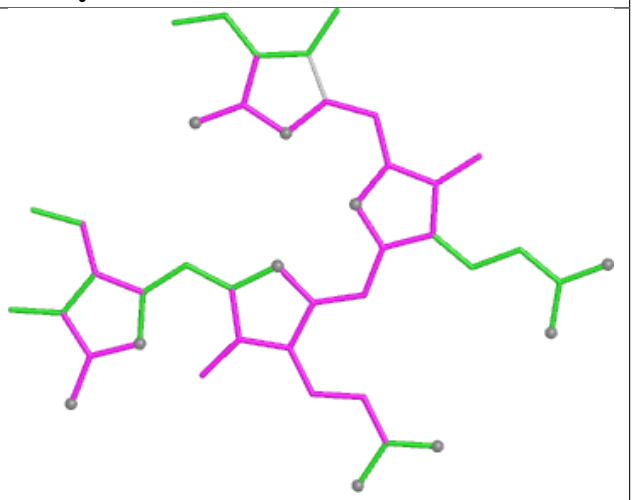

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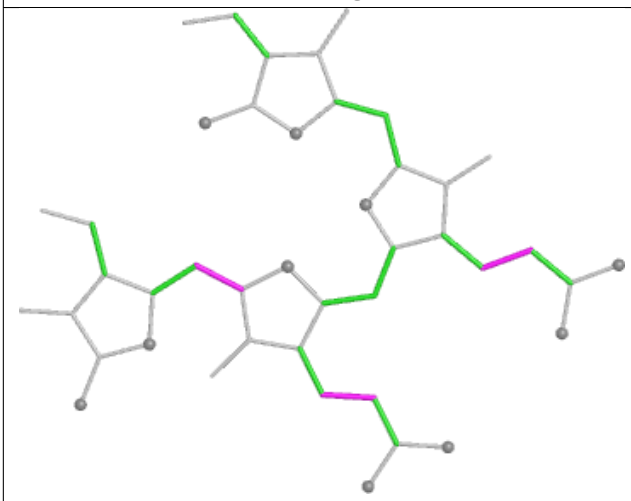

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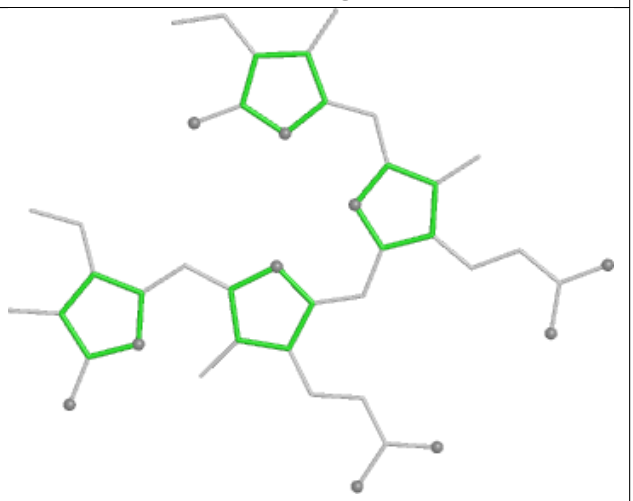
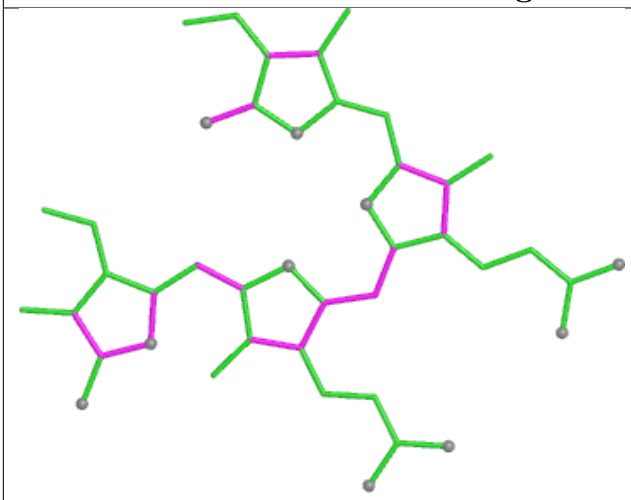


Rings

Ligand PEB ZF 201



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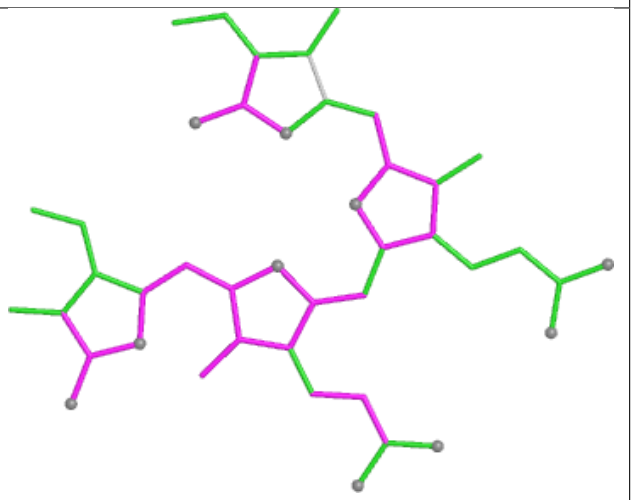

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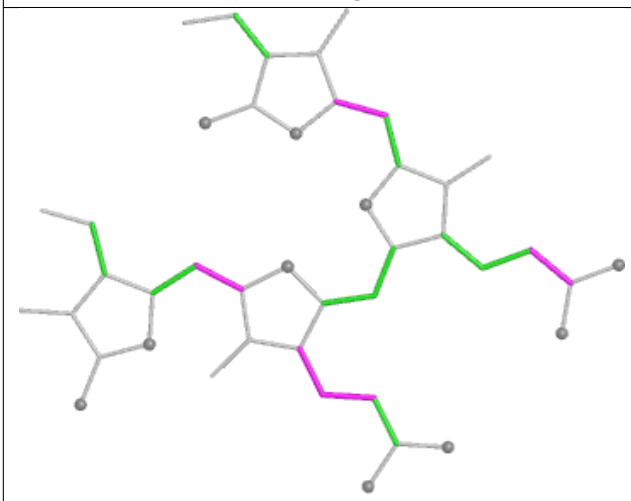

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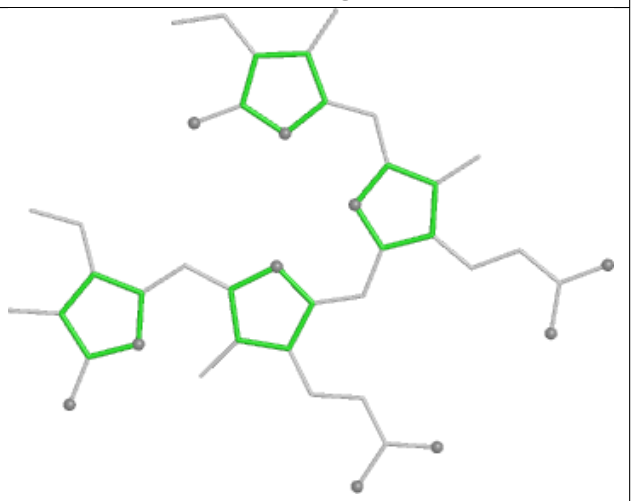
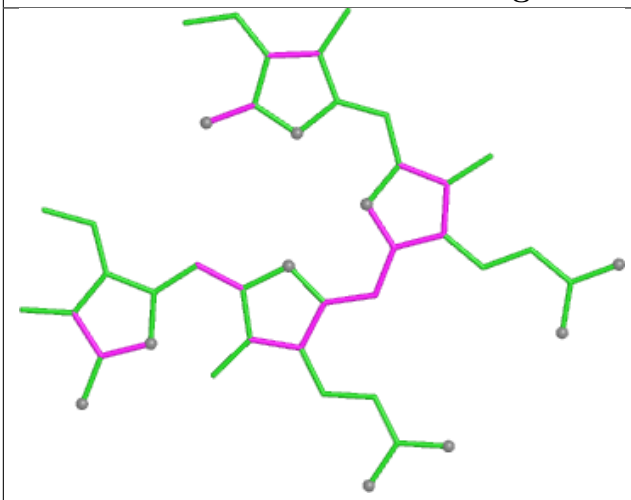


Rings

Ligand PEB CP 203



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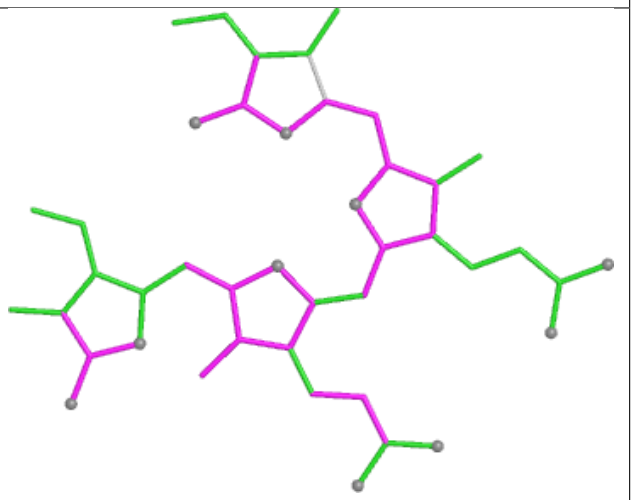

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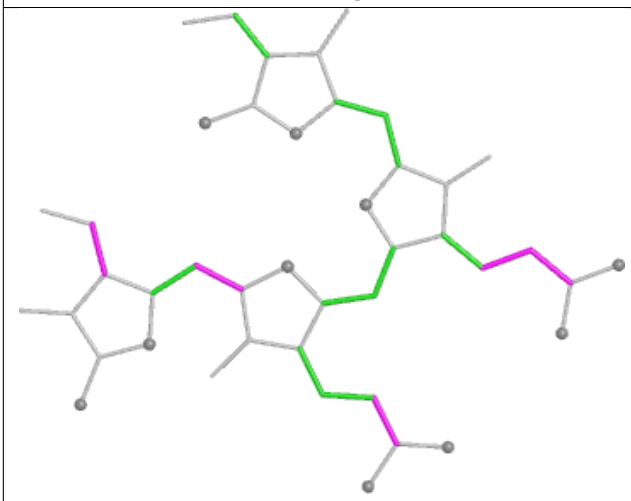

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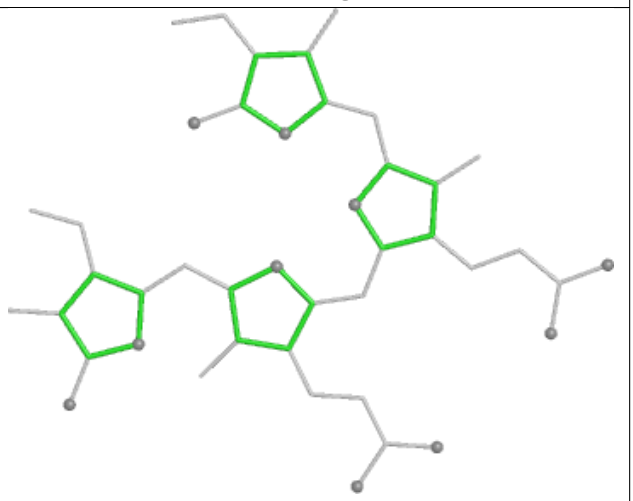
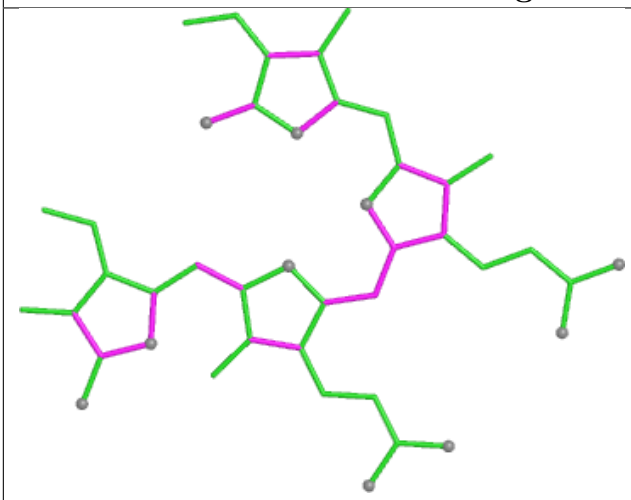


Rings

Ligand PEB O4 202



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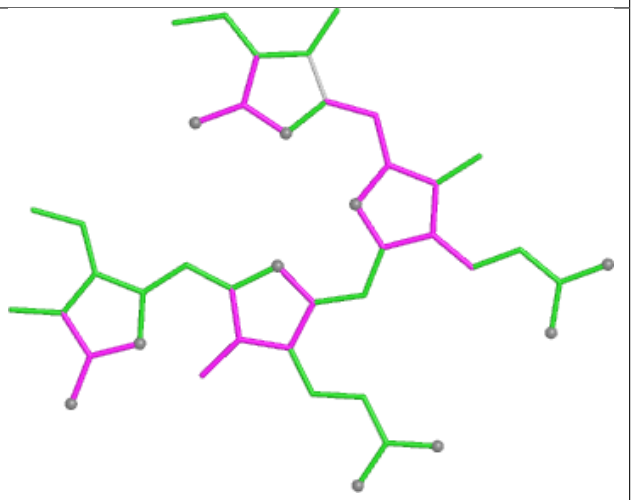

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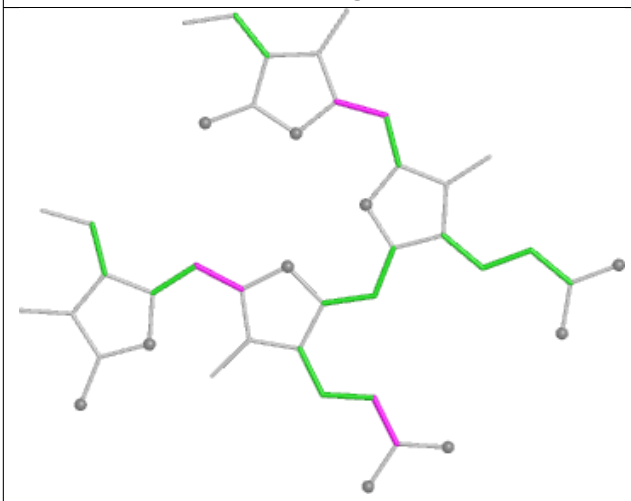

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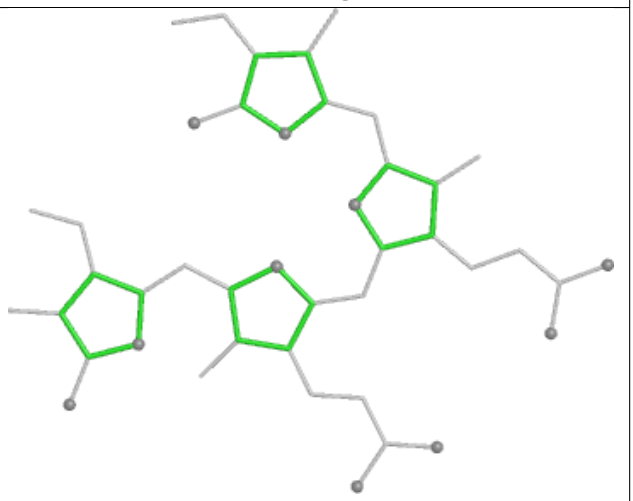
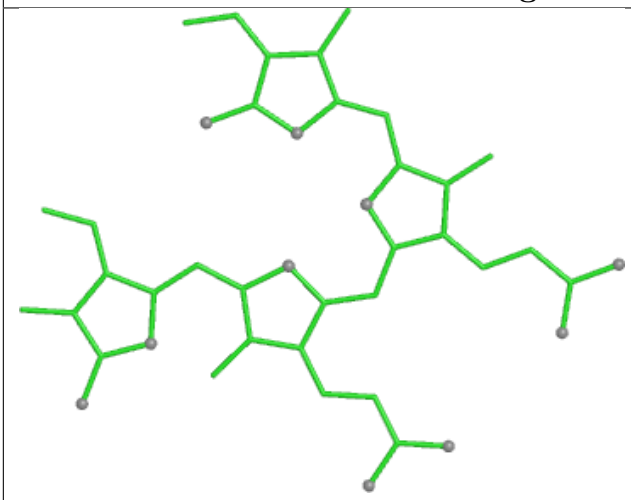


Rings

Ligand PEB k4 202



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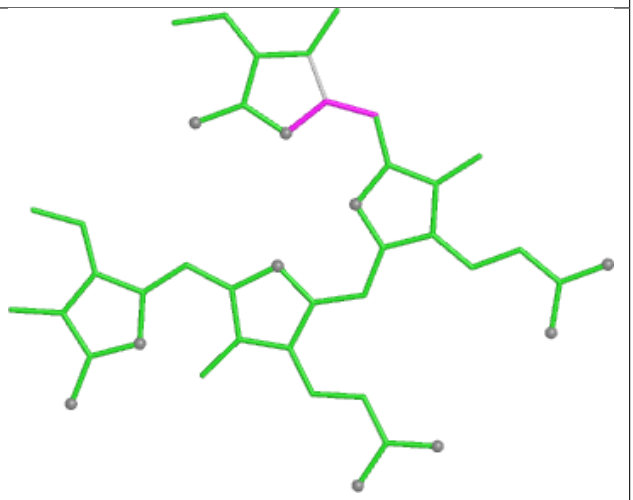

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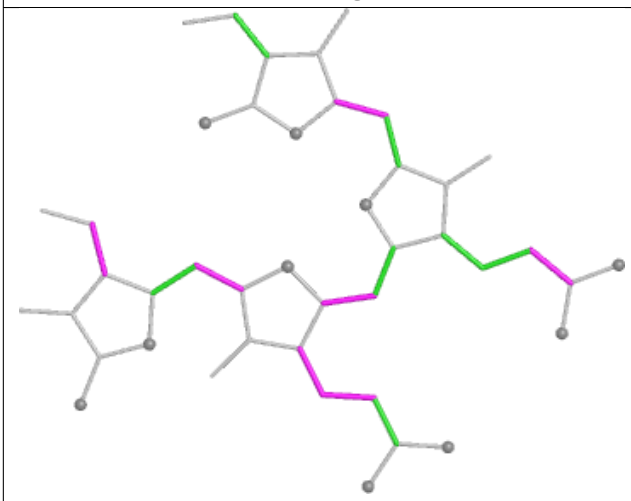

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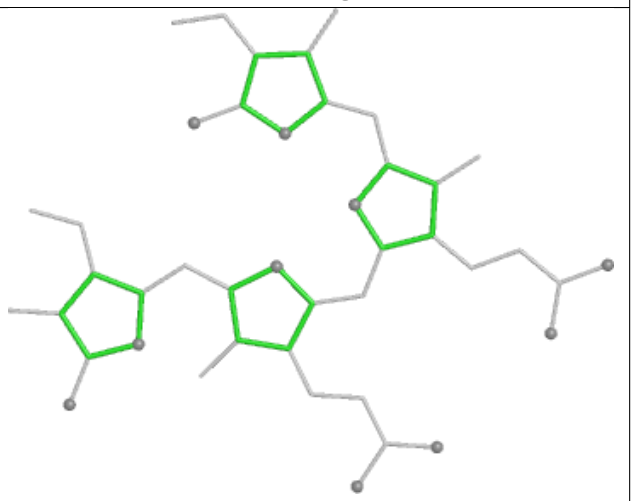
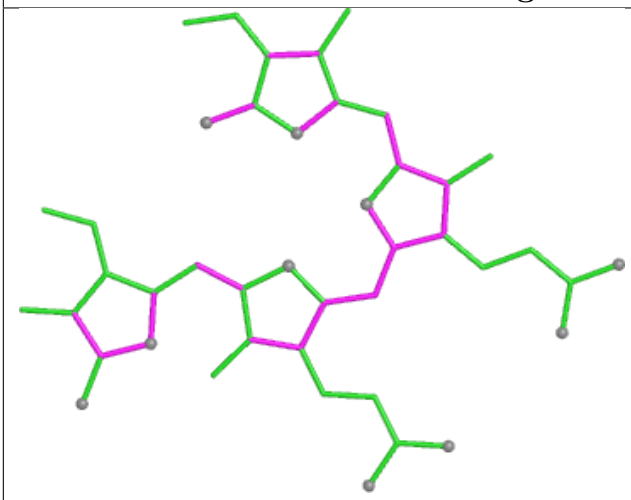


Rings

Ligand PEB xF 302



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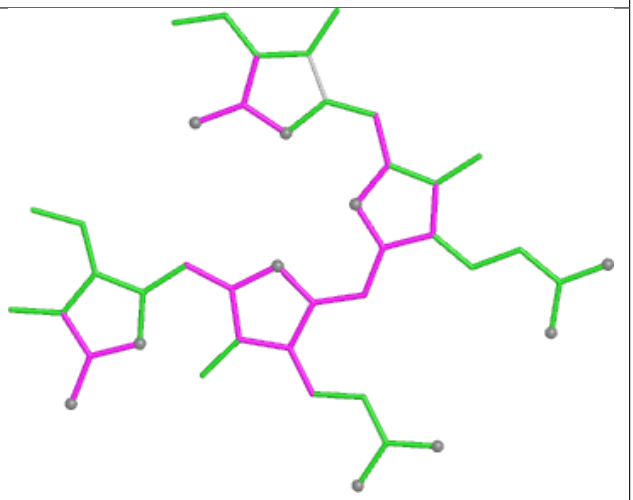
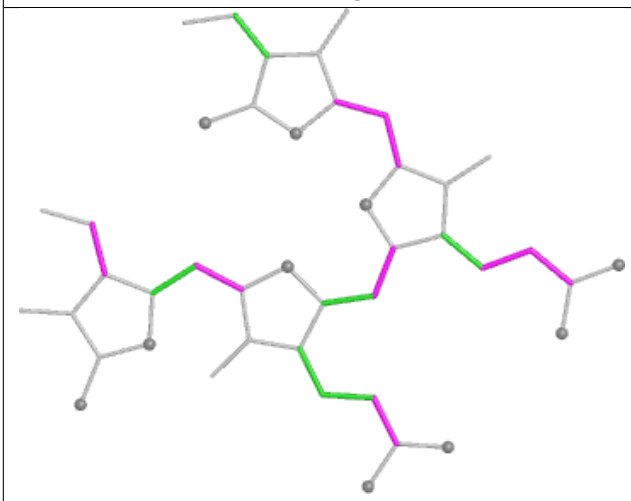


Bond angles



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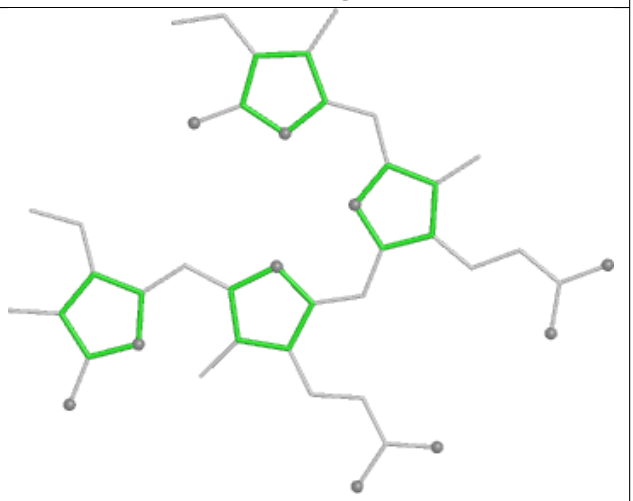
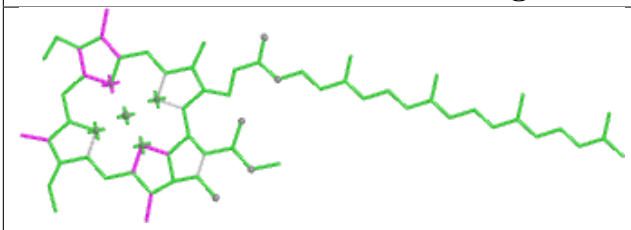


Rings

Ligand CLA BN 810



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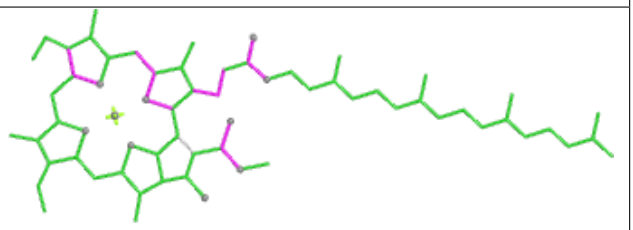
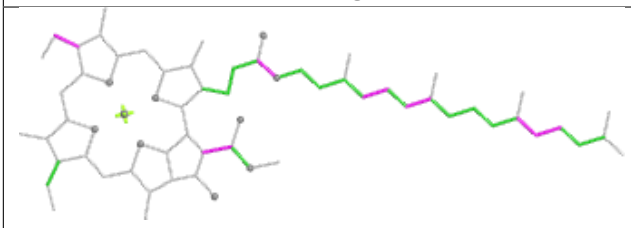


Bond angles



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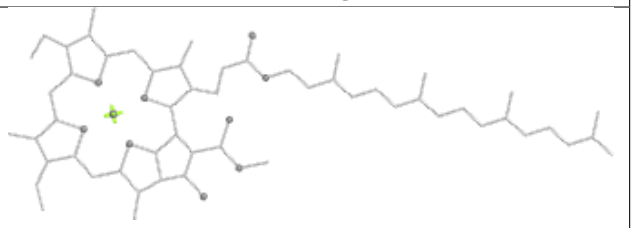
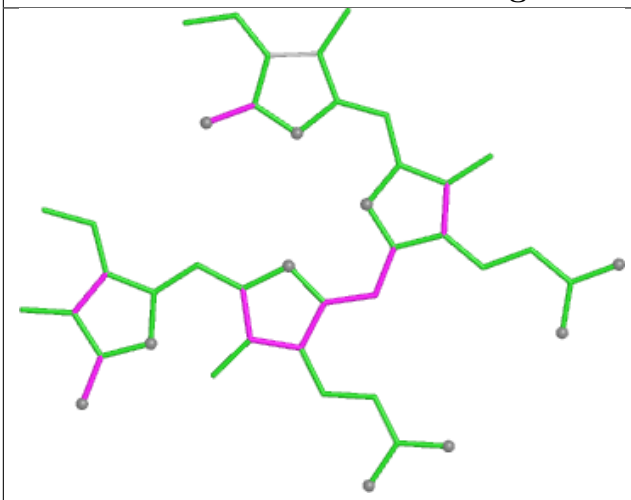
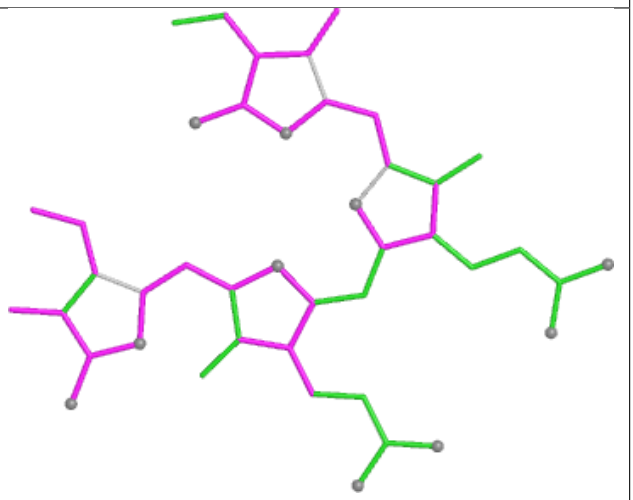


Rings

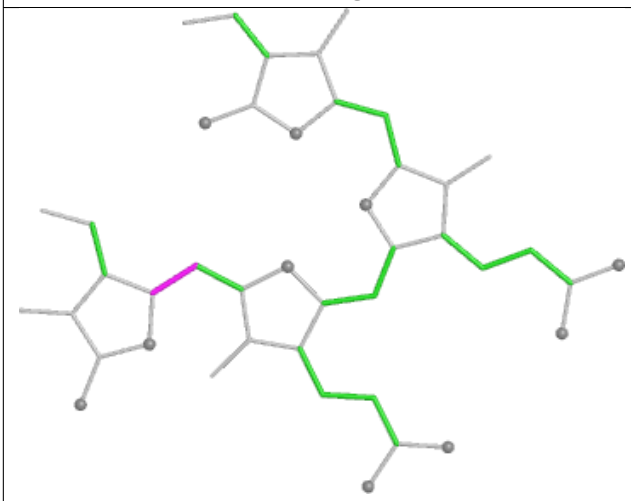
Ligand PUB AO 302



Bond lengths



Bond angles



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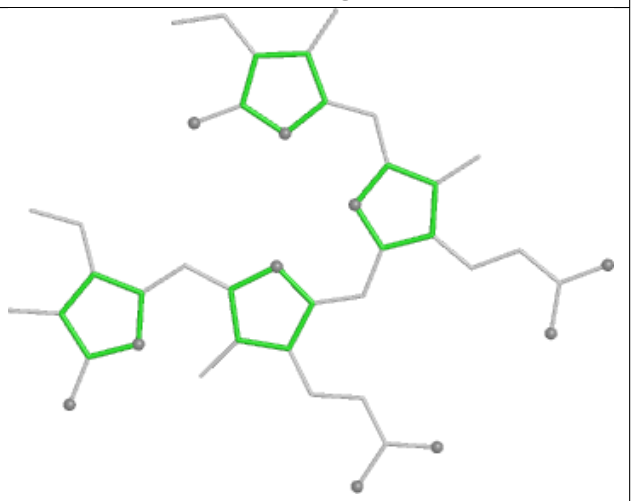
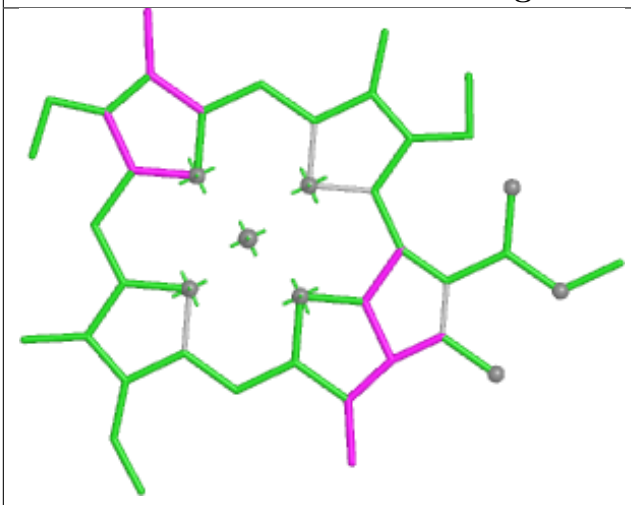


Rings

Ligand CLA 4N 604



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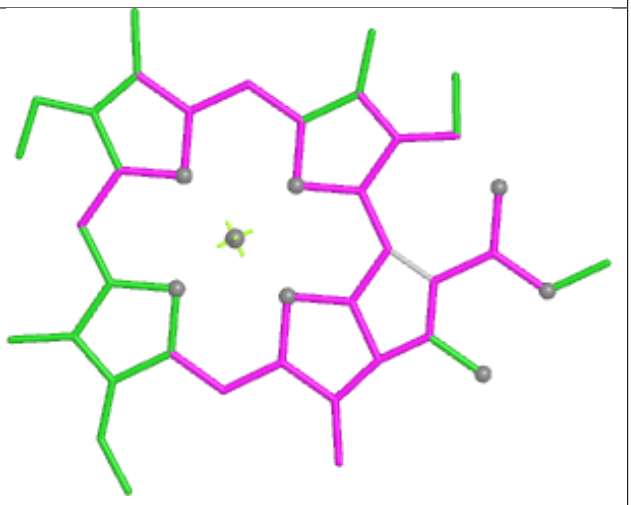

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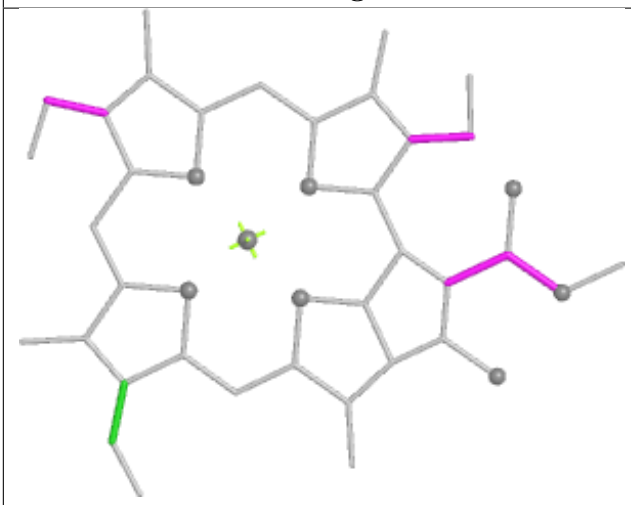
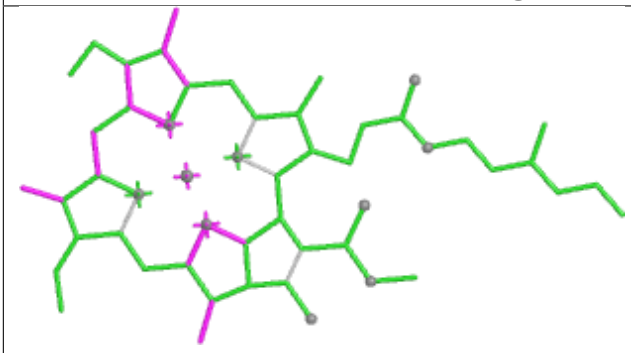


Torsions



Rings

Ligand CLA AN 803



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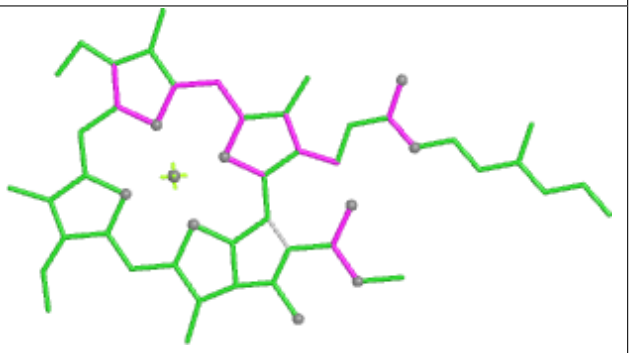

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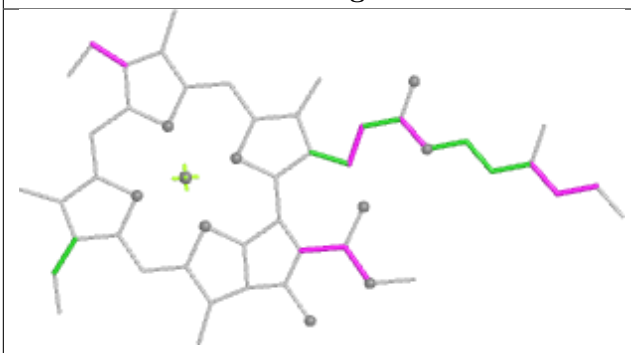

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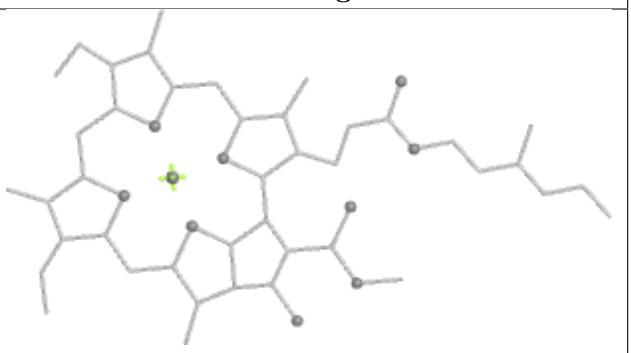
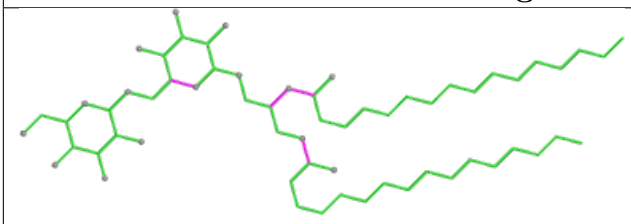


Rings

Ligand DGD c6 601



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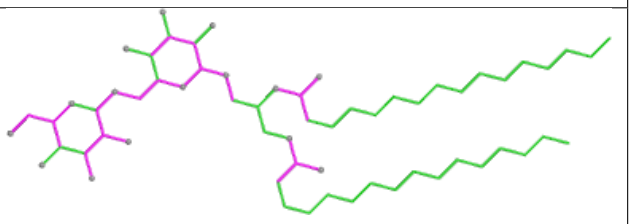

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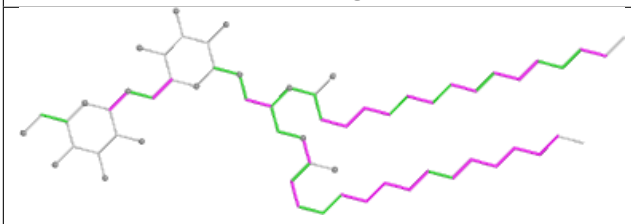

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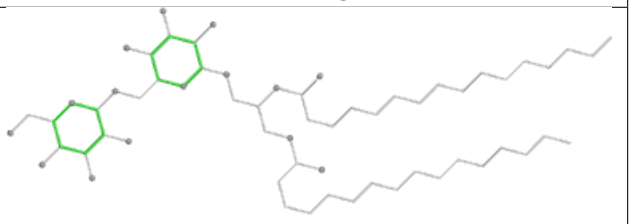
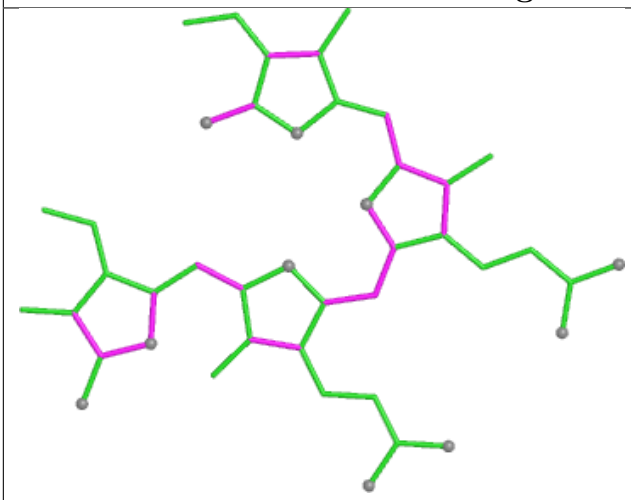


Rings

Ligand PEB TJ 201



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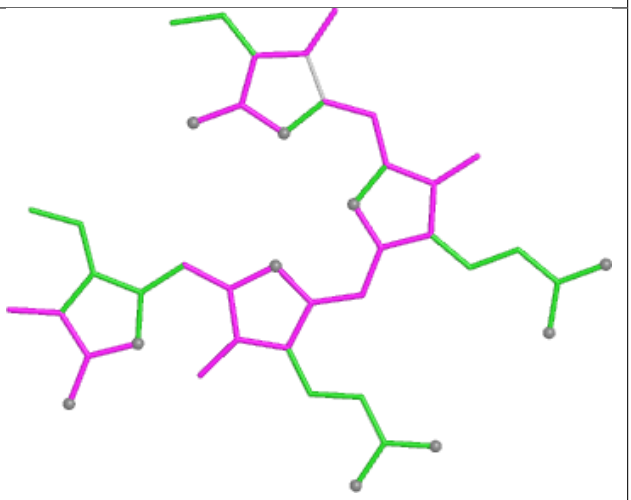

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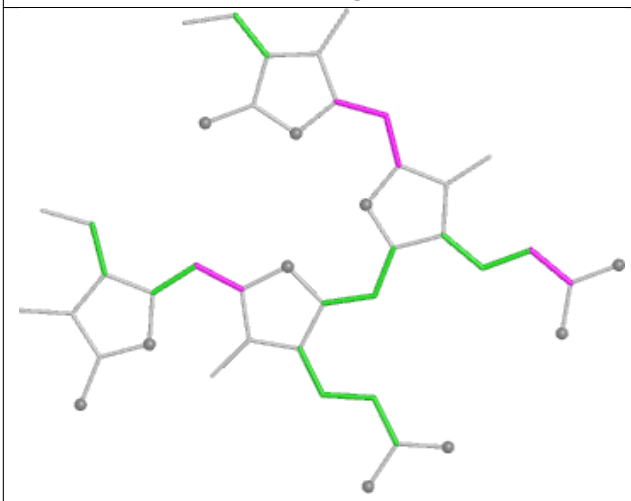

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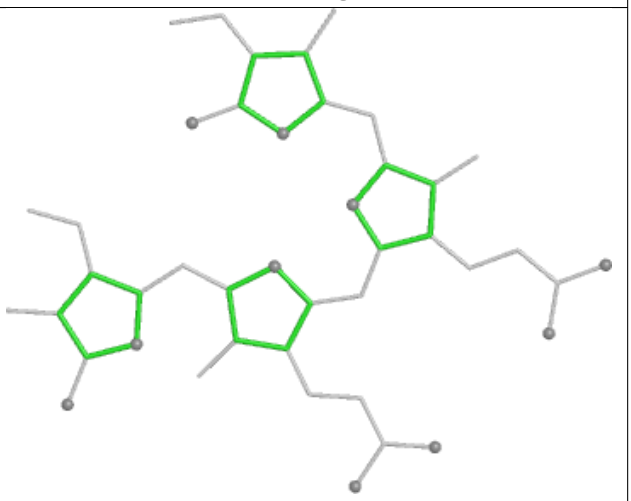
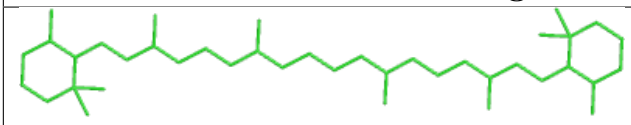


Rings

Ligand BCR AN 845



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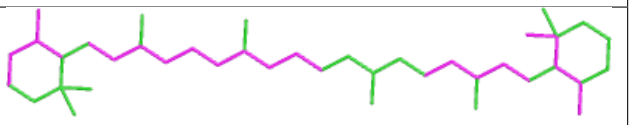

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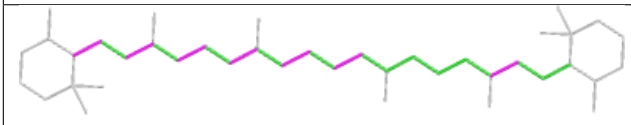

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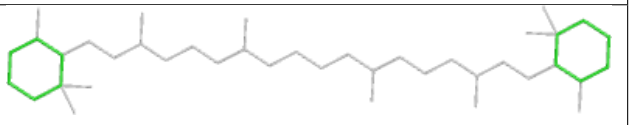
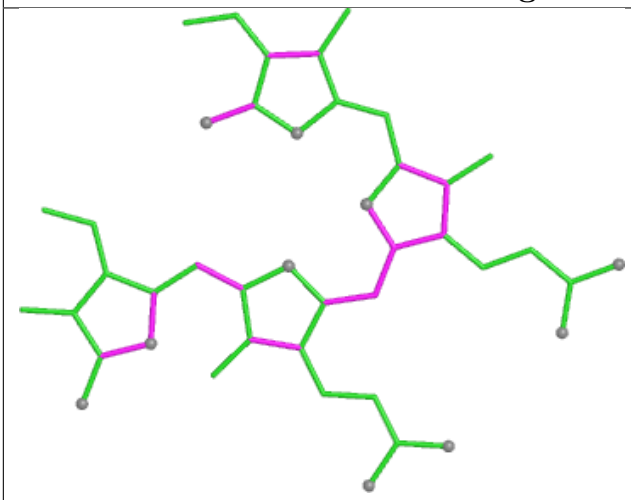


Rings

Ligand PEB TI 202



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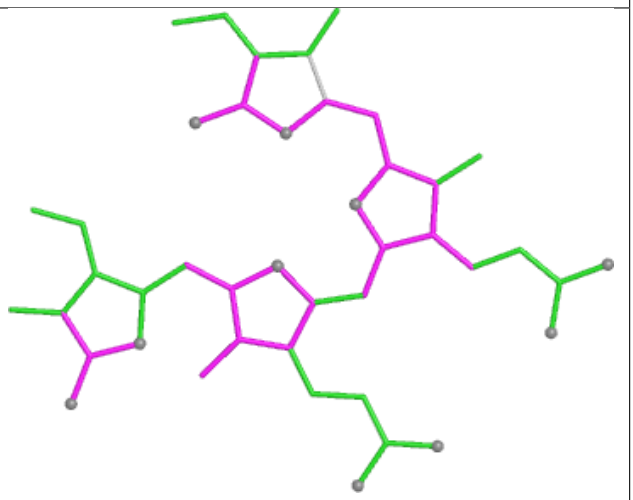

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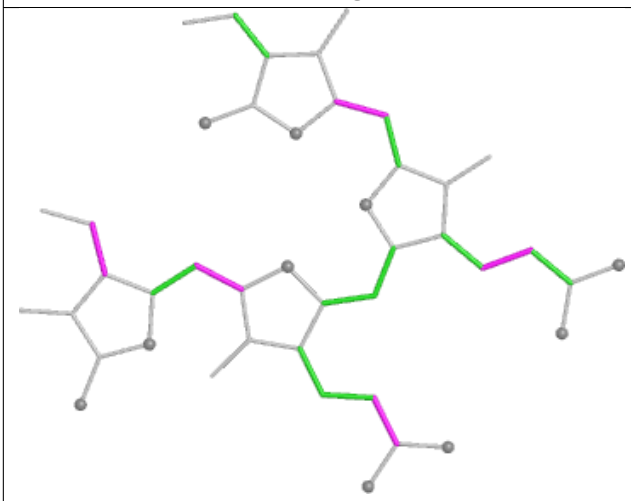

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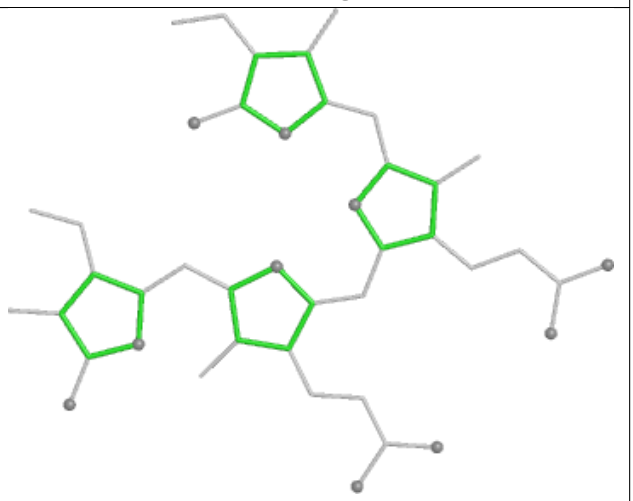
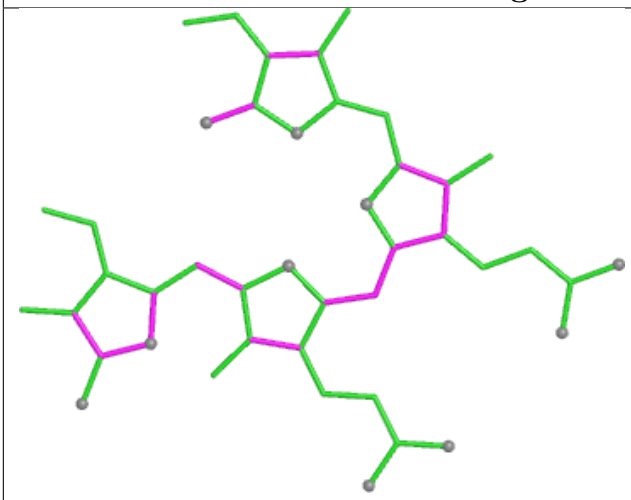


Rings

Ligand PEB SM 203



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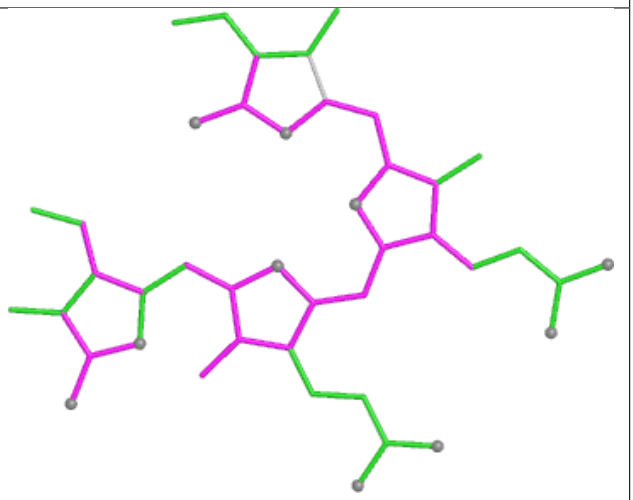

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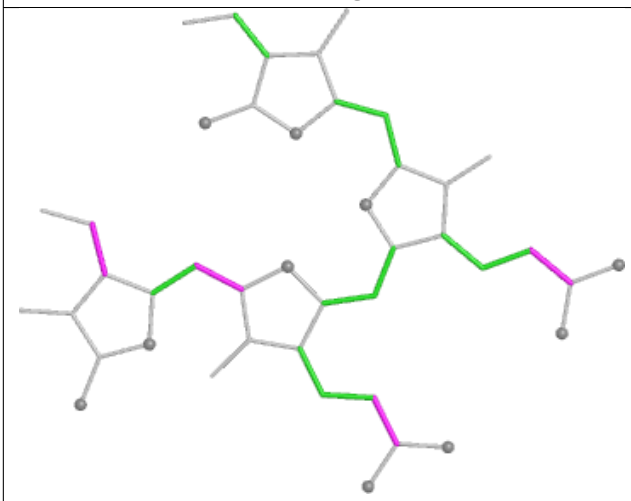

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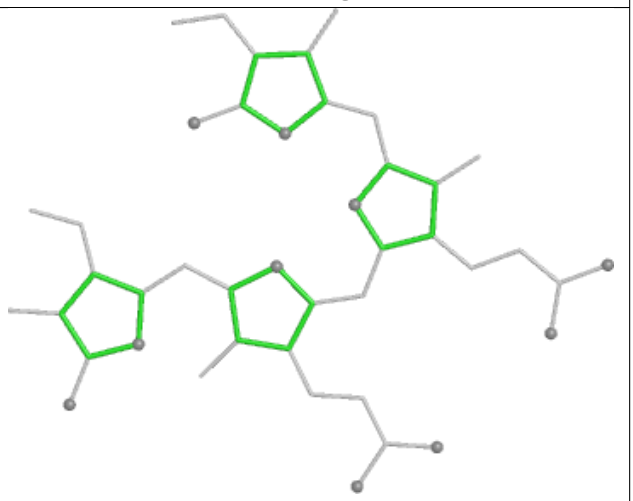
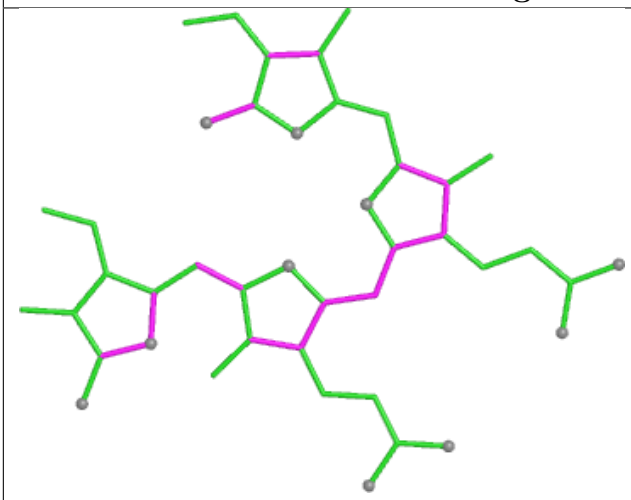


Rings

Ligand PEB LQ 201



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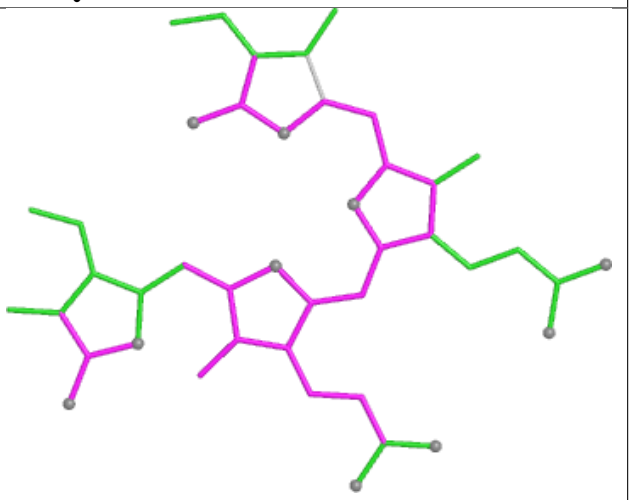

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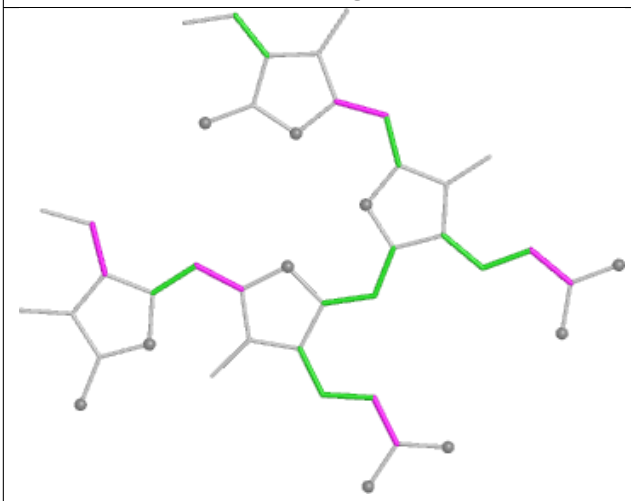

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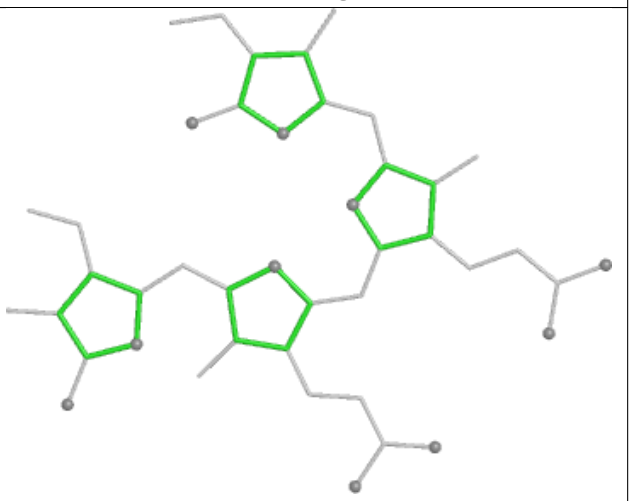
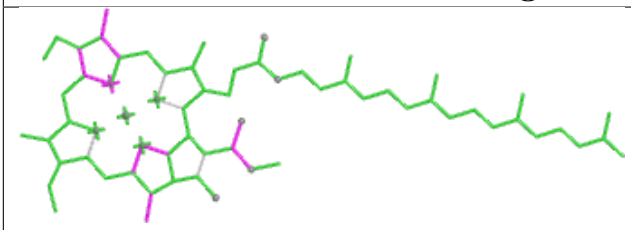


Rings

Ligand CLA 32 304



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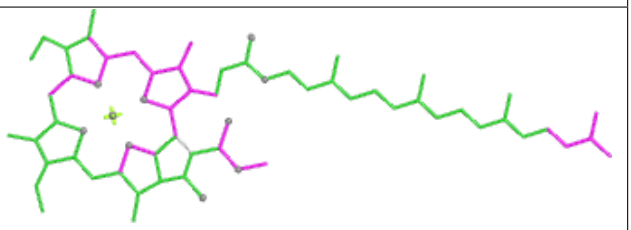

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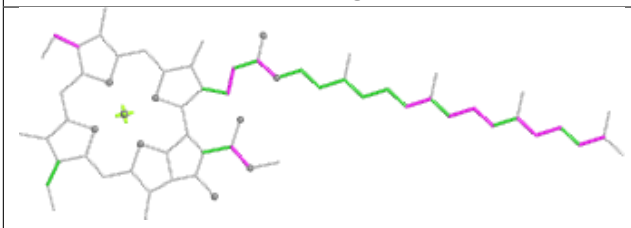

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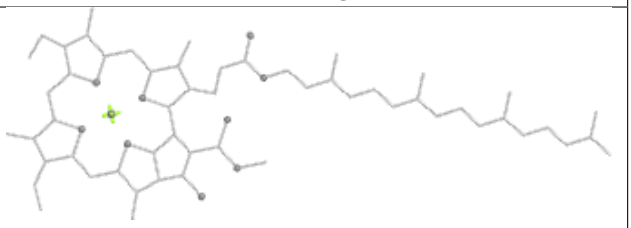
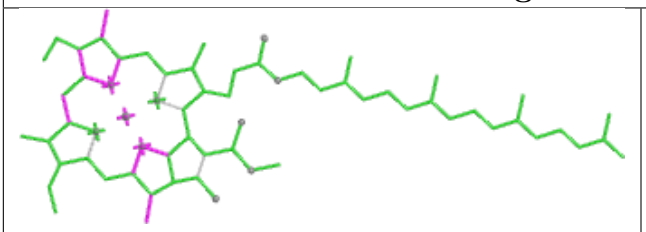


Rings

Ligand CLA A2 821



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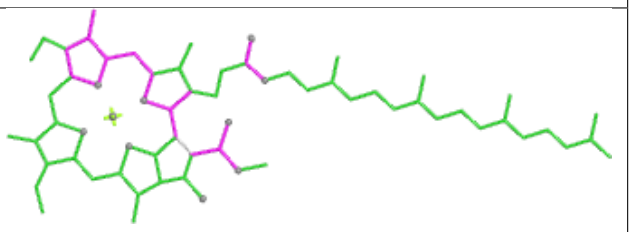

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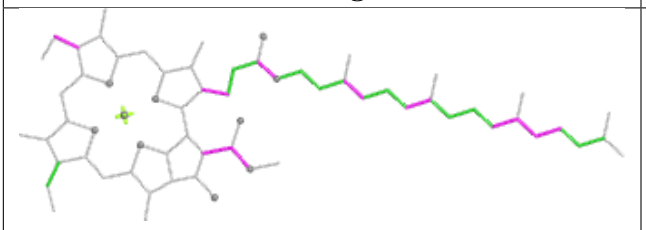

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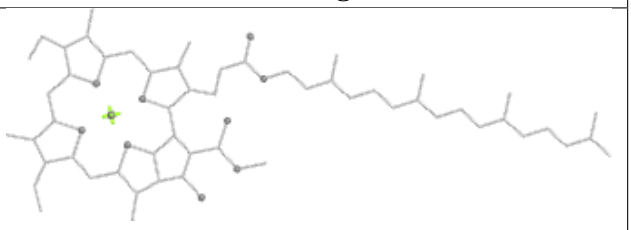
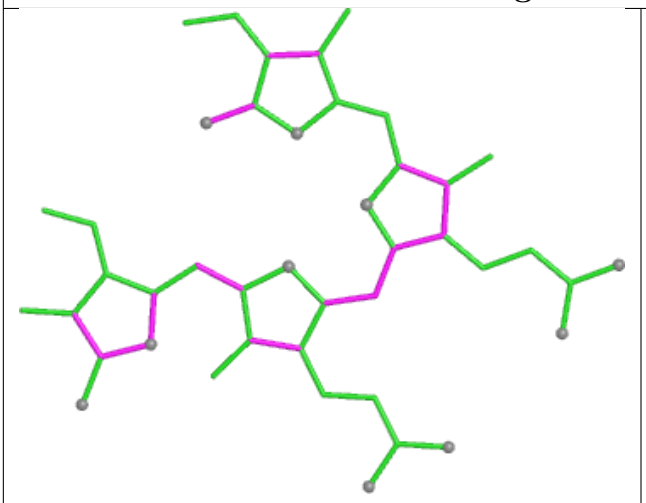


Rings

Ligand PEB bO 202



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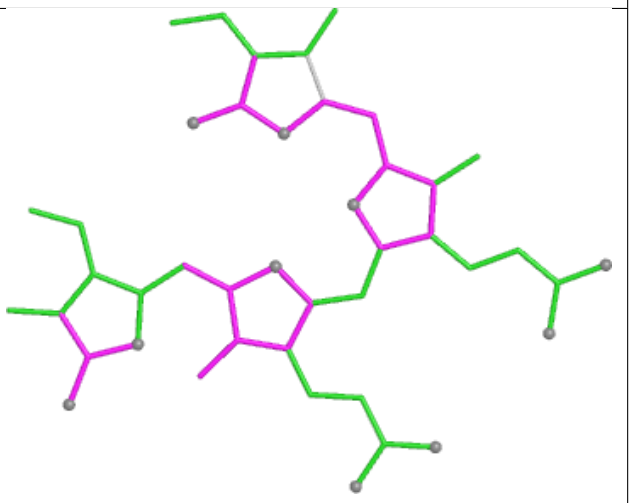

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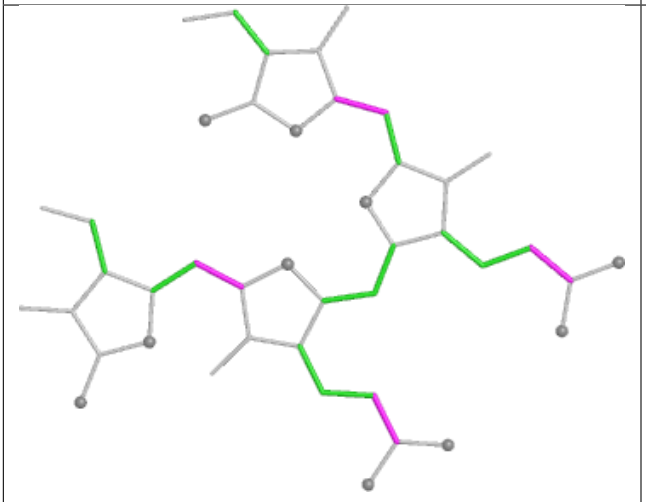

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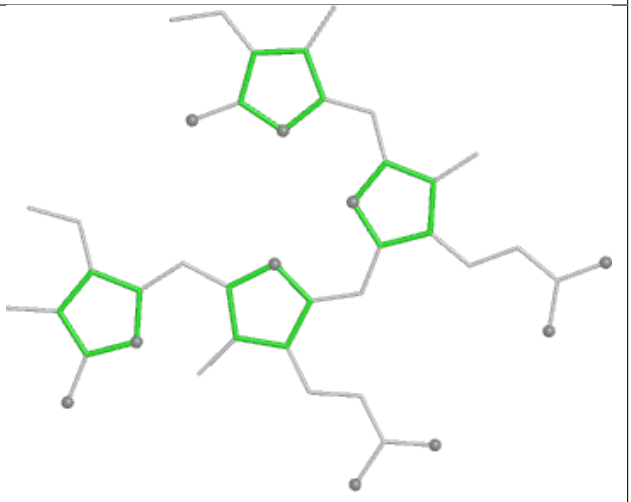
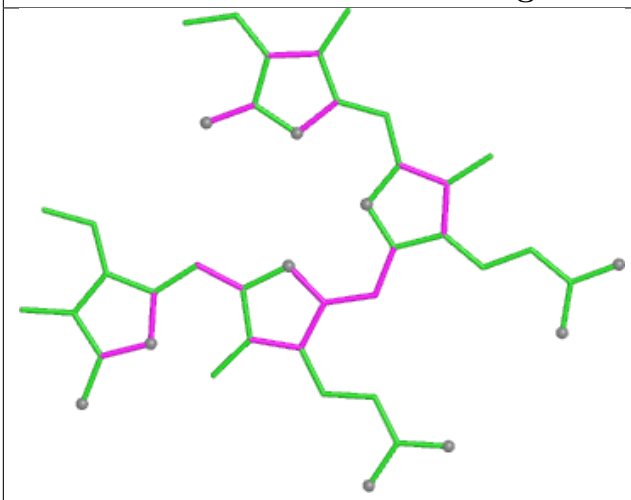


Rings

Ligand PEB HI 202



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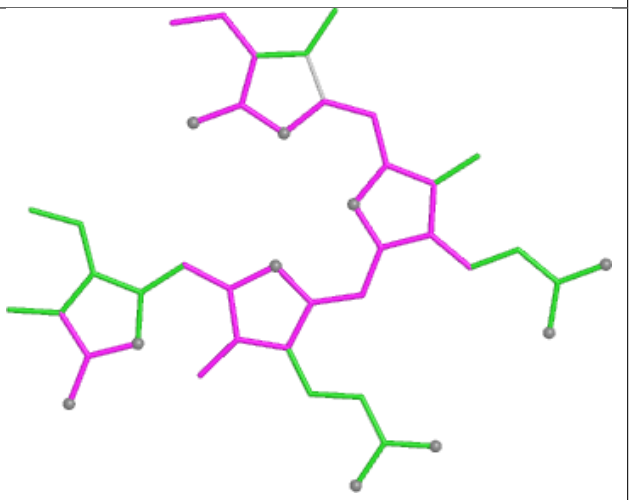

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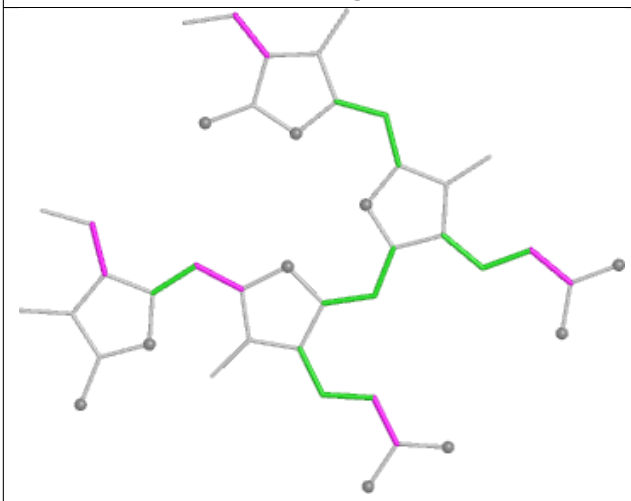

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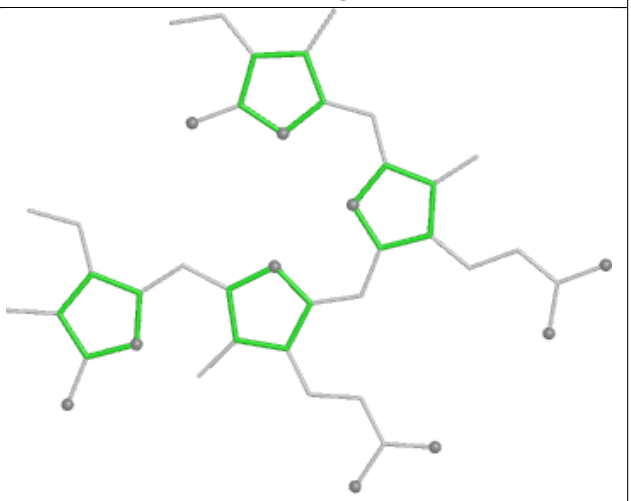
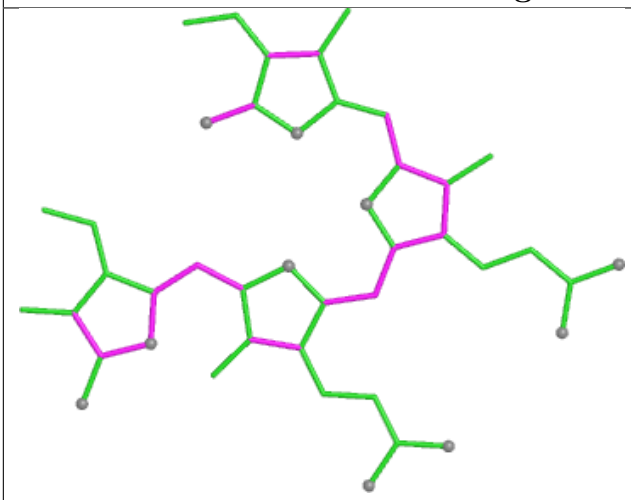


Rings

Ligand PEB hO 201



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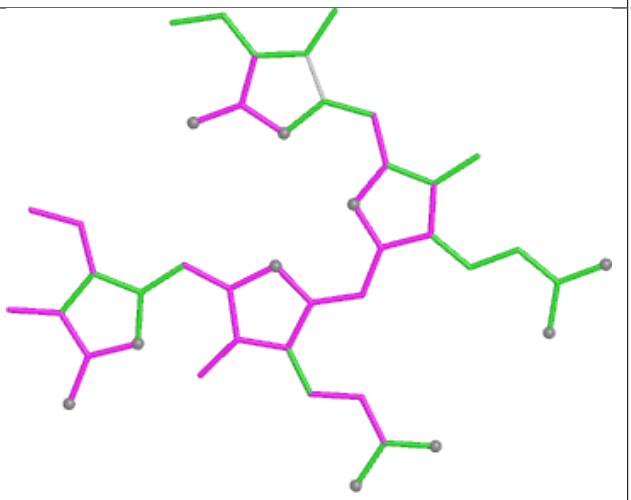

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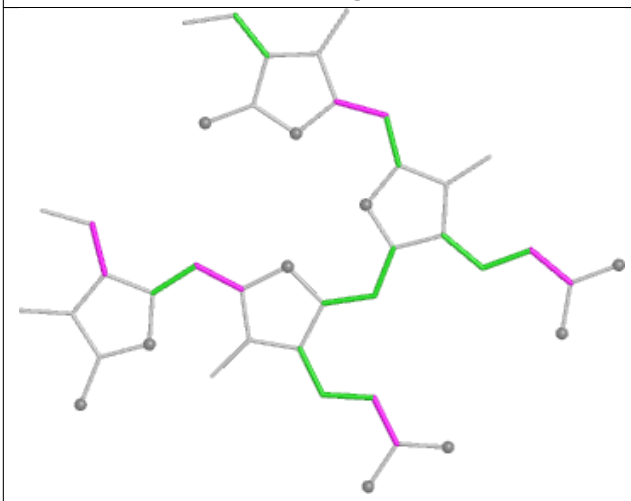

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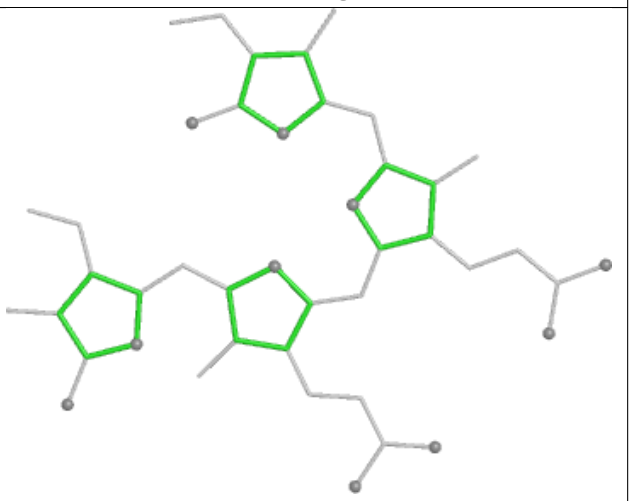
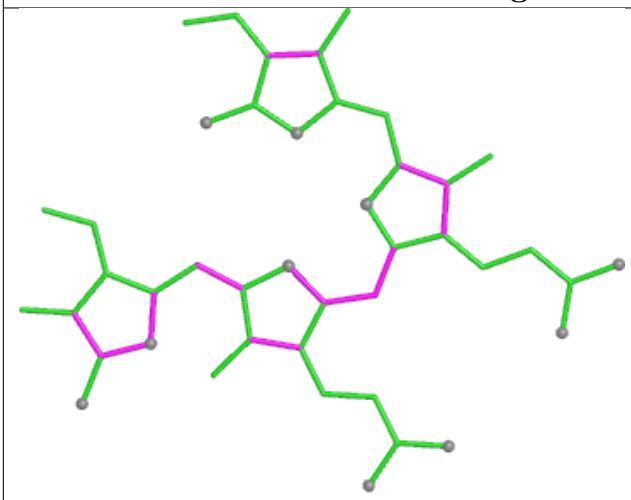


Rings

Ligand PEB UA 201



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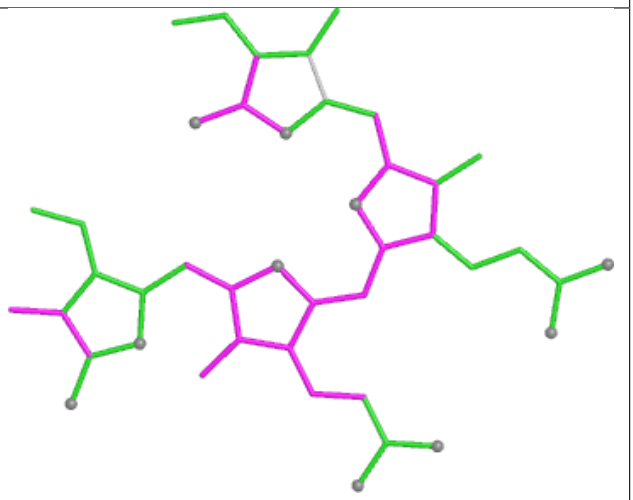
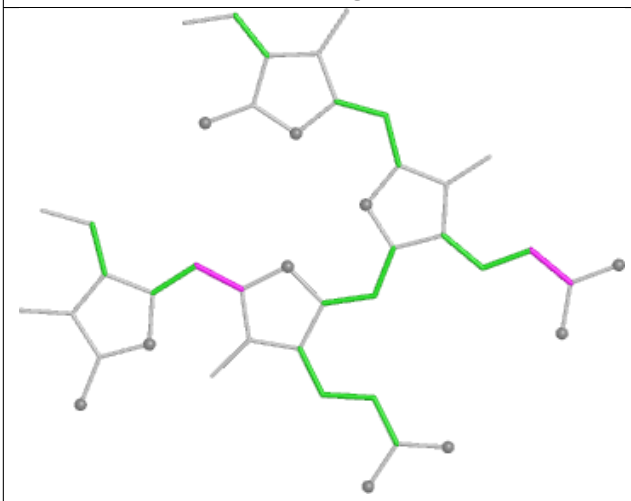


Bond angles



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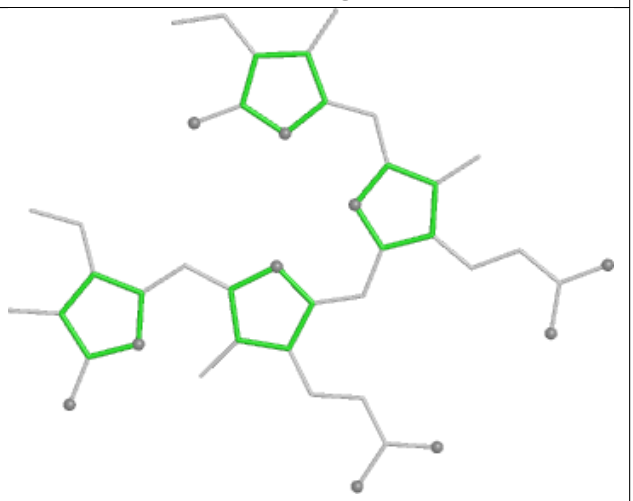
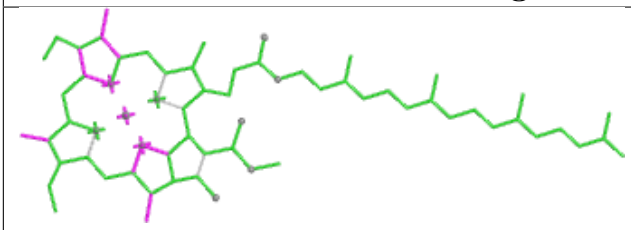


Rings

Ligand CLA BN 813



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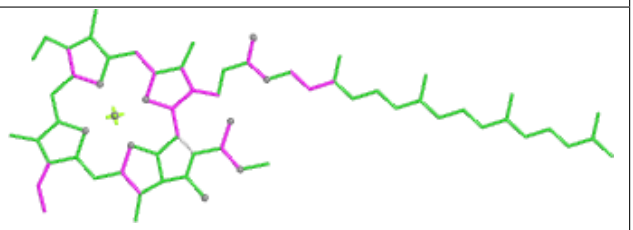
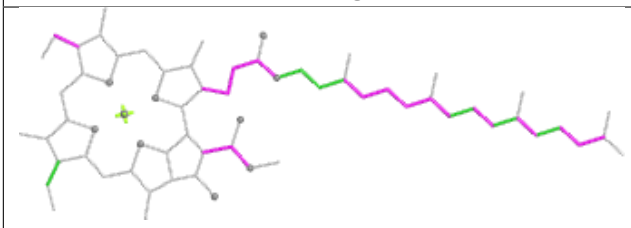


Bond angles



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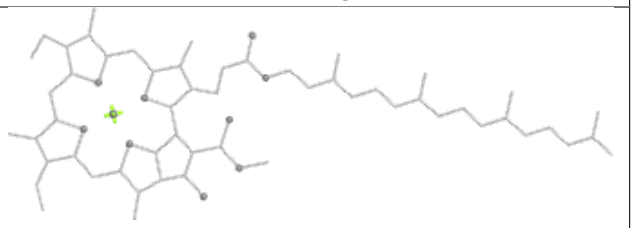
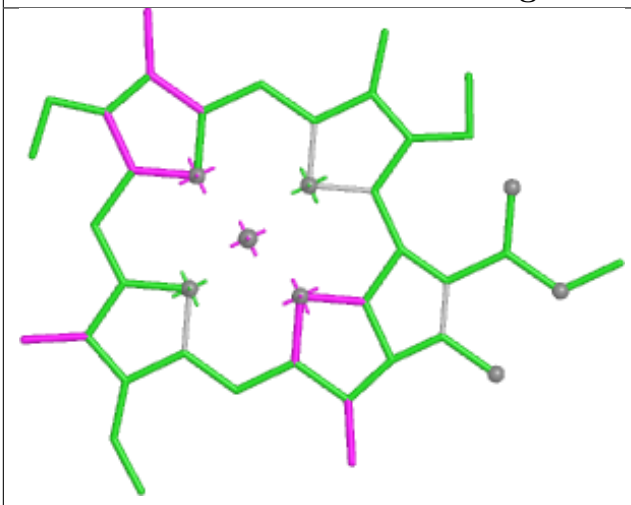


Rings

Ligand CLA 72 604



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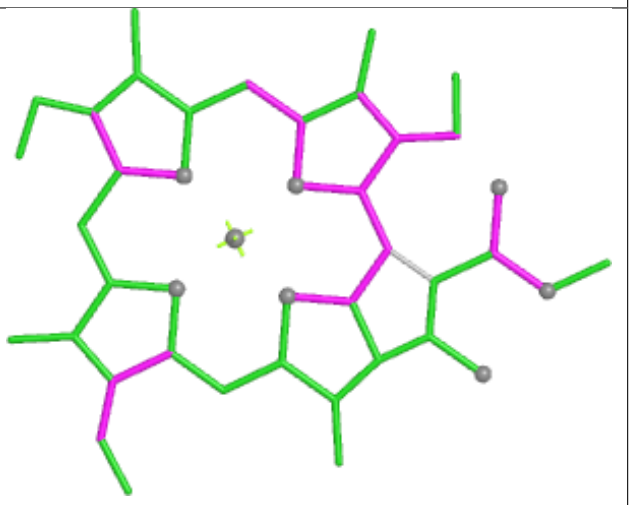

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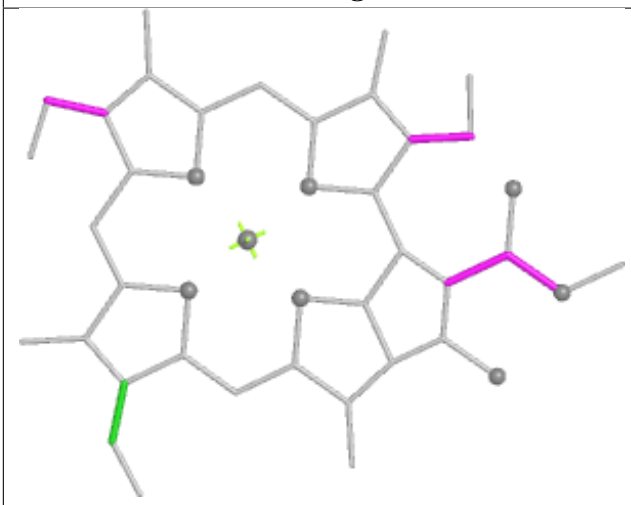
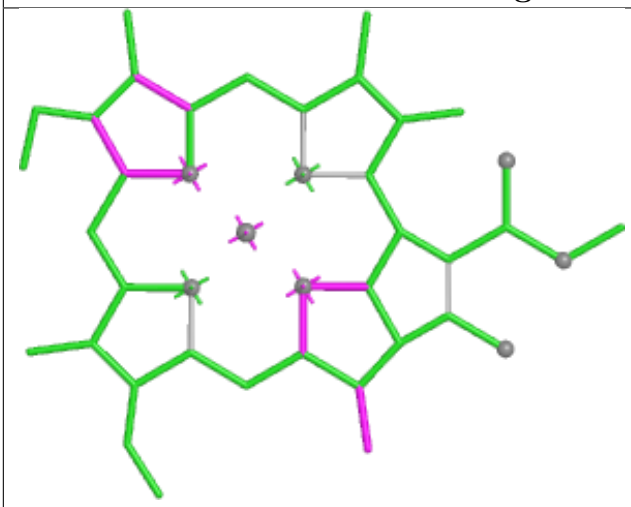


Torsions



Rings

Ligand CLA 3N 310



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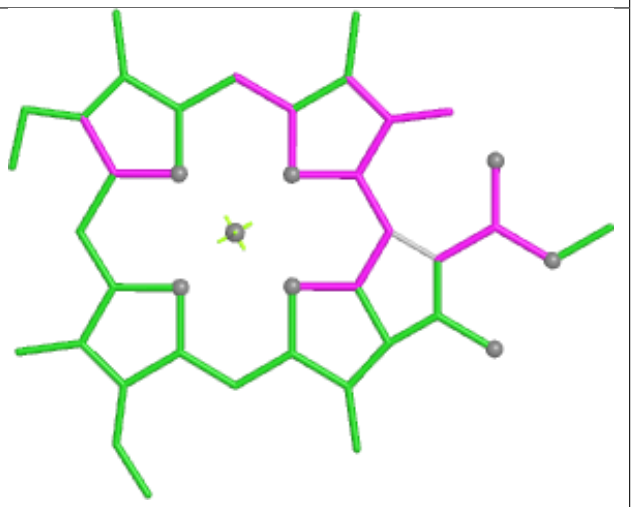

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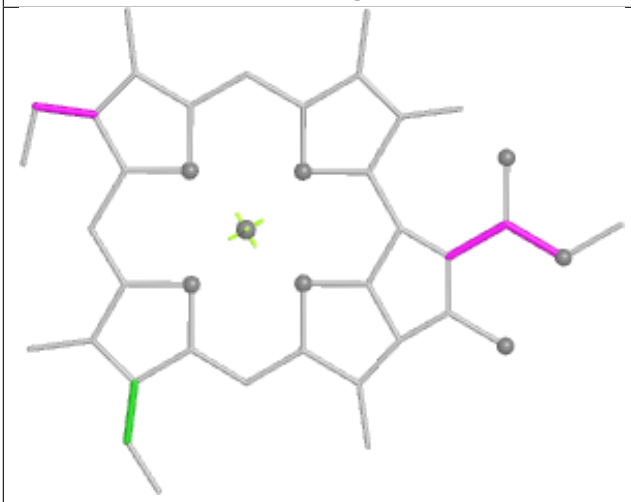

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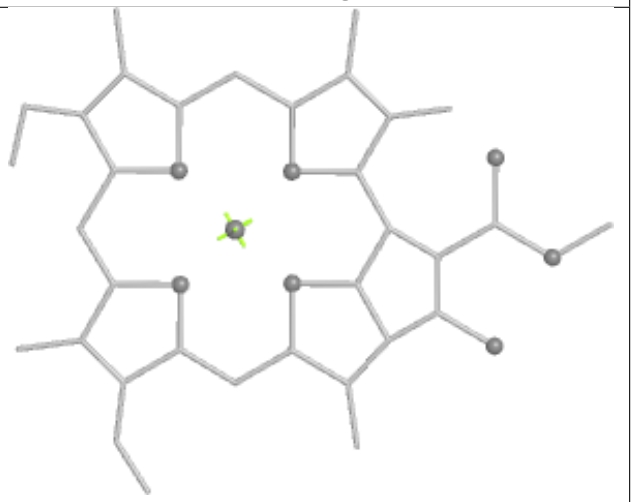
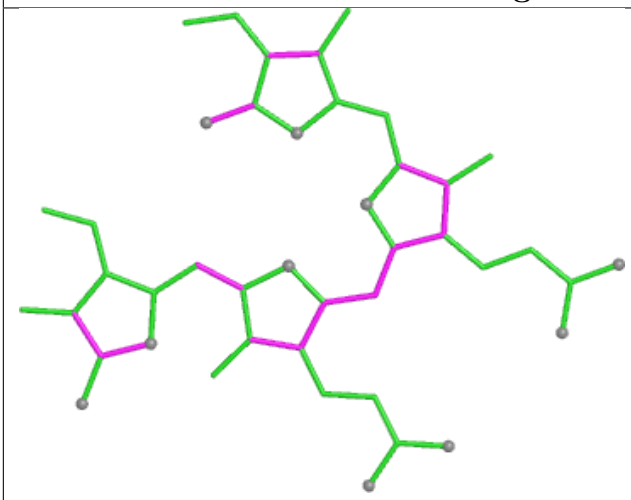


Rings

Ligand PEB PA 202



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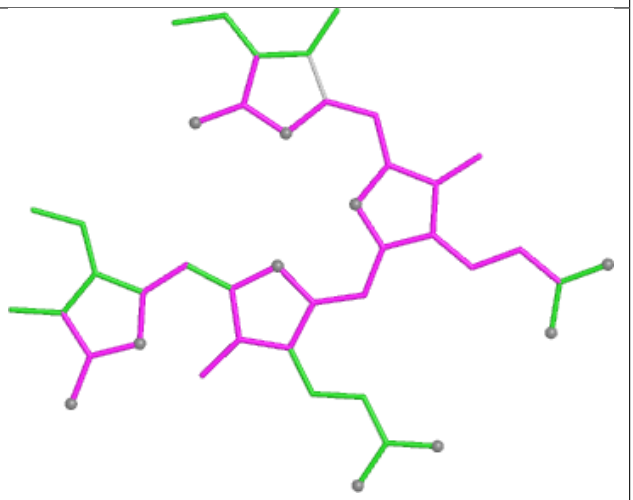

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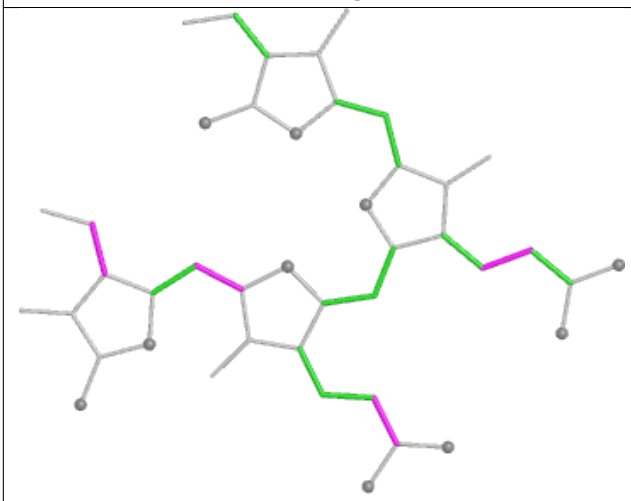

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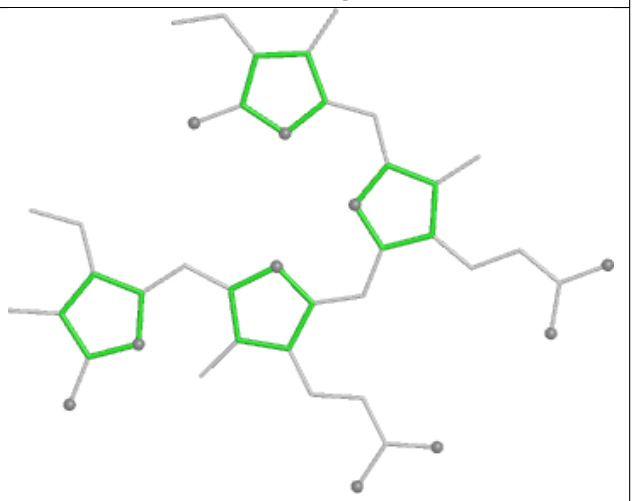
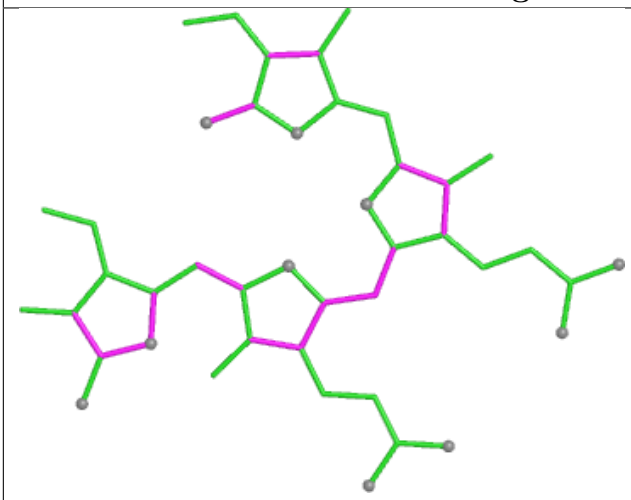


Rings

Ligand PEB PO 202



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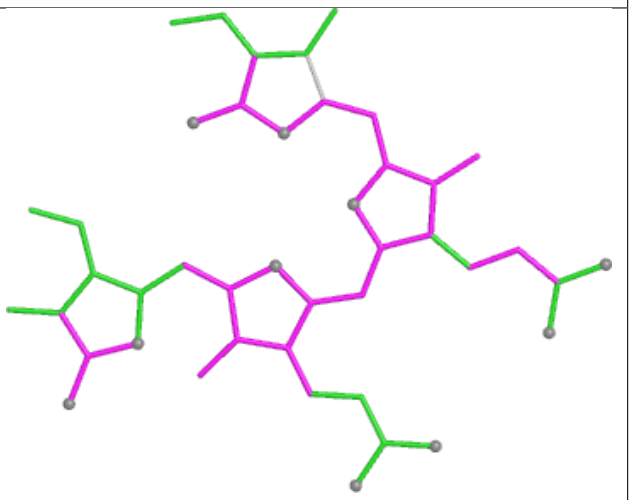

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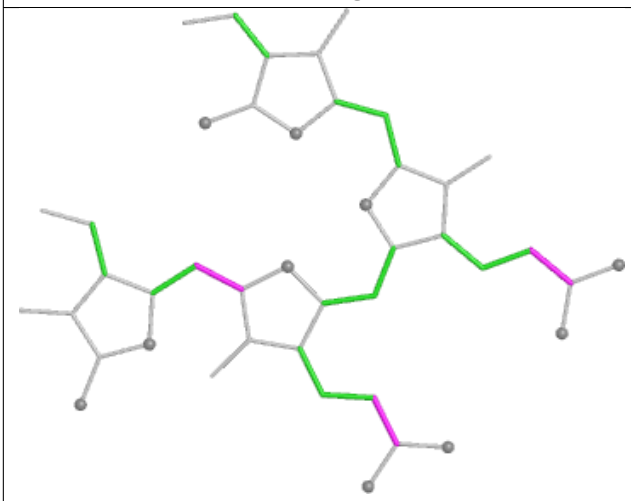

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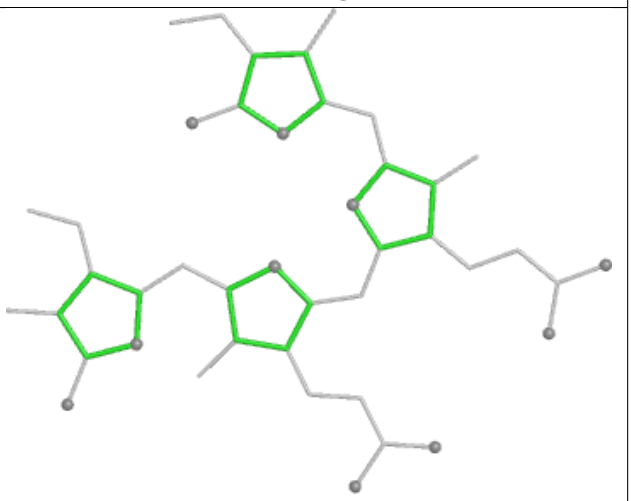
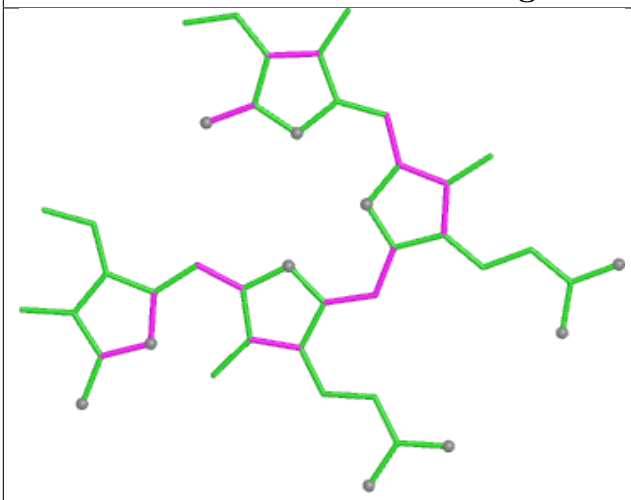


Rings

Ligand PEB fH 202



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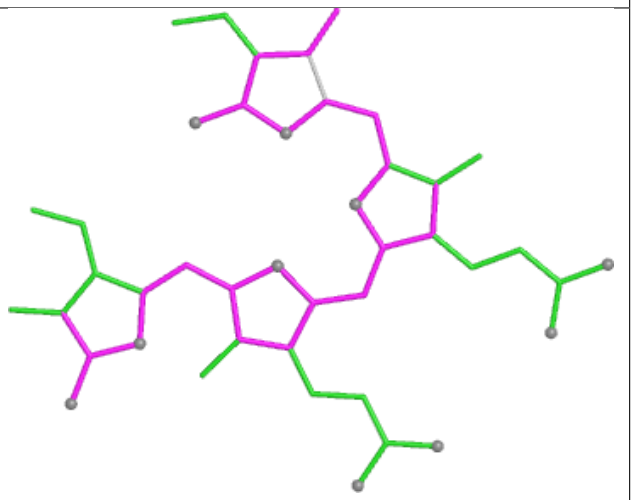

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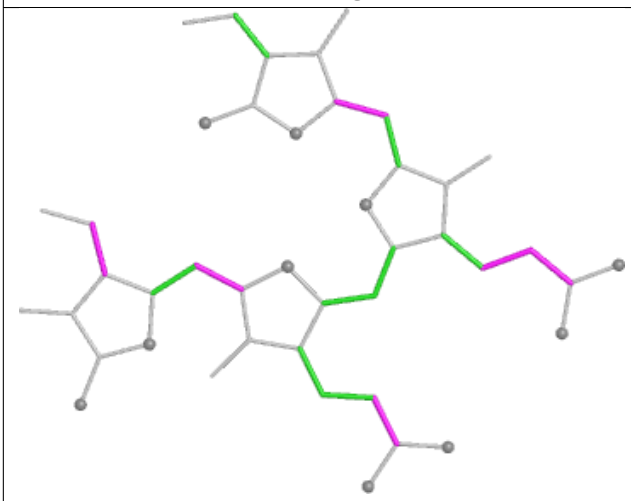

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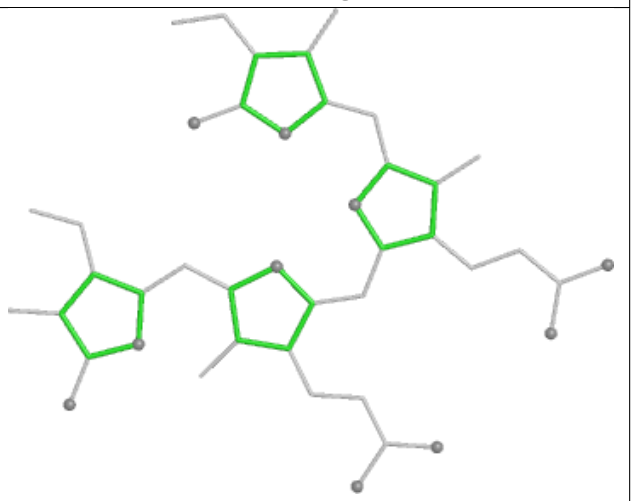
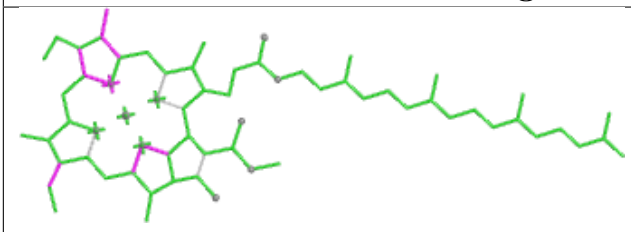


Rings

Ligand CLA L2 203



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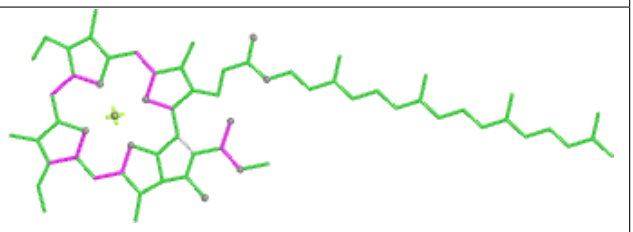

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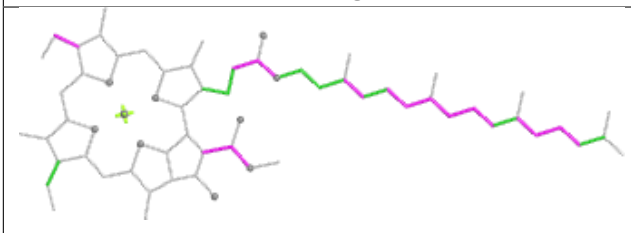

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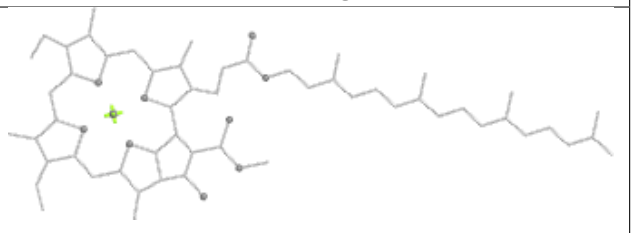
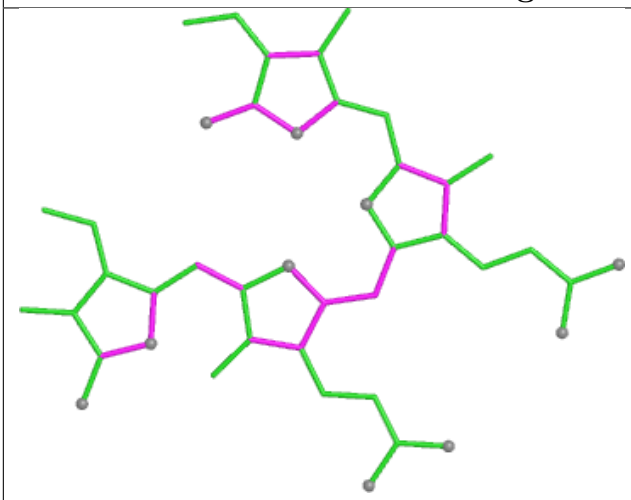


Rings

Ligand PEB KI 201



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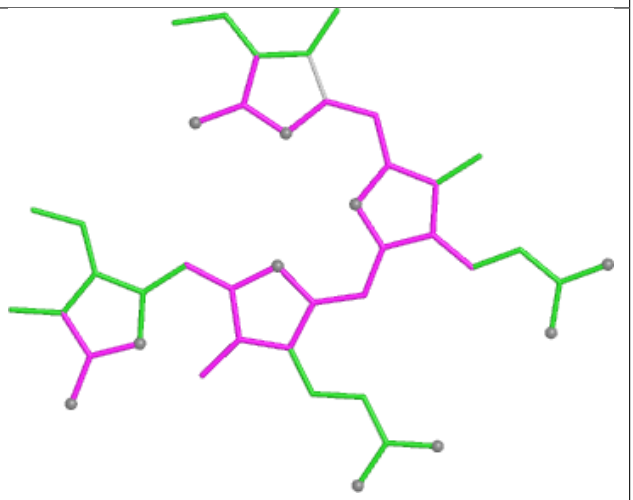

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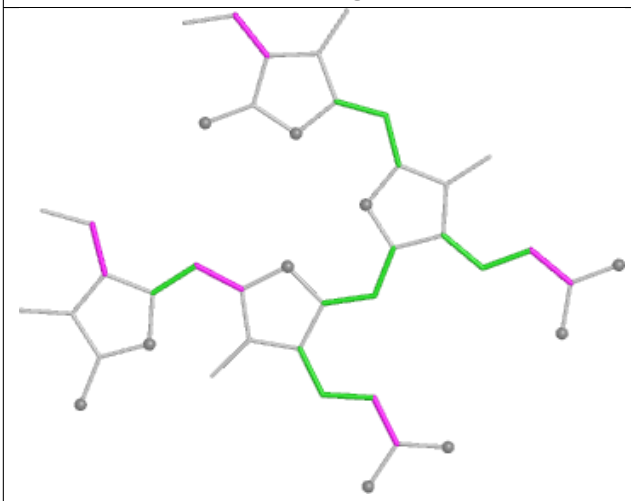

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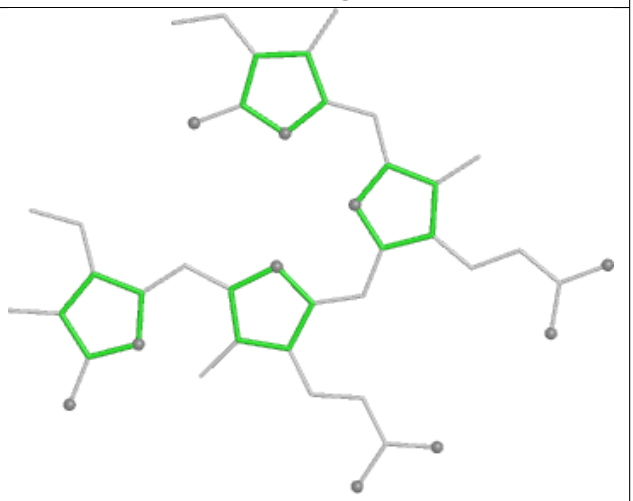
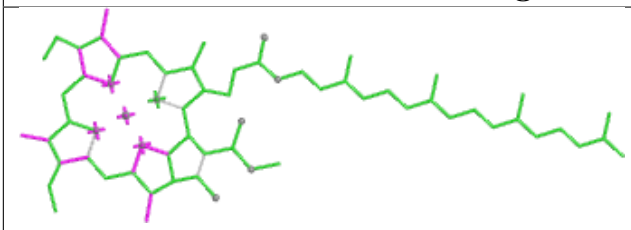


Rings

Ligand CLA 8N 303



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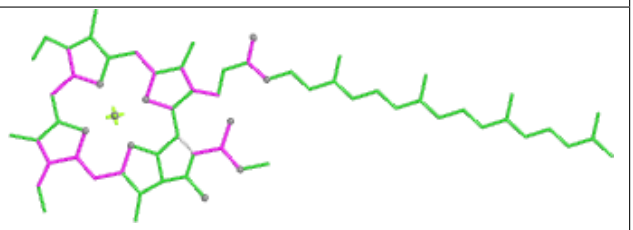

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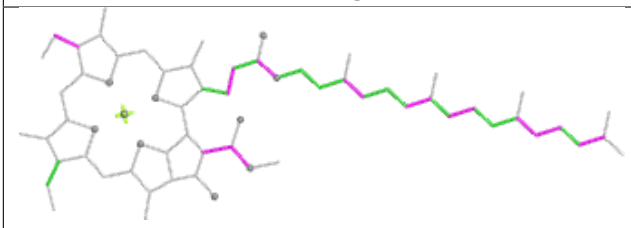

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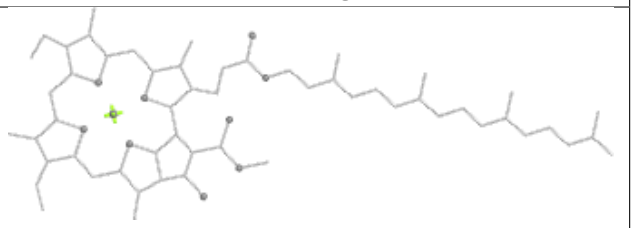
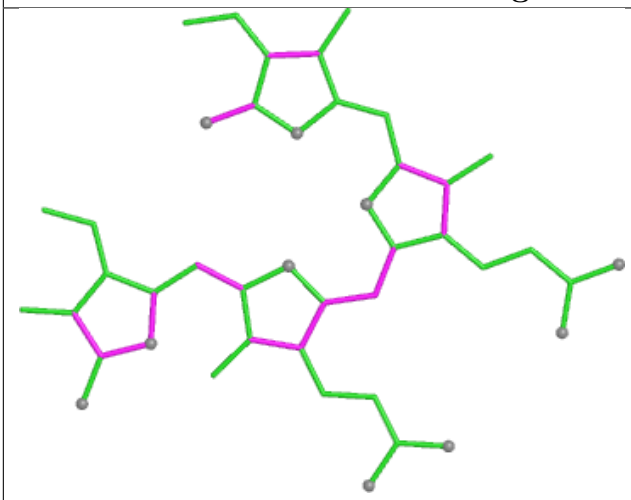


Rings

Ligand PEB UP 201



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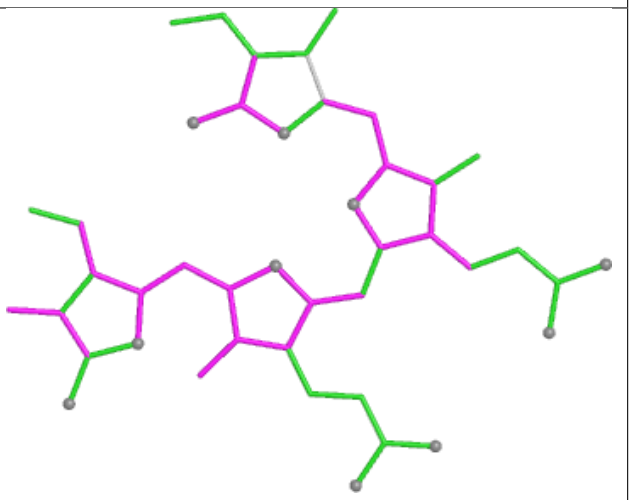

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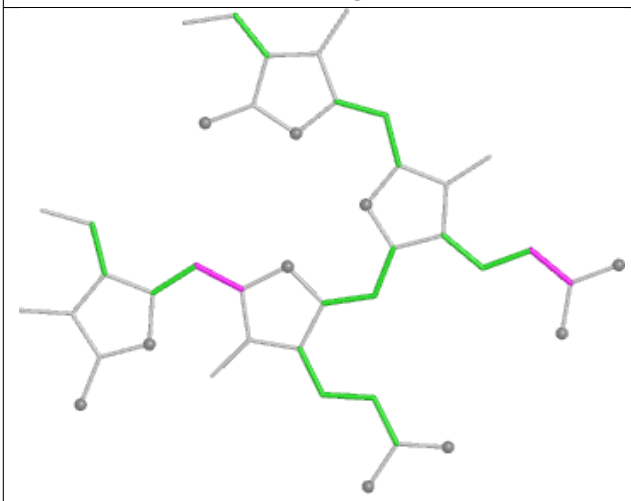

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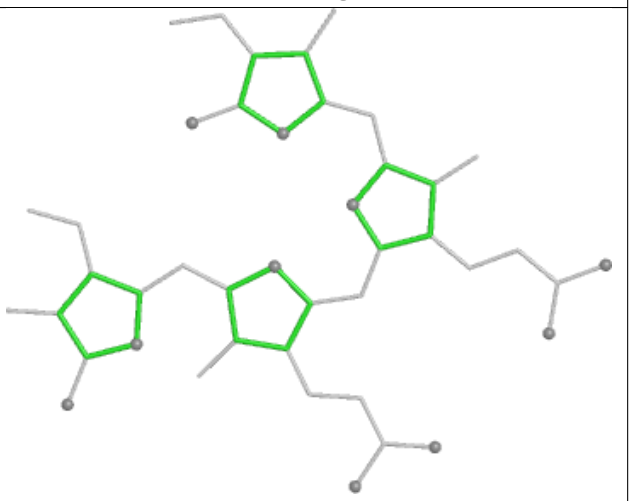
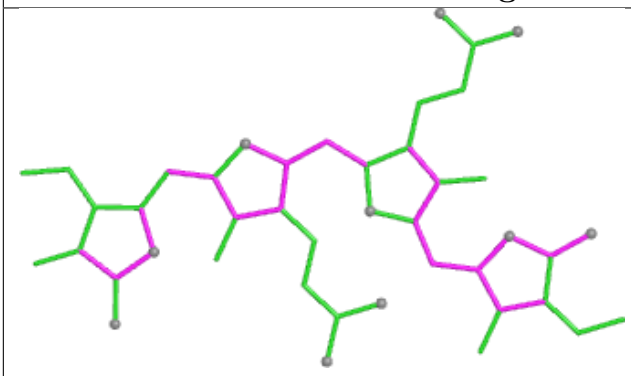


Rings

Ligand CYC NO 1001



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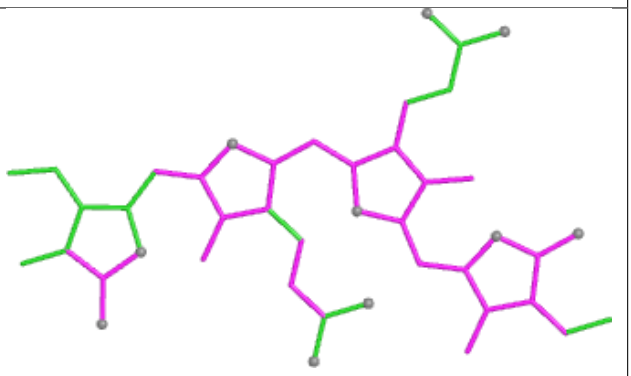

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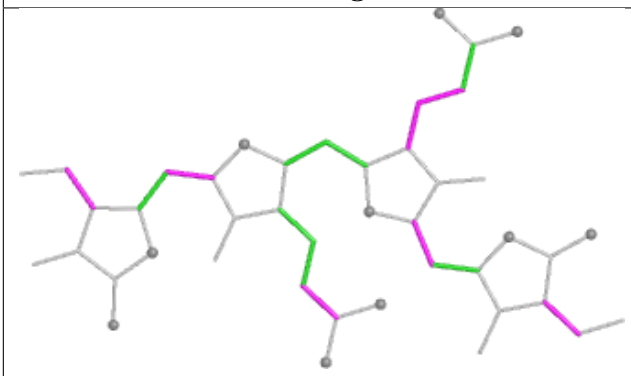

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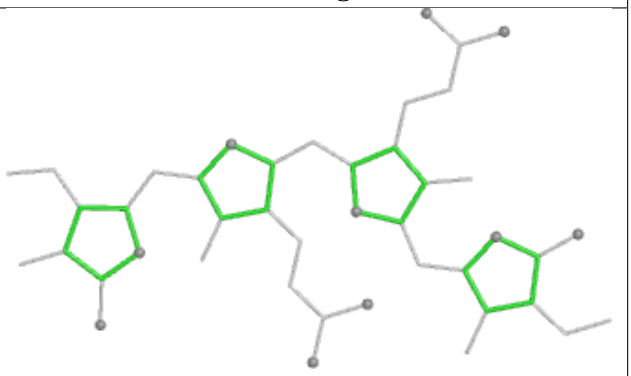
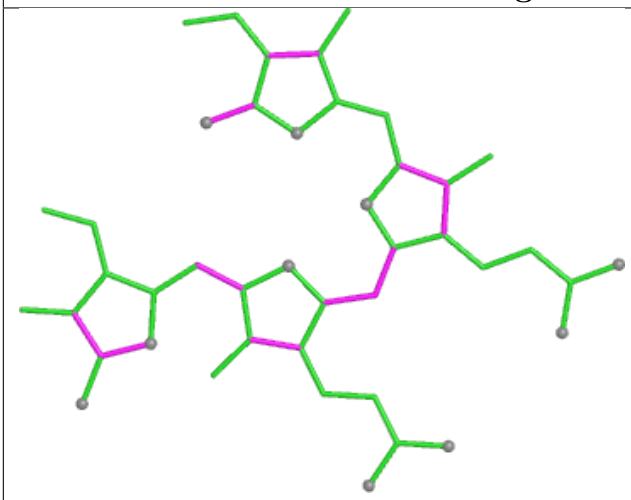


Rings

Ligand PEB FA 201



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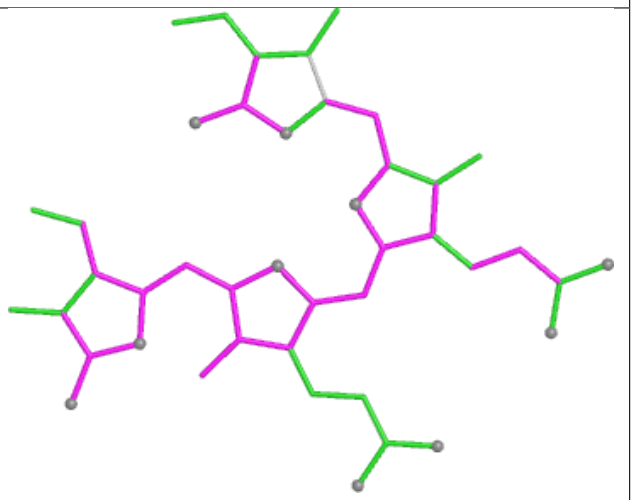

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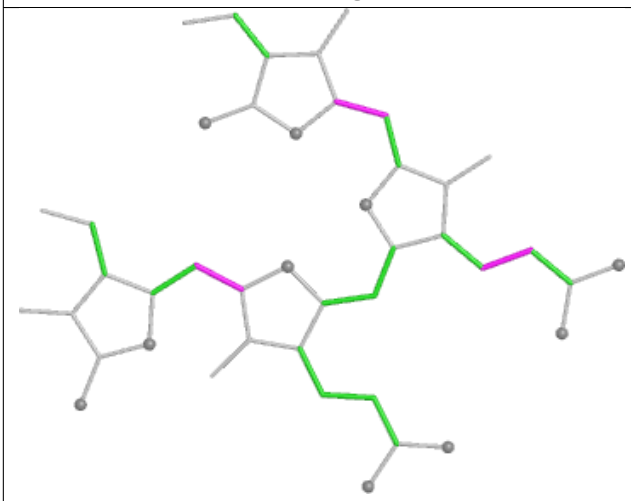

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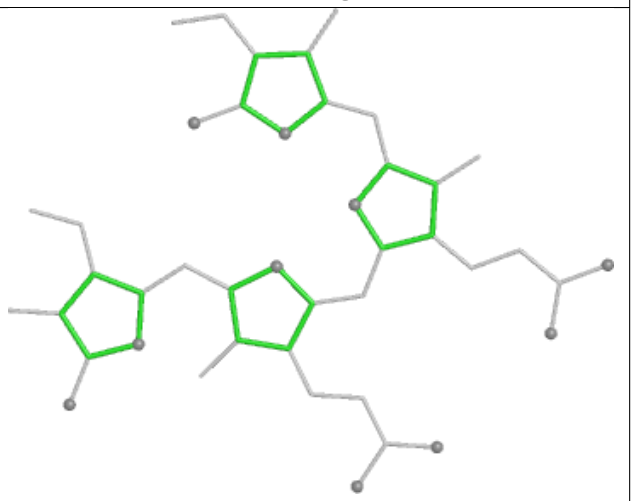
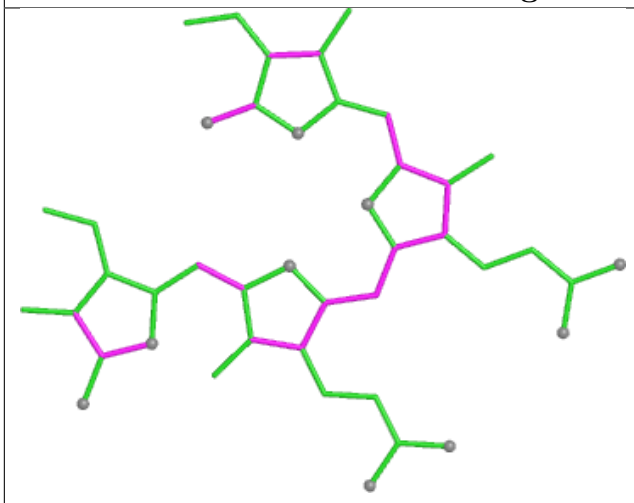


Rings

Ligand PEB g1 202



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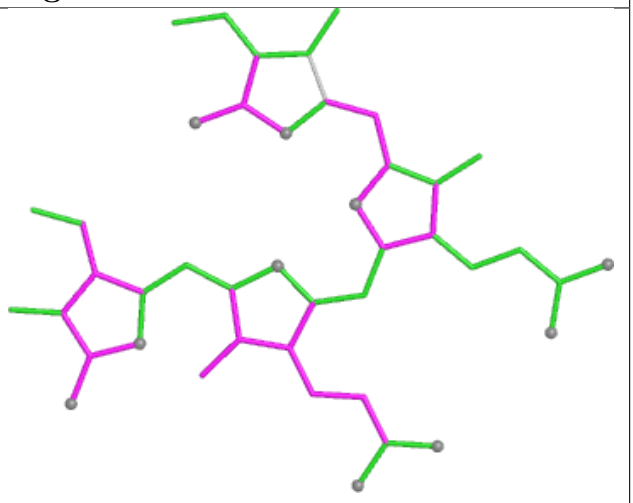
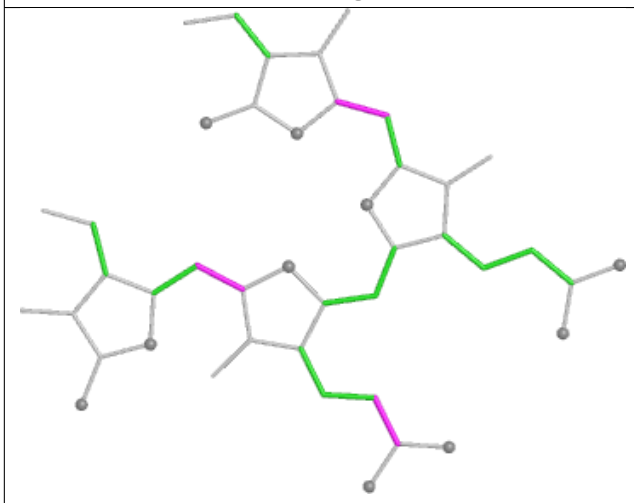


Bond angles



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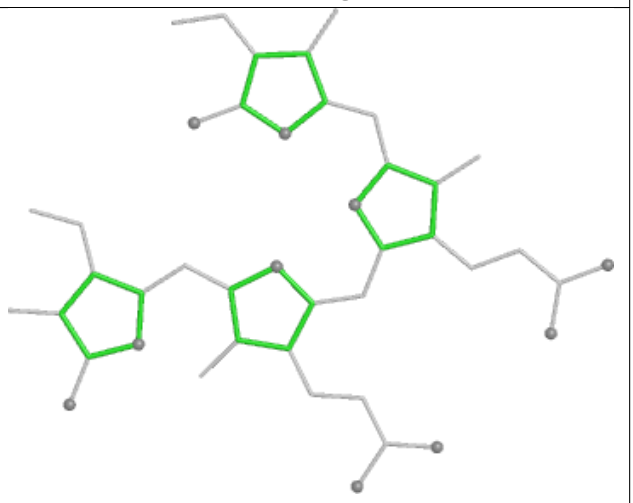
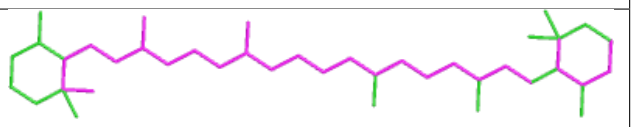


Rings

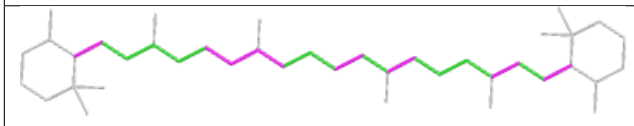
Ligand BCR K2 102



Bond lengths



Bond angles



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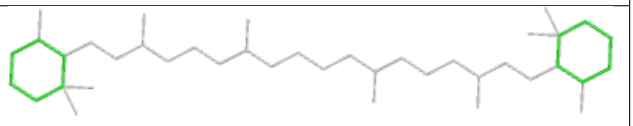
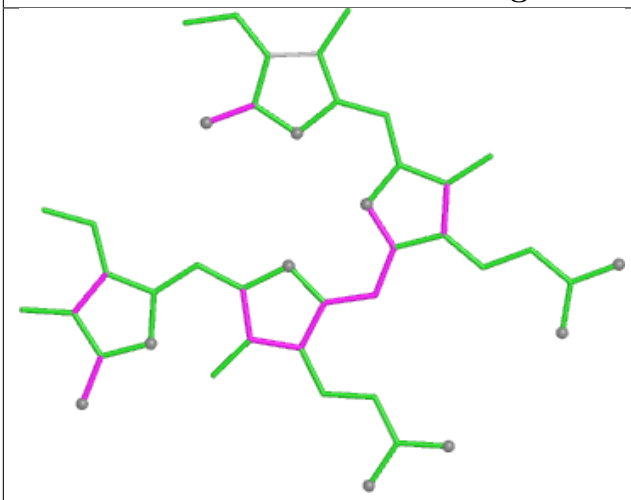
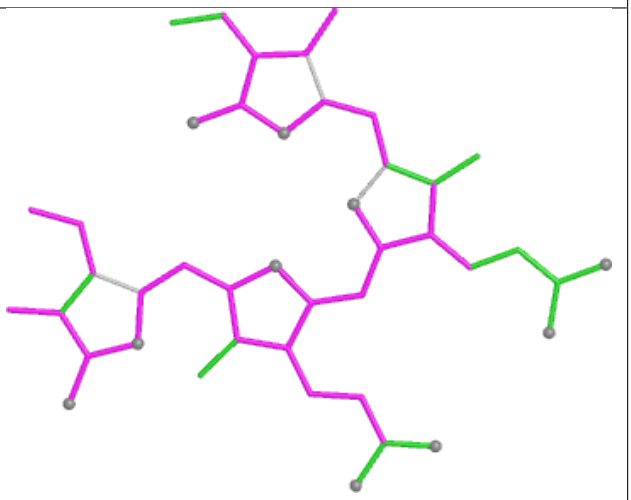


Rings

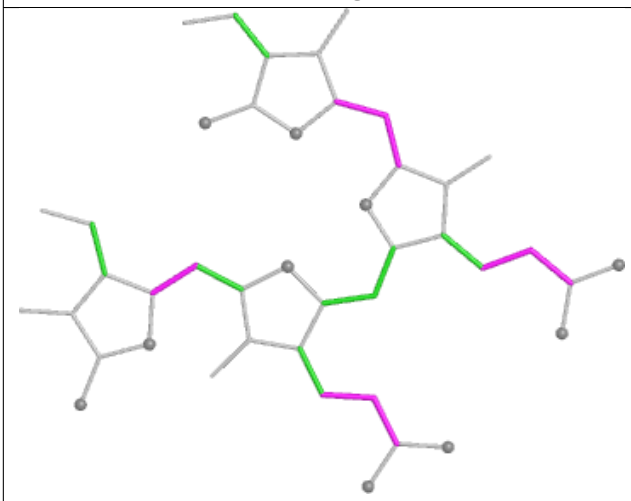
Ligand PUB AE 302



Bond lengths



Bond angles



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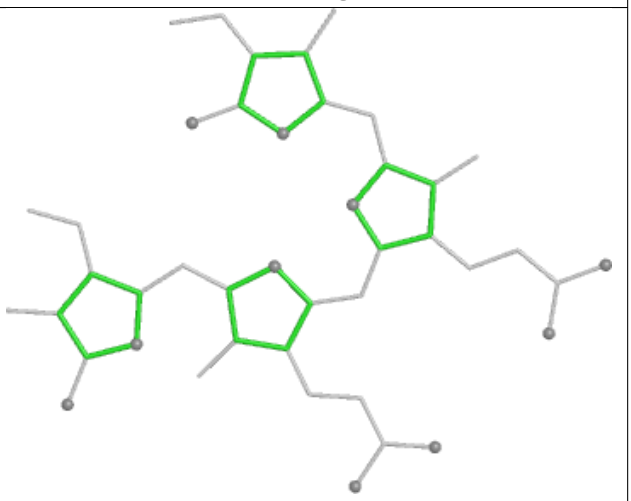
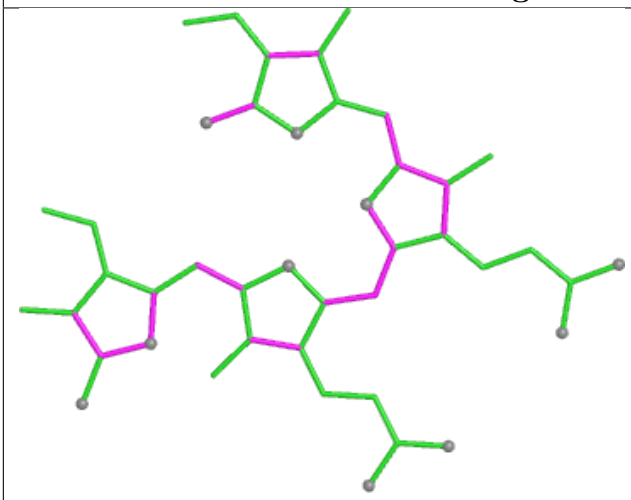
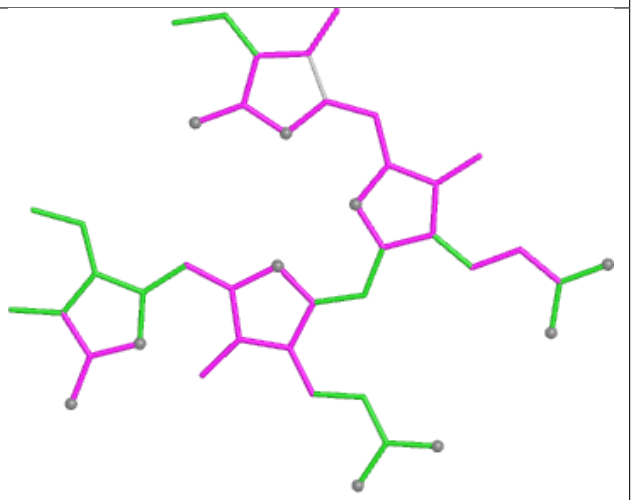


Rings

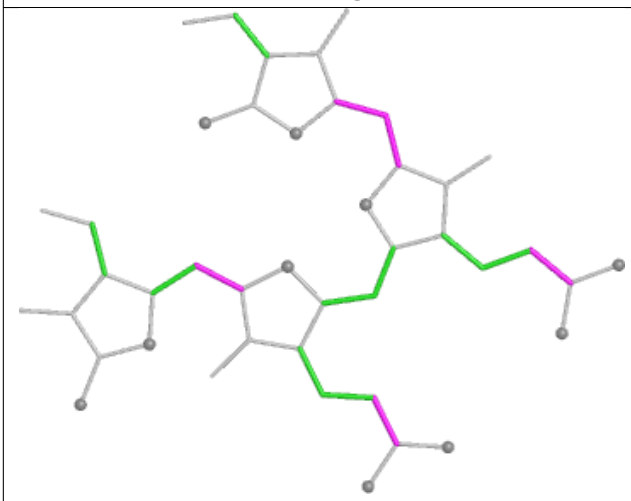
Ligand PEB OP 201



Bond lengths



Bond angles



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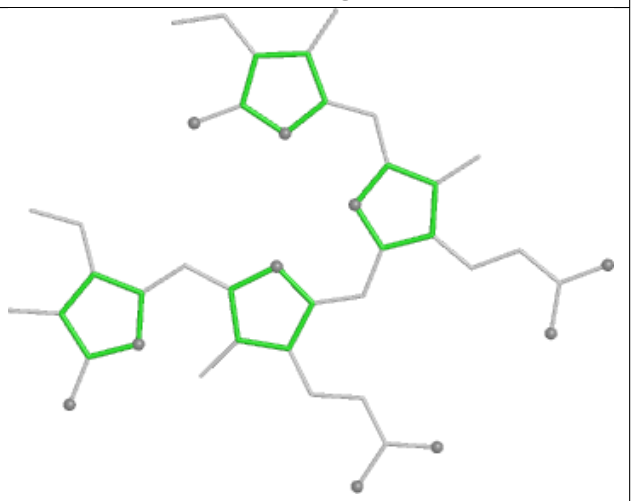
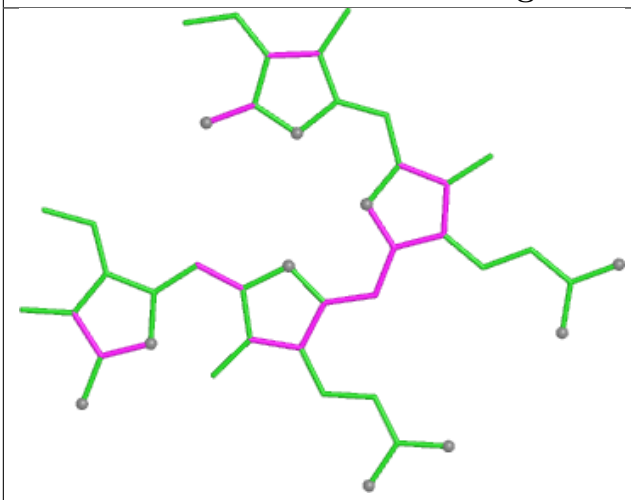
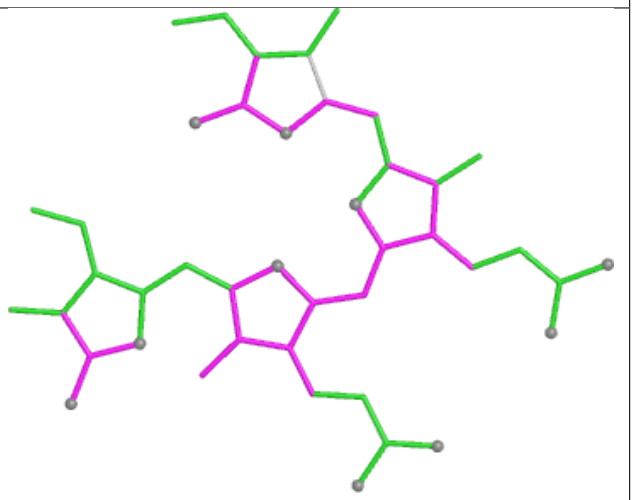


Rings

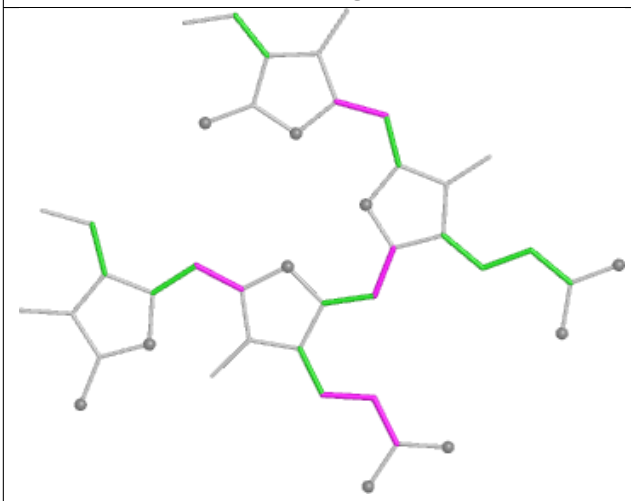
Ligand PEB vF 202



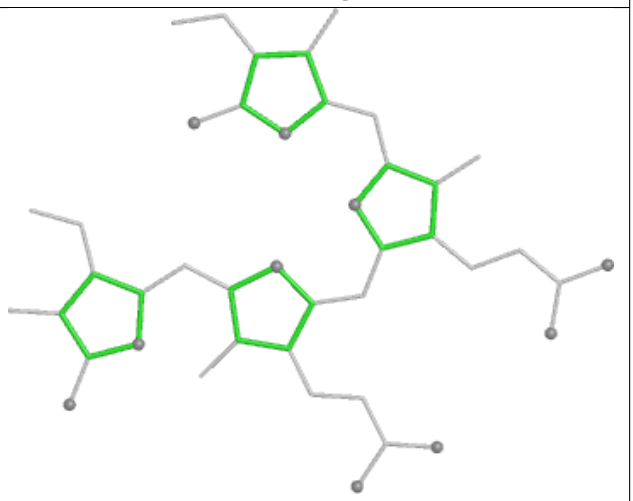
Bond lengths



Bond angles

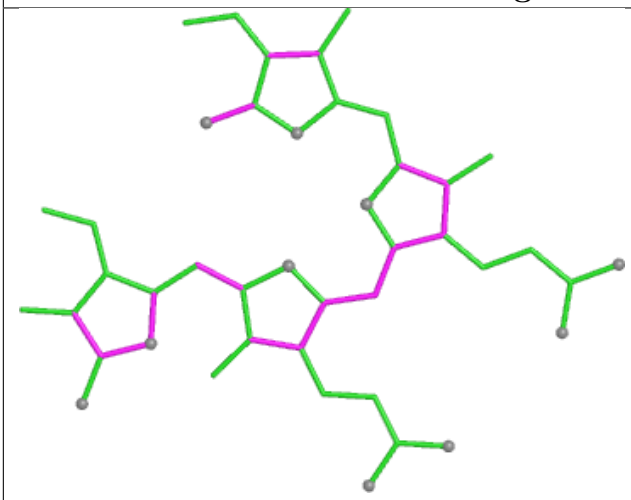


Torsions



Rings

Ligand PEB kG 201



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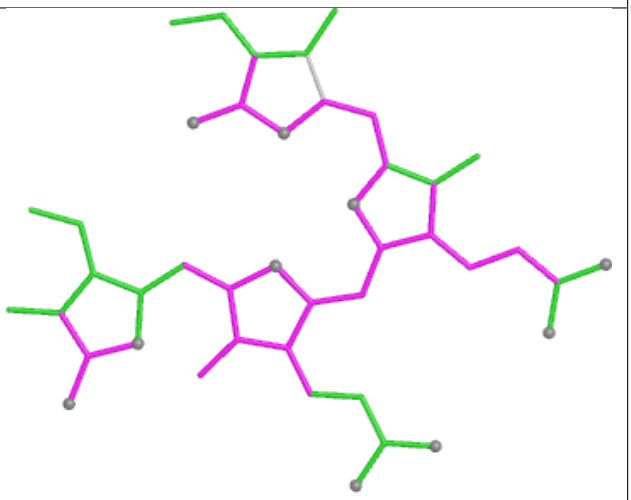

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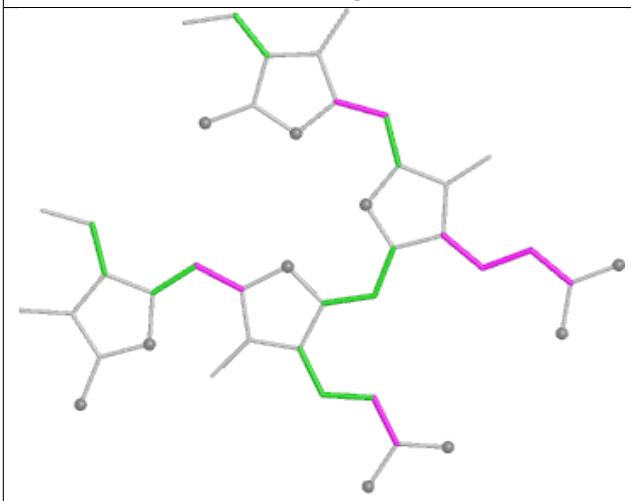

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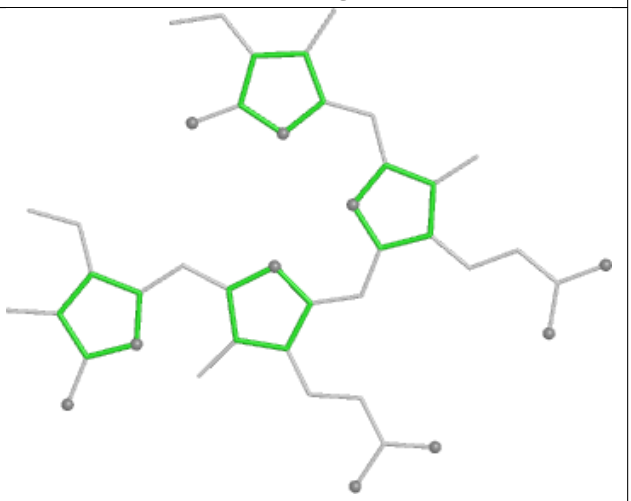
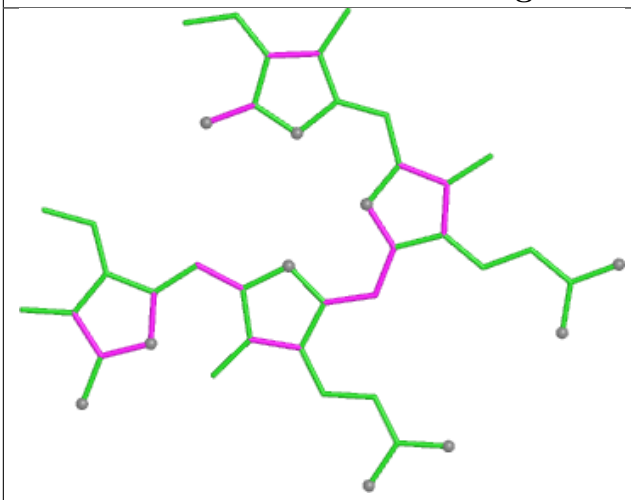


Rings

Ligand PEB V7 201



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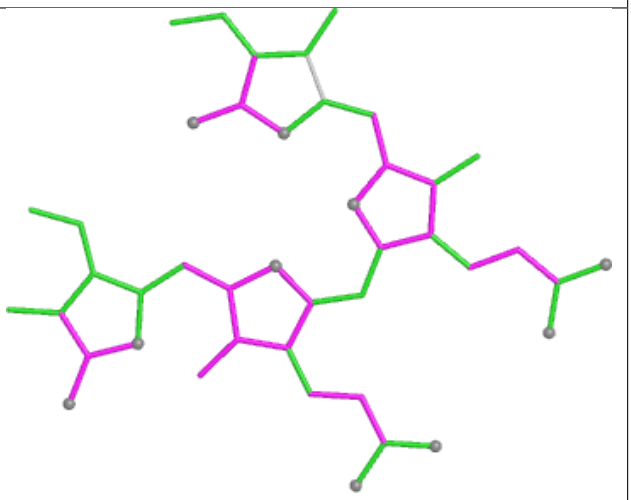
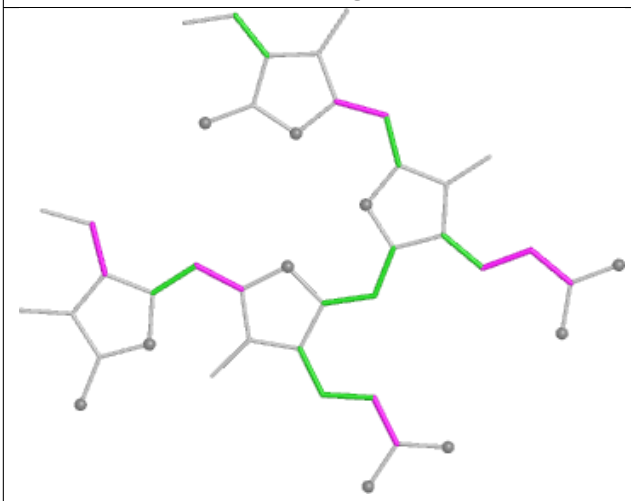


Bond angles



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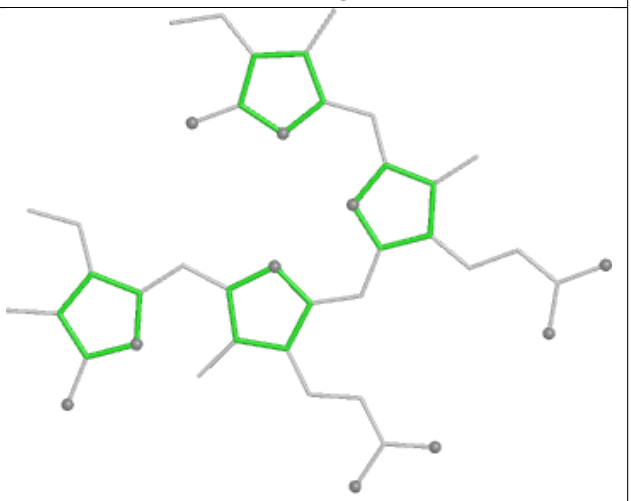
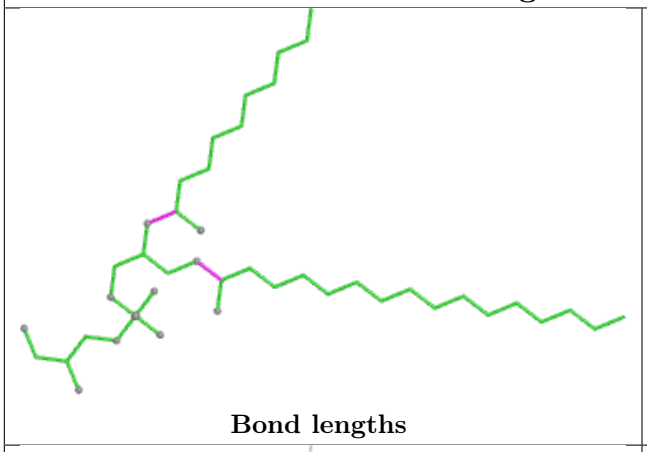


Rings

Ligand LHG a6 610



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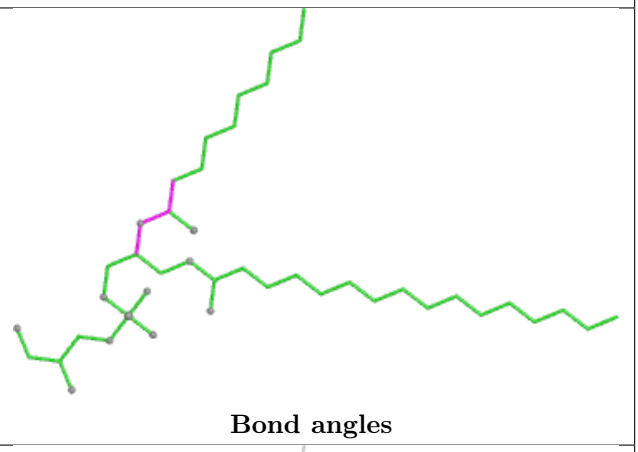

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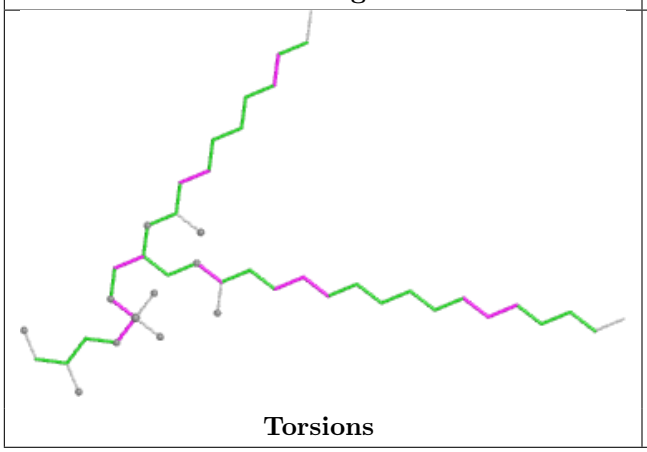

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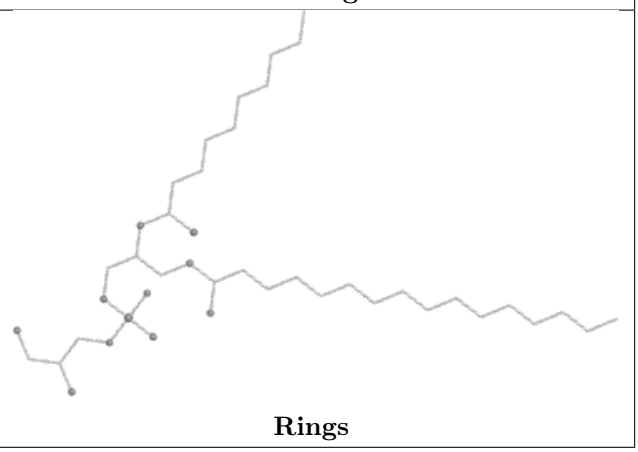
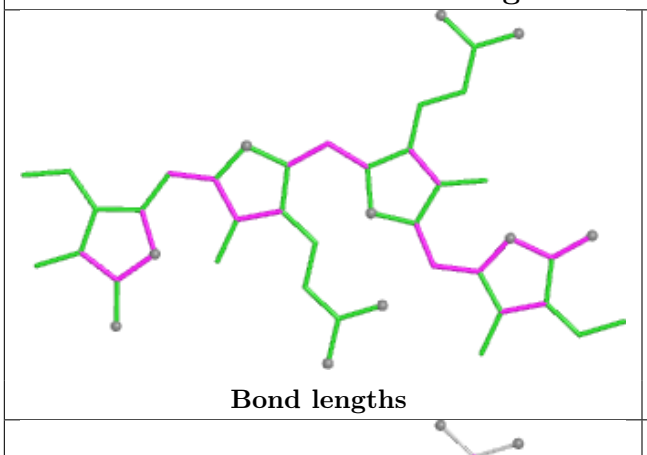


Rings

Ligand CYC FO 1001



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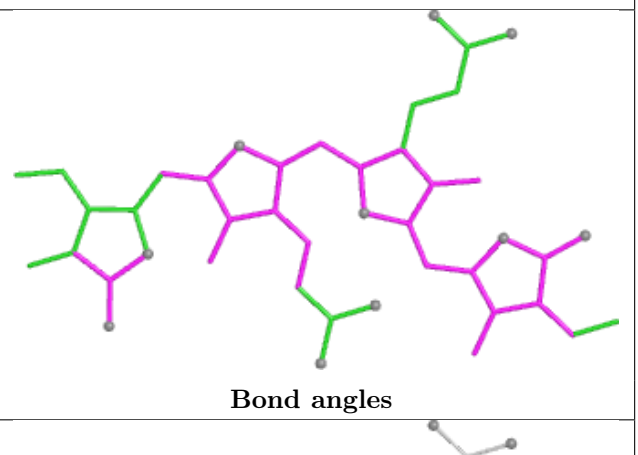

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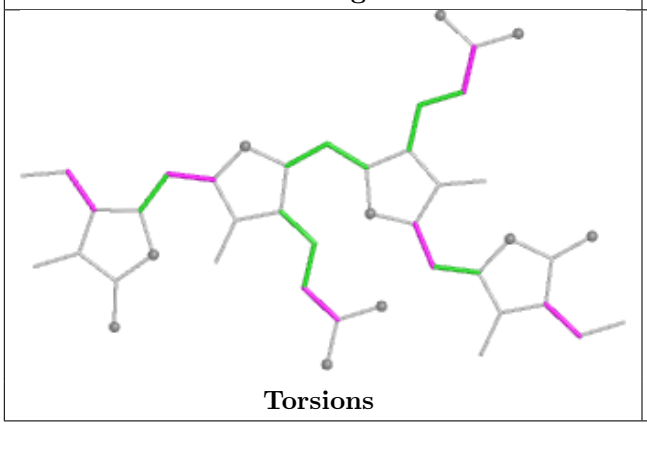

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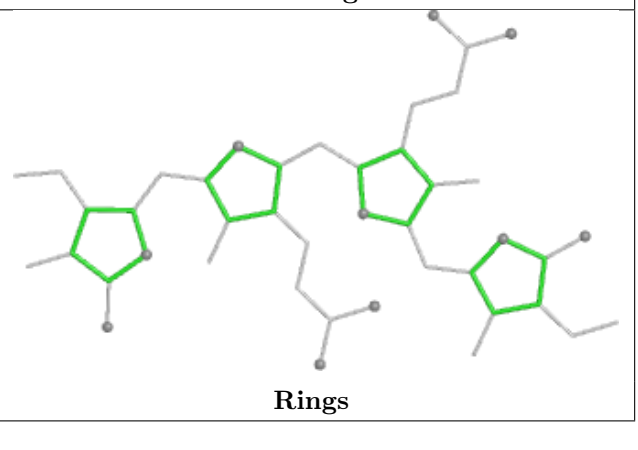
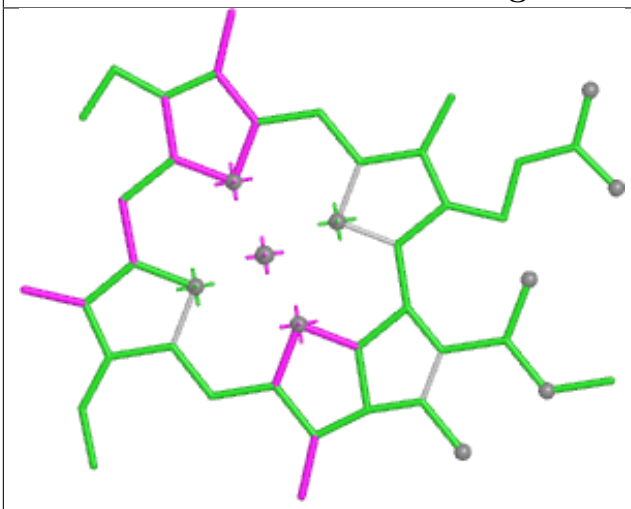


Rings

Ligand CLA KN 102



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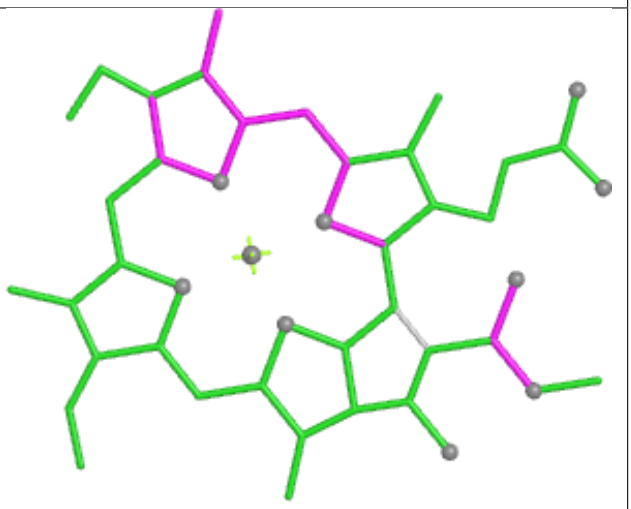

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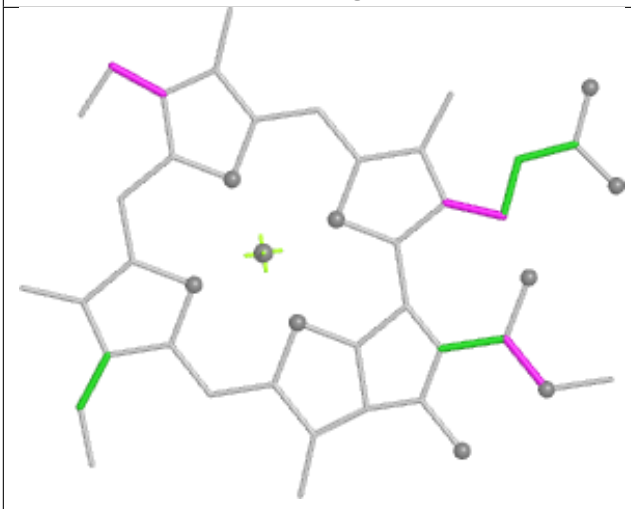
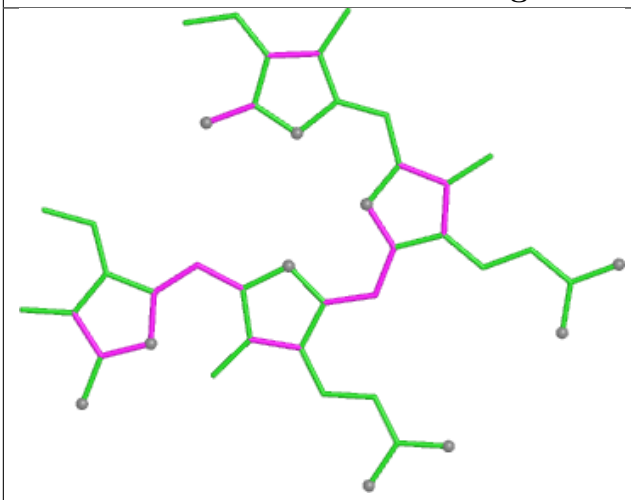


Torsions



Rings

Ligand PEB W4 201



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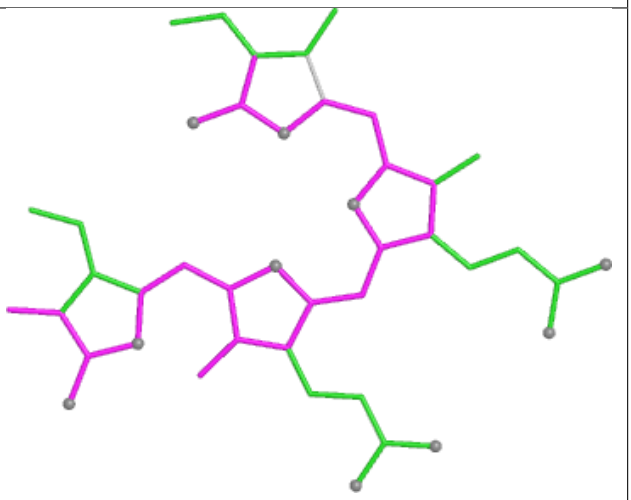

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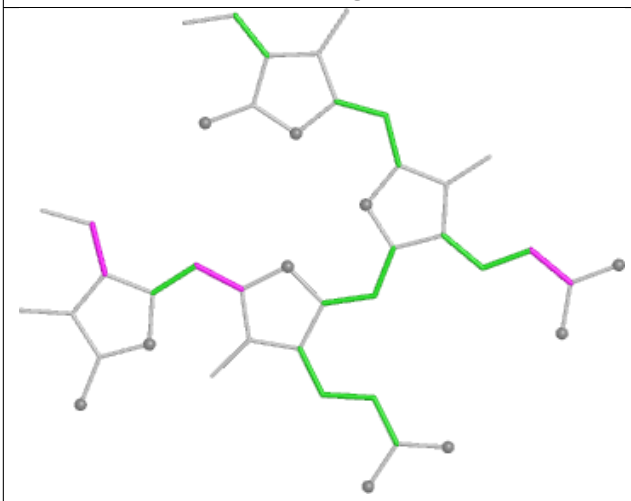

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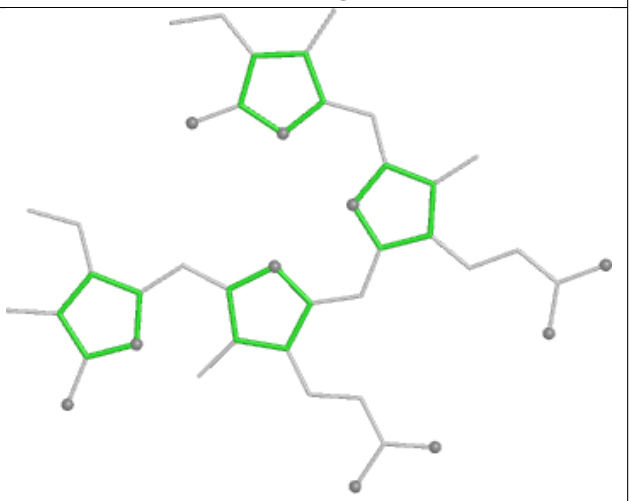
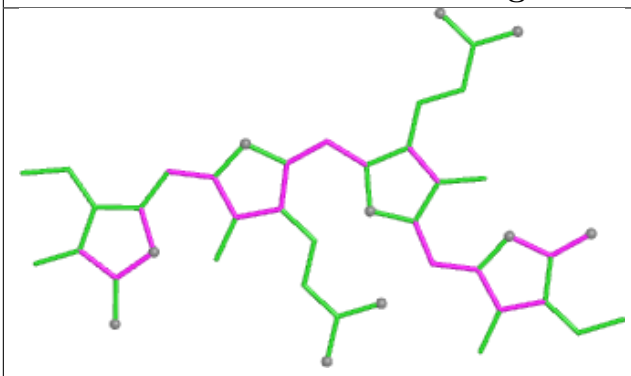


Rings

Ligand CYC g3 1001



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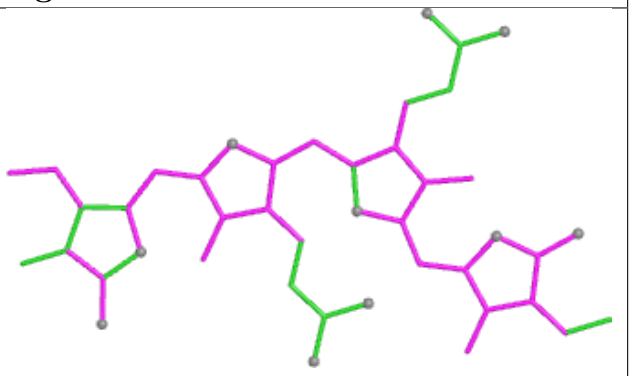

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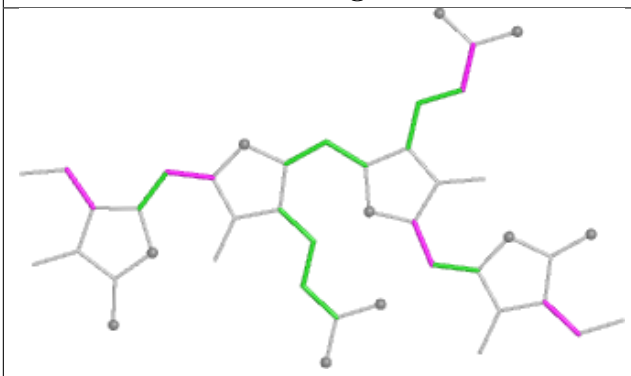

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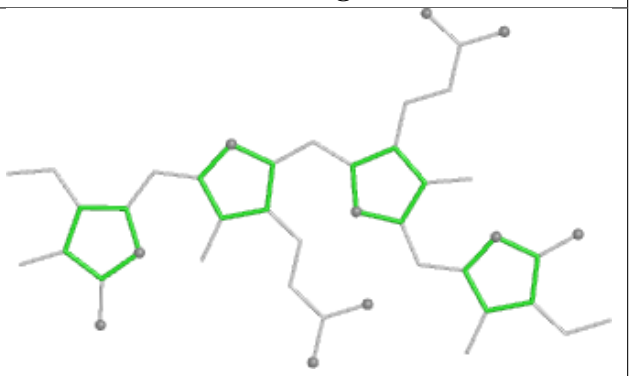
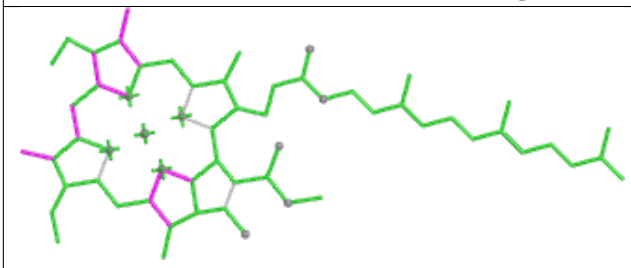


Rings

Ligand CLA CL 513



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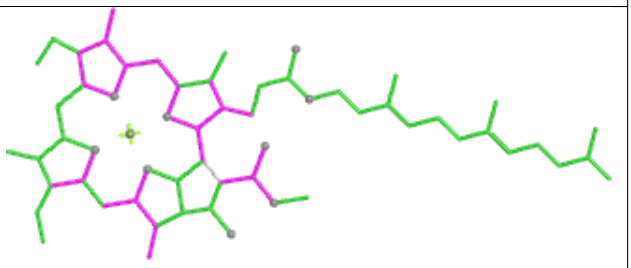

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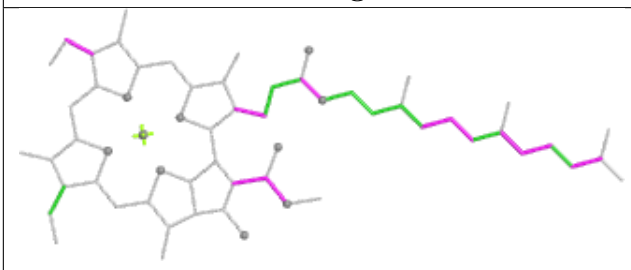

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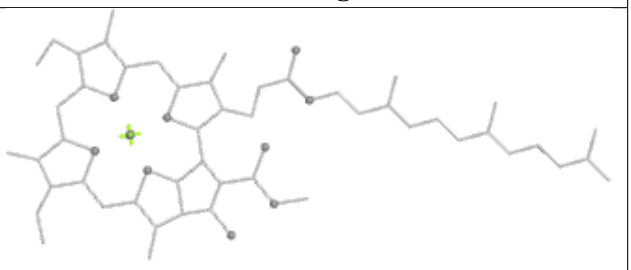
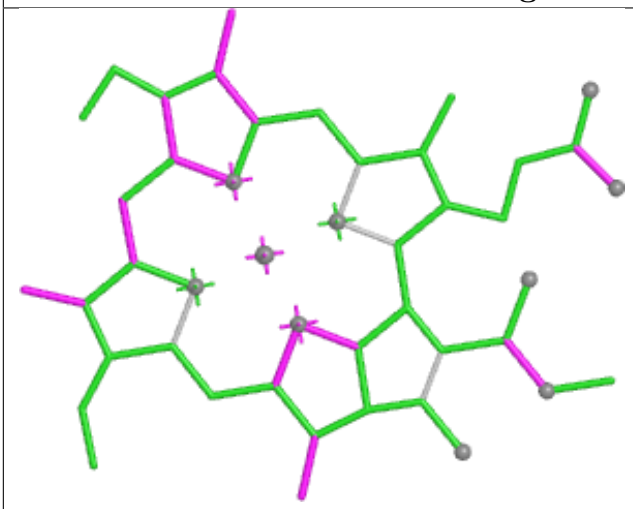


Rings

Ligand CLA 82 305



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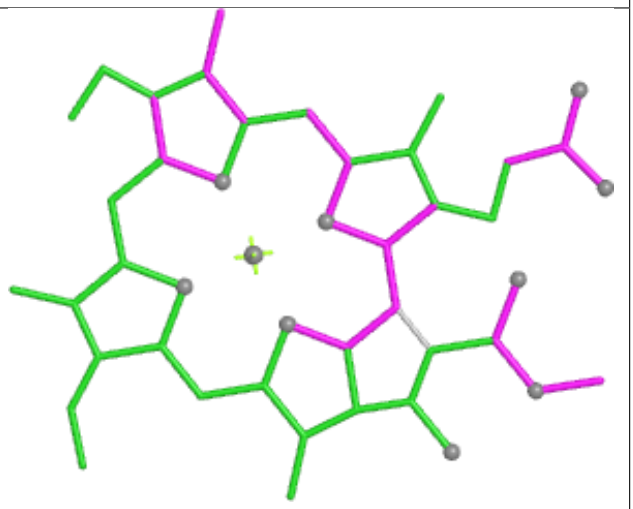
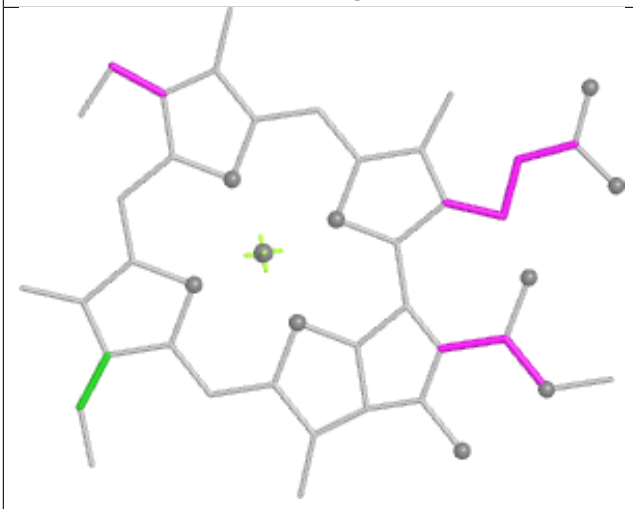


Bond angles

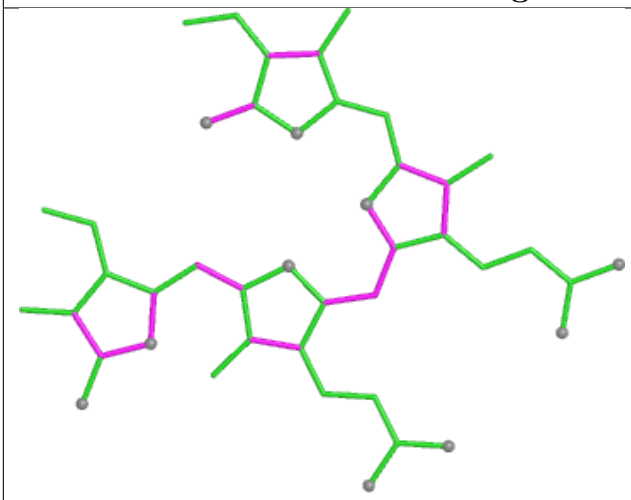


Torsions



Rings

Ligand PEB DB 203



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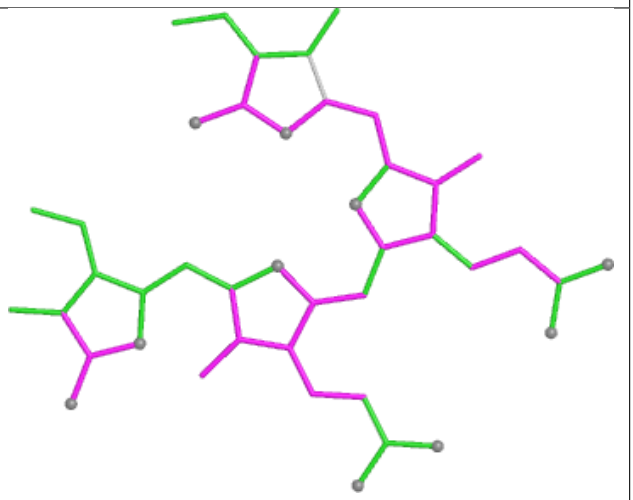
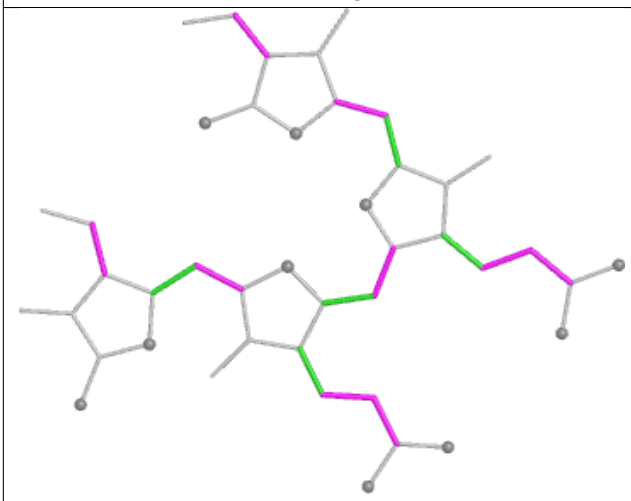


Bond angles



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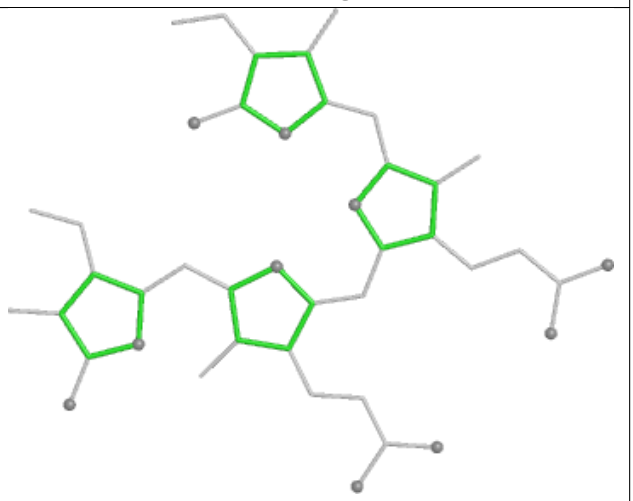
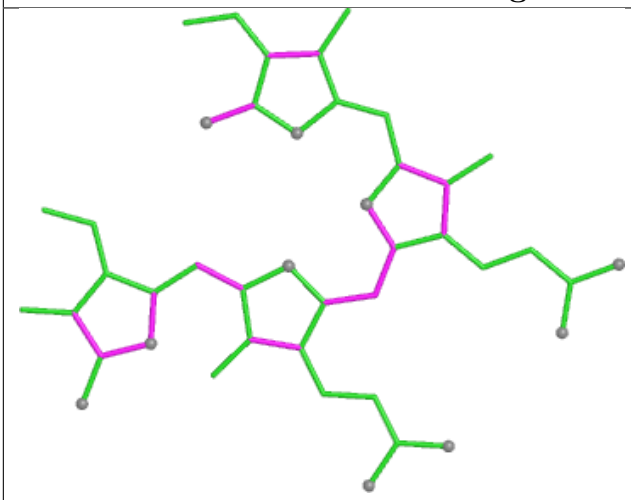


Rings

Ligand PEB mO 201



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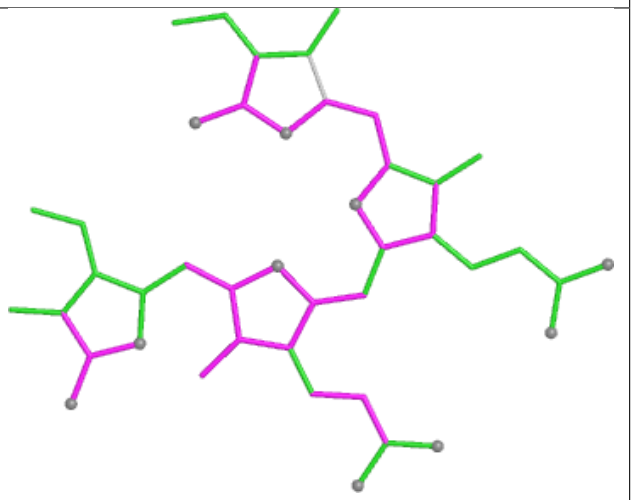
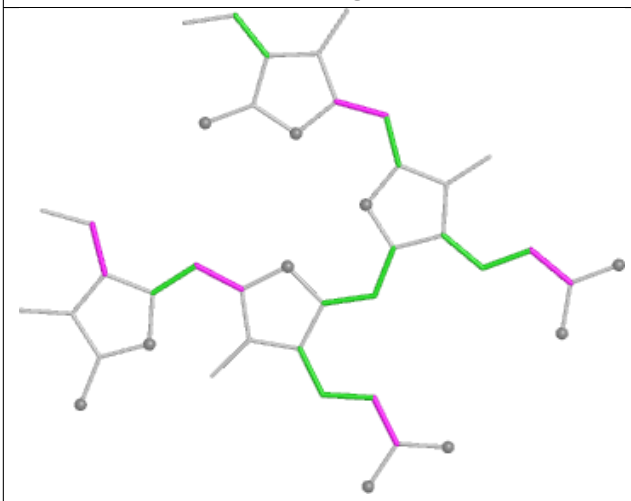


Bond angles



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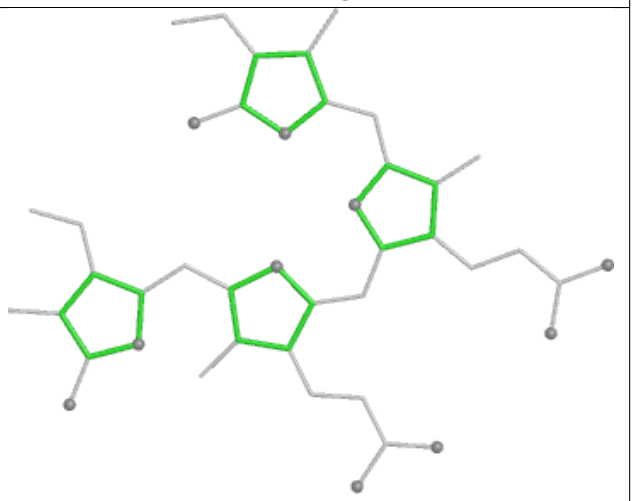
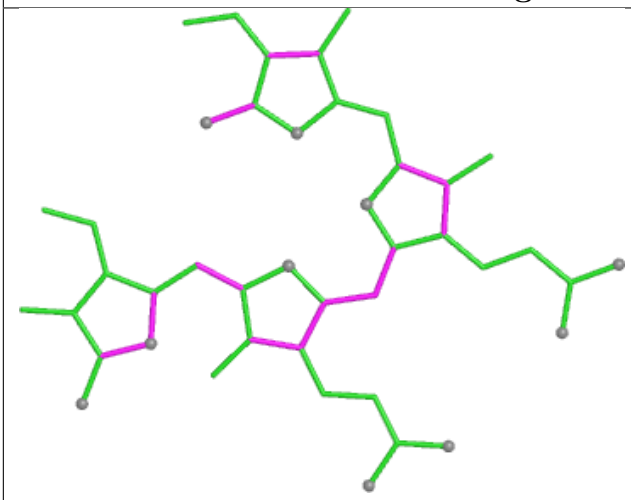


Rings

Ligand PEB H5 202



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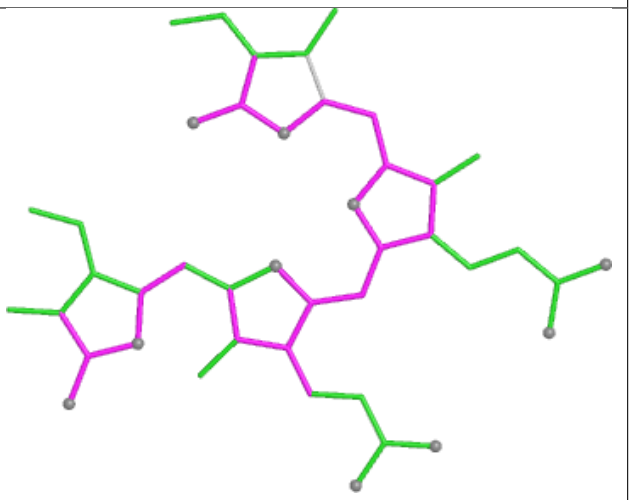
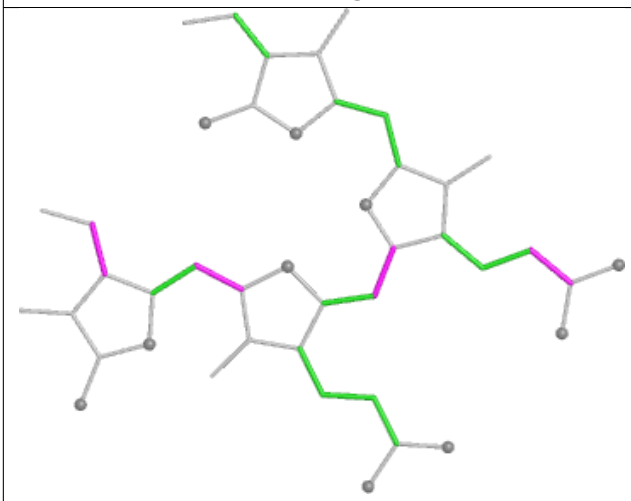


Bond angles



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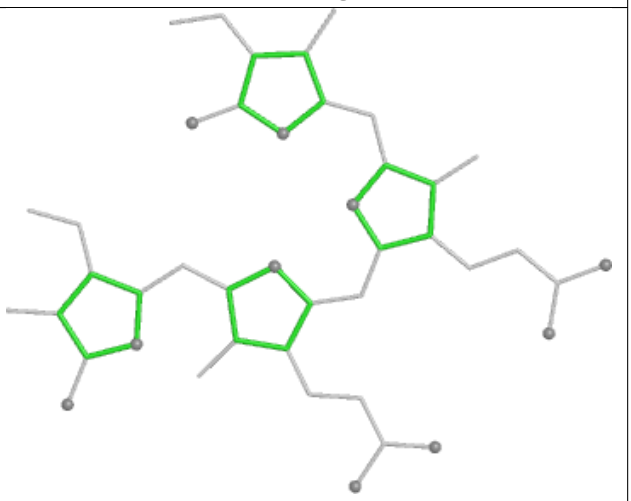
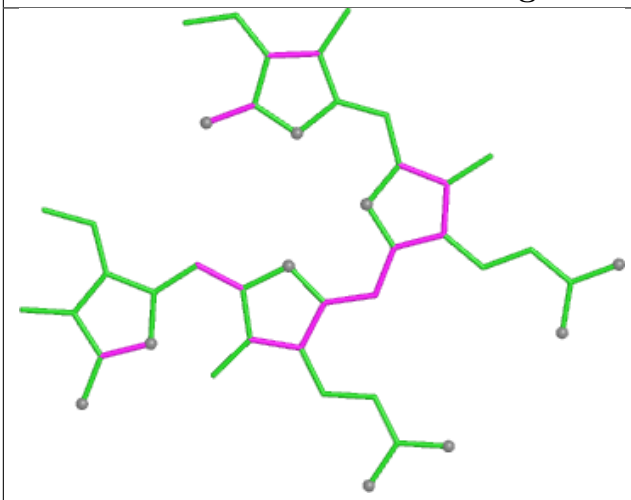


Rings

Ligand PEB d1 203



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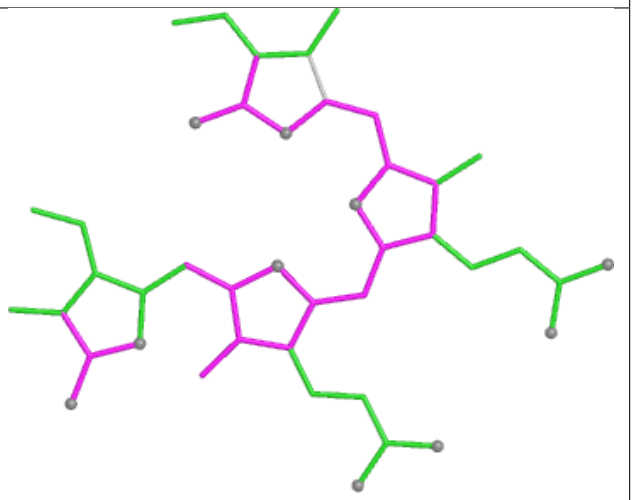
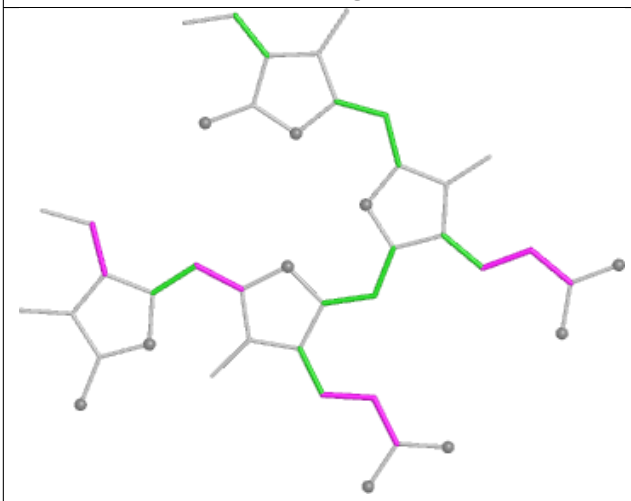


Bond angles



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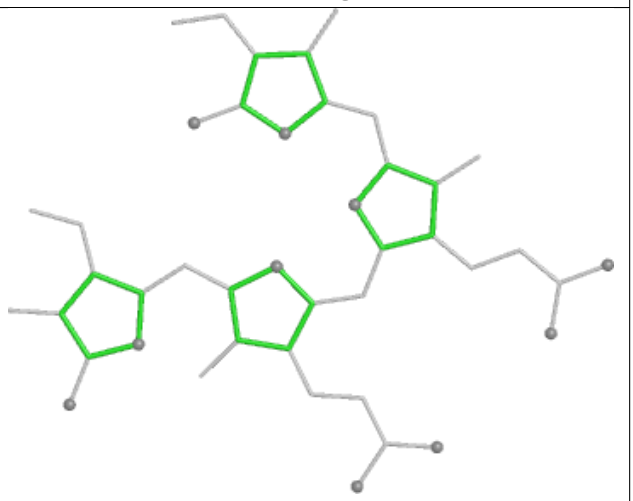
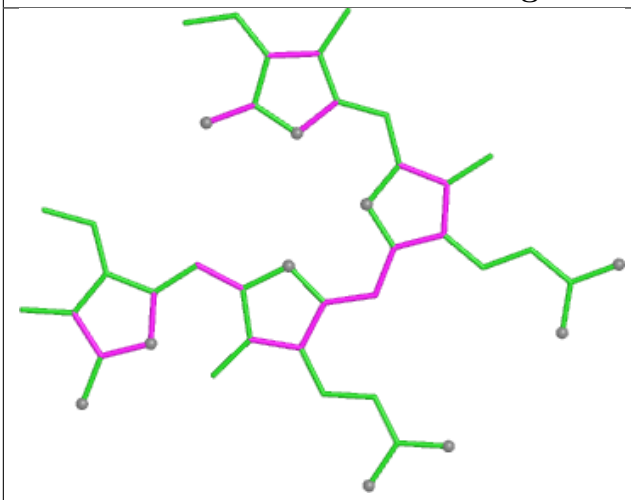


Rings

Ligand PEB lE 201



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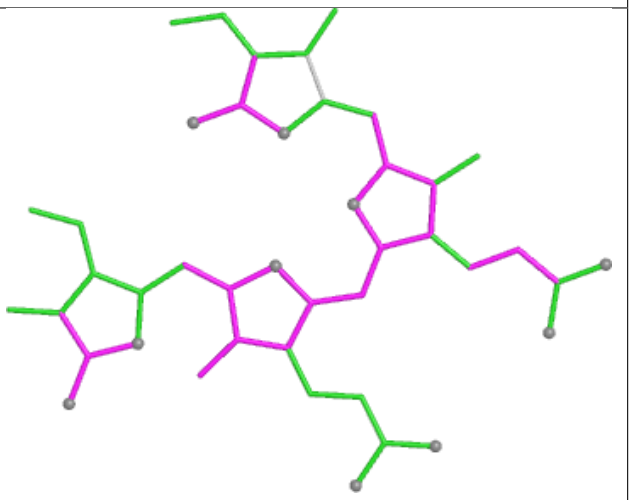
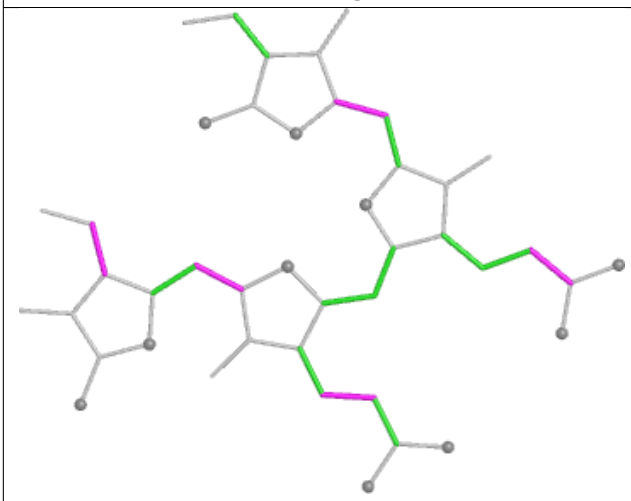


Bond angles



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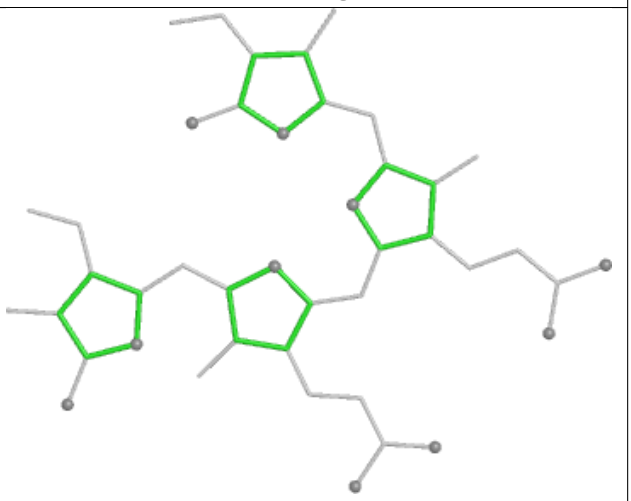
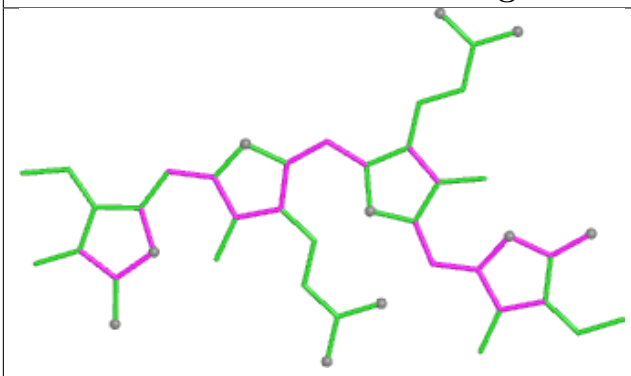
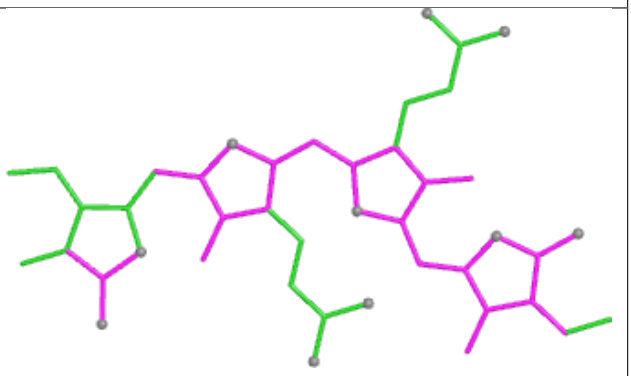


Rings

Ligand CYC DH 1001



Bond lengths



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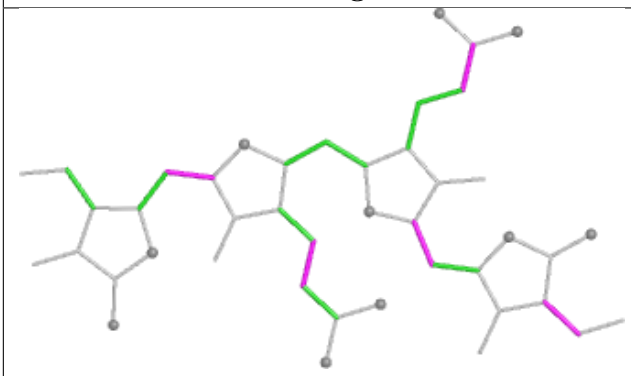

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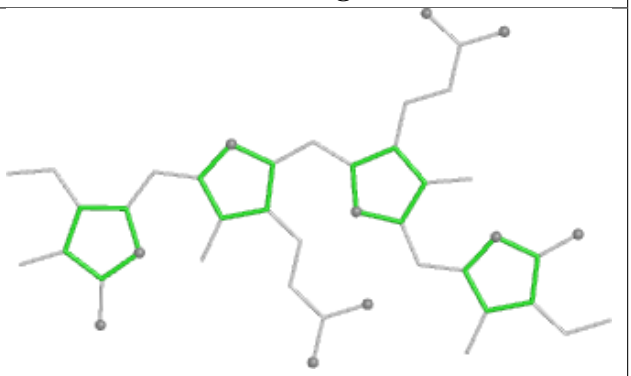
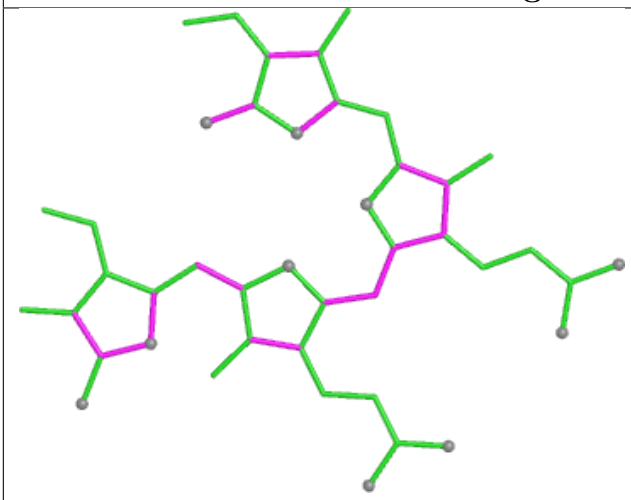


Rings

Ligand PEB l4 202



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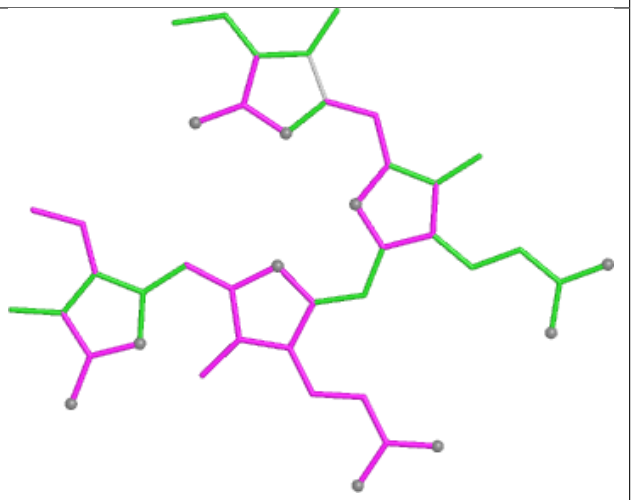

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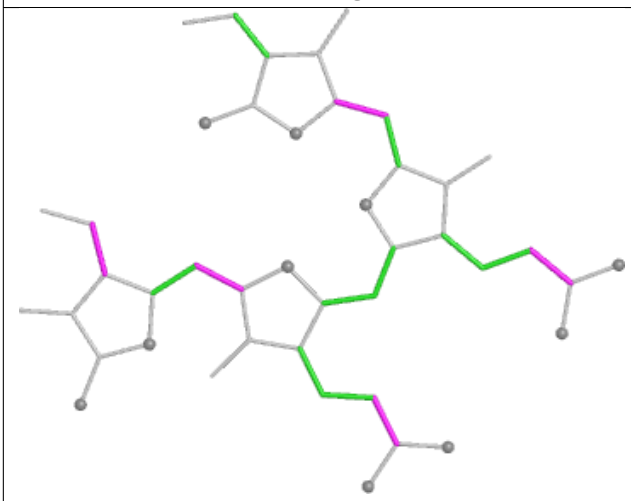

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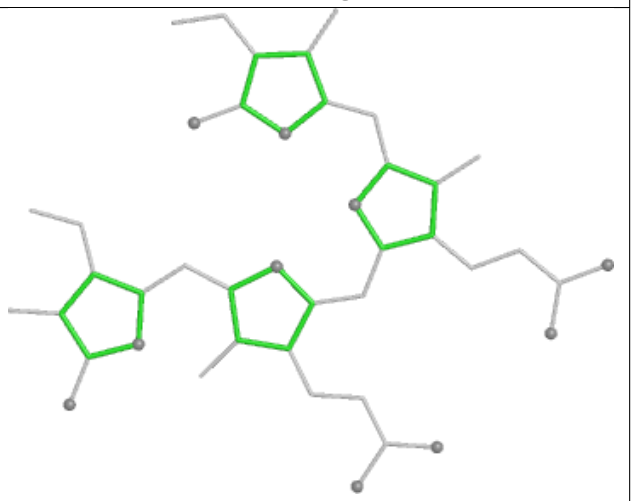
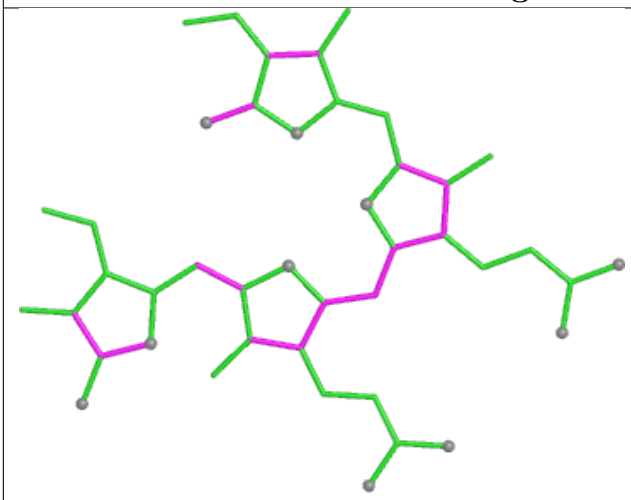


Rings

Ligand PEB XQ 203



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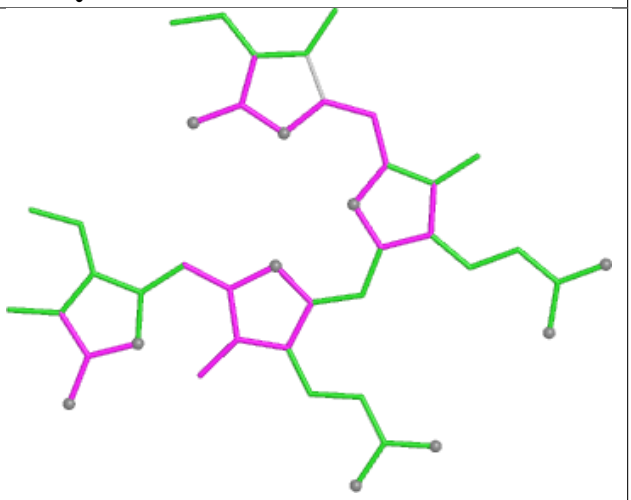

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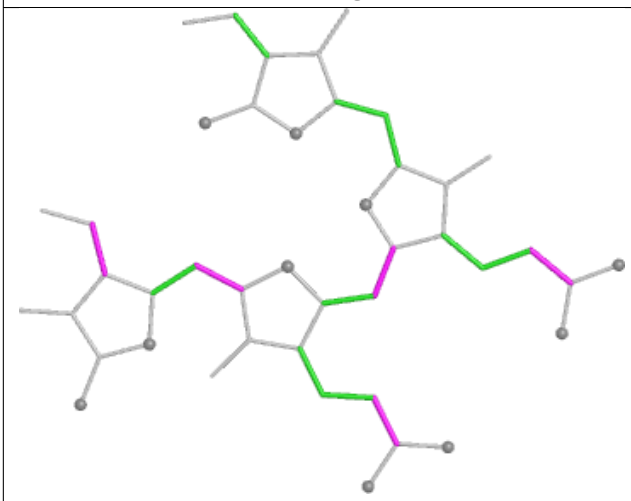

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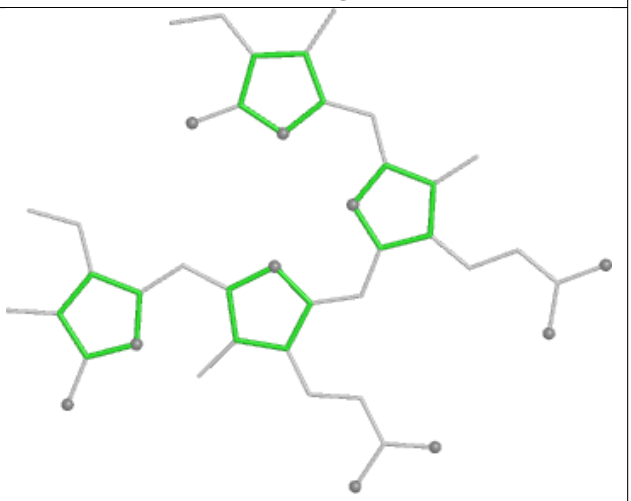

Rings

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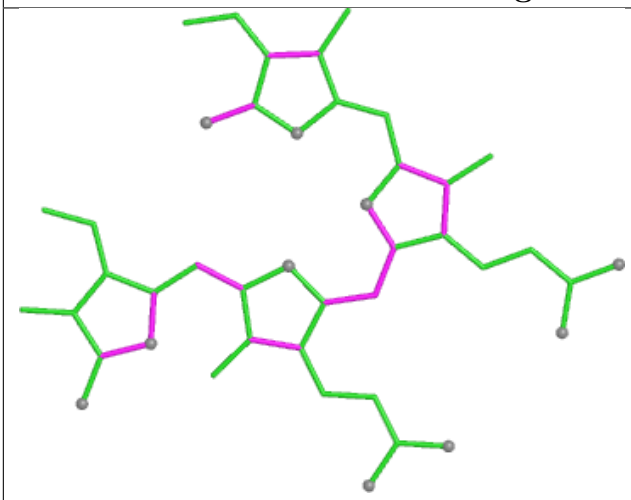

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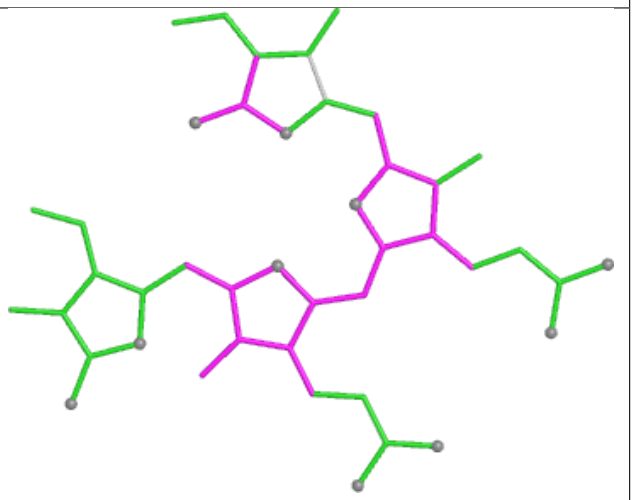

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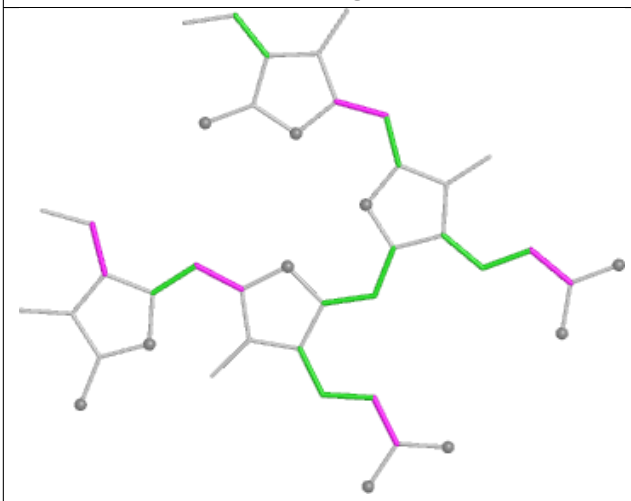

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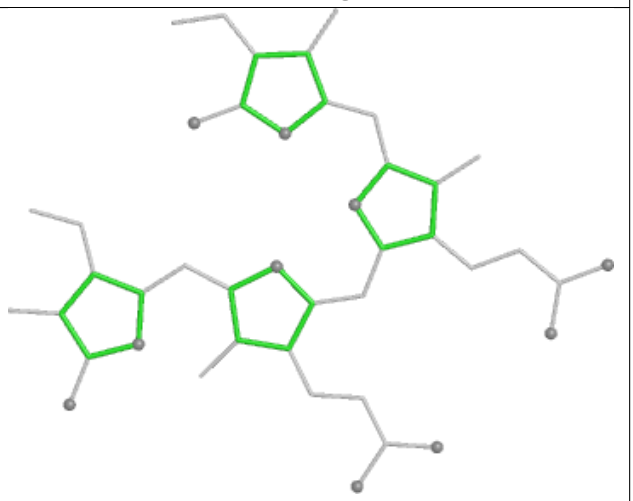
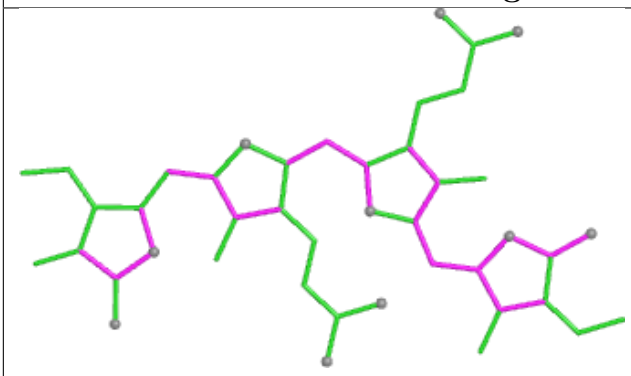


Rings

Ligand CYC JO 1001



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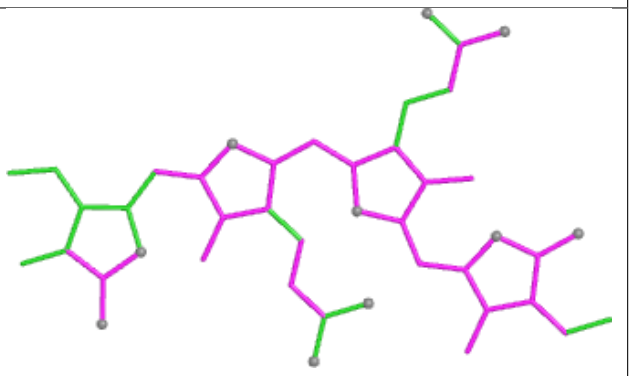

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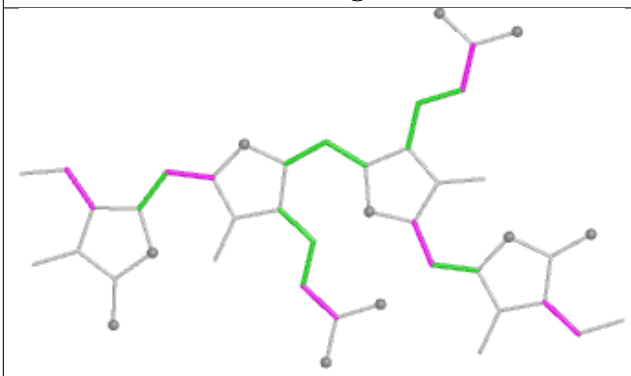

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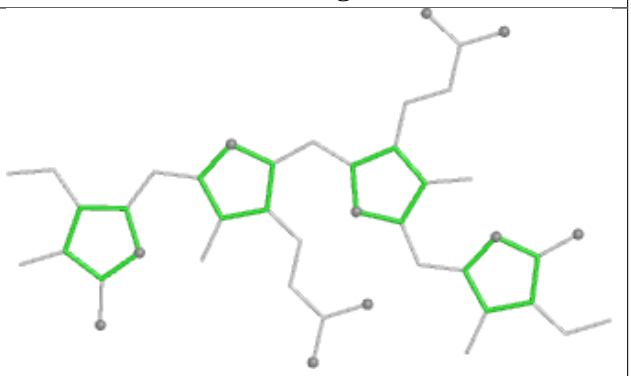
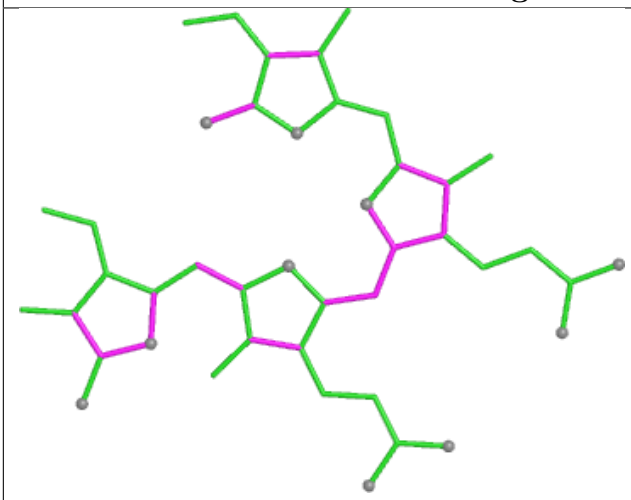


Rings

Ligand PEB GB 201



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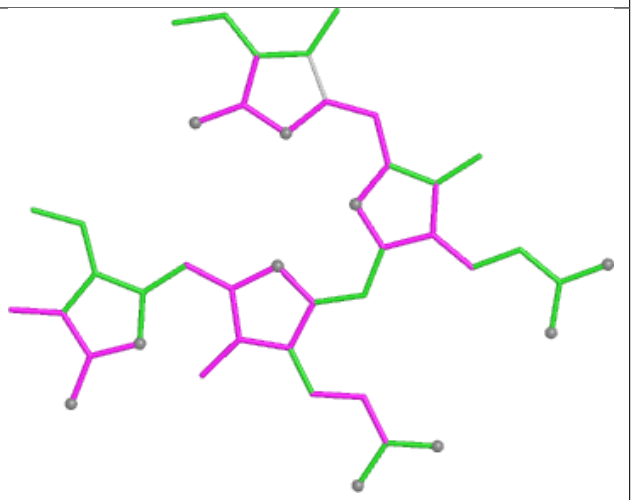

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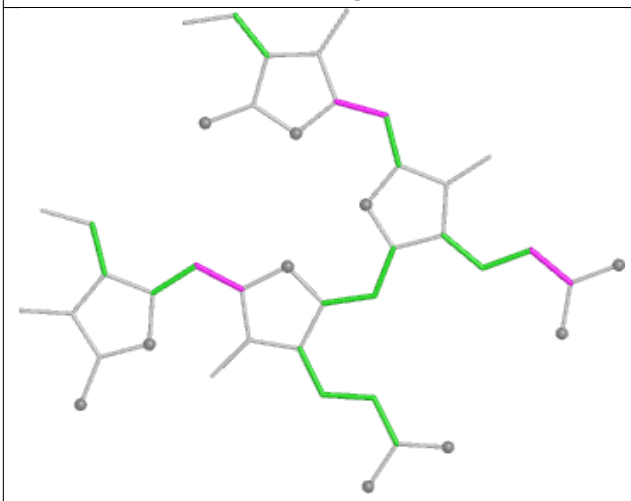

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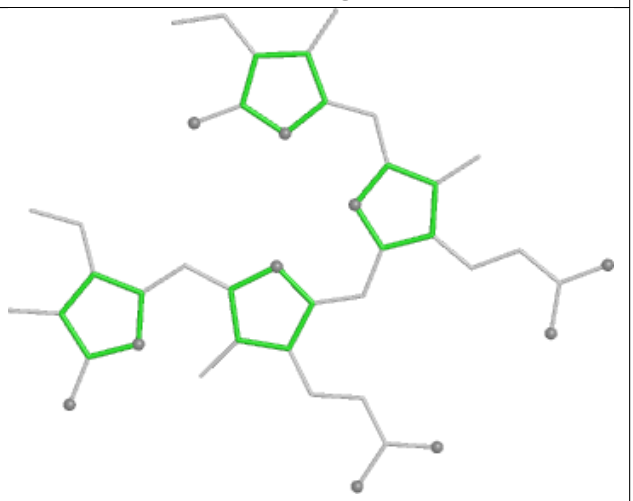
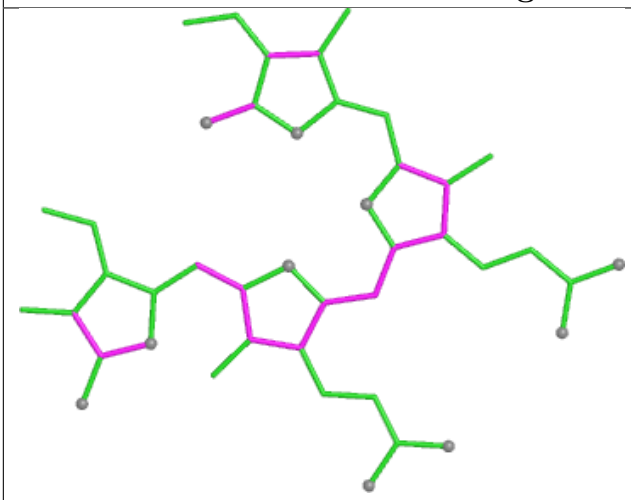


Rings

Ligand PEB qF 201



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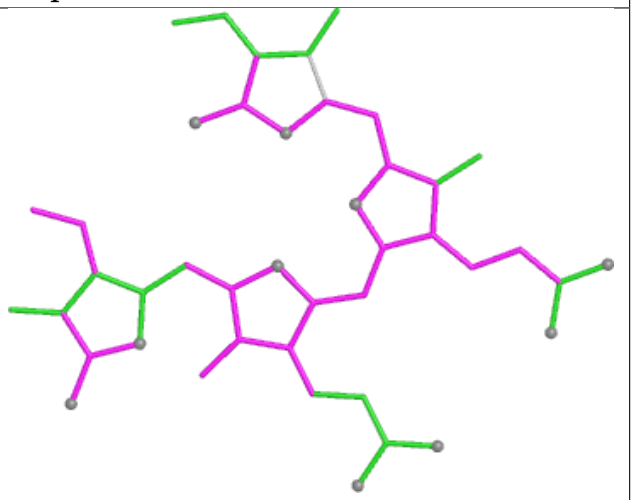
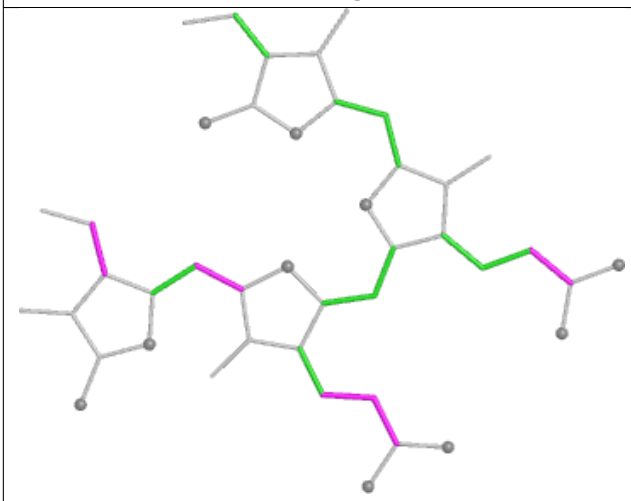


Bond angles



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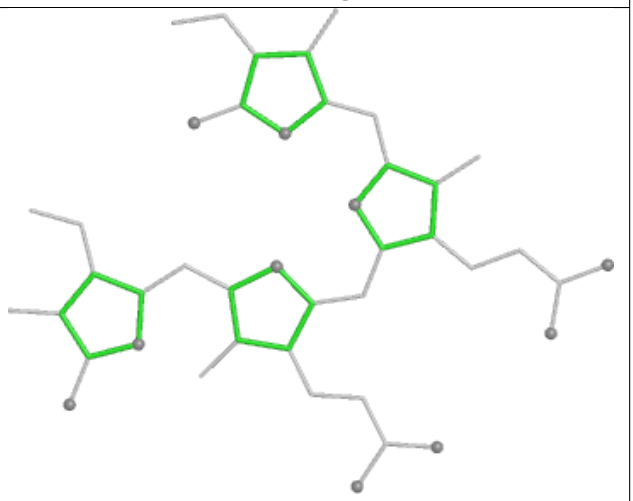
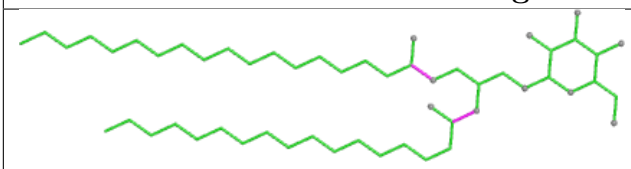


Rings

Ligand LMG dL 407



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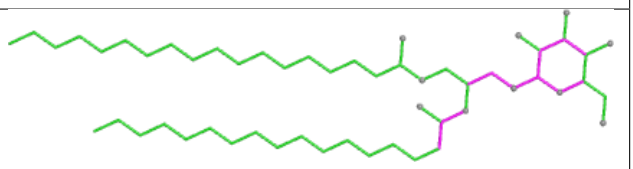

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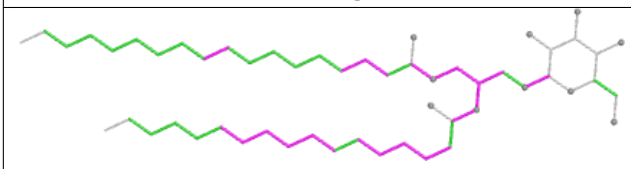

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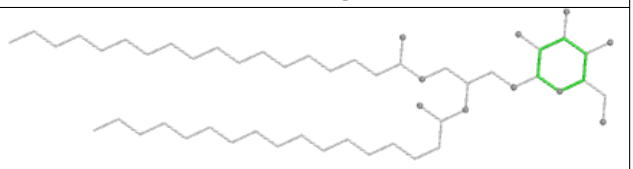
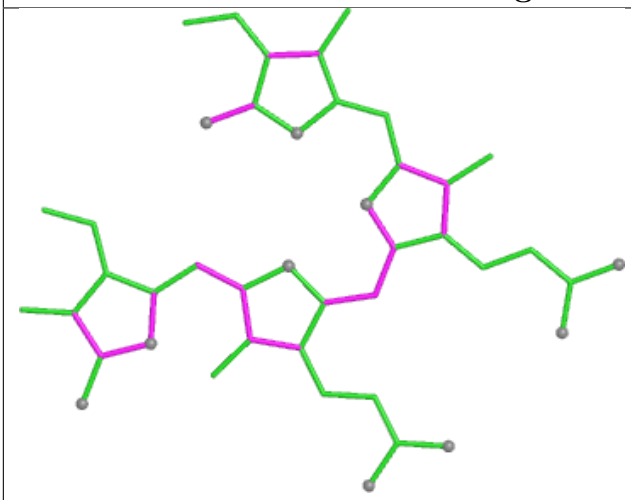


Rings

Ligand PEB G5 201



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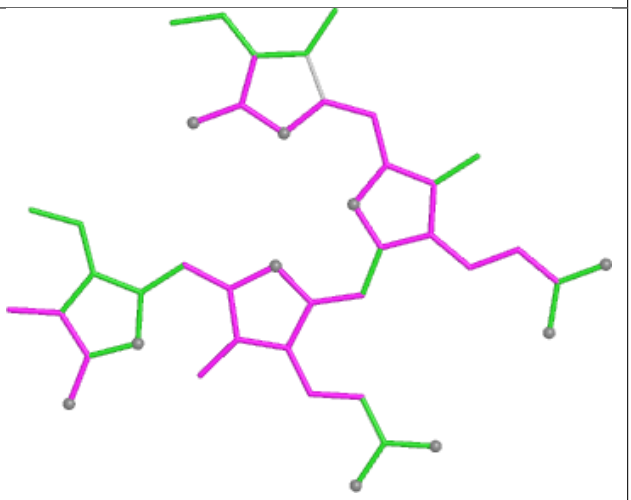

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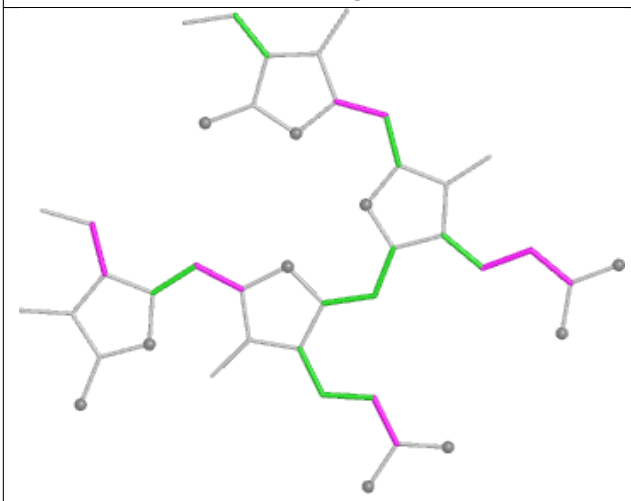

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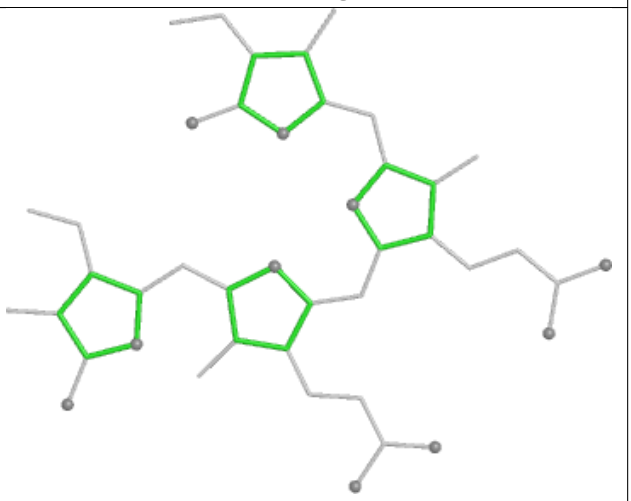
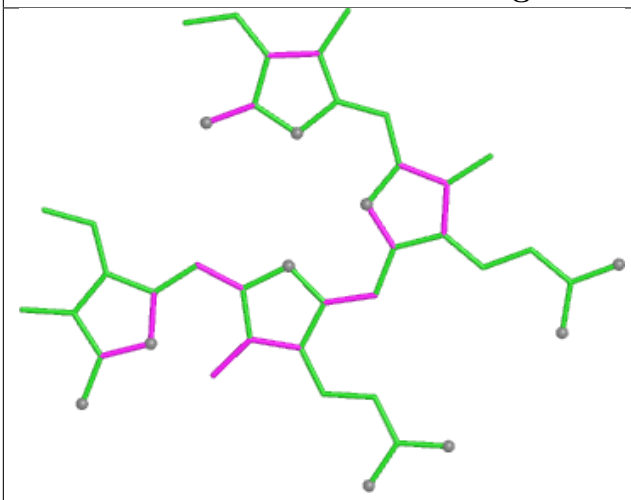


Rings

Ligand PEB UF 201



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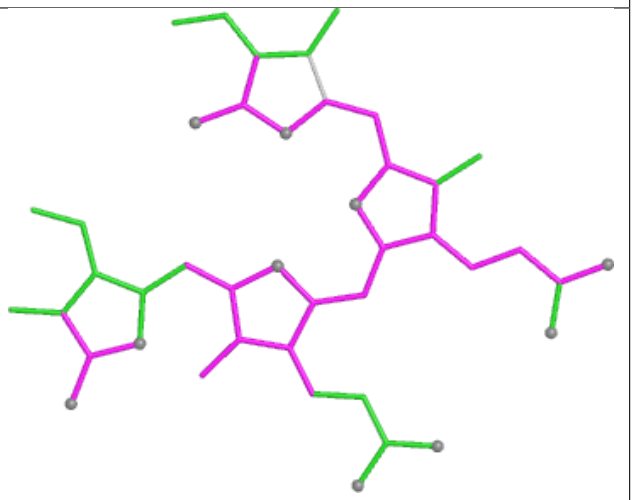
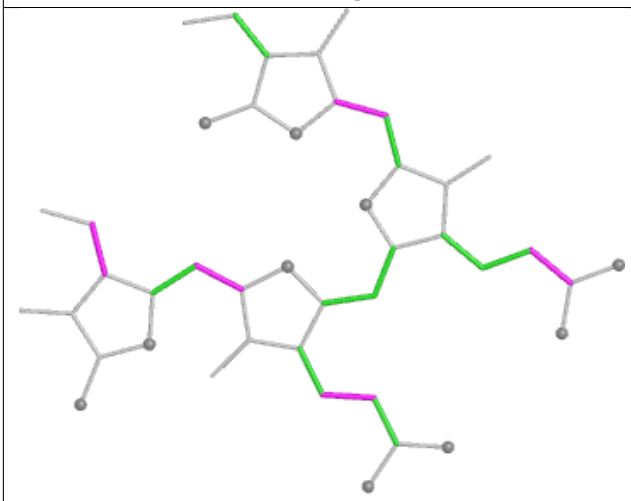


Bond angles



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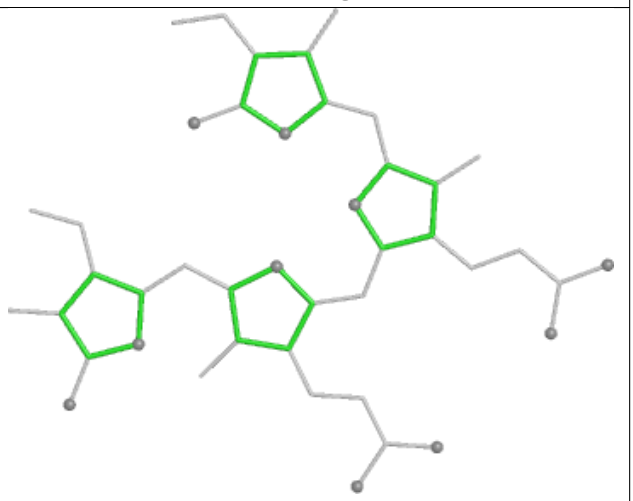
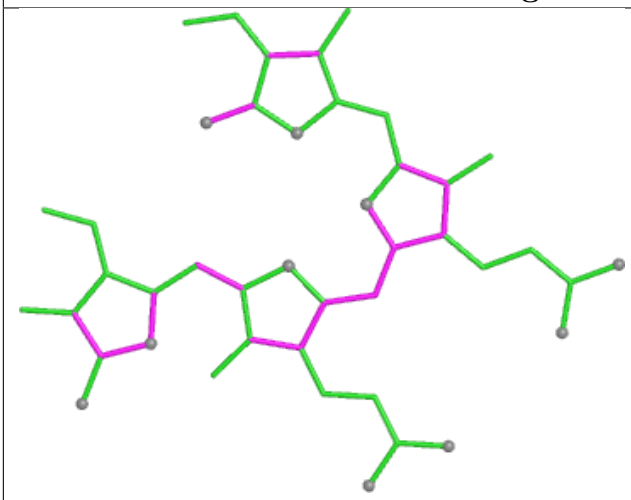


Rings

Ligand PEB t8 201



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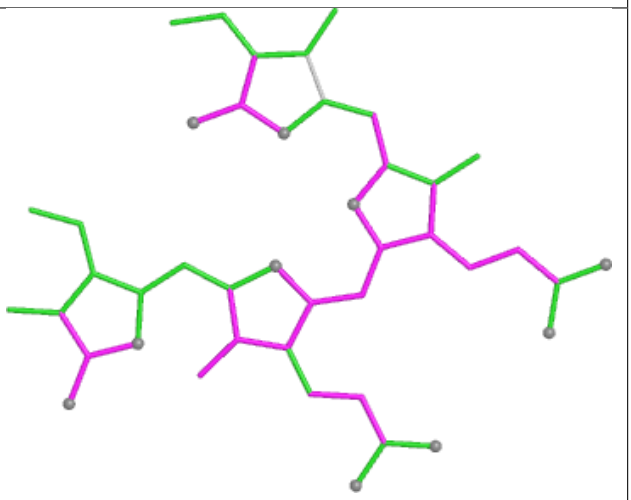
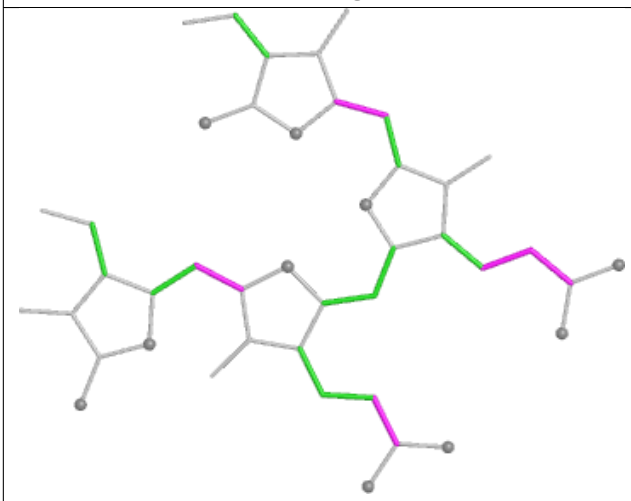


Bond angles



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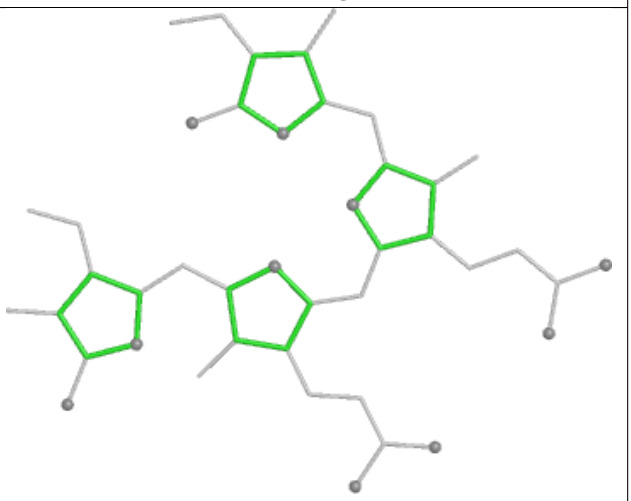
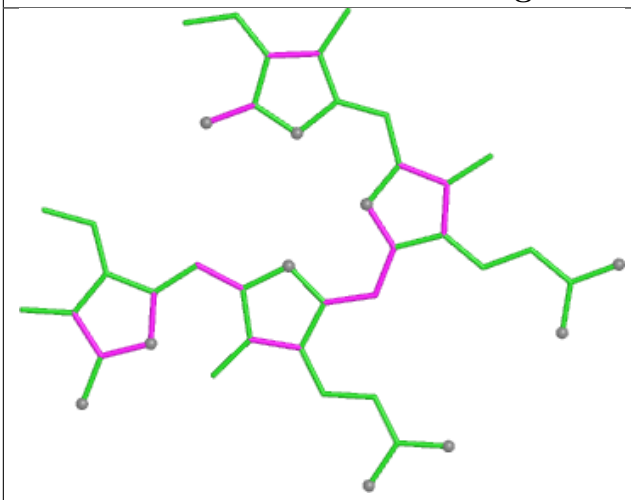


Rings

Ligand PEB N7 203



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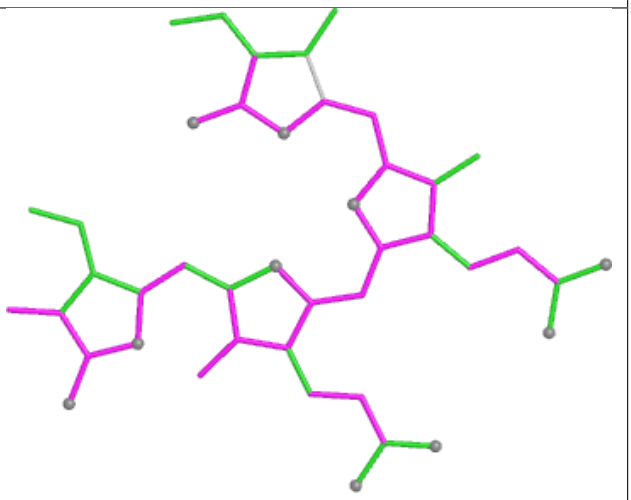

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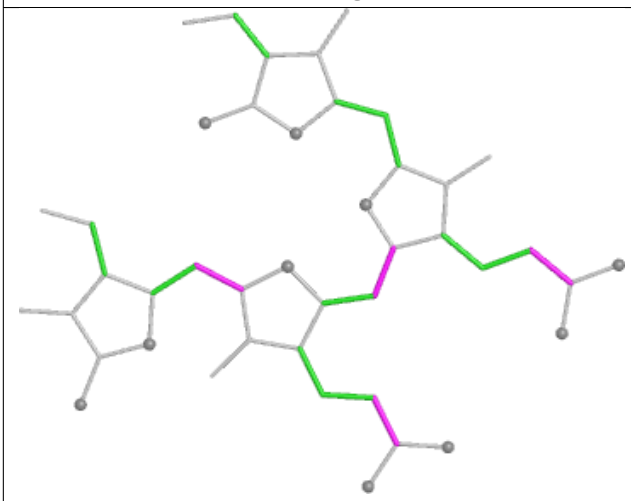

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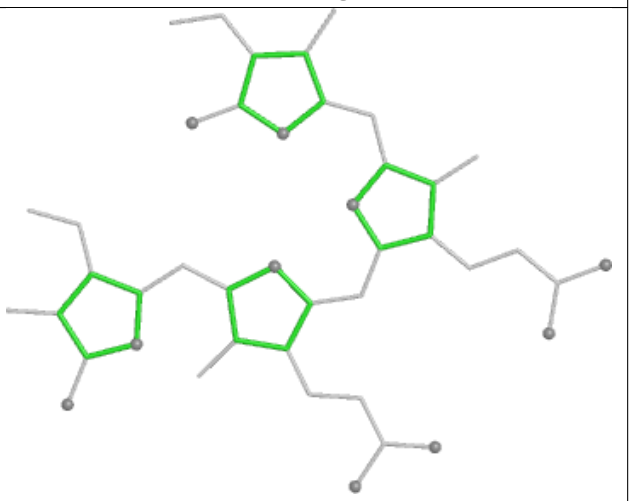
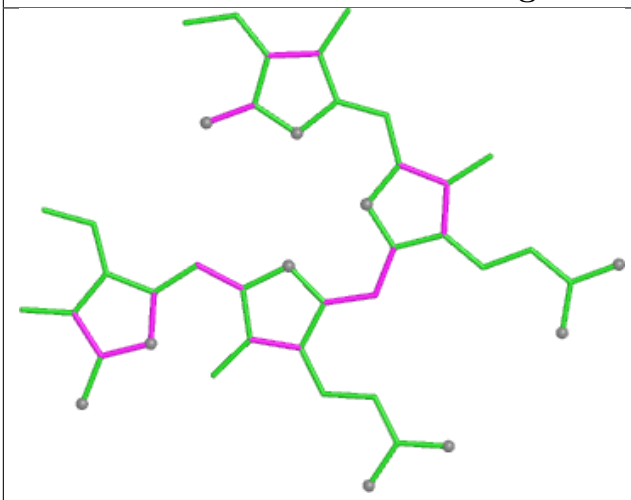


Rings

Ligand PEB d4 201



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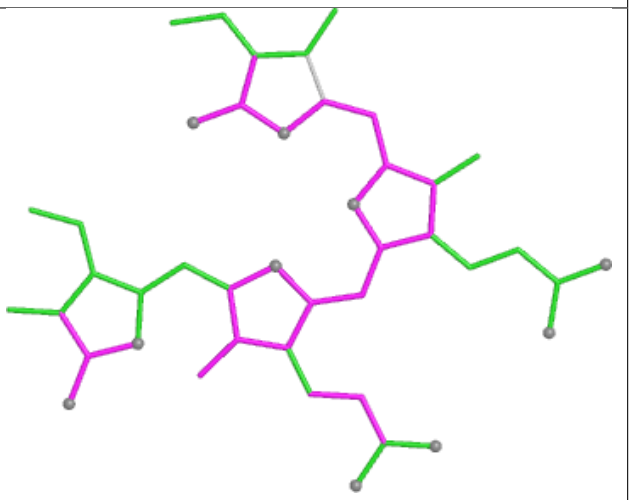
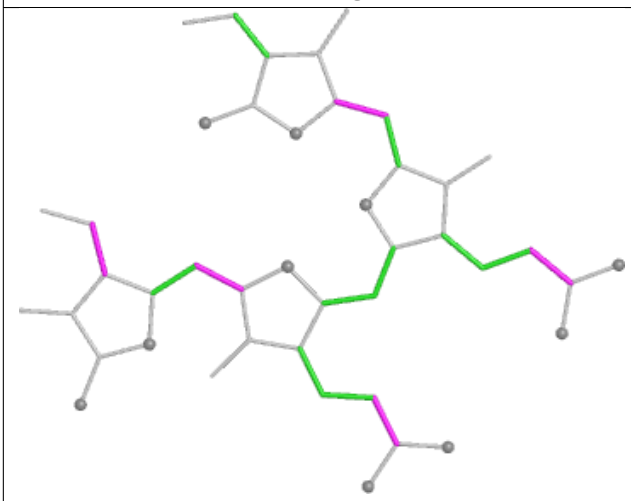


Bond angles



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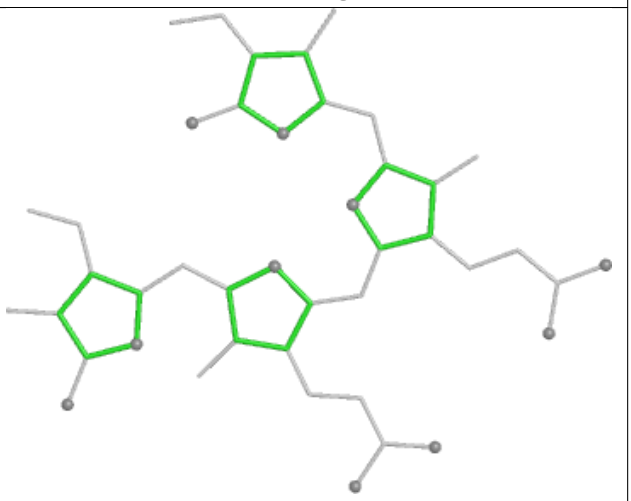
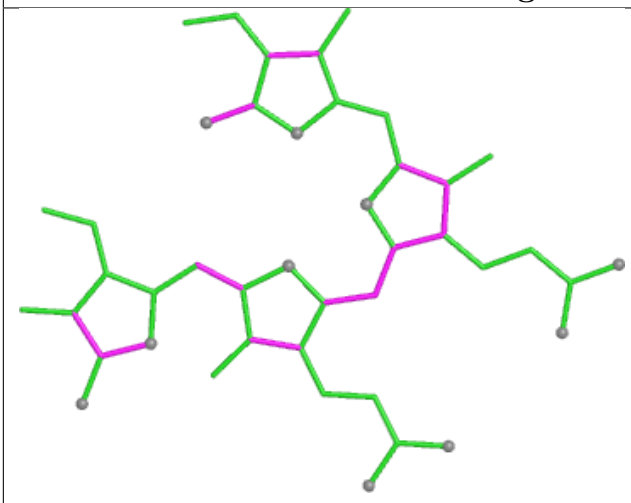


Rings

Ligand PEB OI 203



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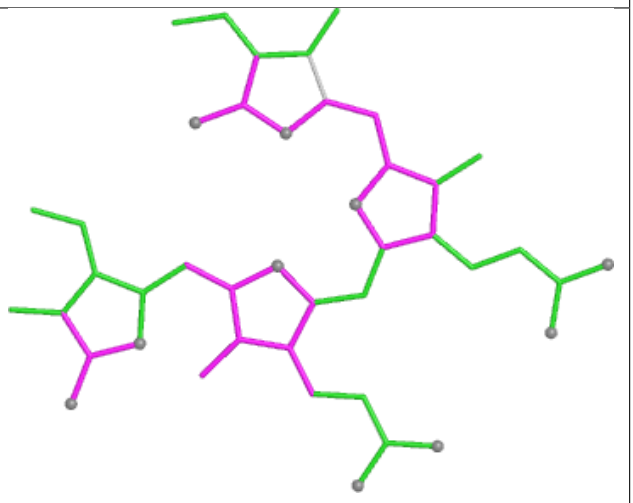
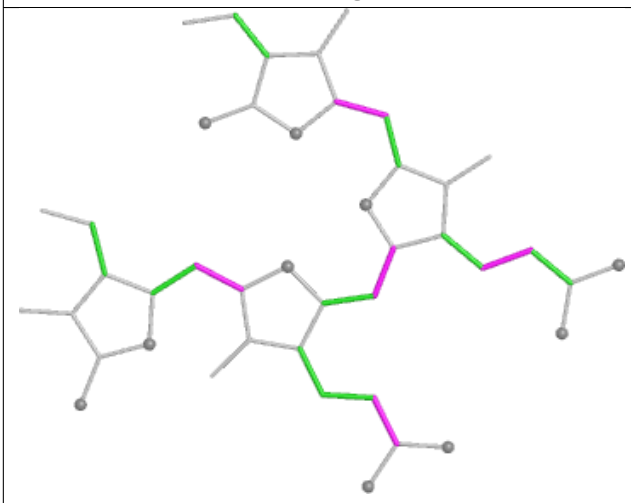


Bond angles



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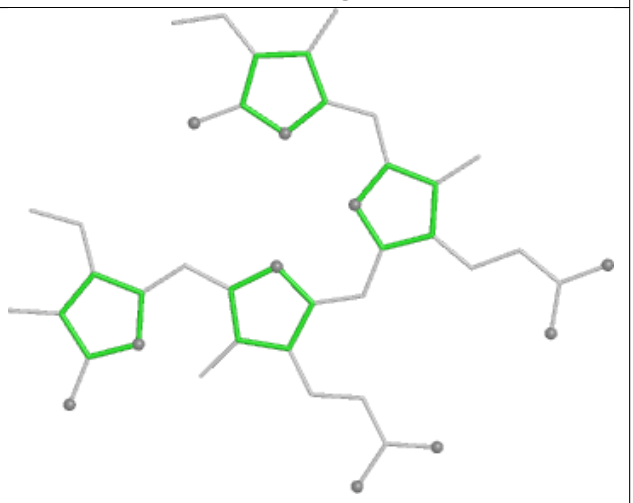
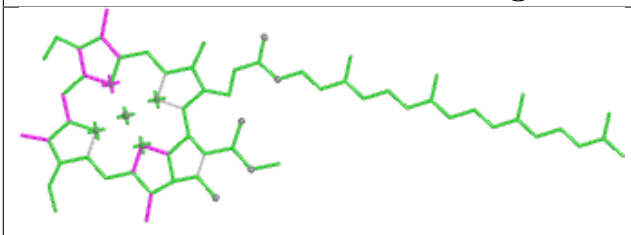


Rings

Ligand CLA AN 835



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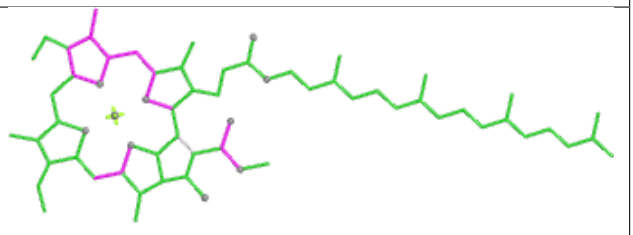
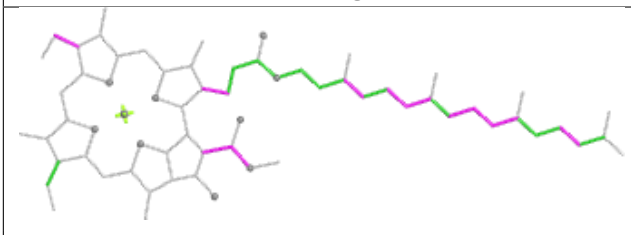
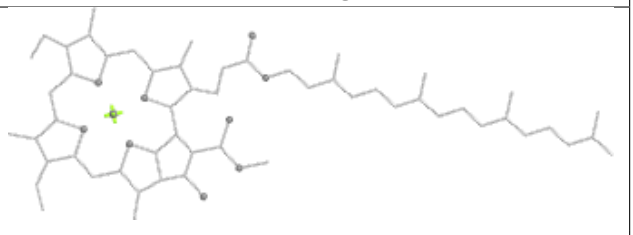


Bond angles

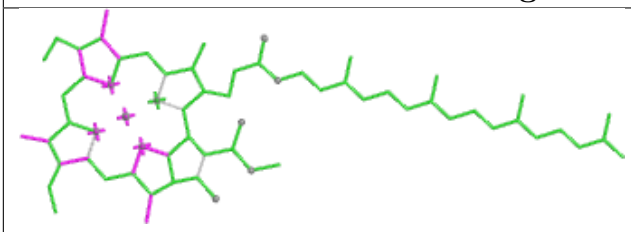


Torsions



Rings

Ligand CLA 82 302



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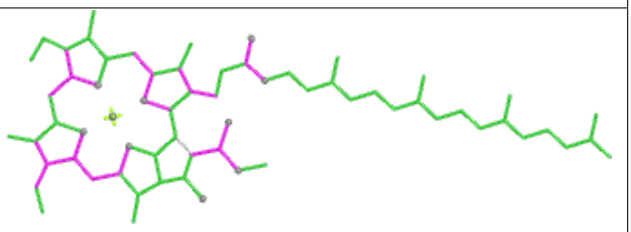
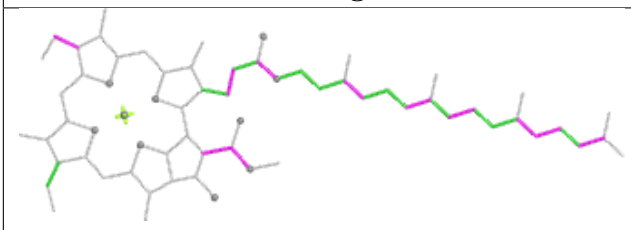


Bond angles



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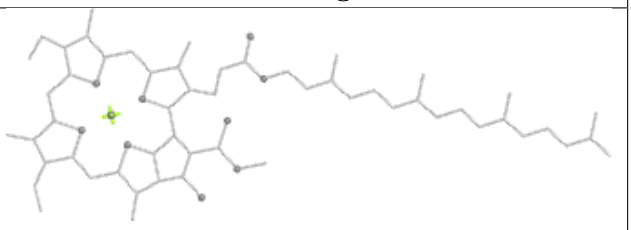
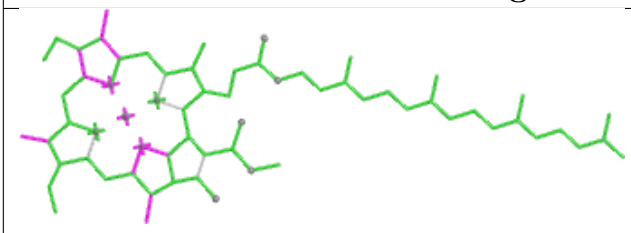


Rings

Ligand CLA AN 805



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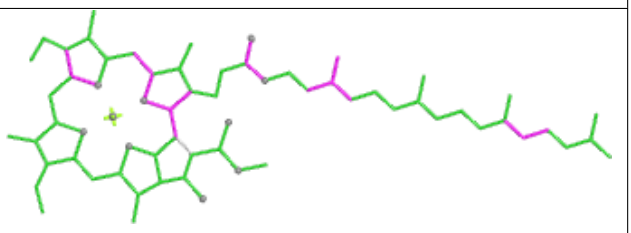

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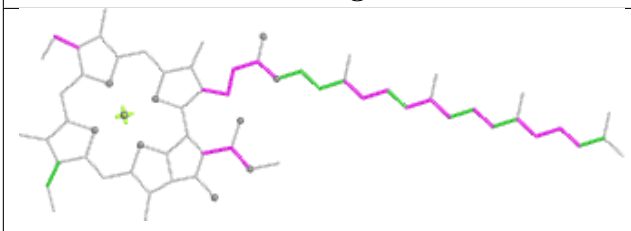

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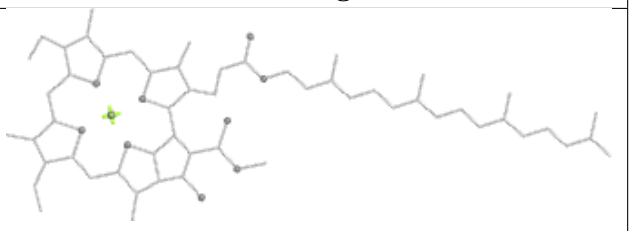
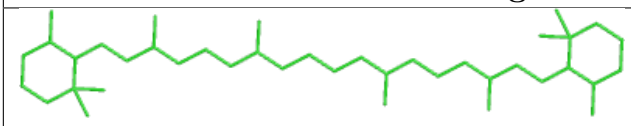


Rings

Ligand BCR BN 841



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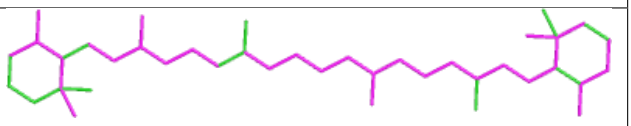

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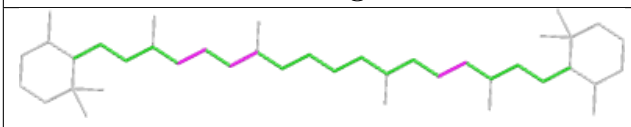

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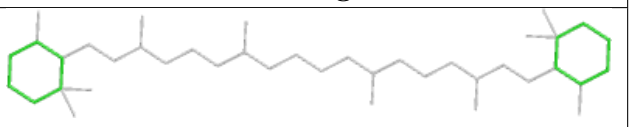
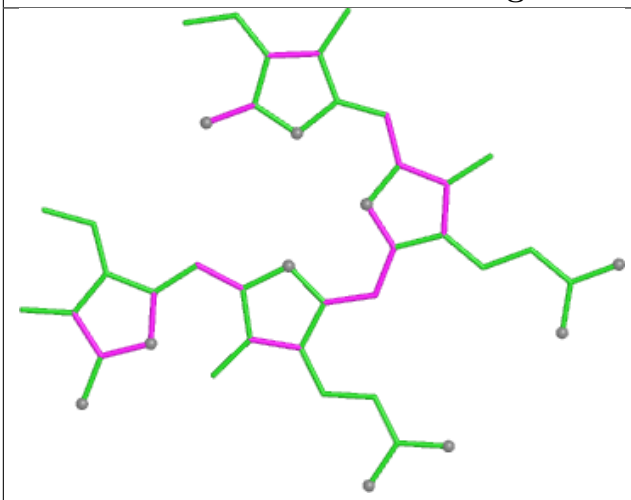


Rings

Ligand PEB WP 201



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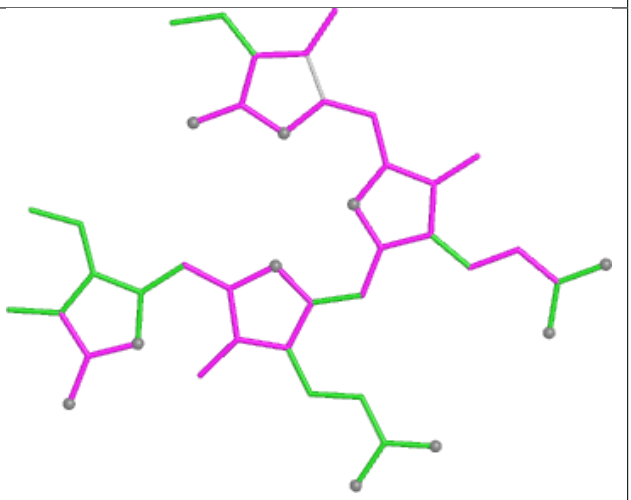
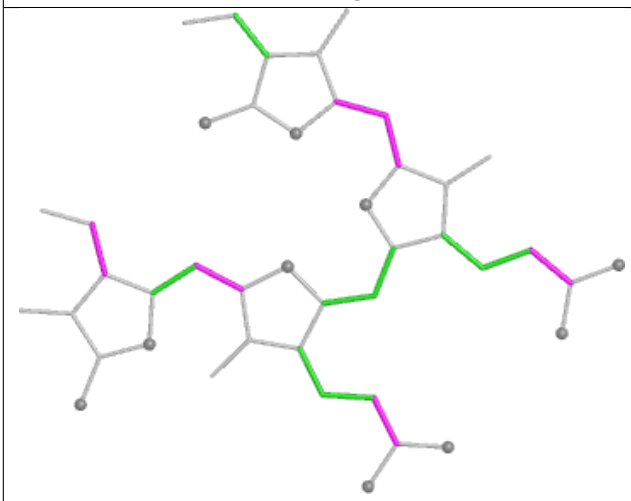


Bond angles



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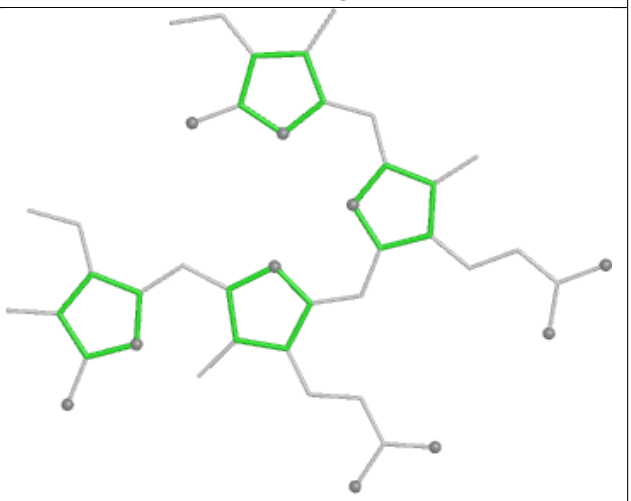
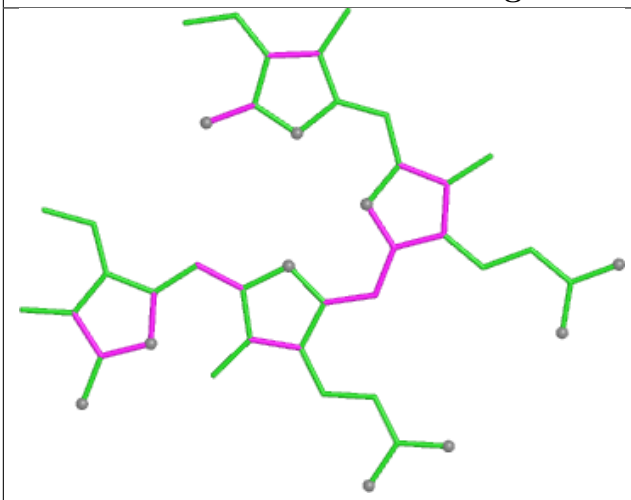


Rings

Ligand PEB LO 1002



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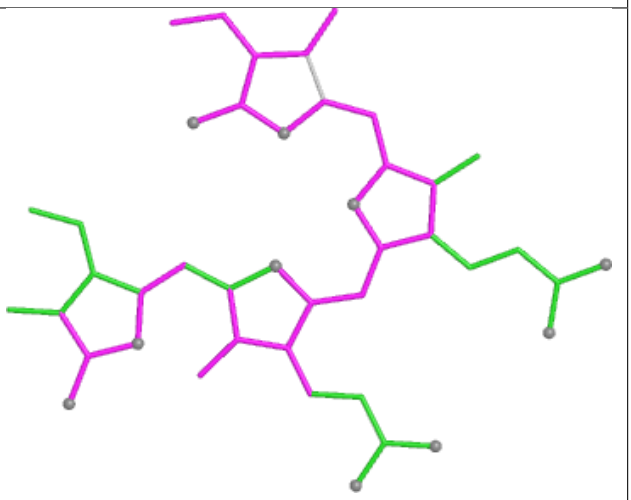
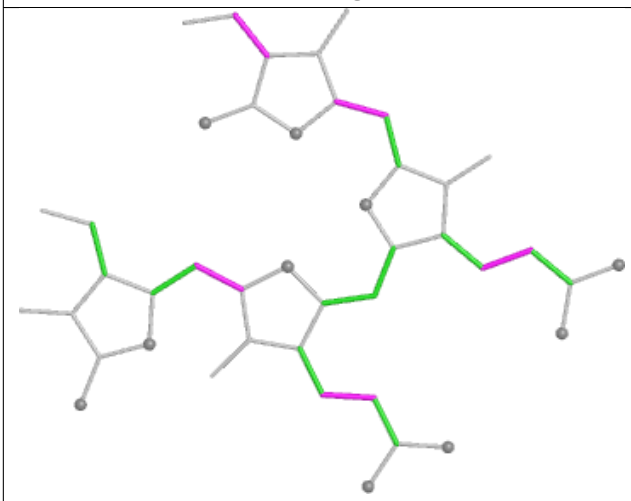


Bond angles



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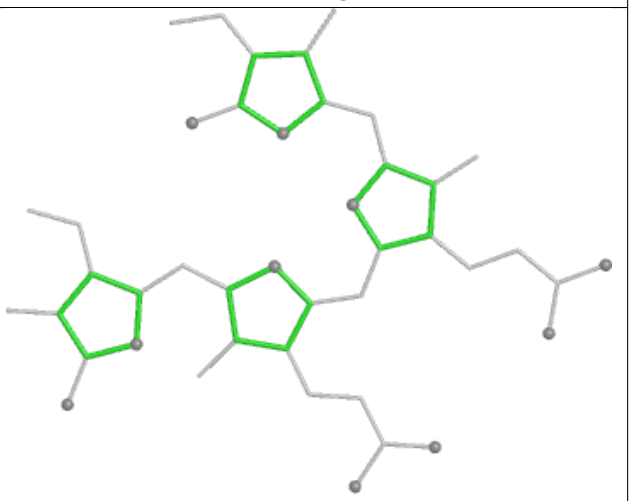
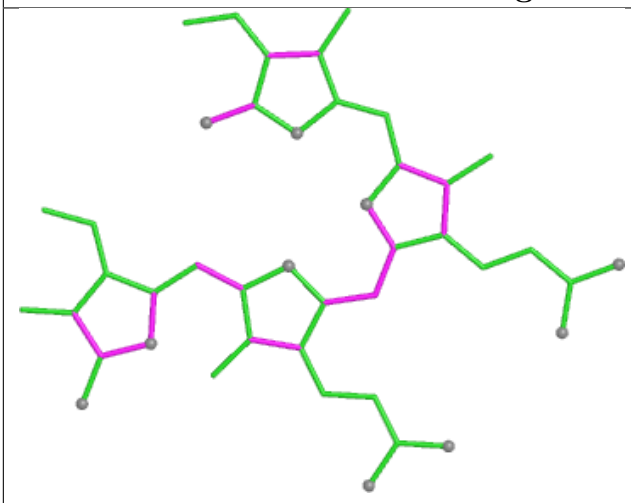


Rings

Ligand PEB Y5 201



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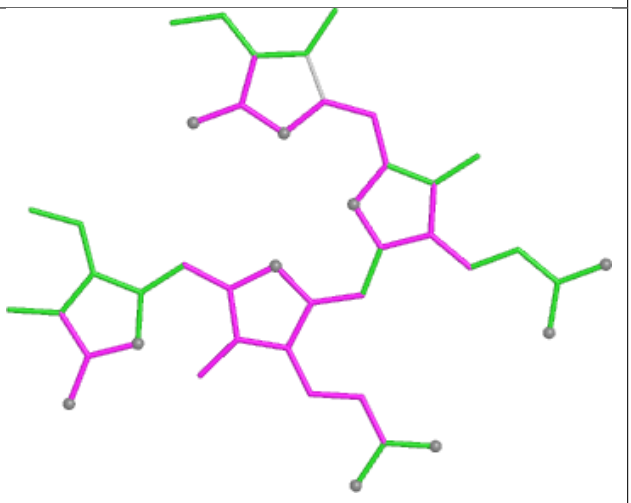
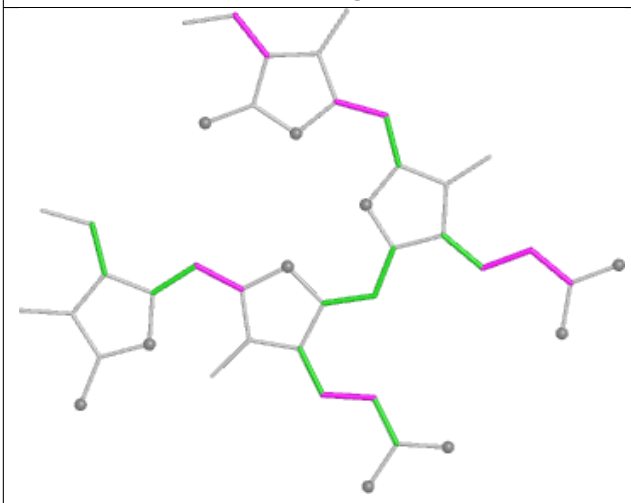


Bond angles



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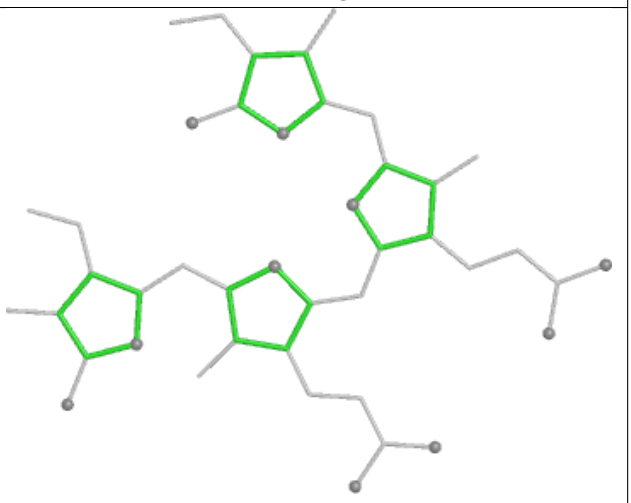
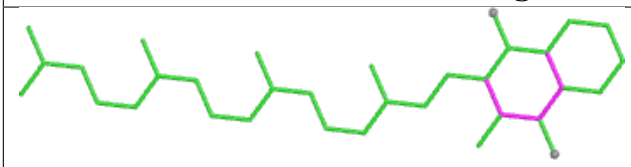


Rings

Ligand PQN B2 837



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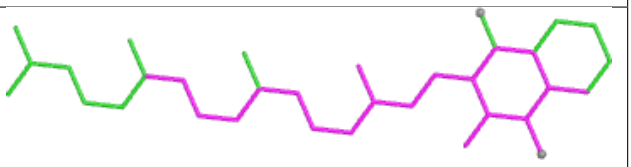

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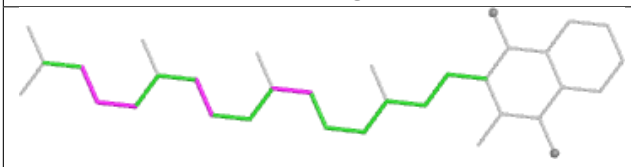

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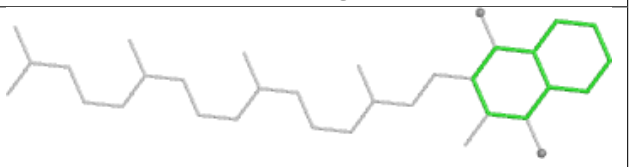
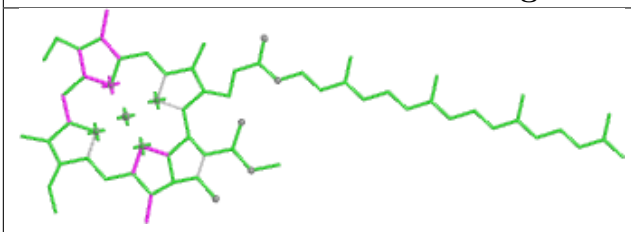


Rings

Ligand CLA c6 606



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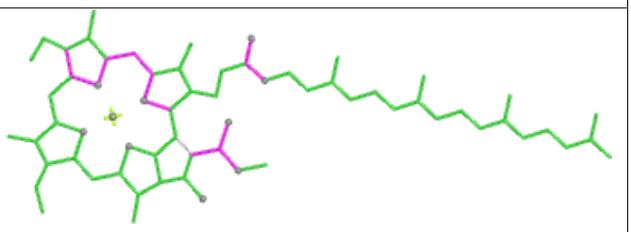

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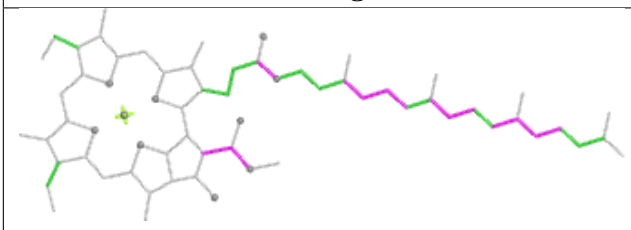

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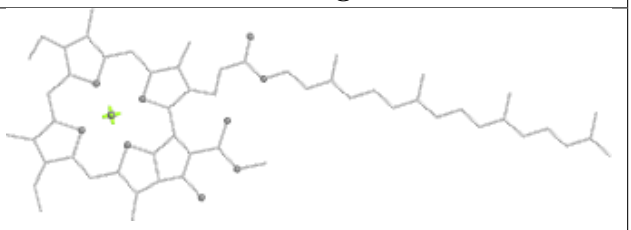
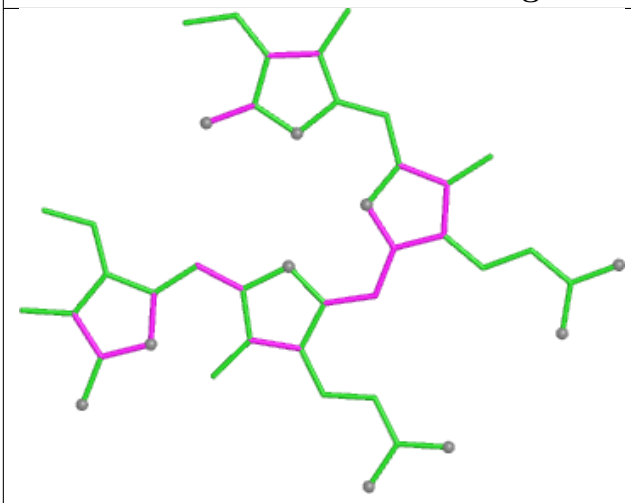


Rings

Ligand PEB I5 202



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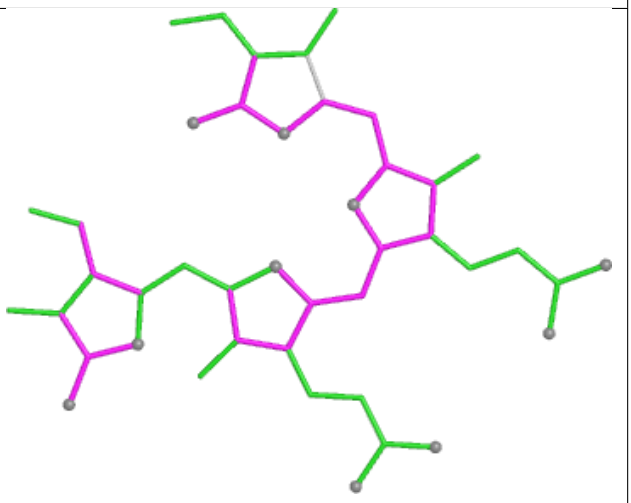
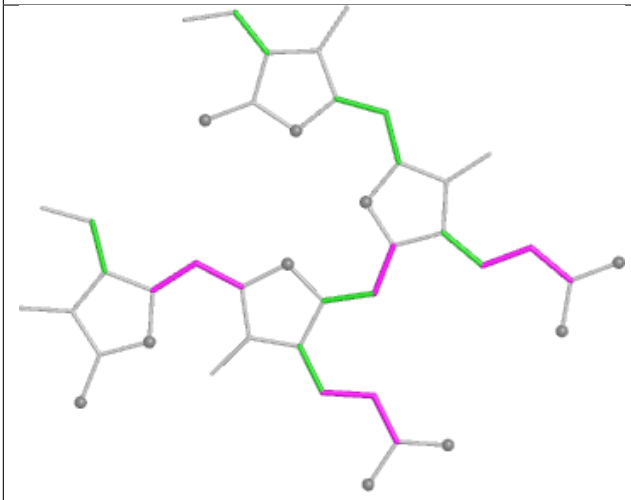


Bond angles



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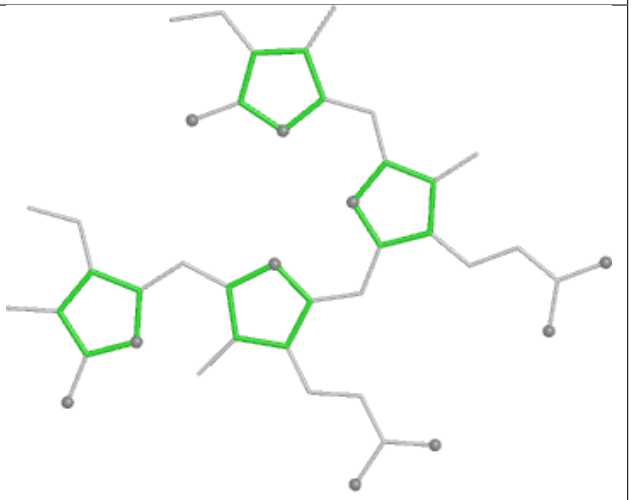
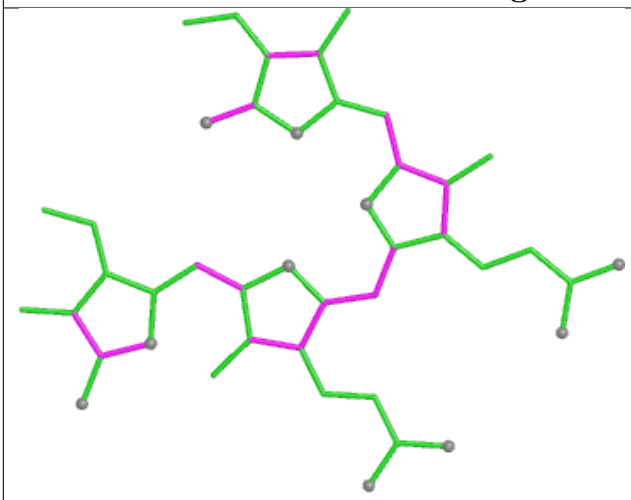


Rings

Ligand PEB DQ 203



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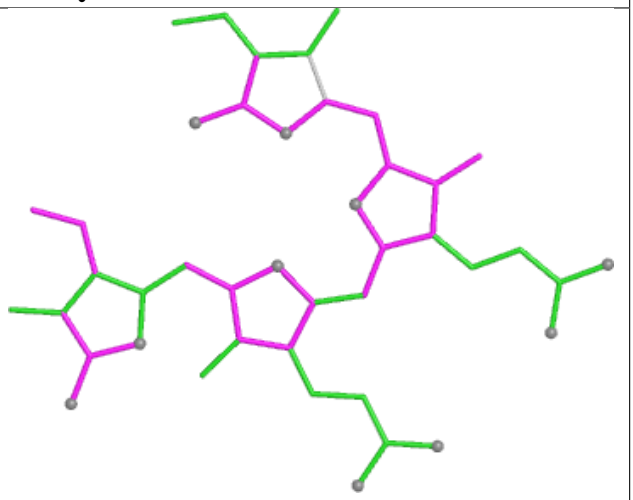

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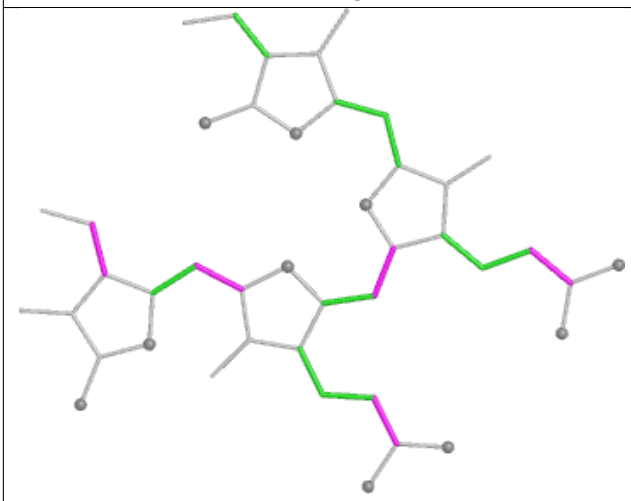

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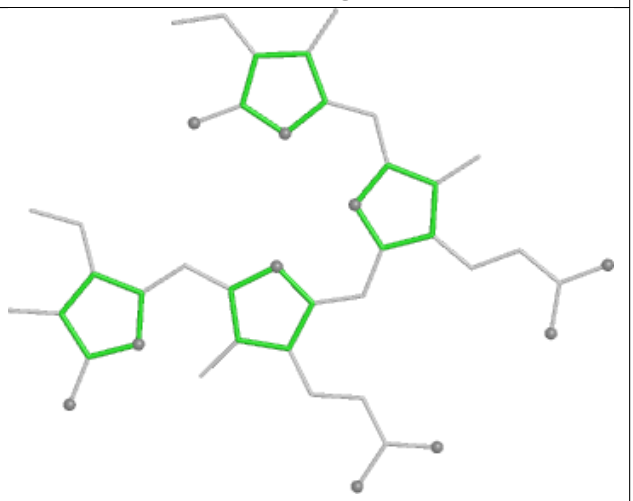
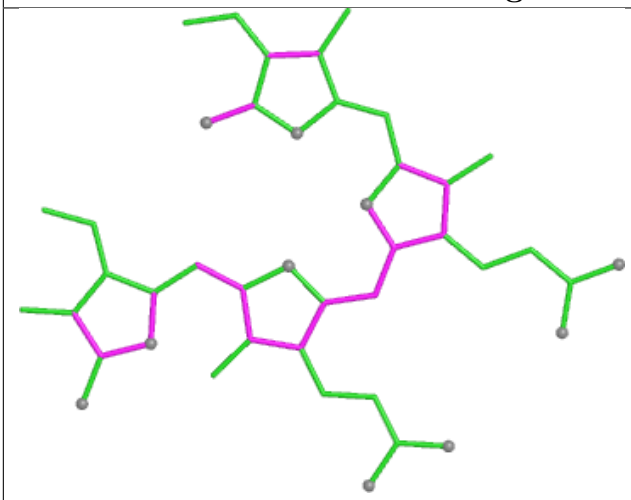


Rings

Ligand PEB mM 202



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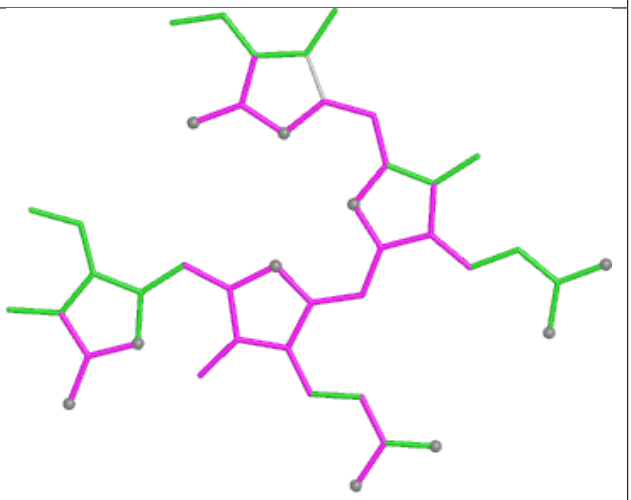
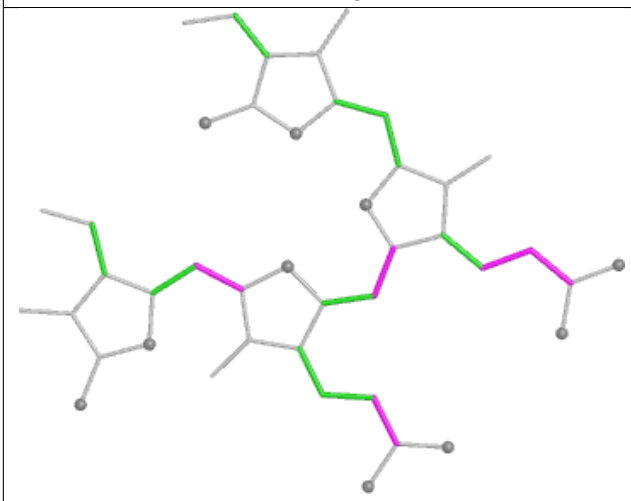


Bond angles



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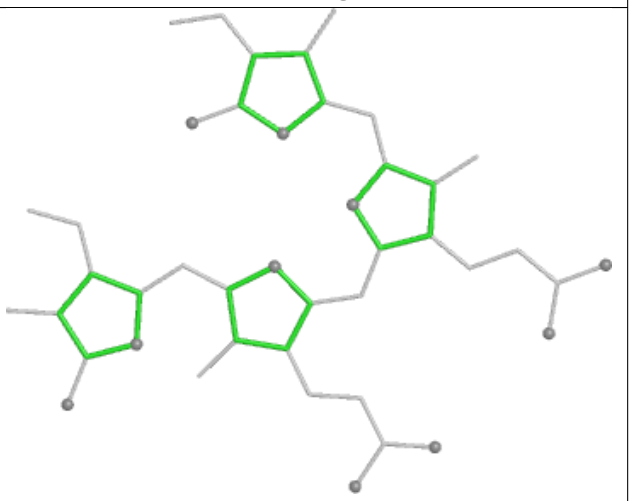
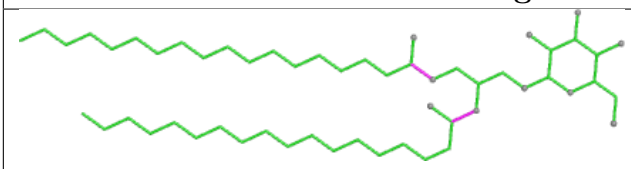


Rings

Ligand LMG k6 101



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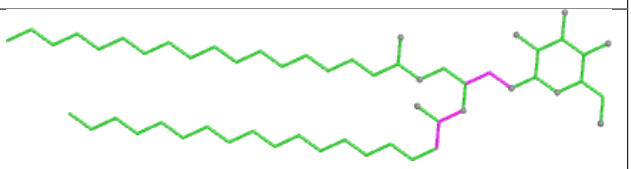
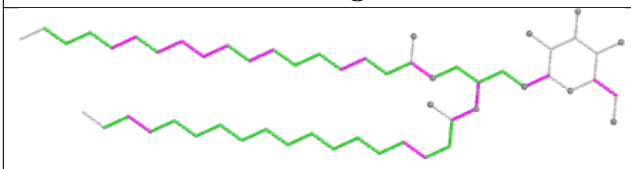


Bond angles



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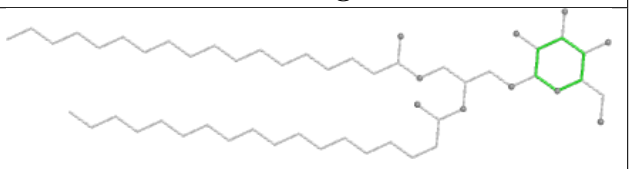
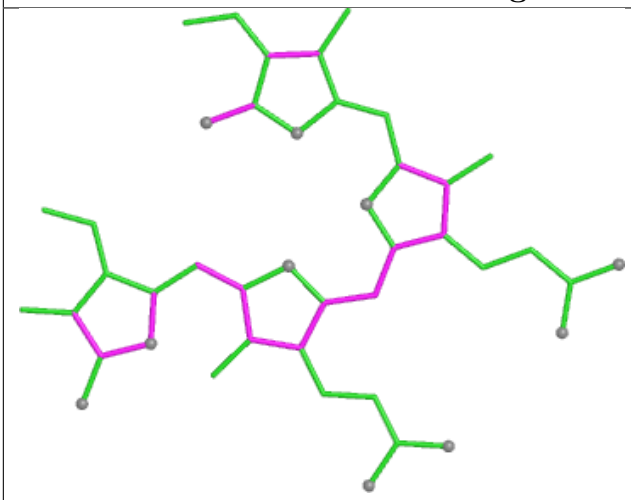


Rings

Ligand PEB MF 203



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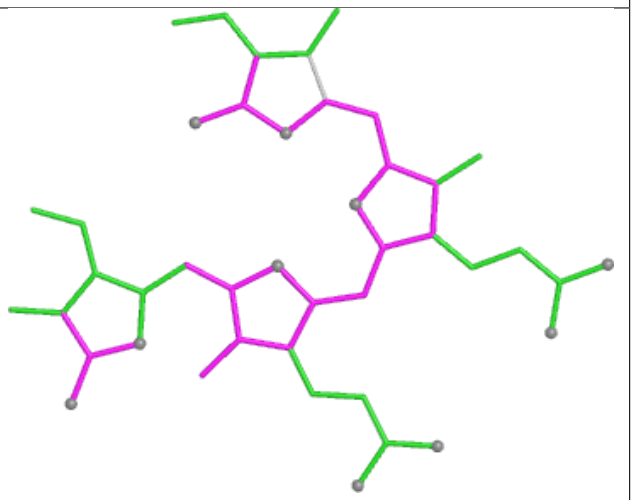
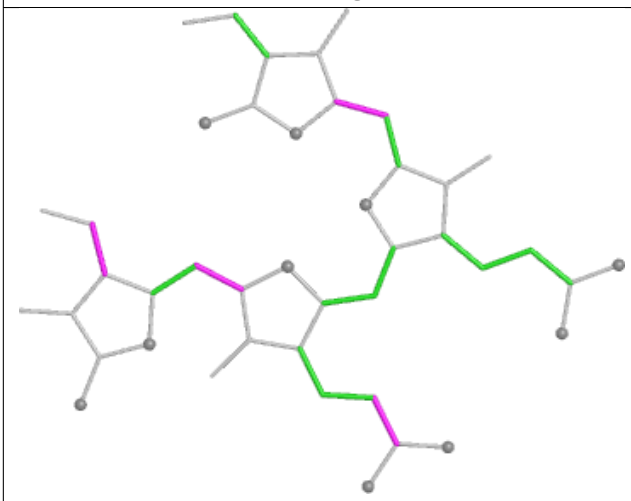


Bond angles



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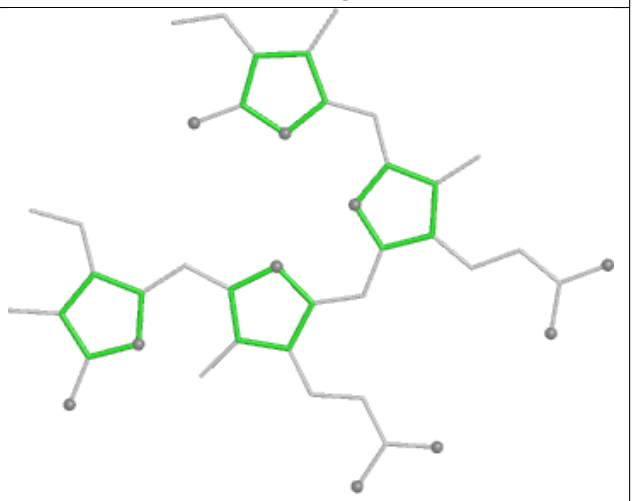
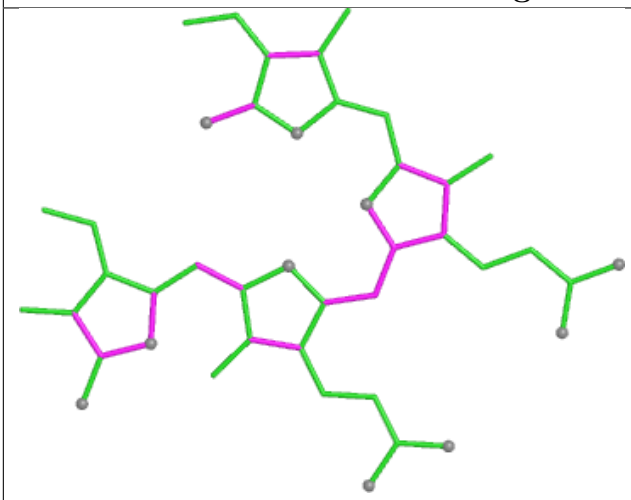


Rings

Ligand PEB PP 202



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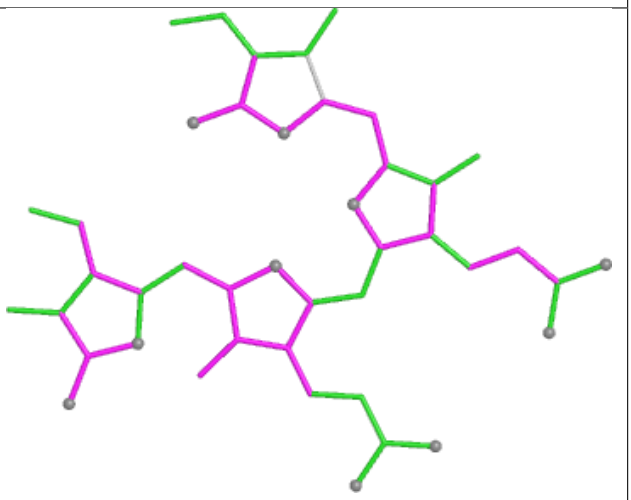
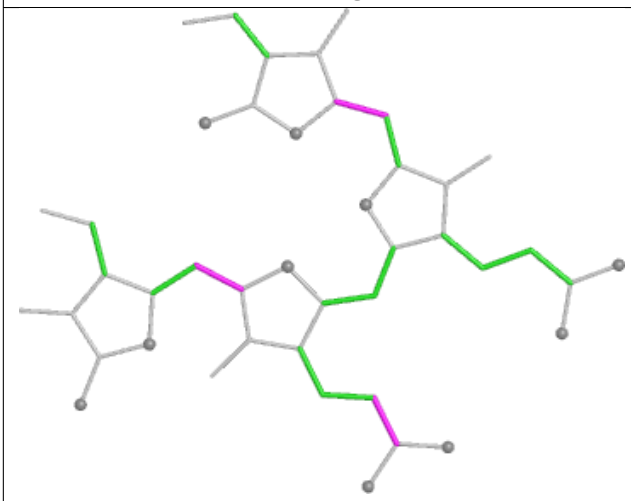


Bond angles



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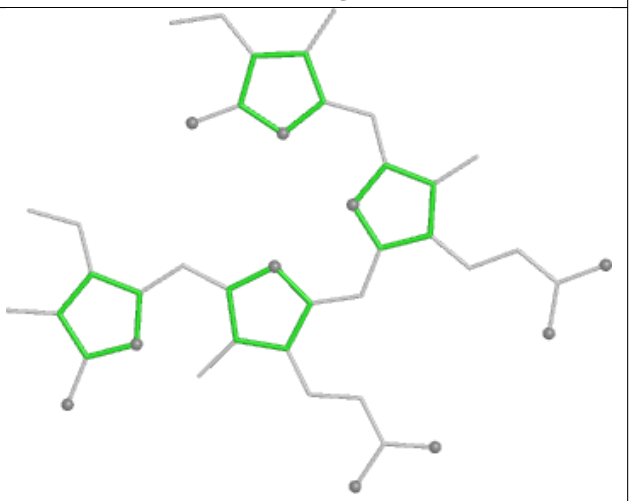
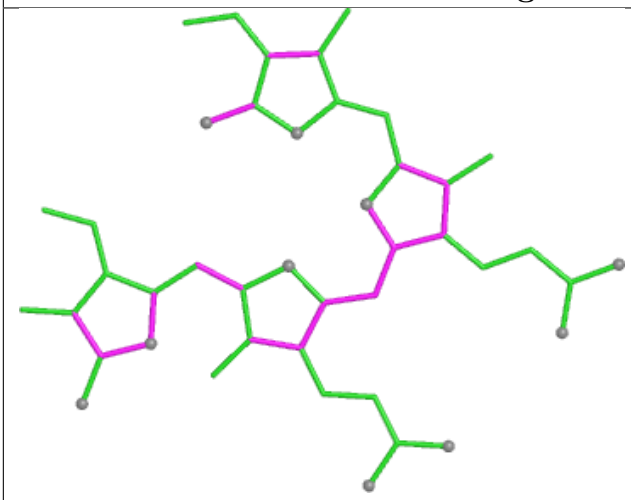
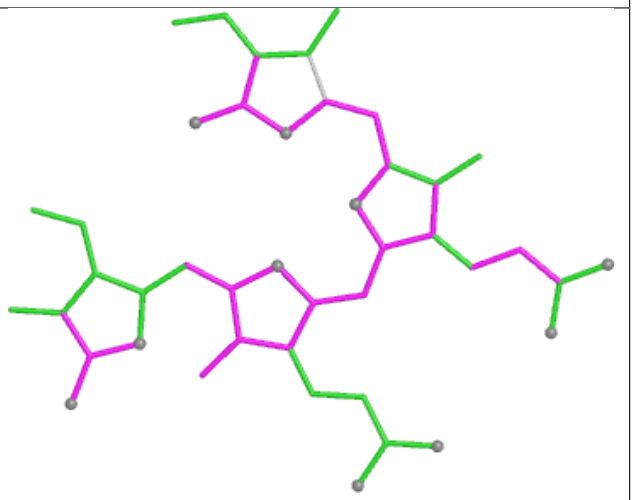


Rings

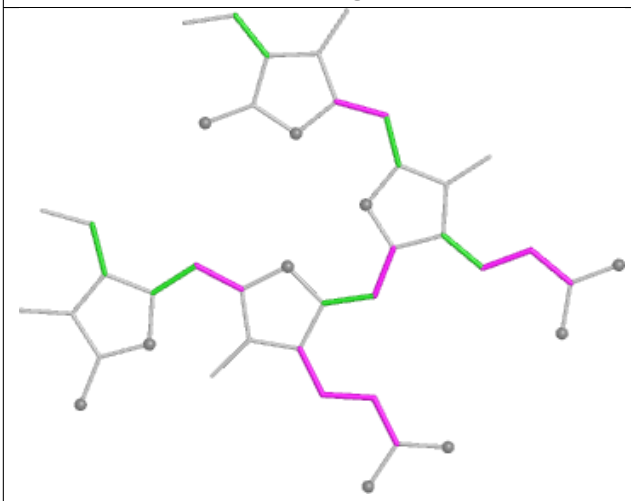
Ligand PEB aE 202



Bond lengths



Bond angles



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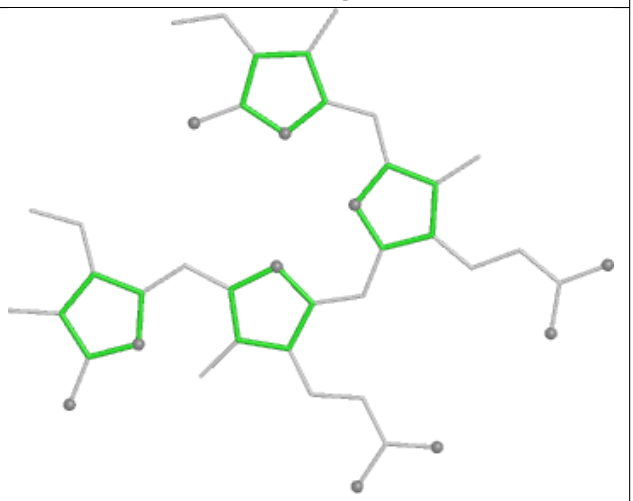
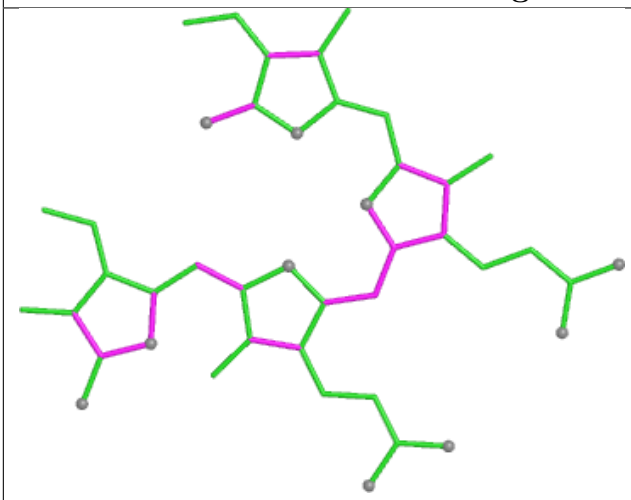


Rings

Ligand PEB DP 201



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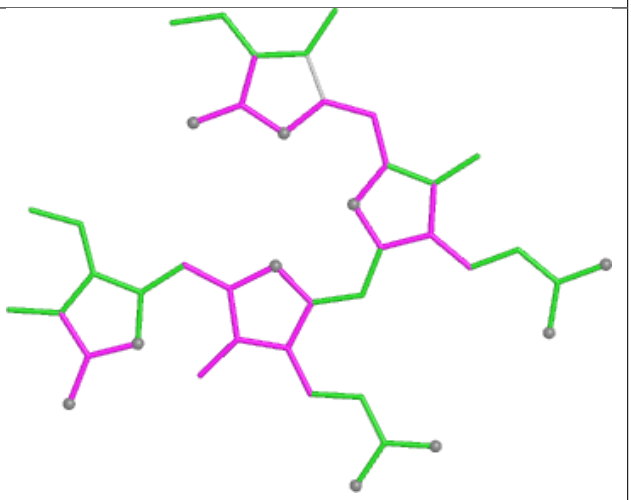

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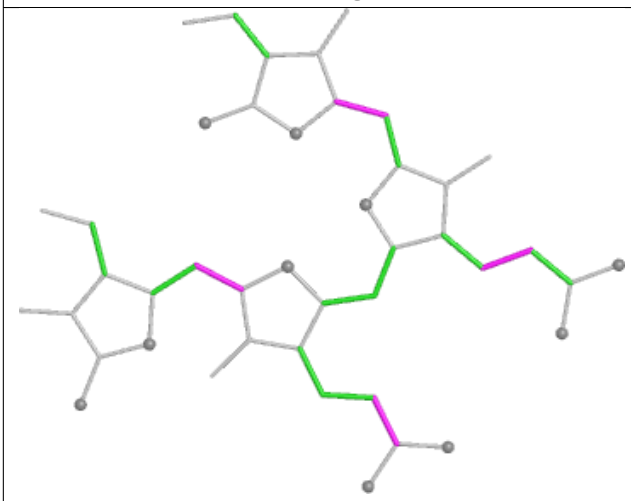

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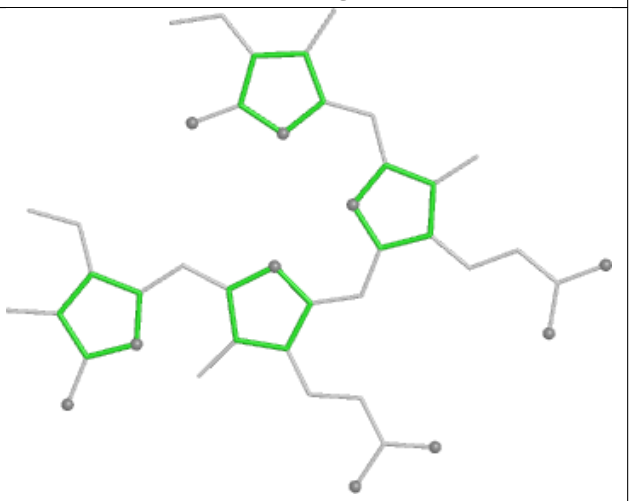
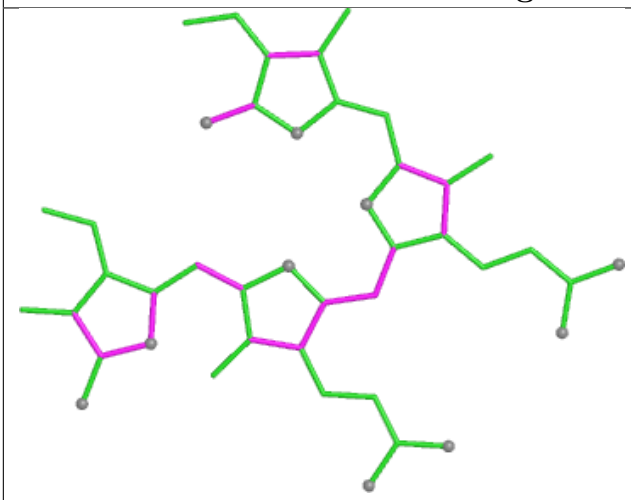


Rings

Ligand PEB P4 202



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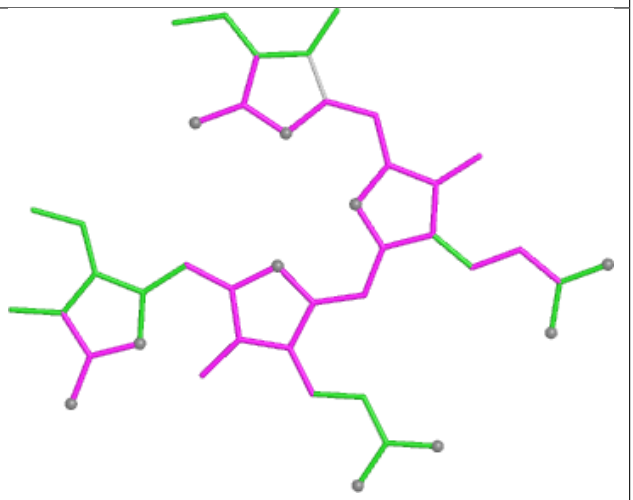

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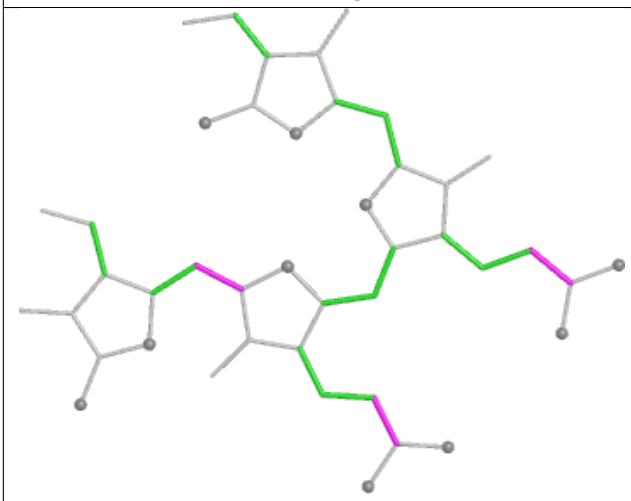

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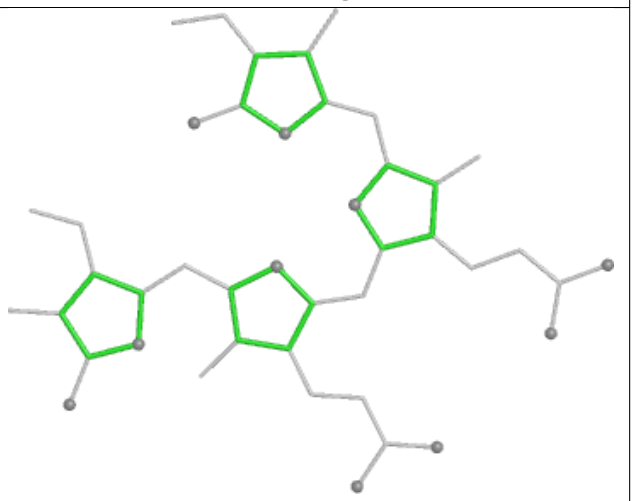
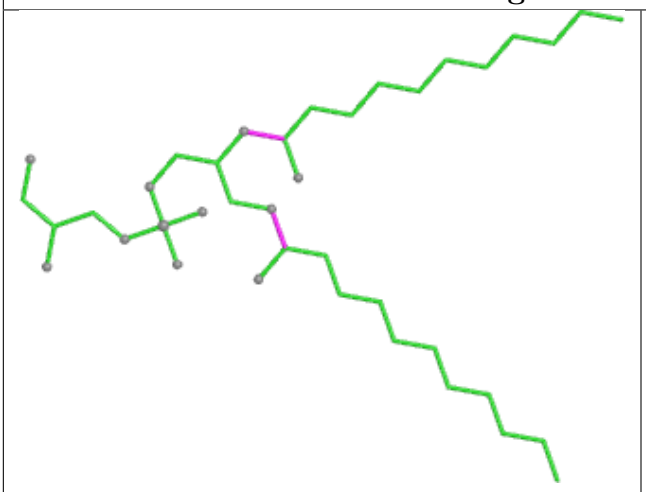


Rings

Ligand LHG ML 102



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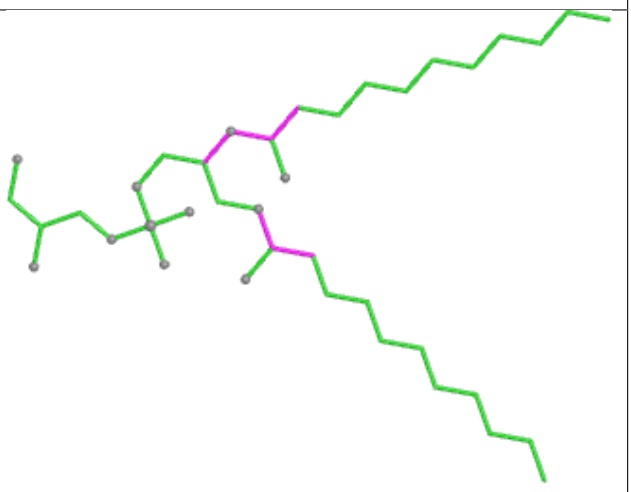

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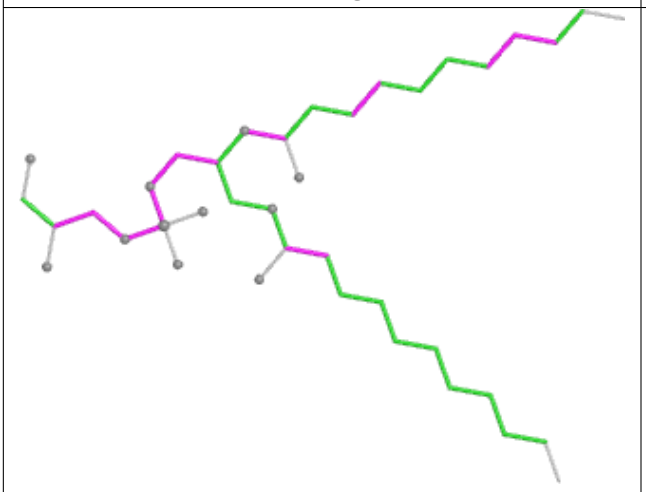

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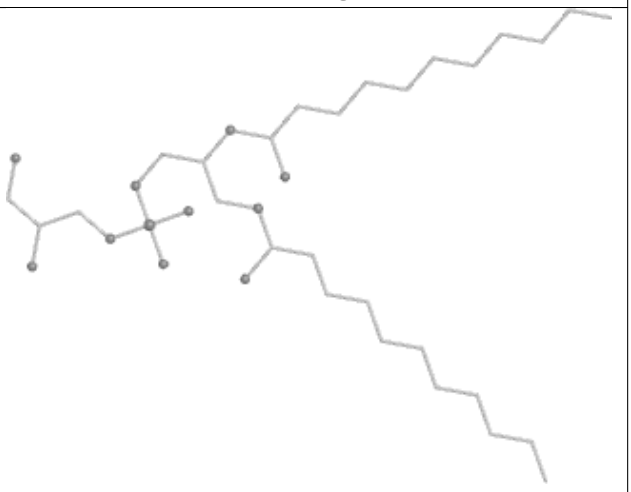
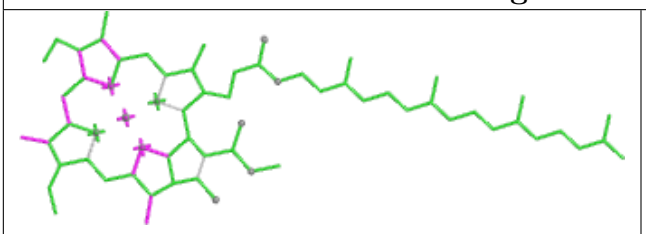


Rings

Ligand CLA BN 805



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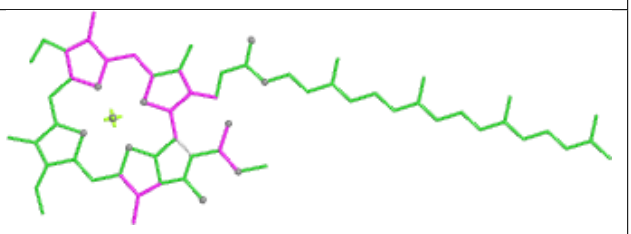

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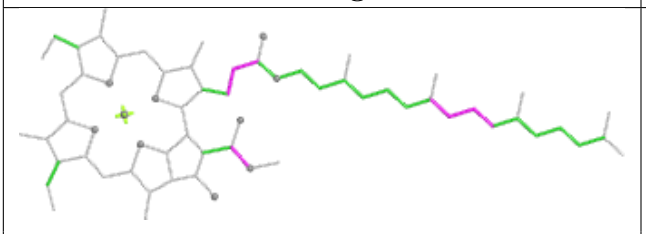

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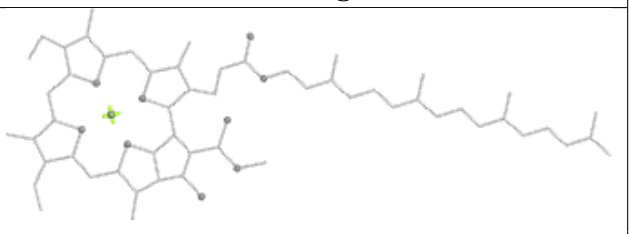
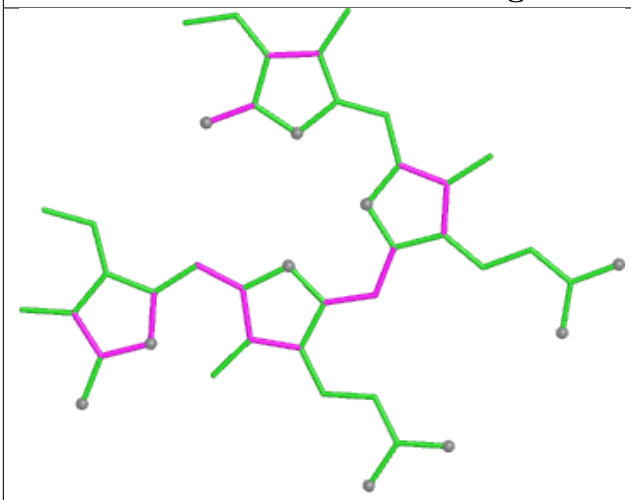


Rings

Ligand PEB RM 201



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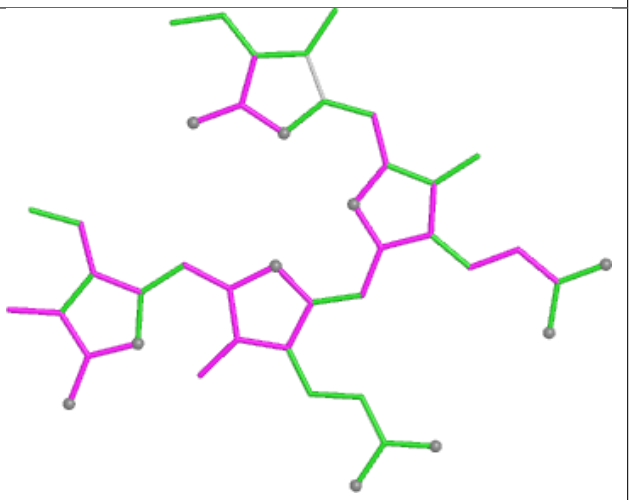

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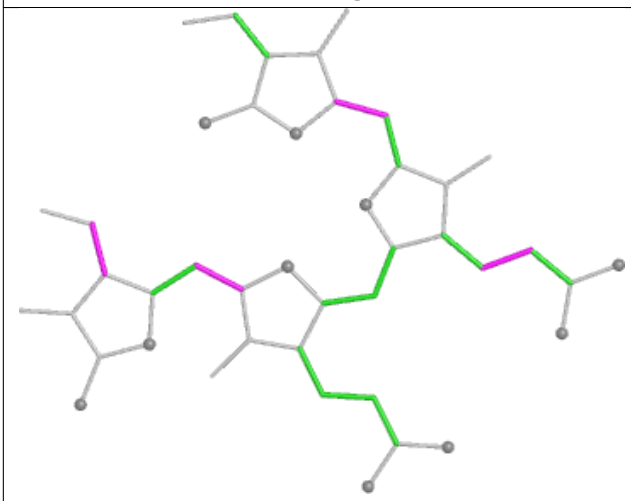

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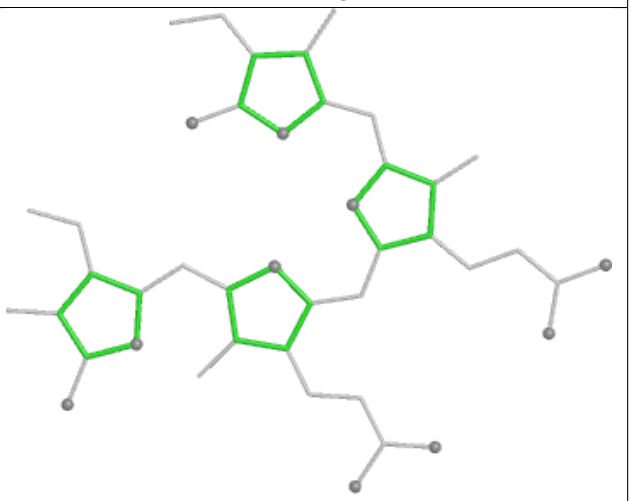
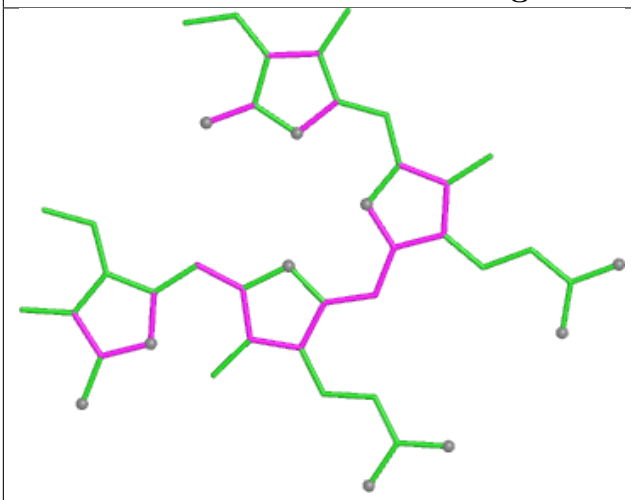


Rings

Ligand PEB mE 201



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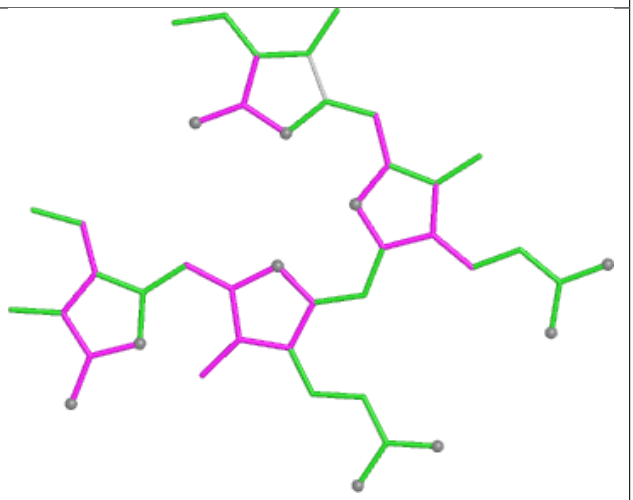

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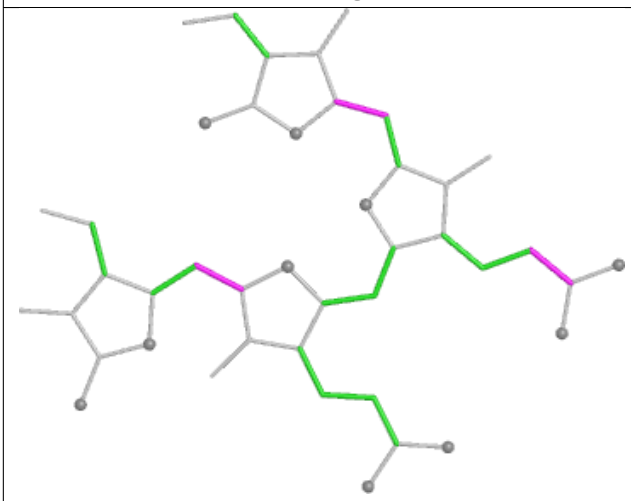

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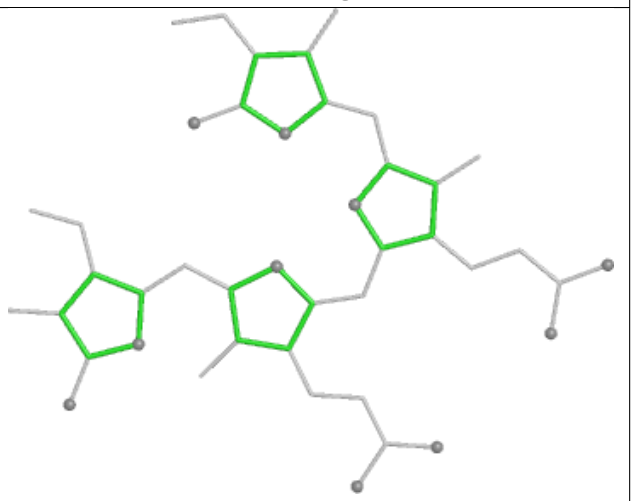
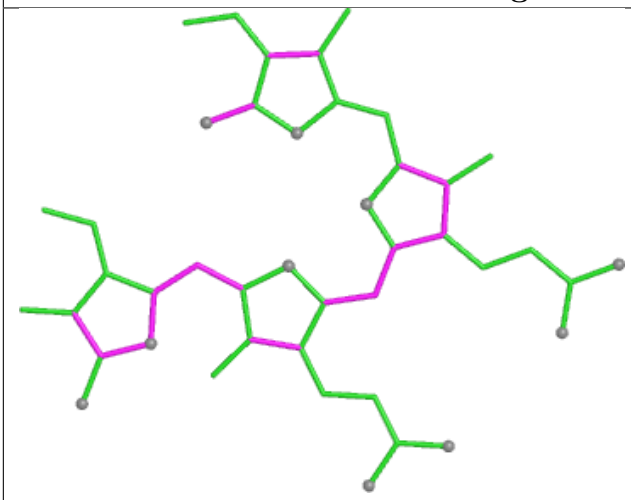


Rings

Ligand PEB OO 201



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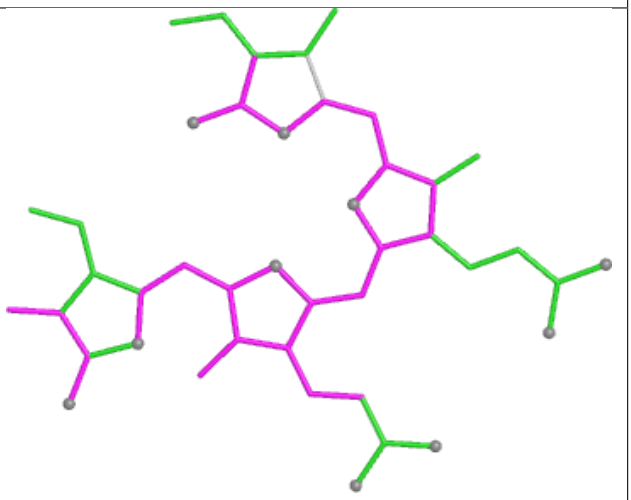

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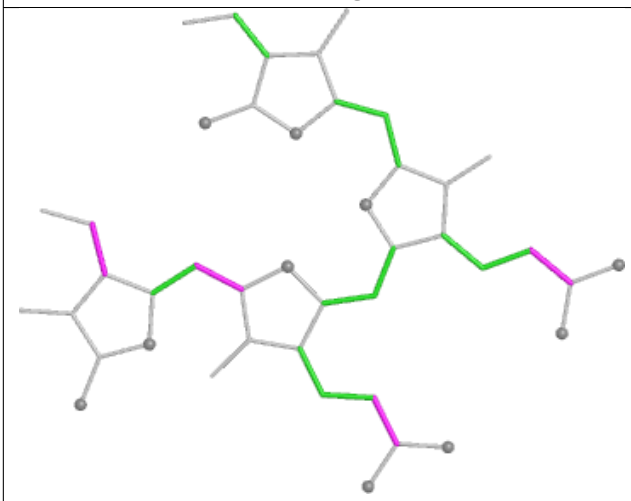

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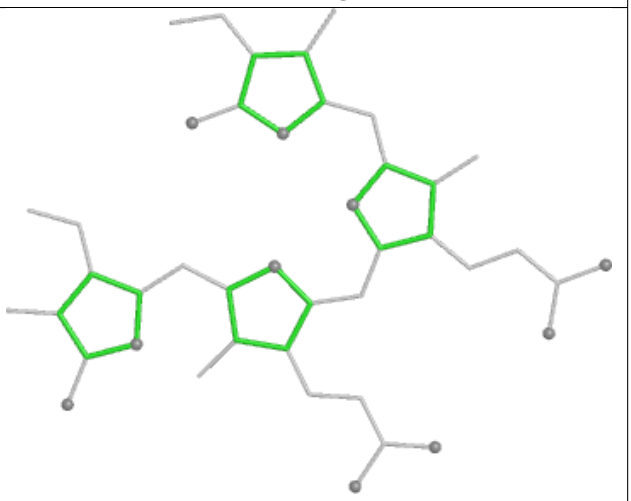
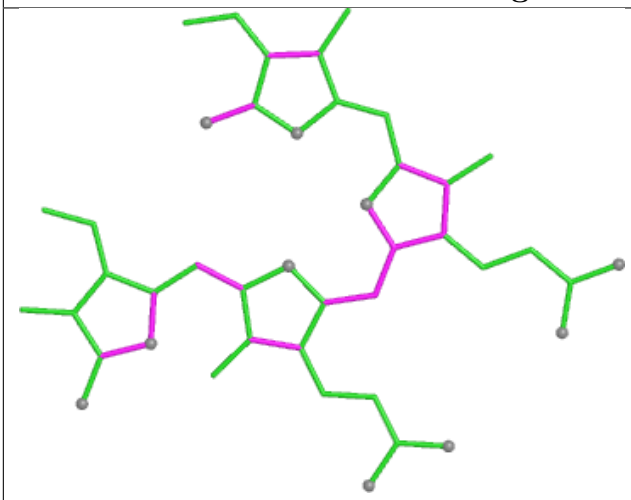


Rings

Ligand PEB AQ 301



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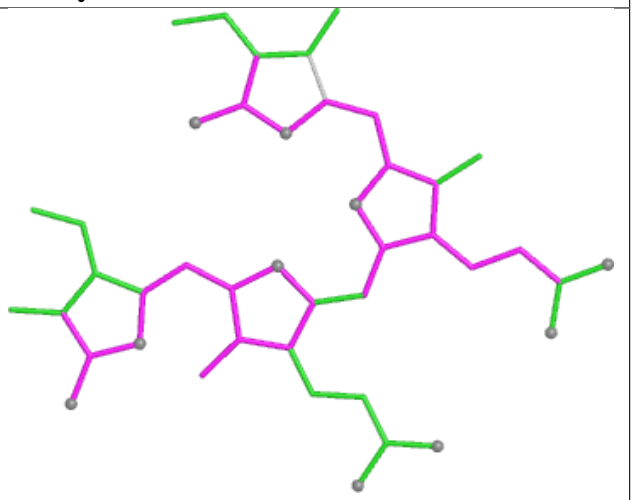

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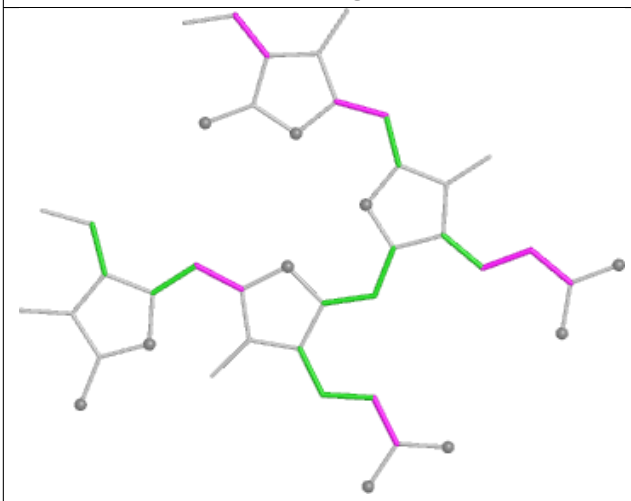

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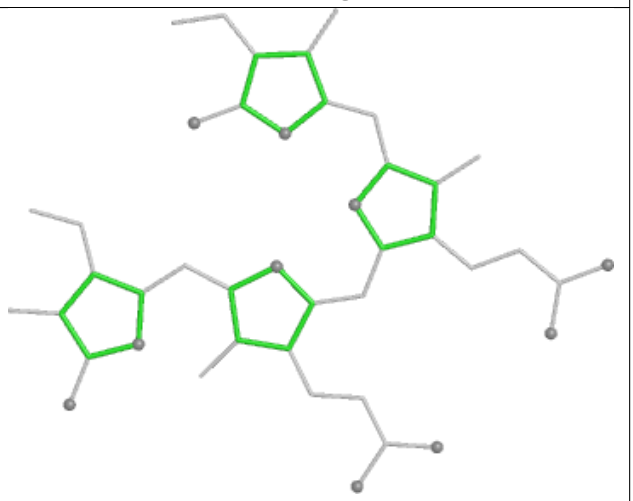
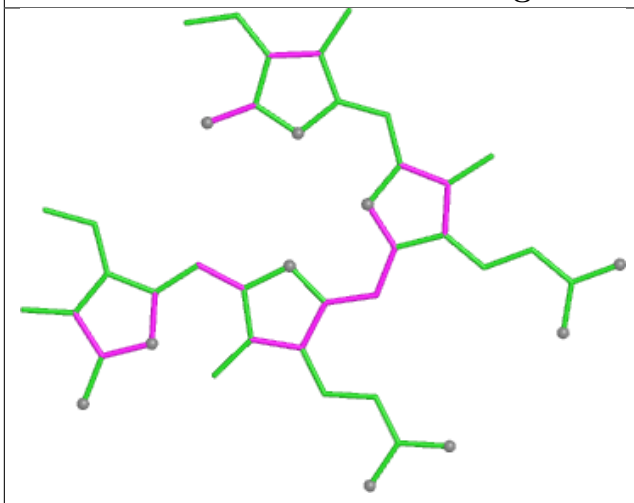


Rings

Ligand PEB BP 201



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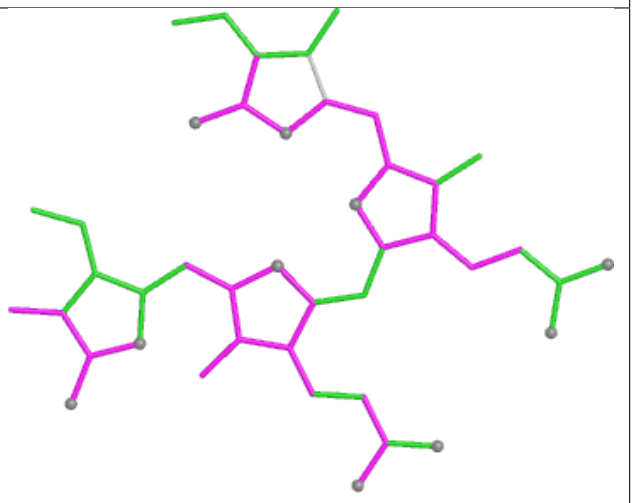

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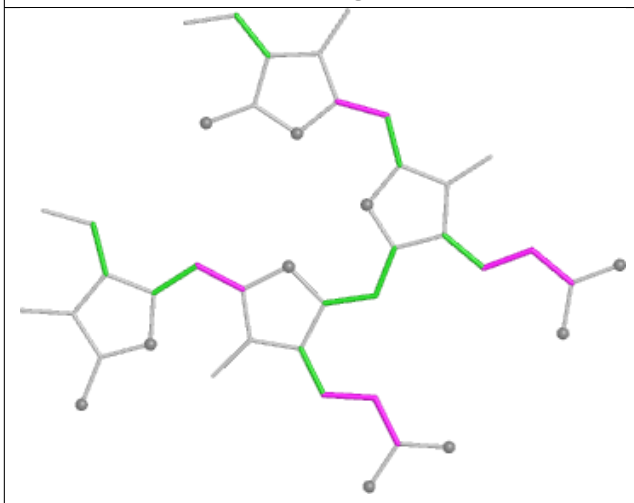

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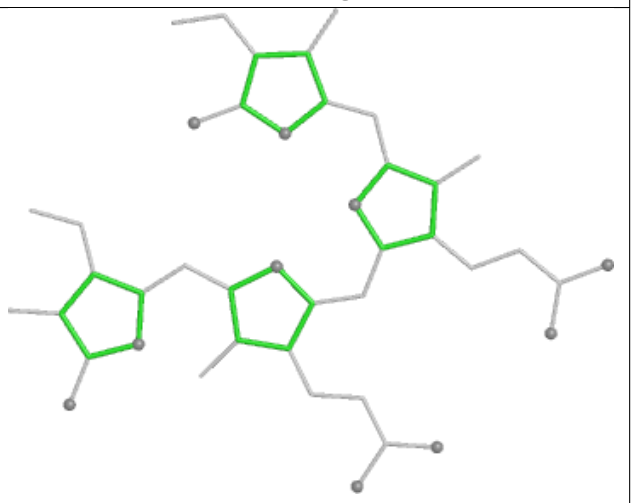
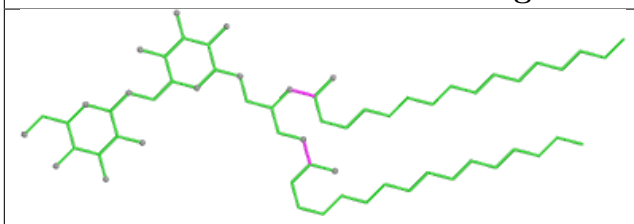


Rings

Ligand DGD JL 101



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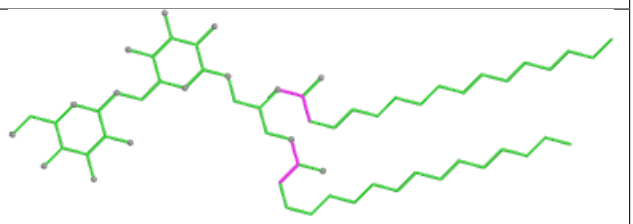
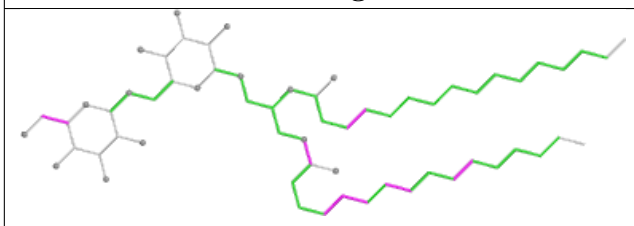


Bond angles



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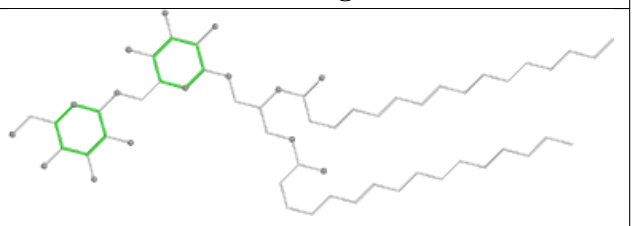
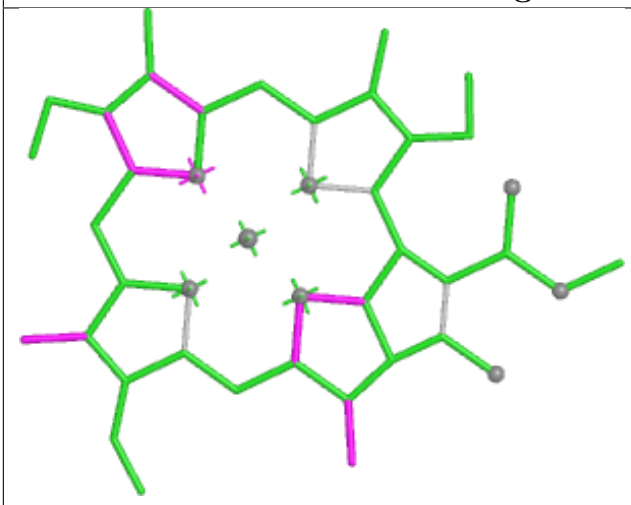


Rings

Ligand CLA 8N 307



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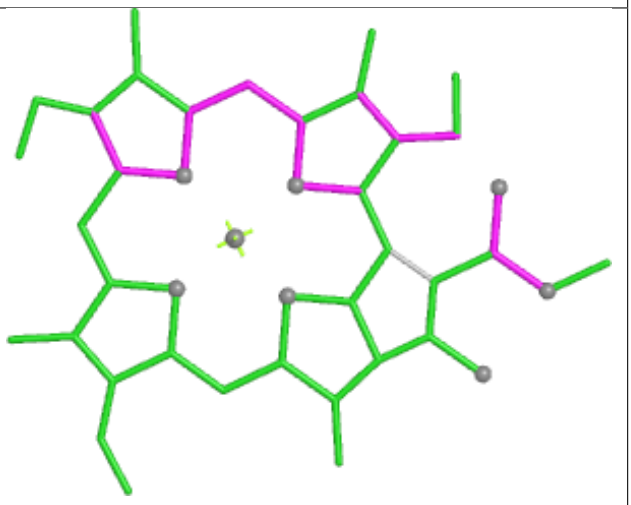

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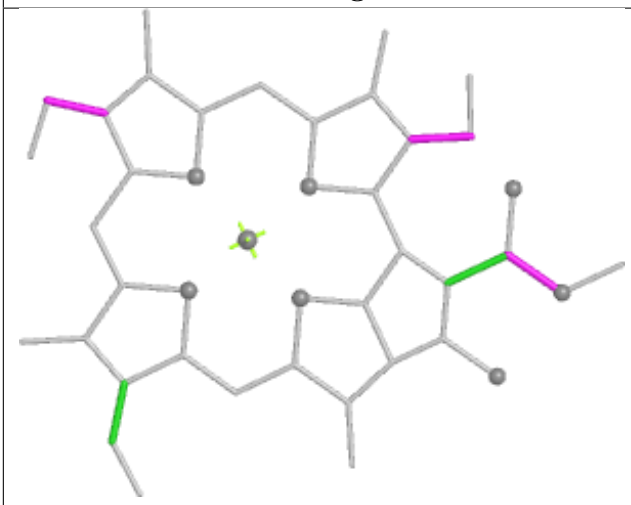
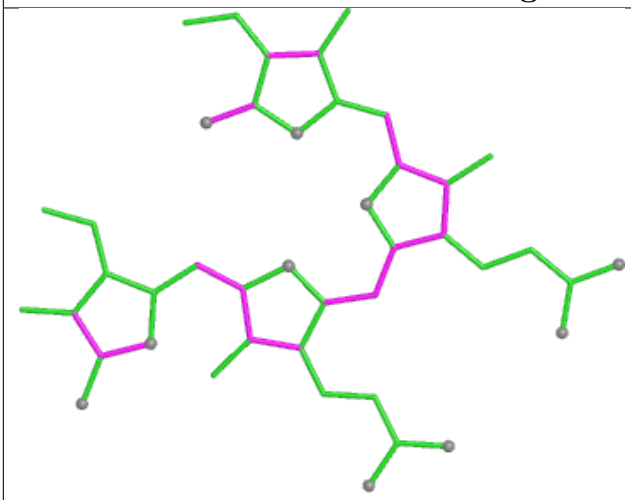


Torsions



Rings

Ligand PEB a1 202



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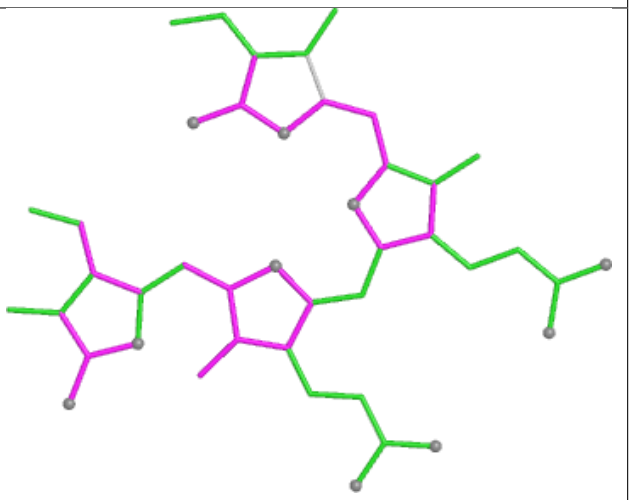
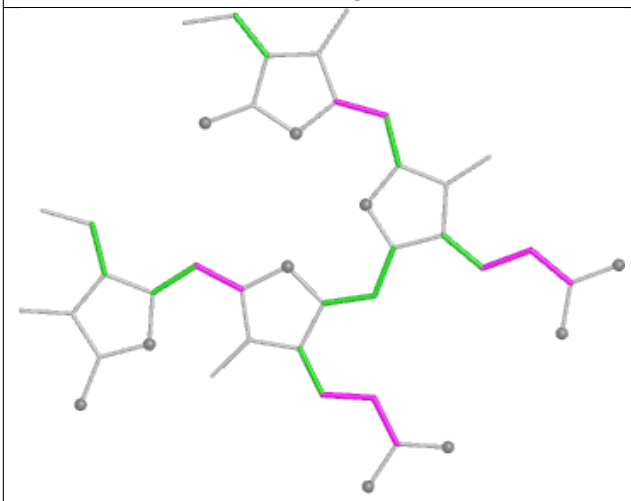


Bond angles



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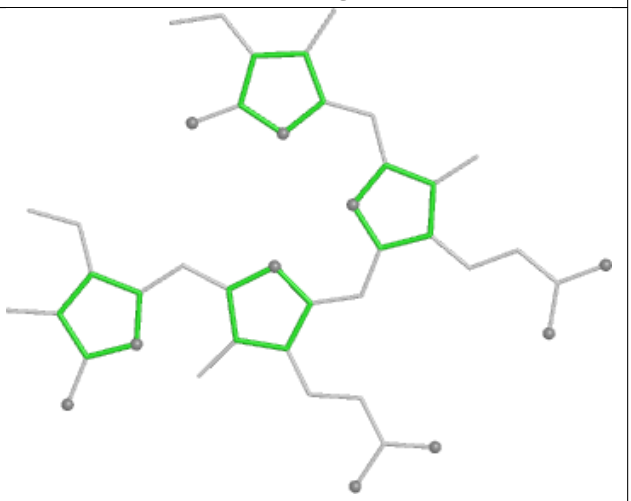
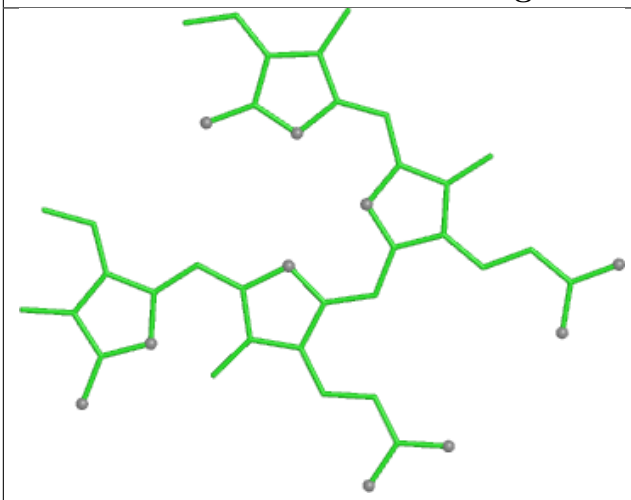


Rings

Ligand PEB kO 203



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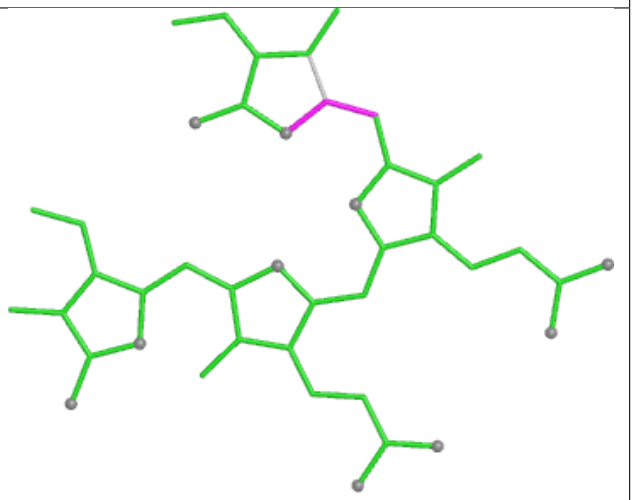
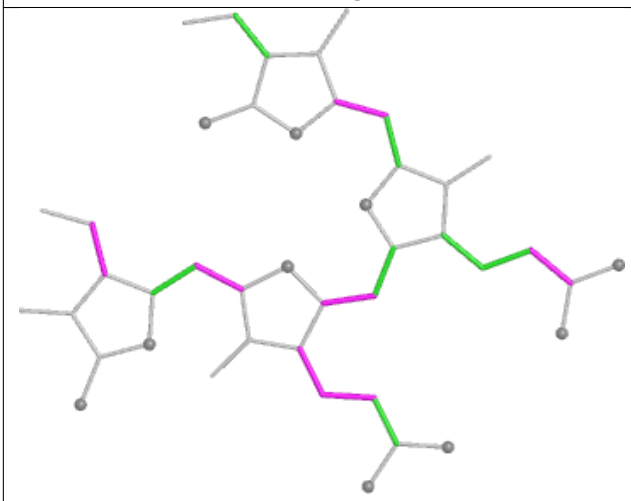


Bond angles



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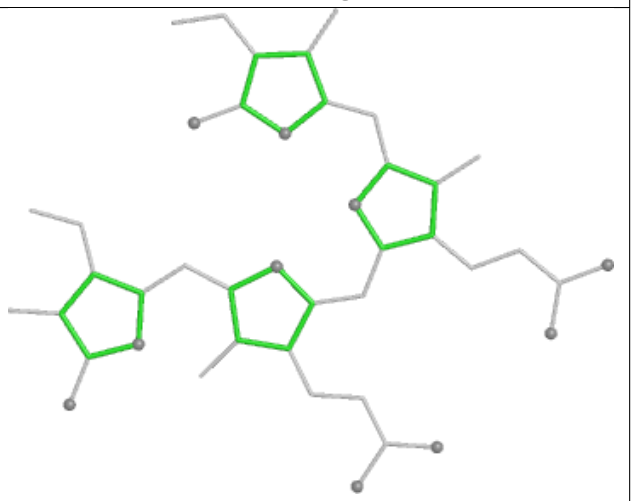
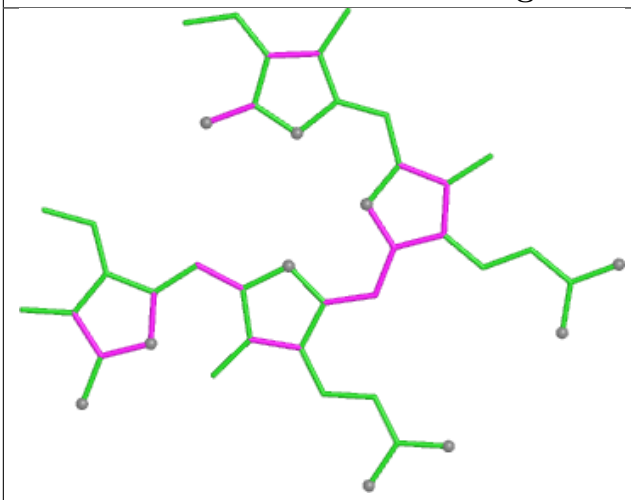


Rings

Ligand PEB EJ 203



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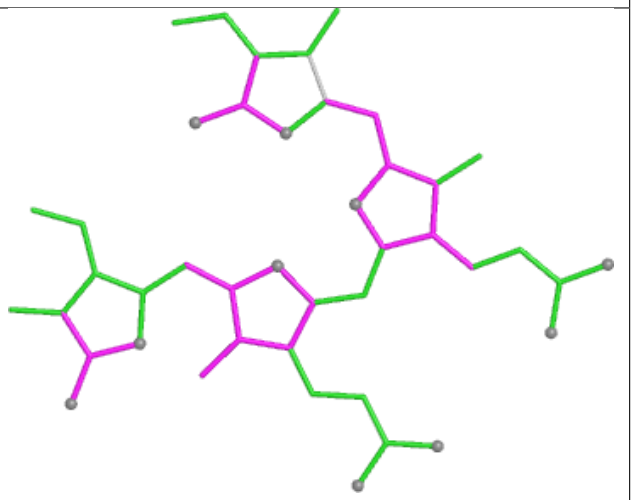
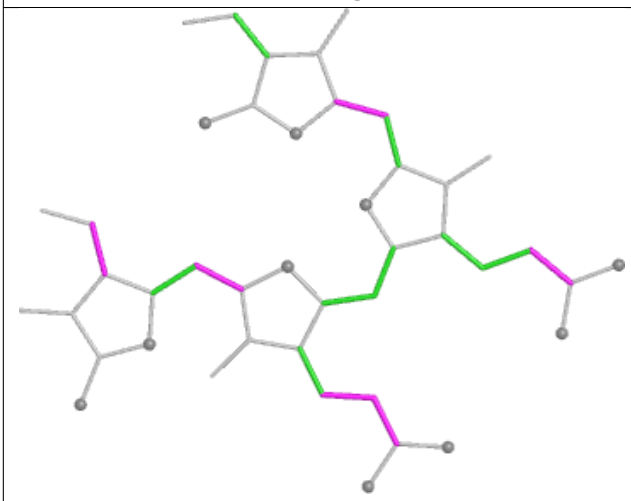


Bond angles



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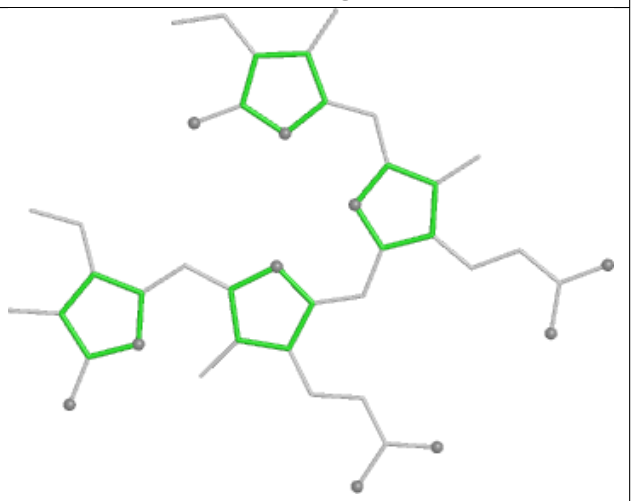
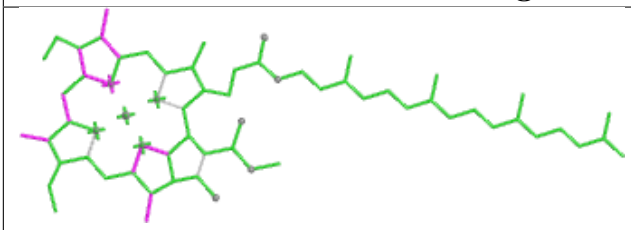


Rings

Ligand CLA C6 517



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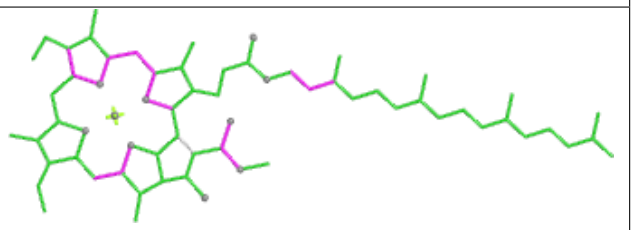

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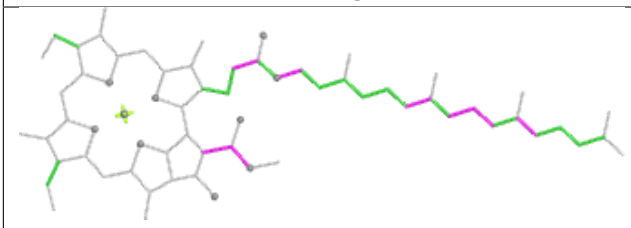
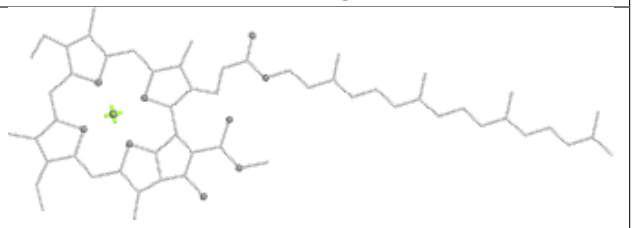
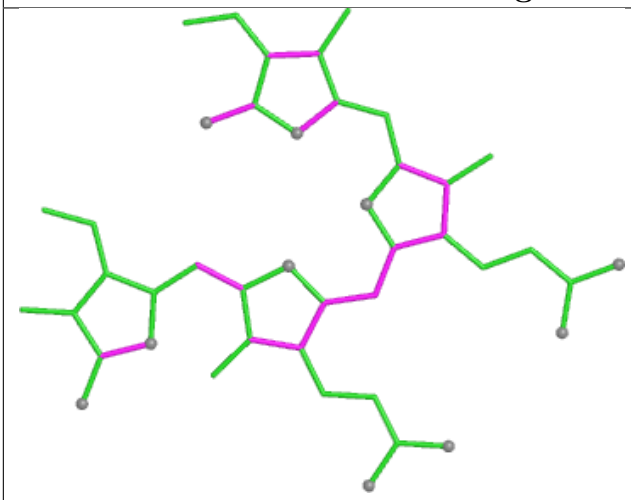


Torsions



Rings

Ligand PEB D7 202



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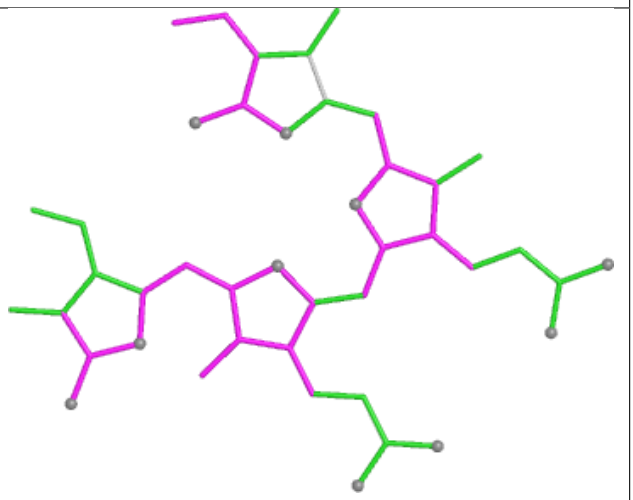

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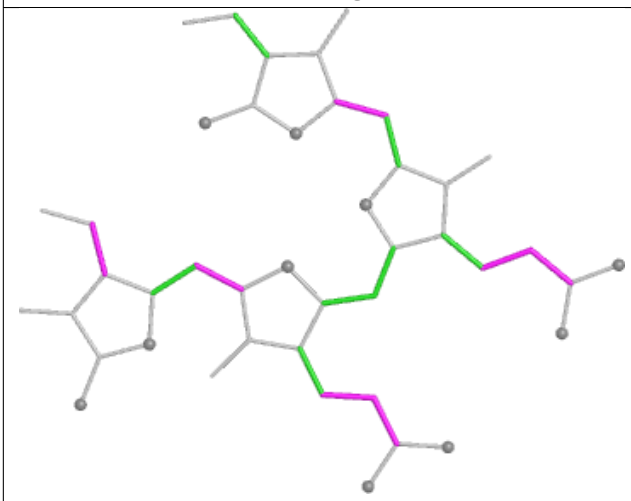

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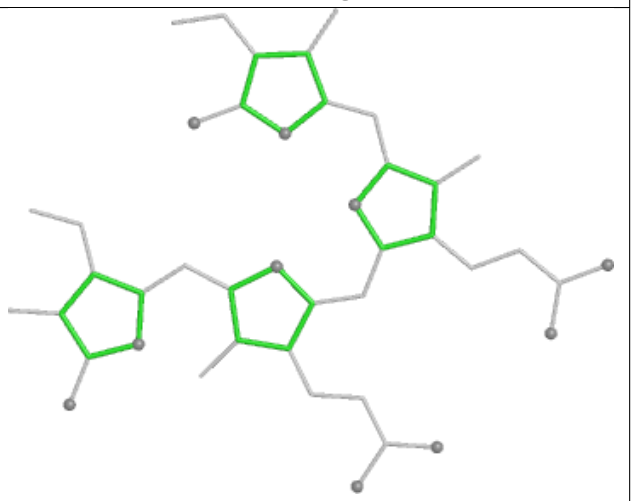
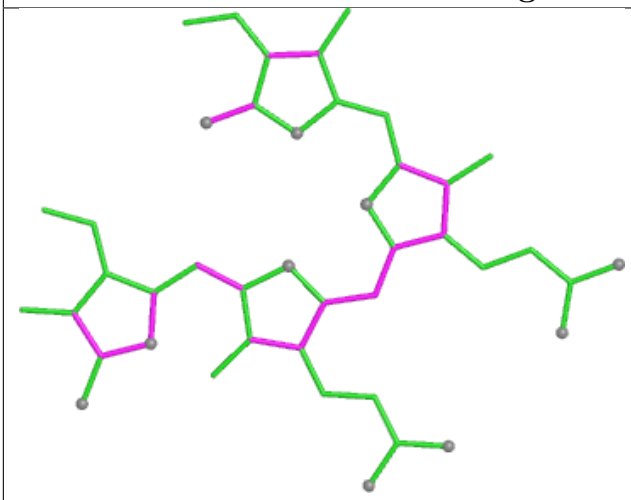


Rings

Ligand PEB hJ 202



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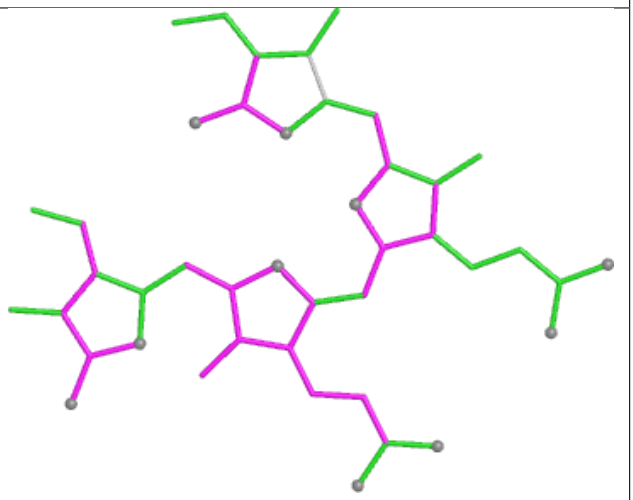

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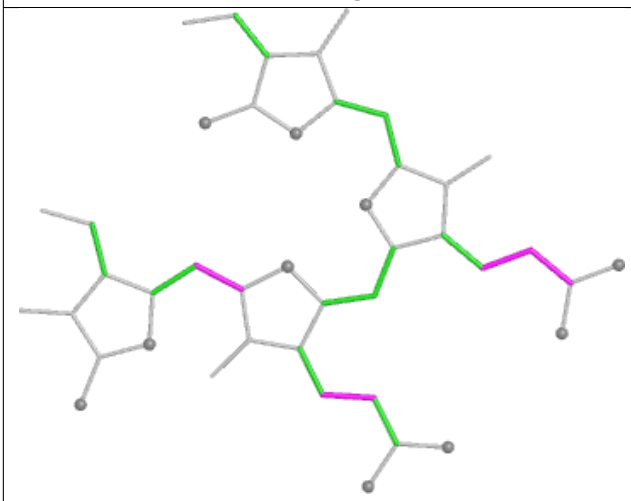

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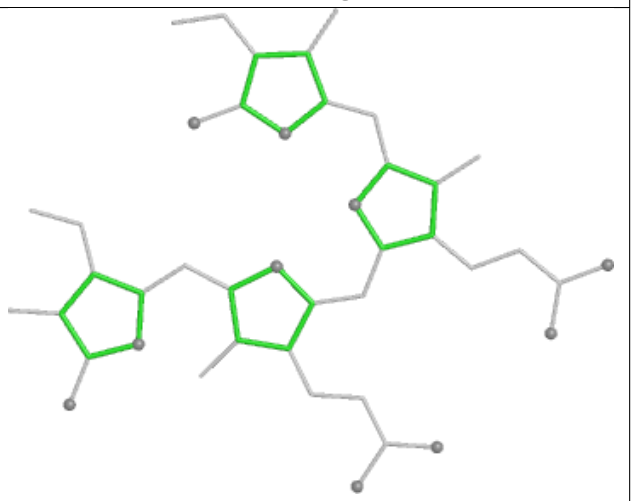
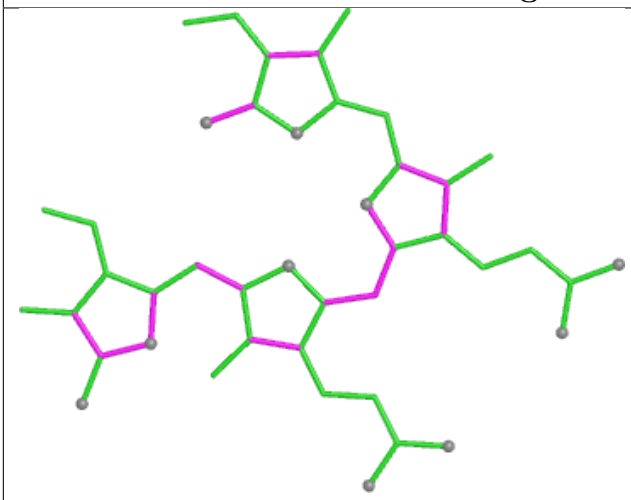


Rings

Ligand PEB LI 202



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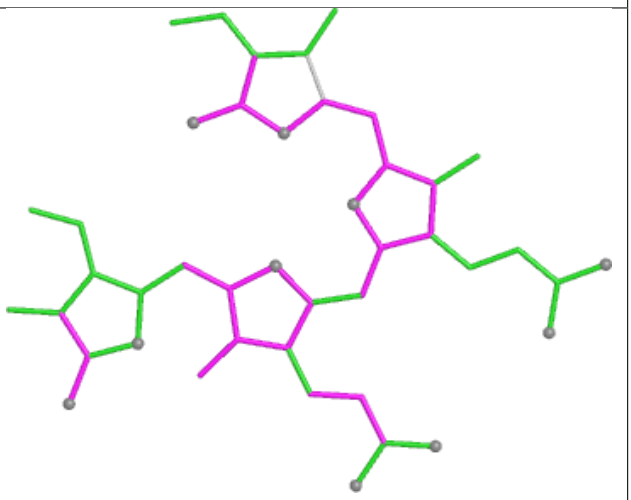

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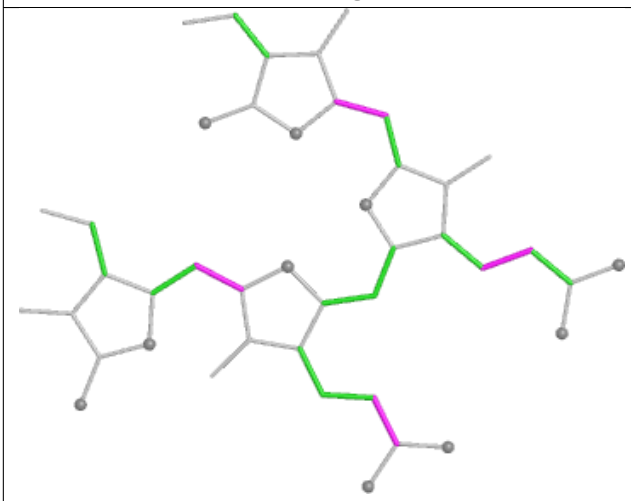

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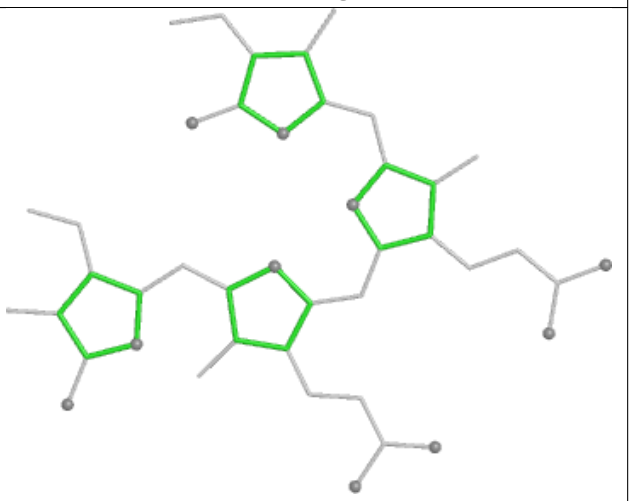
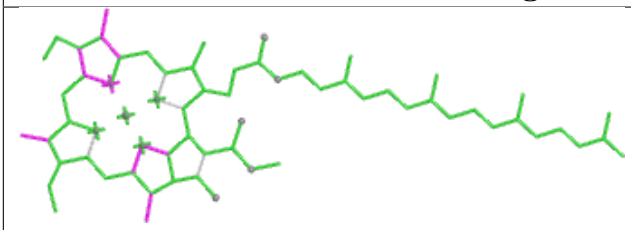


Rings

Ligand CLA I2 103



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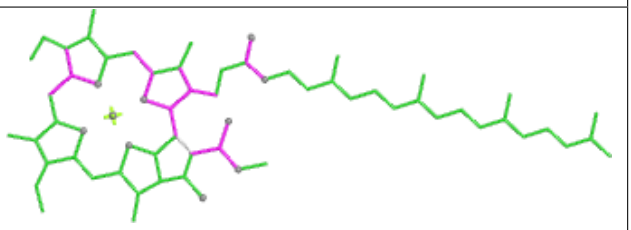

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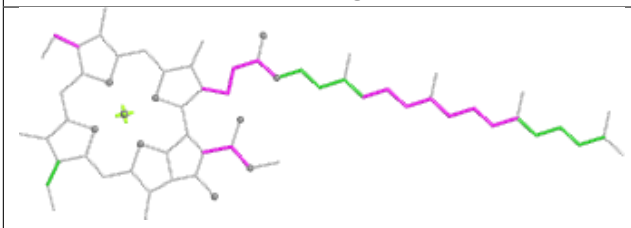

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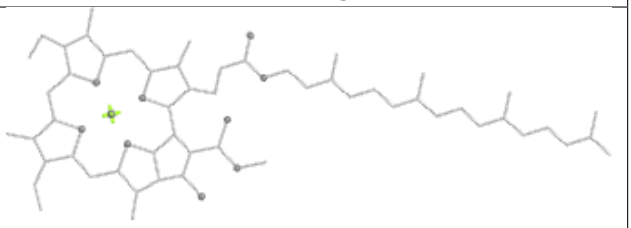
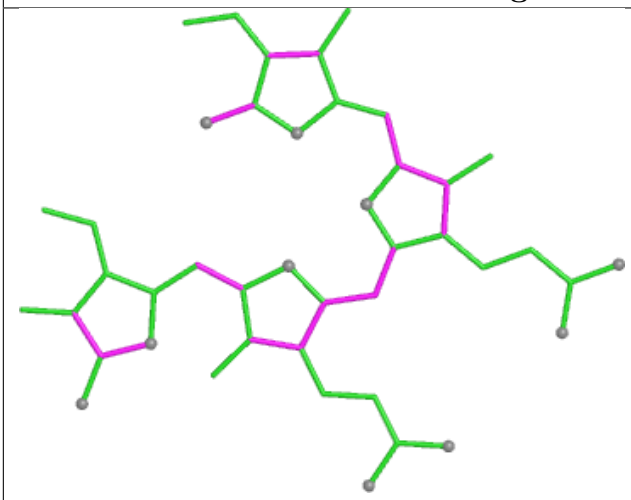


Rings

Ligand PEB DD 203



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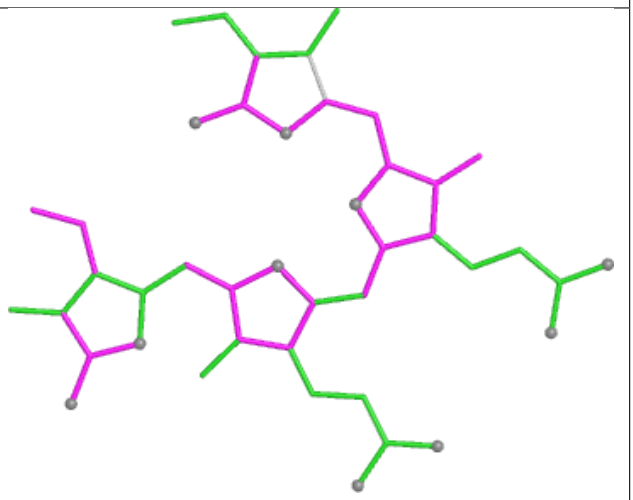

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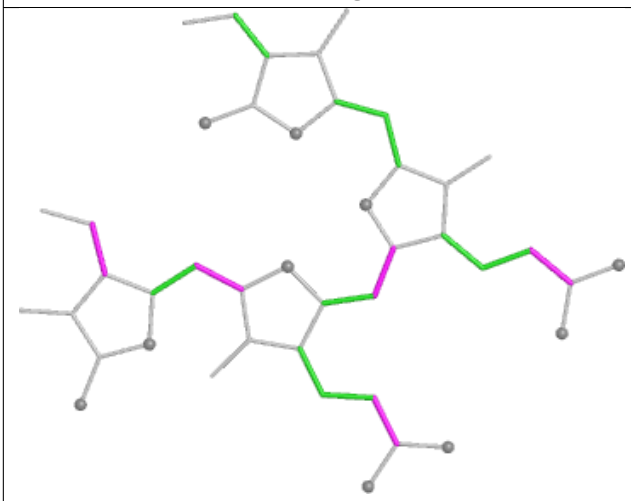

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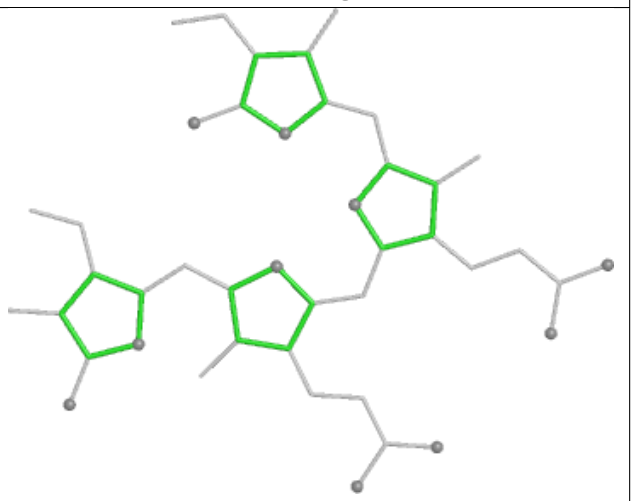

Rings

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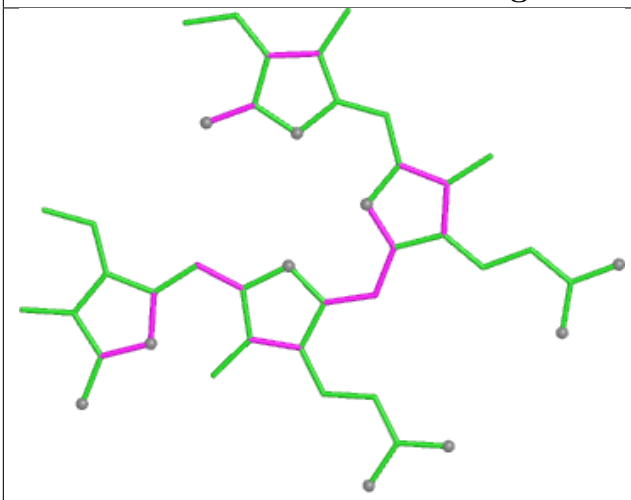

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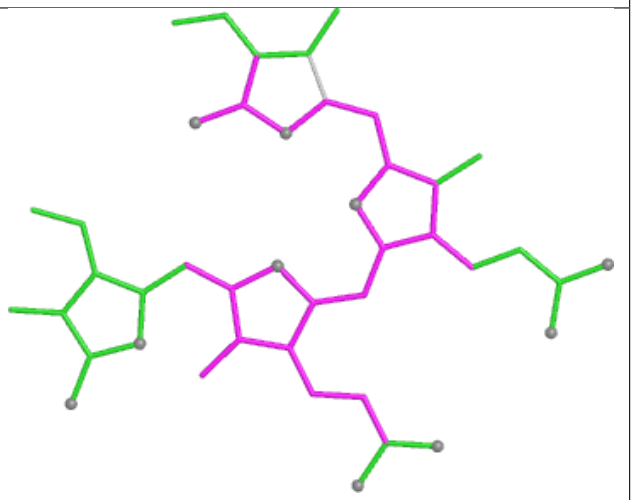

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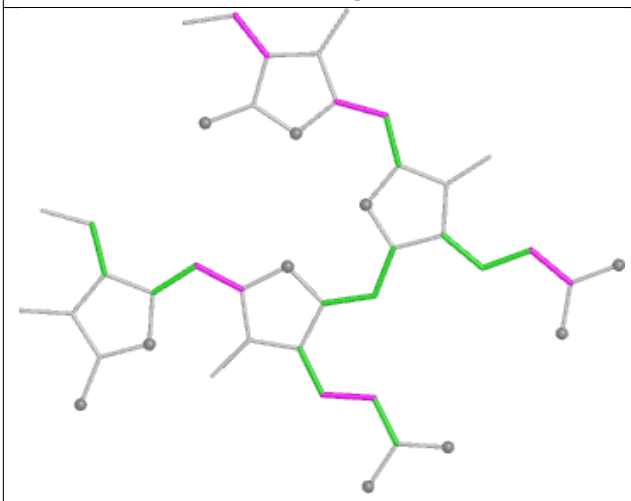

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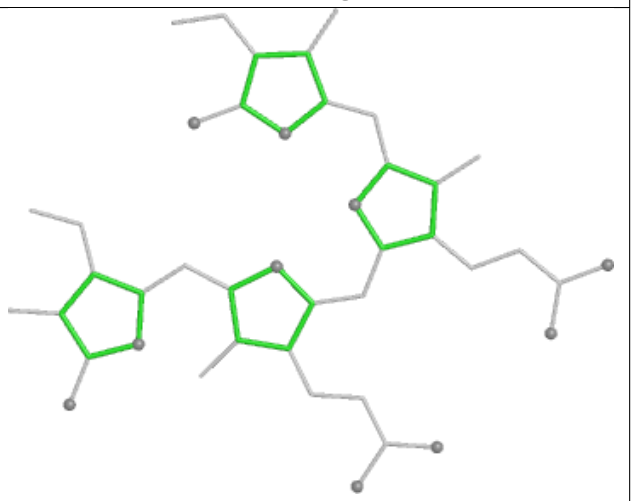
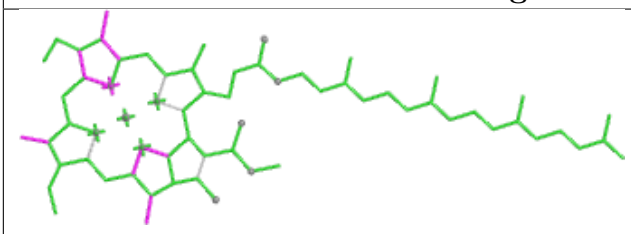


Rings

Ligand CLA AN 809



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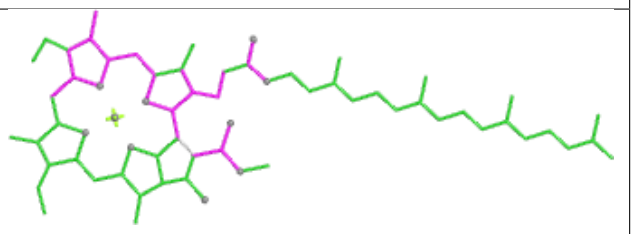

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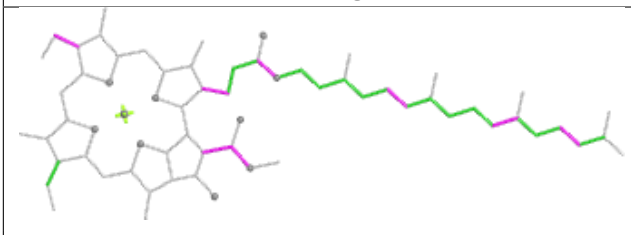

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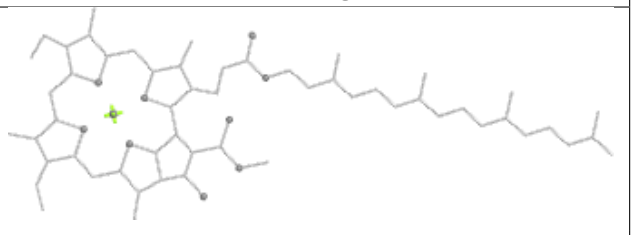
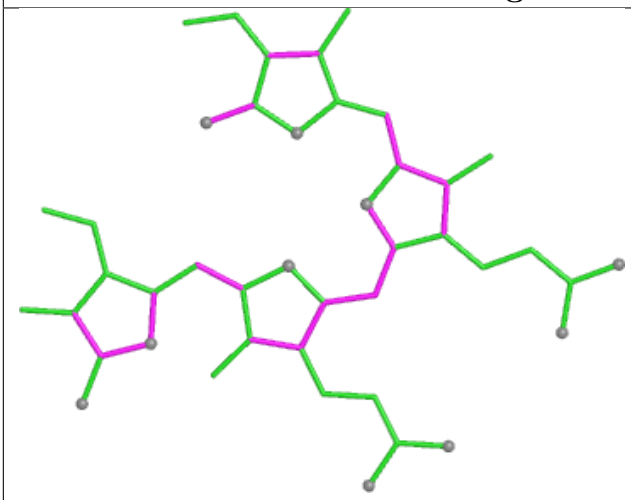


Rings

Ligand PEB JO 1002



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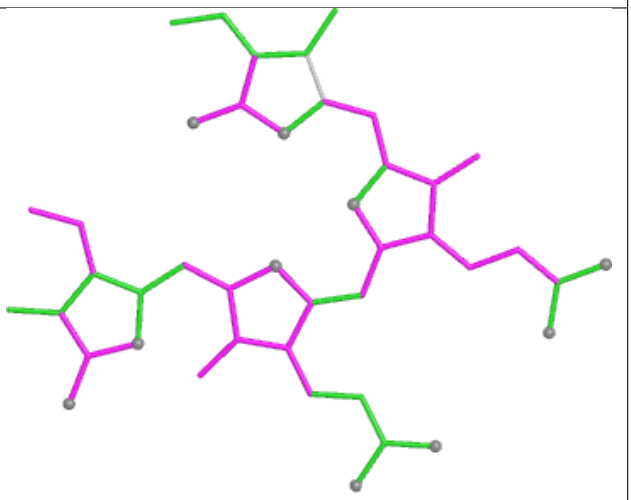

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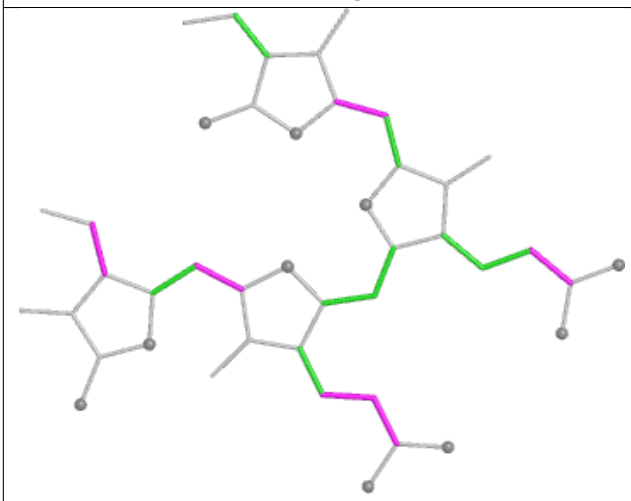

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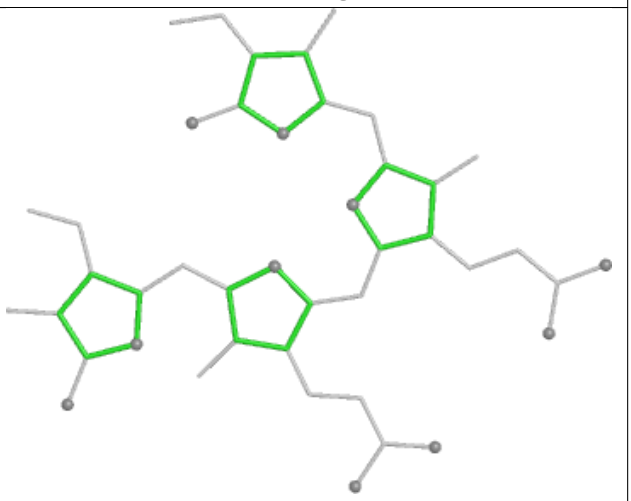
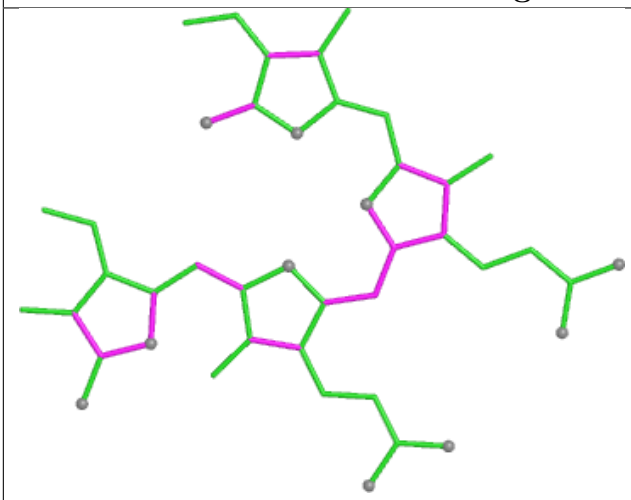


Rings

Ligand PEB PE 201



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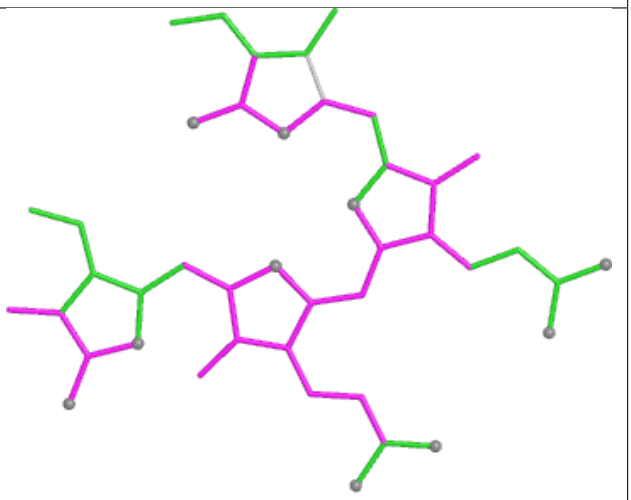

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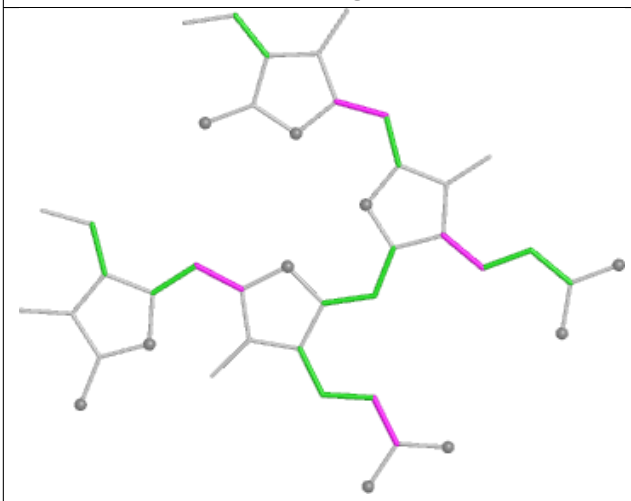

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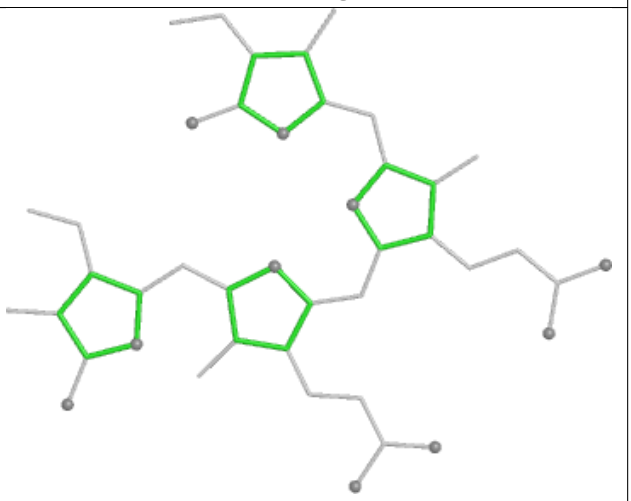
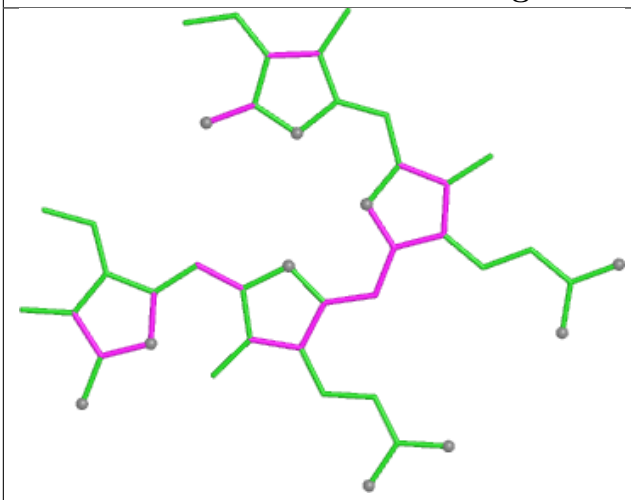


Rings

Ligand PEB RP 201



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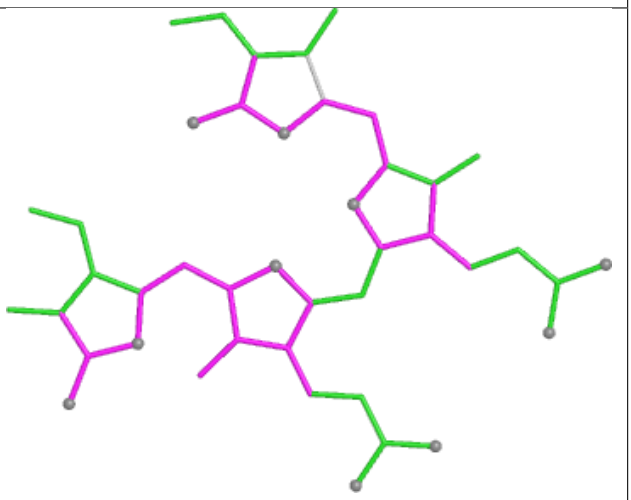

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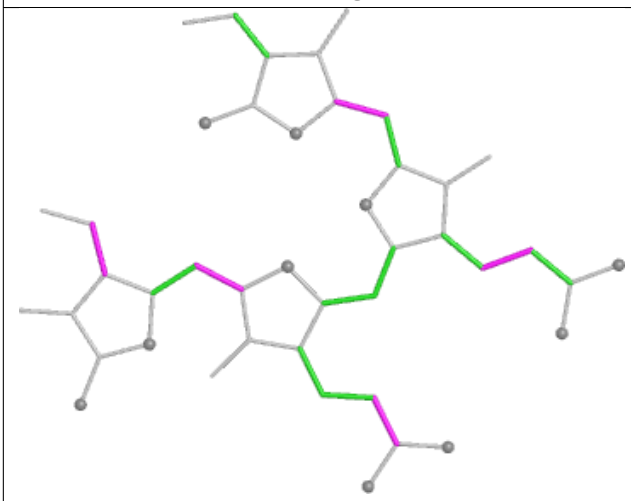

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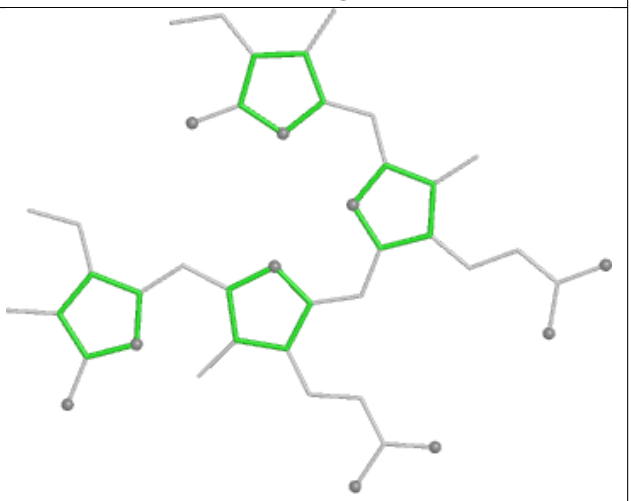
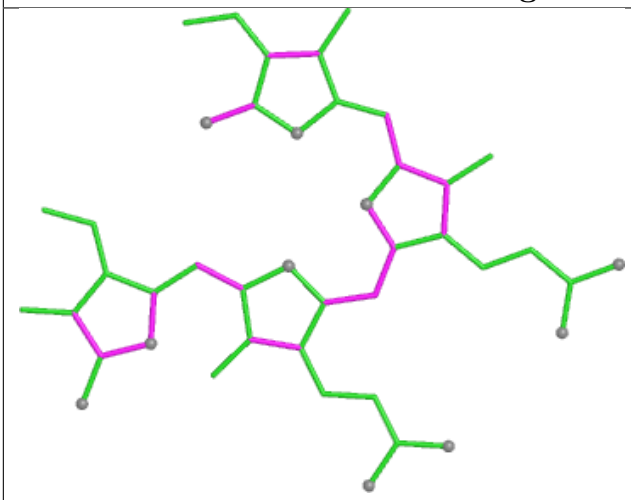


Rings

Ligand PEB JJ 201



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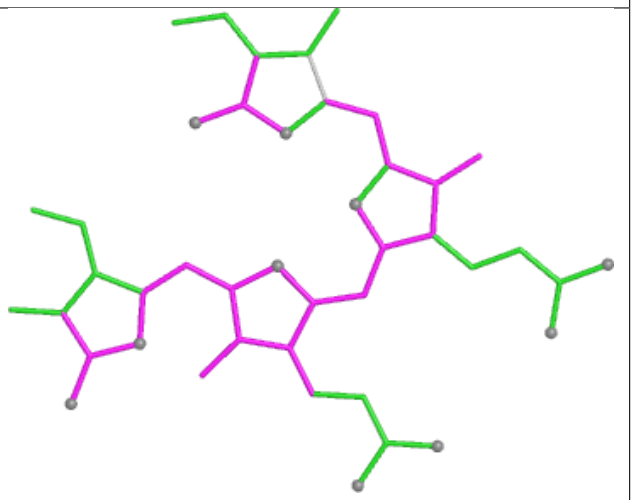

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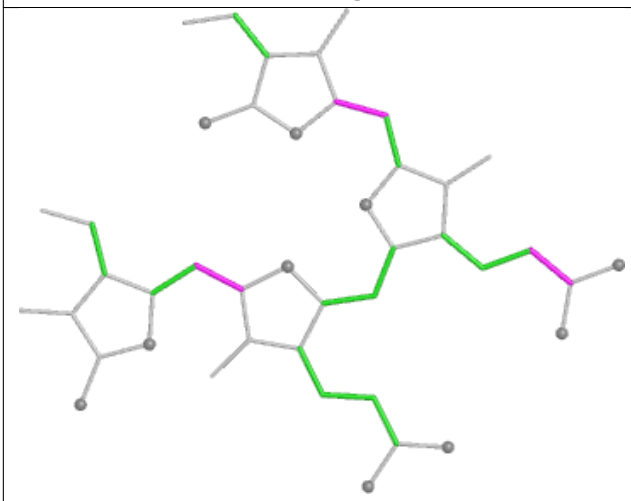

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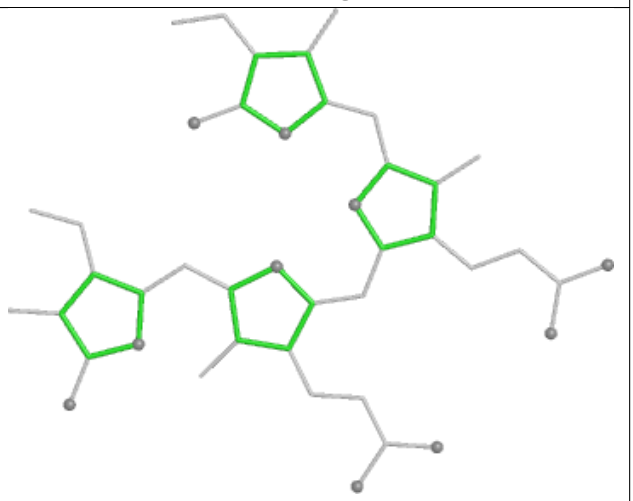
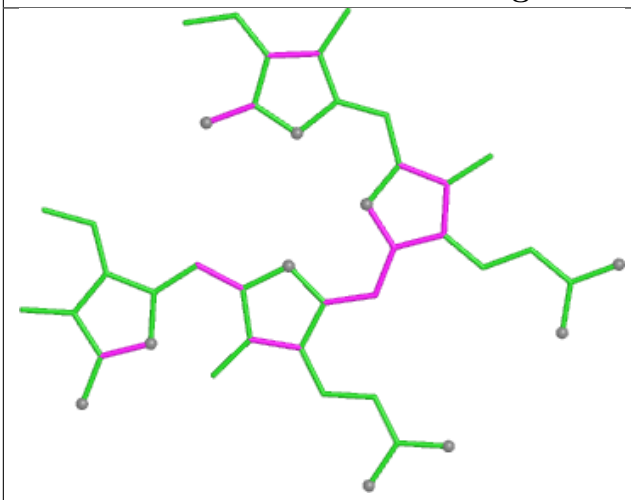


Rings

Ligand PEB PO 203



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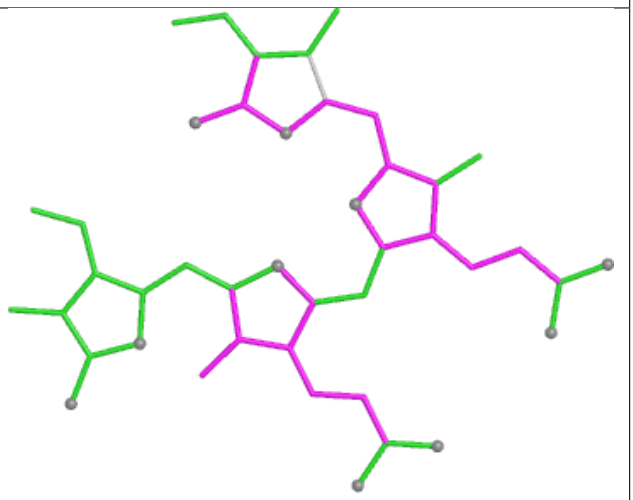

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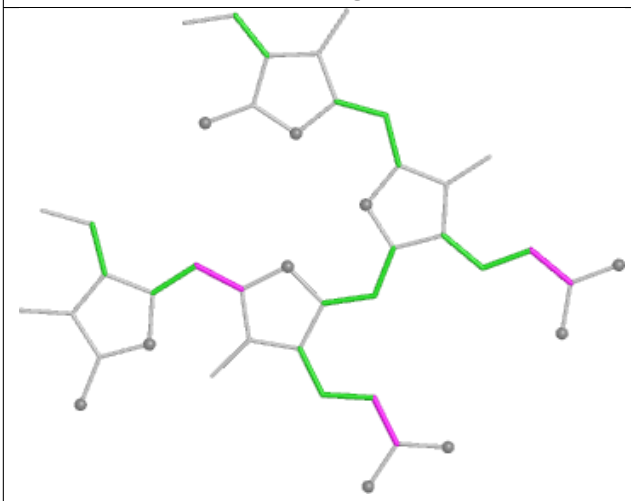

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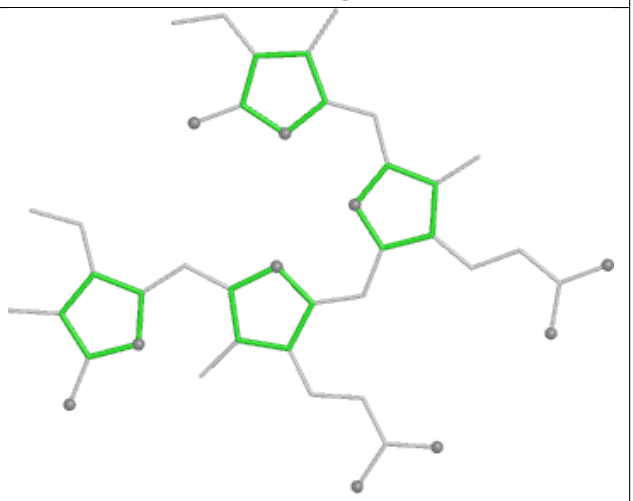
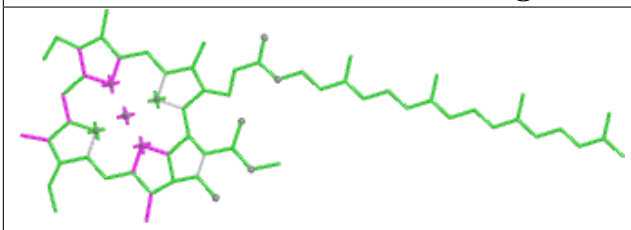


Rings

Ligand CLA A2 849



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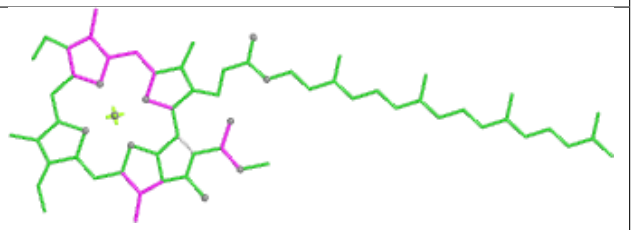
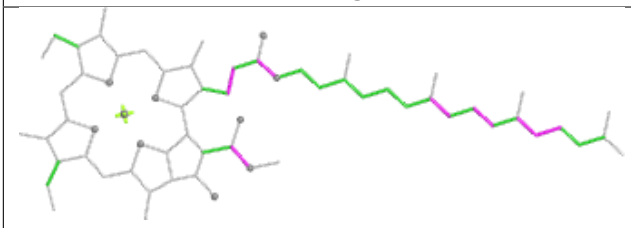


Bond angles



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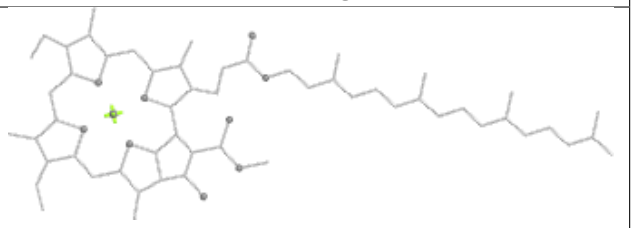
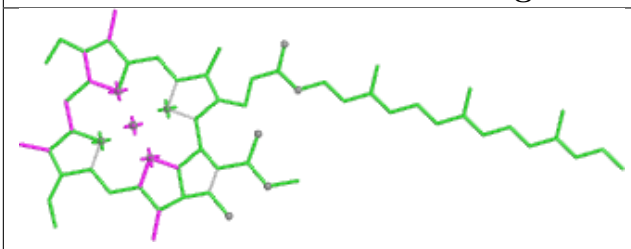
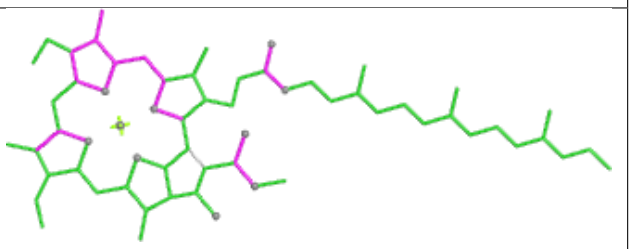
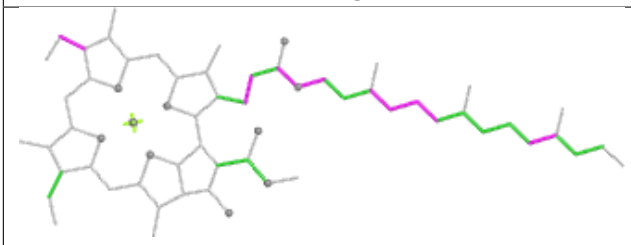
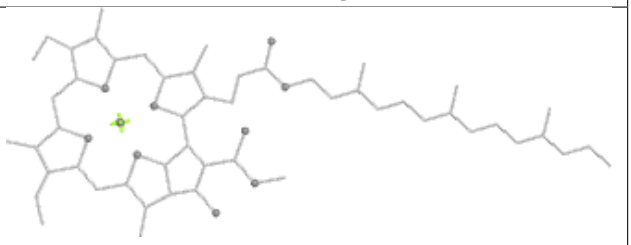
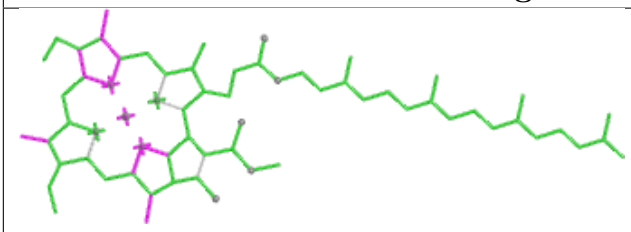
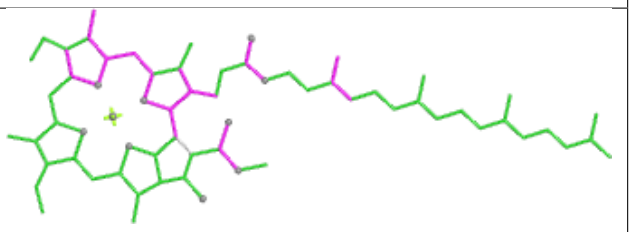
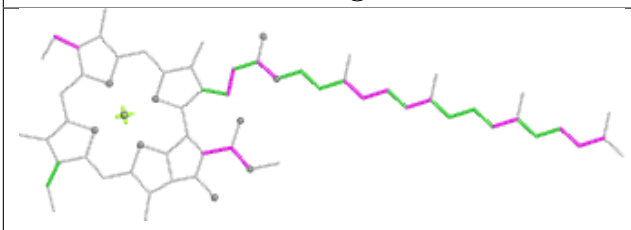
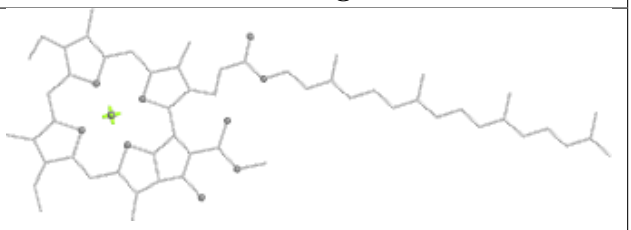
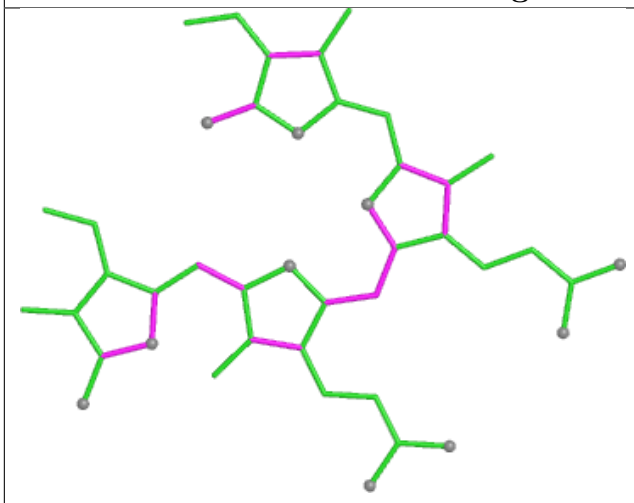


Rings

Ligand CLA A2 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEB QK 201



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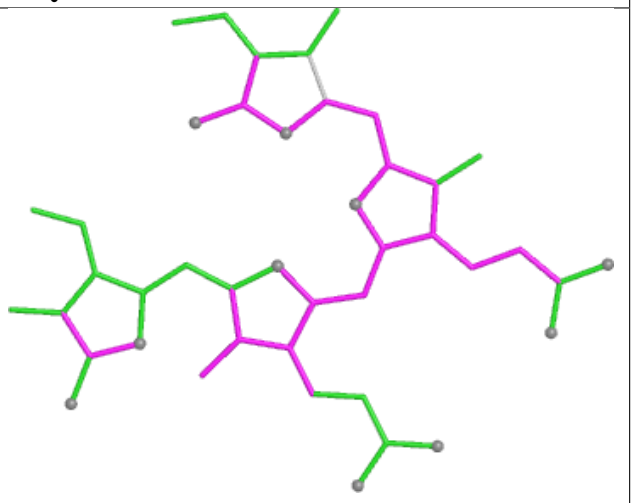

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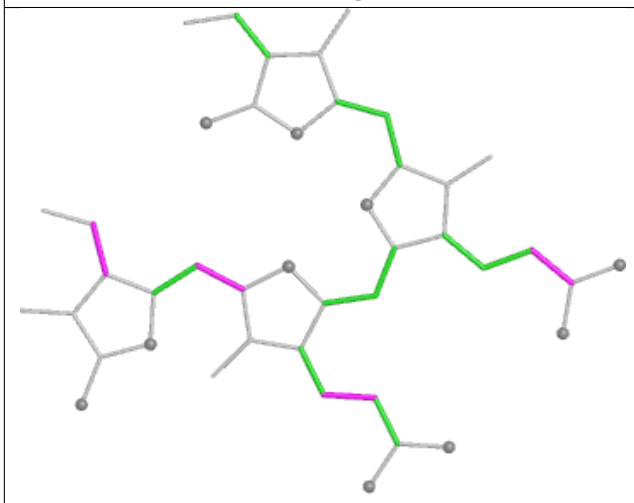

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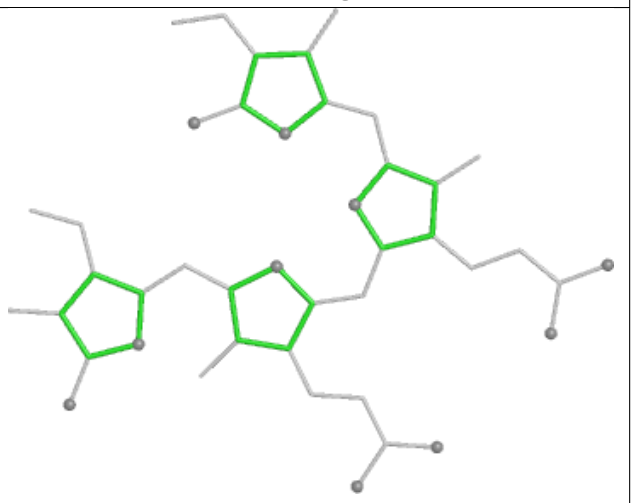
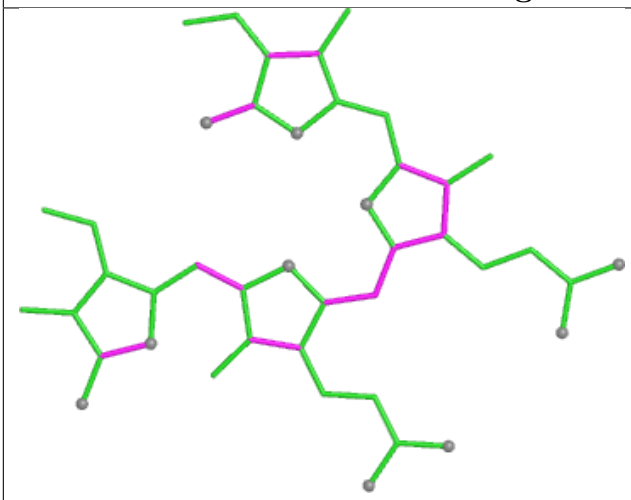


Rings

Ligand PEB aH 201



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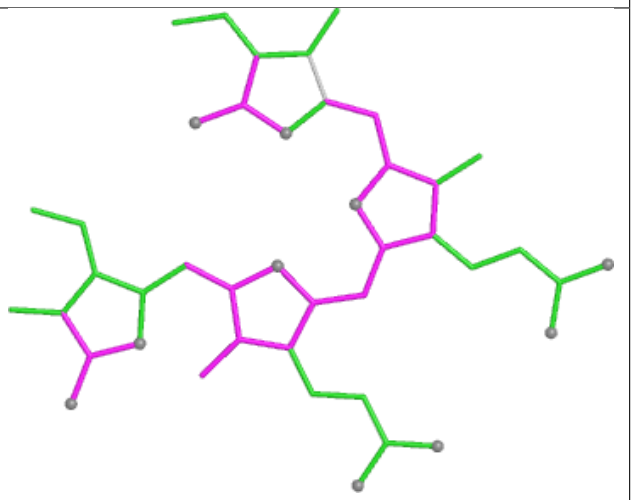
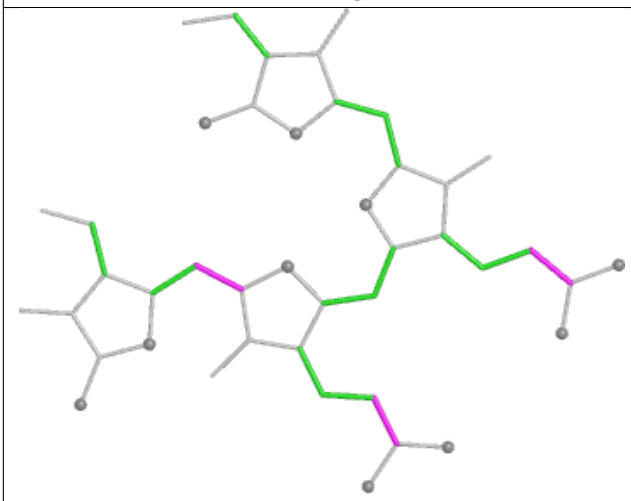


Bond angles



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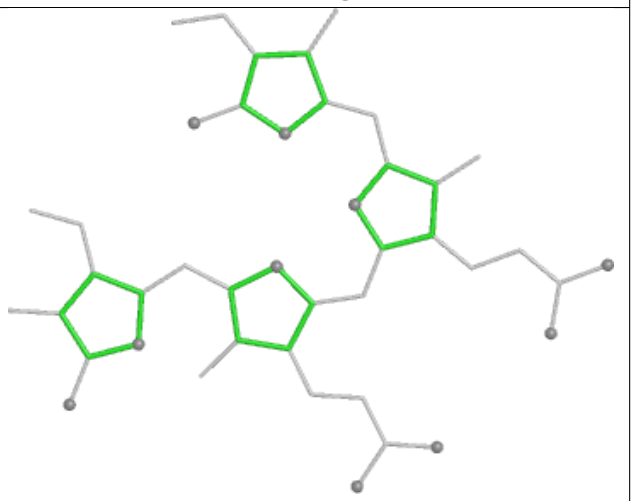
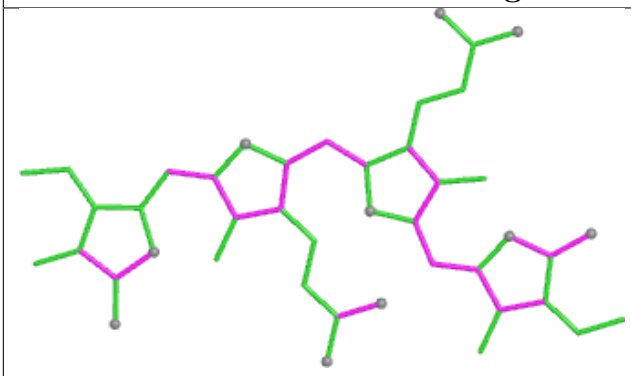


Rings

Ligand CYC w3 1001



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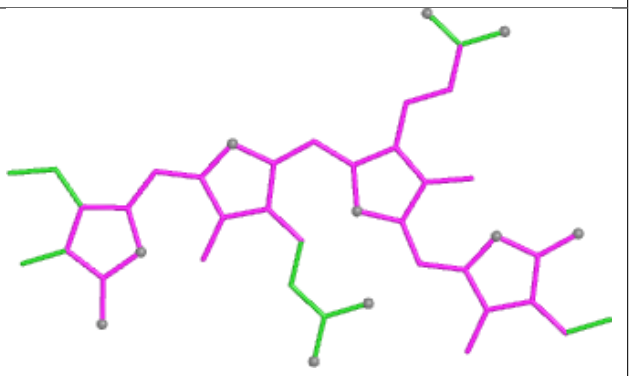
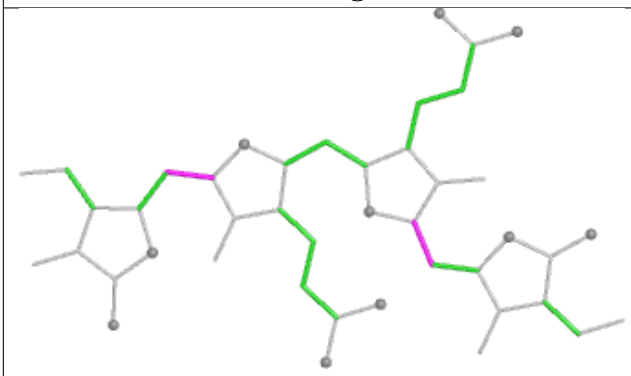


Bond angles



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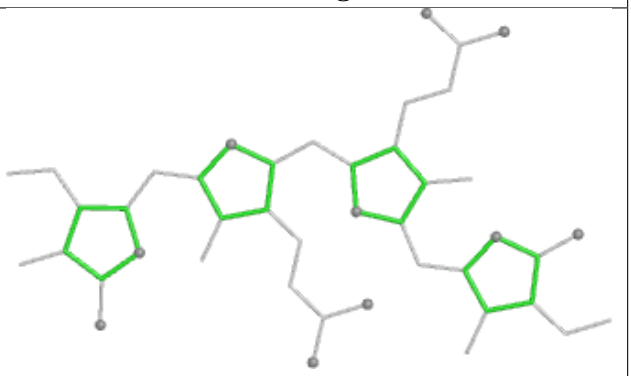
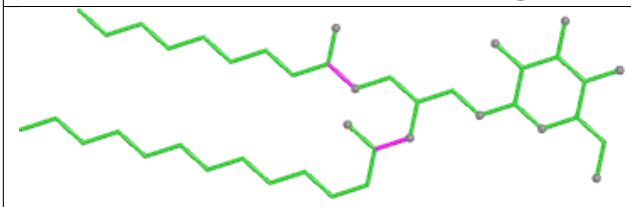


Rings

Ligand LMG bL 623



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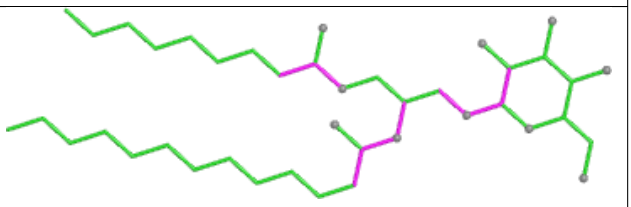
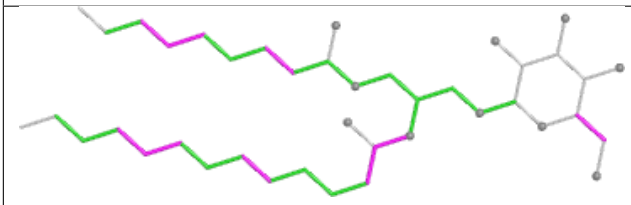


Bond angles



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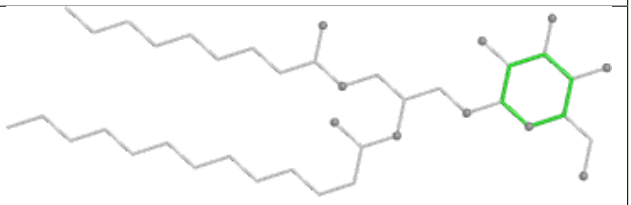
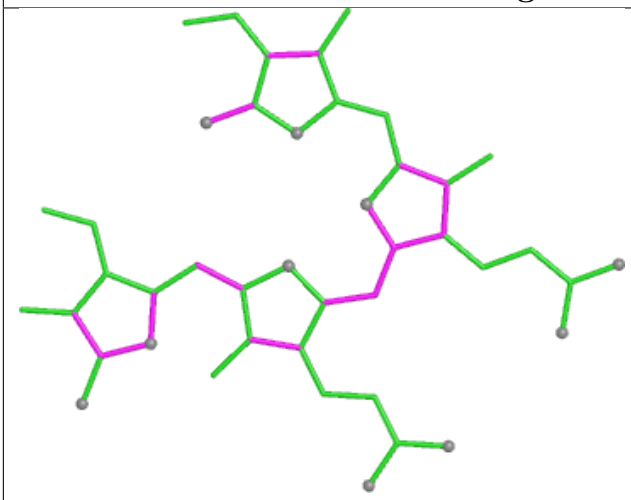


Rings

Ligand PEB gF 202



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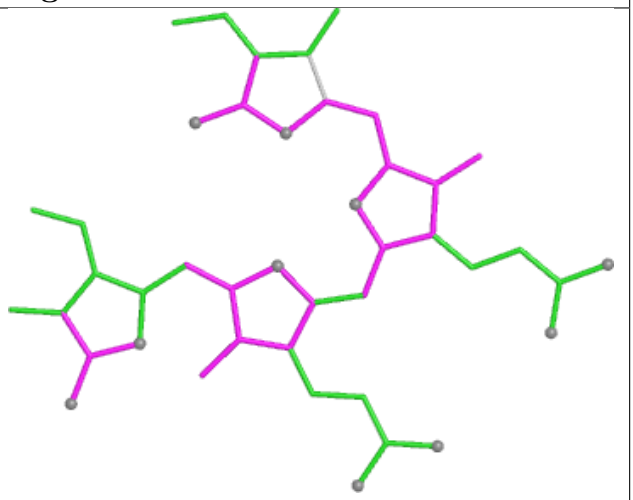
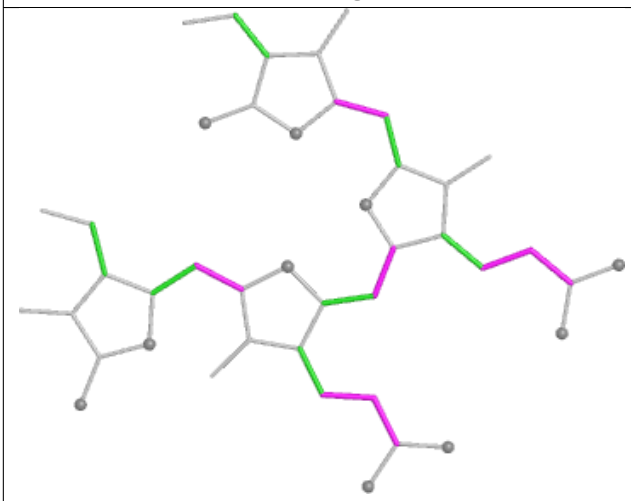


Bond angles



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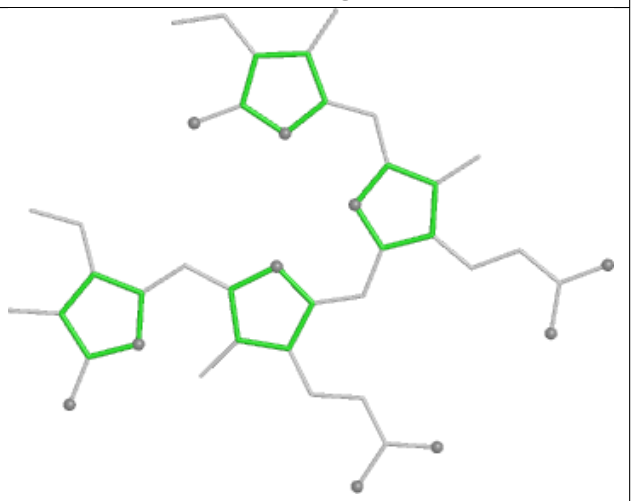
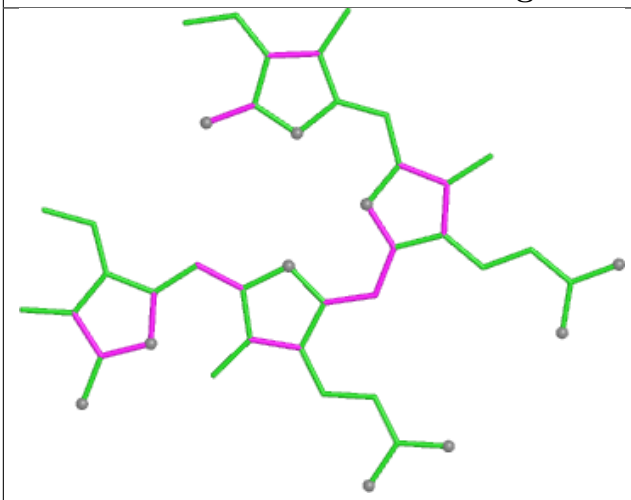


Rings

Ligand PEB P4 201



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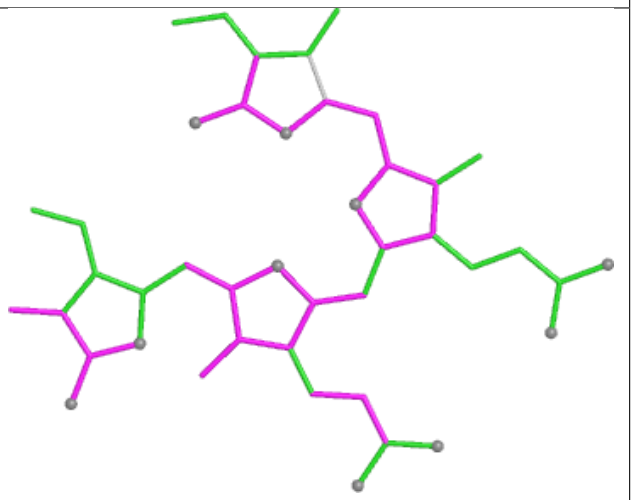

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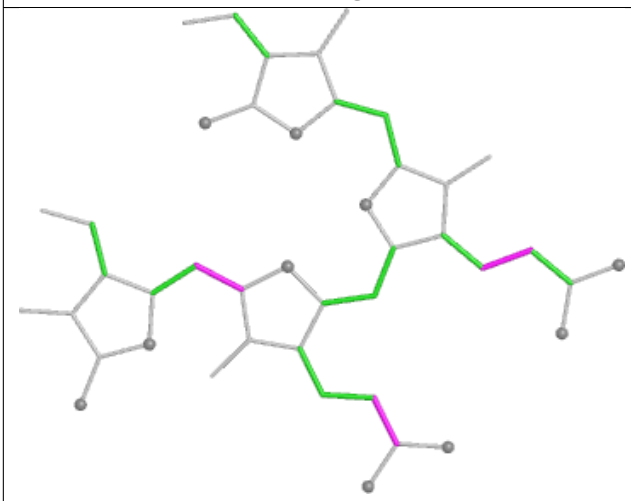

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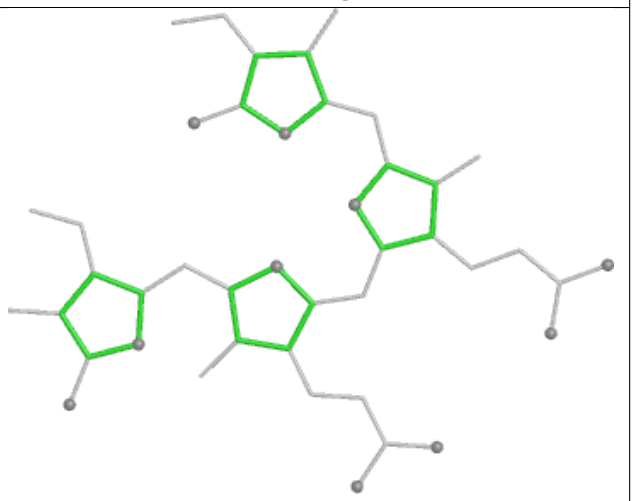
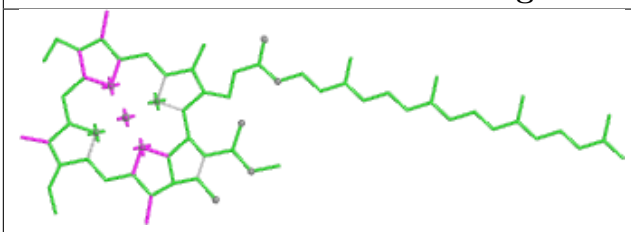


Rings

Ligand CLA bL 617



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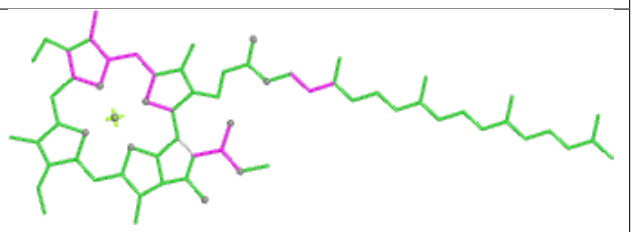
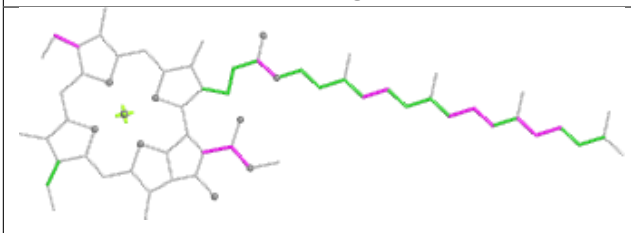


Bond angles



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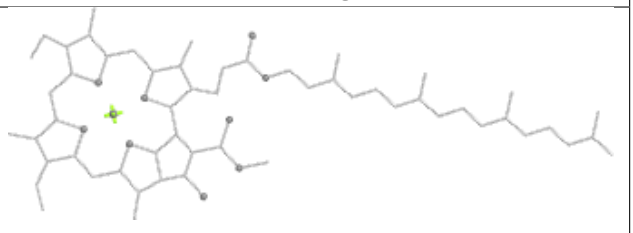
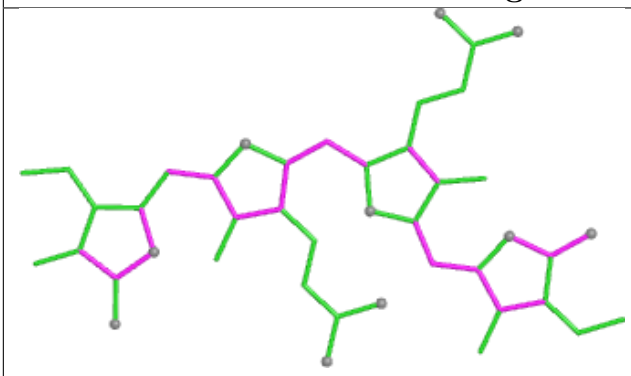


Rings

Ligand CYC F1 1001



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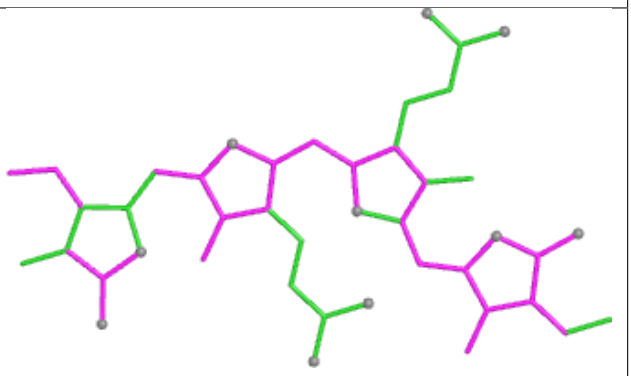

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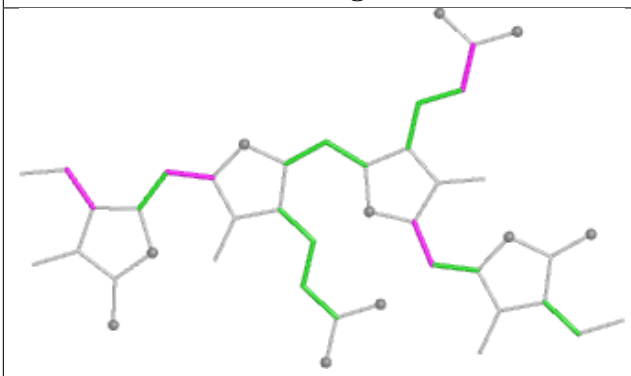

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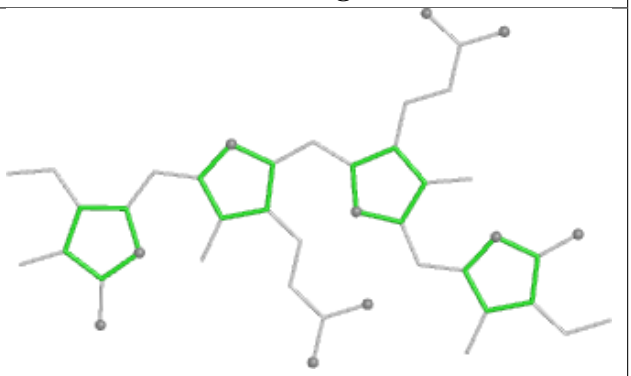
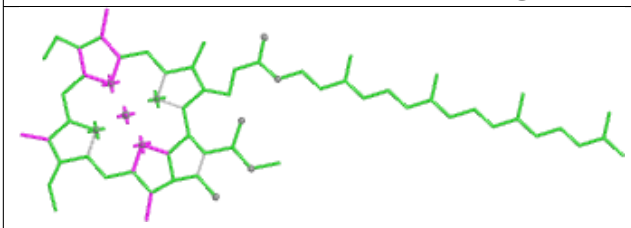


Rings

Ligand CLA CL 503



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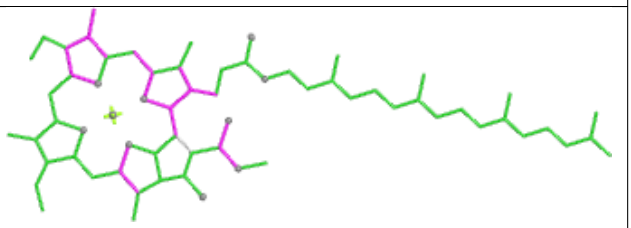
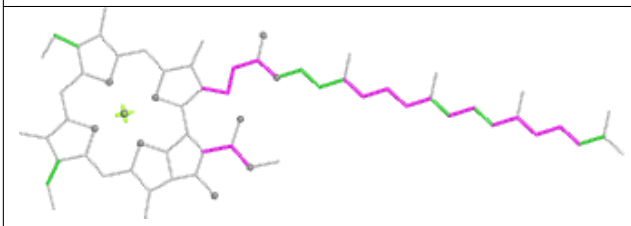


Bond angles



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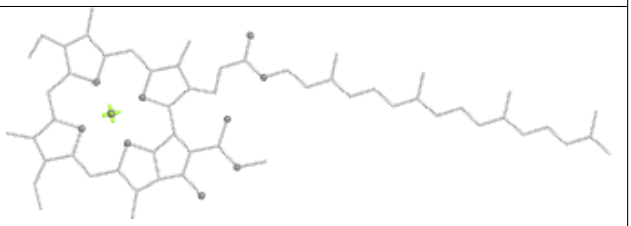
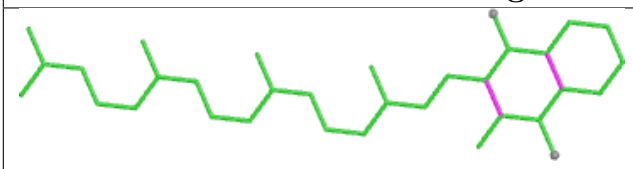


Rings

Ligand PQN AN 842



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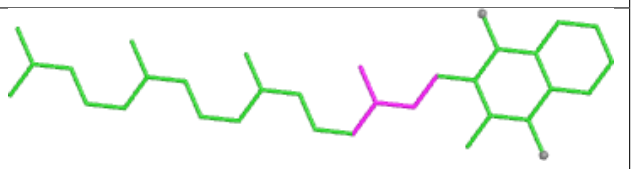
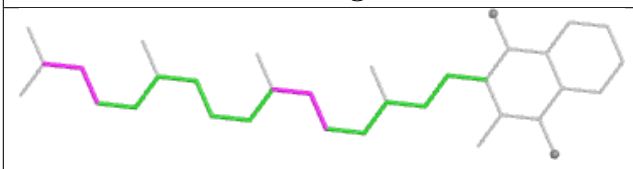


Bond angles



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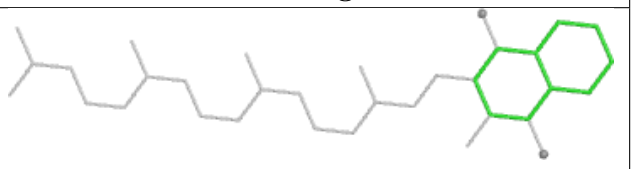
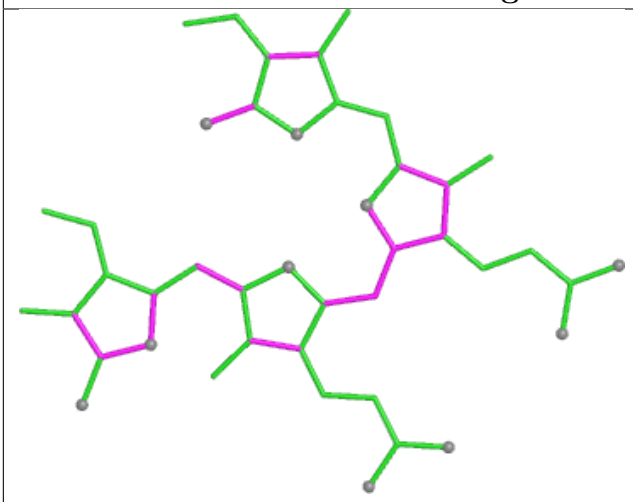


Rings

Ligand PEB HO 1002



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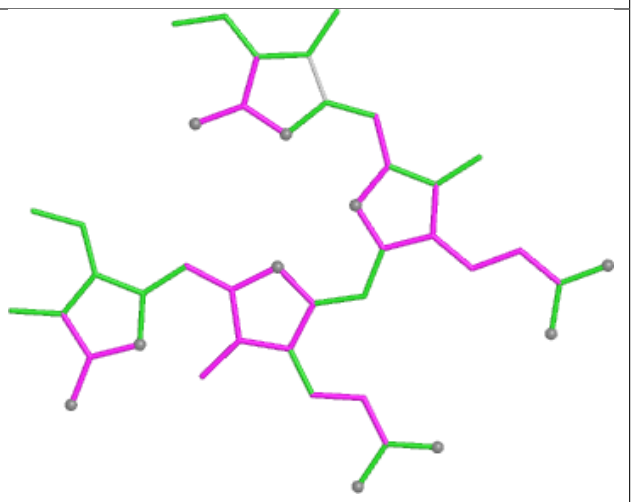
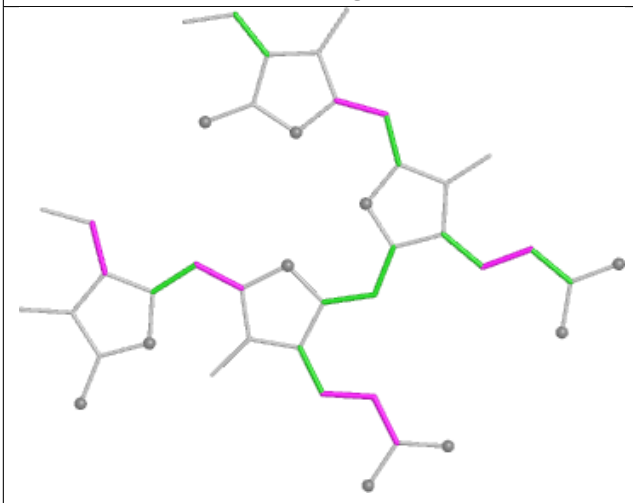


Bond angles



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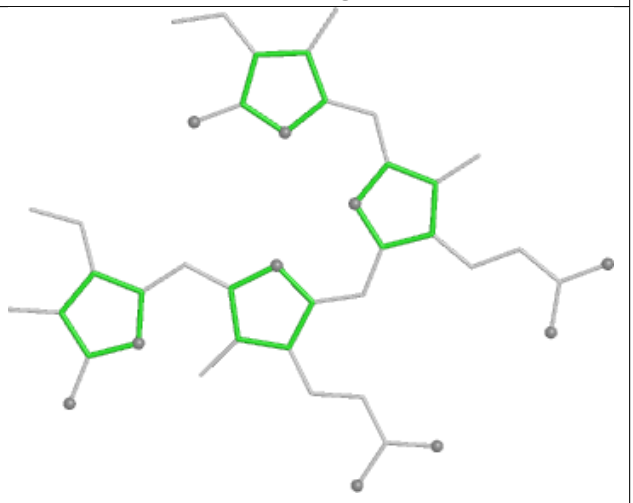
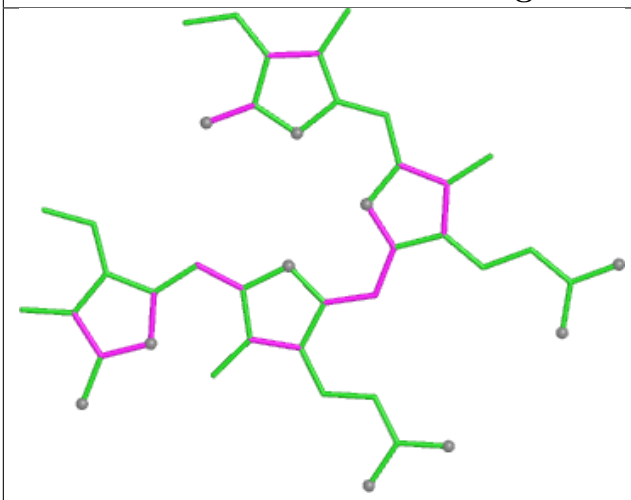
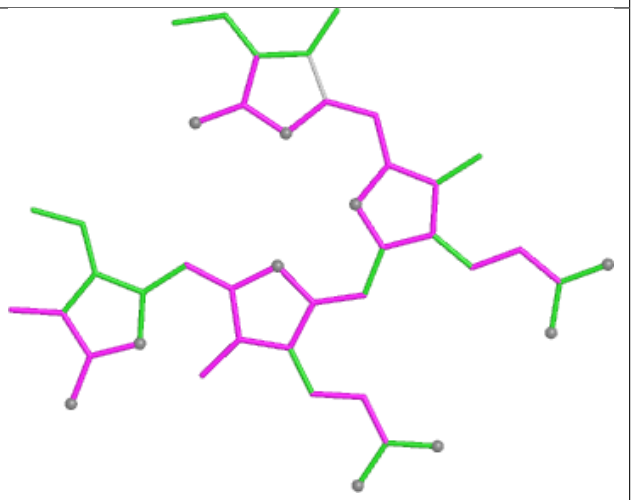


Rings

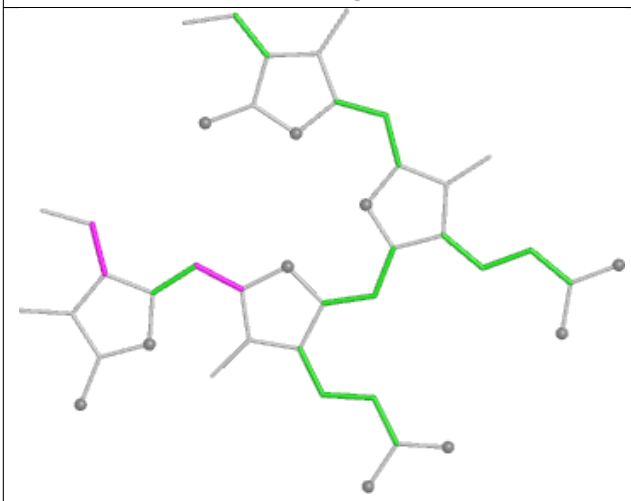
Ligand PEB V4 201



Bond lengths



Bond angles



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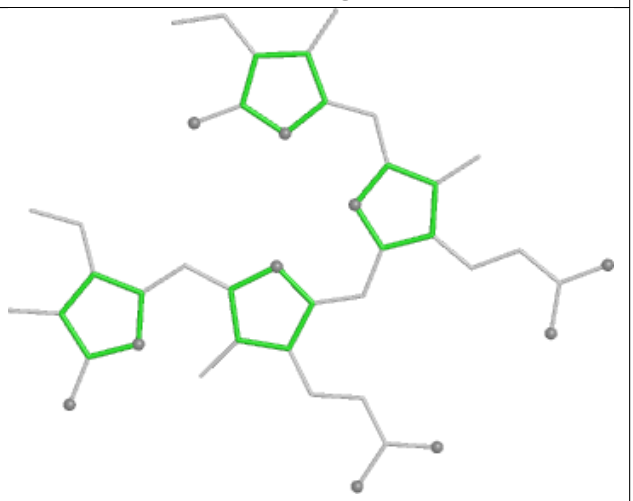
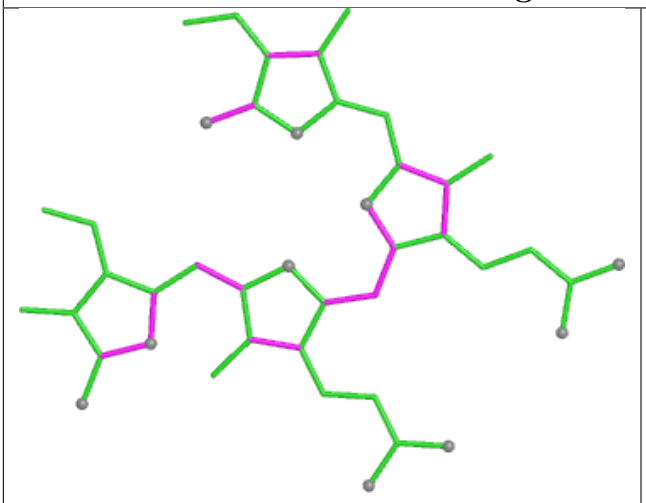
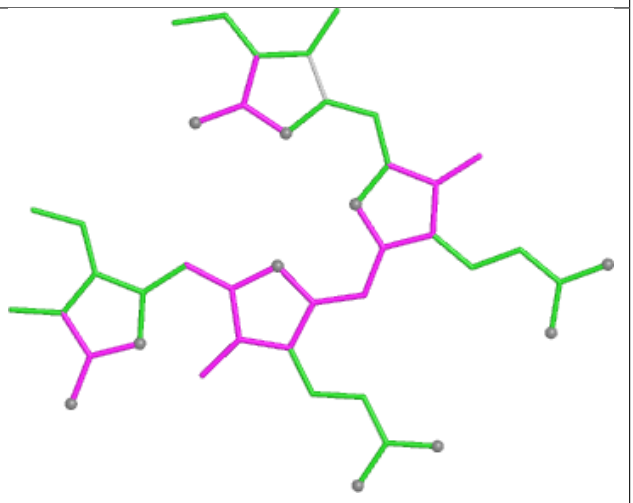


Rings

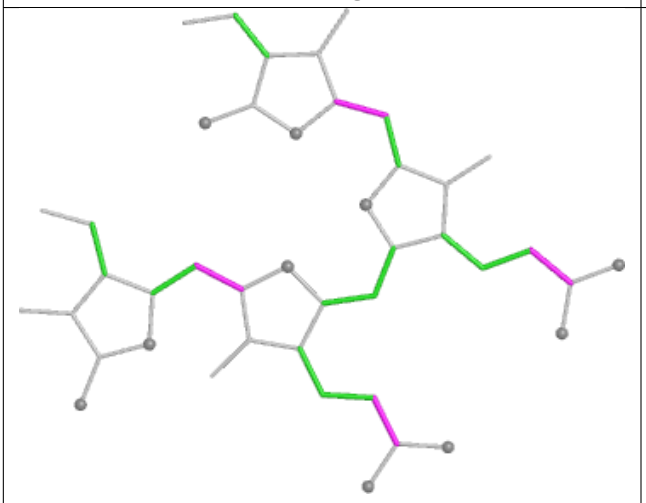
Ligand PEB AJ 302



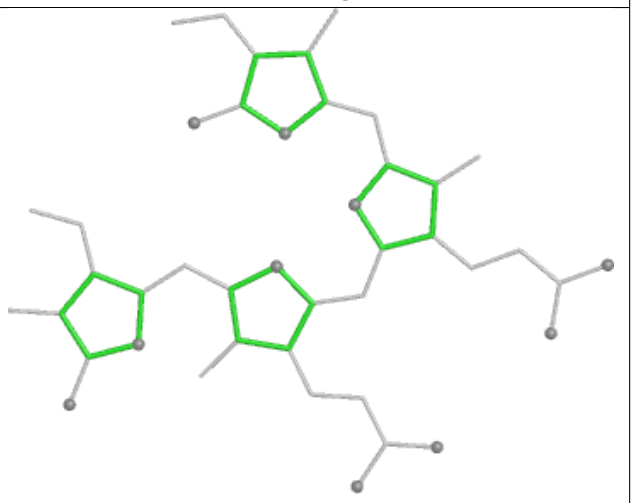
Bond lengths



Bond angles

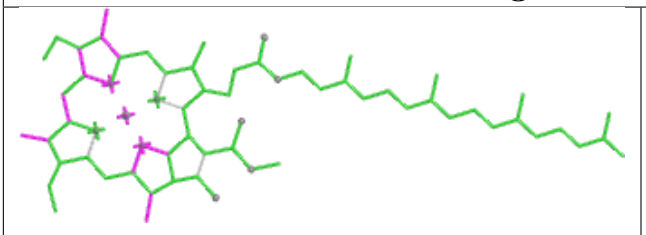


Torsions



Rings

Ligand CLA AN 838



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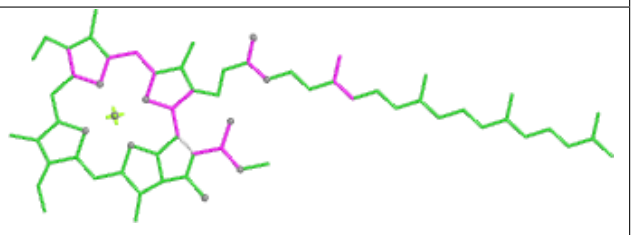

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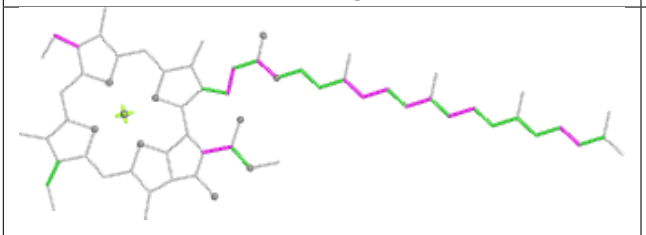

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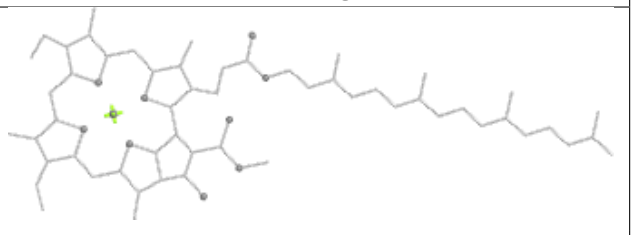
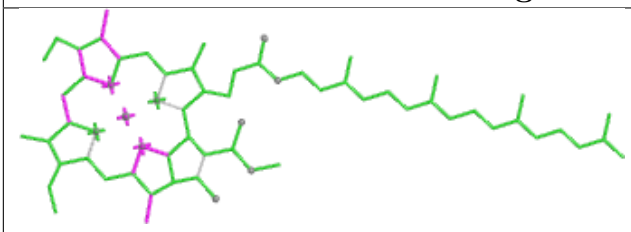


Rings

Ligand CLA B2 818



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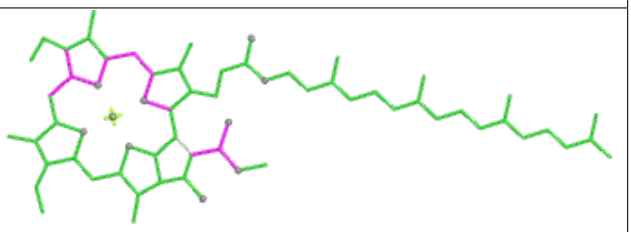

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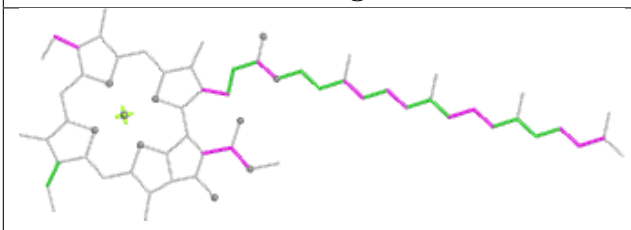

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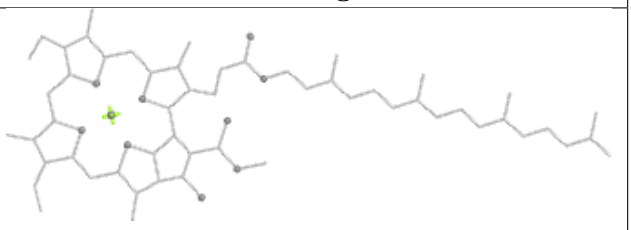
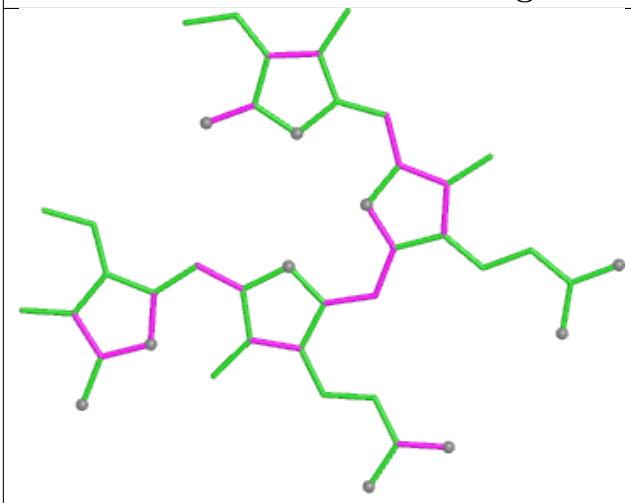


Rings

Ligand PEB gB 203



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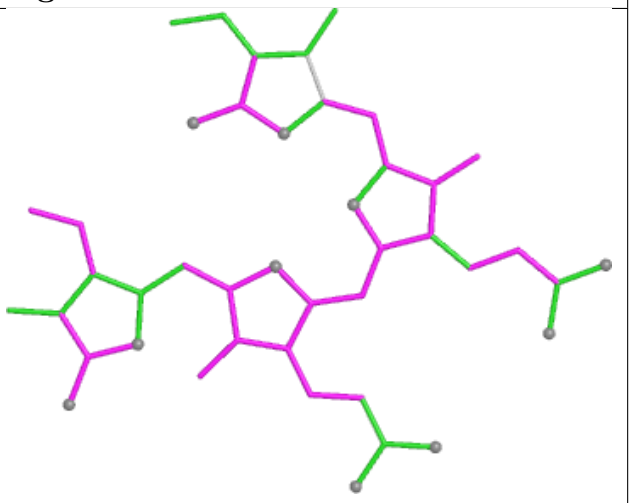

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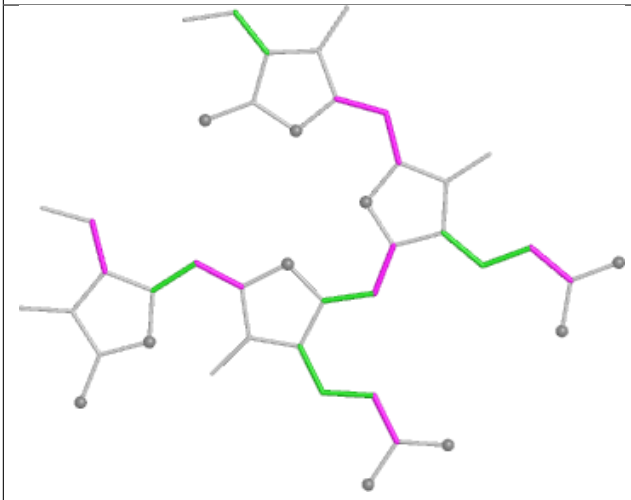

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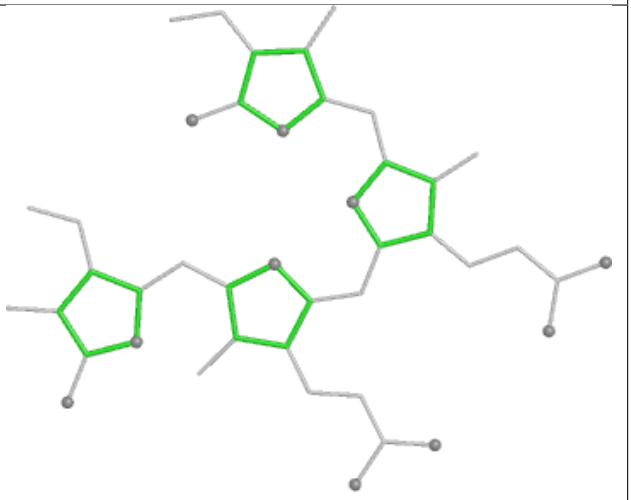
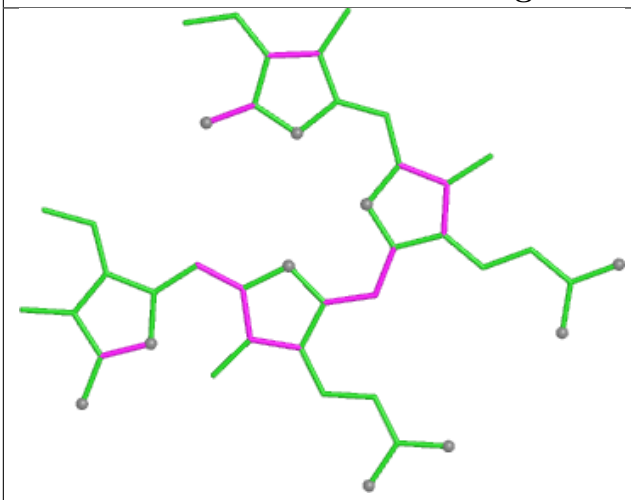


Rings

Ligand PEB aK 203



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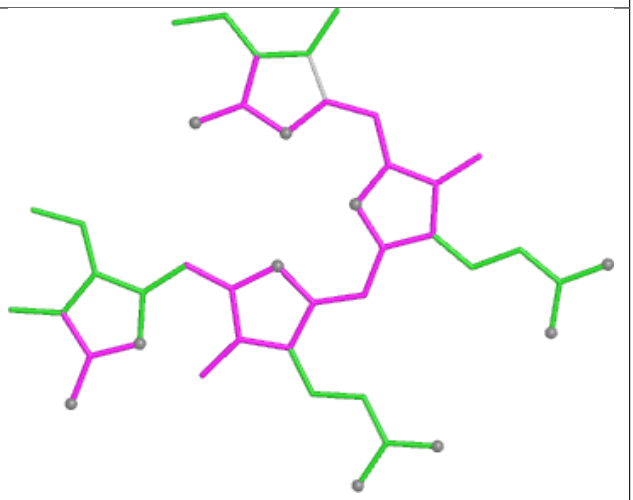

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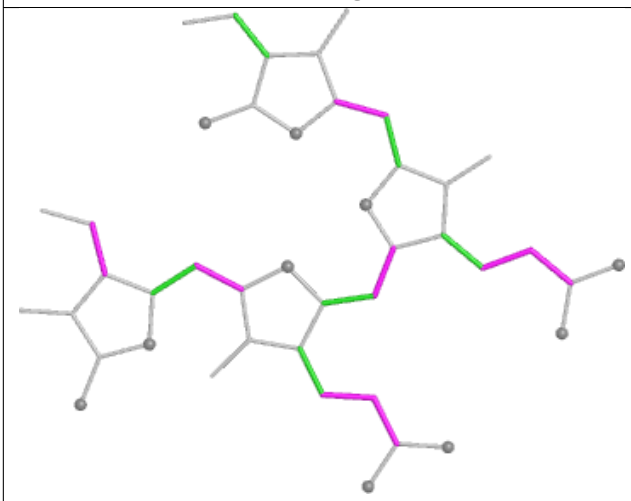

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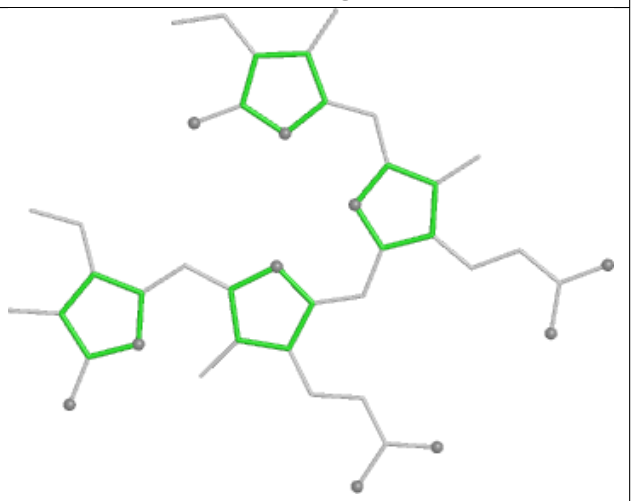
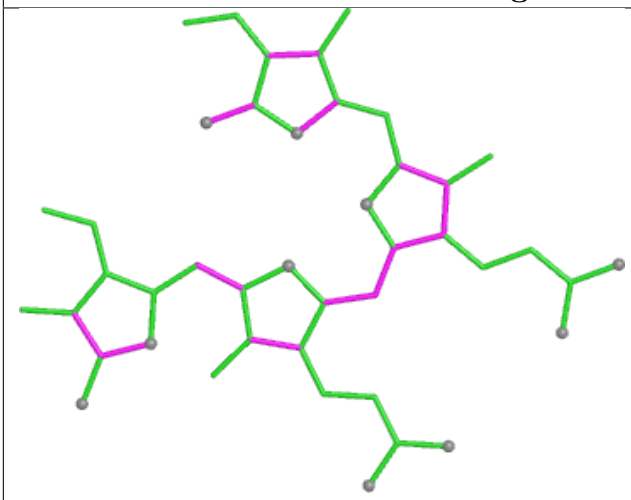


Rings

Ligand PEB QQ 201



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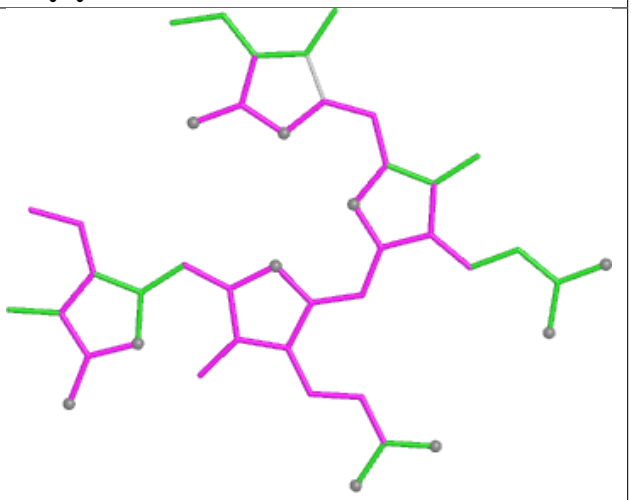

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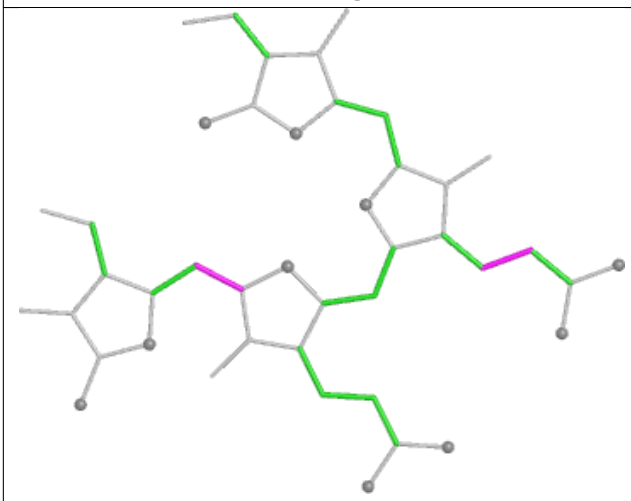

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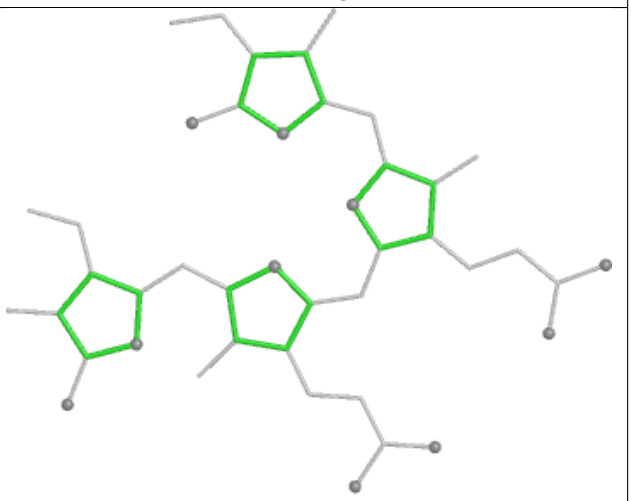

Rings

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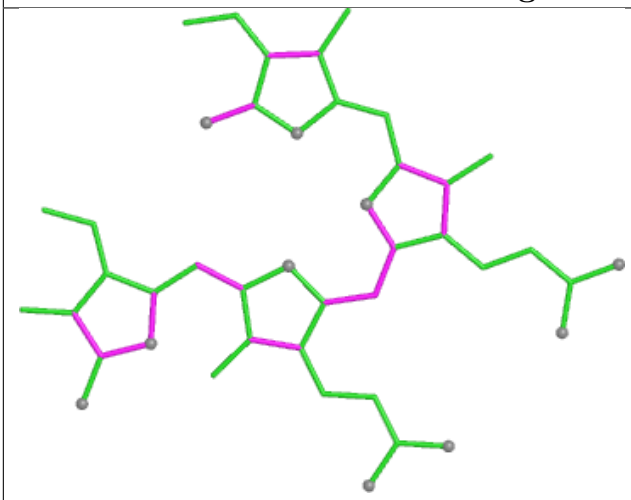

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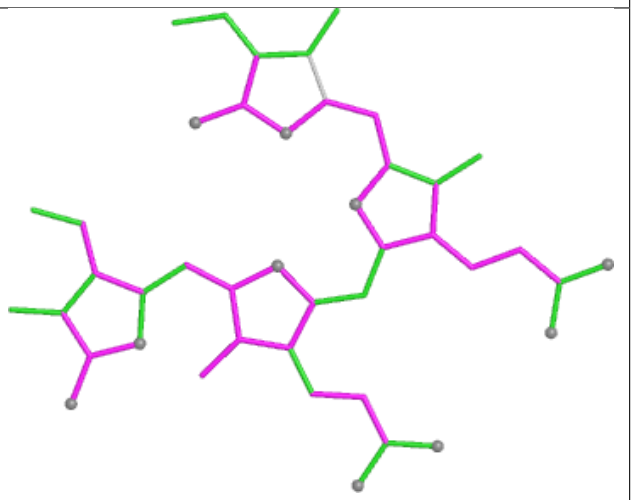

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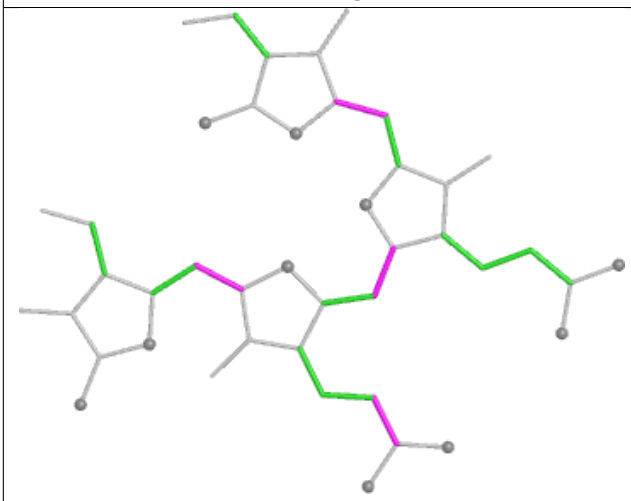

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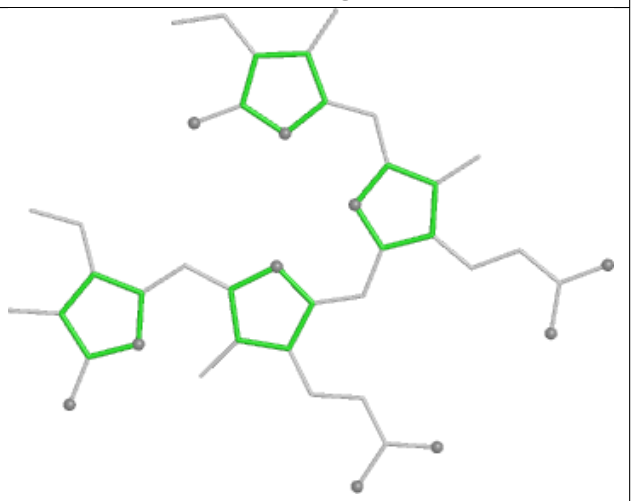
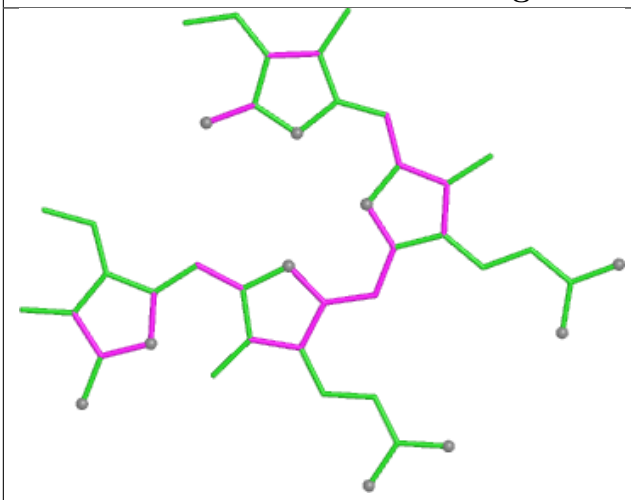


Rings

Ligand PEB FD 203



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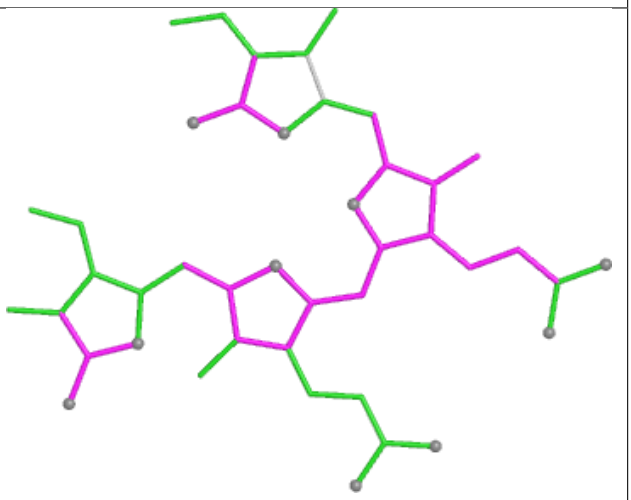

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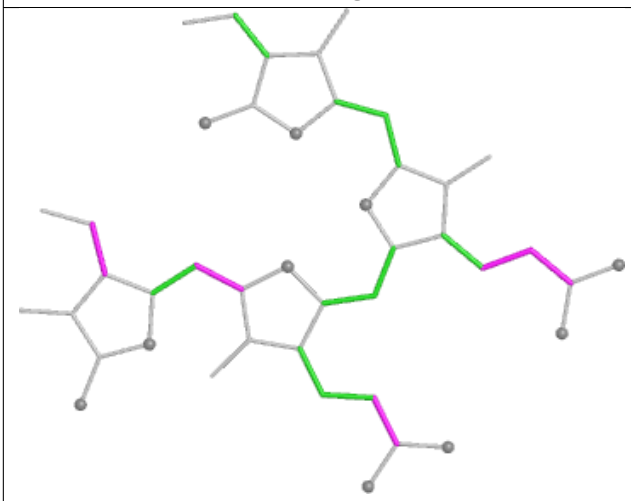

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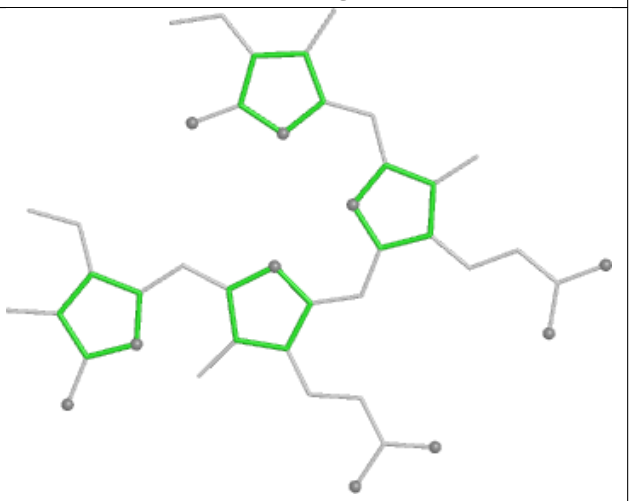
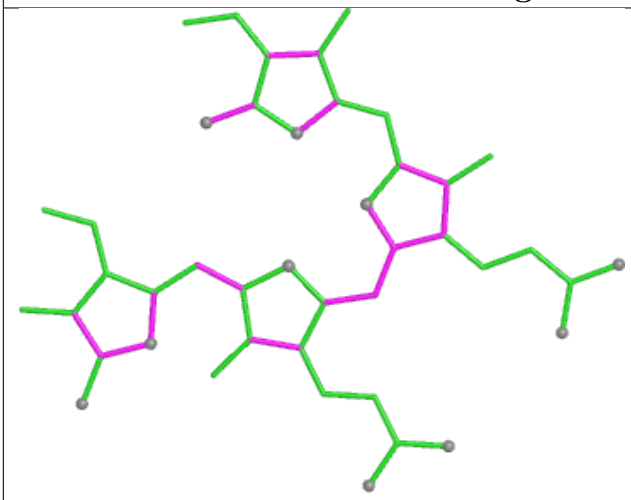


Rings

Ligand PEB N9 201



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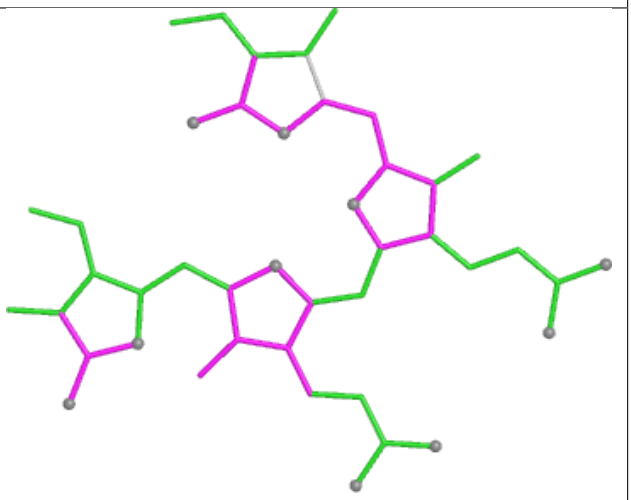

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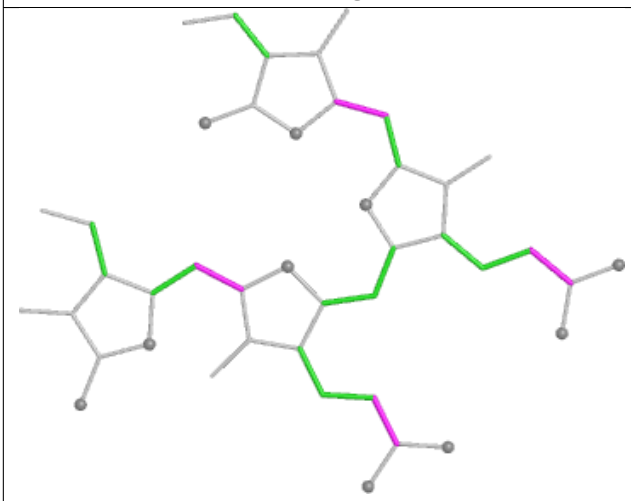

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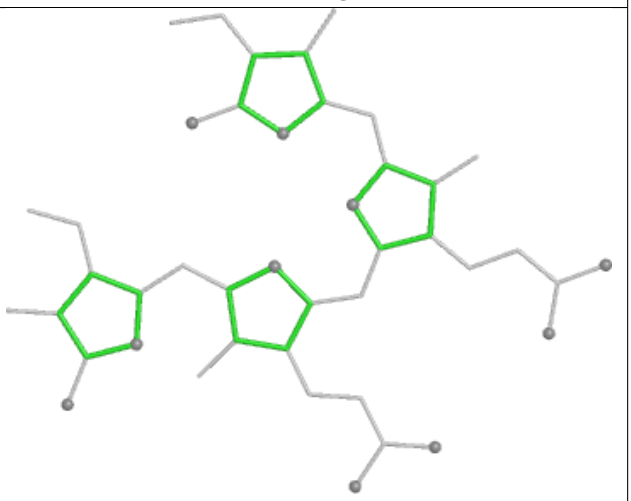
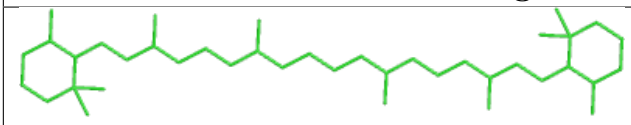


Rings

Ligand BCR B2 843



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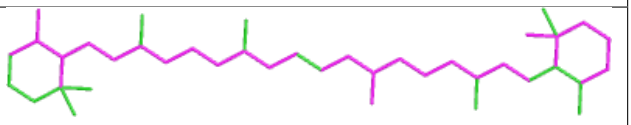

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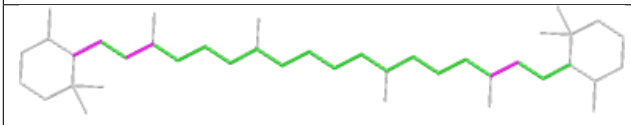

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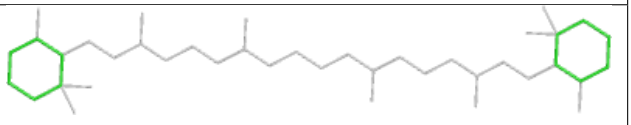
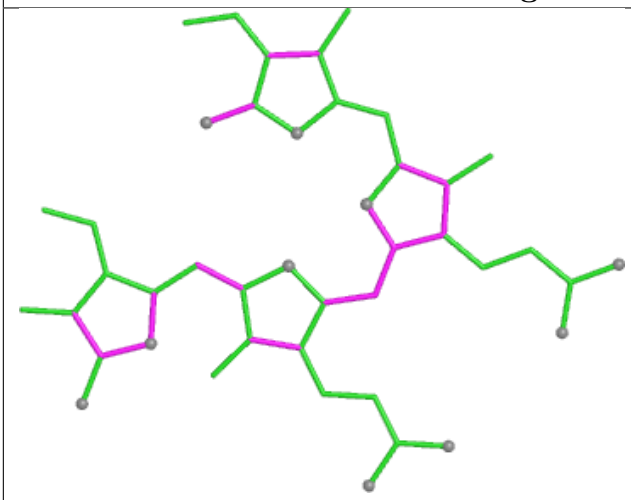


Rings

Ligand PEB LI 201



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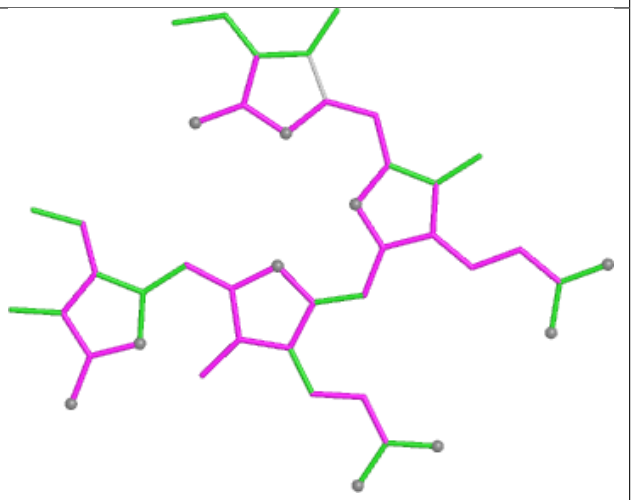

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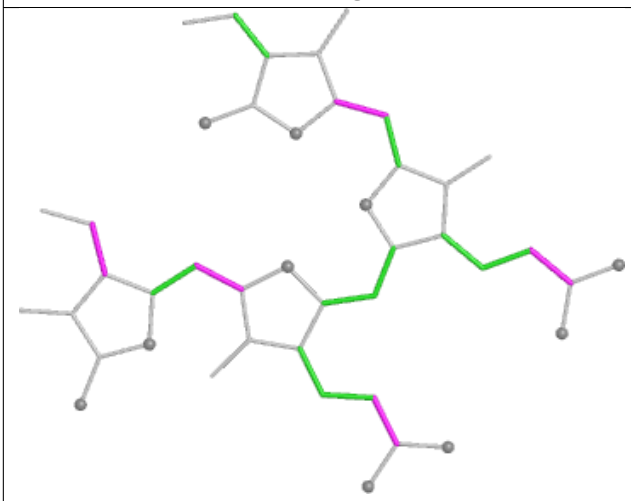

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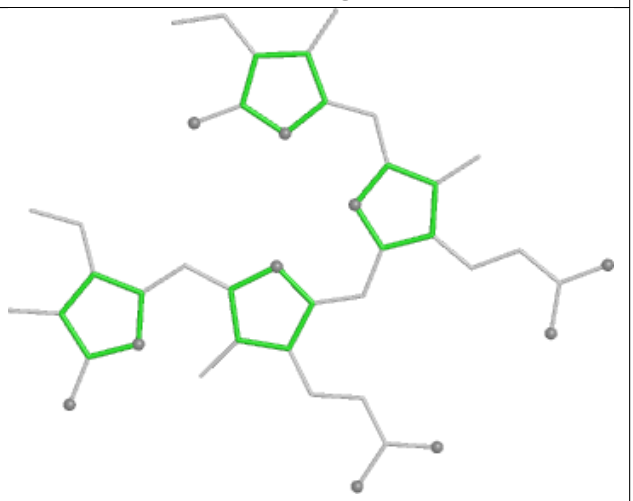
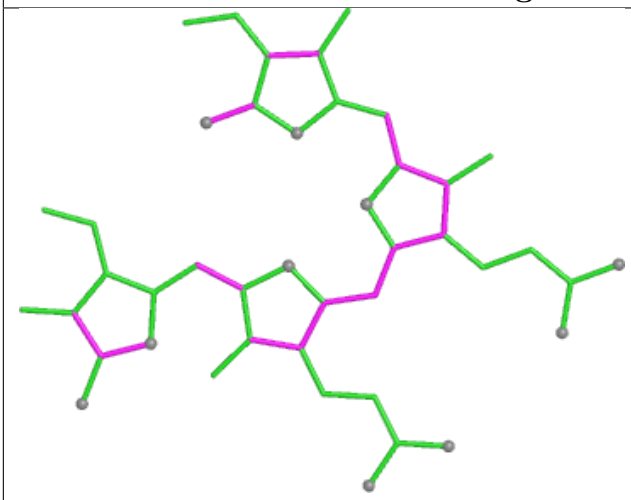


Rings

Ligand PEB R1 202



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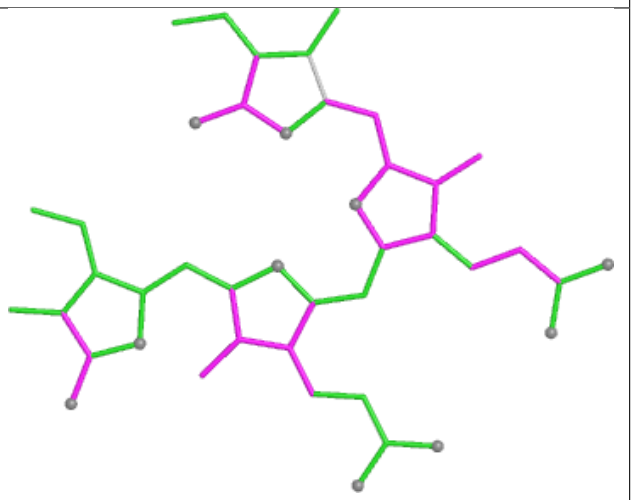

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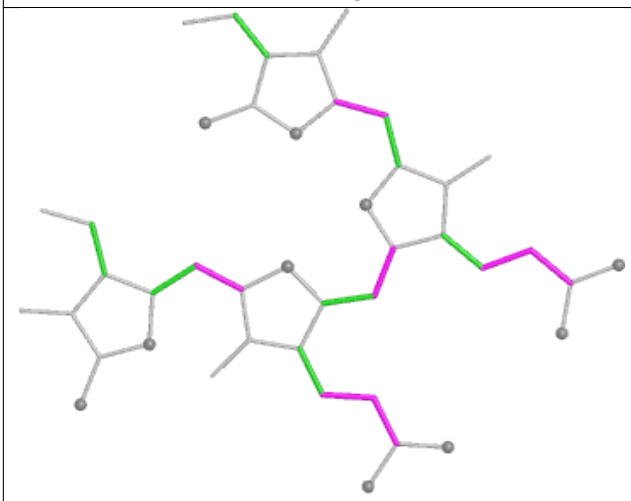

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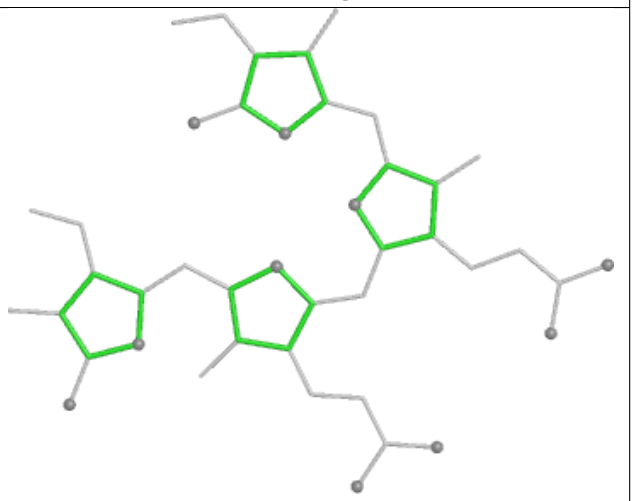
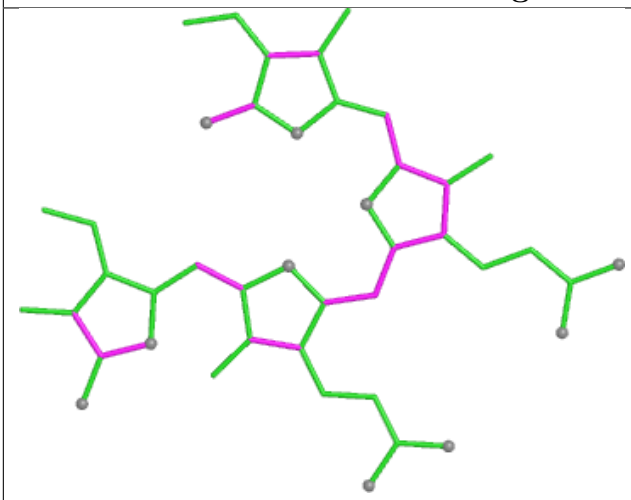


Rings

Ligand PEB TQ 202



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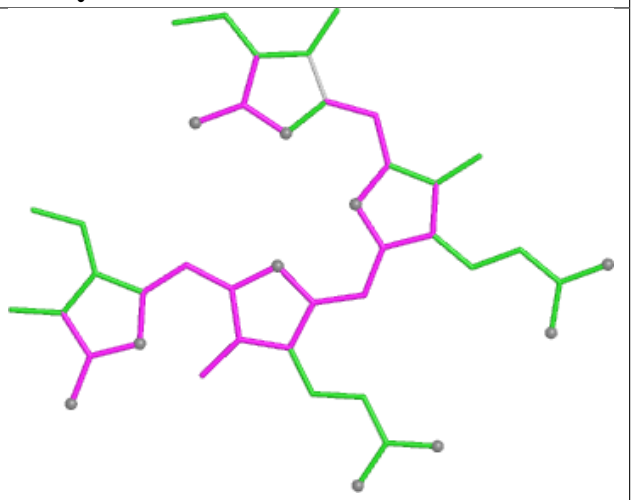

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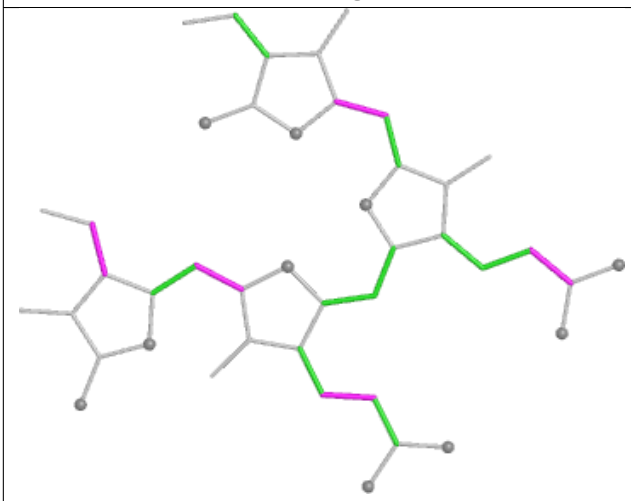

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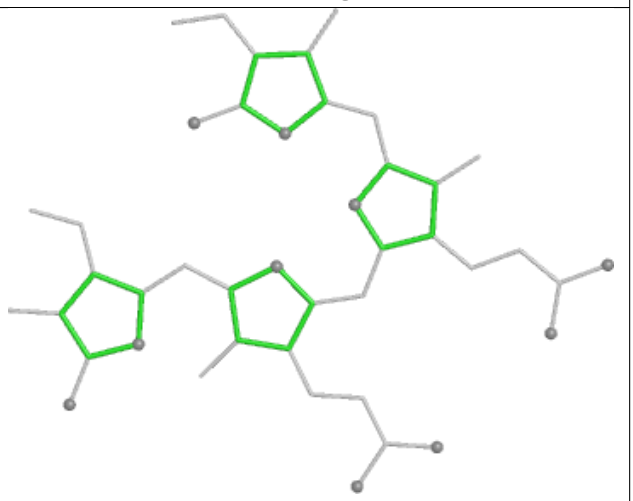
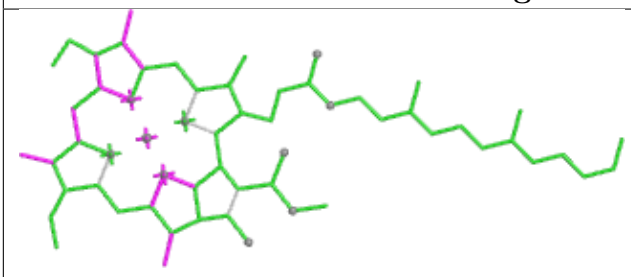


Rings

Ligand CLA BL 604



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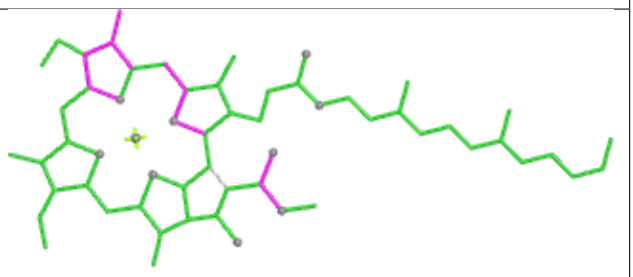
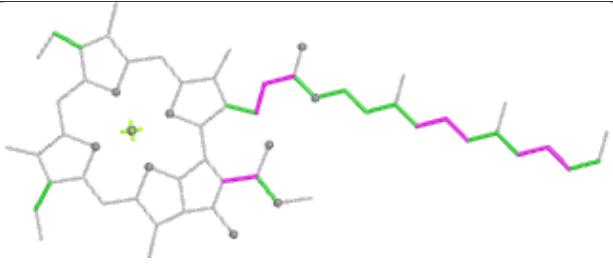


Bond angles



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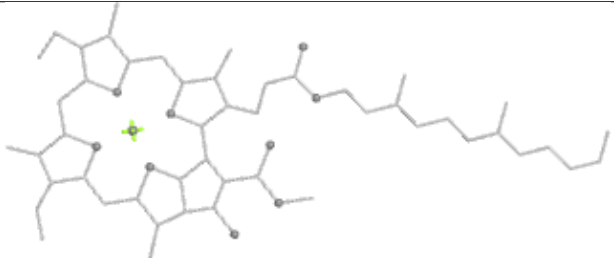
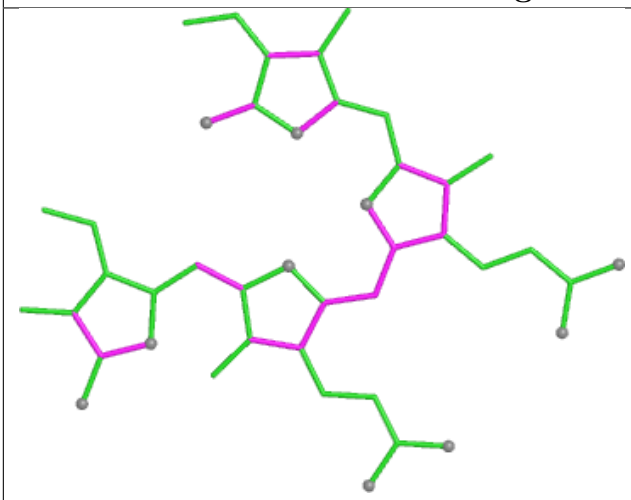


Rings

Ligand PEB G9 202



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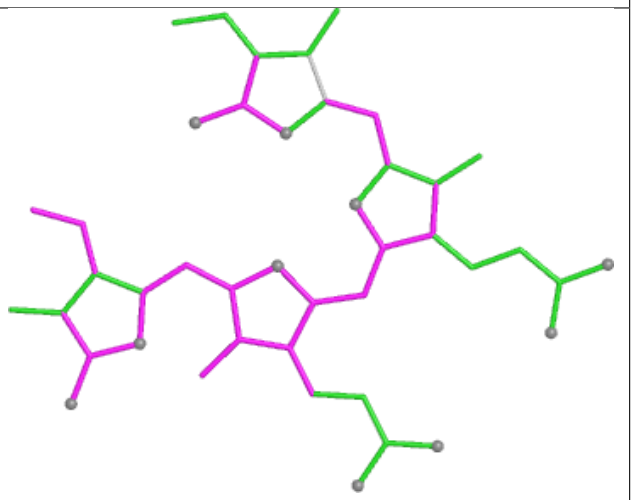
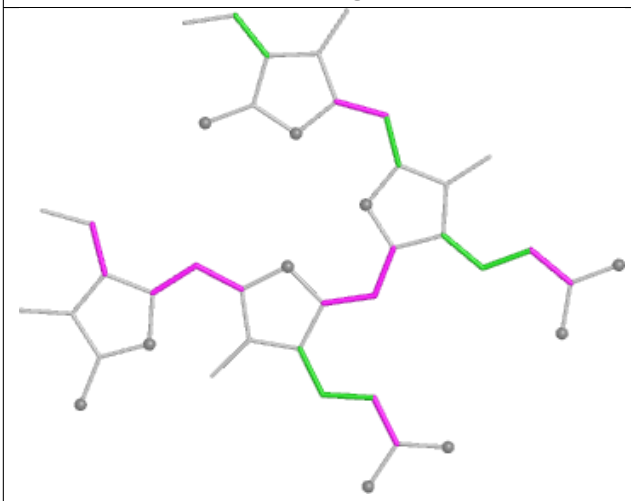


Bond angles



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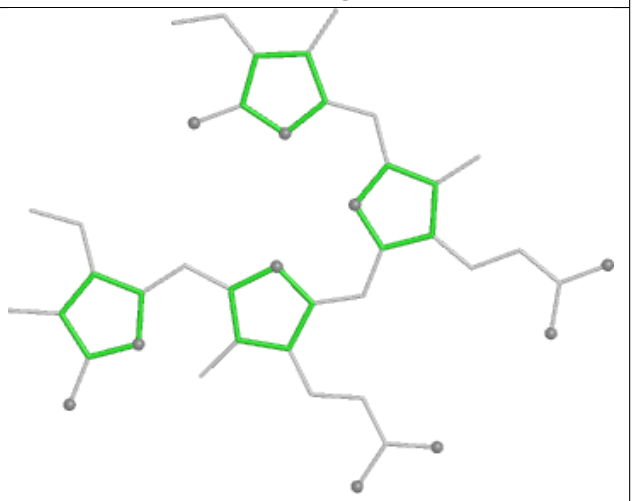
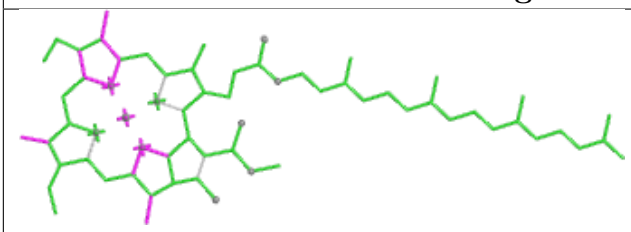
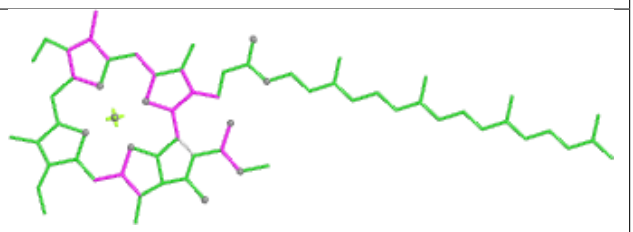


Rings

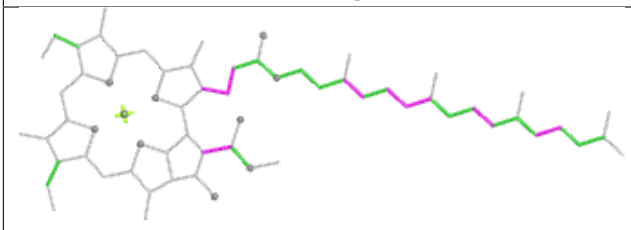
Ligand CLA A2 826



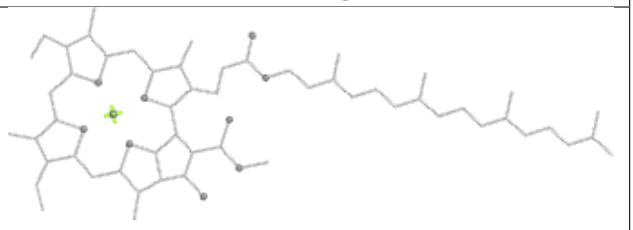
Bond lengths



Bond angles

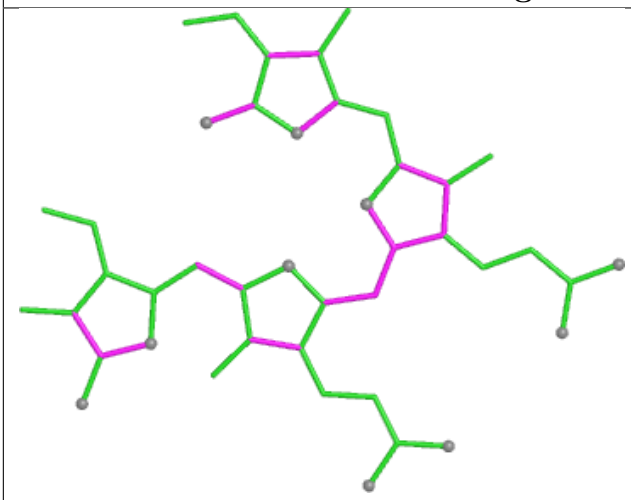


Torsions



Rings

Ligand PEB K7 202



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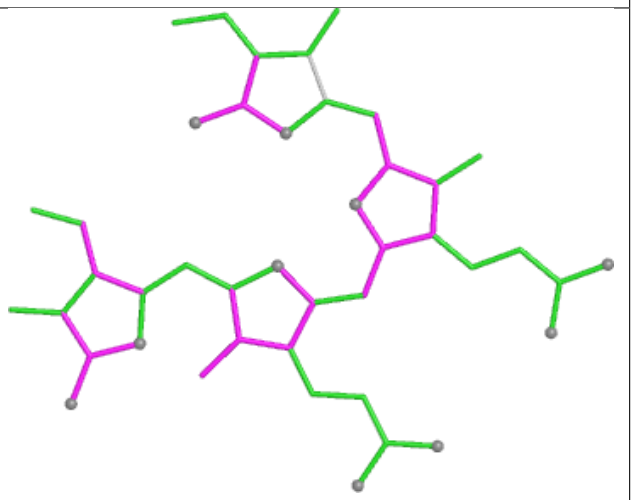

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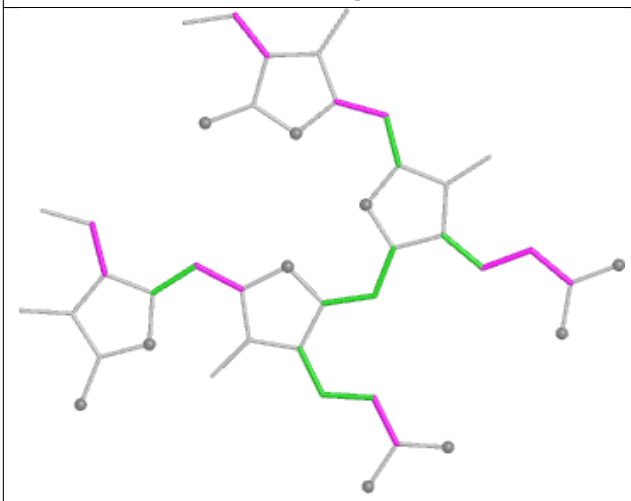

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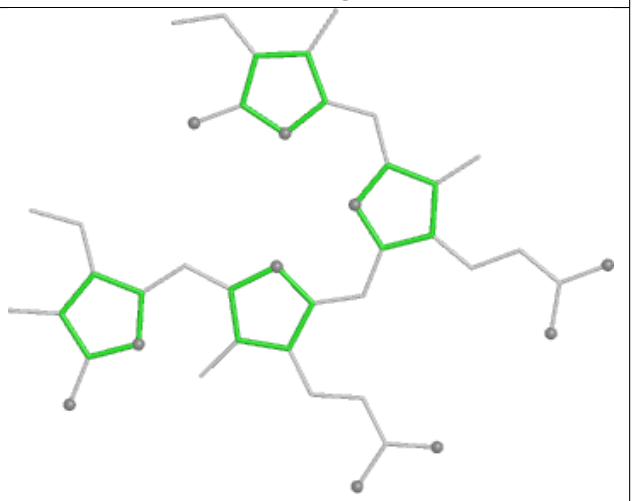
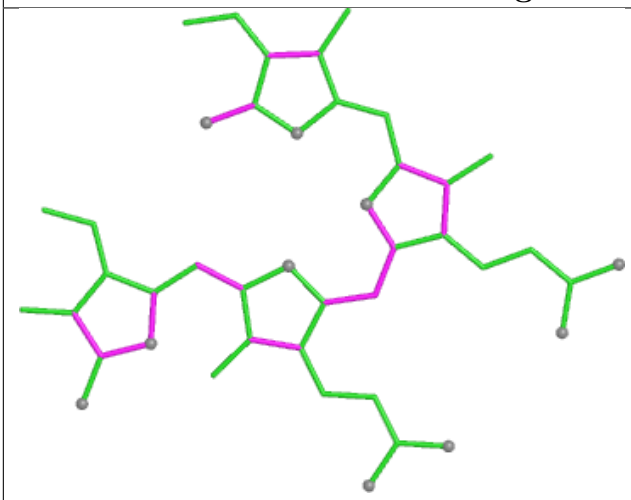


Rings

Ligand PEB SB 201



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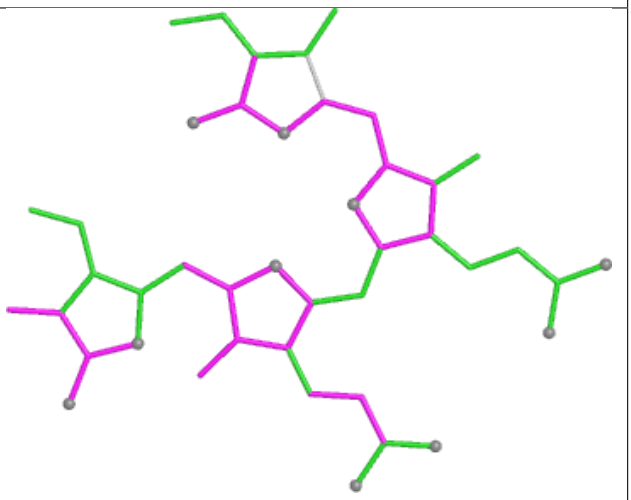

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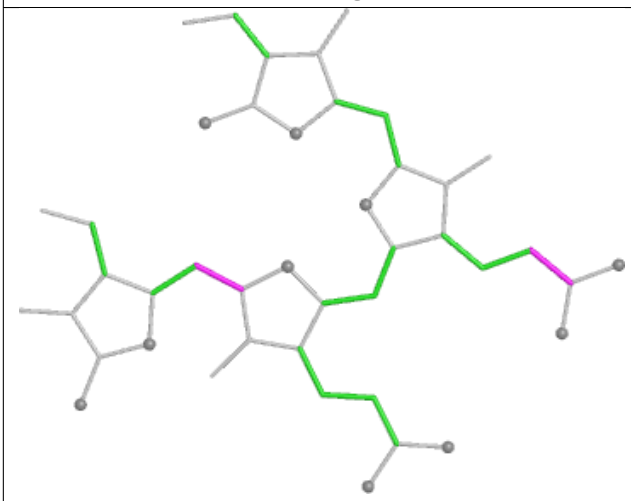

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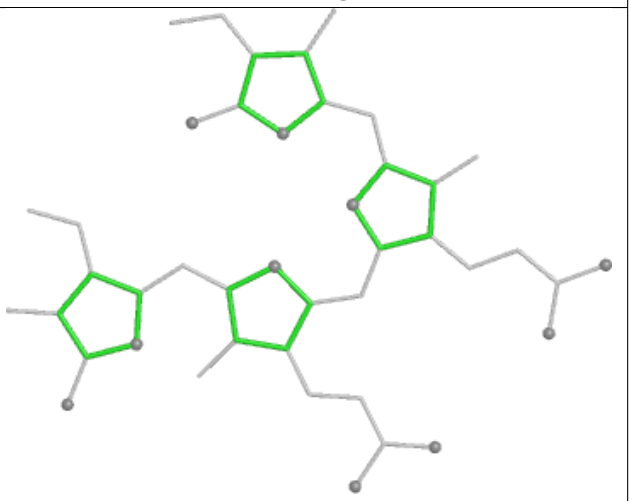
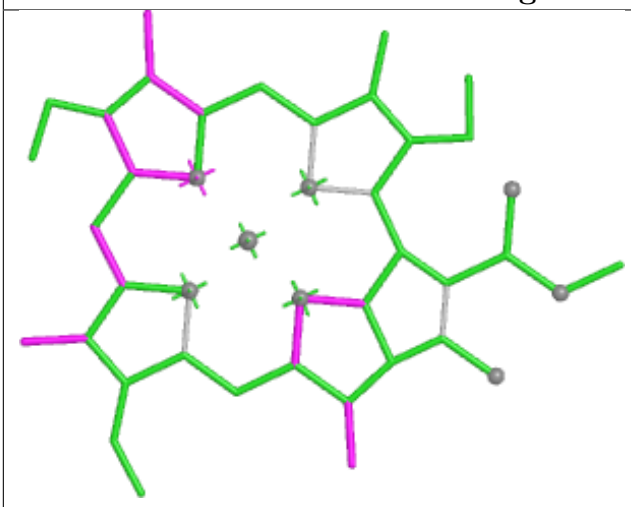


Rings

Ligand CLA J2 101



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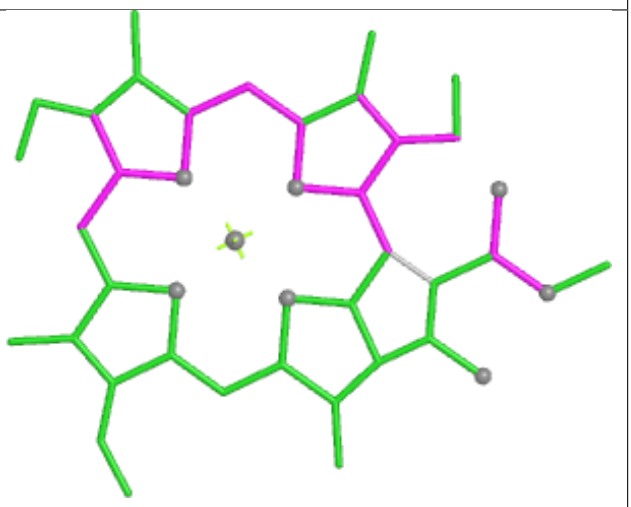

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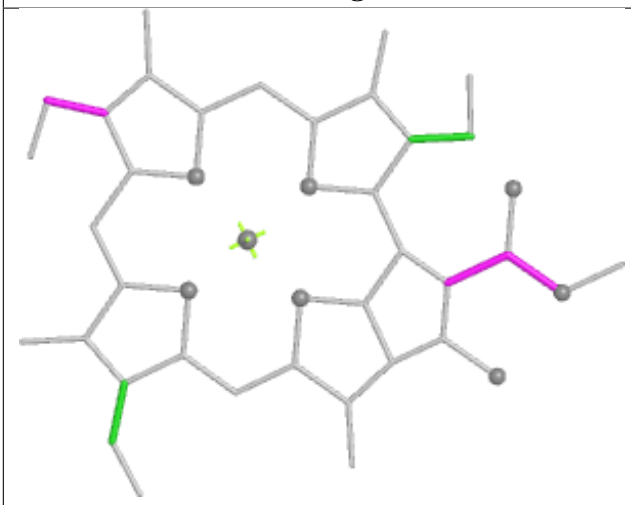
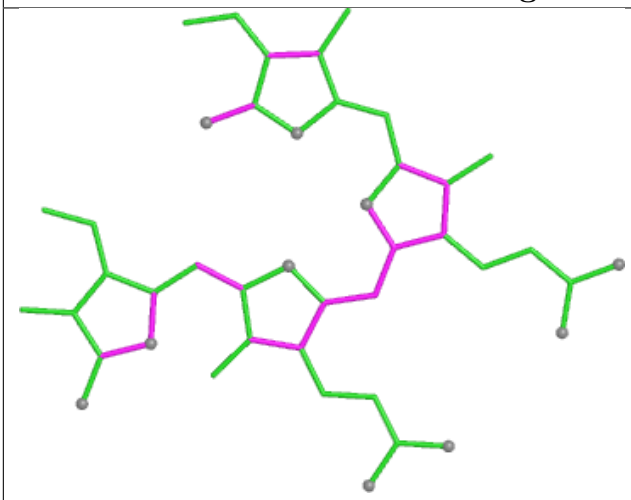


Torsions



Rings

Ligand PEB k1 201



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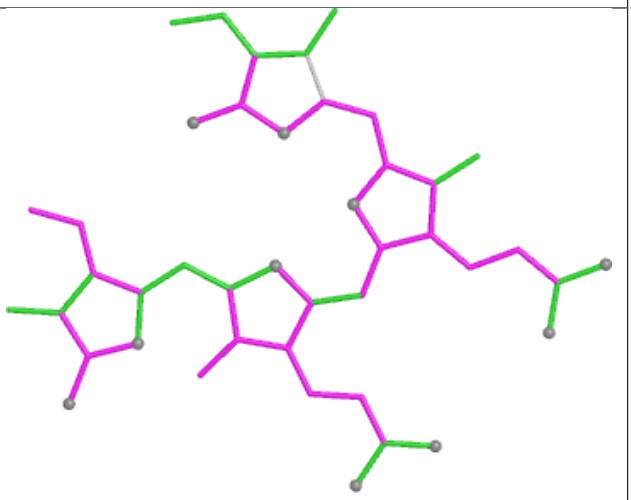
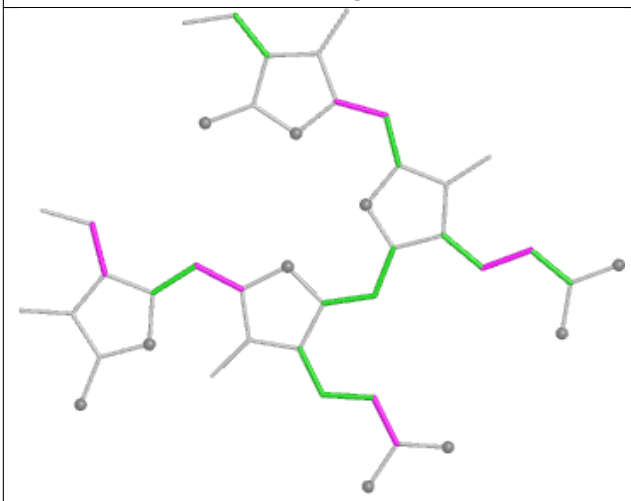


Bond angles



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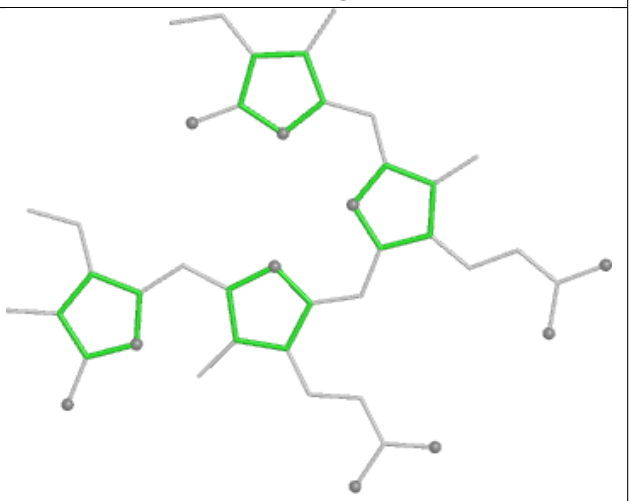
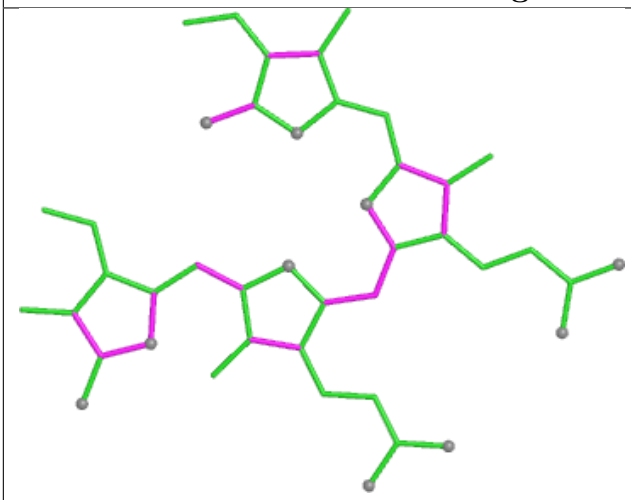


Rings

Ligand PEB PG 202



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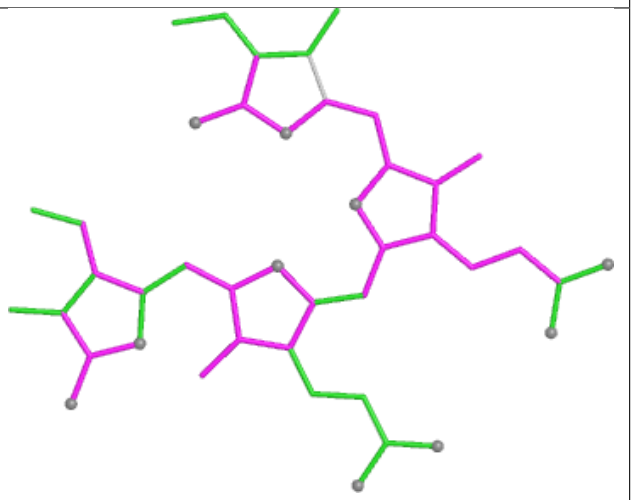

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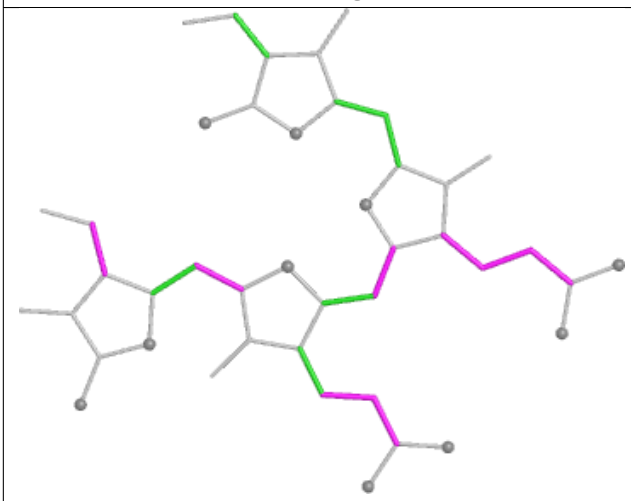

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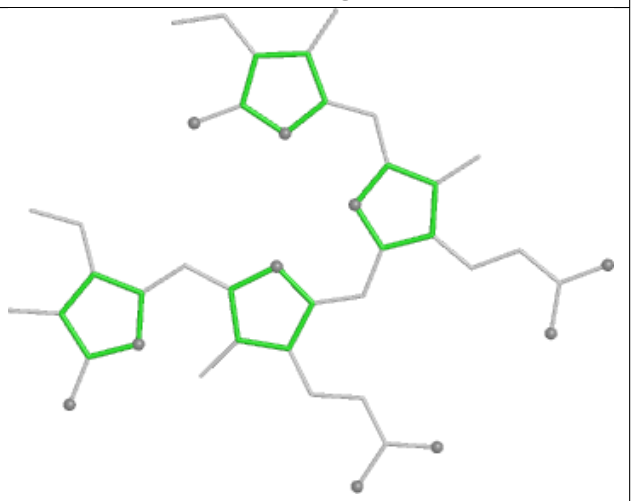
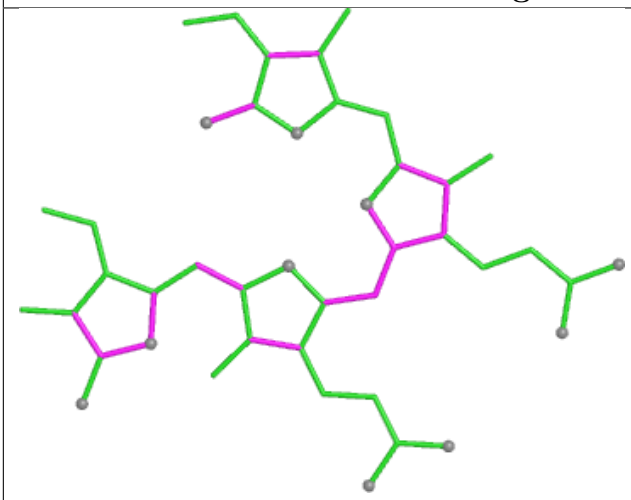


Rings

Ligand PEB WI 203



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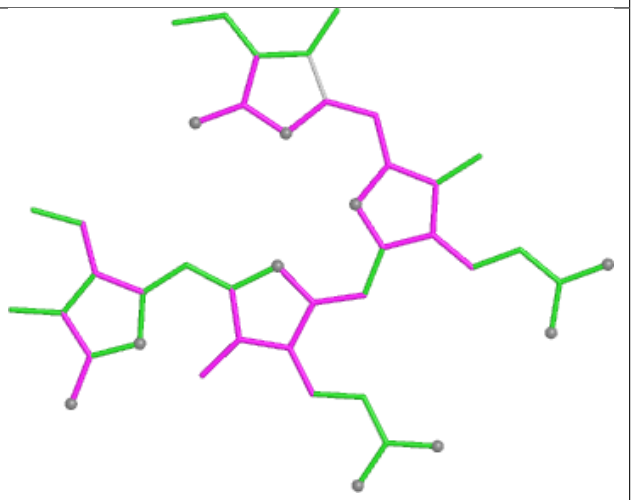
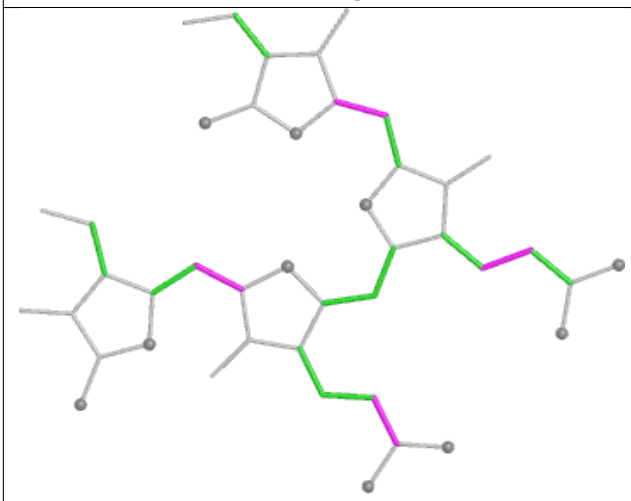


Bond angles



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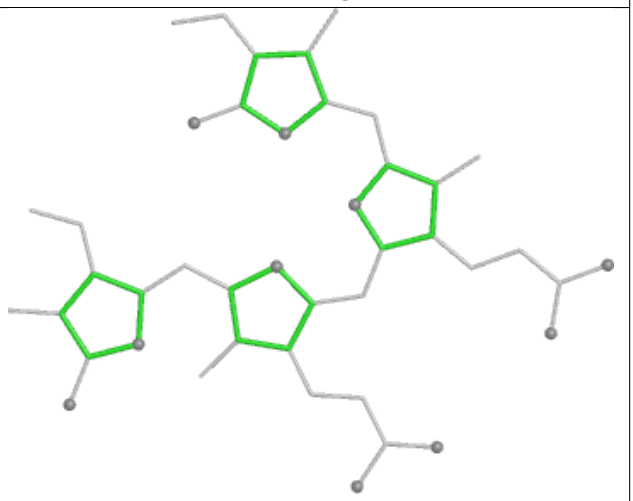
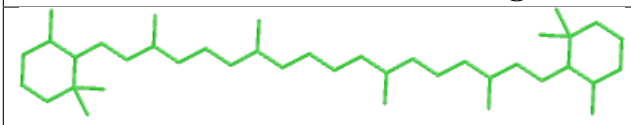


Rings

Ligand BCR AN 846



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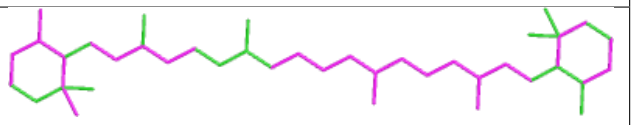

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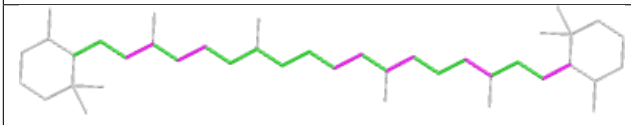

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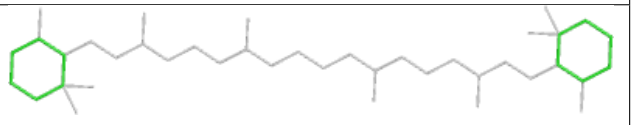
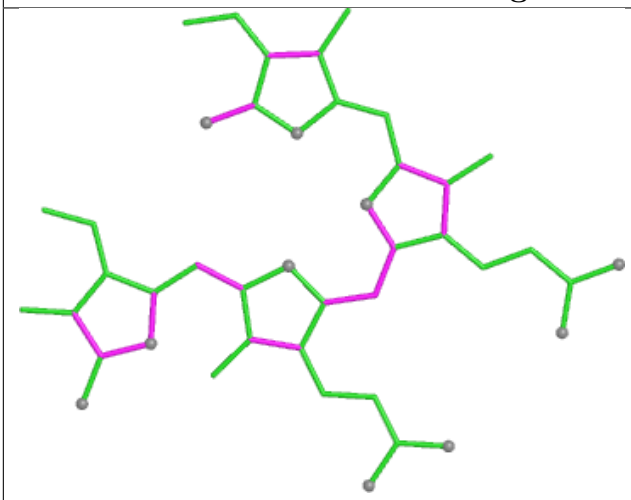


Rings

Ligand PEB YG 201



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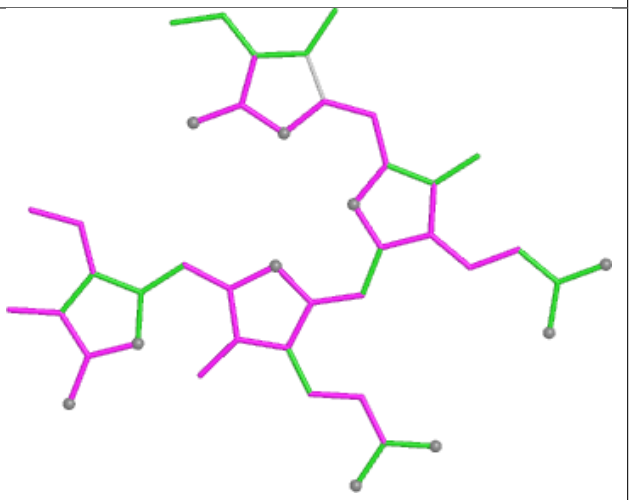

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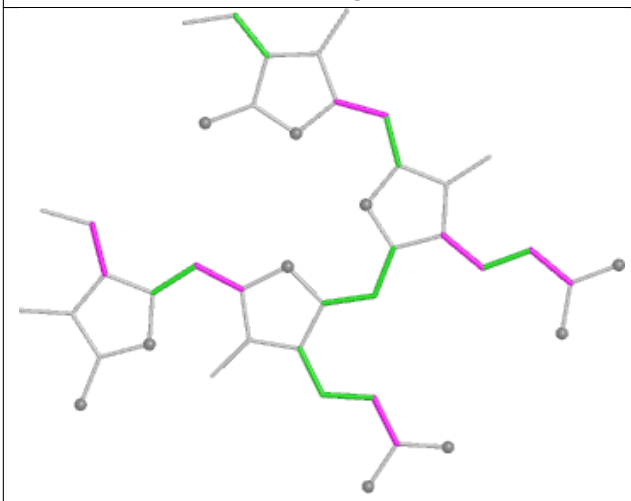

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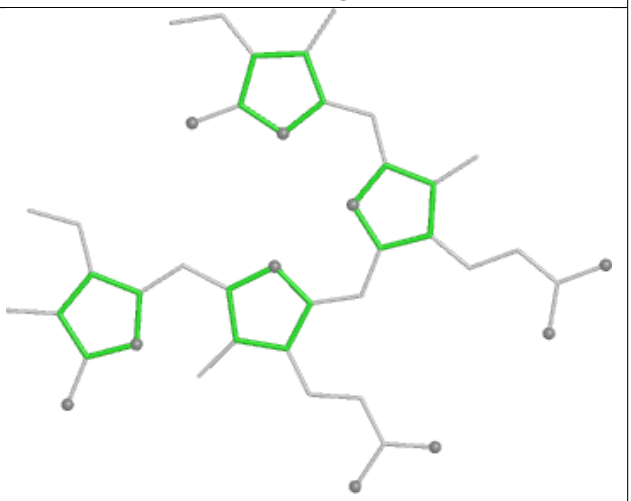
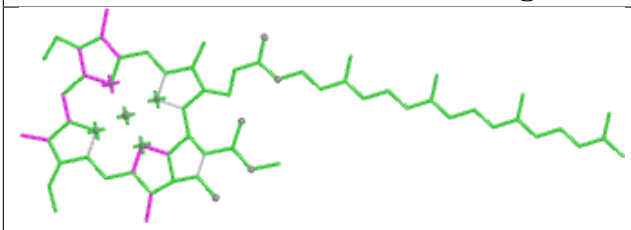


Rings

Ligand CLA b6 604



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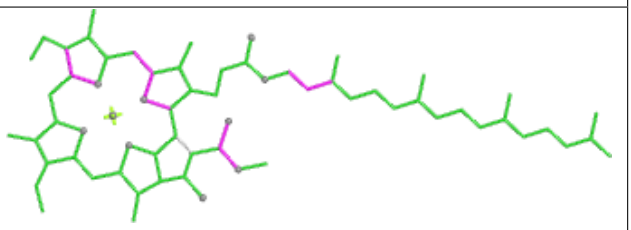
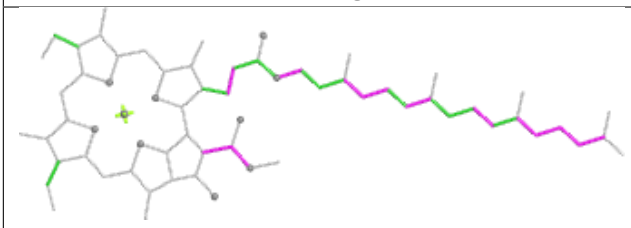


Bond angles



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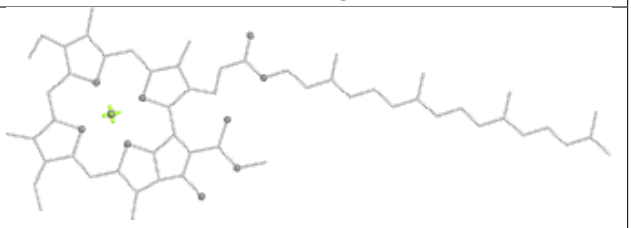
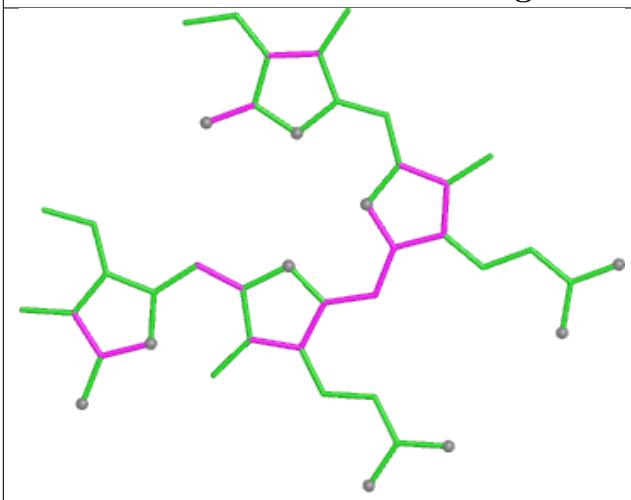


Rings

Ligand PEB N9 202



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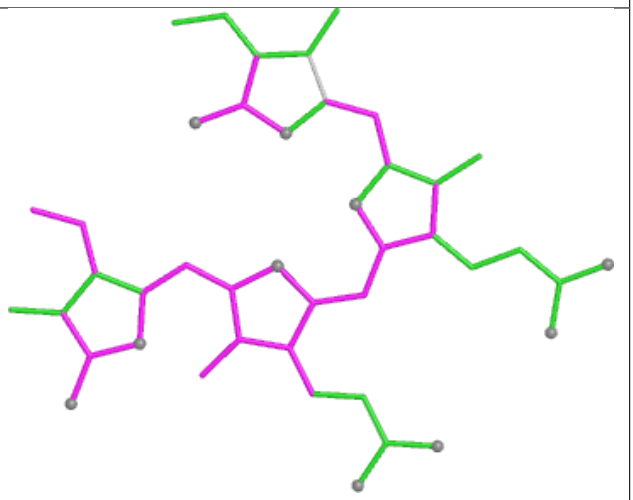

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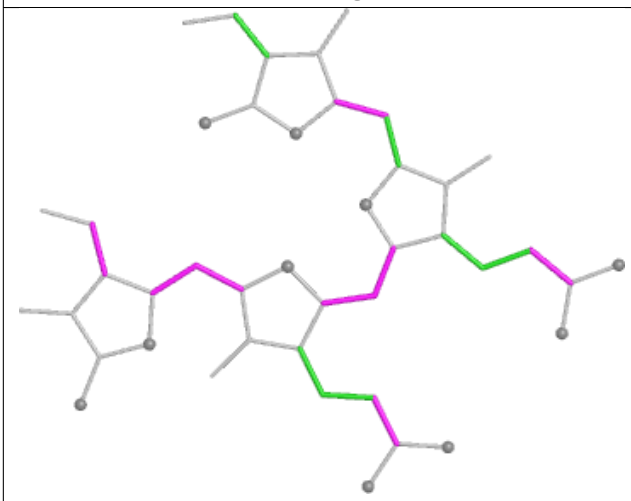

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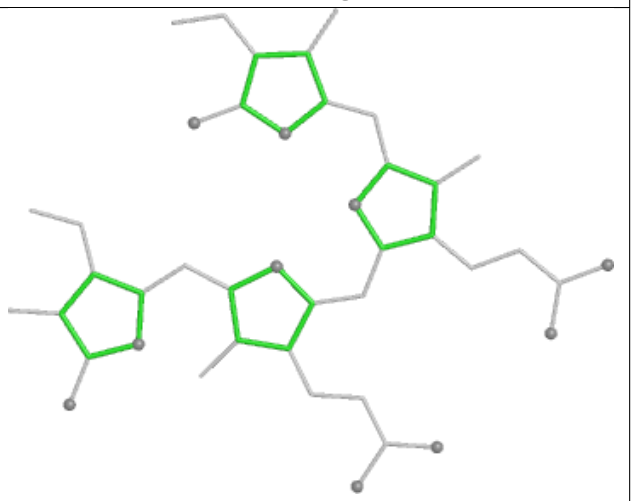
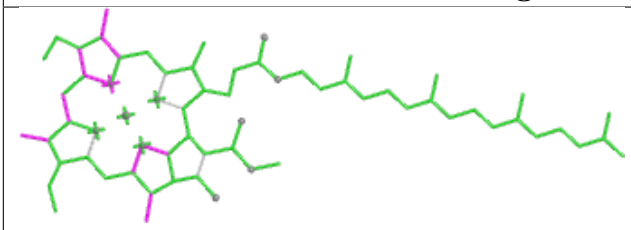


Rings

Ligand CLA B6 614



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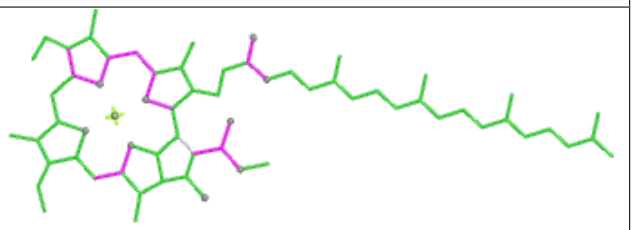

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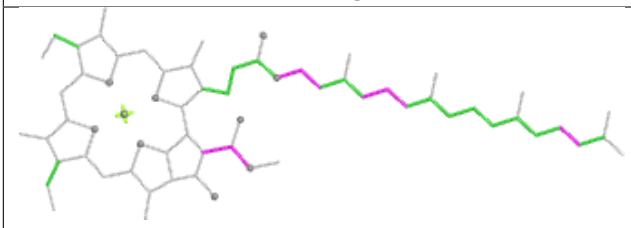

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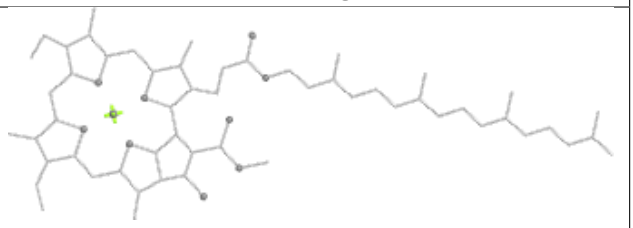
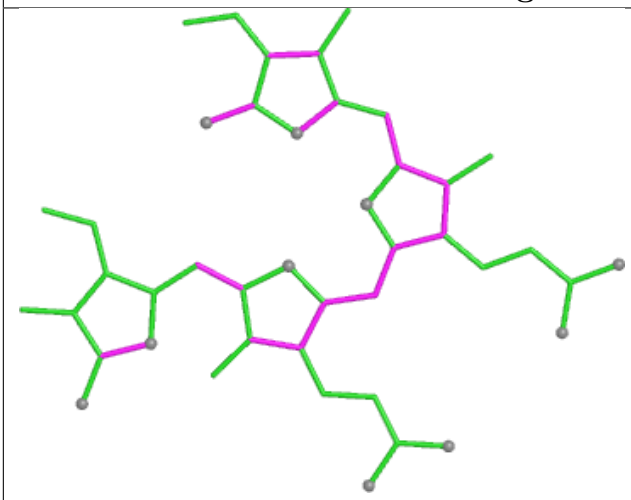


Rings

Ligand PEB tK 202



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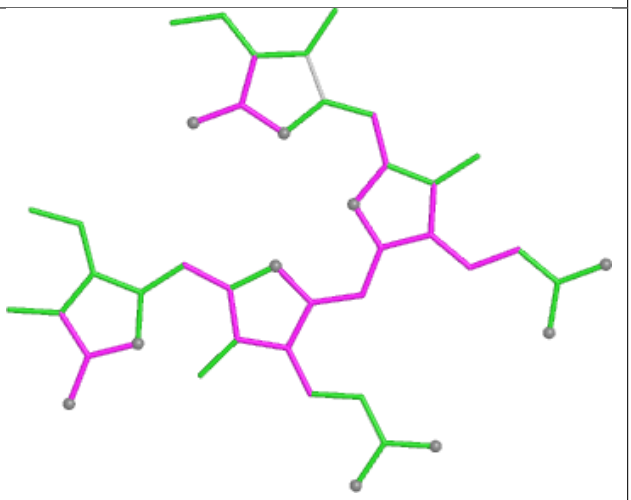
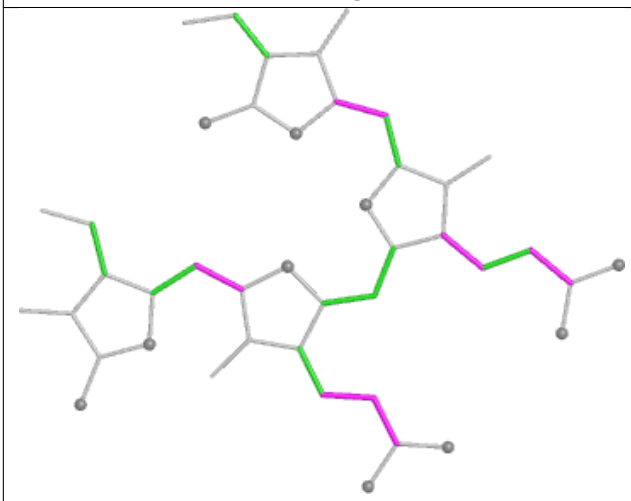


Bond angles



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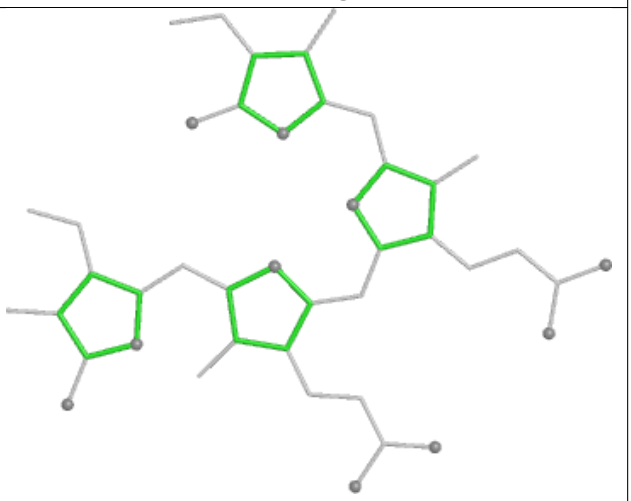
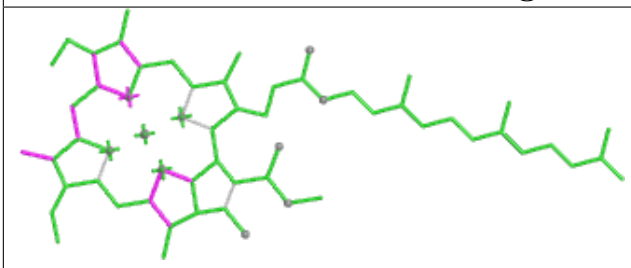


Rings

Ligand CLA cL 515



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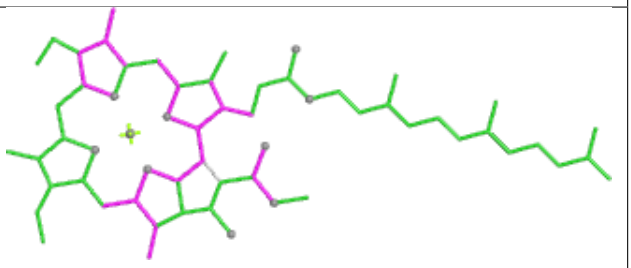
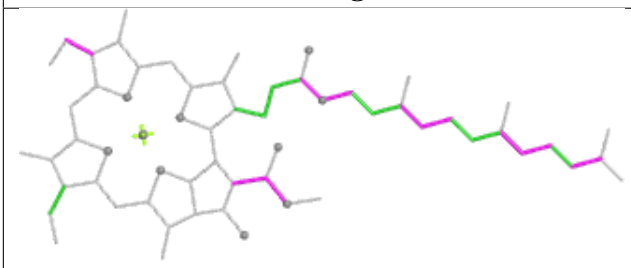


Bond angles



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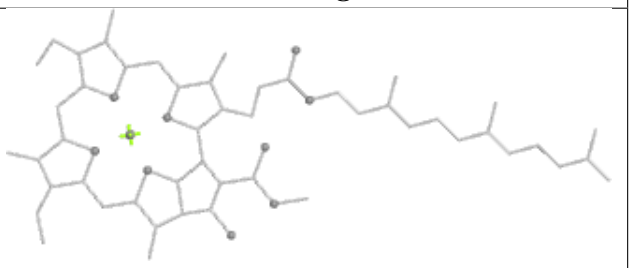
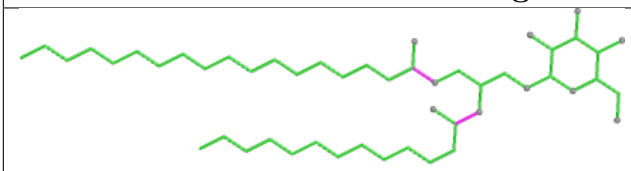
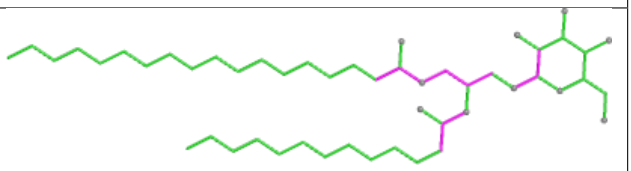
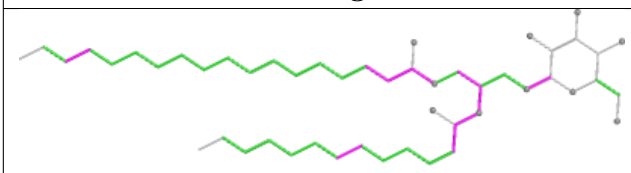
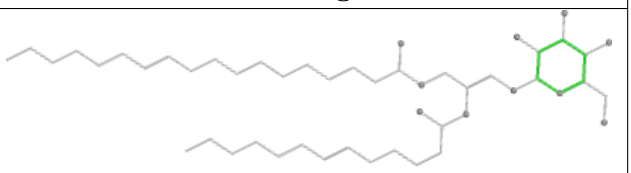
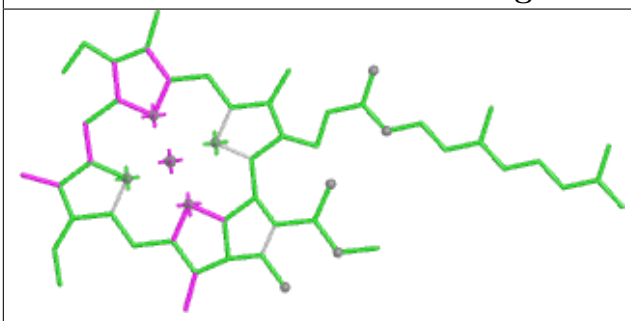
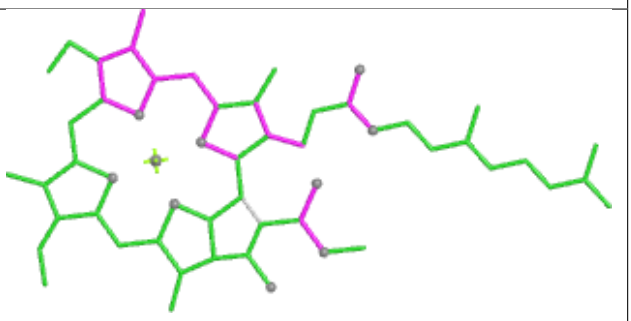
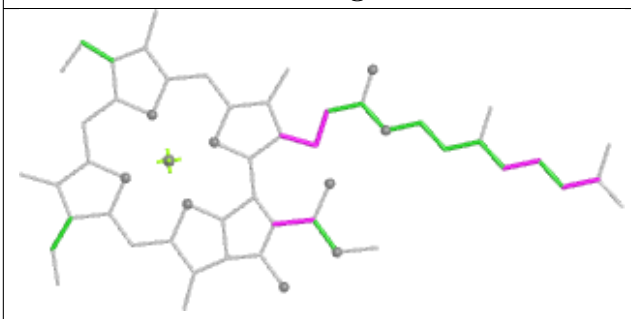
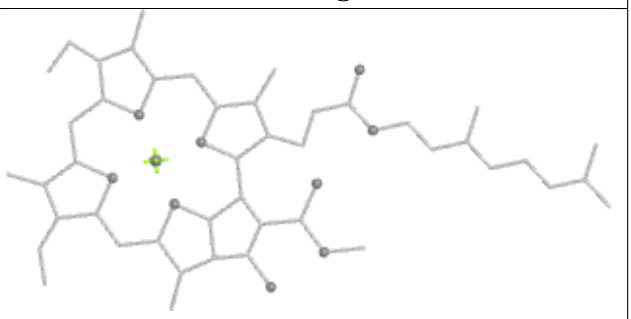


Rings

Ligand LMG bL 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

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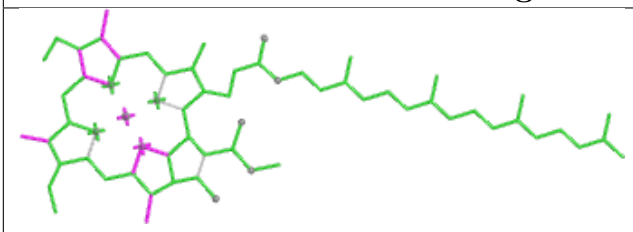

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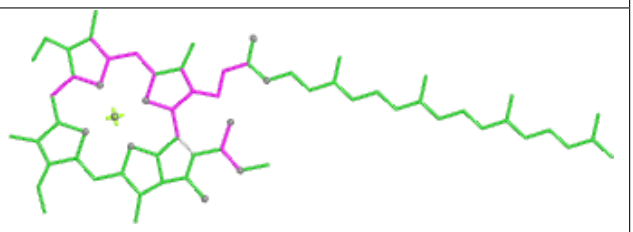

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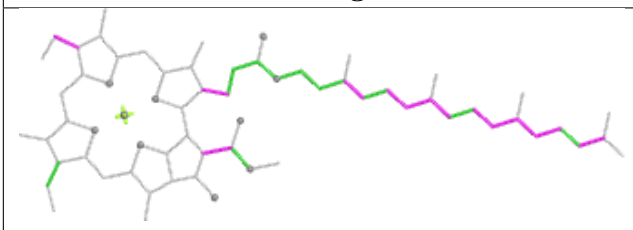

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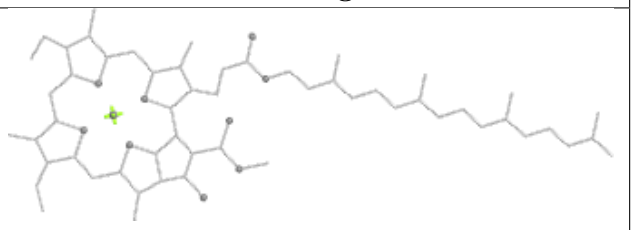
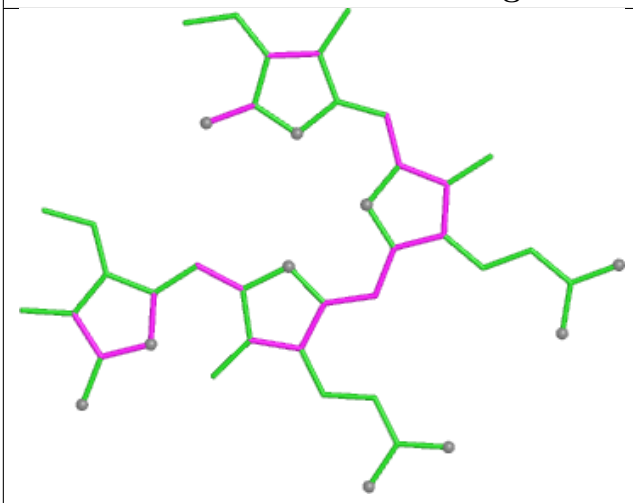


Rings

Ligand PEB HE 1002



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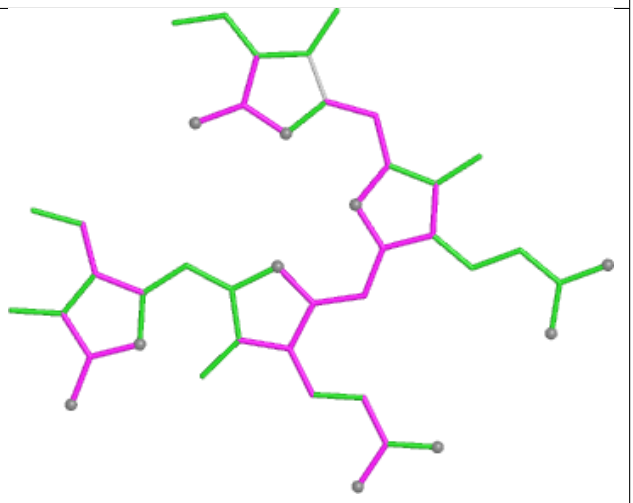

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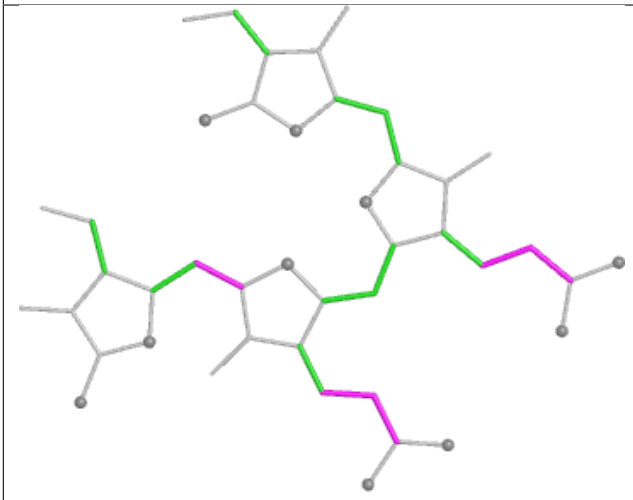

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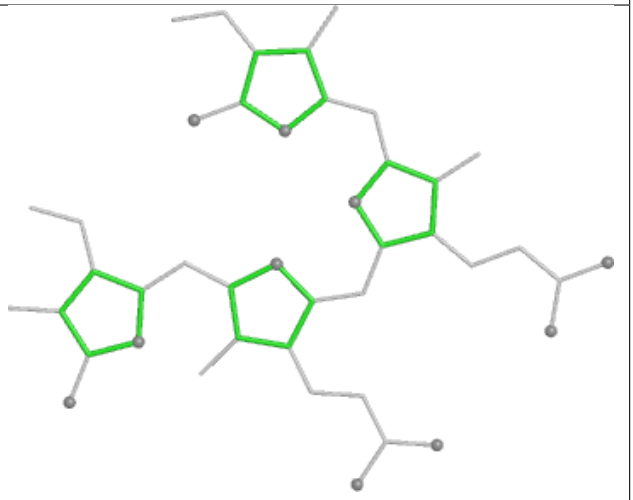
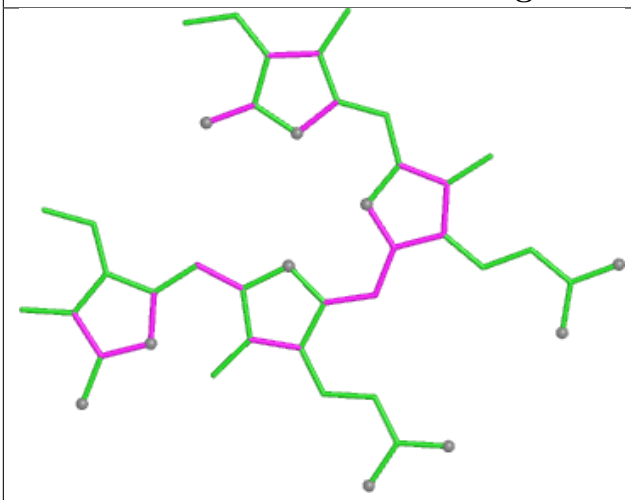


Rings

Ligand PEB A7 202



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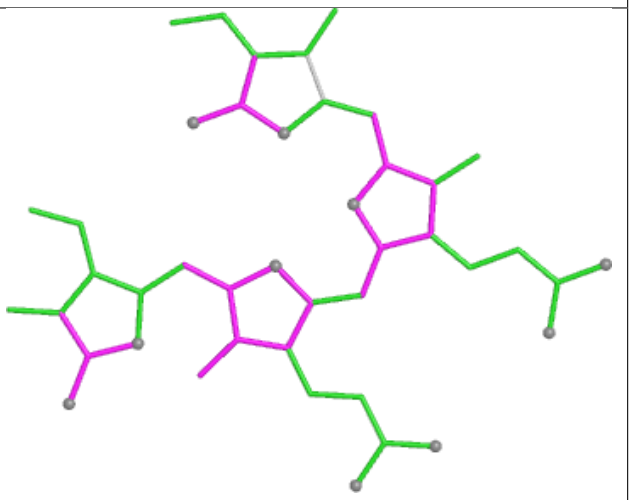

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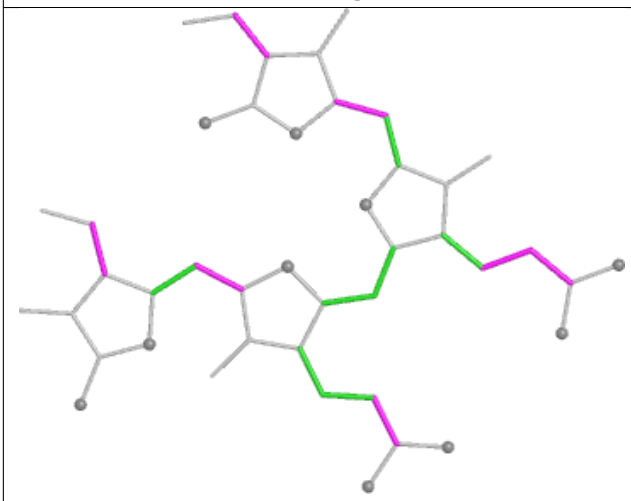

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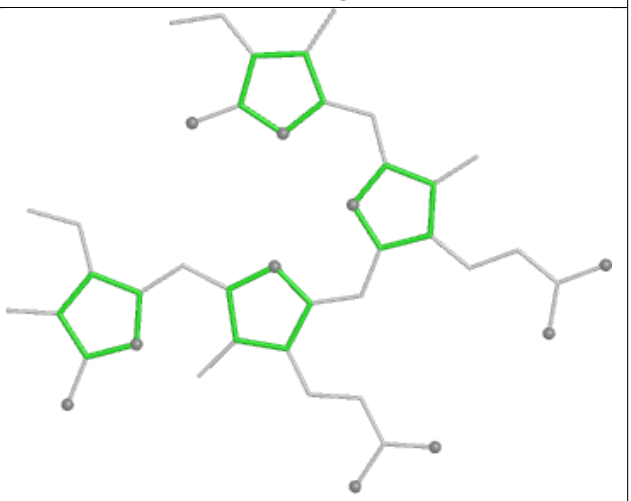

Rings

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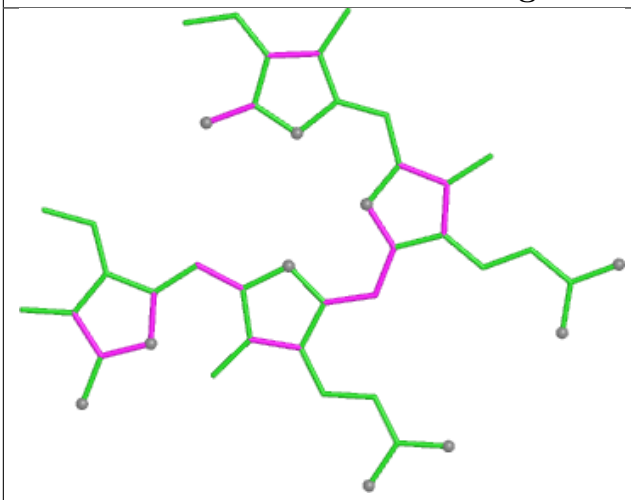

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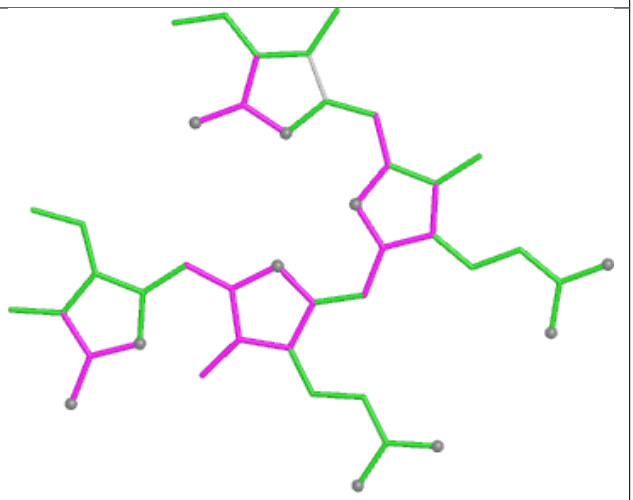

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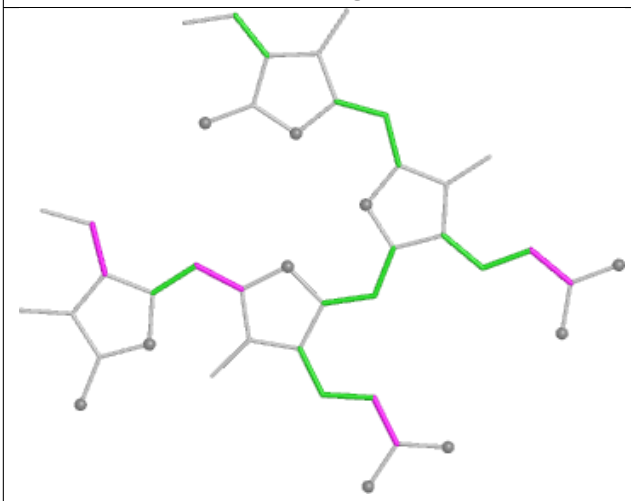

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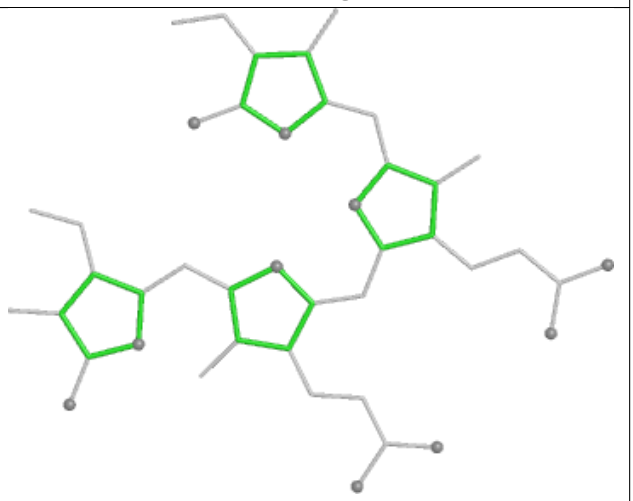

Rings

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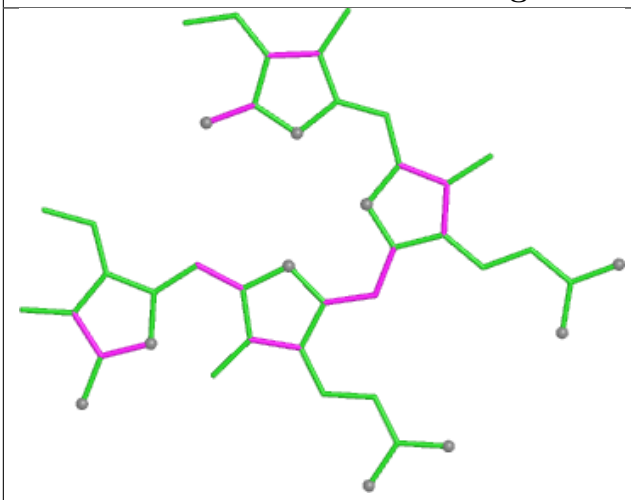

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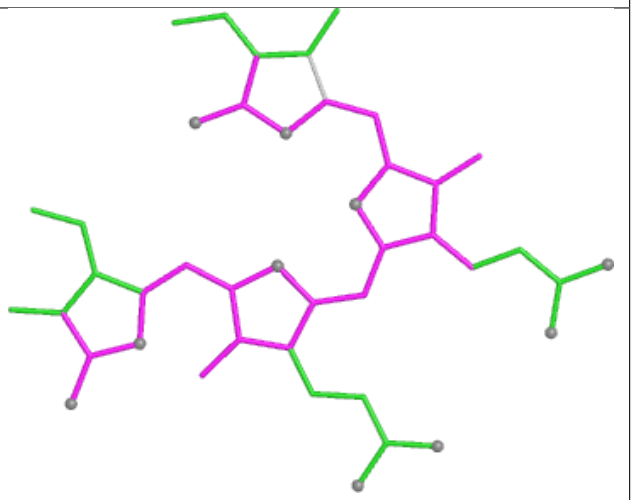

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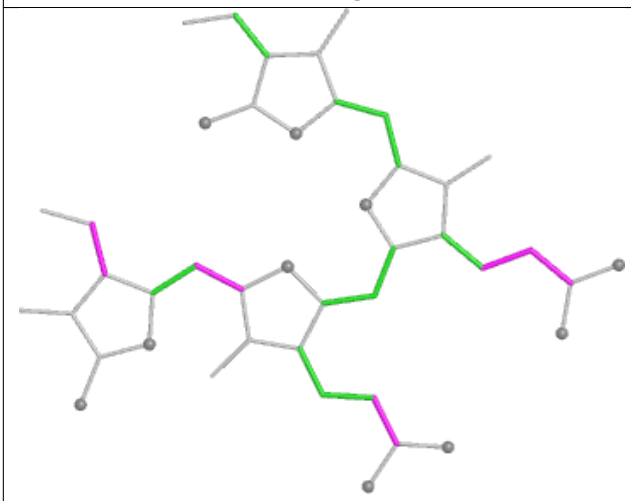

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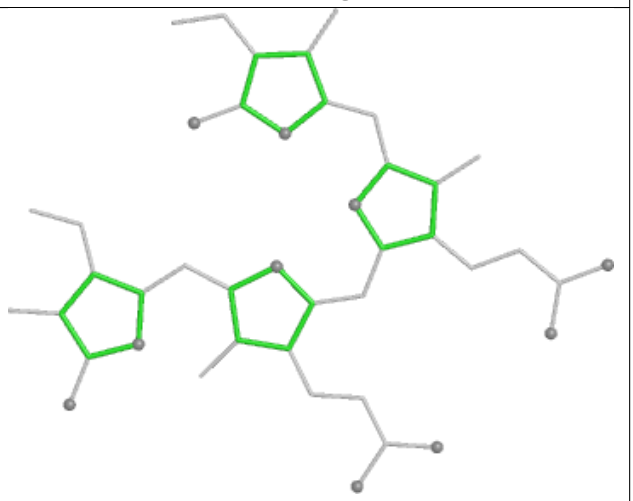
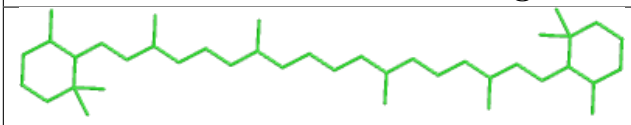


Rings

Ligand BCR B2 842



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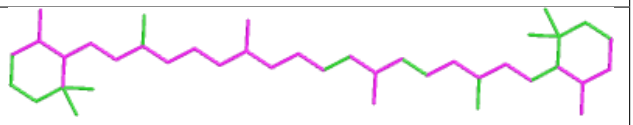

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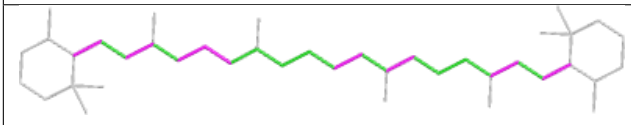

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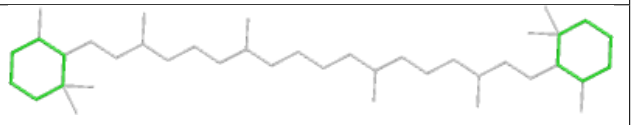
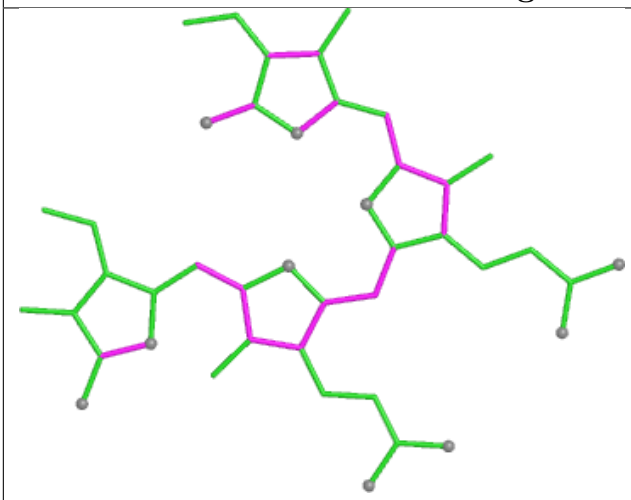


Rings

Ligand PEB oF 201



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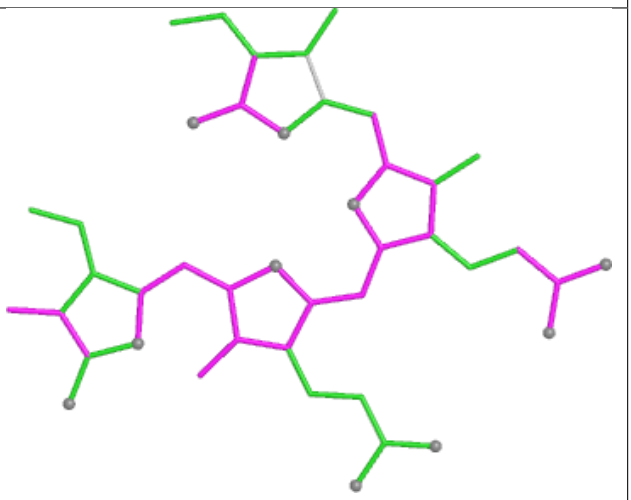

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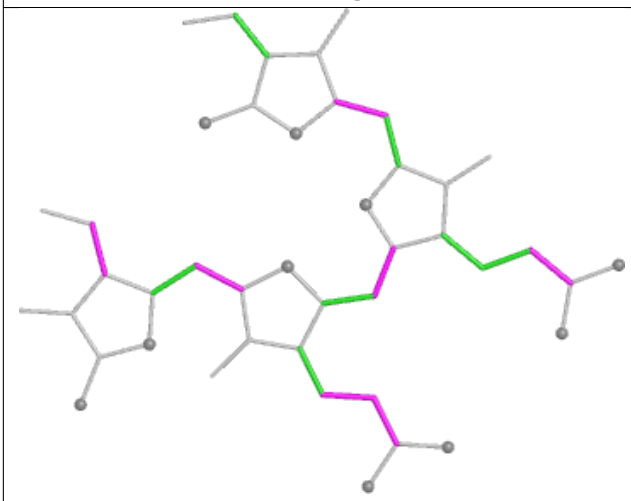

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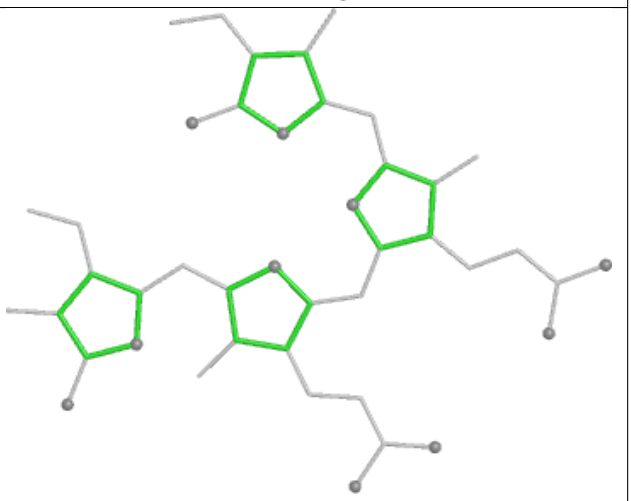

Rings

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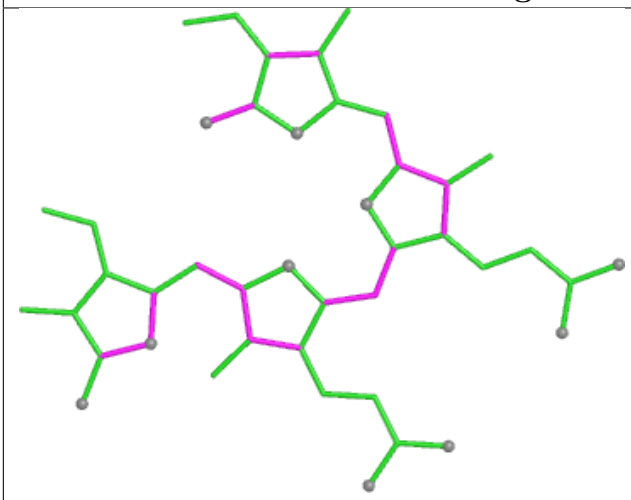

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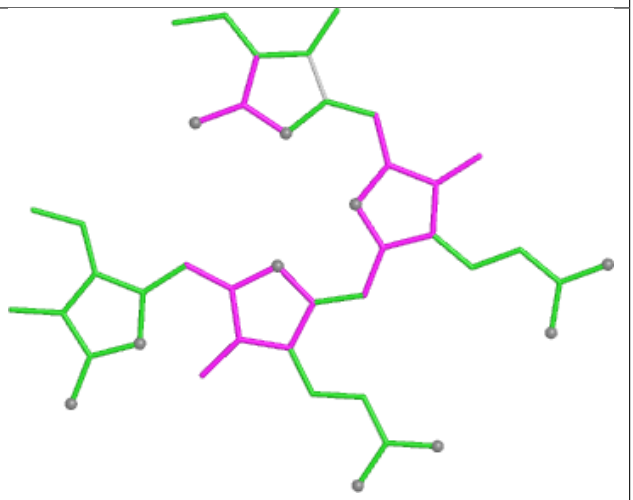

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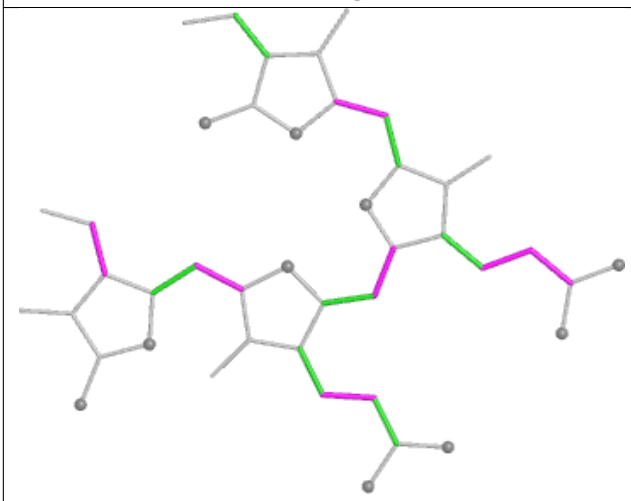

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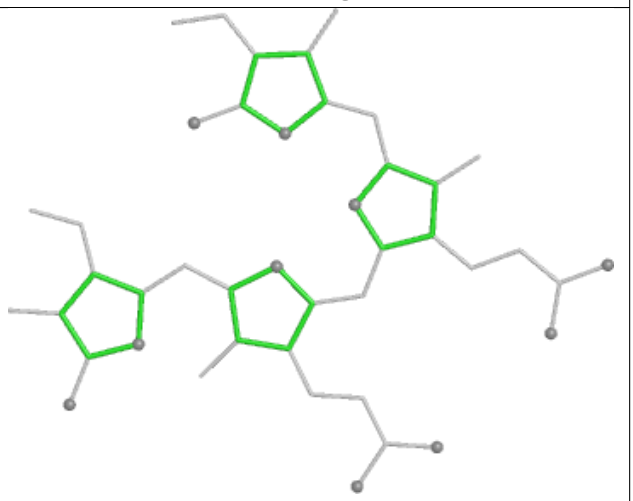
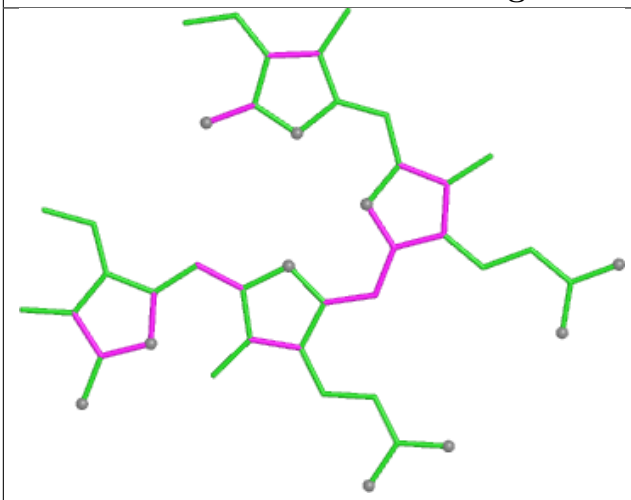


Rings

Ligand PEB BM 301



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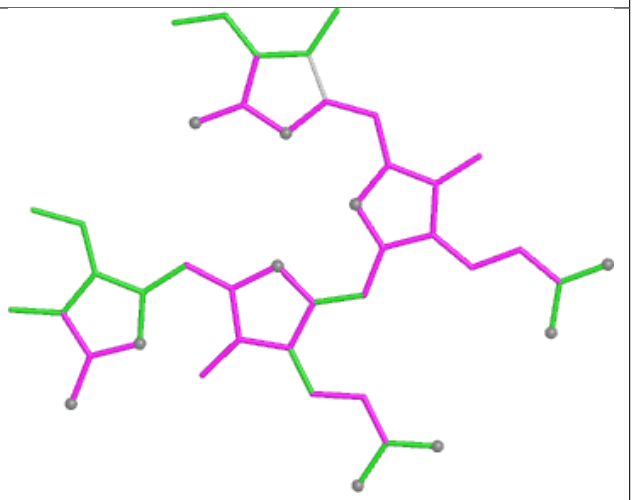

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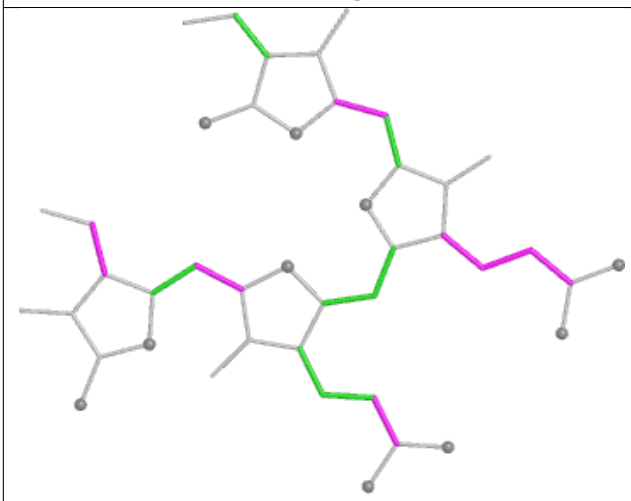

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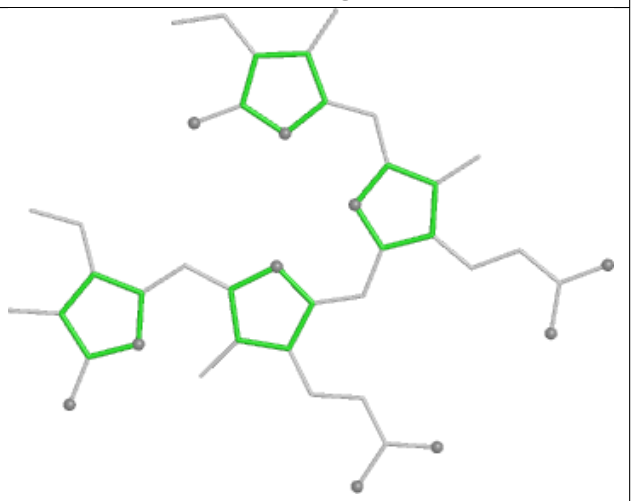
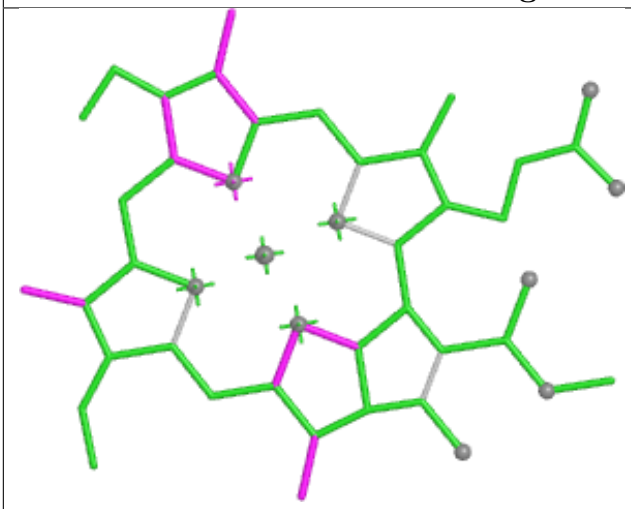


Rings

Ligand CLA 32 313



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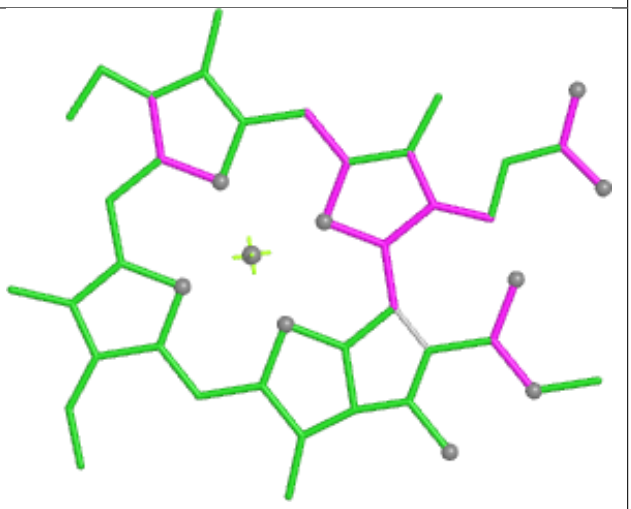

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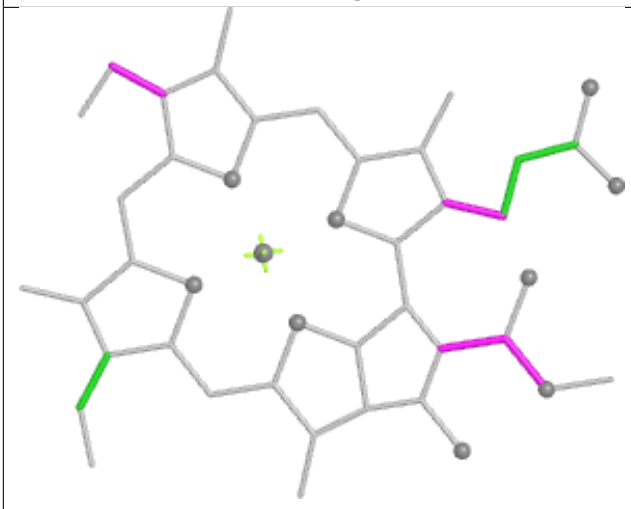
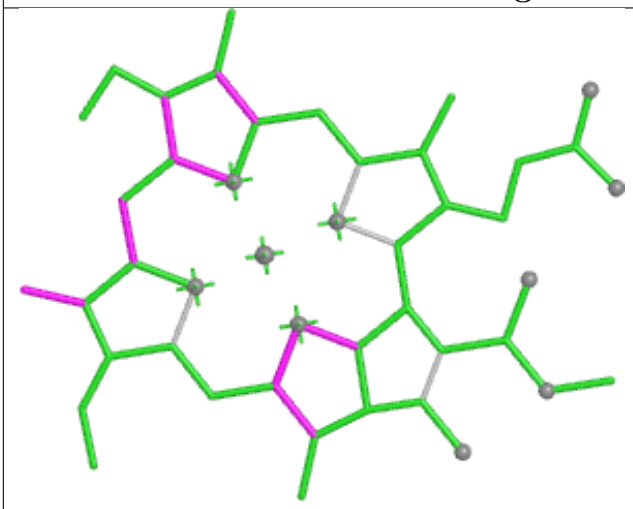


Torsions



Rings

Ligand CLA 6N 612



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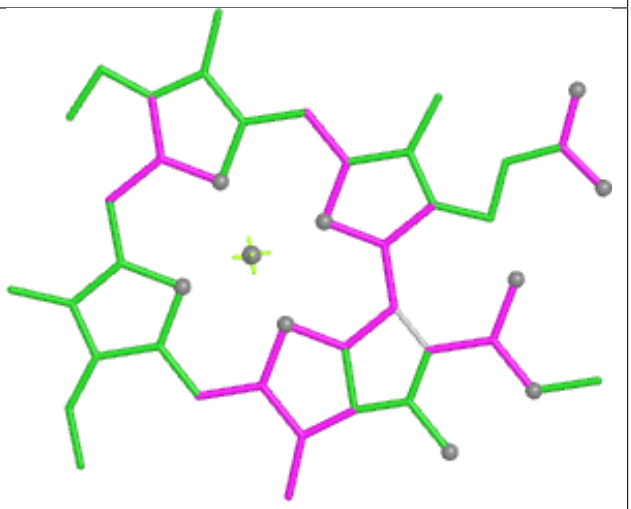
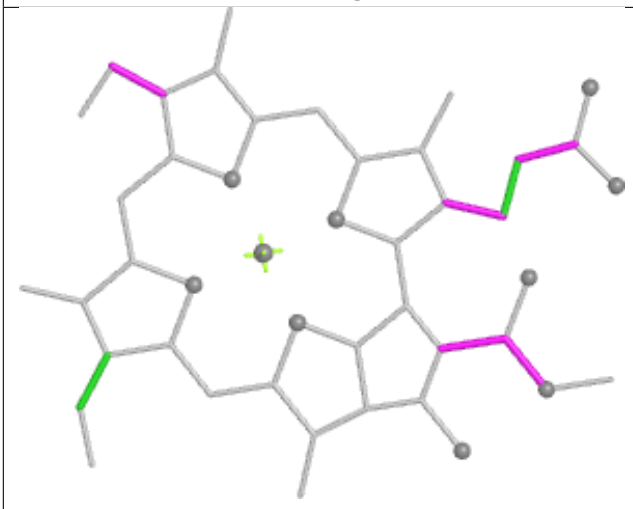


Bond angles

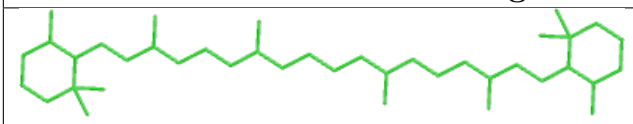


Torsions



Rings

Ligand BCR BN 842



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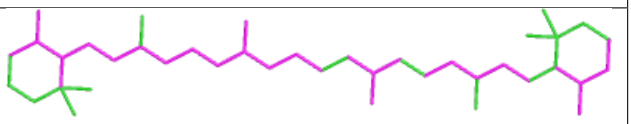

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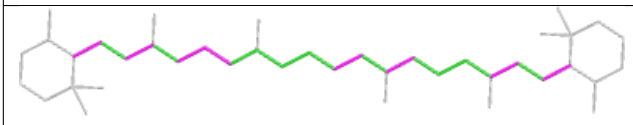

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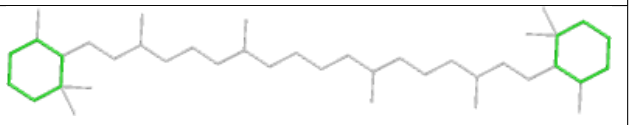
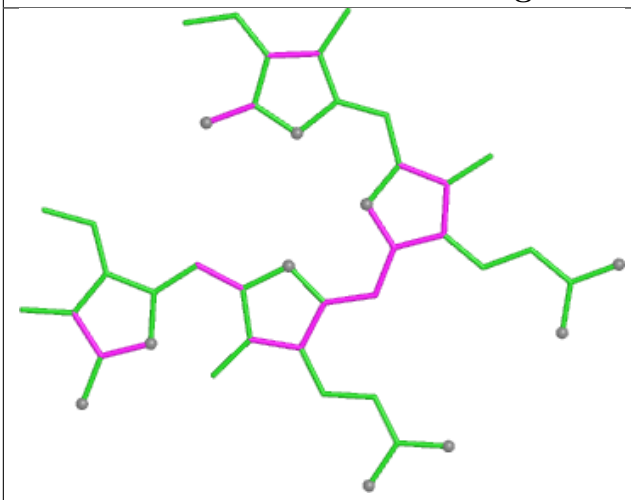


Rings

Ligand PEB G9 201



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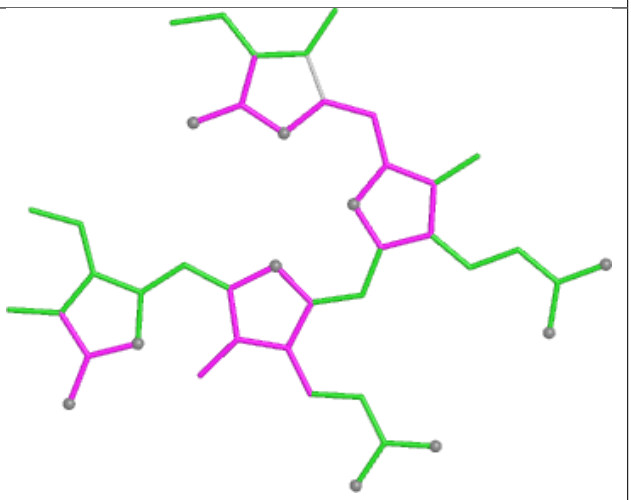

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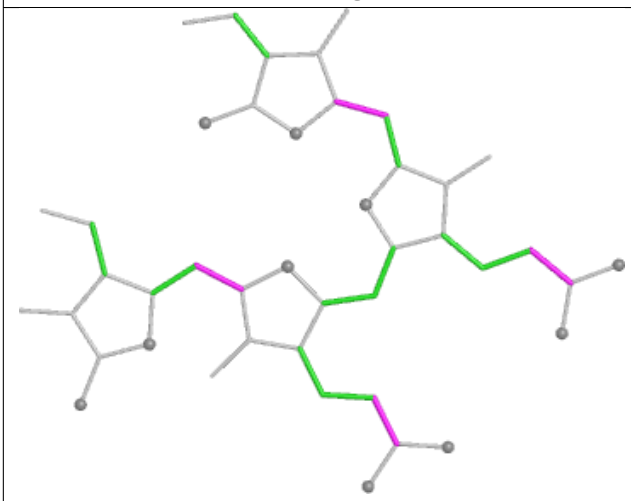

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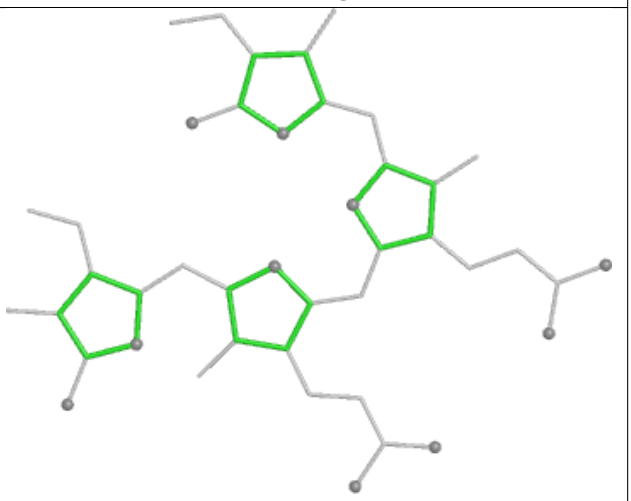

Rings

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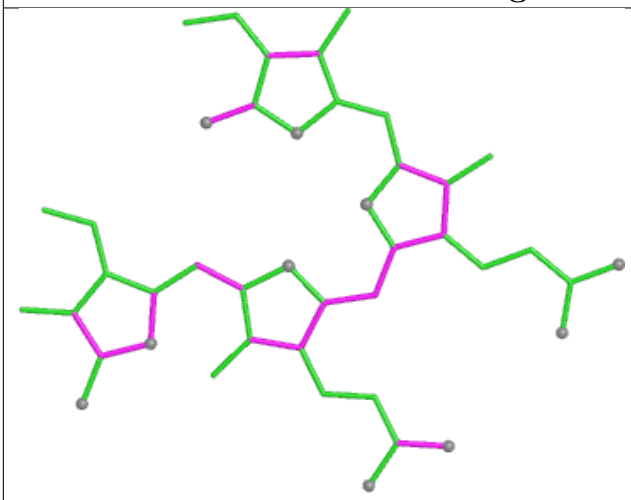

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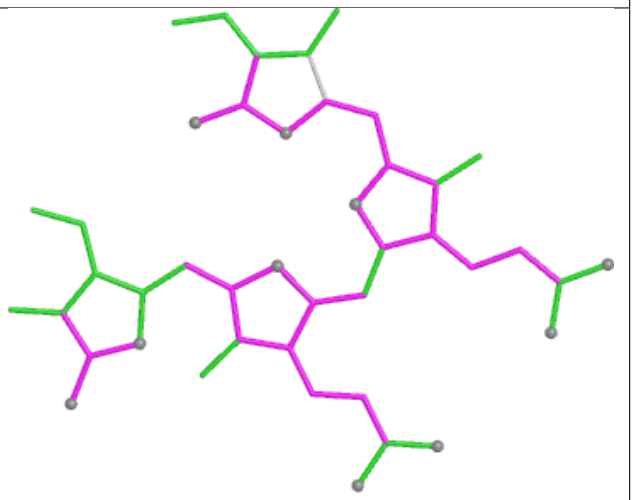
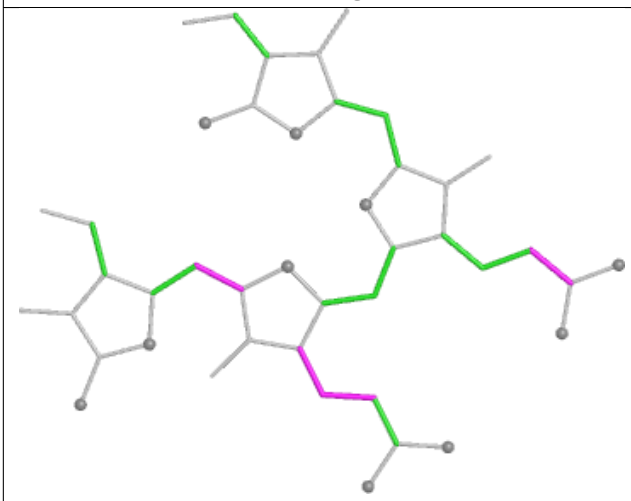
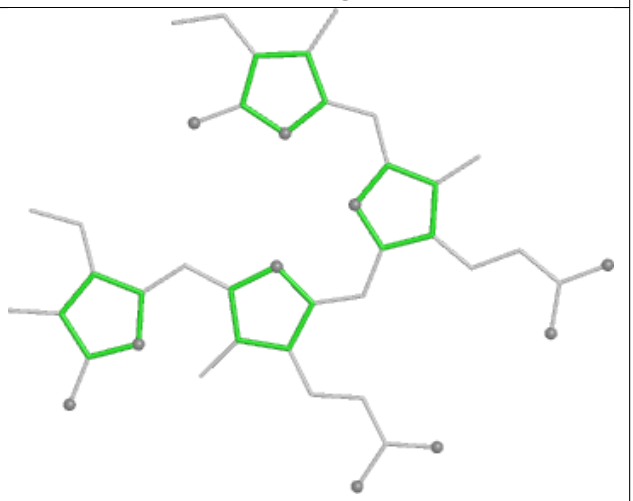


Bond angles

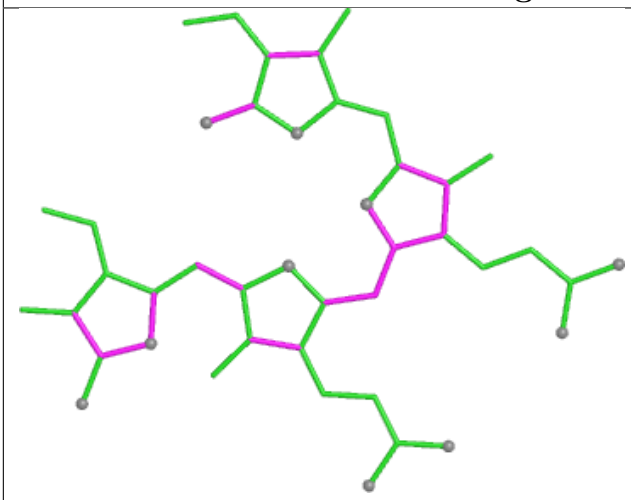


Torsions



Rings

Ligand PEB RJ 202



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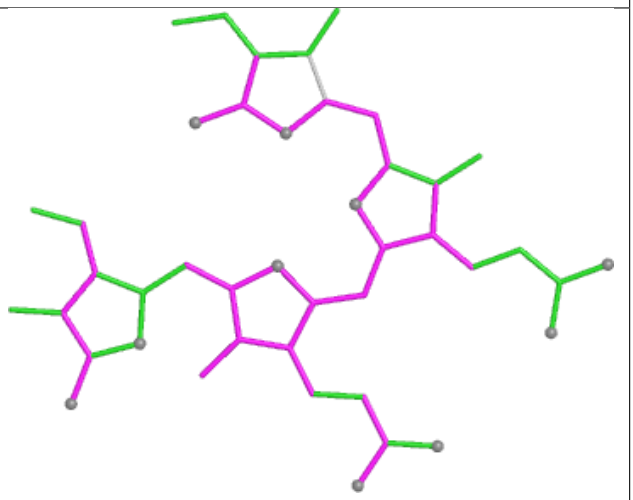
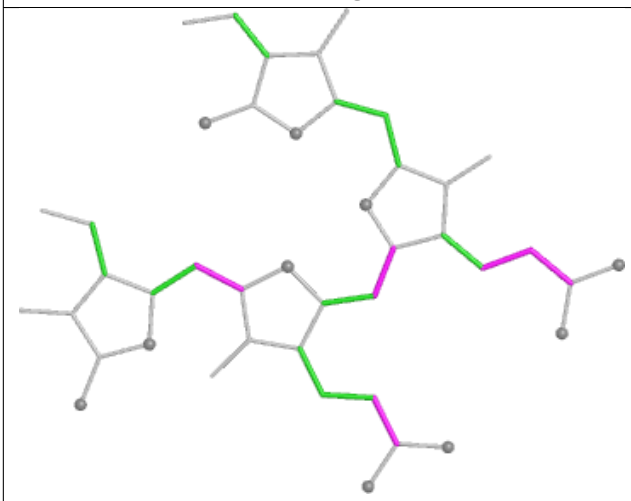


Bond angles



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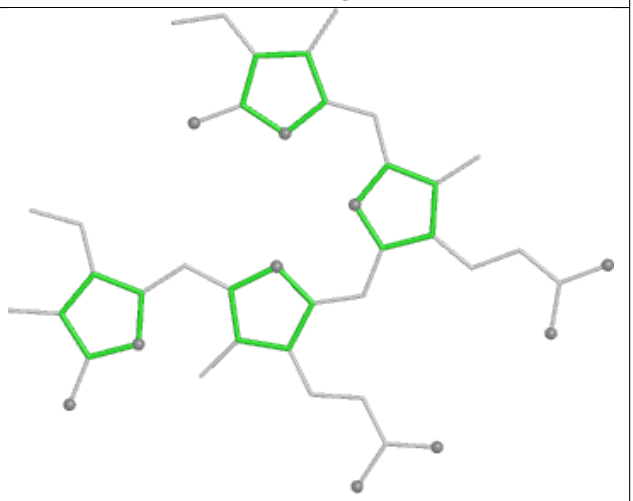
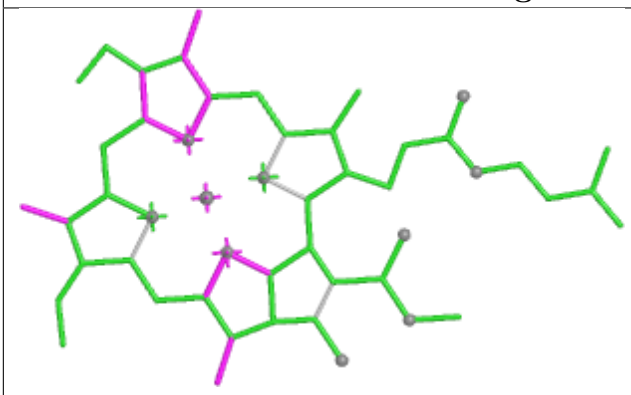


Rings

Ligand CLA A2 832



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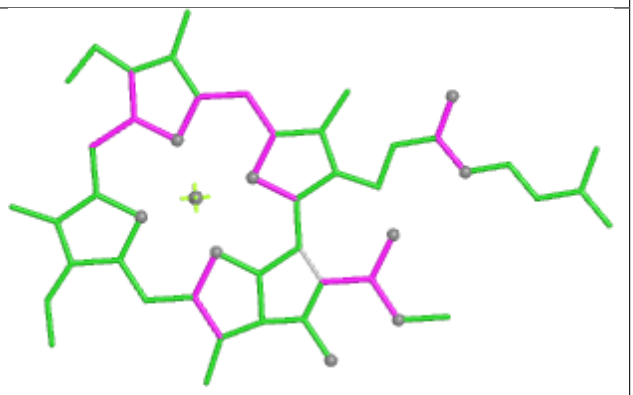
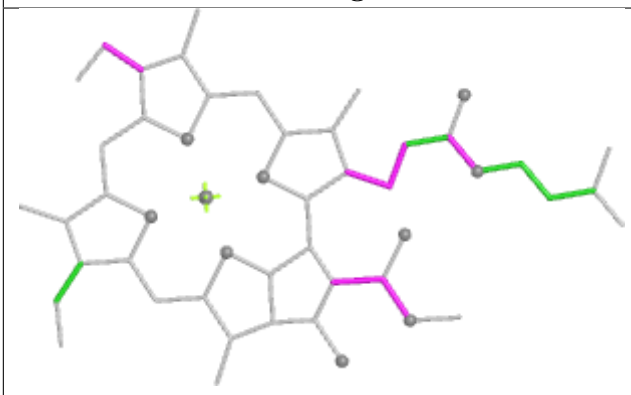


Bond angles



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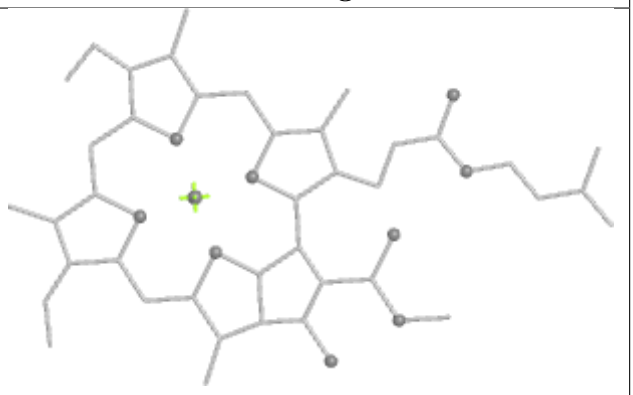
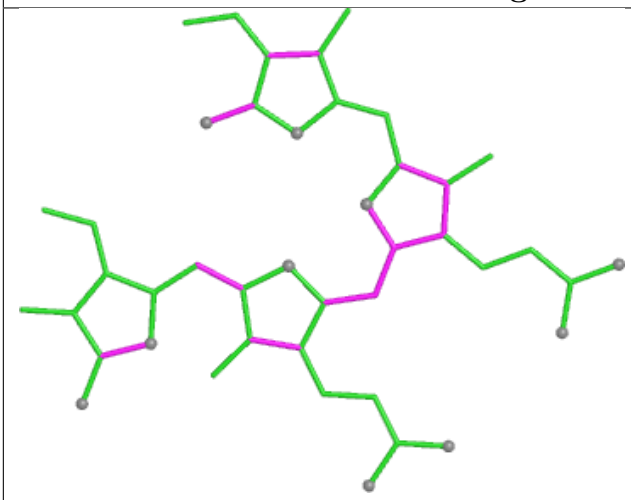


Rings

Ligand PEB ND 203



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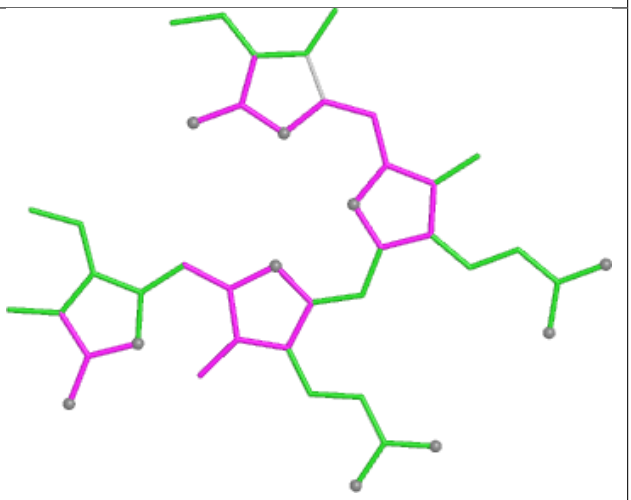

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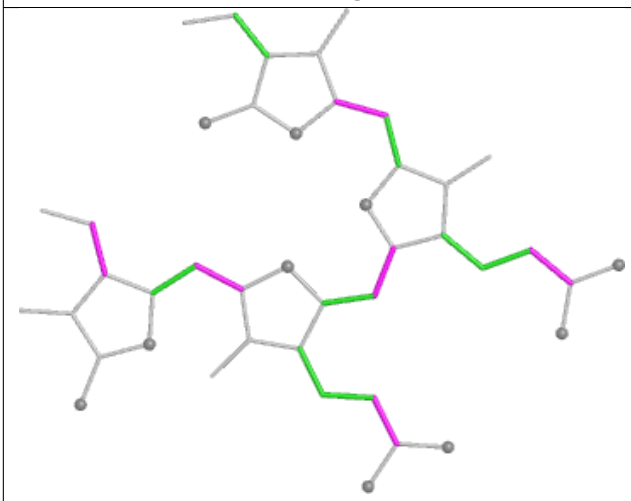

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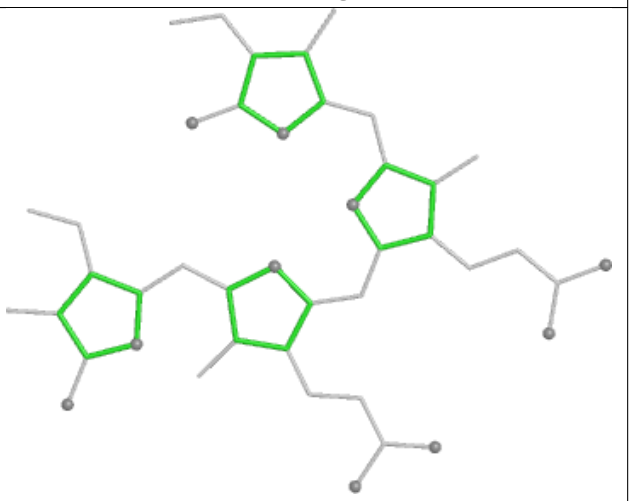
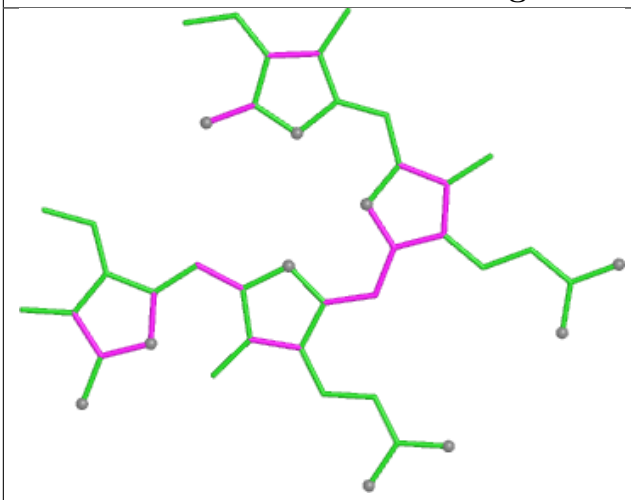


Rings

Ligand PEB L4 1002



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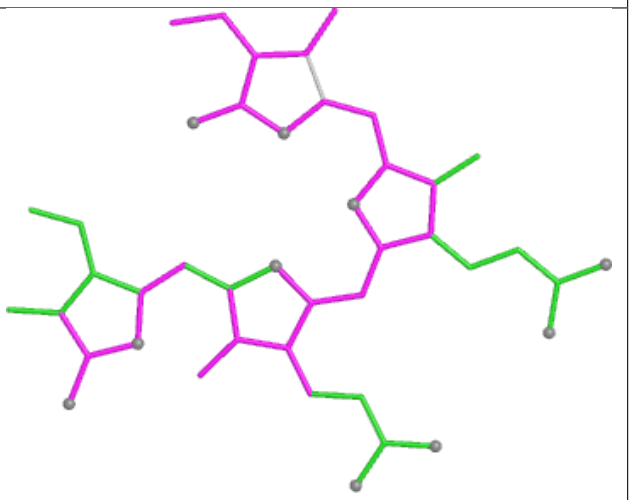
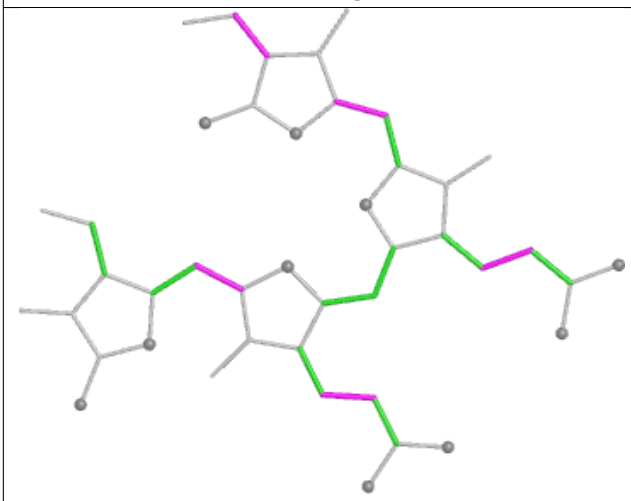


Bond angles



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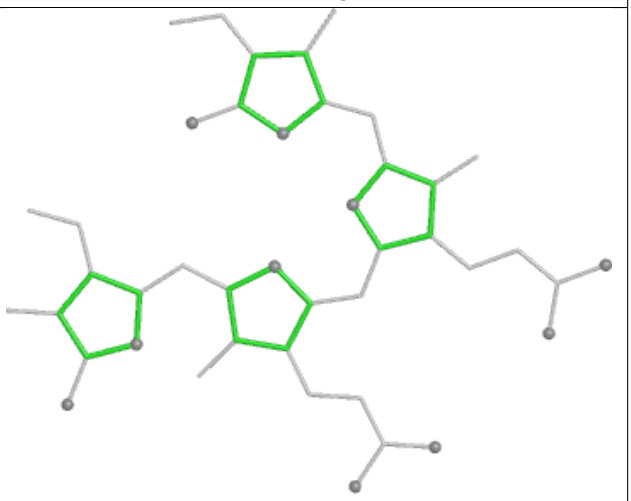
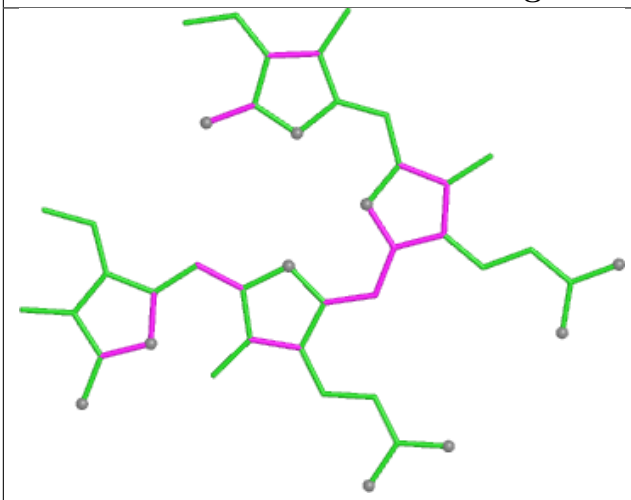


Rings

Ligand PEB II 202



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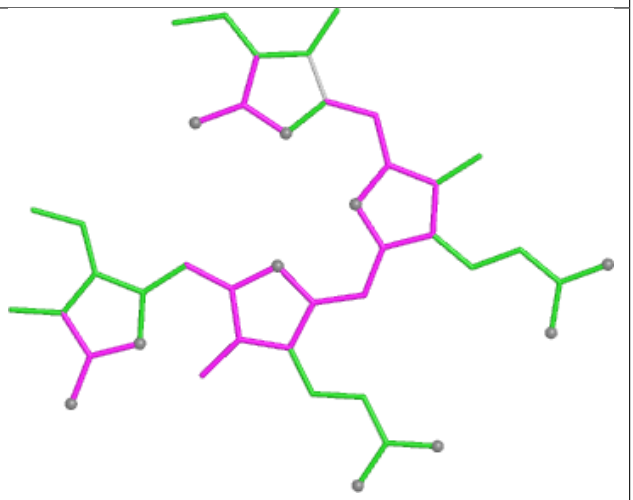

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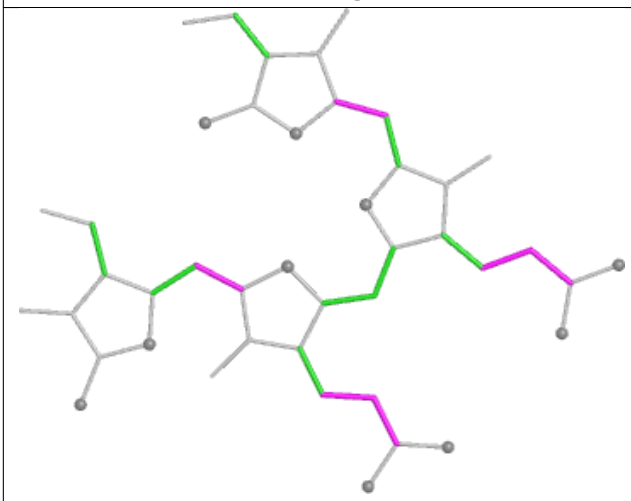

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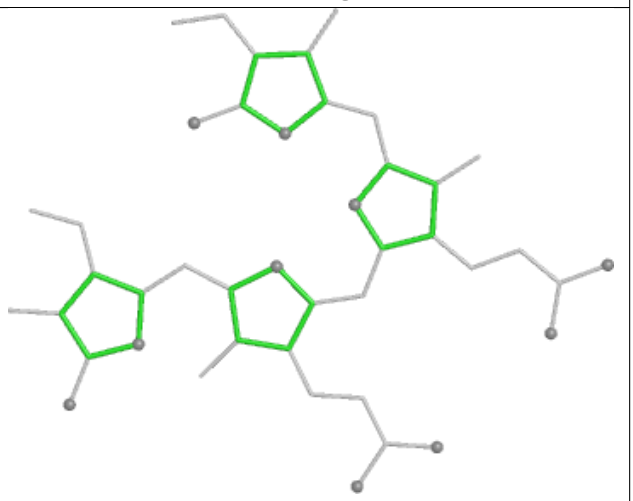
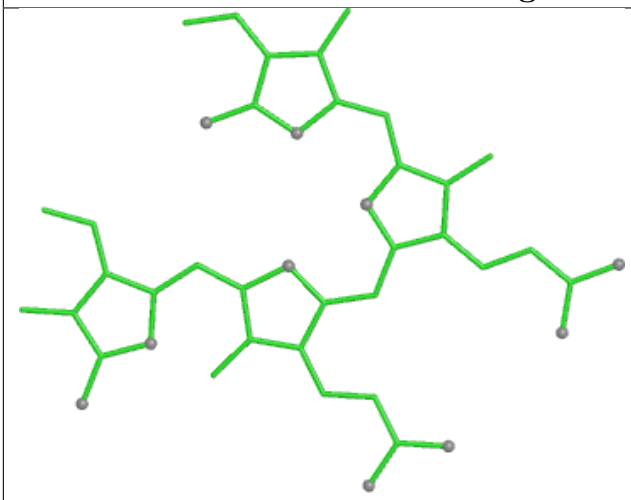


Rings

Ligand PEB h1 203



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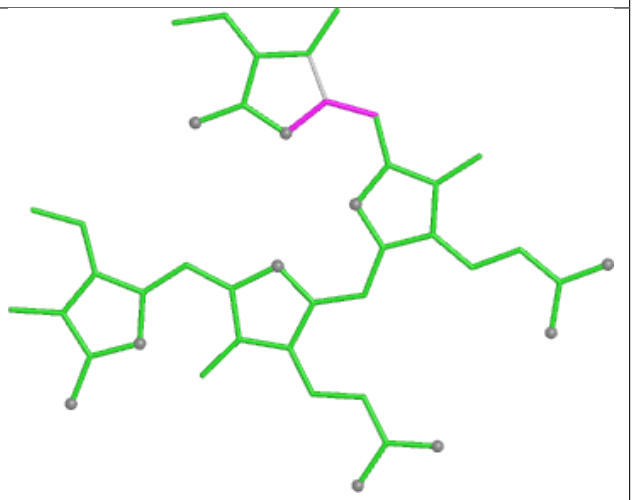
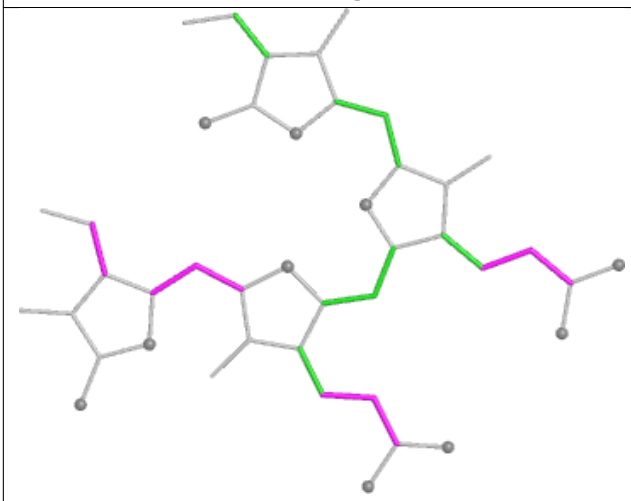


Bond angles



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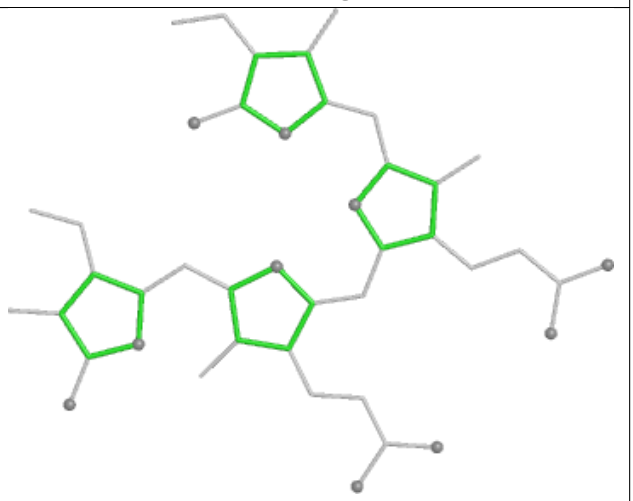
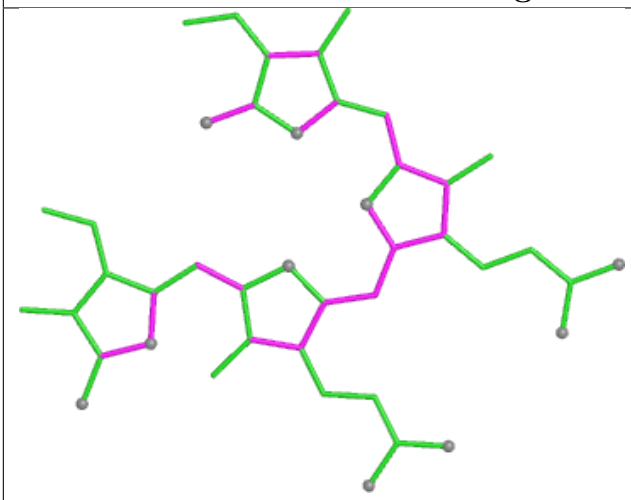


Rings

Ligand PEB xK 302



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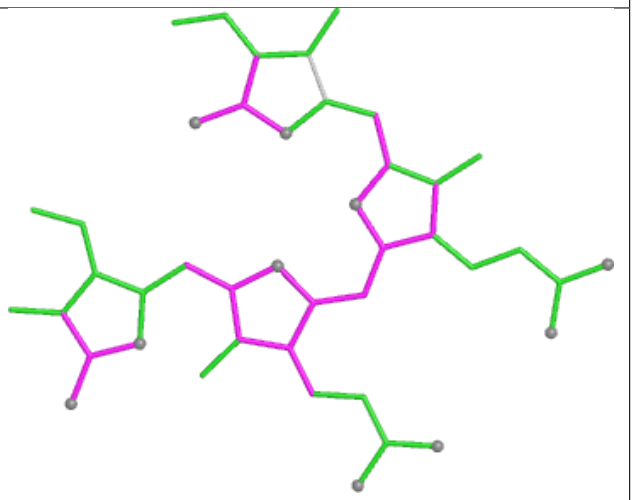

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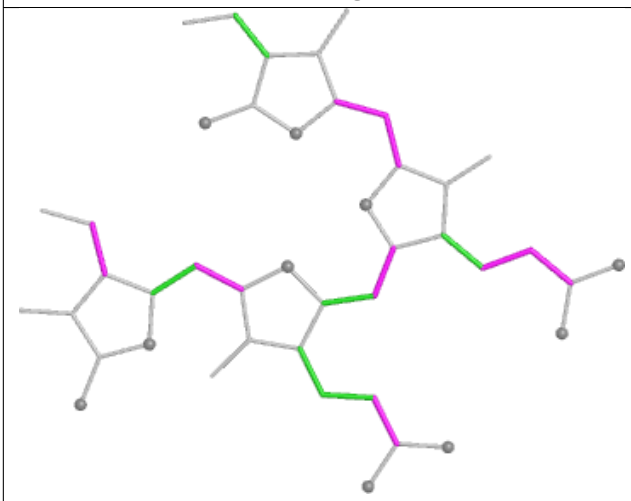

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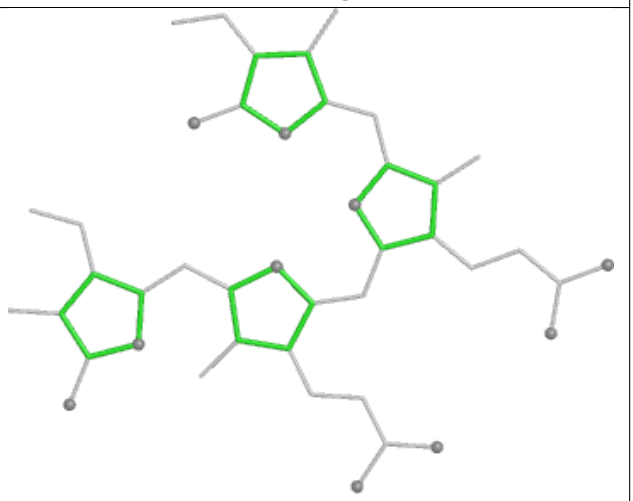
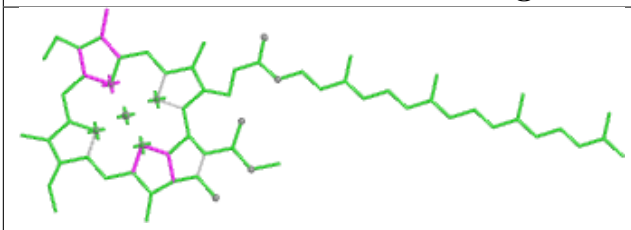


Rings

Ligand CLA B2 836



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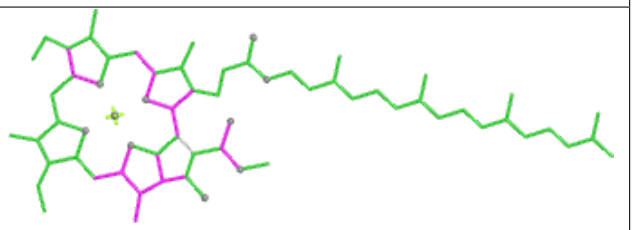

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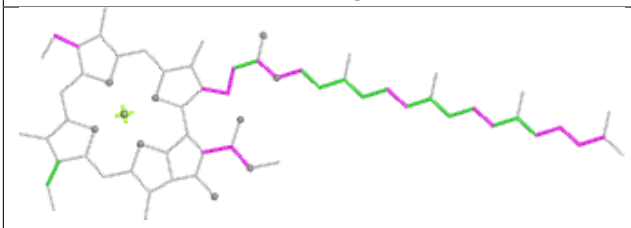

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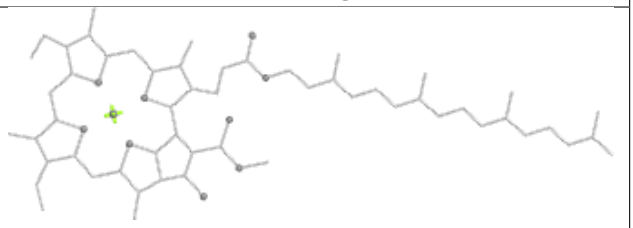
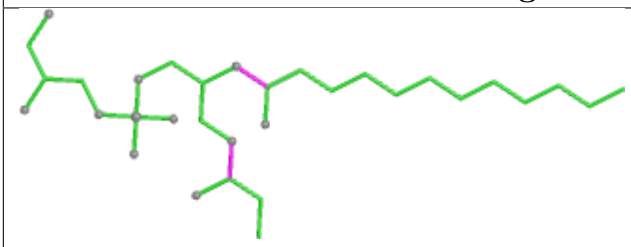


Rings

Ligand LHG c6 619



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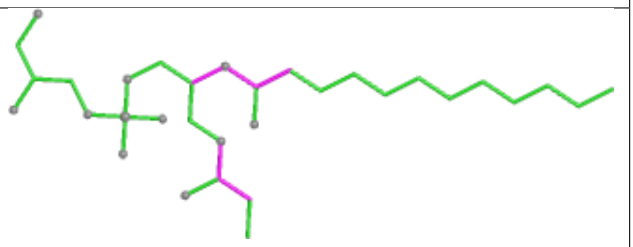

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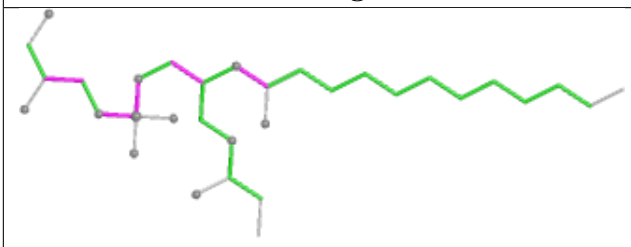

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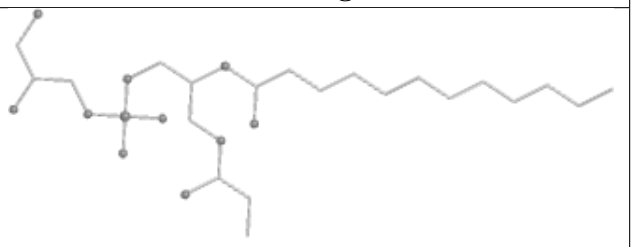
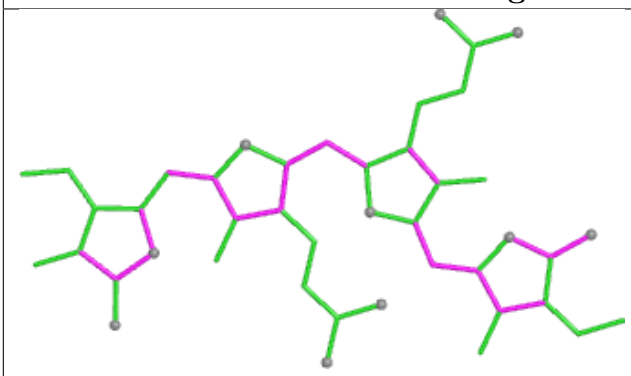


Rings

Ligand CYC J3 1001



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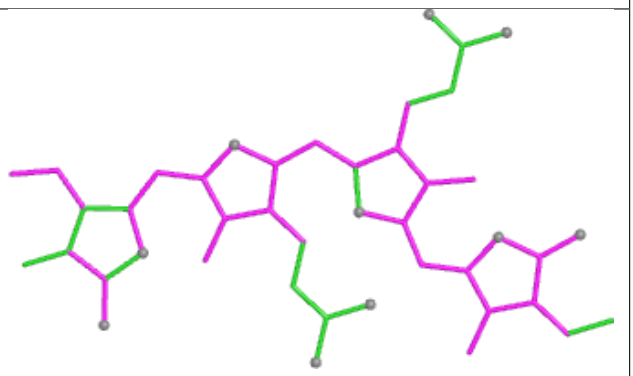
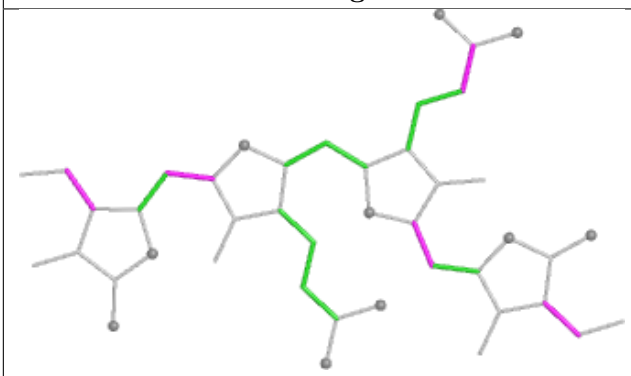


Bond angles



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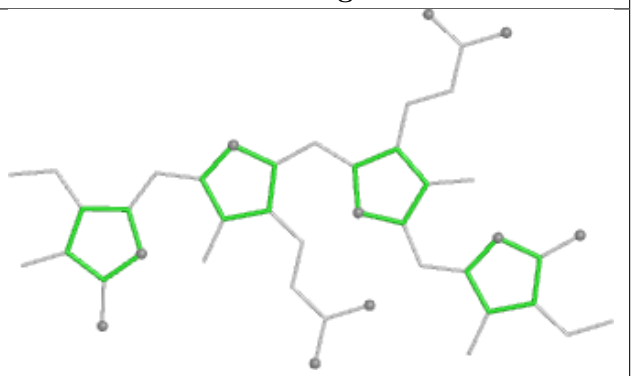
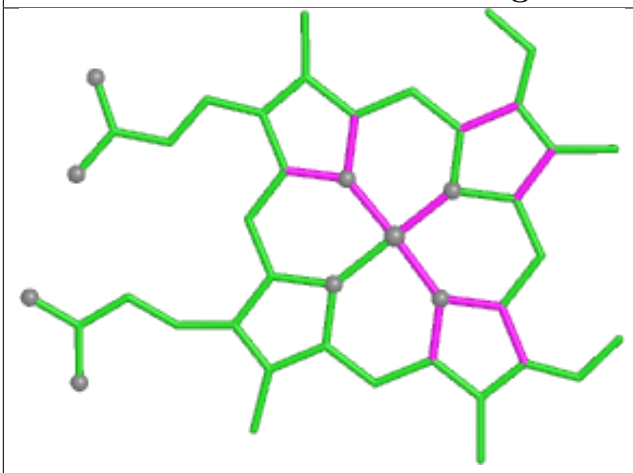


Rings

Ligand HEM vL 201



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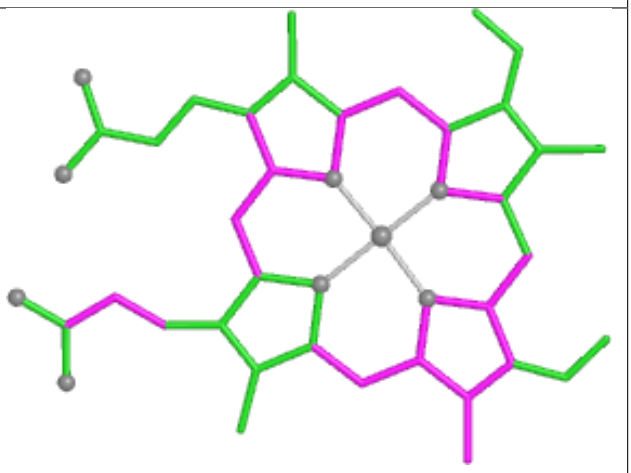
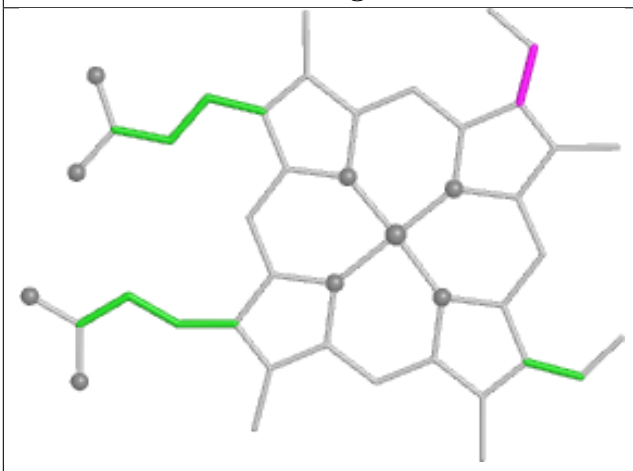


Bond angles



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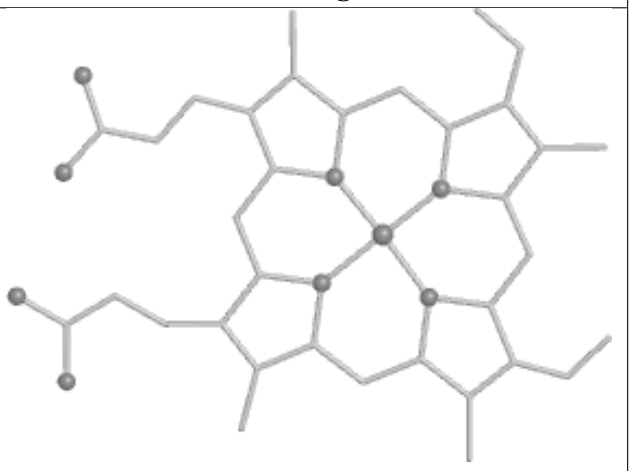
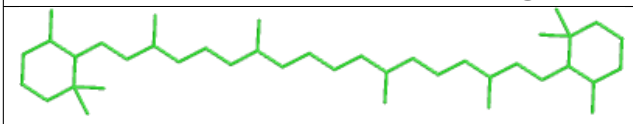


Rings

Ligand BCR fL 101



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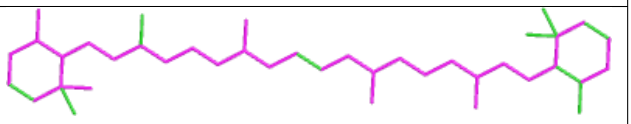
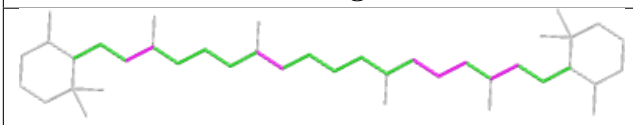


Bond angles



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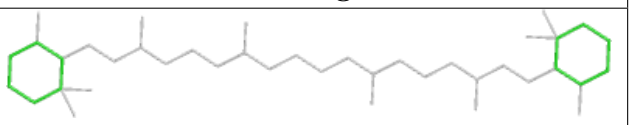
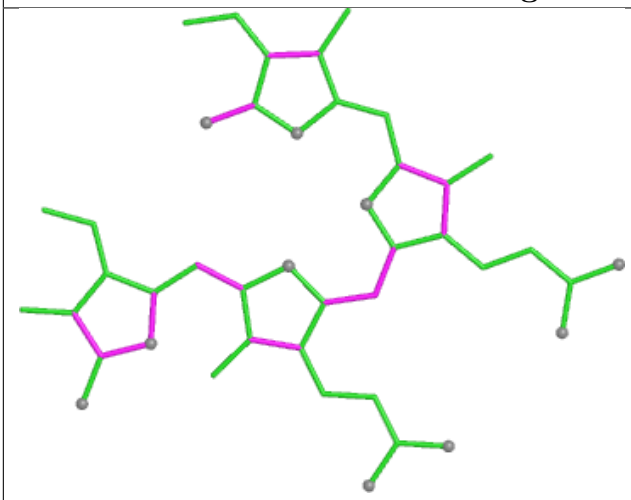


Rings

Ligand PEB c4 201



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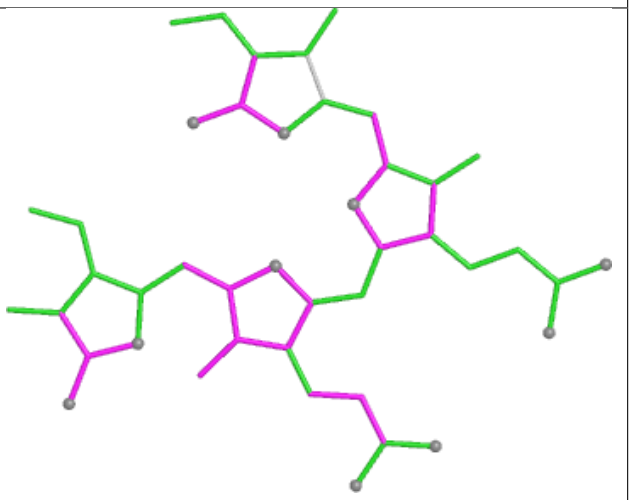
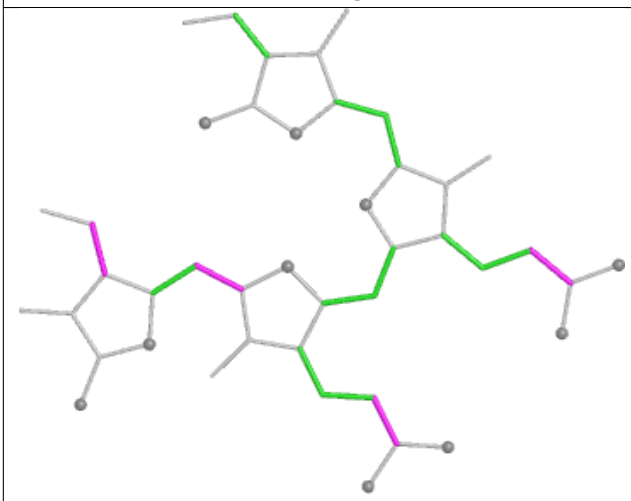


Bond angles



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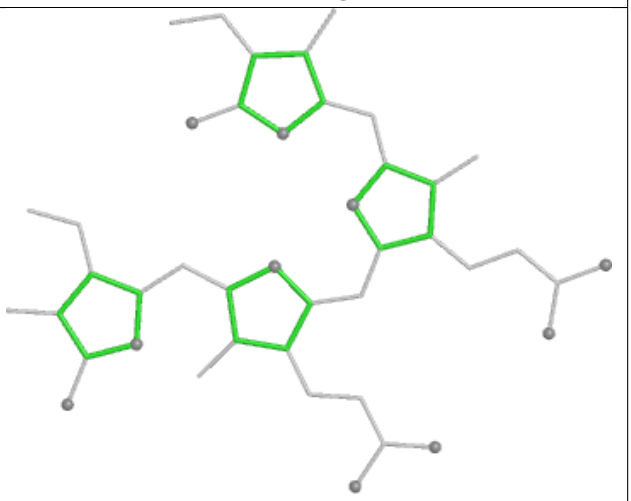
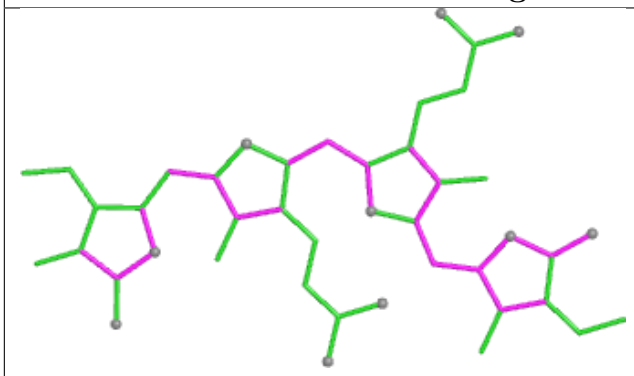
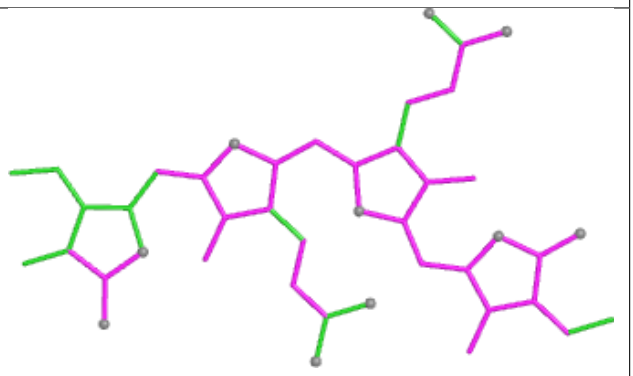


Rings

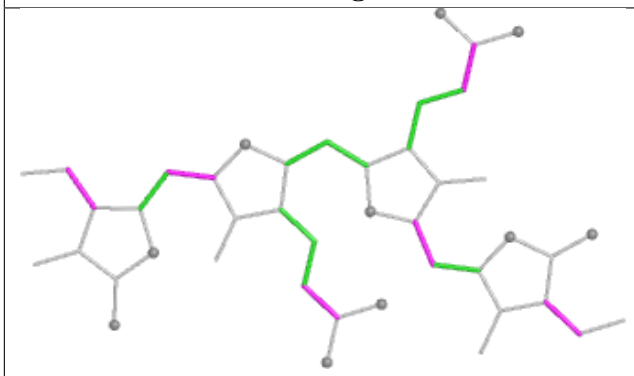
Ligand CYC J4 1001



Bond lengths



Bond angles



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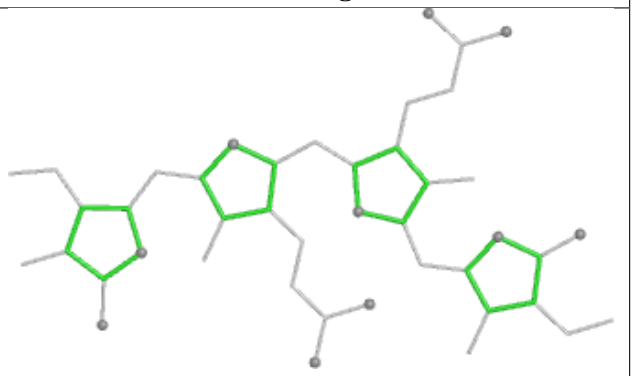
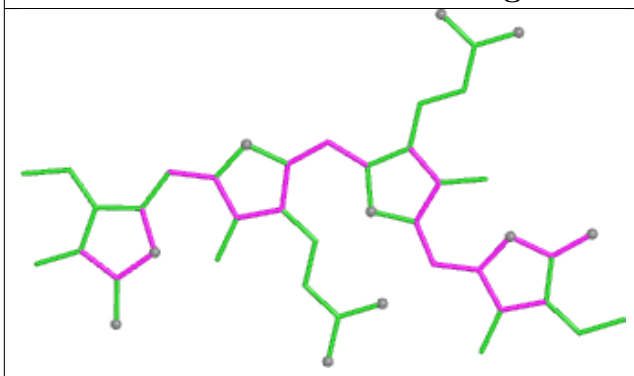
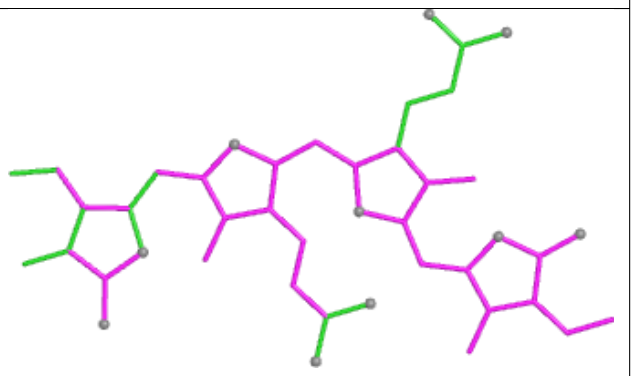


Rings

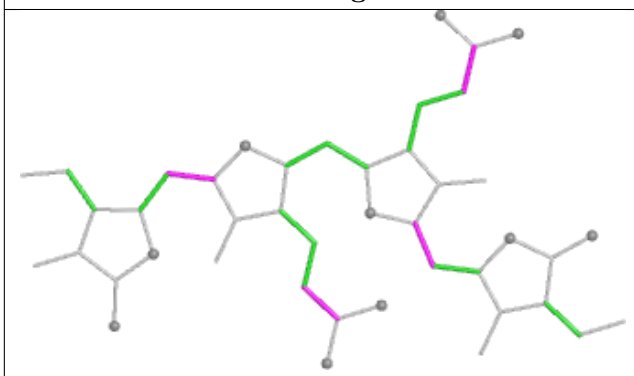
Ligand CYC JH 1001



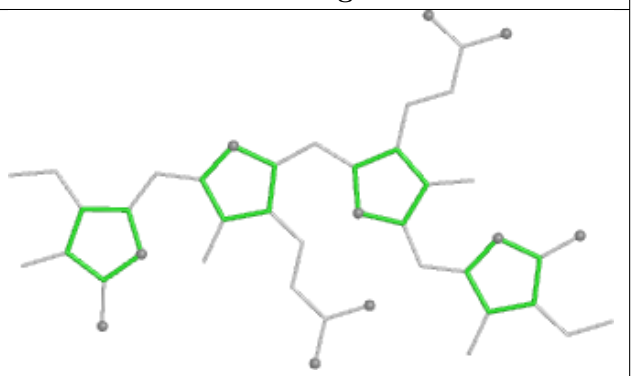
Bond lengths



Bond angles

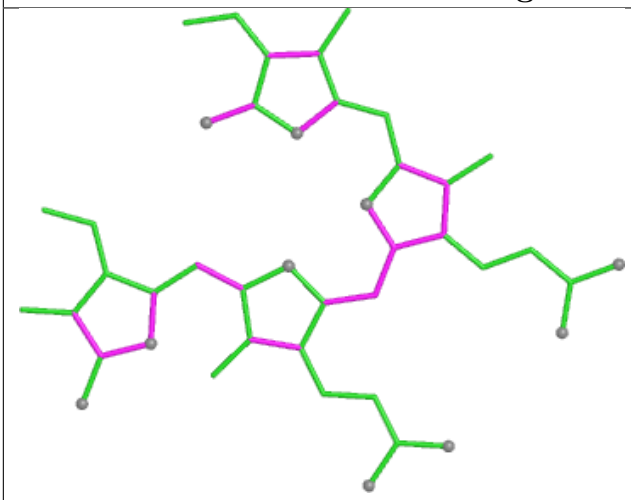


Torsions



Rings

Ligand PEB T9 201



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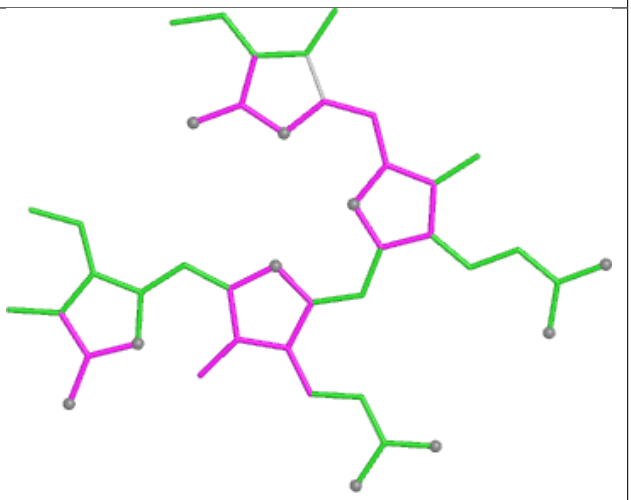

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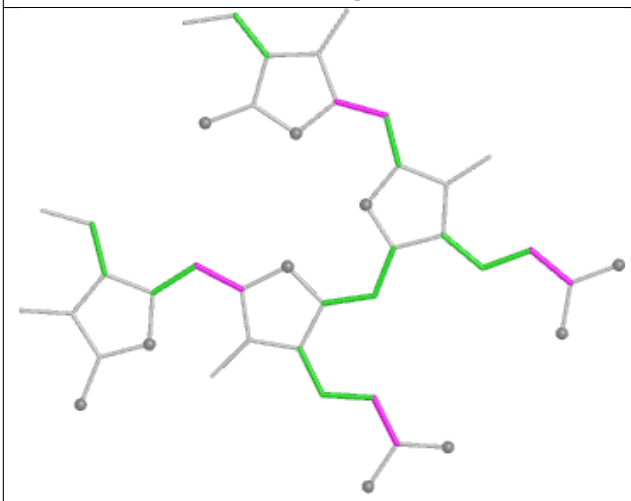

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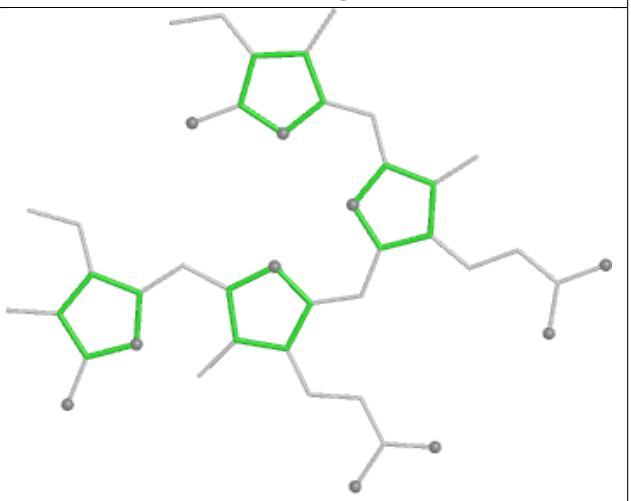
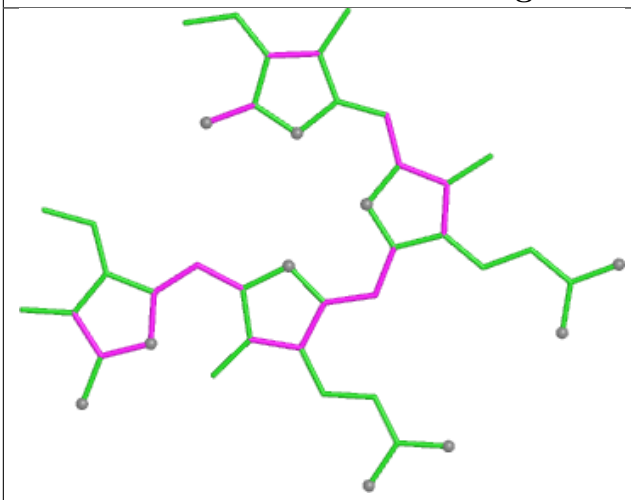


Rings

Ligand PEB eK 201



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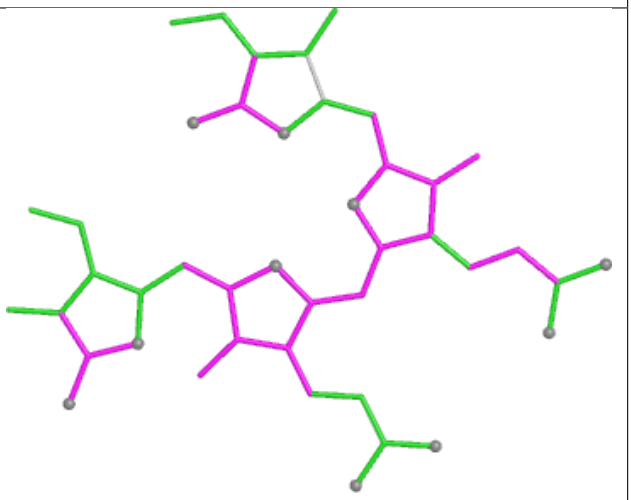

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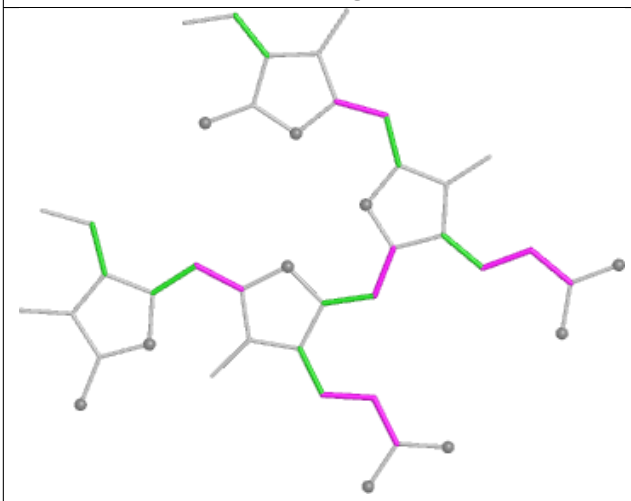

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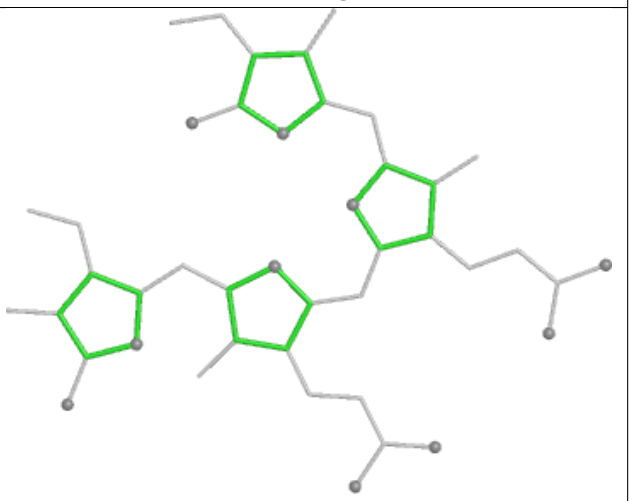
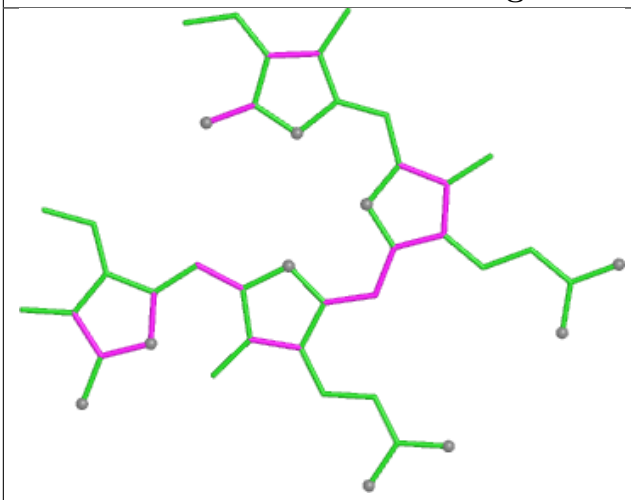


Rings

Ligand PEB GM 201



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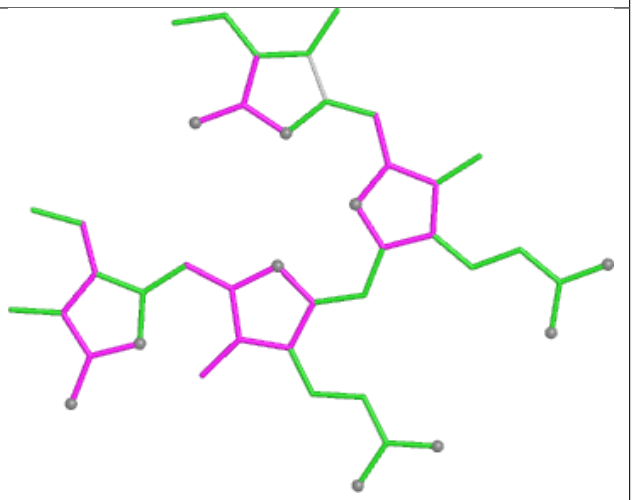

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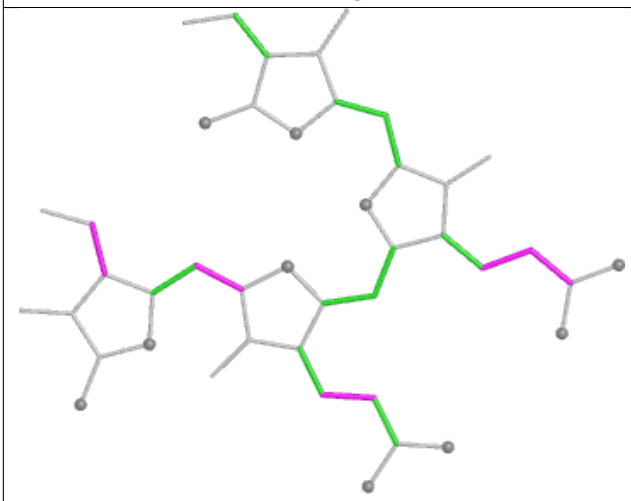

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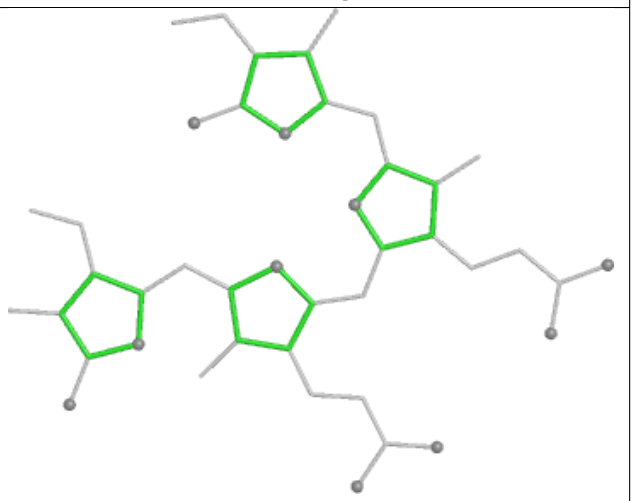
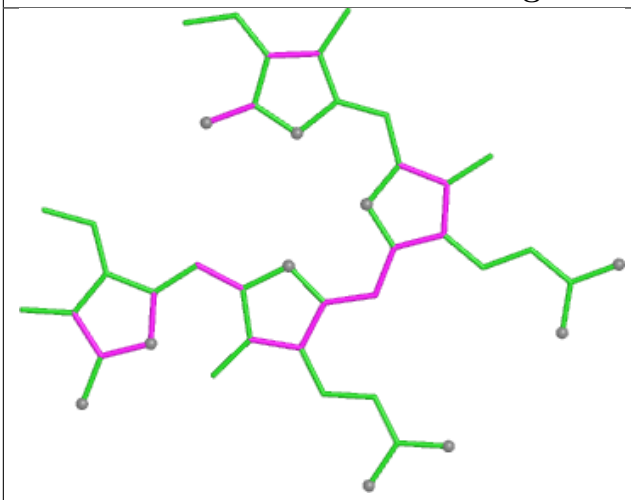


Rings

Ligand PEB jJ 203



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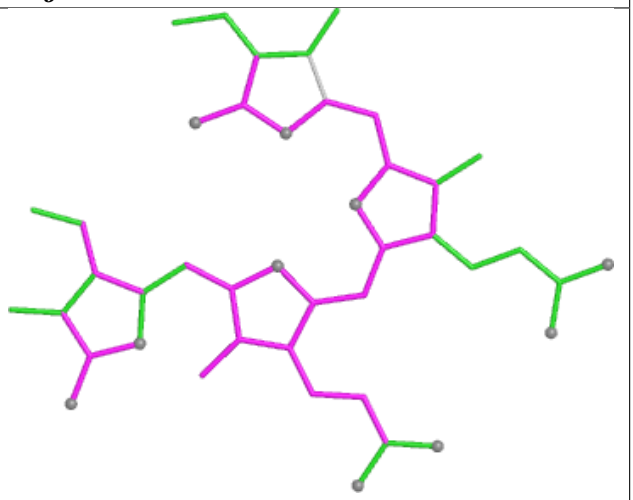

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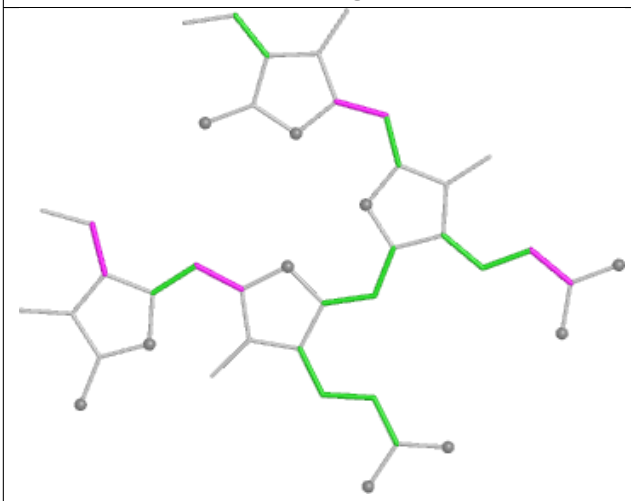

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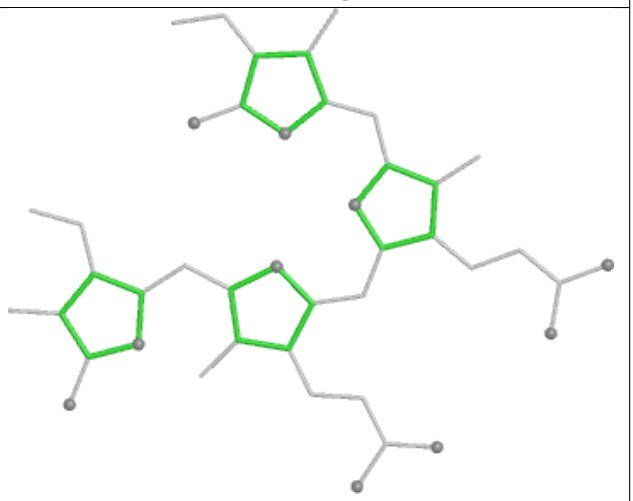

Rings

Ligand BCR b6 602



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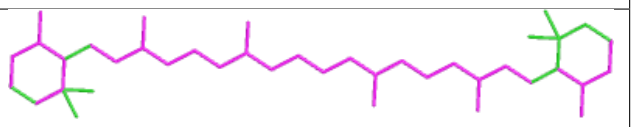

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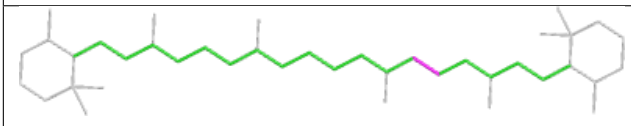

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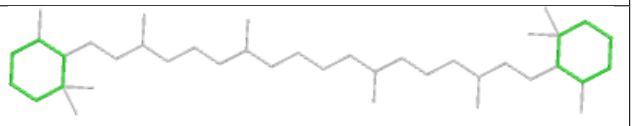
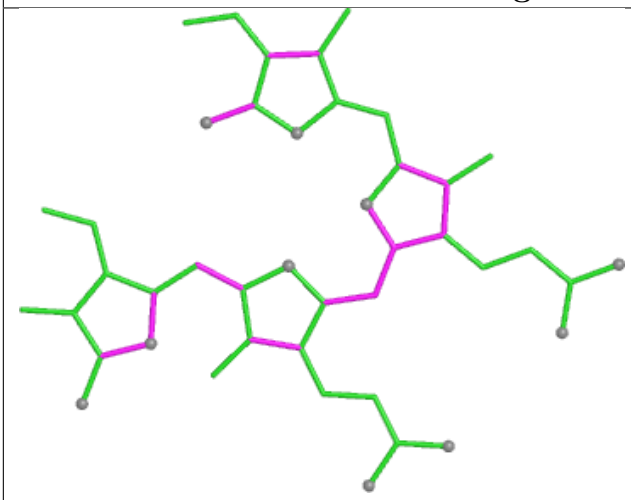


Rings

Ligand PEB wF 302



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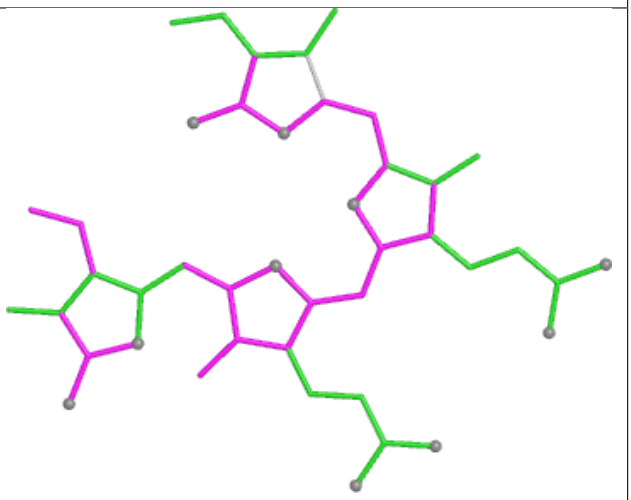
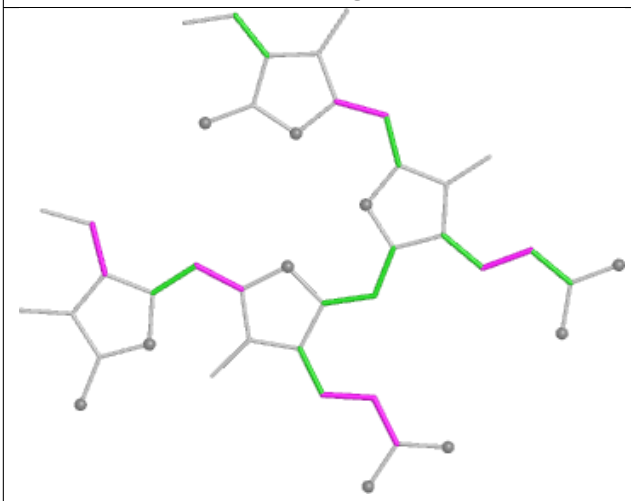


Bond angles



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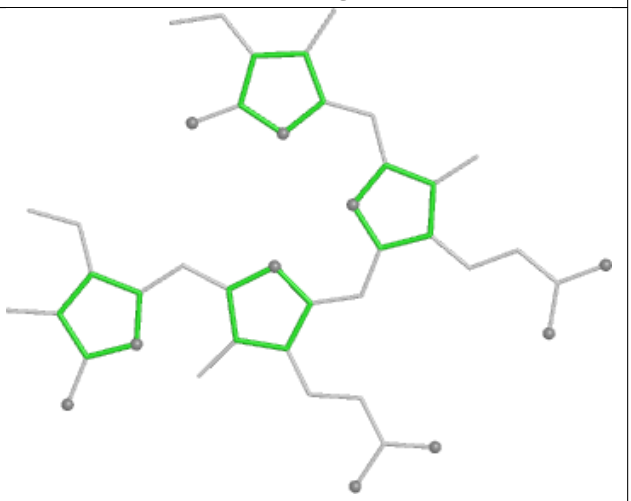
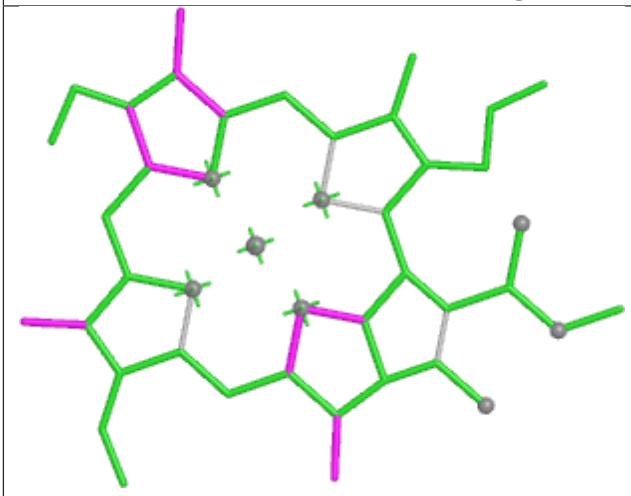


Rings

Ligand CLA BN 821



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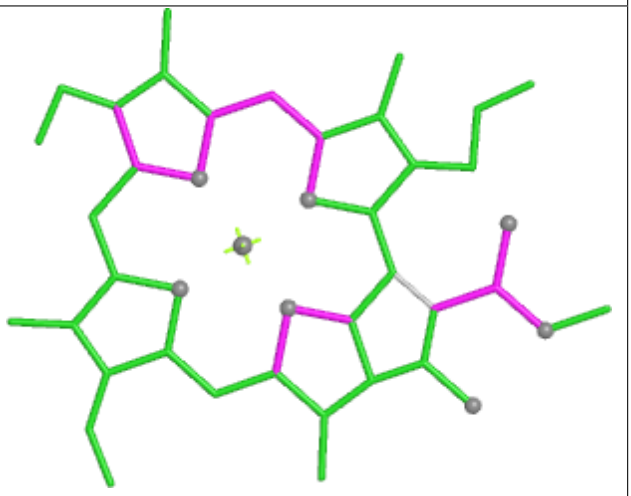

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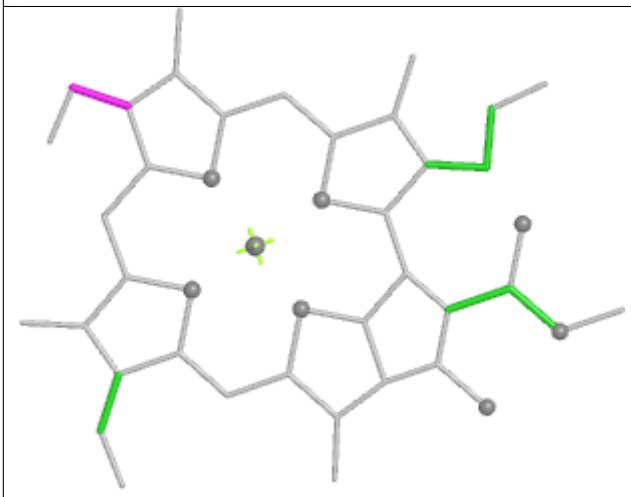

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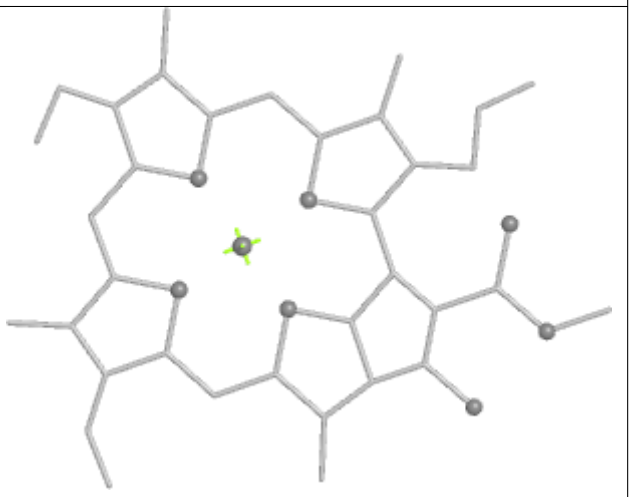
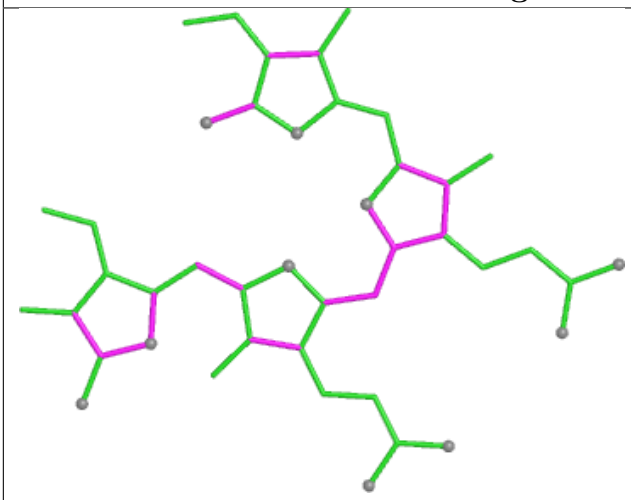


Rings

Ligand PEB XA 201



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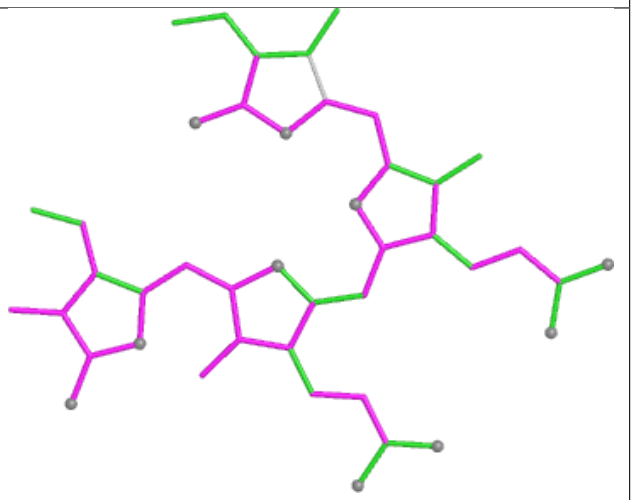

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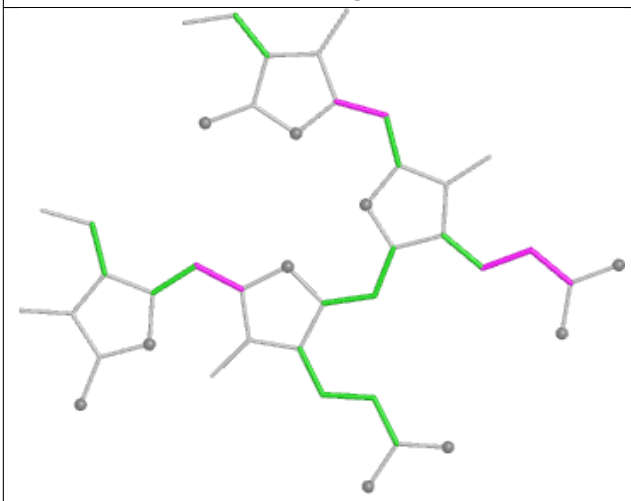

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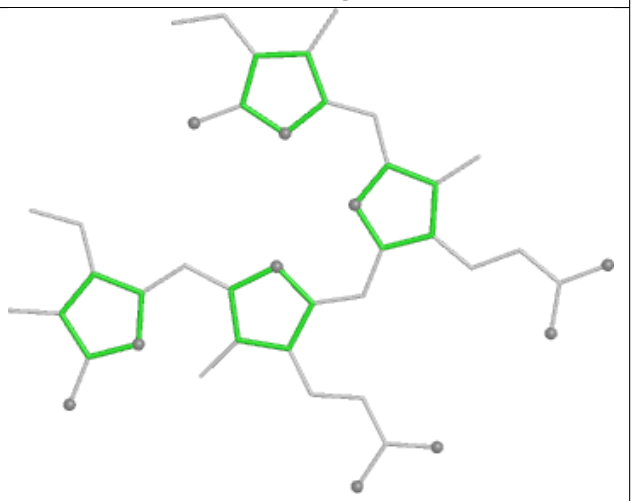
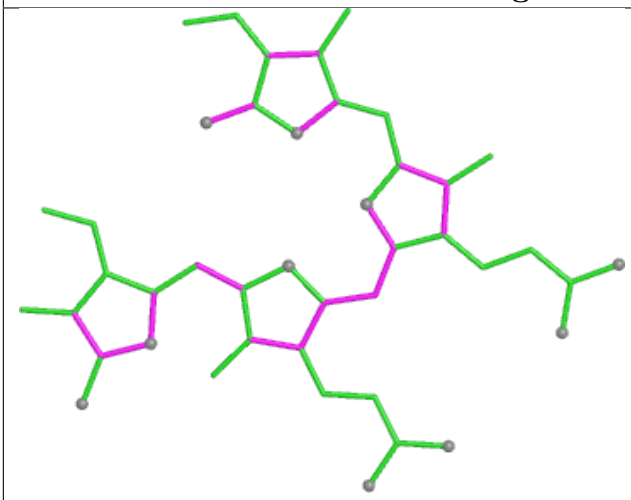


Rings

Ligand PEB QP 202



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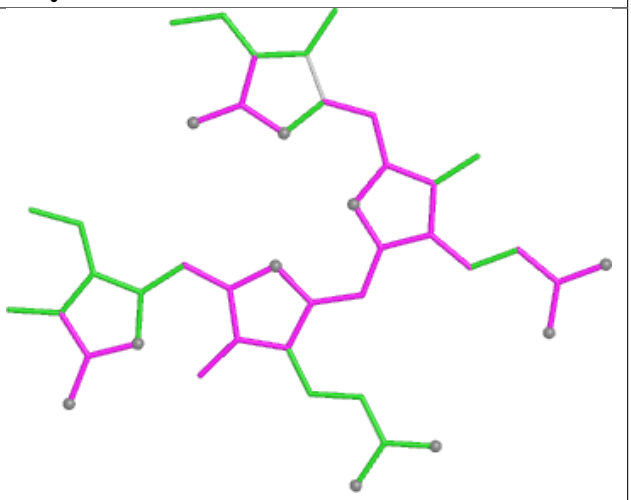

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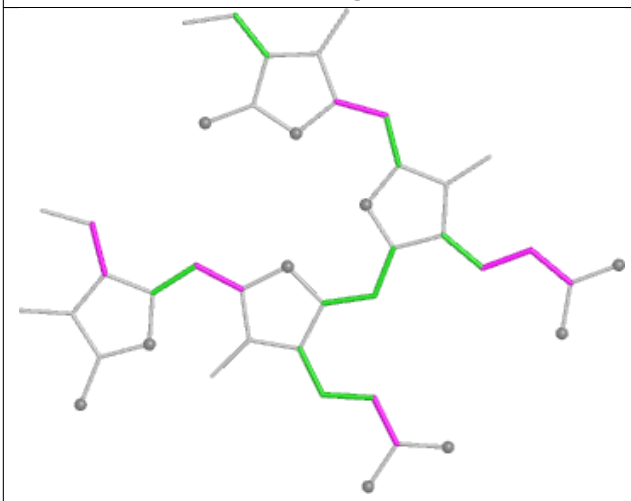

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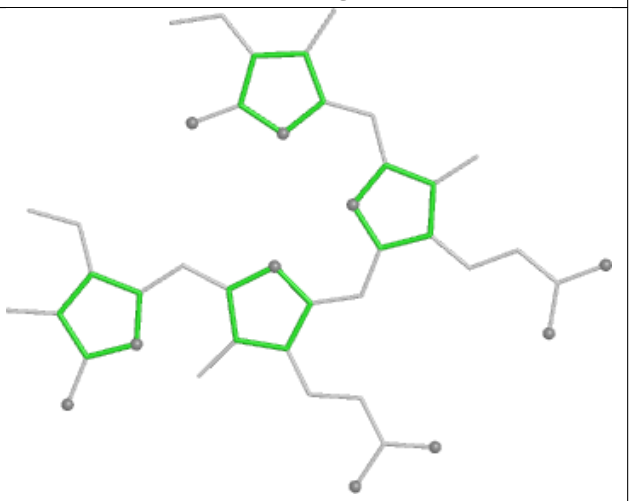
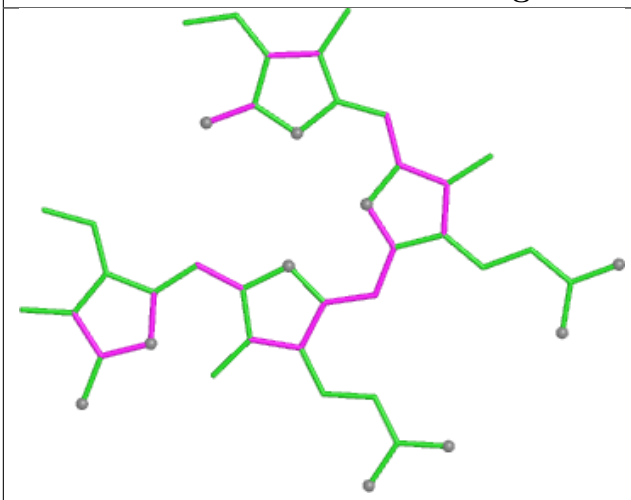


Rings

Ligand PEB CP 201



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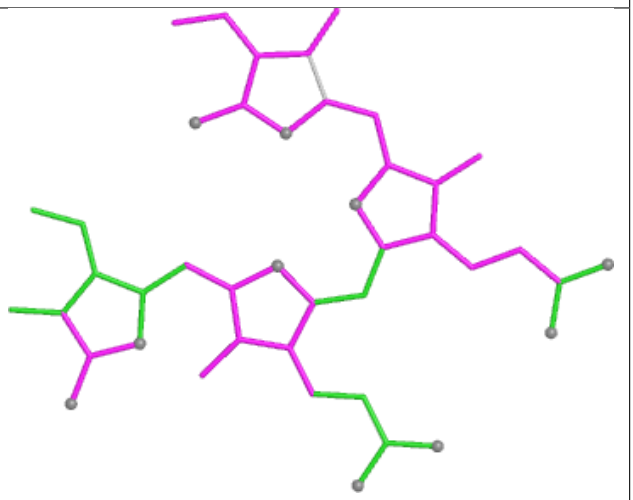
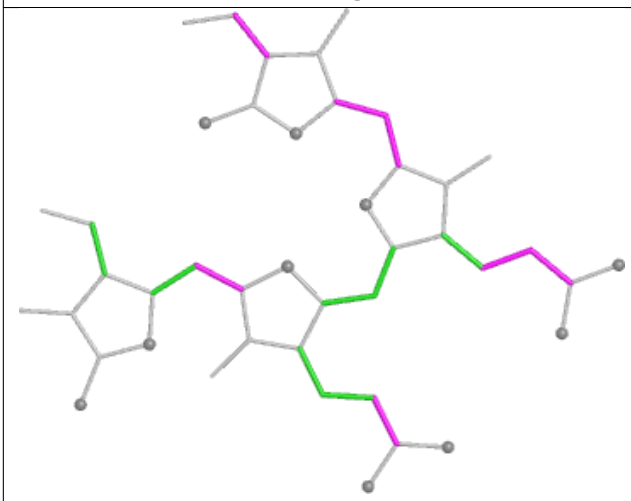


Bond angles



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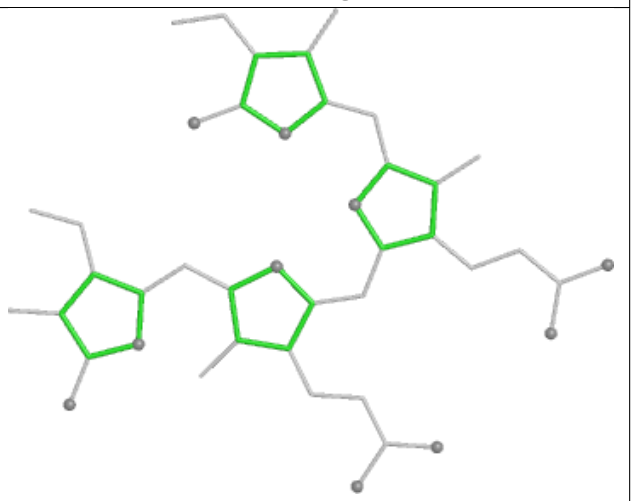
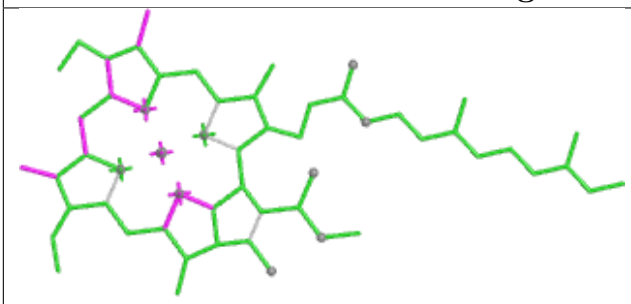
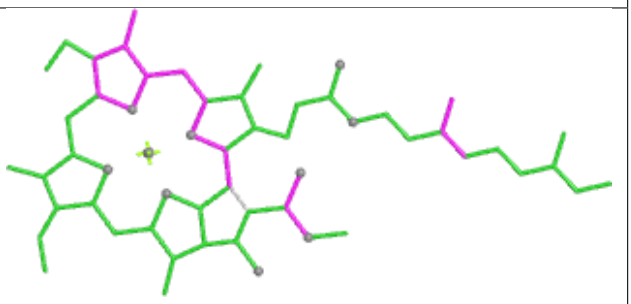
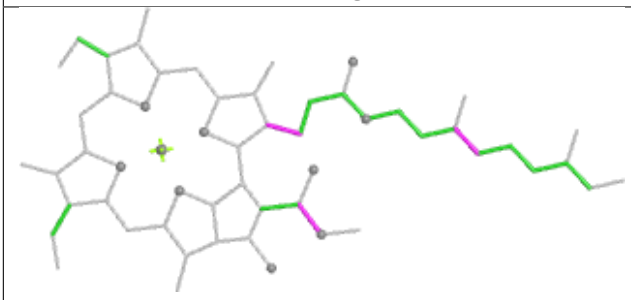
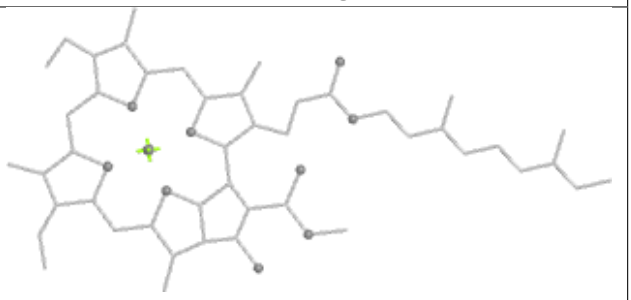
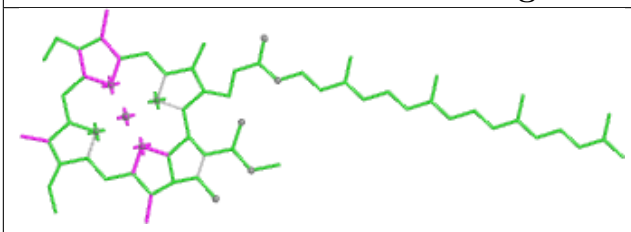
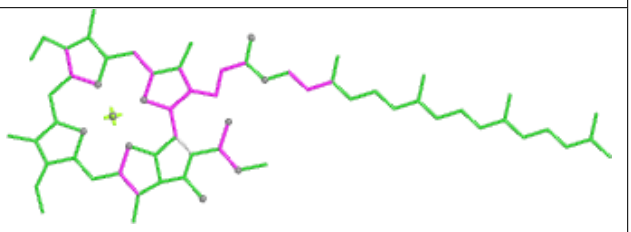
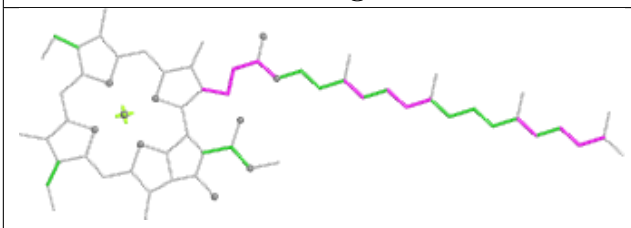
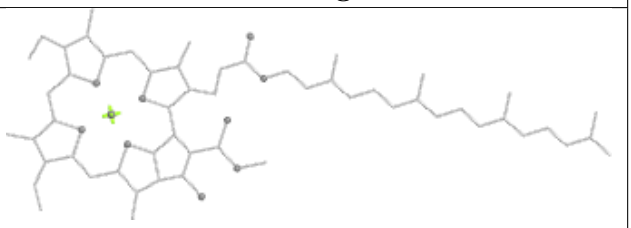
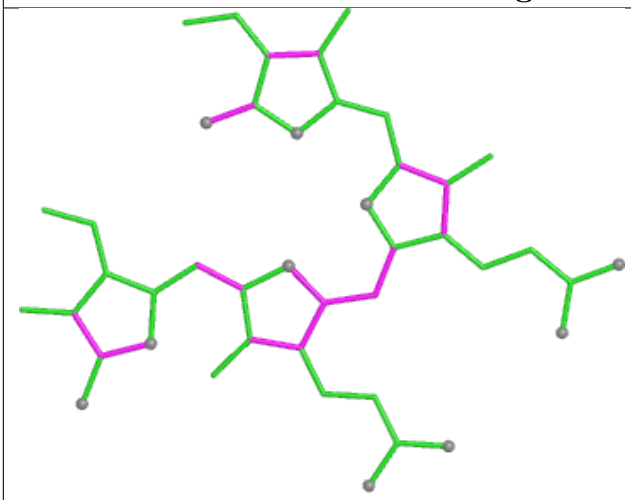


Rings

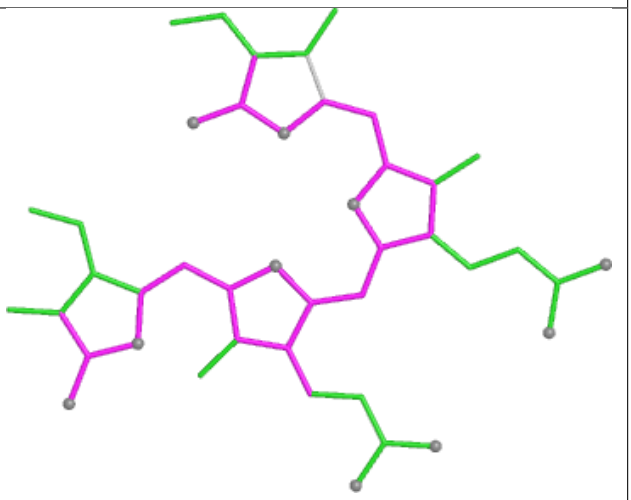
Ligand CLA L2 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b6 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

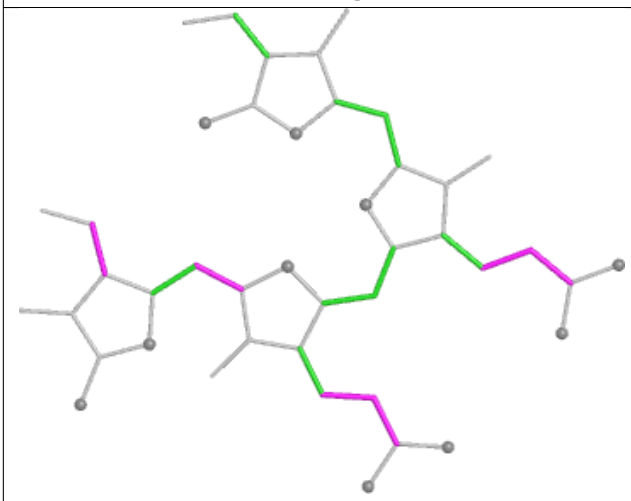
Ligand PEB R7 202



Bond lengths



Bond angles



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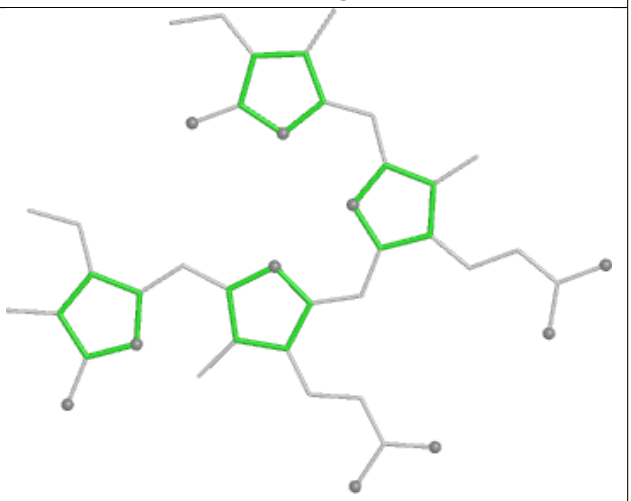
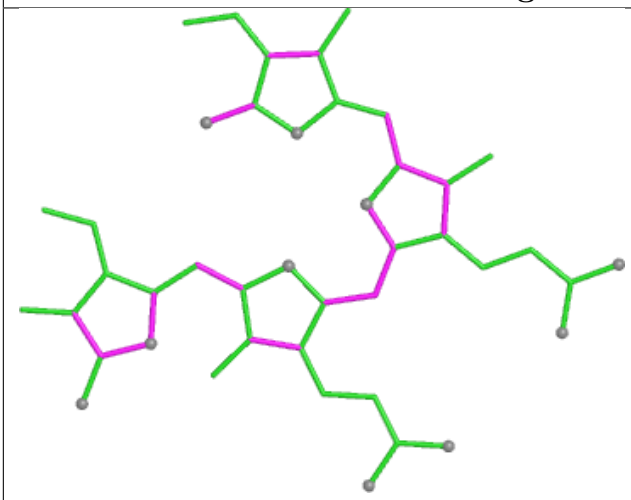


Rings

Ligand PEB JF 202



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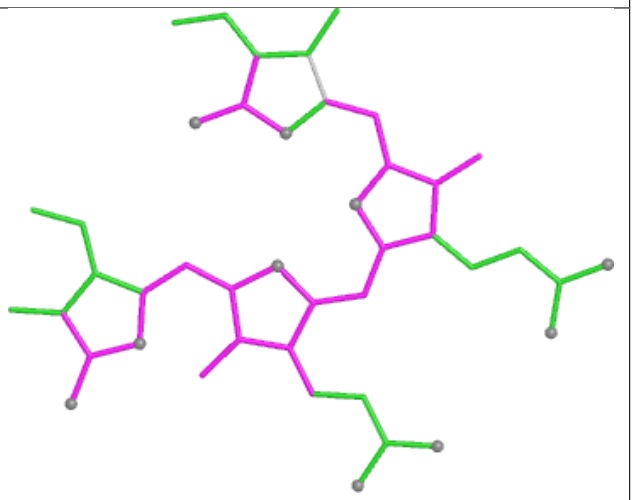
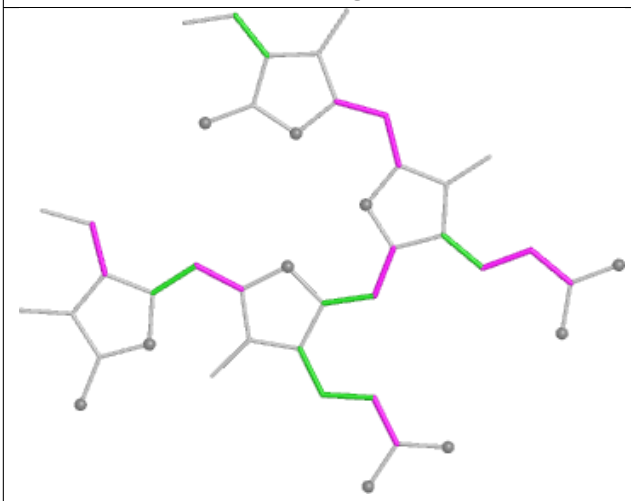


Bond angles



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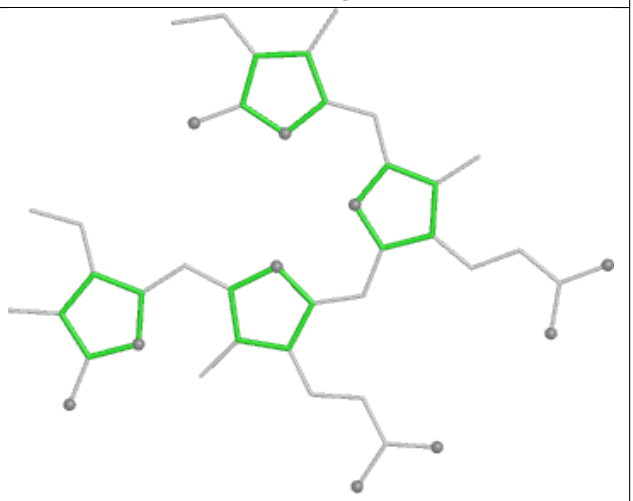
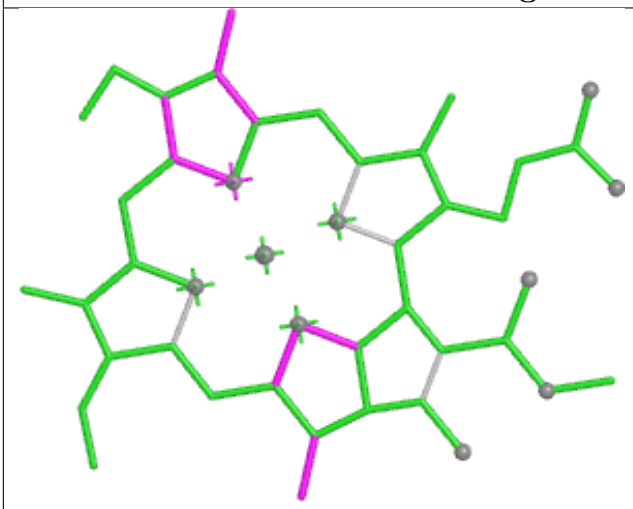
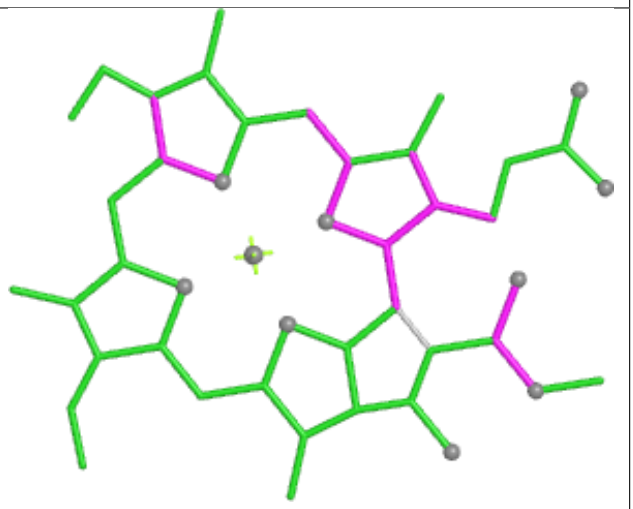


Rings

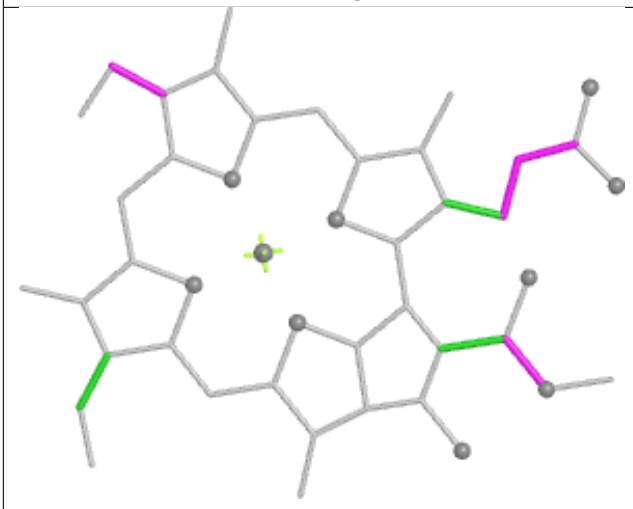
Ligand CLA 82 304



Bond lengths



Bond angles

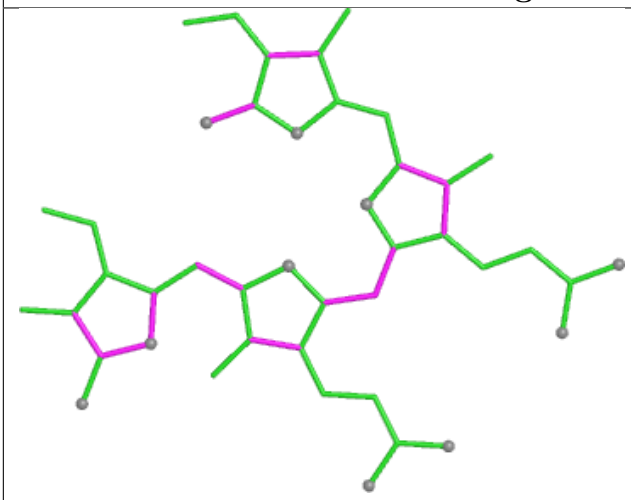


Torsions



Rings

Ligand PEB ZE 201



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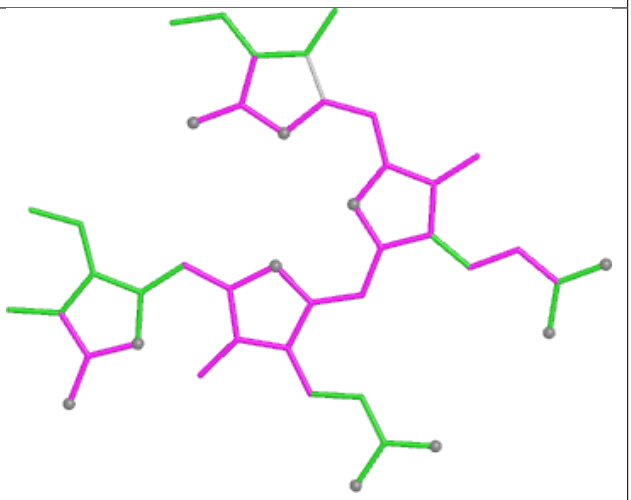

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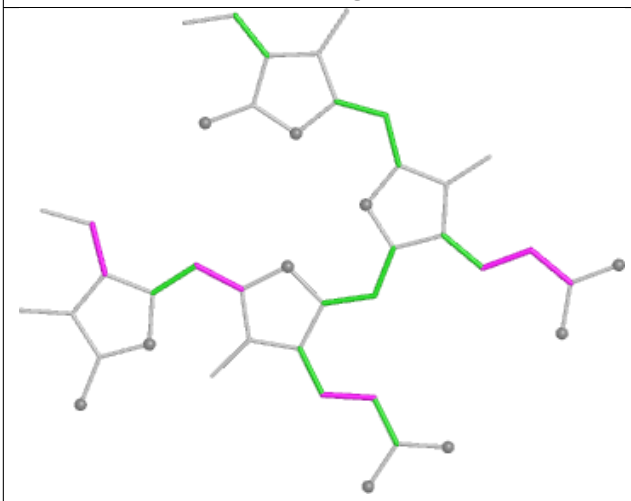

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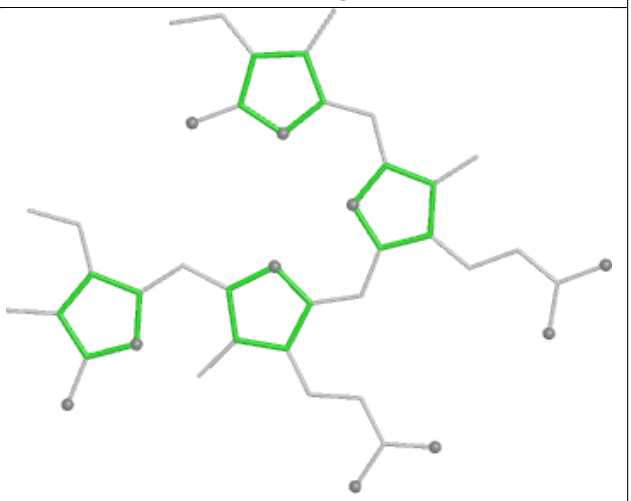
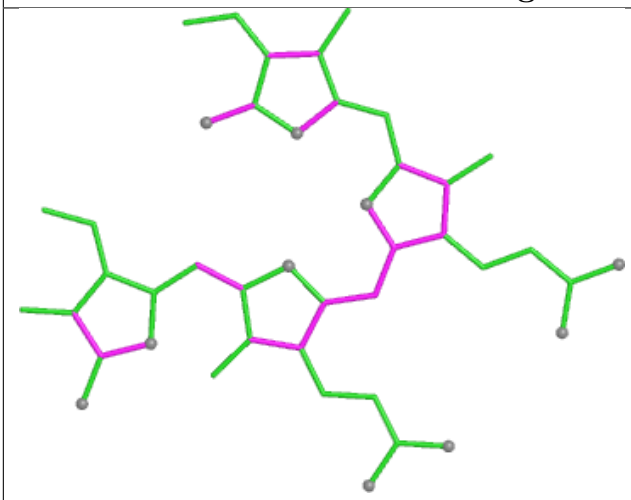


Rings

Ligand PEB tC 201



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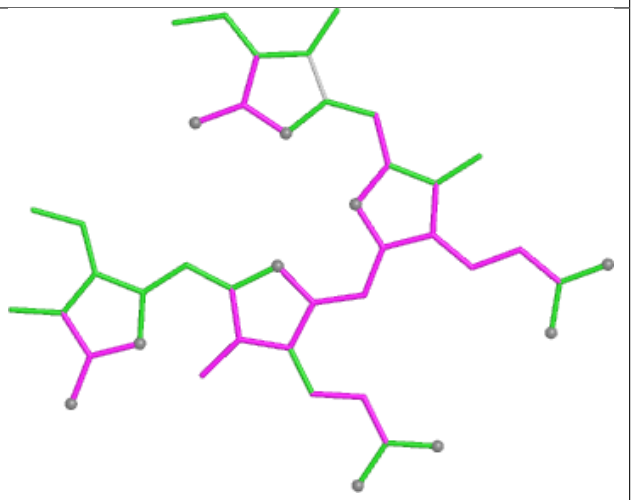

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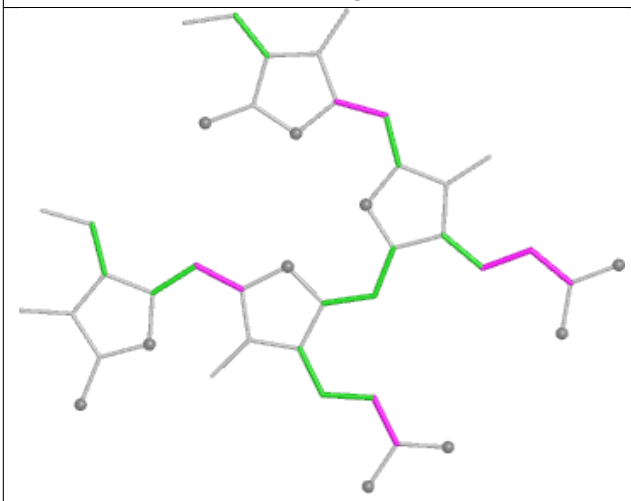

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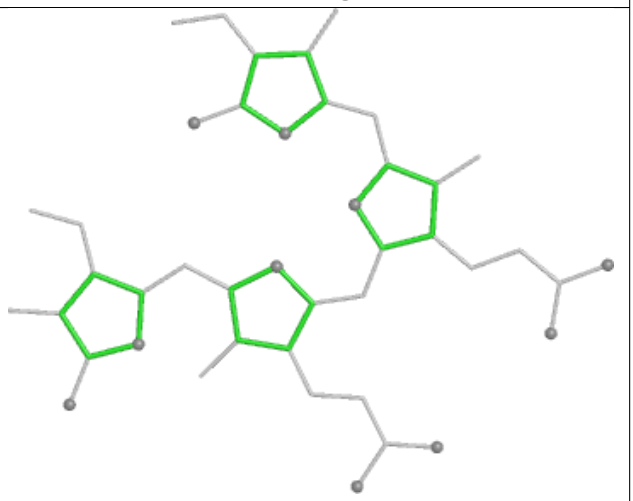
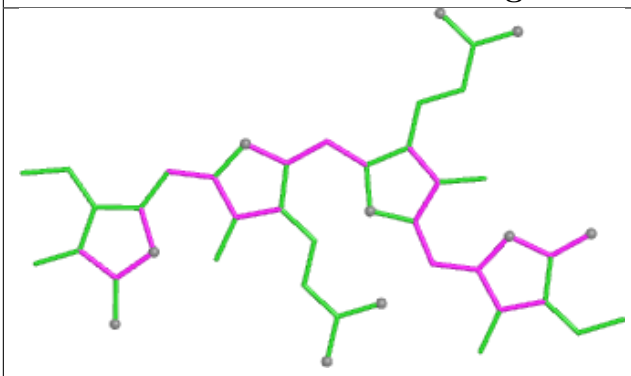


Rings

Ligand CYC E4 1001



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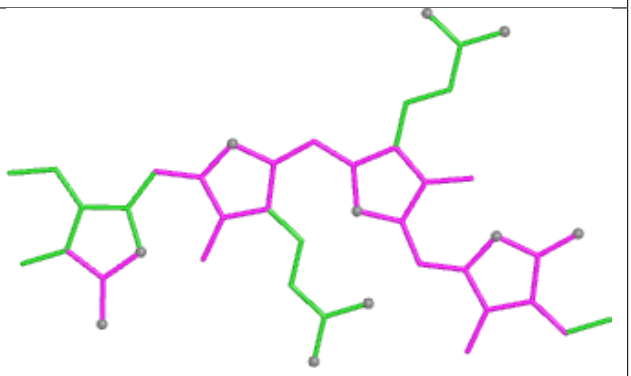

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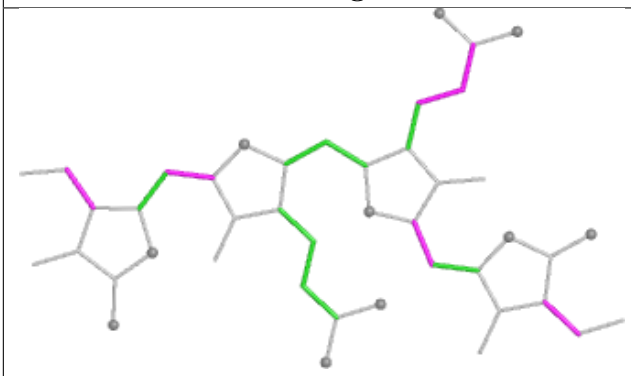

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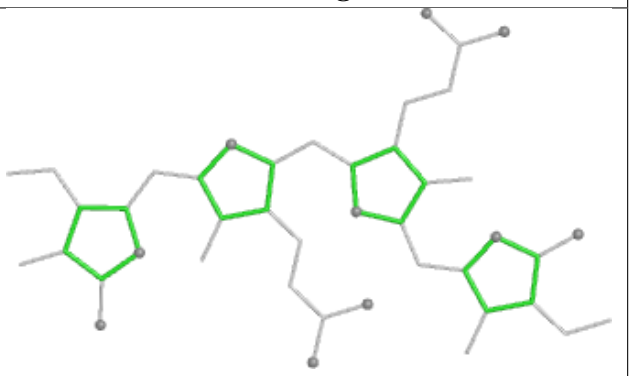
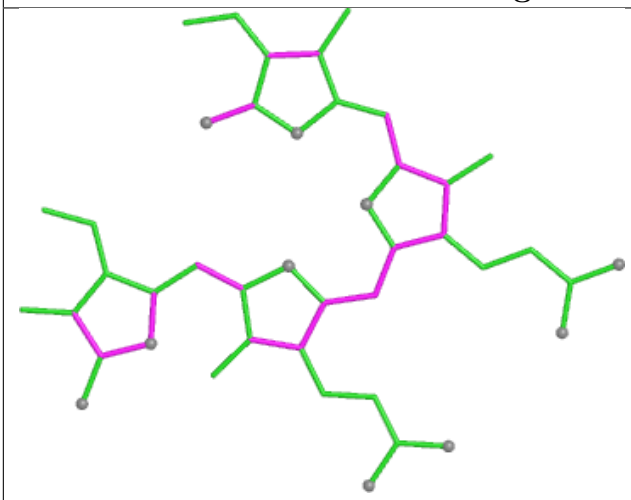


Rings

Ligand PEB hG 201



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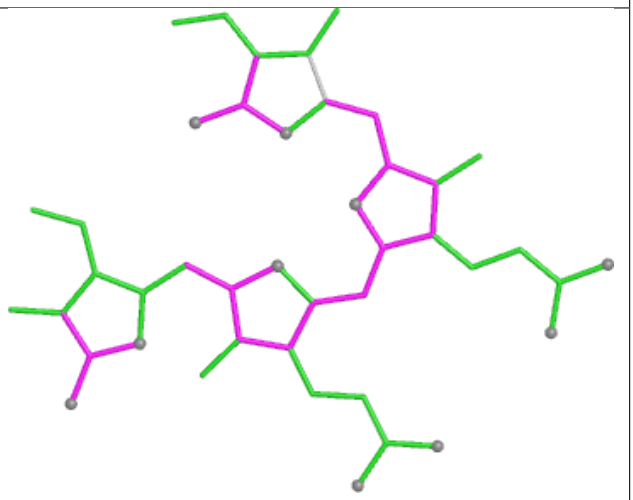

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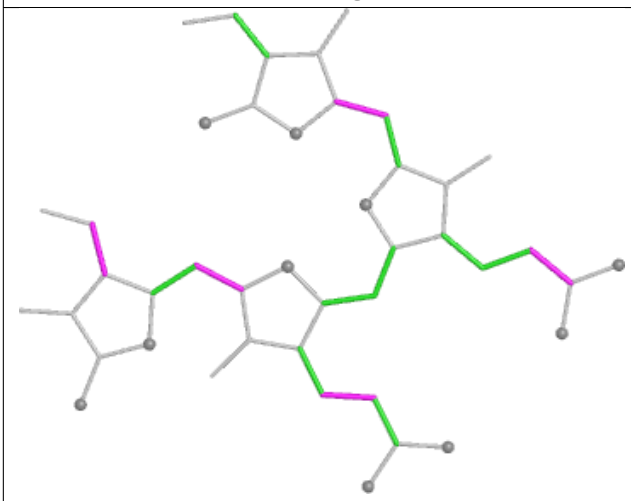

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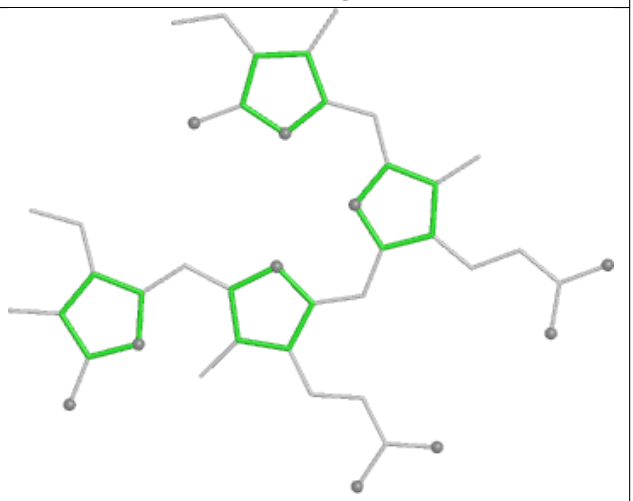
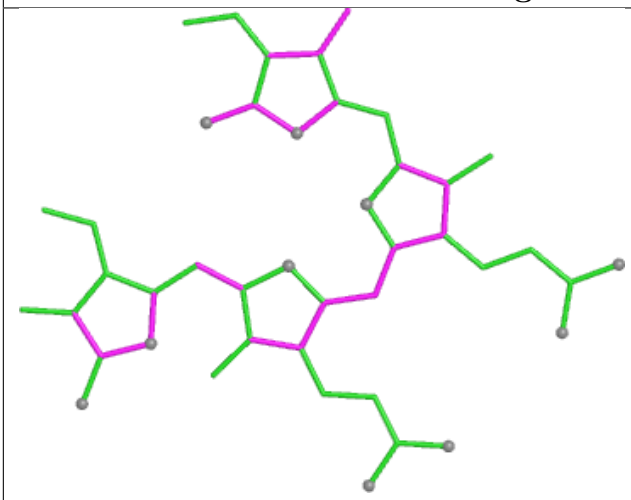


Rings

Ligand PEB H5 201



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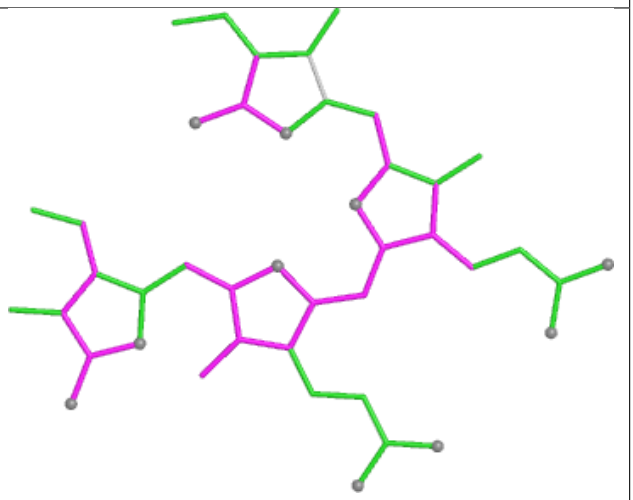

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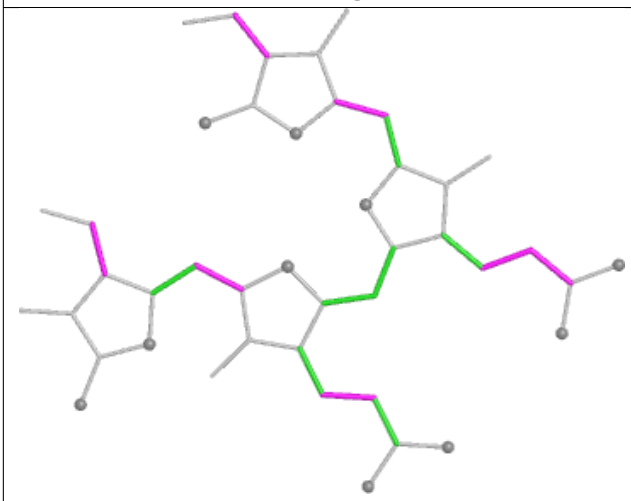

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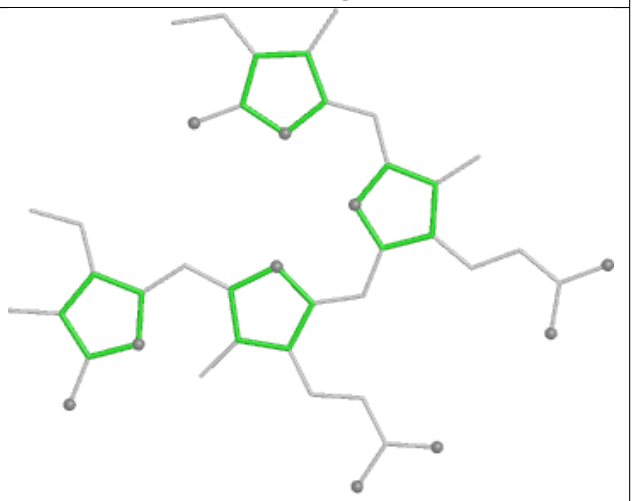
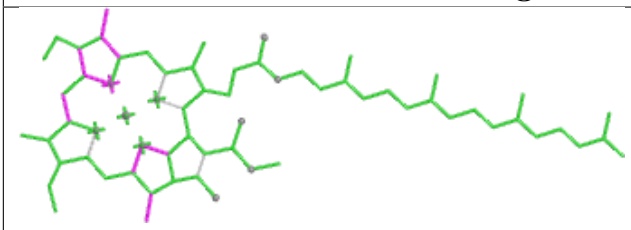


Rings

Ligand CLA C6 511



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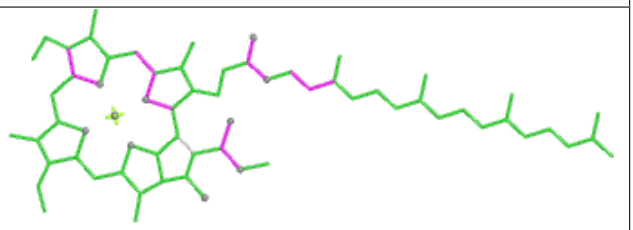

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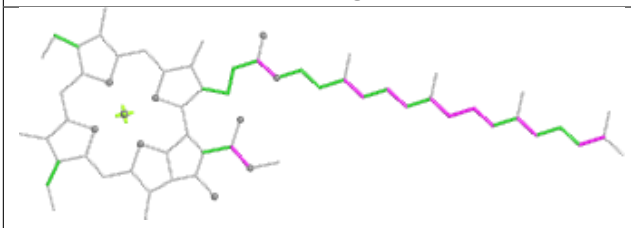

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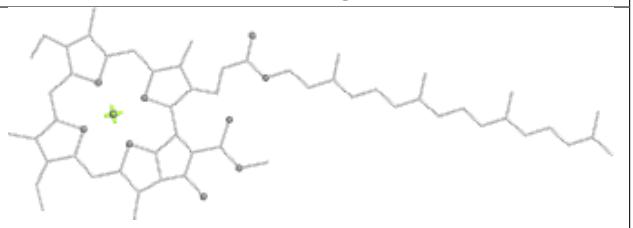
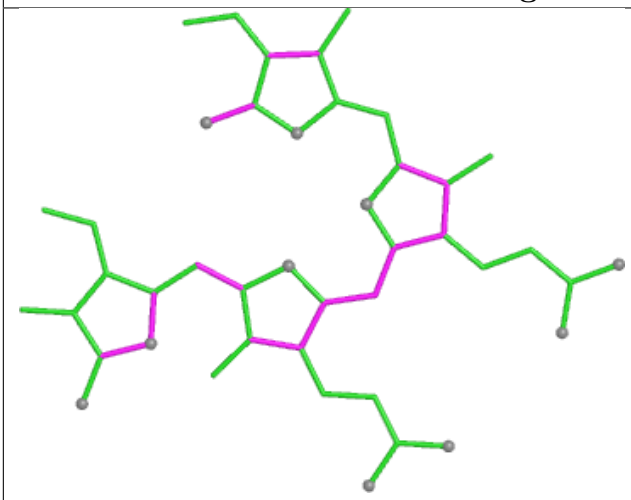


Rings

Ligand PEB 18 201



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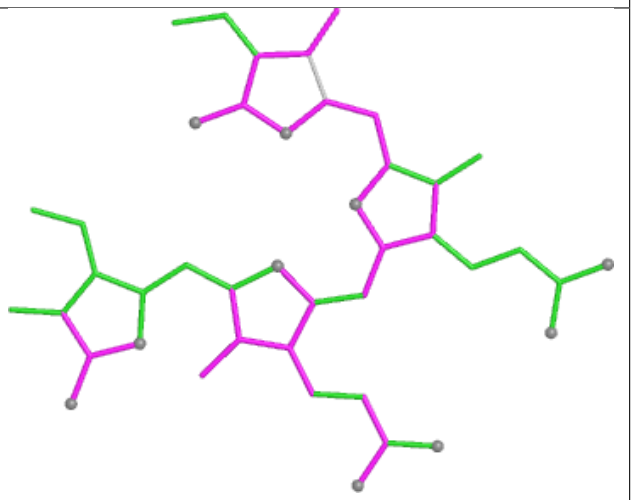

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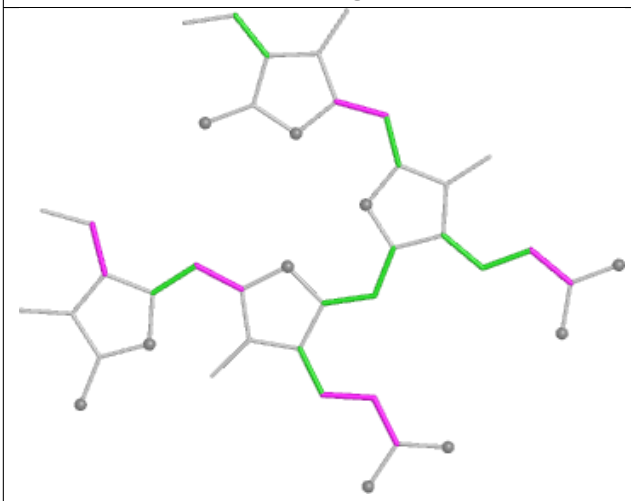

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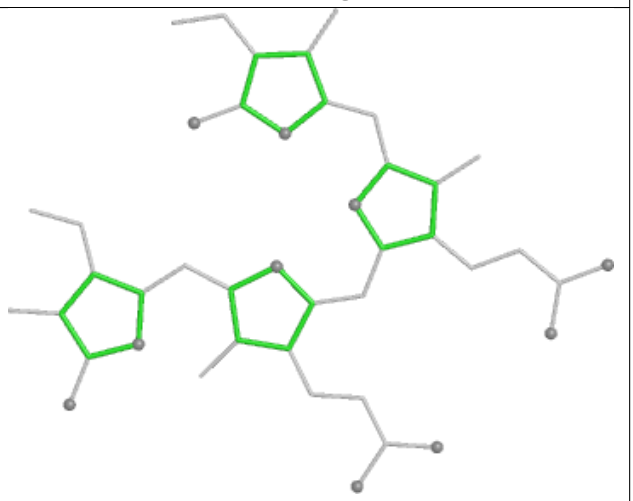
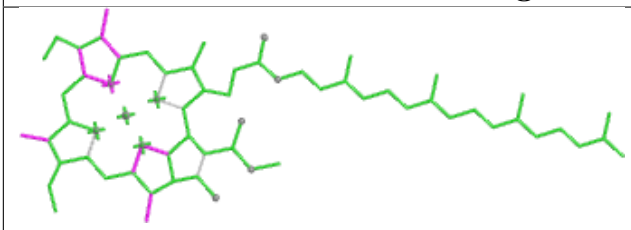


Rings

Ligand CLA B6 608



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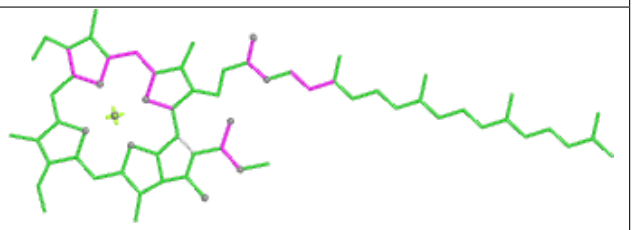

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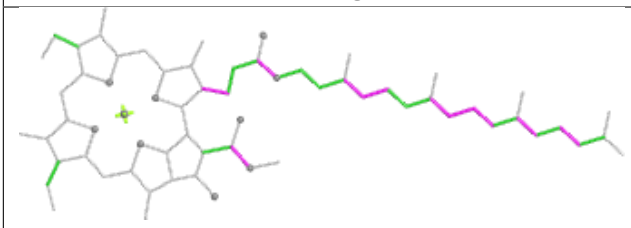

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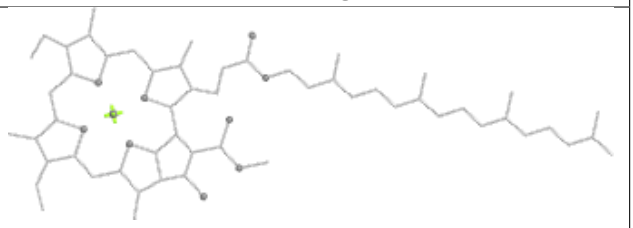
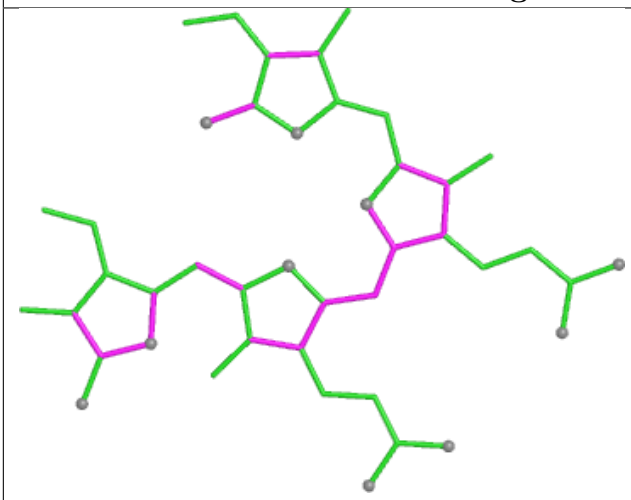


Rings

Ligand PEB YH 201



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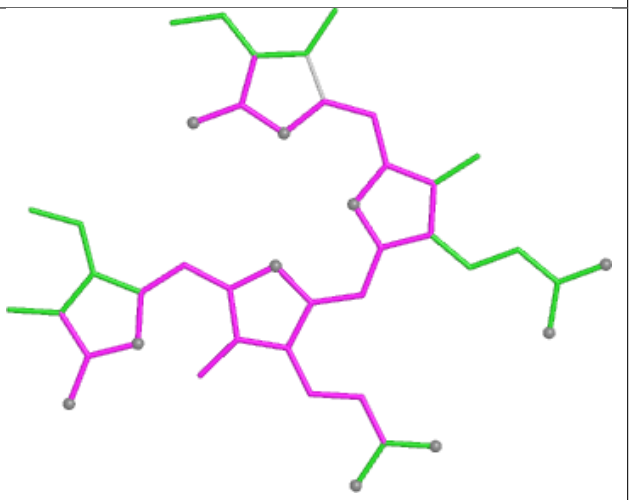

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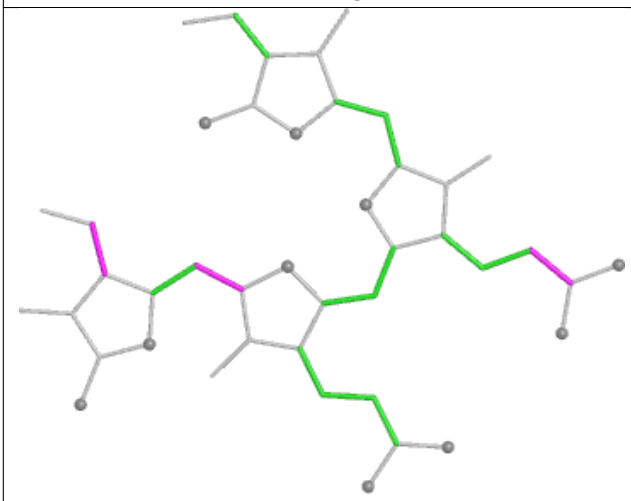

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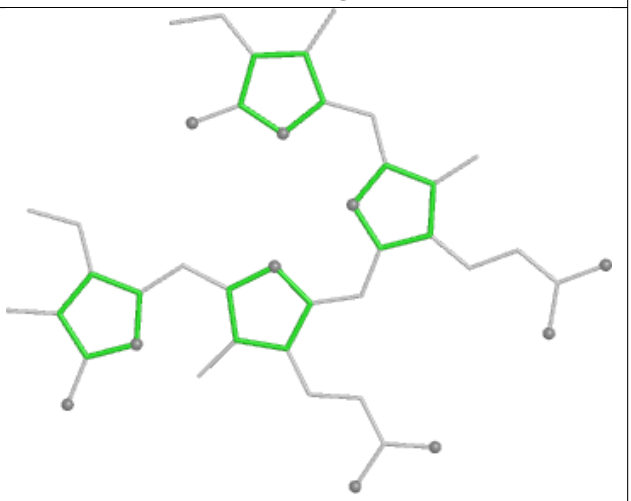
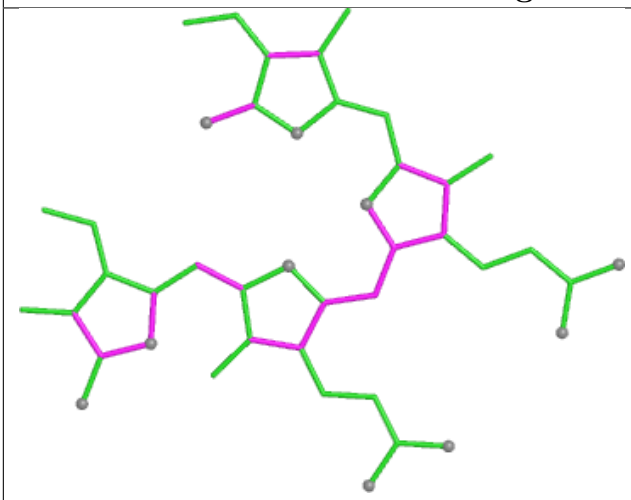


Rings

Ligand PEB LF 202



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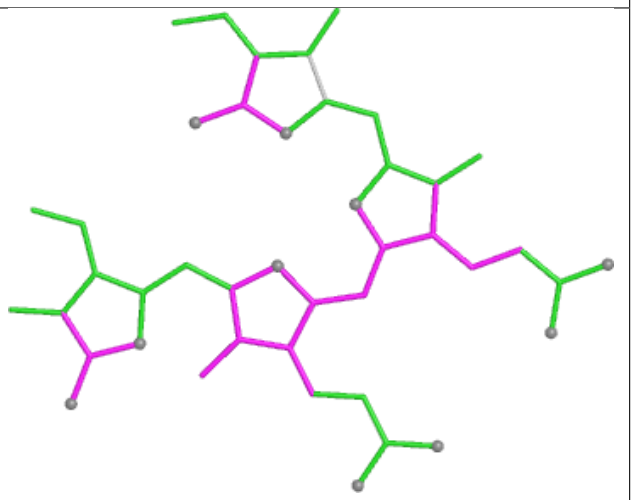

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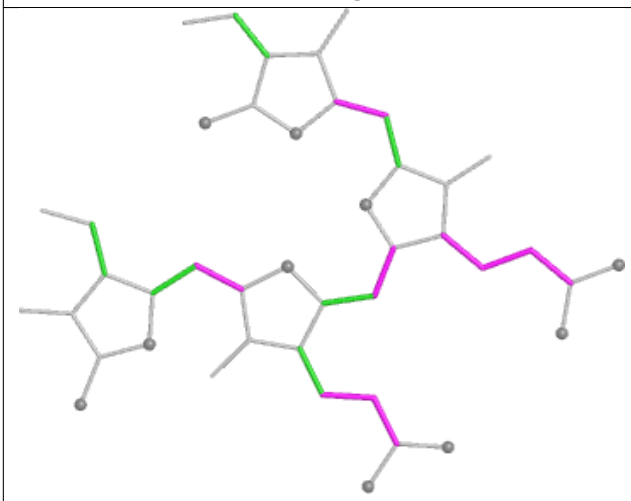

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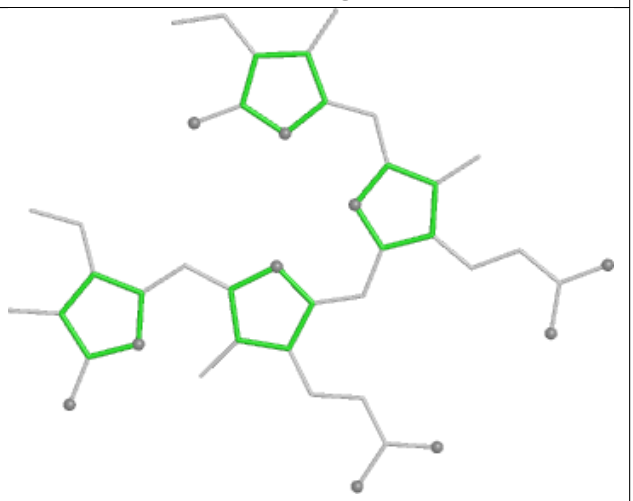
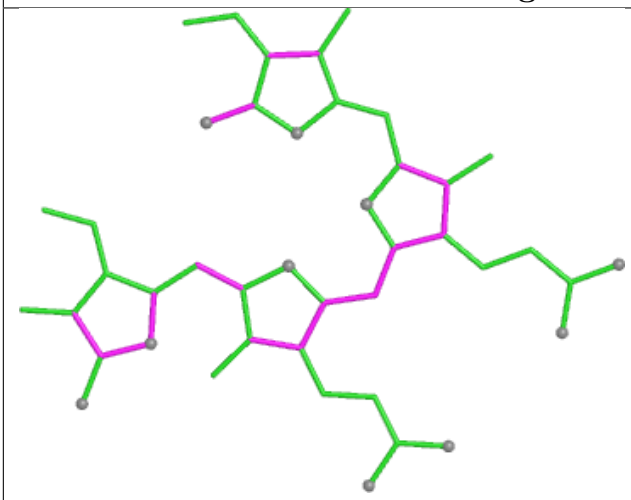


Rings

Ligand PEB dJ 201



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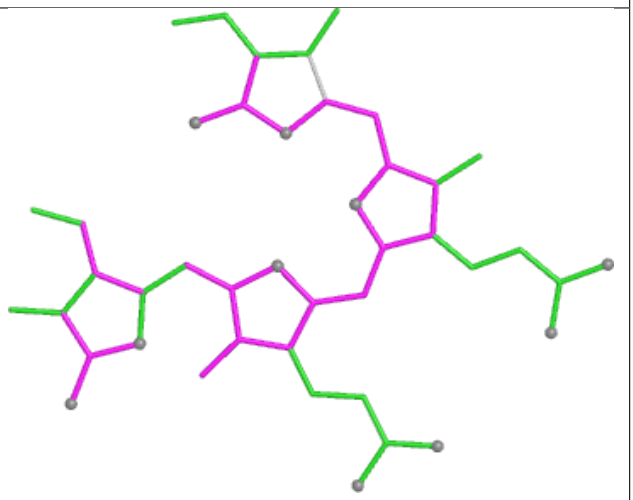

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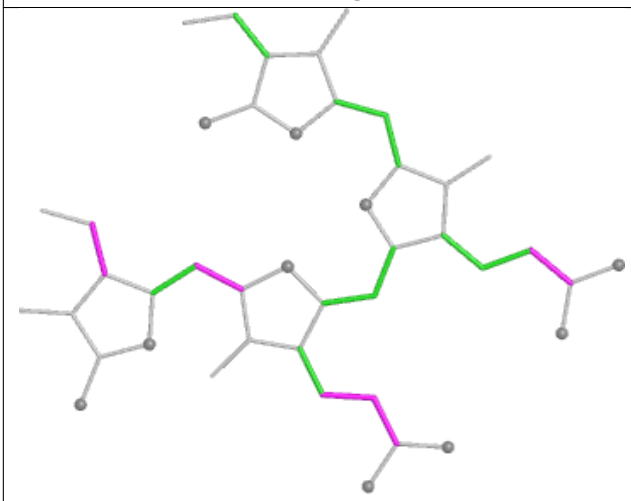

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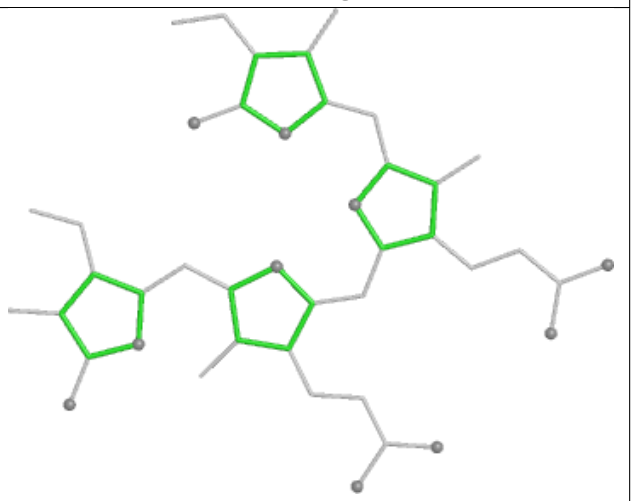
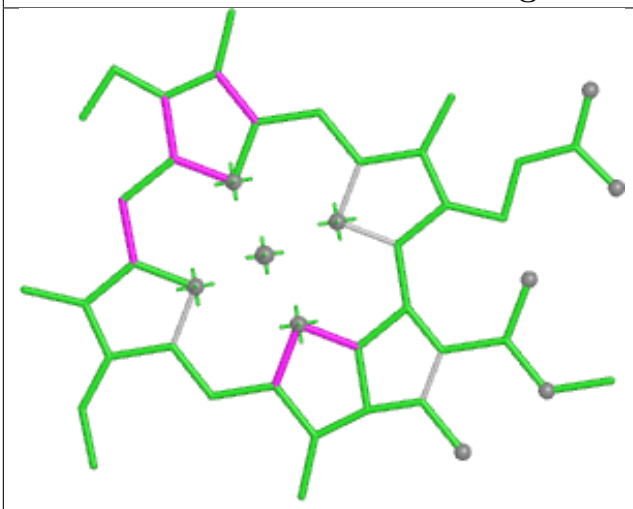


Rings

Ligand CLA 62 312



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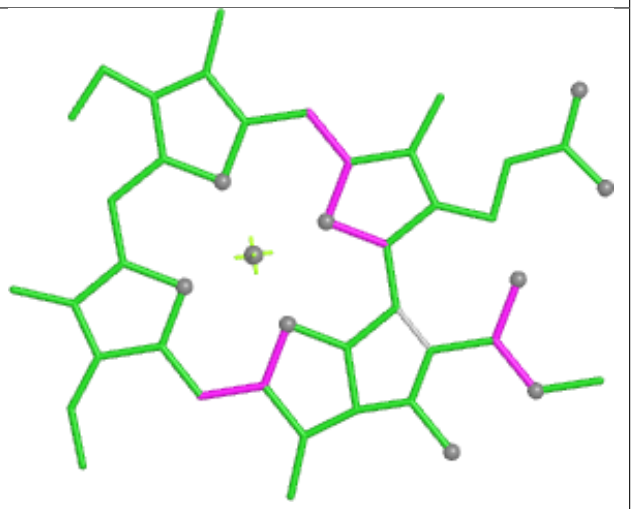
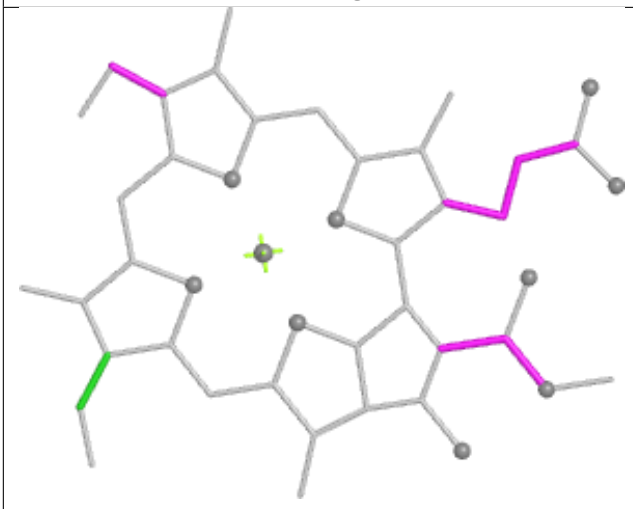


Bond angles

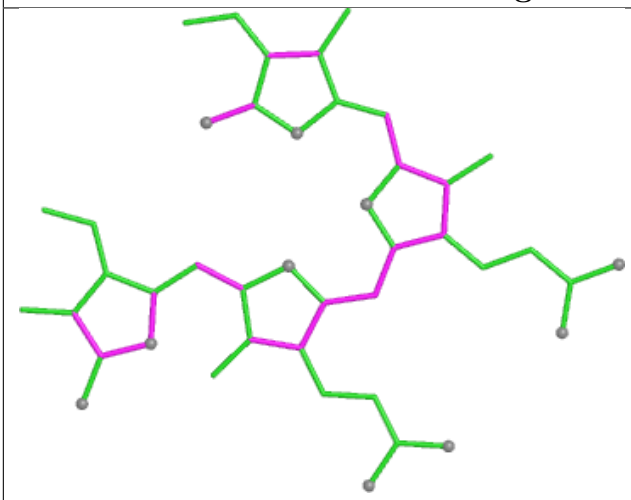


Torsions



Rings

Ligand PEB uC 202



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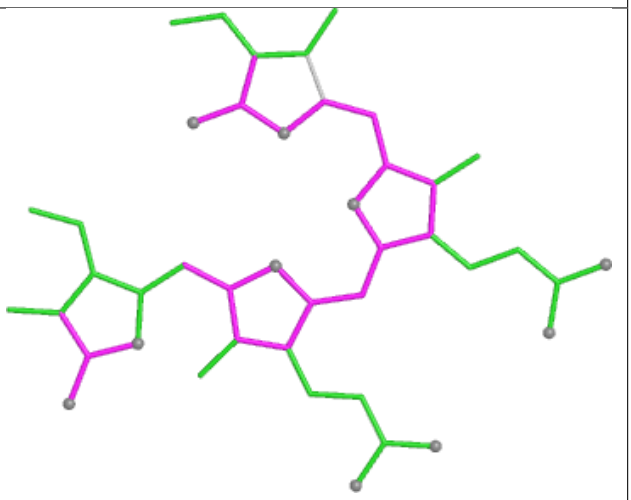
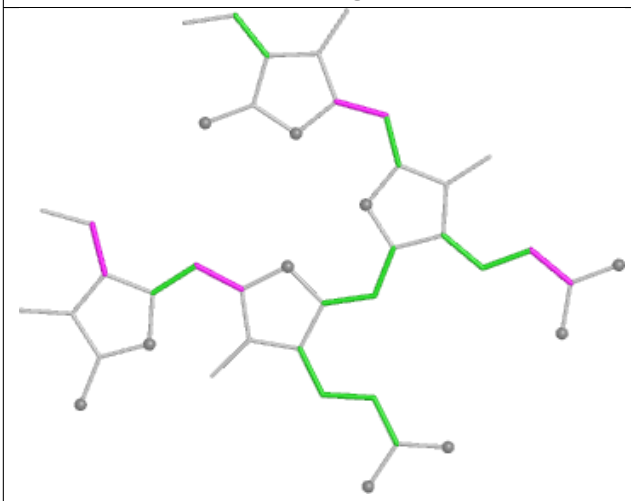


Bond angles



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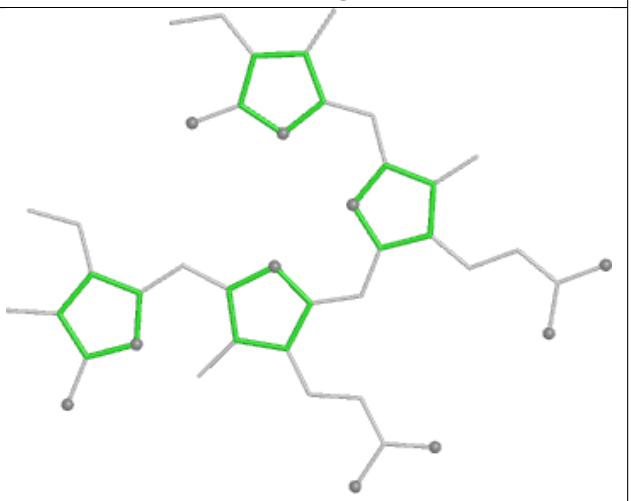
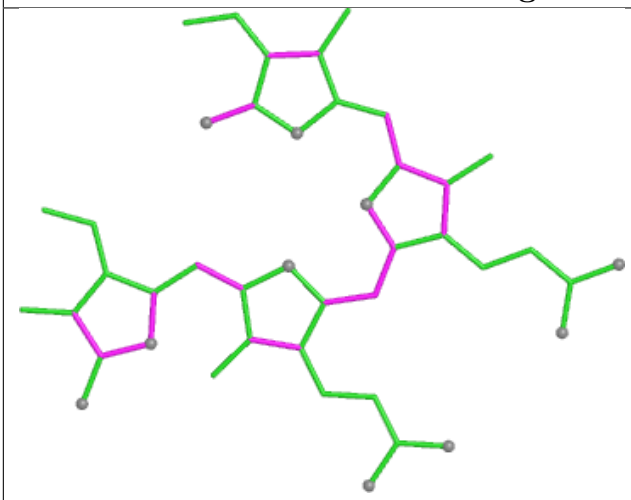


Rings

Ligand PEB IP 203



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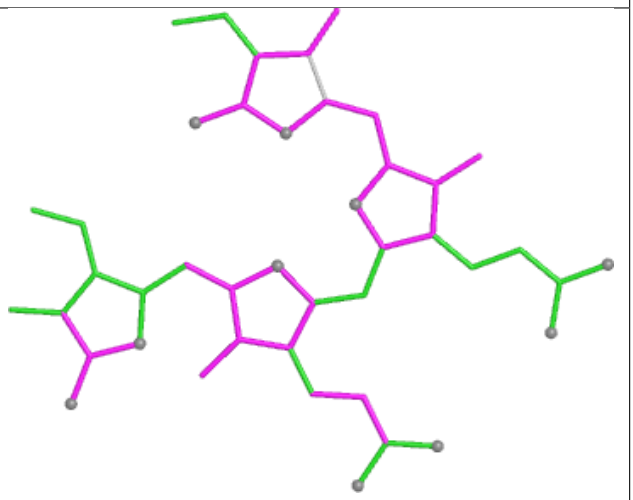
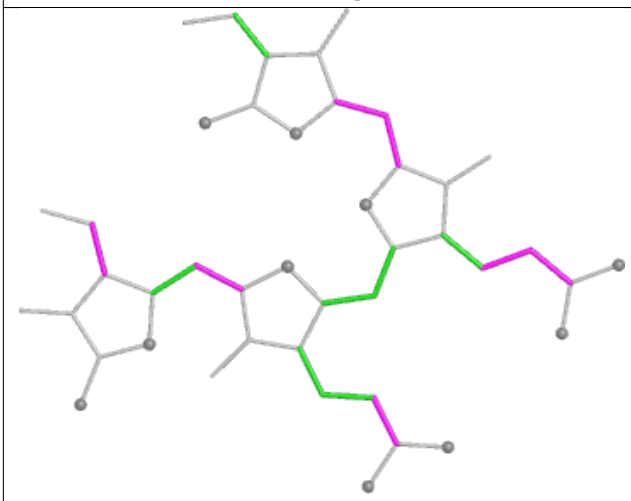


Bond angles



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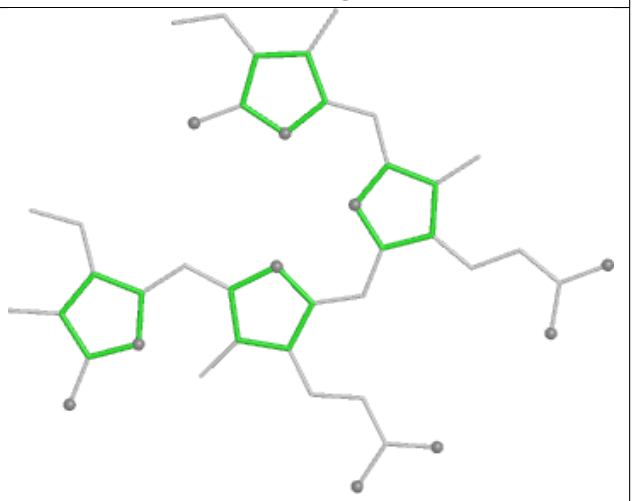
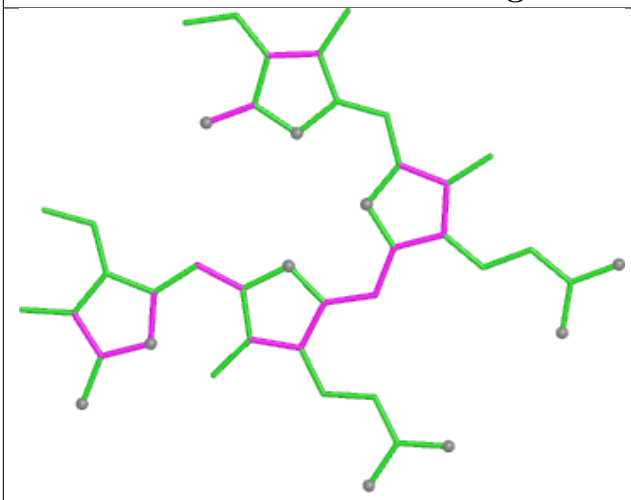
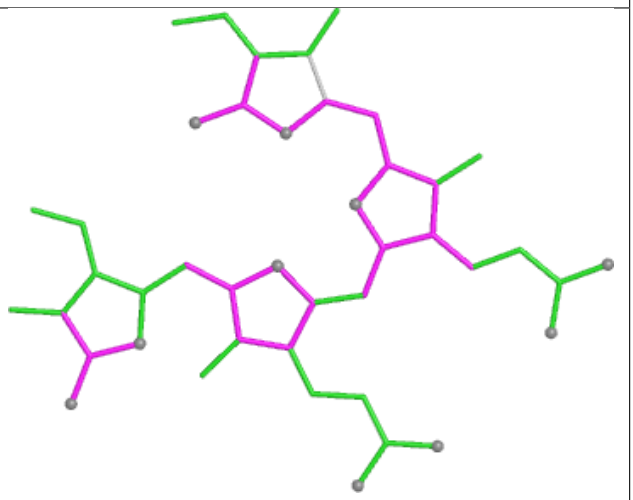


Rings

Ligand PEB KM 202



Bond lengths



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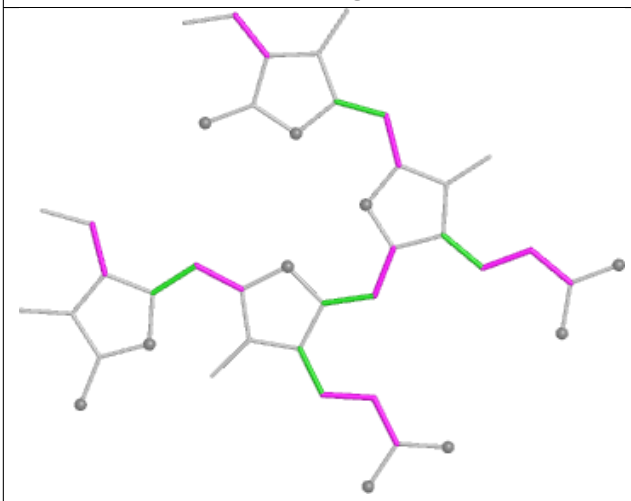

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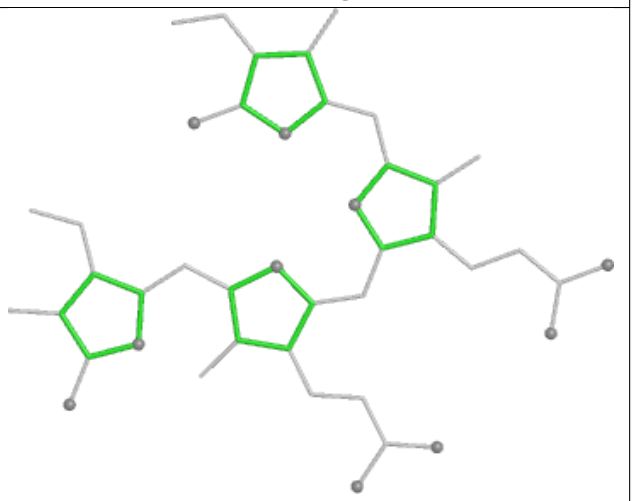
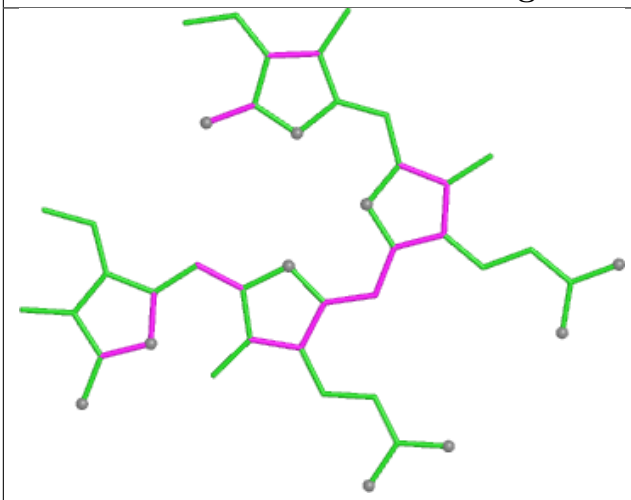


Rings

Ligand PEB jG 202



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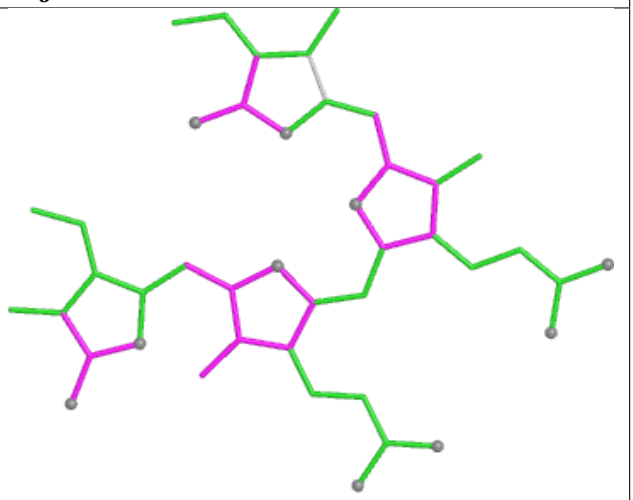

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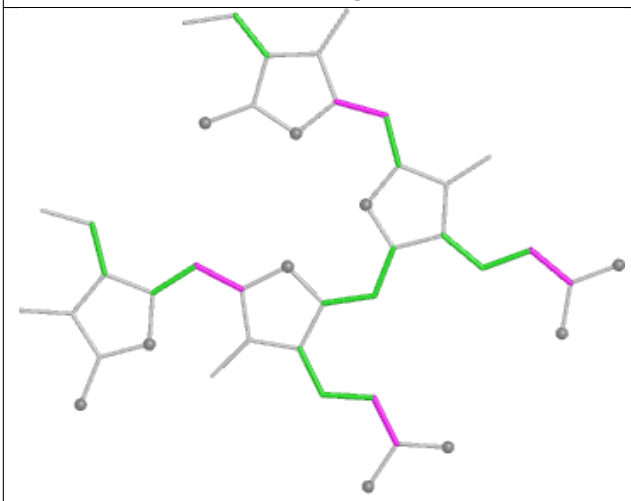

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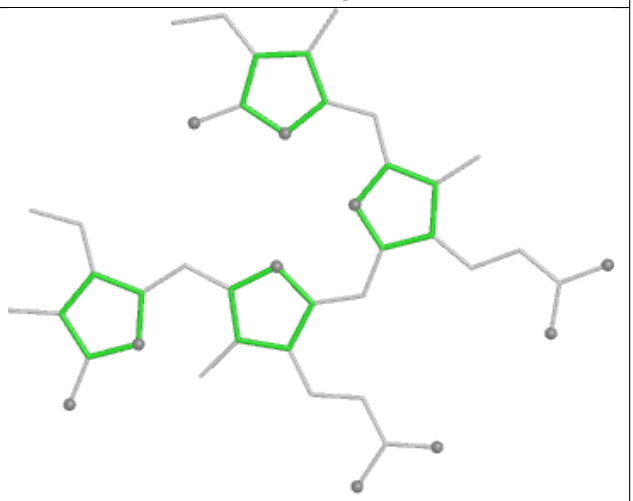
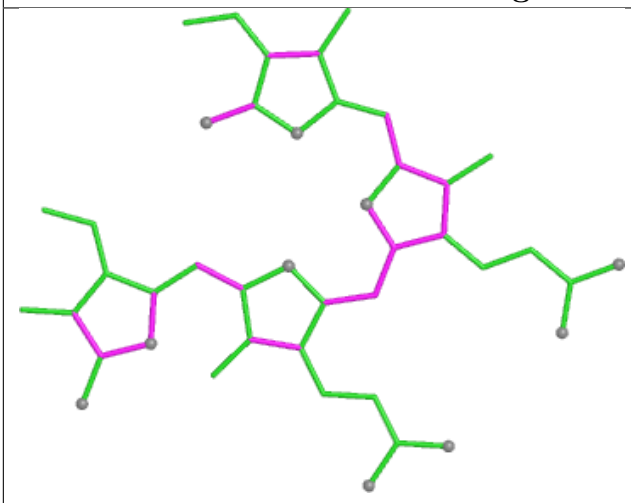


Rings

Ligand PEB NF 202



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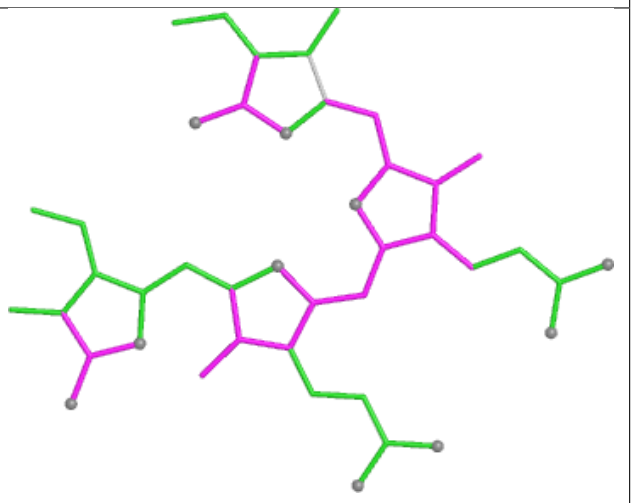

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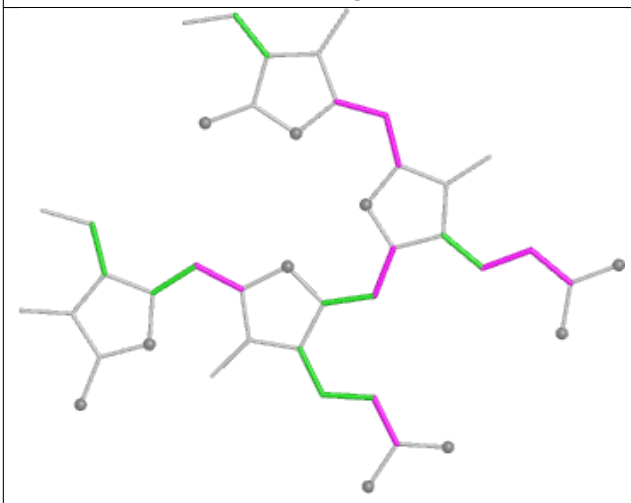

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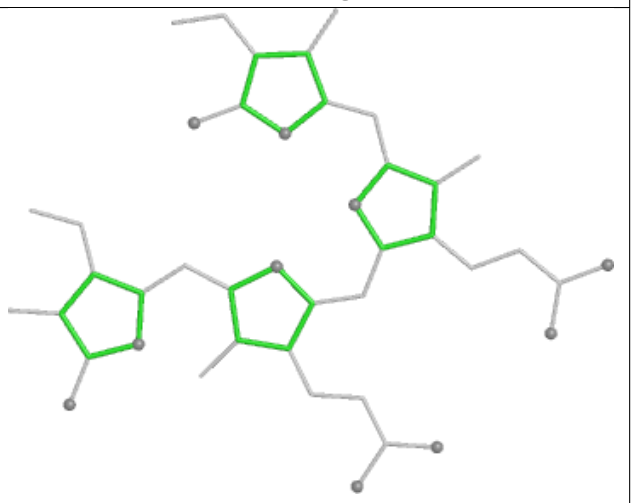
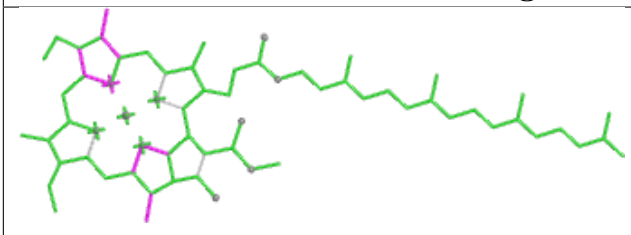


Rings

Ligand CLA cL 513



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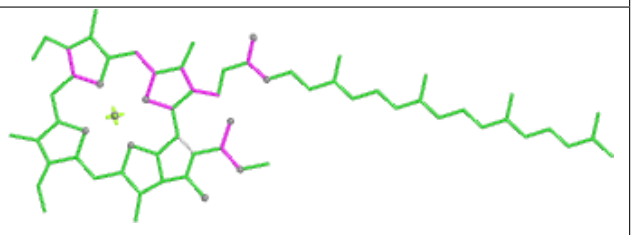

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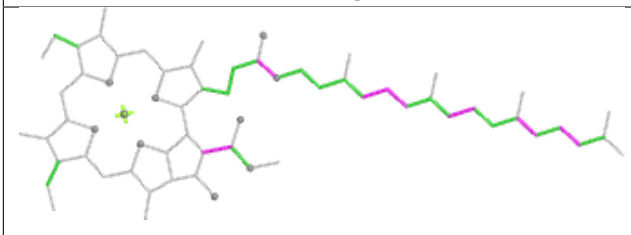

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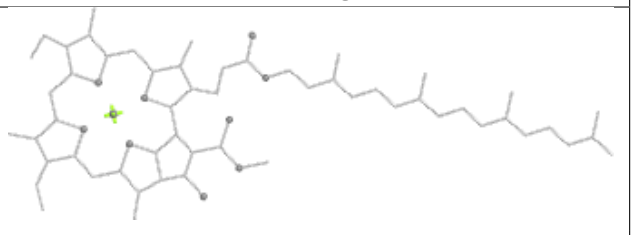
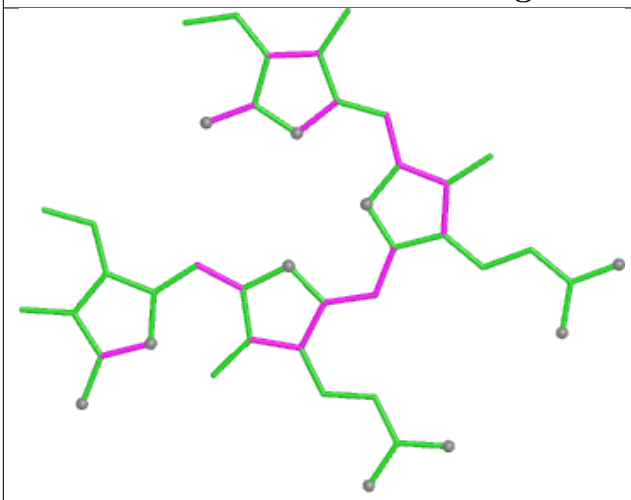


Rings

Ligand PEB JD 202



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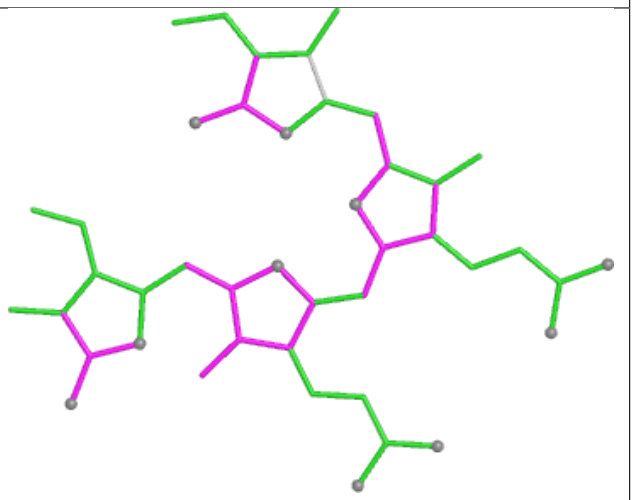

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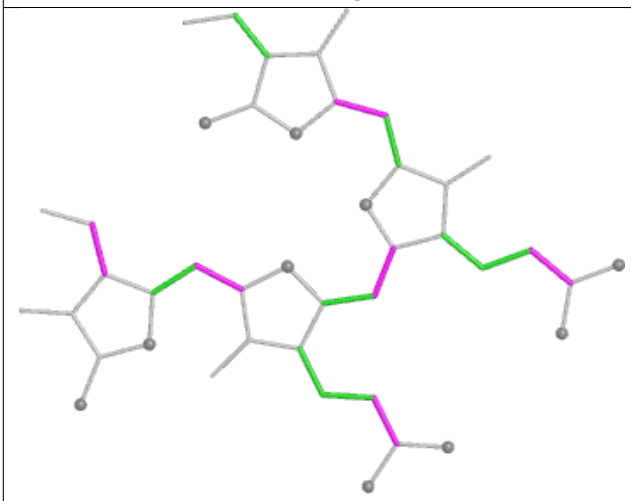

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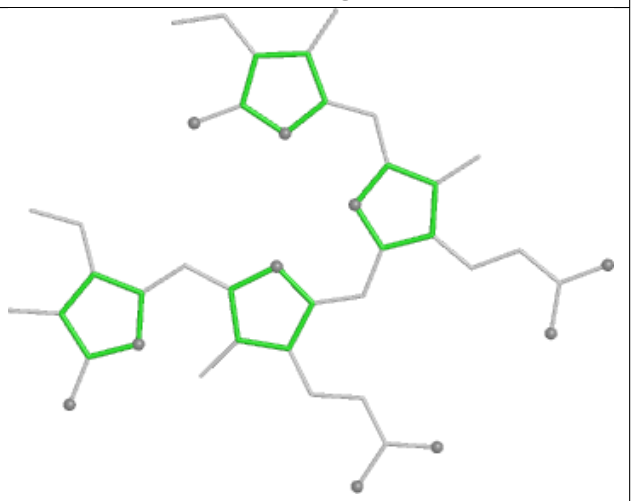
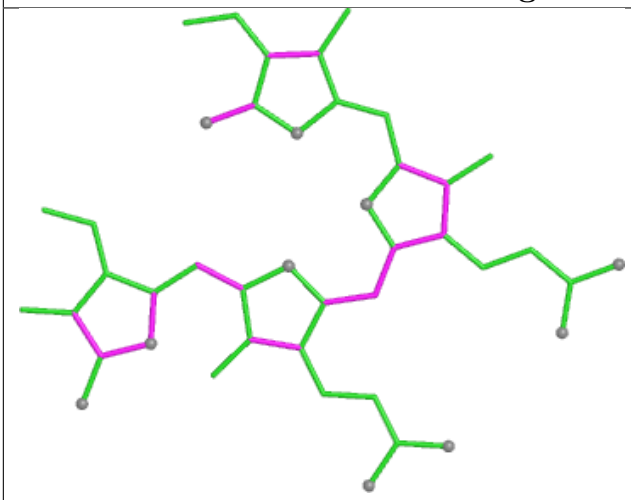


Rings

Ligand PEB S9 203



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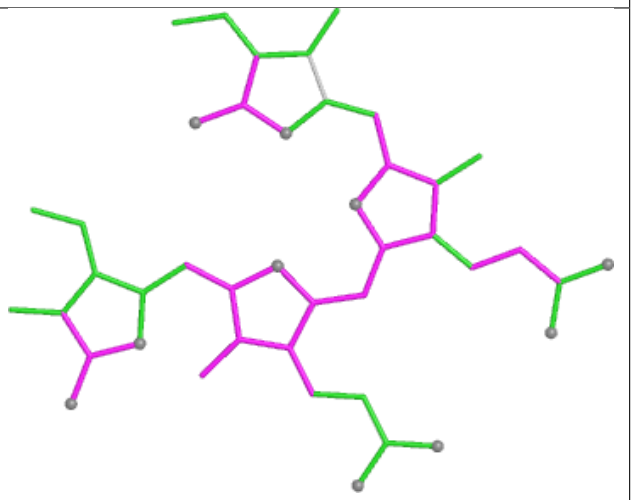

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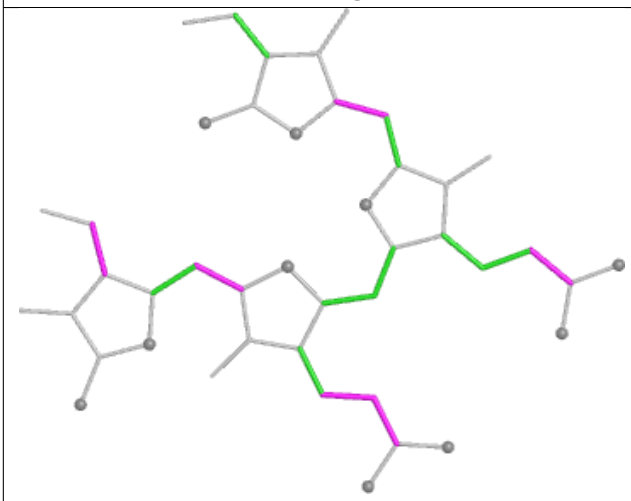

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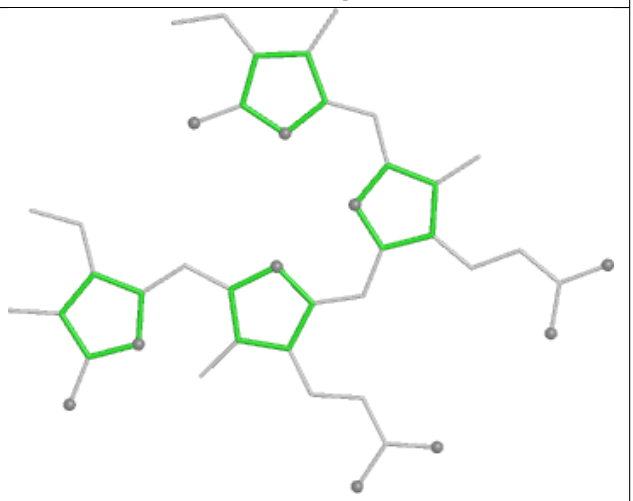
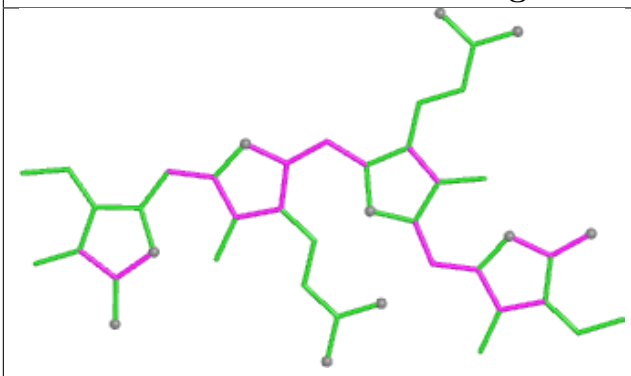


Rings

Ligand CYC M1 201



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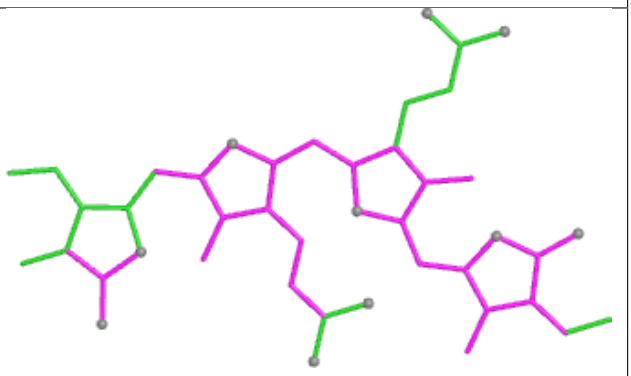

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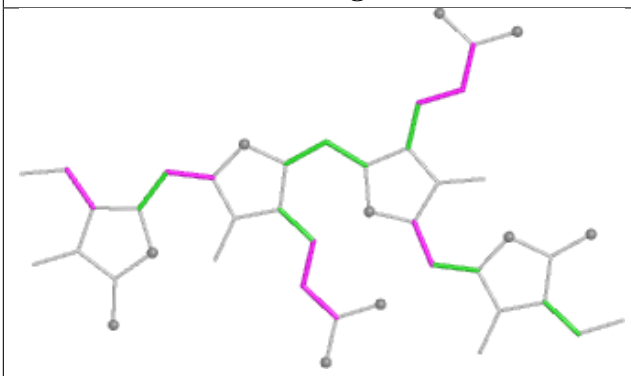

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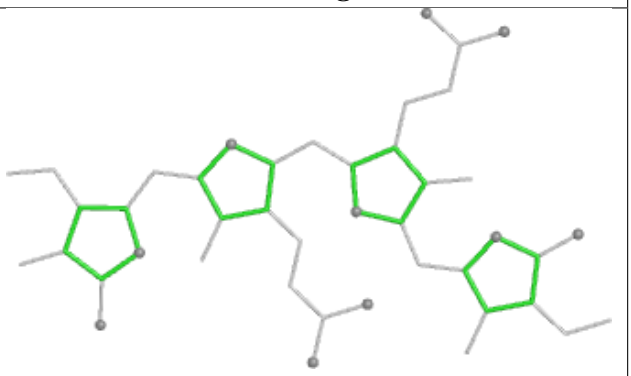
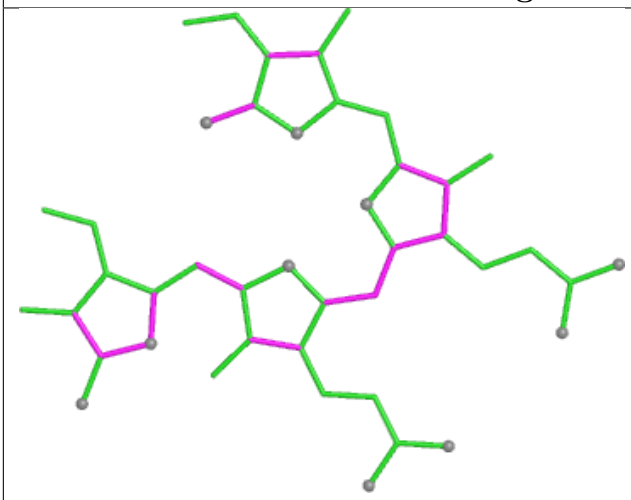


Rings

Ligand PEB eO 202



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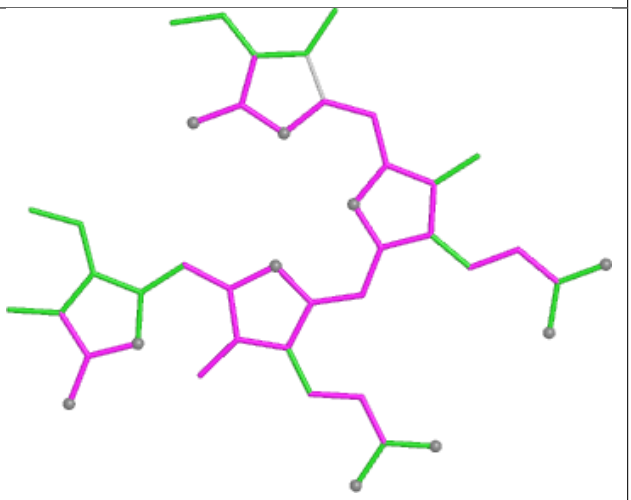

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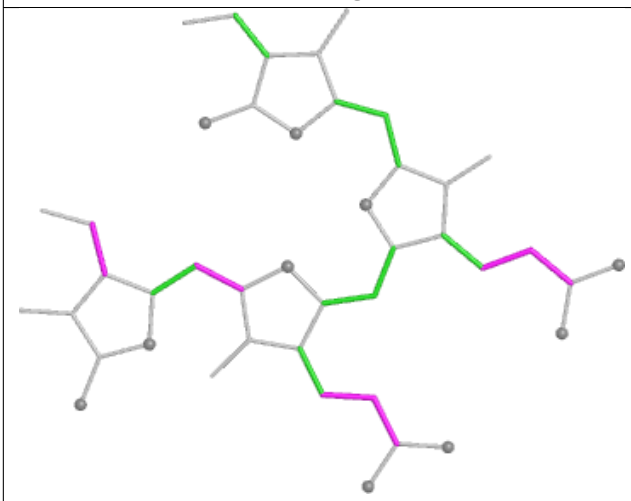

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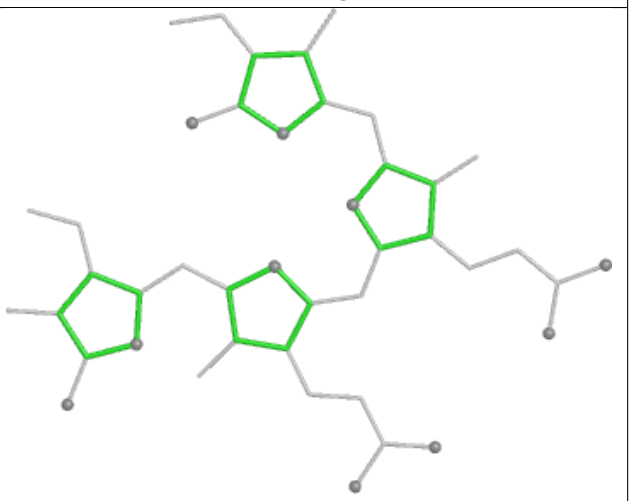
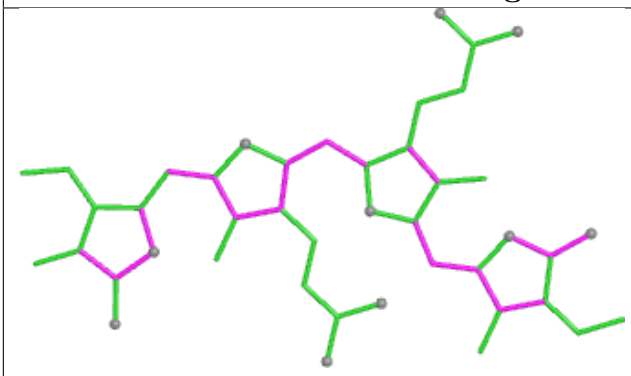


Rings

Ligand CYC C3 1001



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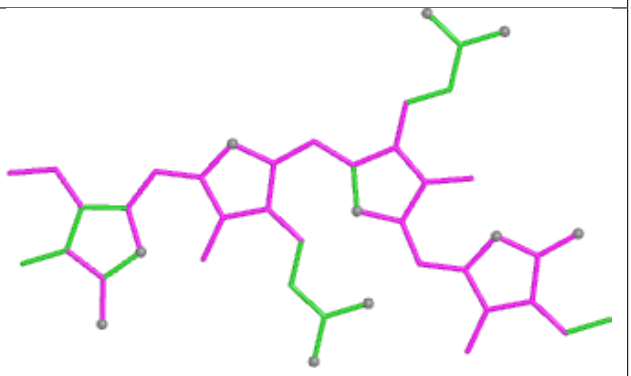

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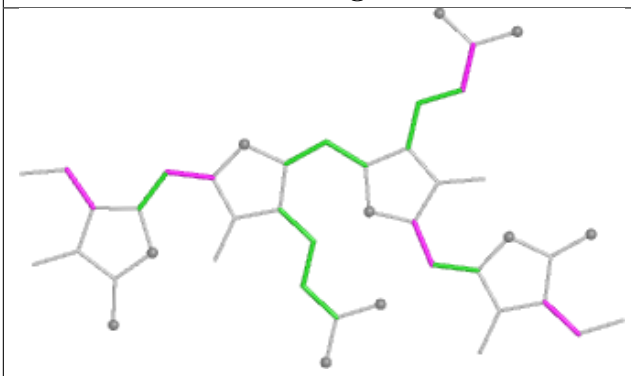

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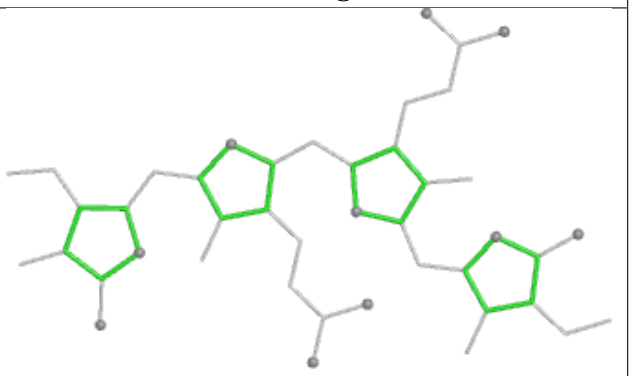
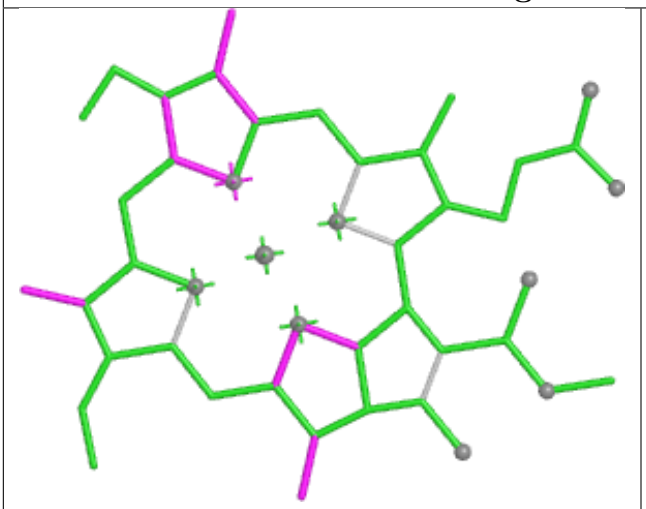


Rings

Ligand CLA A2 816



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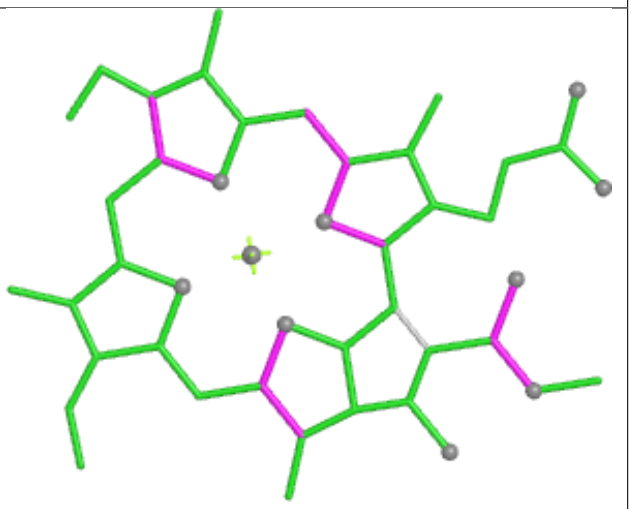

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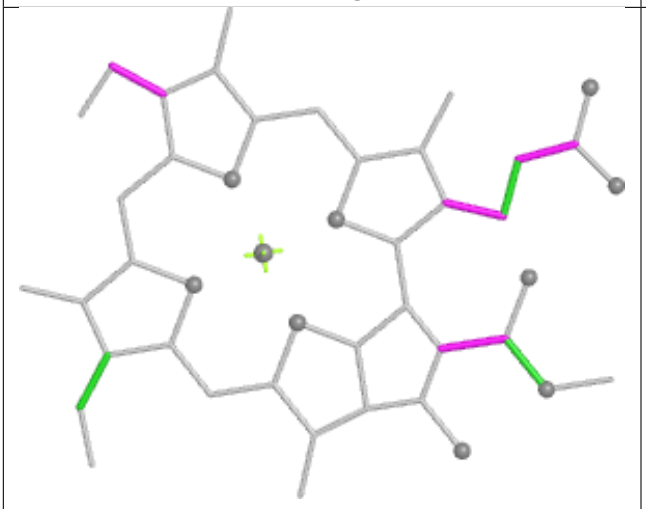
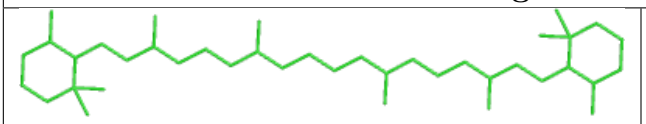


Torsions



Rings

Ligand BCR BL 618



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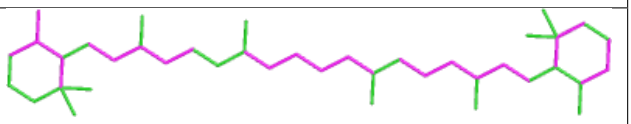

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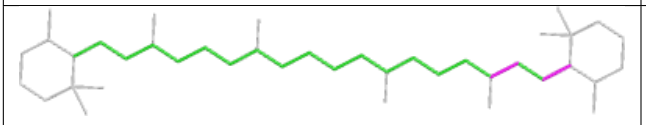

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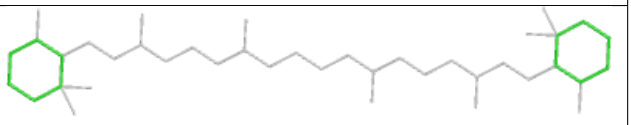
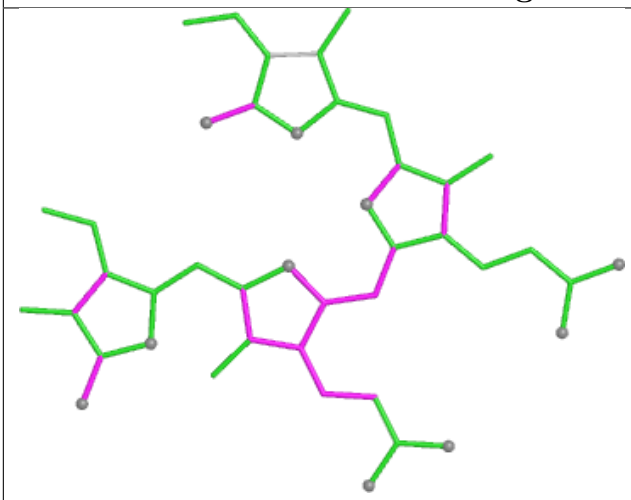


Rings

Ligand PUB Z5 302



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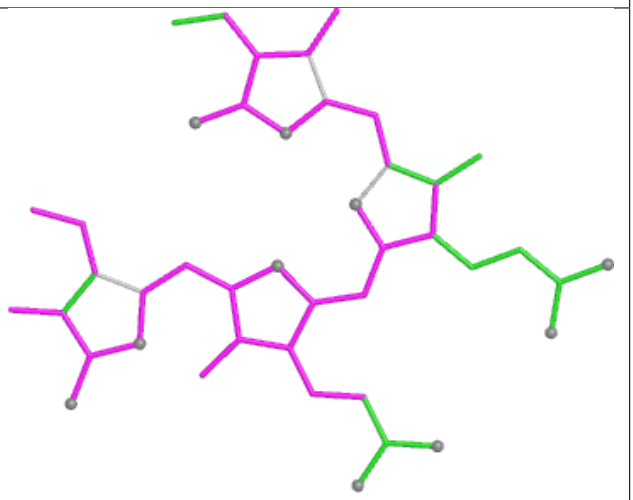

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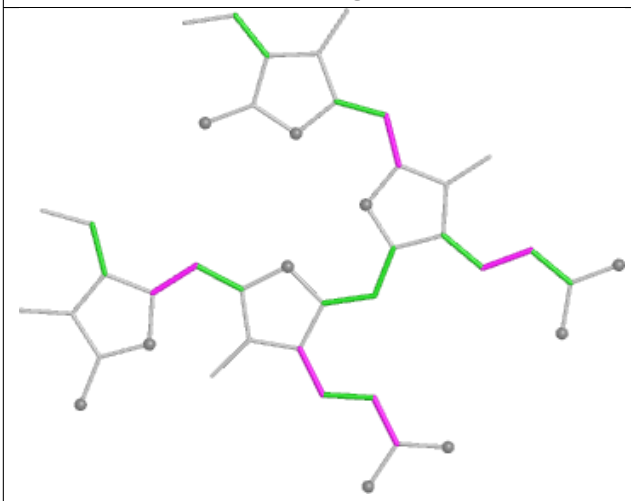

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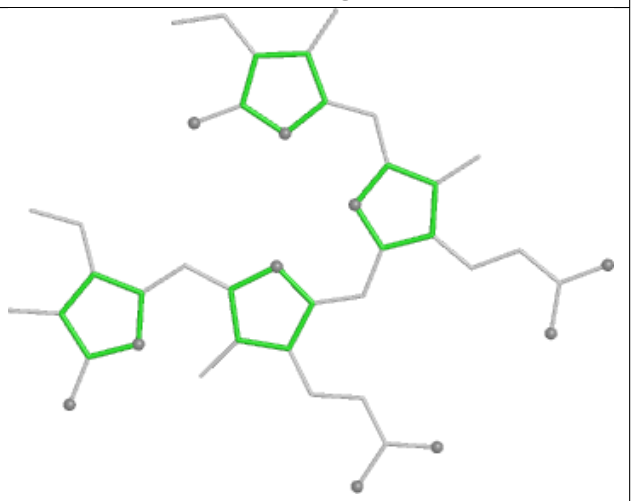
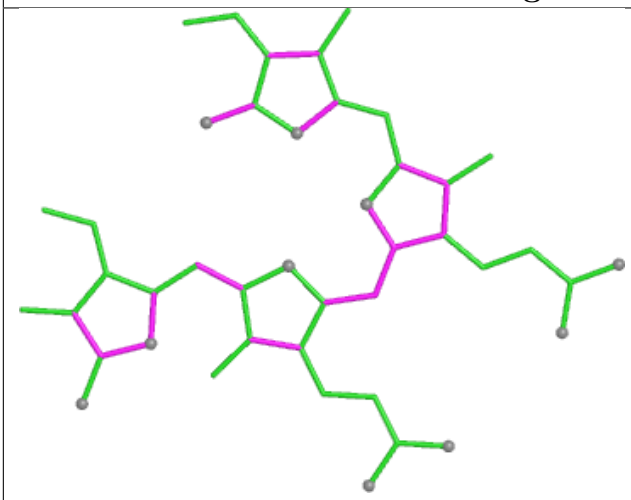


Rings

Ligand PEB j4 202



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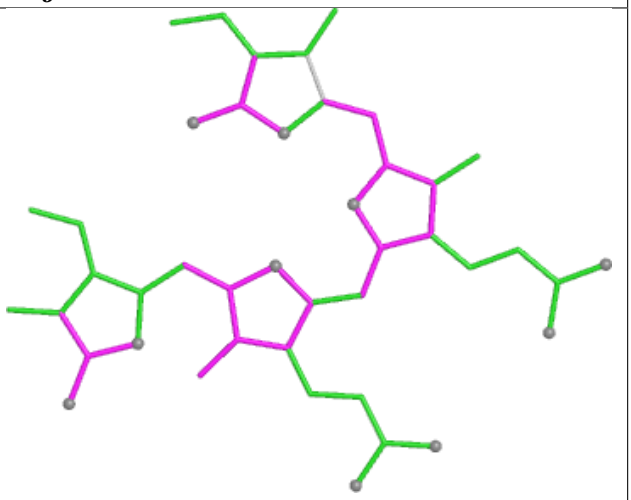
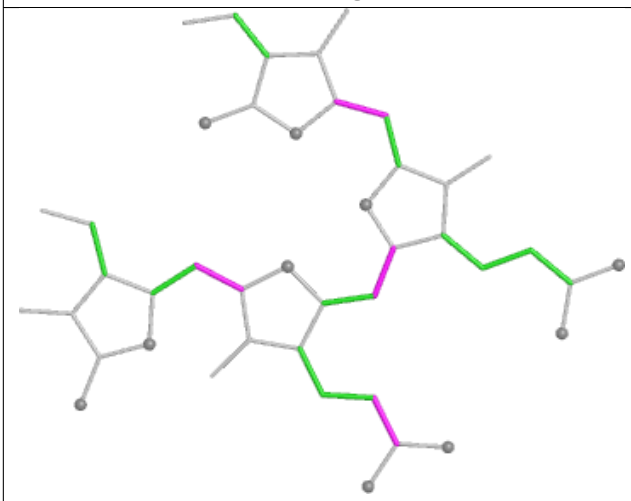


Bond angles



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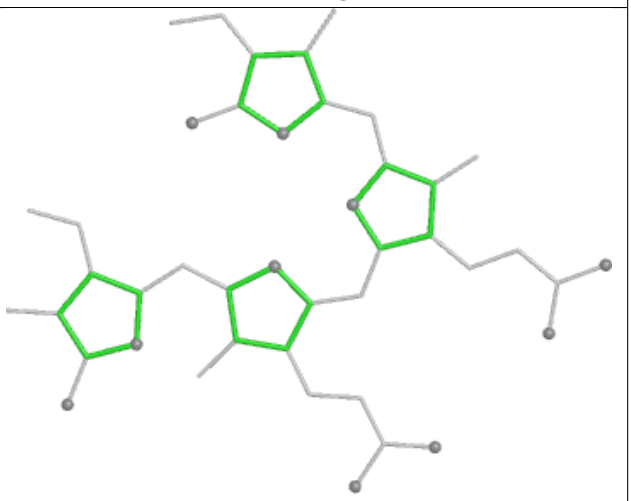
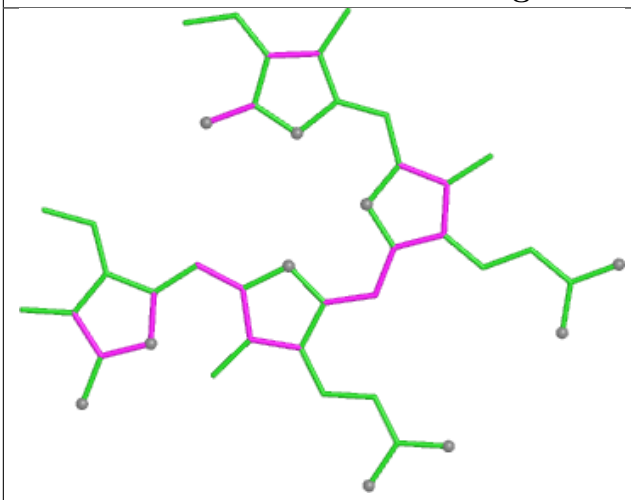


Rings

Ligand PEB ZH 203



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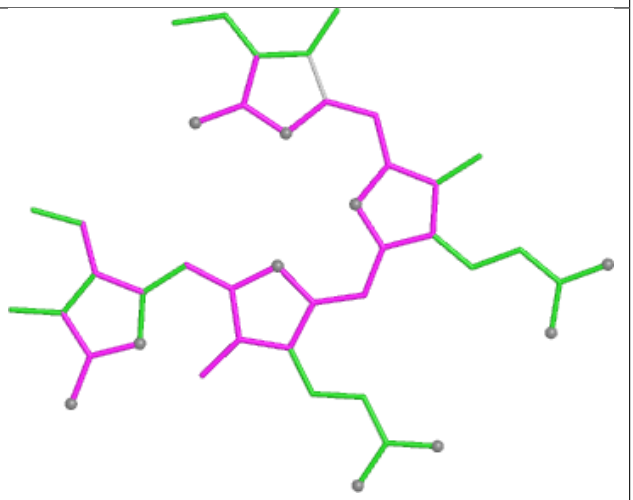
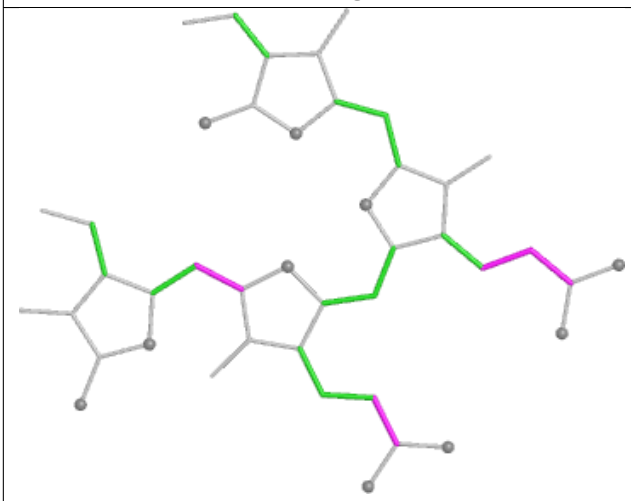


Bond angles



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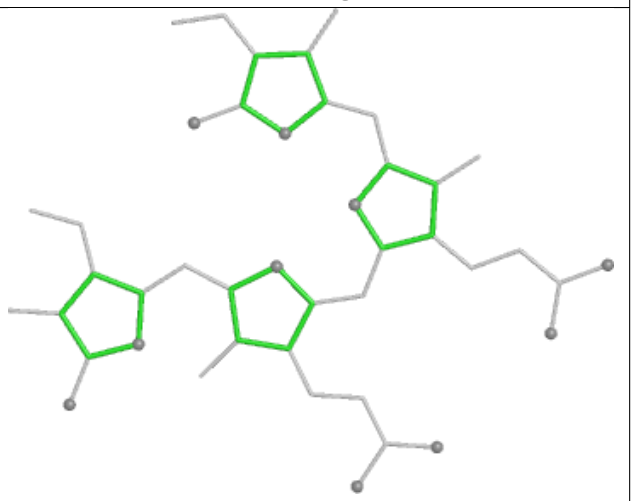
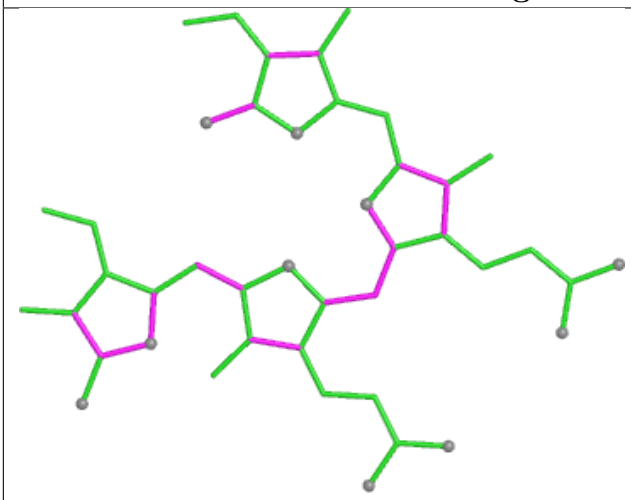


Rings

Ligand PEB VA 201



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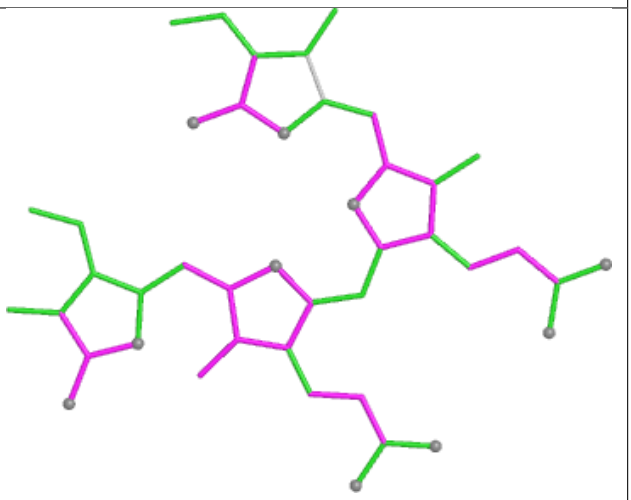
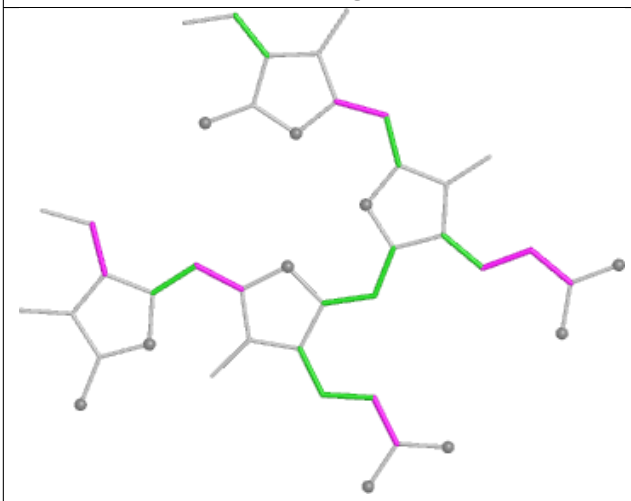


Bond angles



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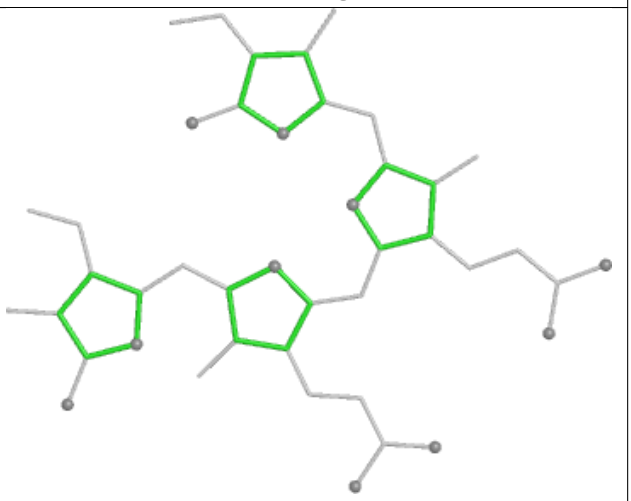
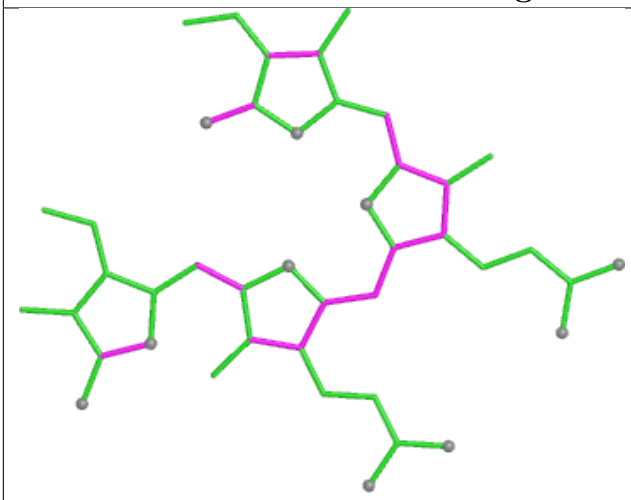


Rings

Ligand PEB JA 202



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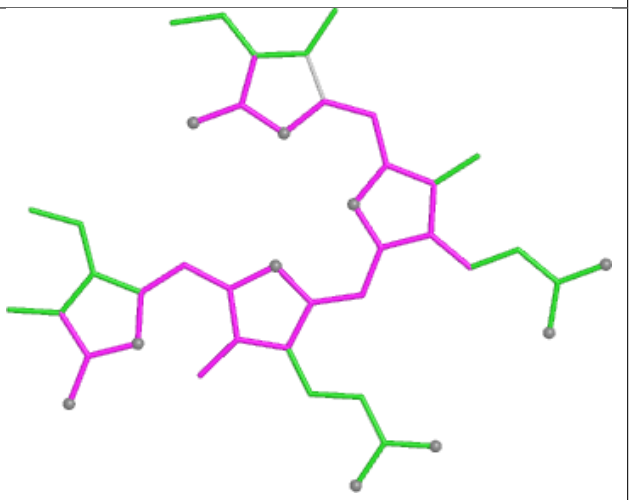

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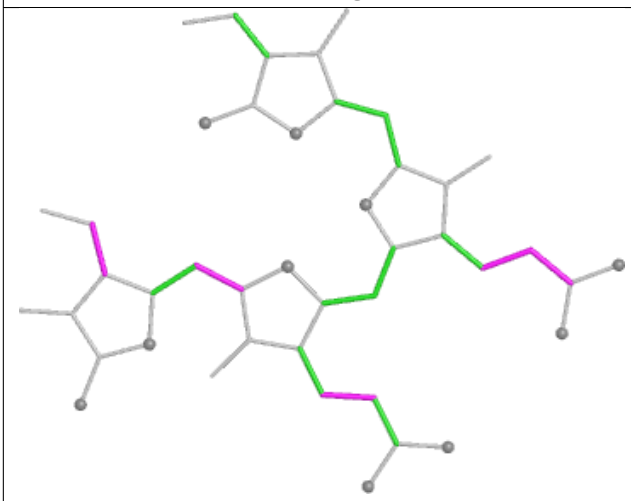

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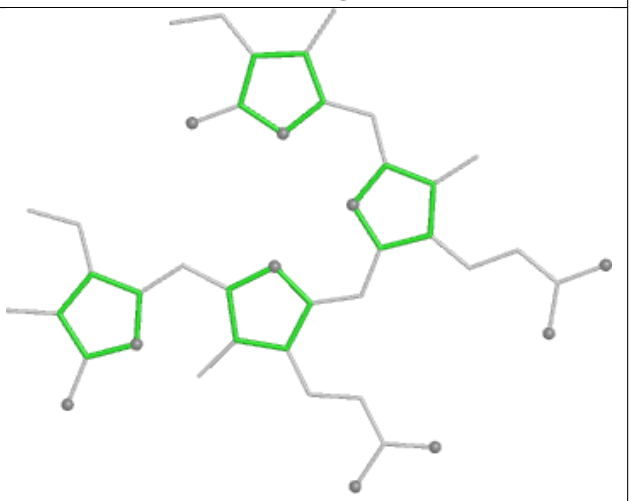
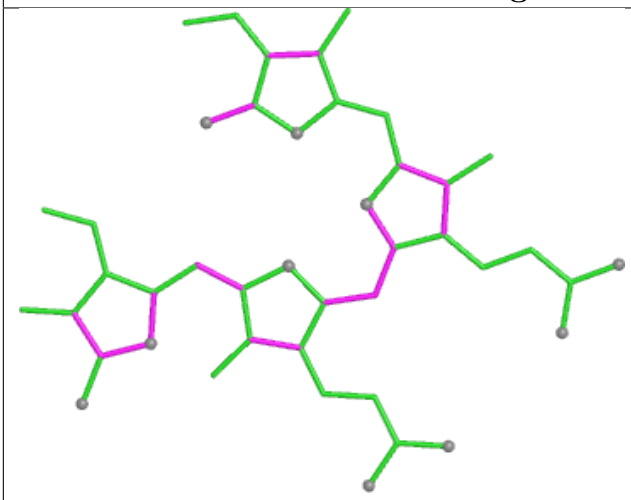


Rings

Ligand PEB NA 201



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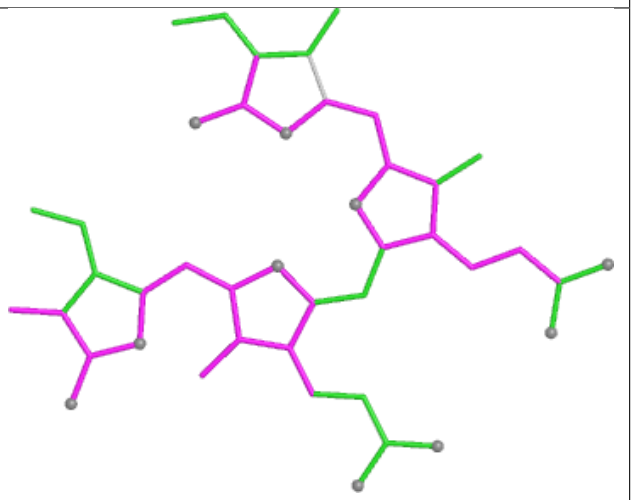

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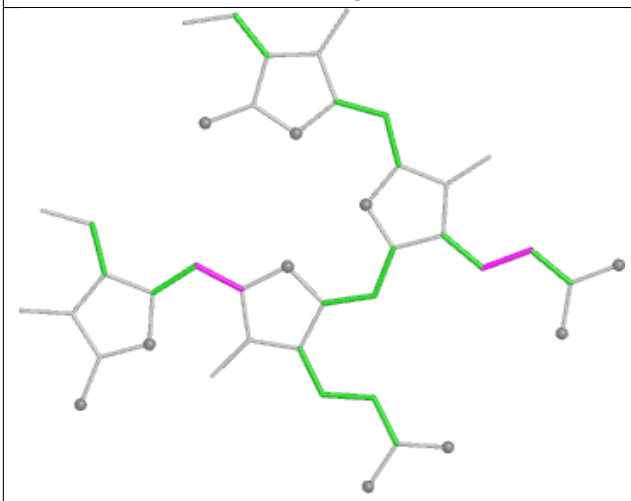

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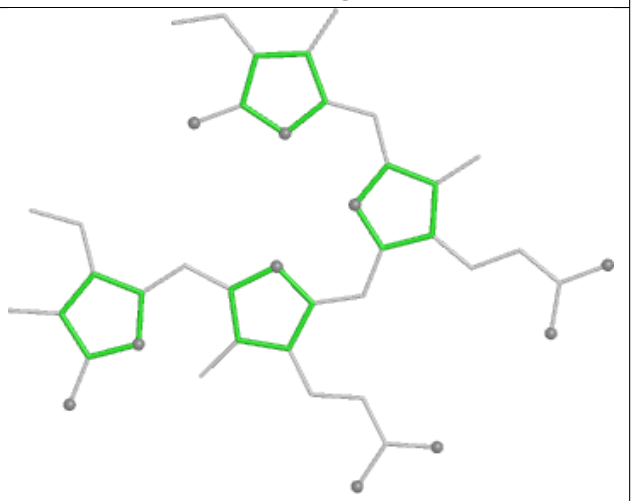
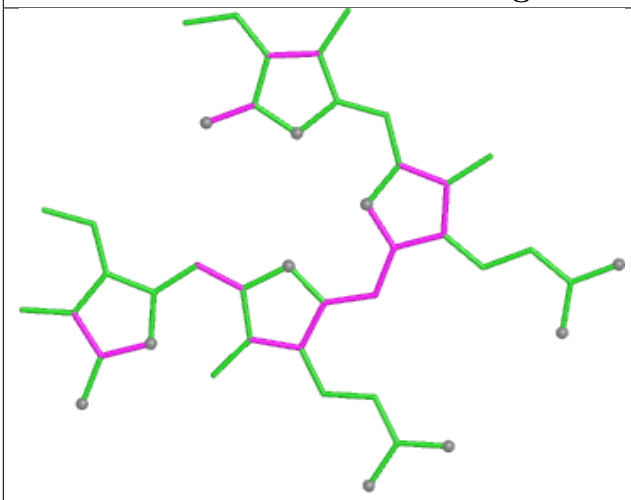


Rings

Ligand PEB cM 202



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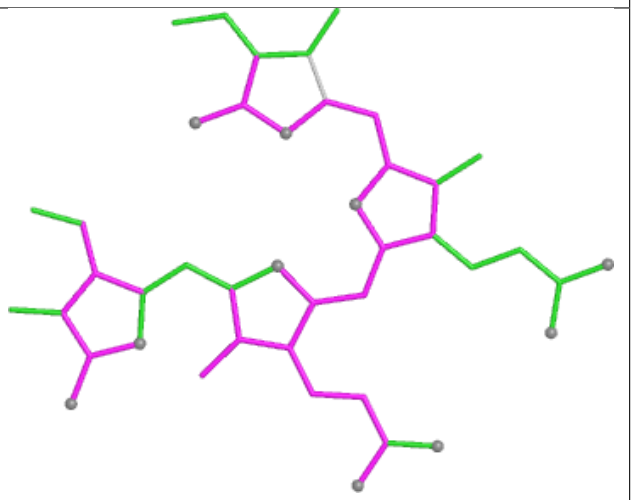

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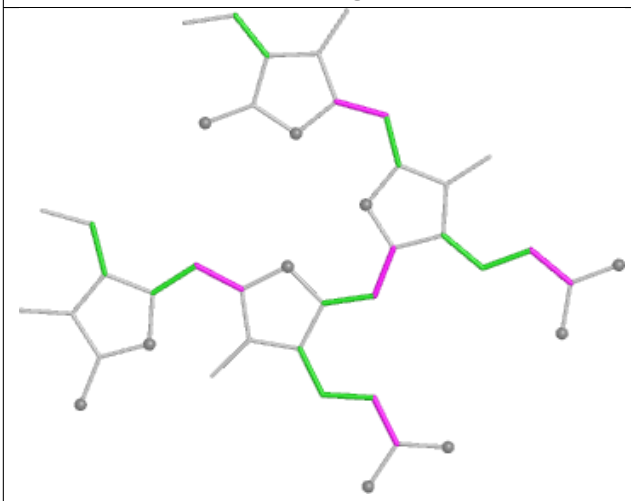

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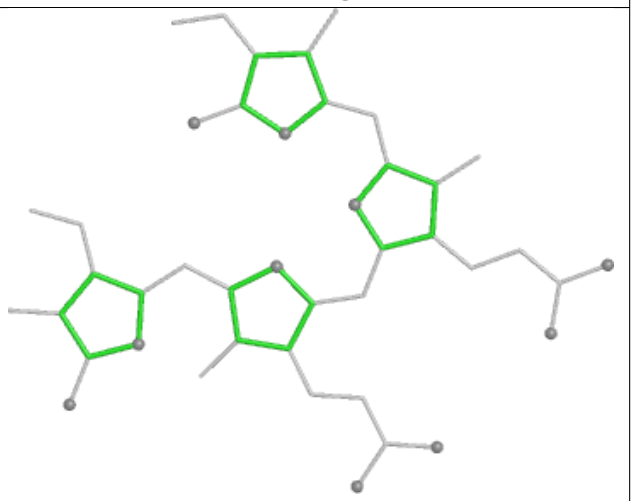
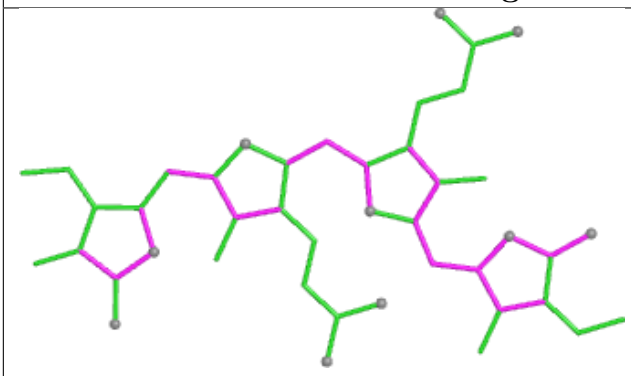


Rings

Ligand CYC LO 1001



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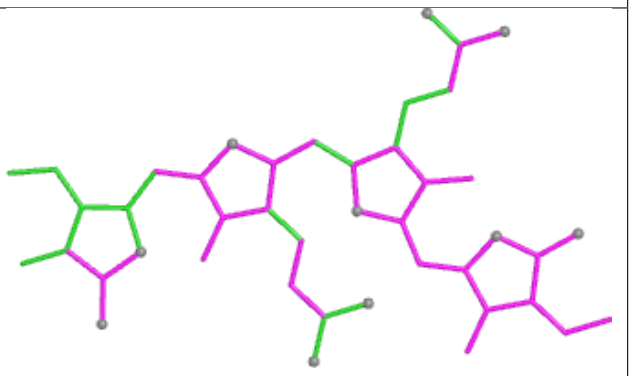

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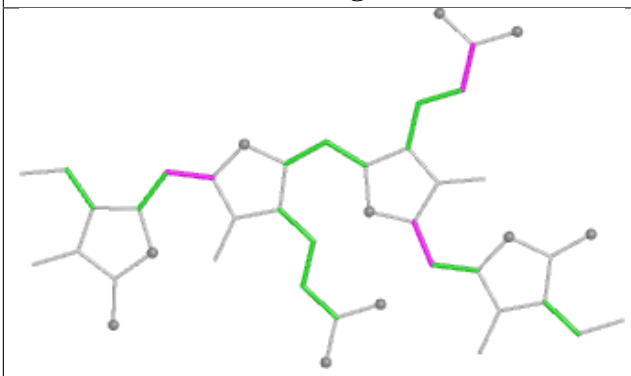

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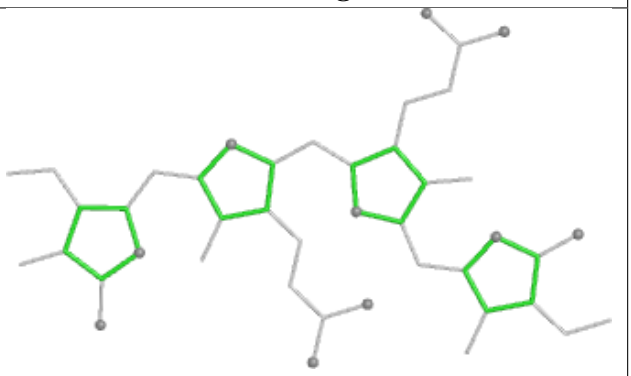
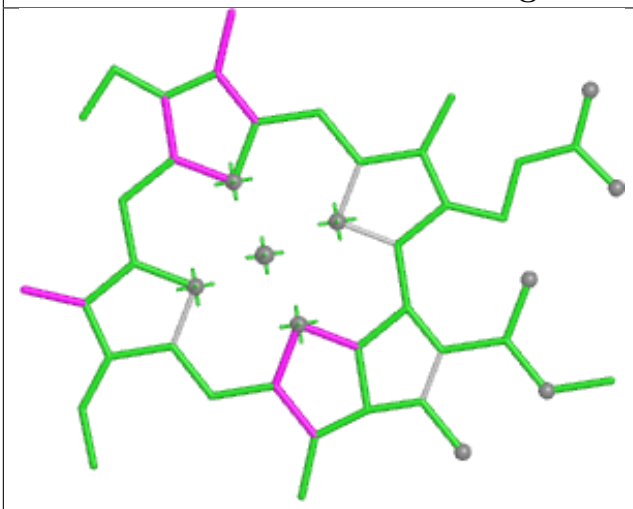


Rings

Ligand CLA 32 302



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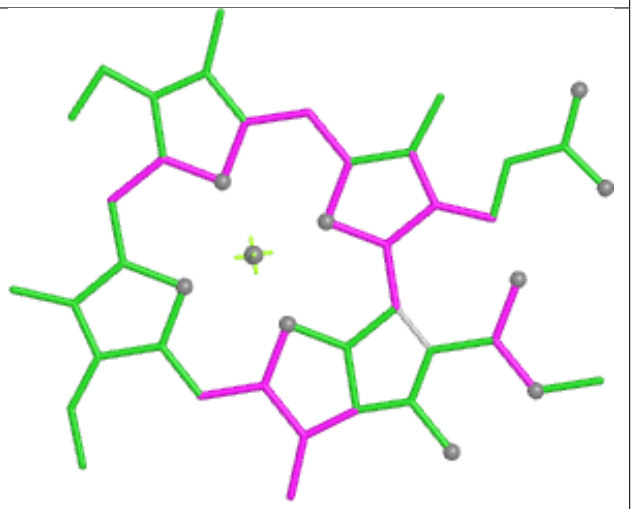

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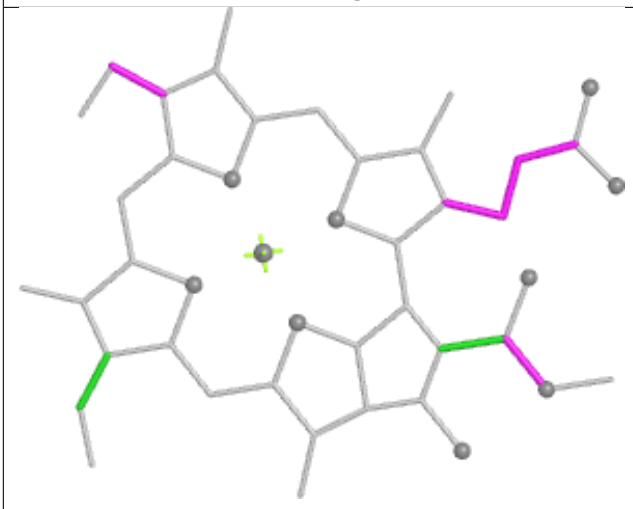
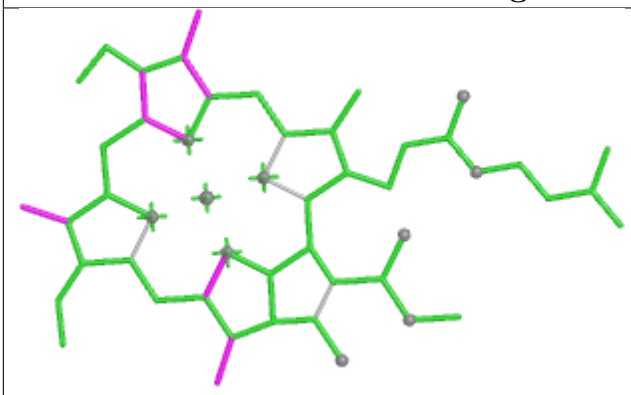


Torsions



Rings

Ligand CLA ON 202



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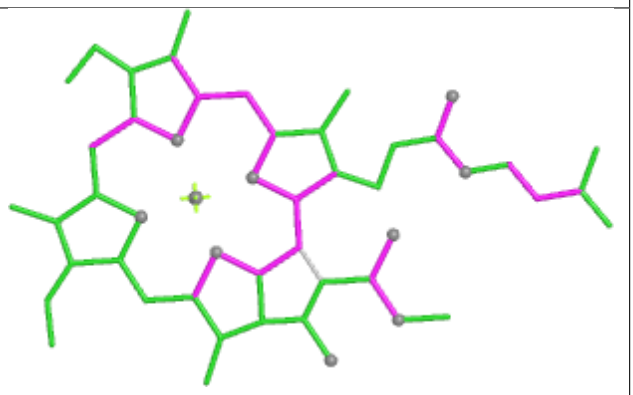

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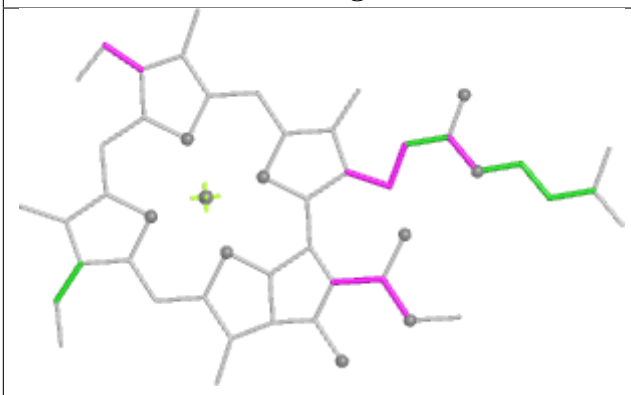

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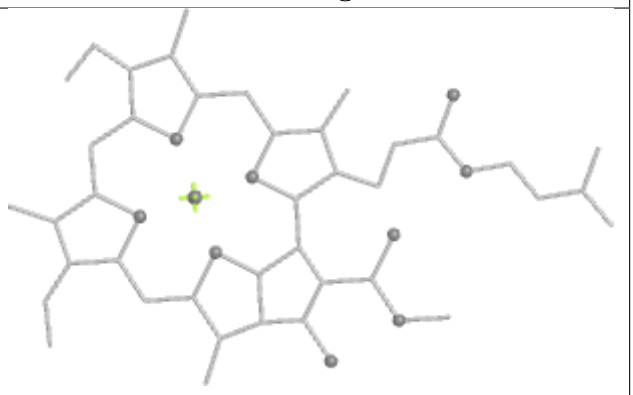
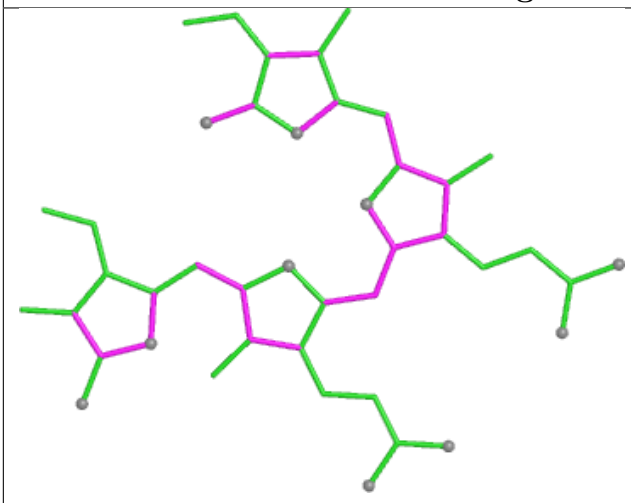


Rings

Ligand PEB rK 202



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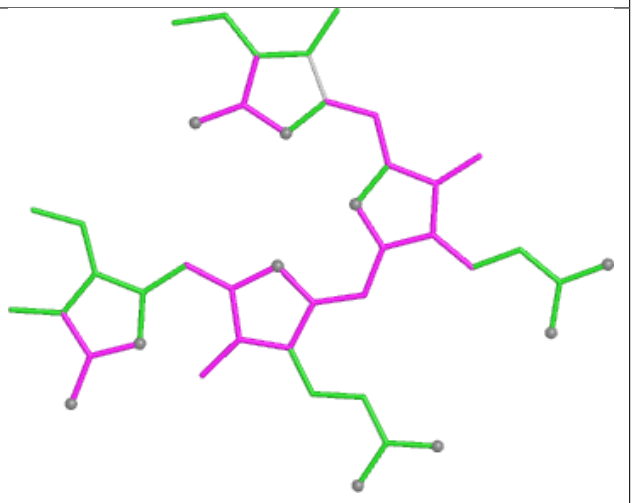

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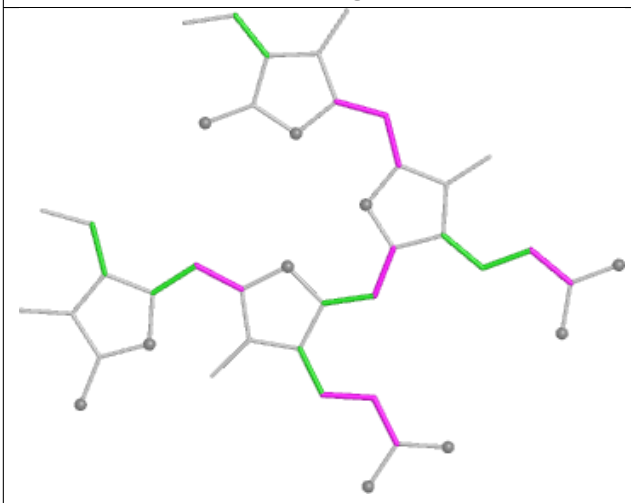

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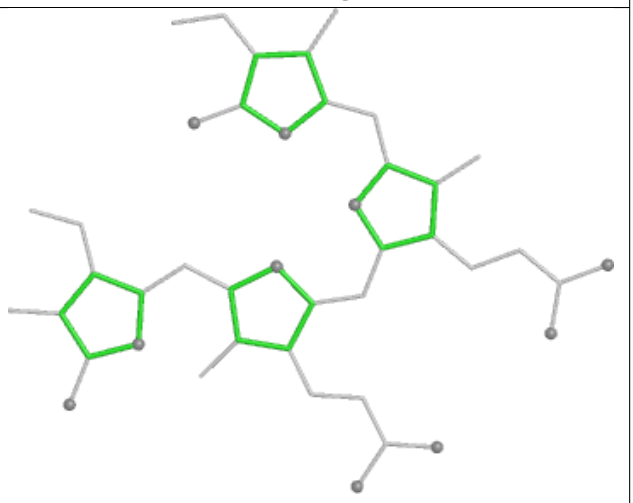
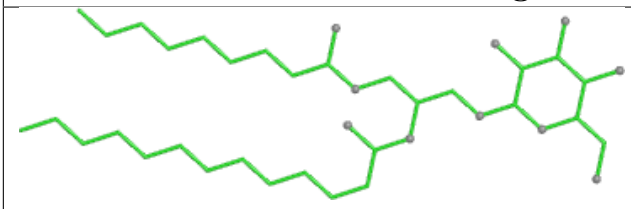


Rings

Ligand LMG bL 610



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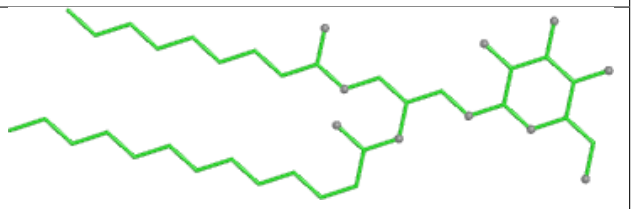

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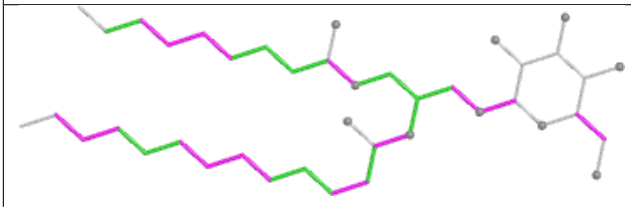

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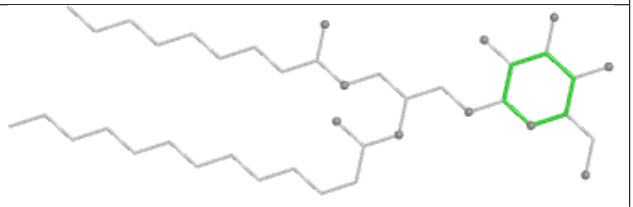
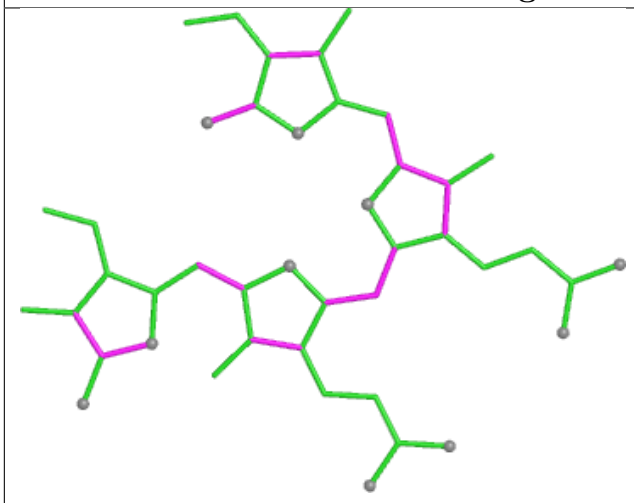


Rings

Ligand PEB Z1 201



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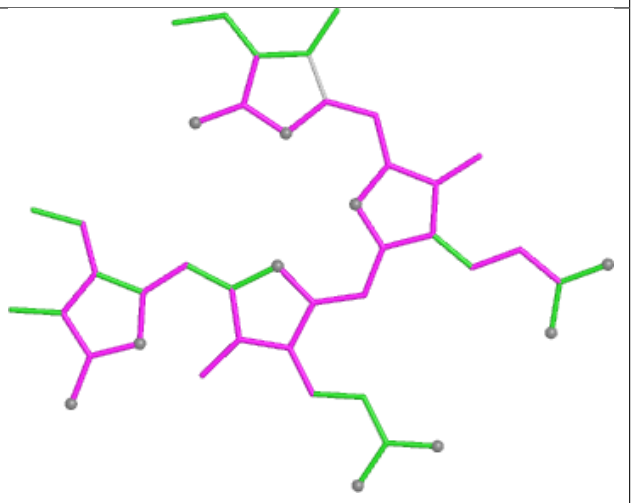

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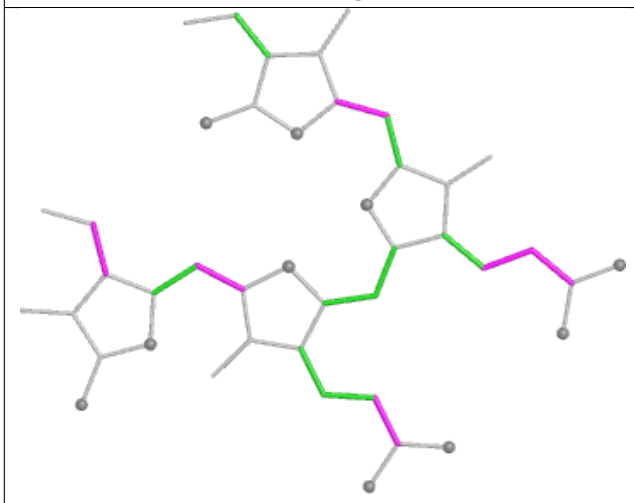

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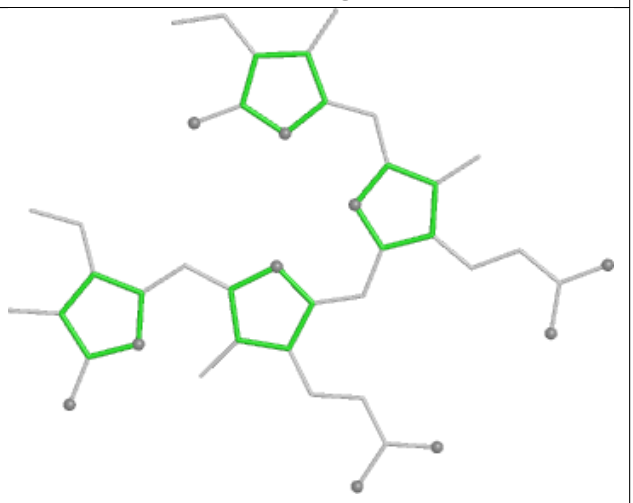

Rings

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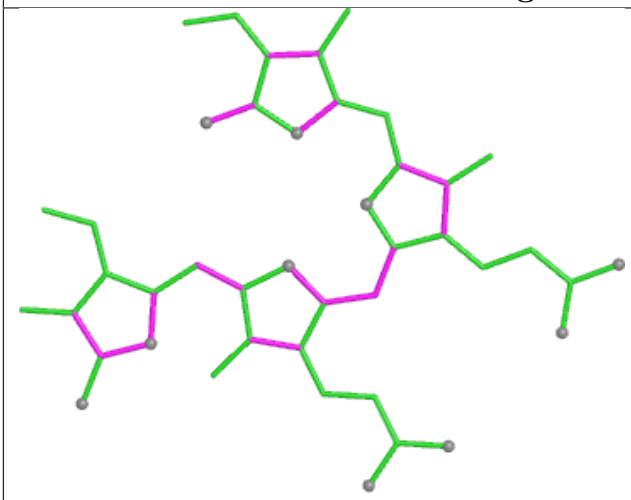

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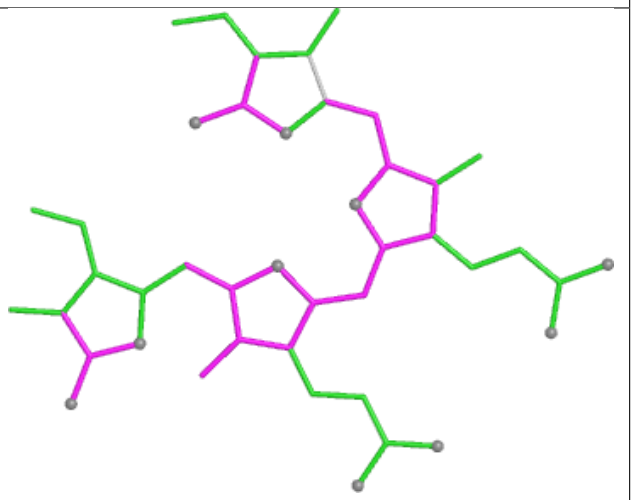

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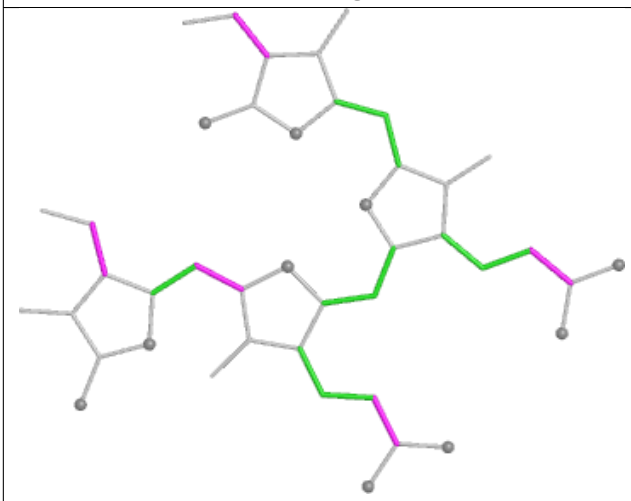

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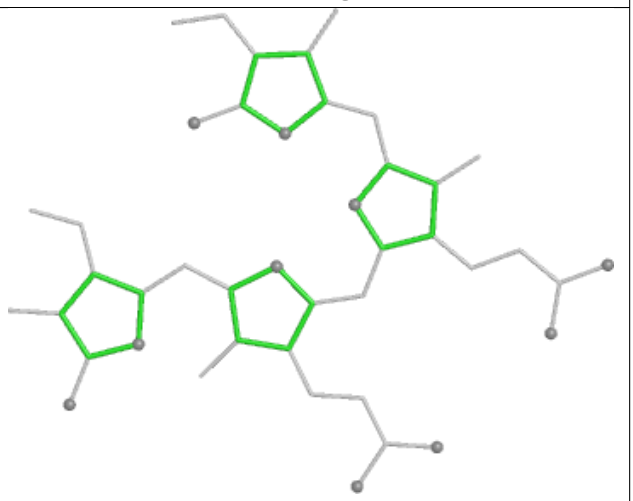

Rings

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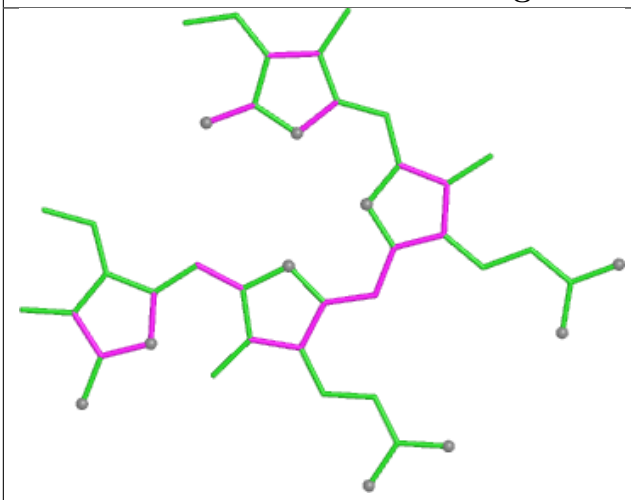

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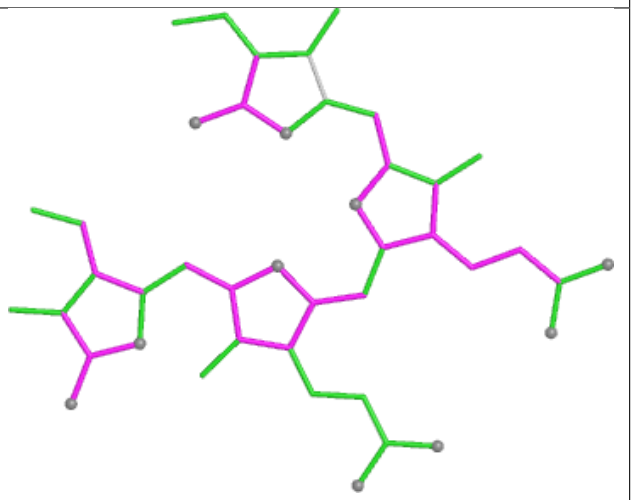

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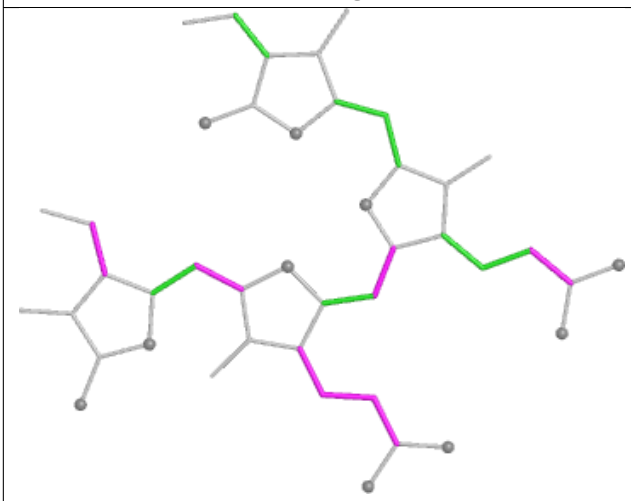

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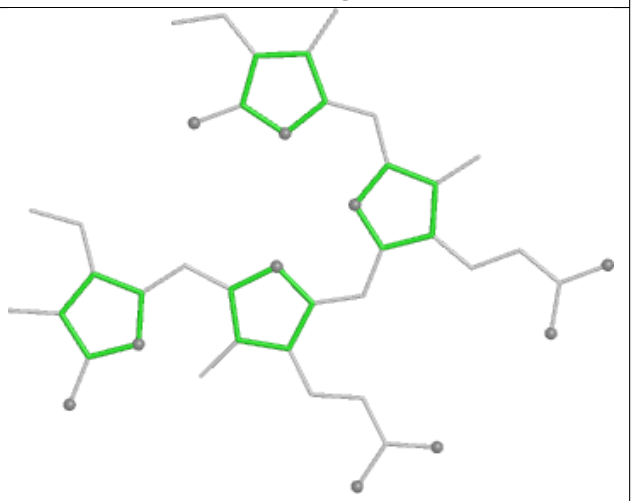
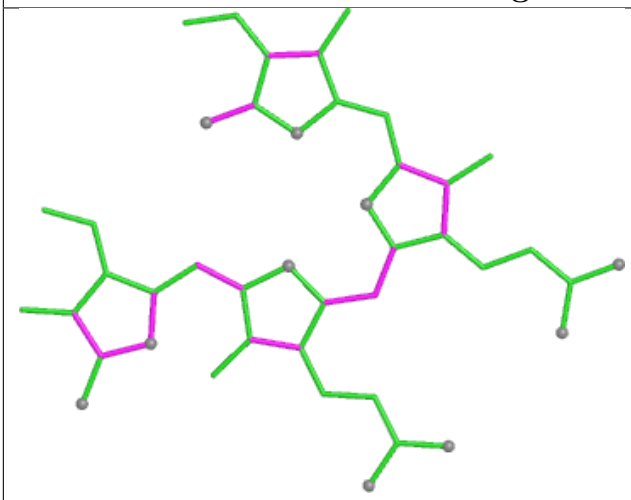


Rings

Ligand PEB M7 201



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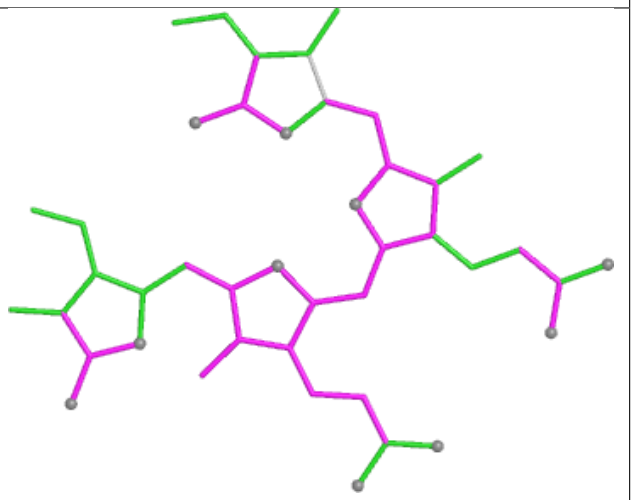

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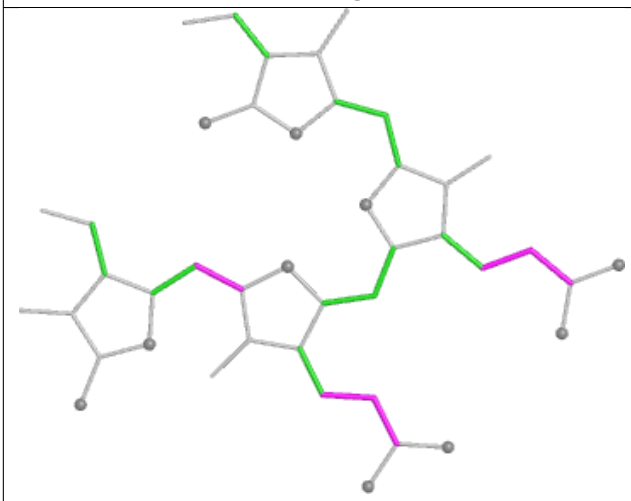

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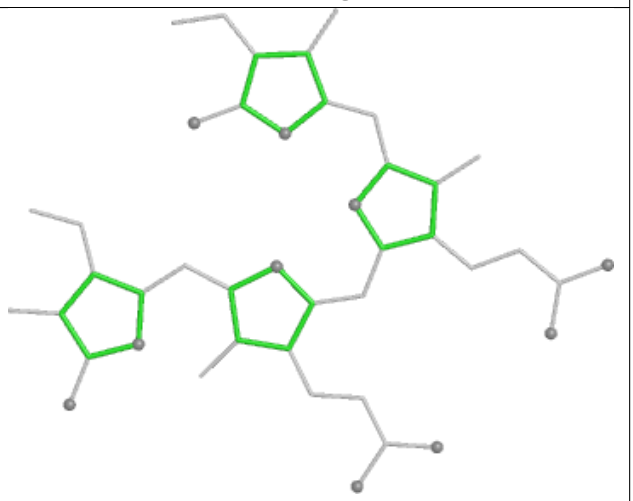
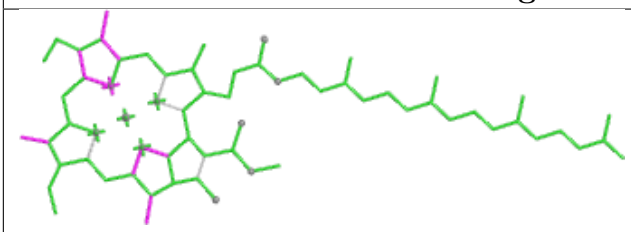


Rings

Ligand CLA b6 617



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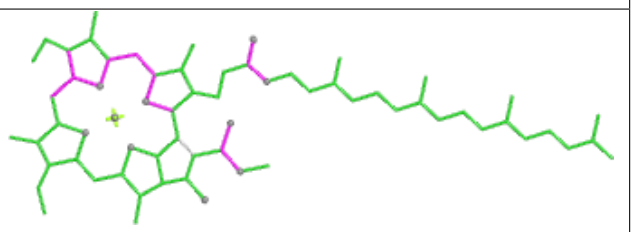
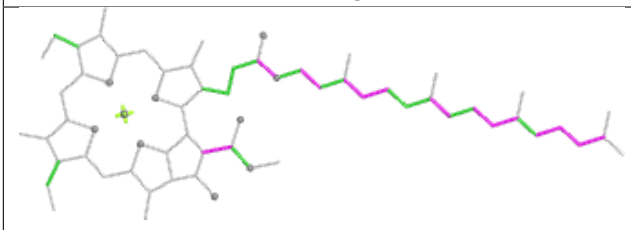


Bond angles



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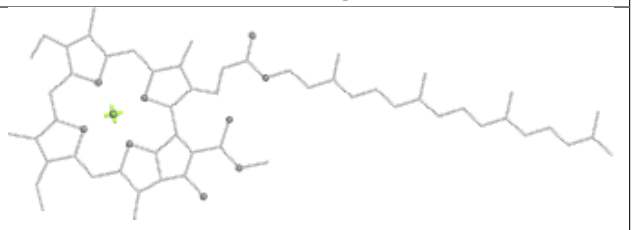
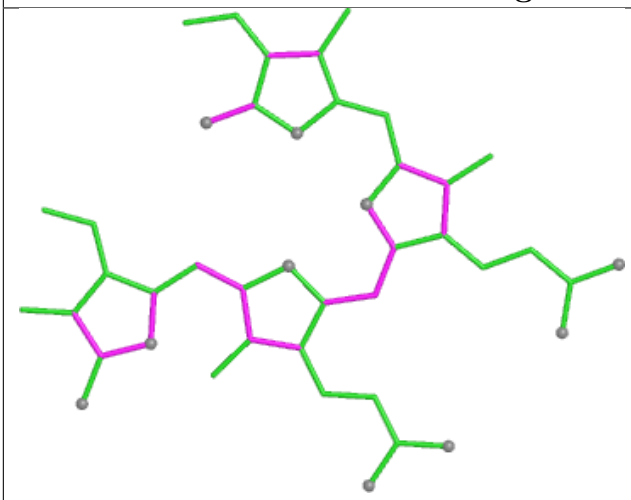


Rings

Ligand PEB ZE 203



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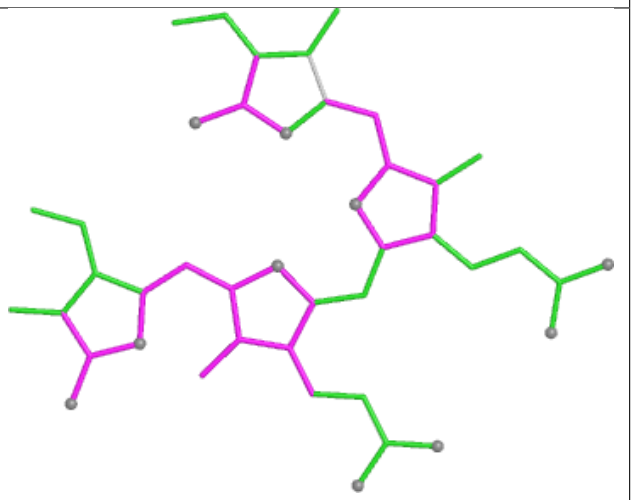
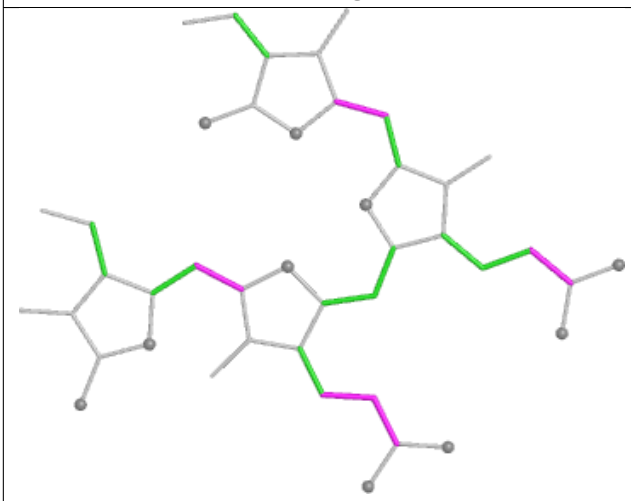


Bond angles



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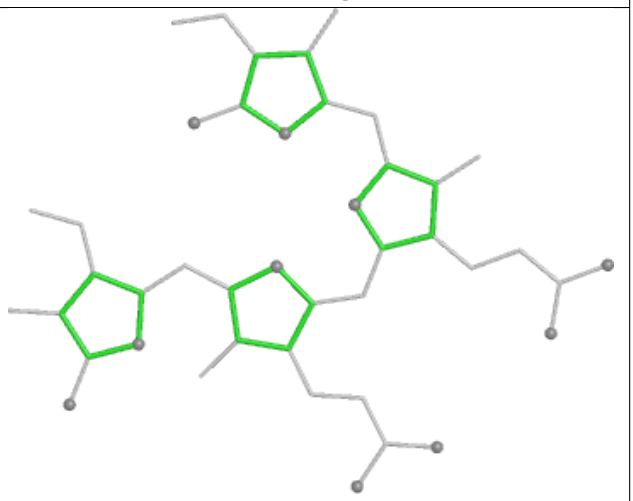
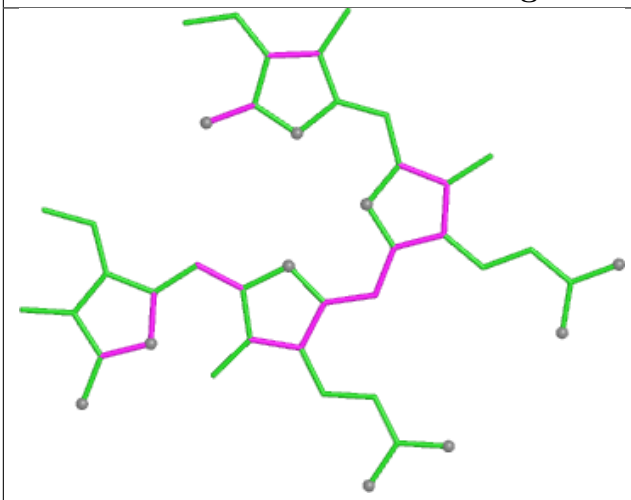


Rings

Ligand PEB jE 202



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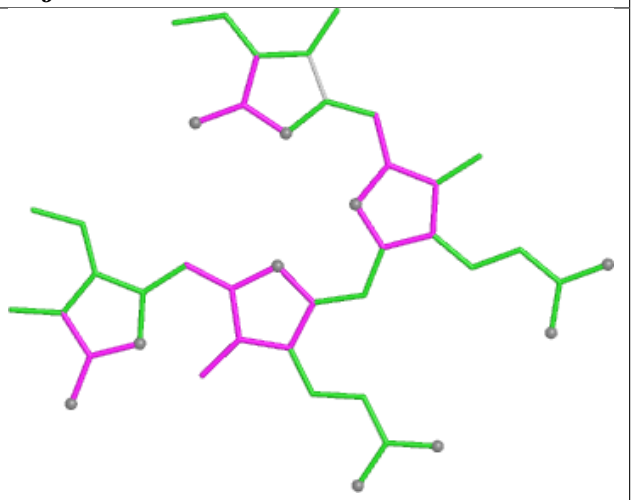
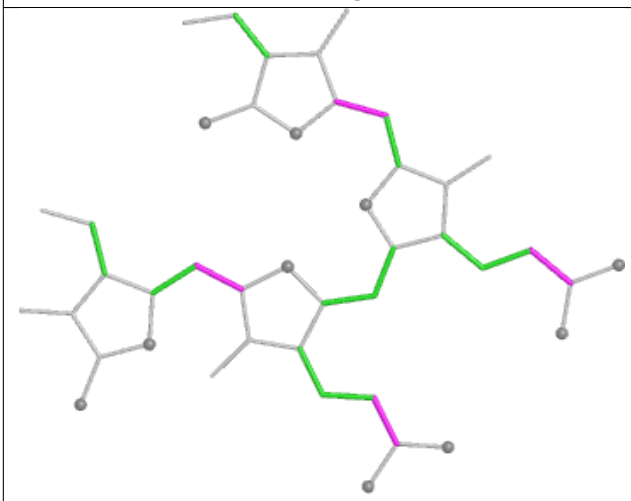


Bond angles



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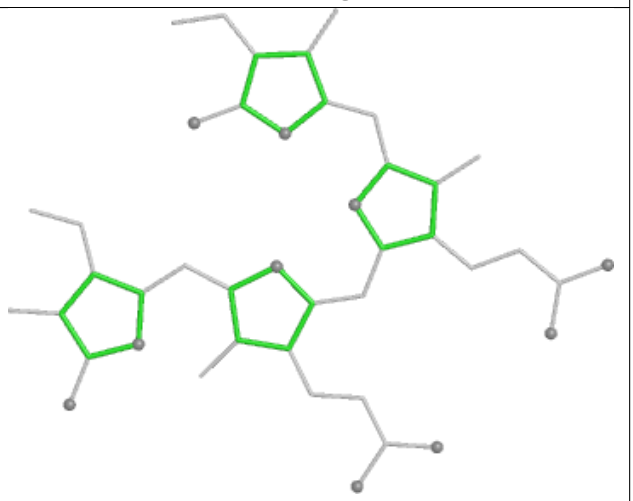
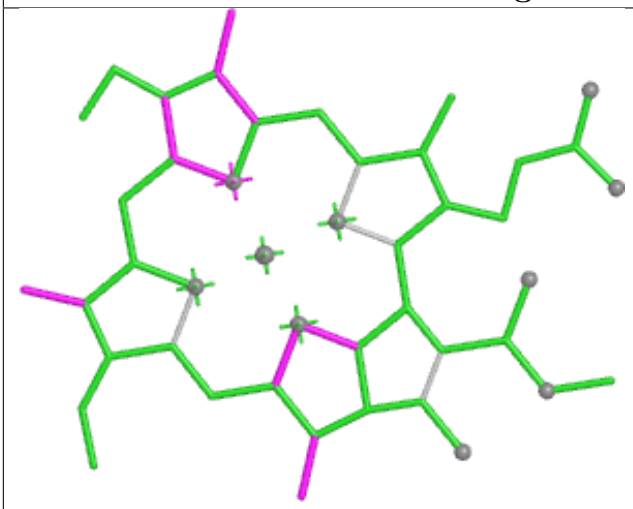


Rings

Ligand CLA 1N 611



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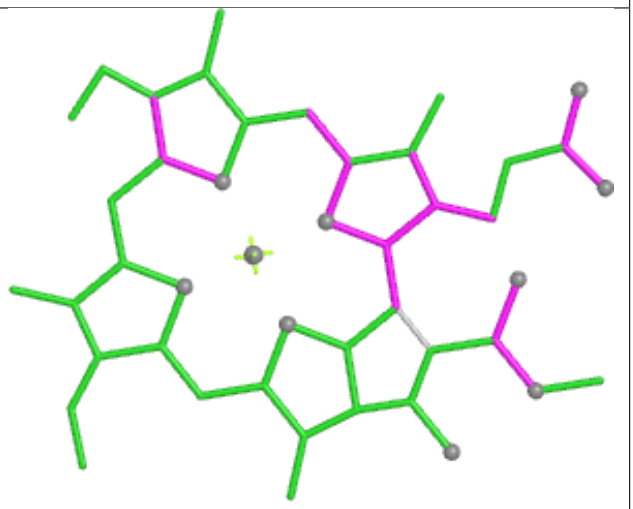
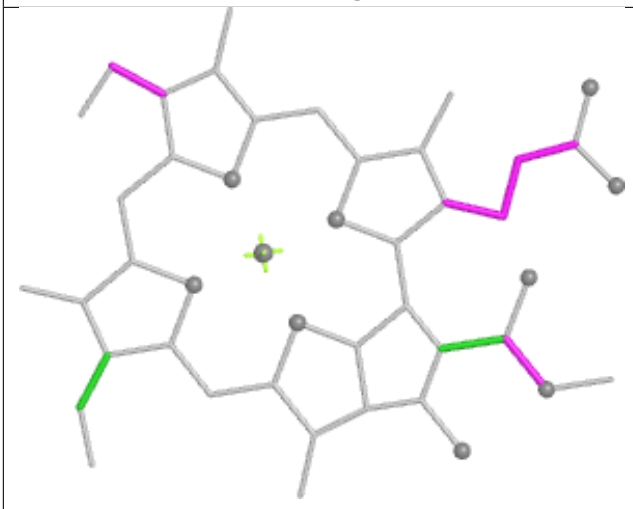


Bond angles

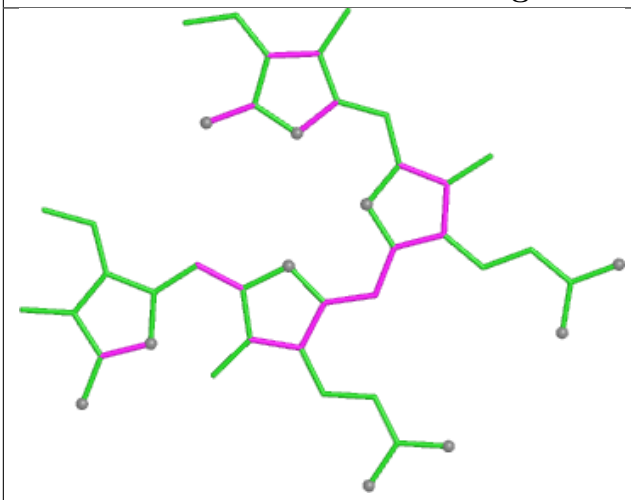


Torsions



Rings

Ligand PEB wC 201



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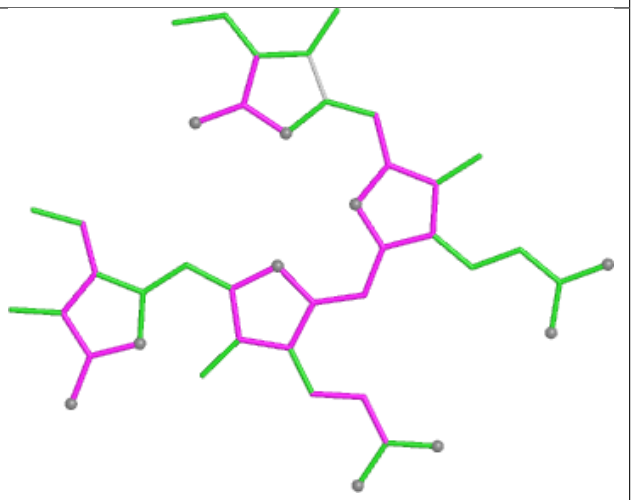

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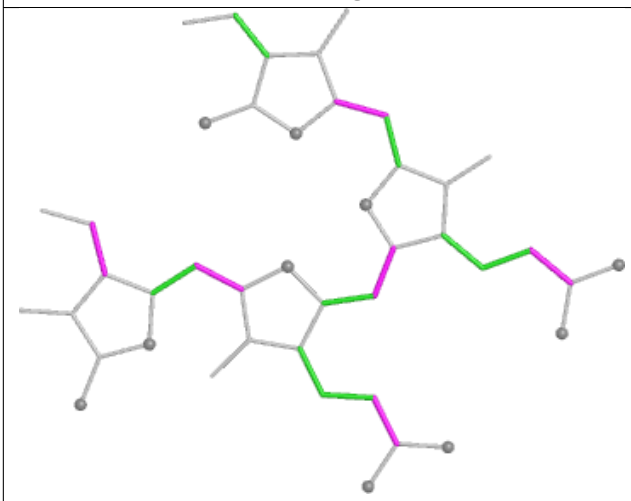

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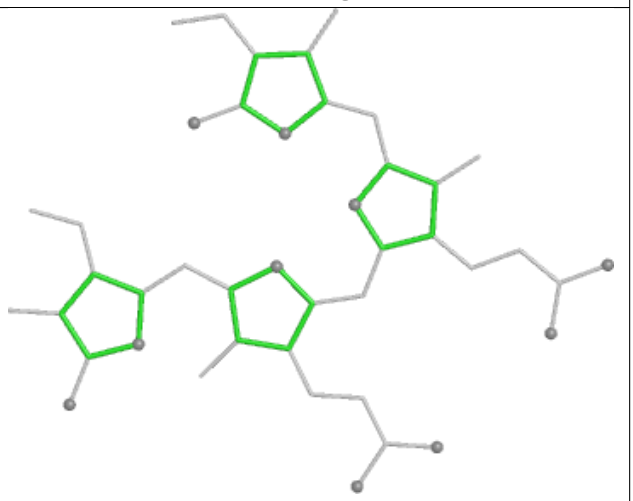
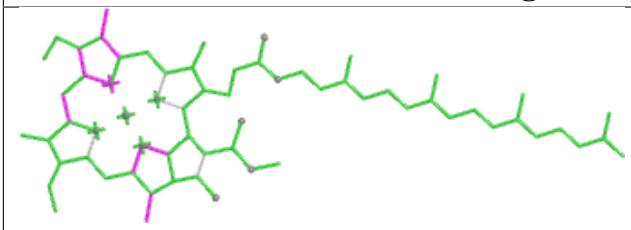


Rings

Ligand CLA c6 608



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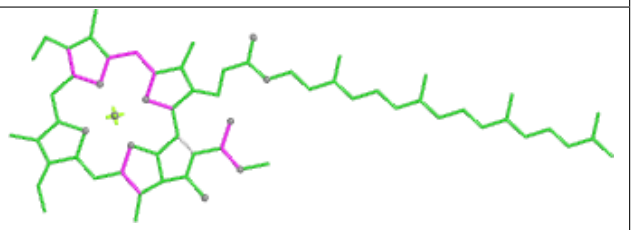

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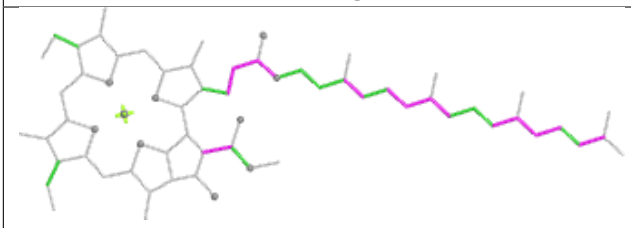

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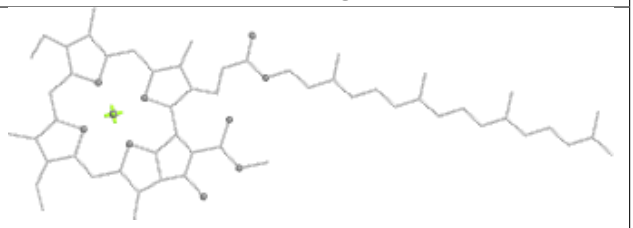
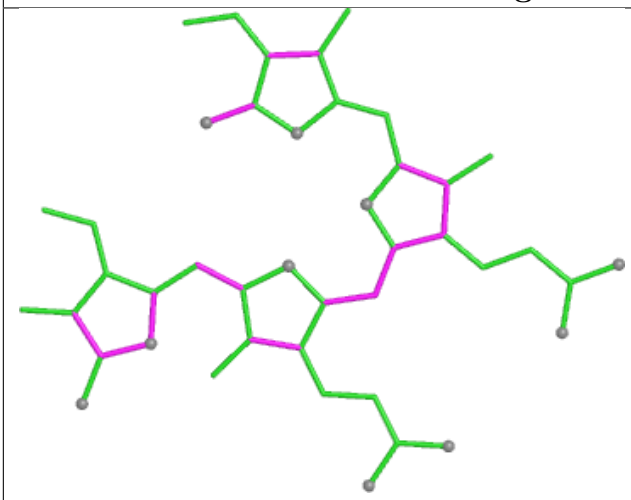


Rings

Ligand PEB DJ 202



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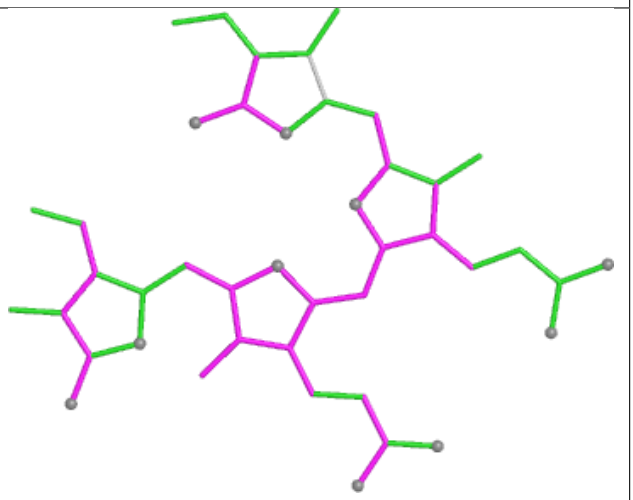

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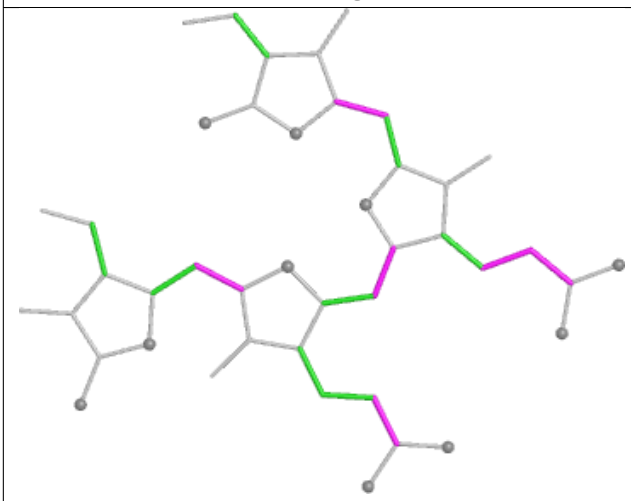

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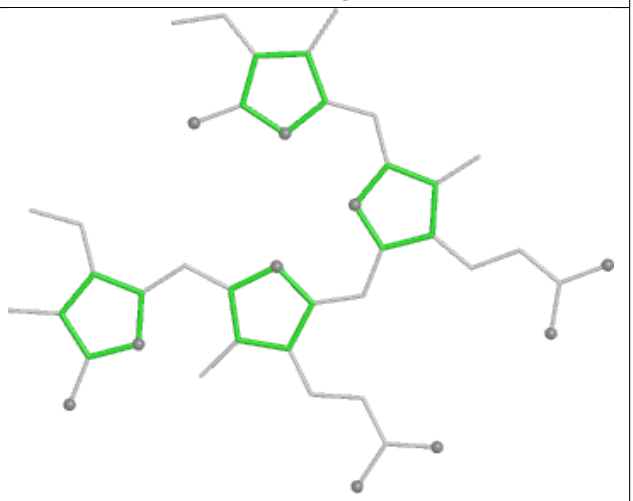
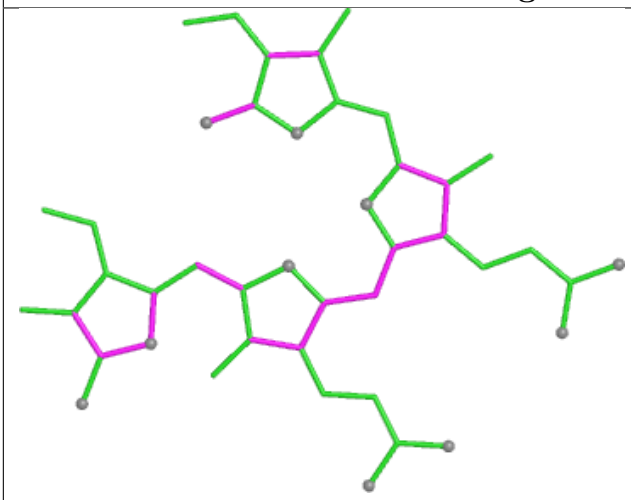


Rings

Ligand PEB hJ 201



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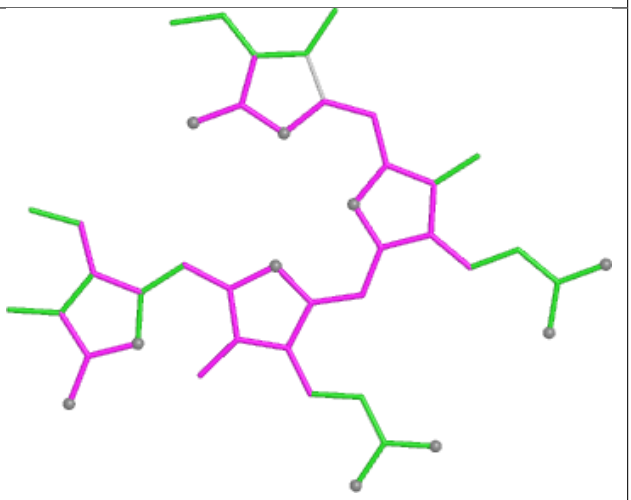

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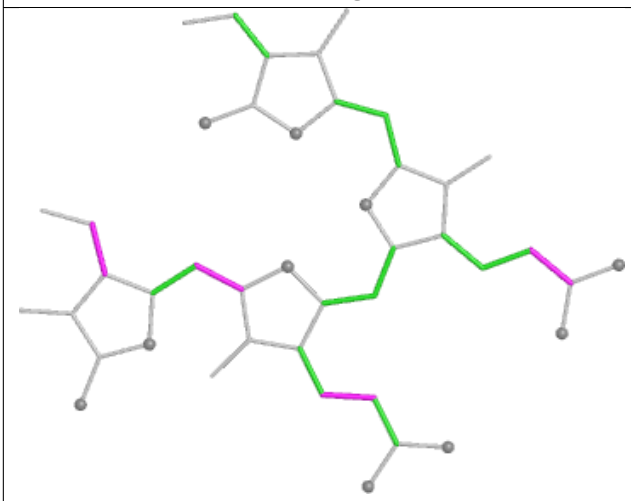

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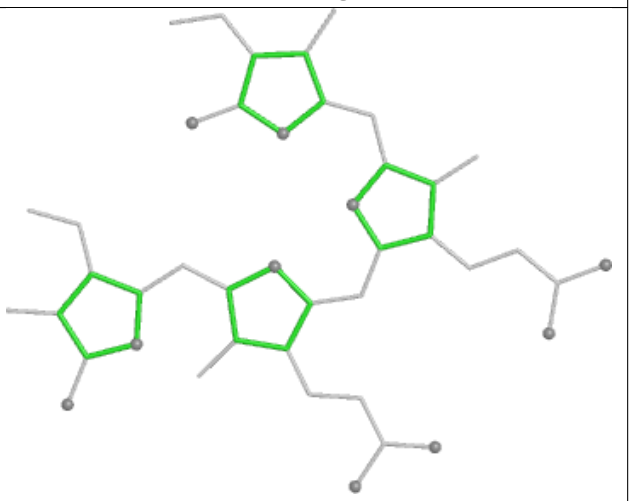

Rings

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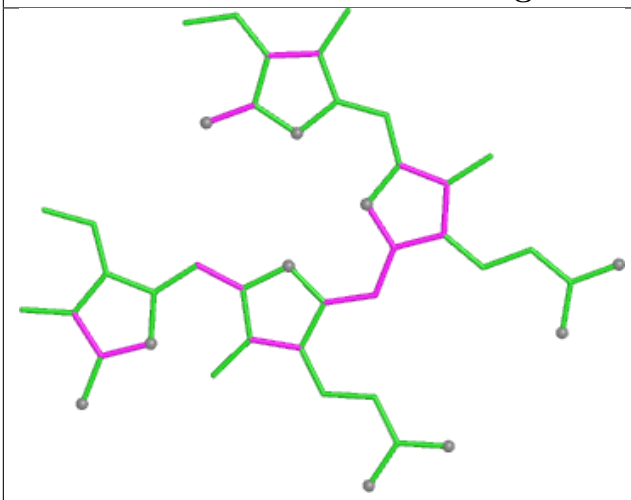

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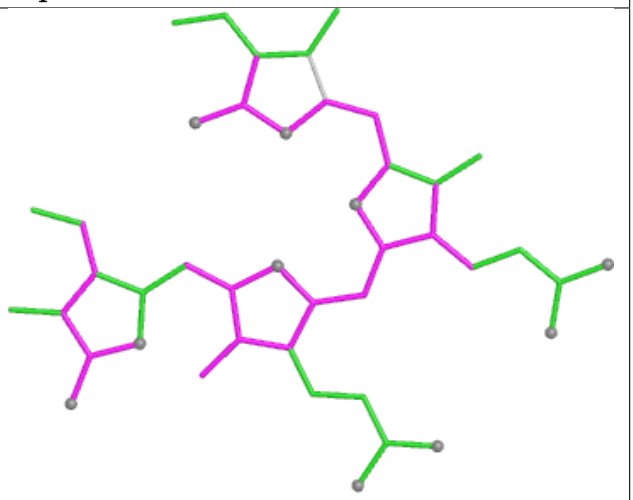

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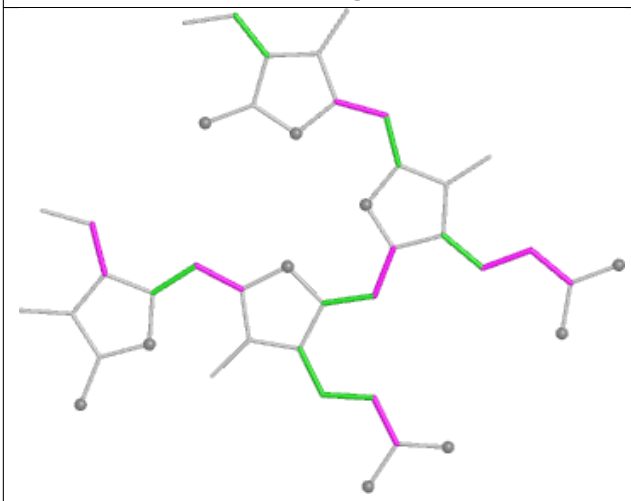

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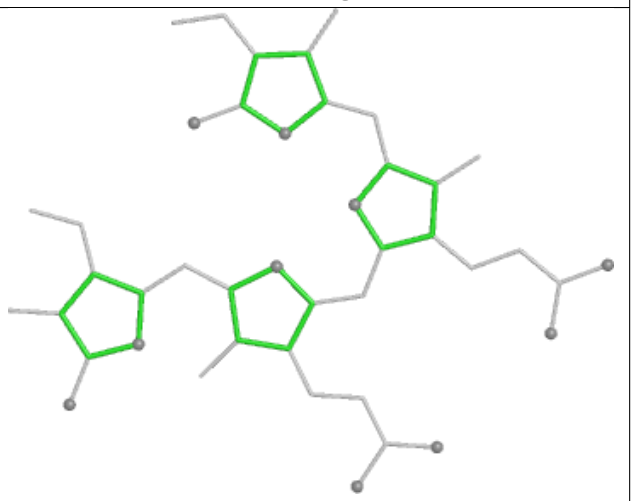
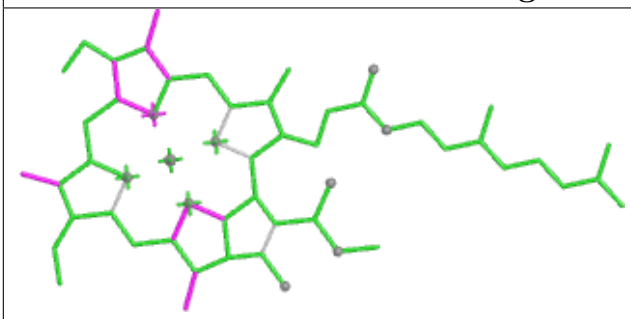


Rings

Ligand CLA cL 516



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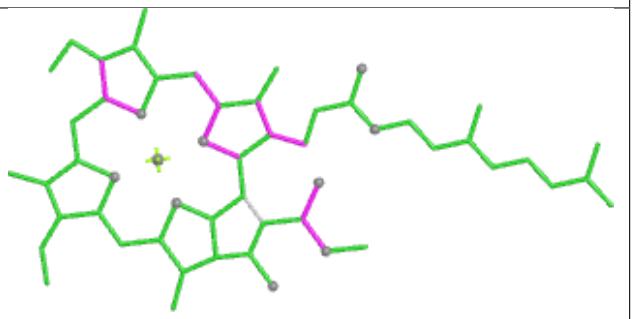

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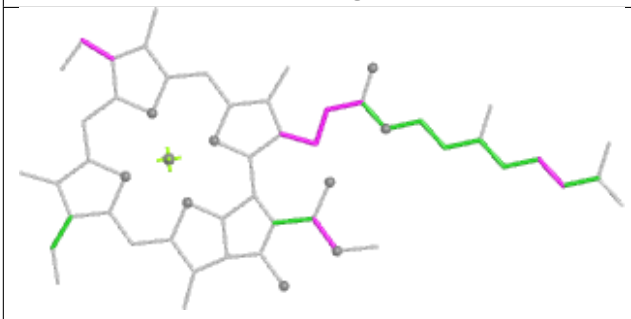

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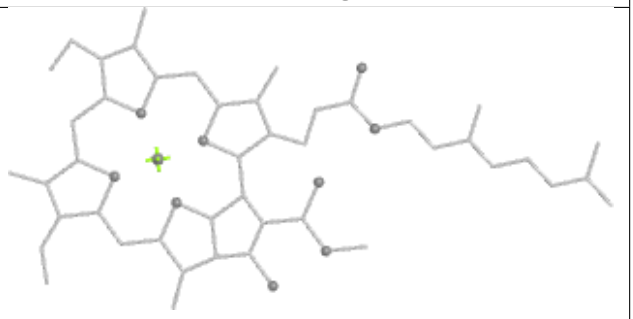
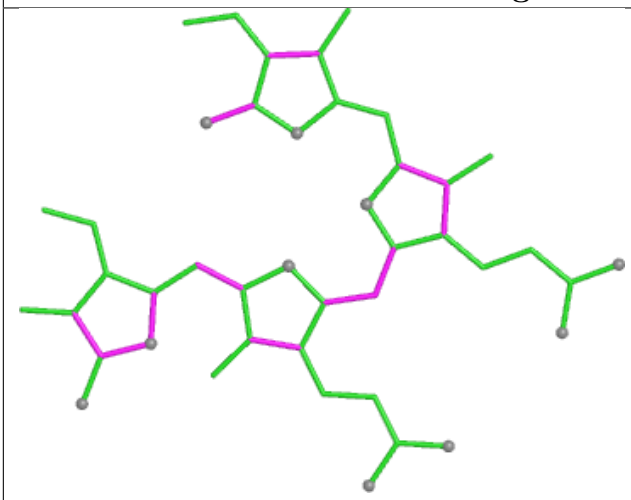


Rings

Ligand PEB KF 201



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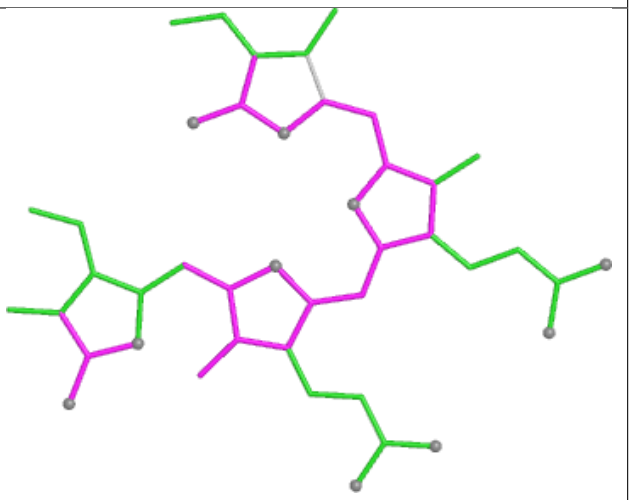

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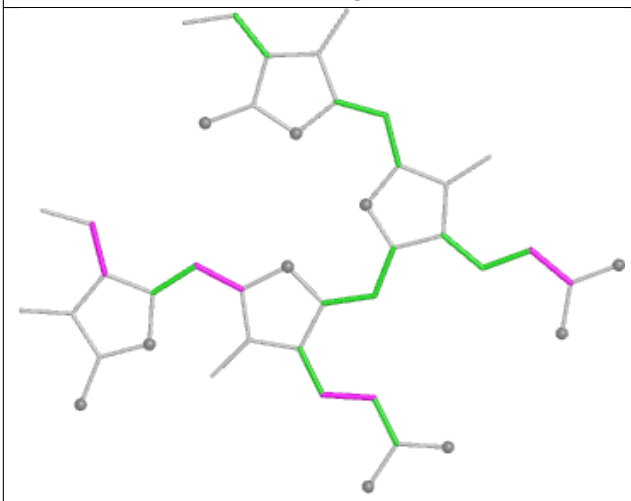

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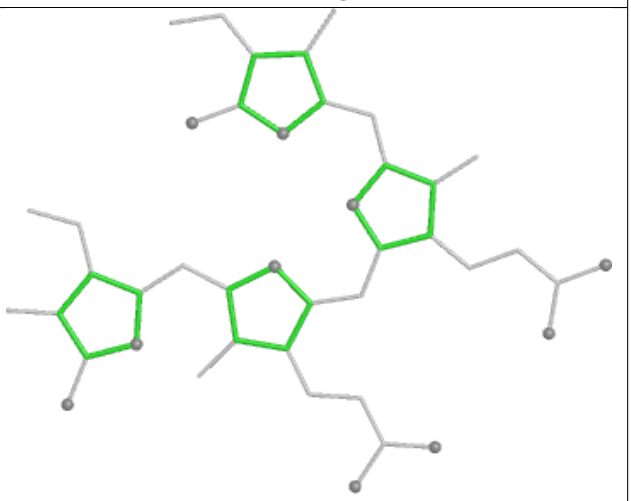
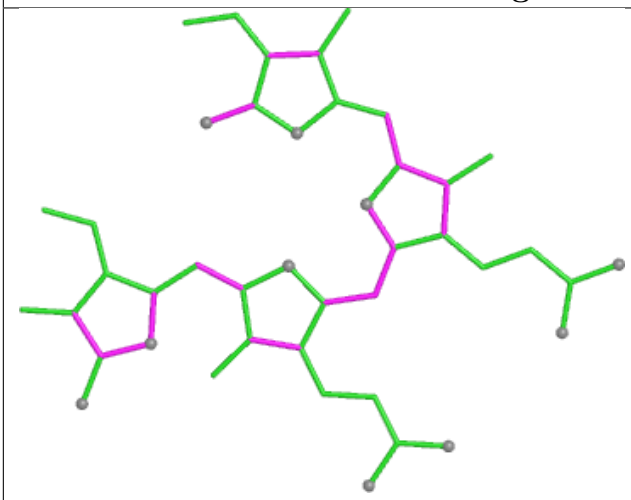


Rings

Ligand PEB YA 301



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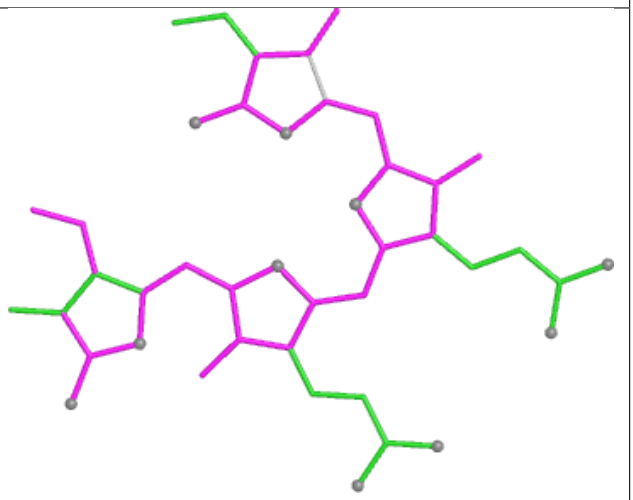

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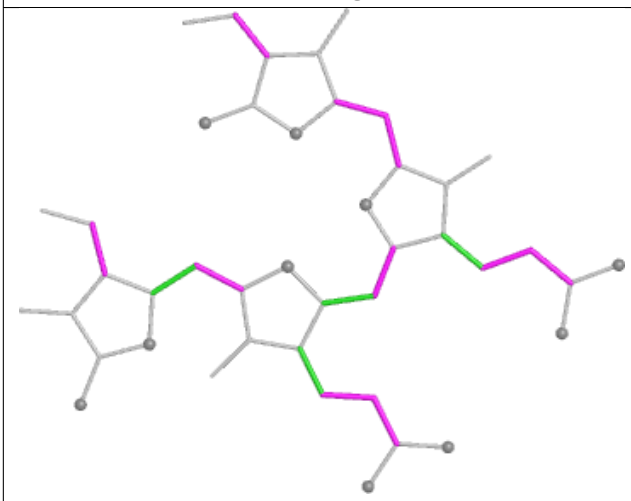

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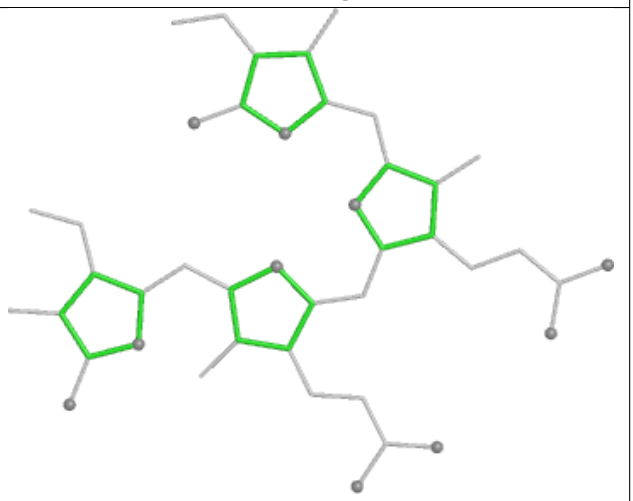
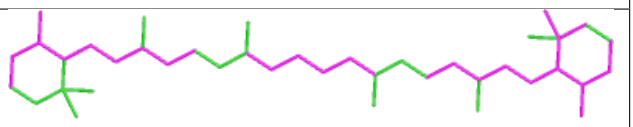


Rings

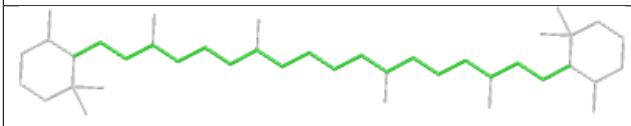
Ligand BCR B6 621



Bond lengths



Bond angles



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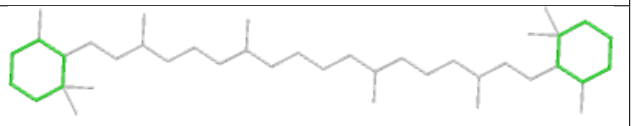
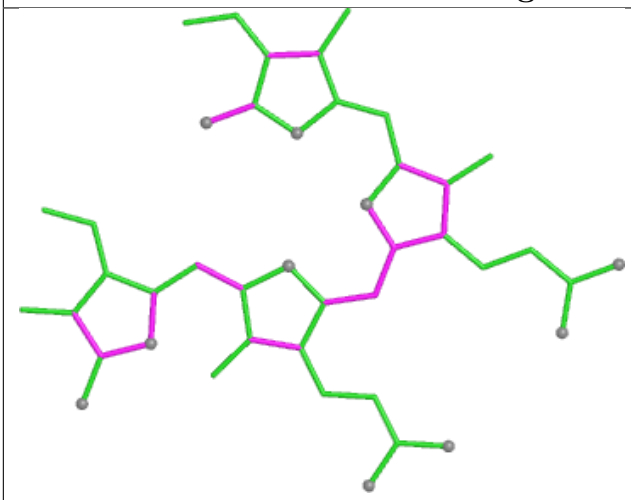


Rings

Ligand PEB VI 202



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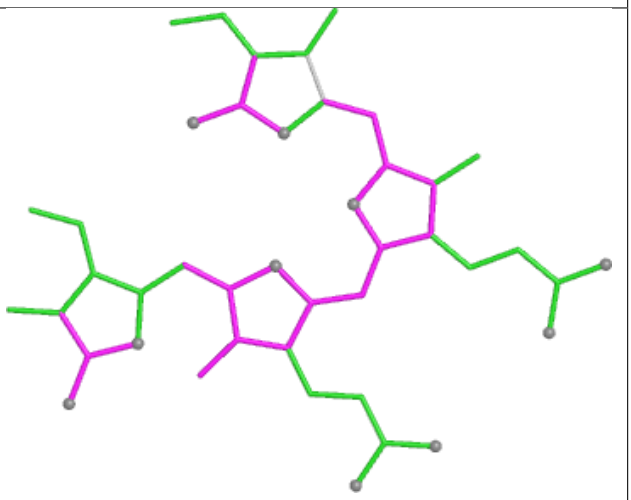

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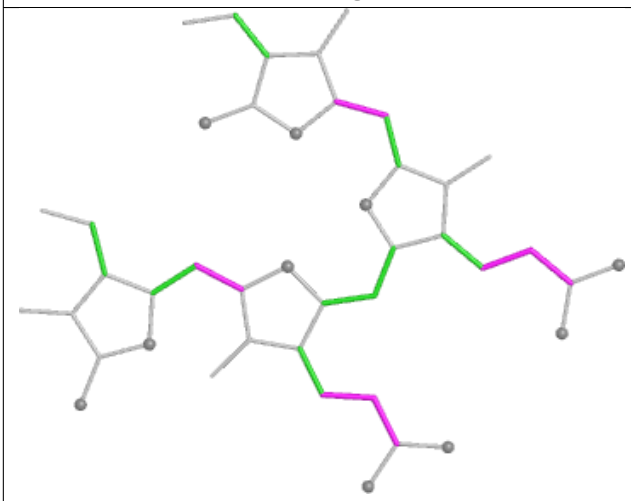

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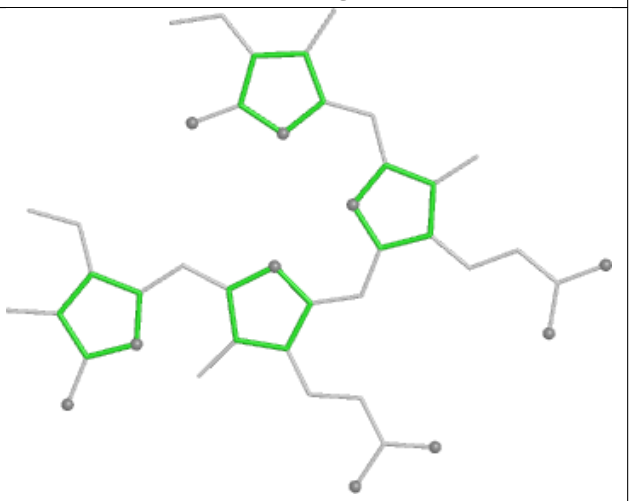
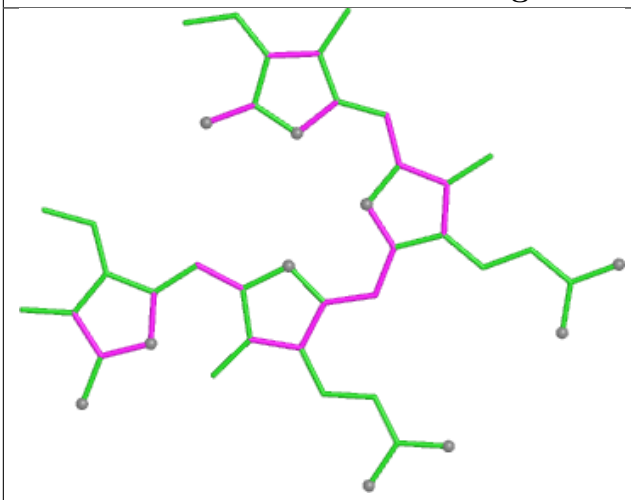


Rings

Ligand PEB TK 202



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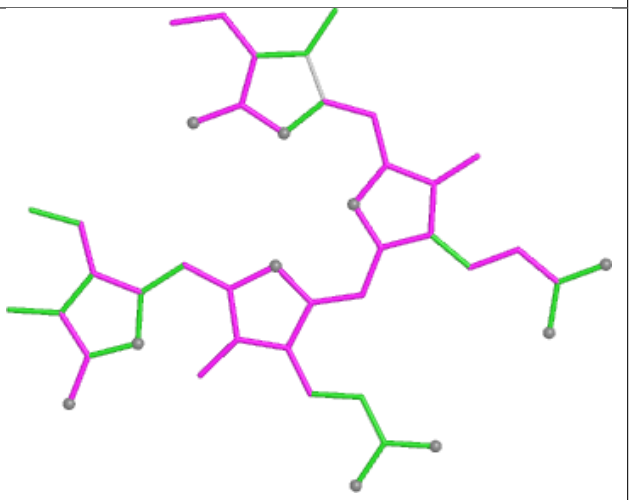
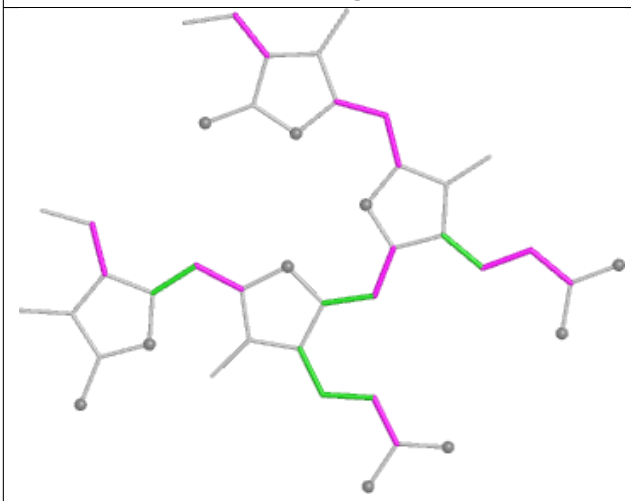


Bond angles



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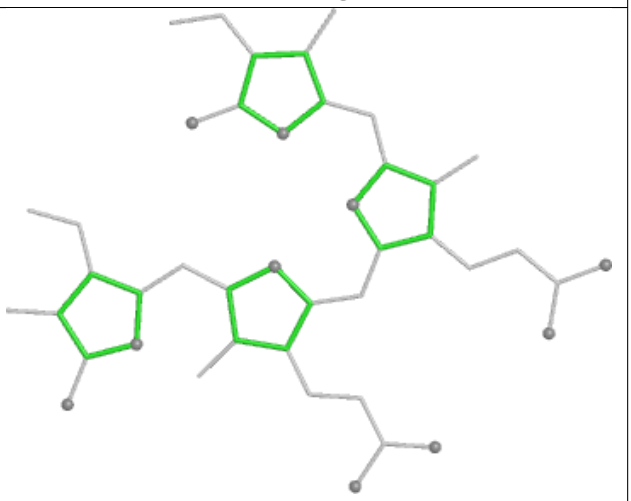
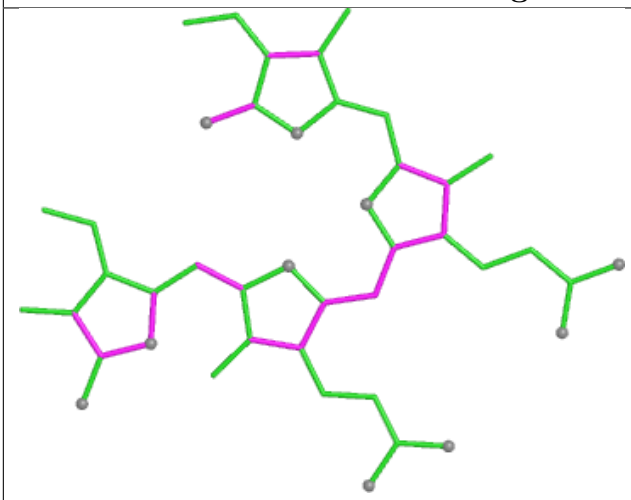


Rings

Ligand PEB AG 301



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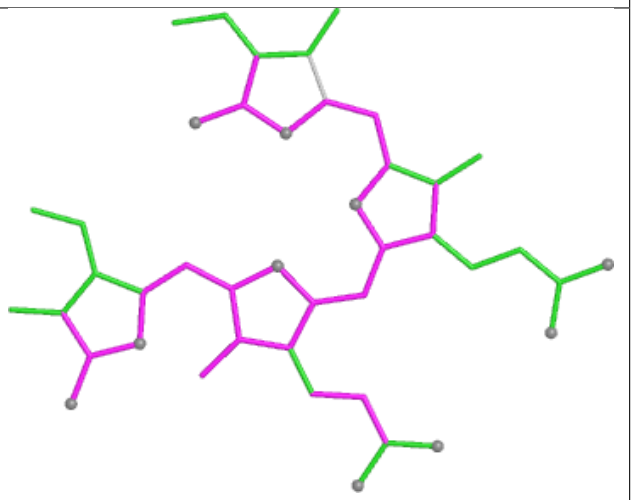
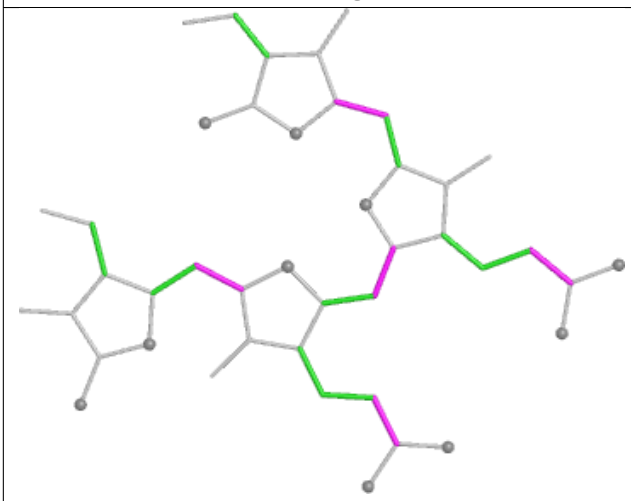


Bond angles



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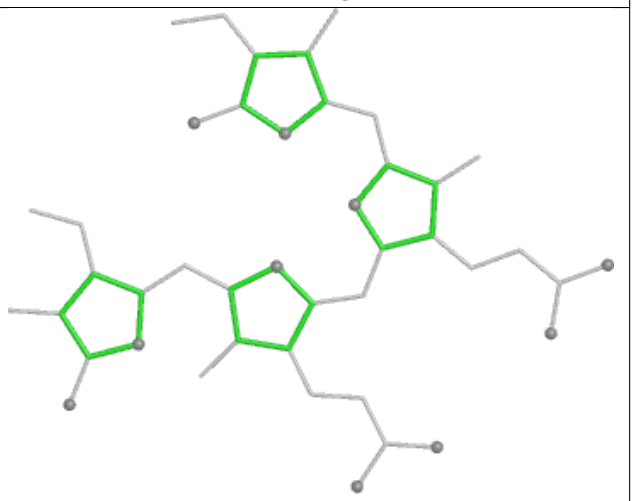
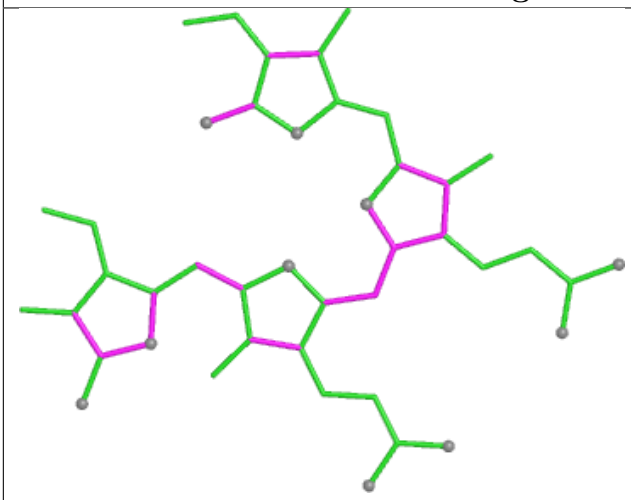


Rings

Ligand PEB YP 502



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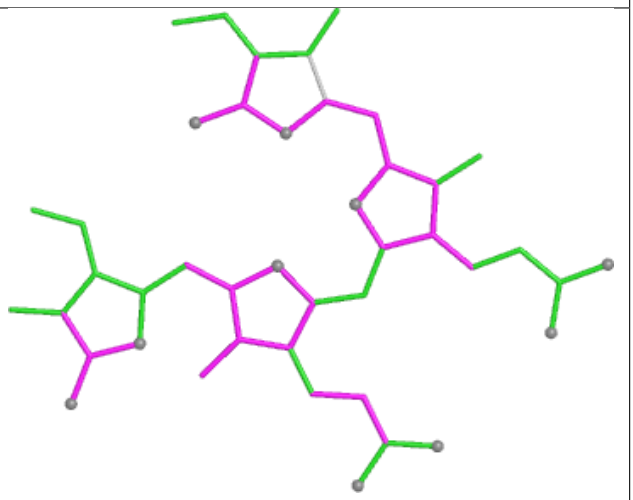
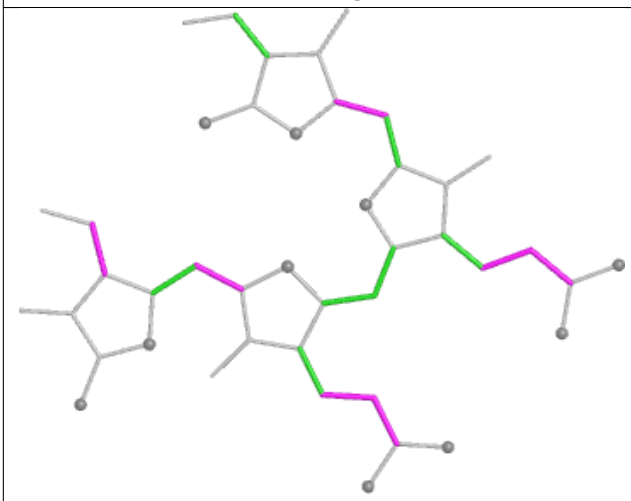


Bond angles



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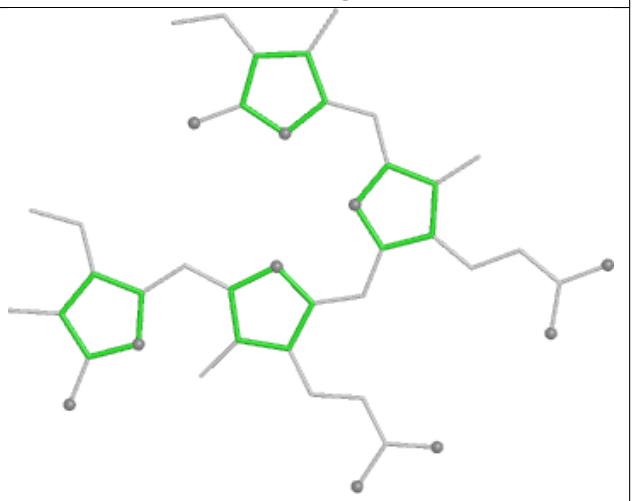
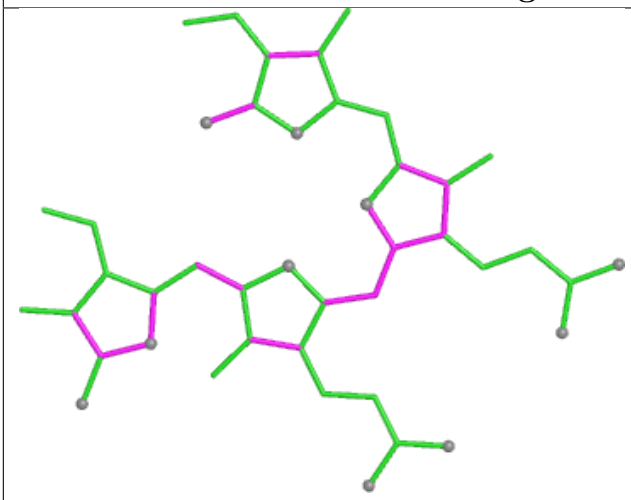


Rings

Ligand PEB SJ 202



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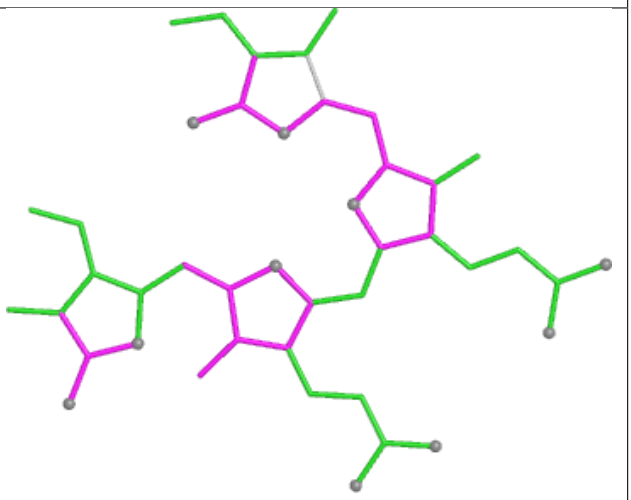
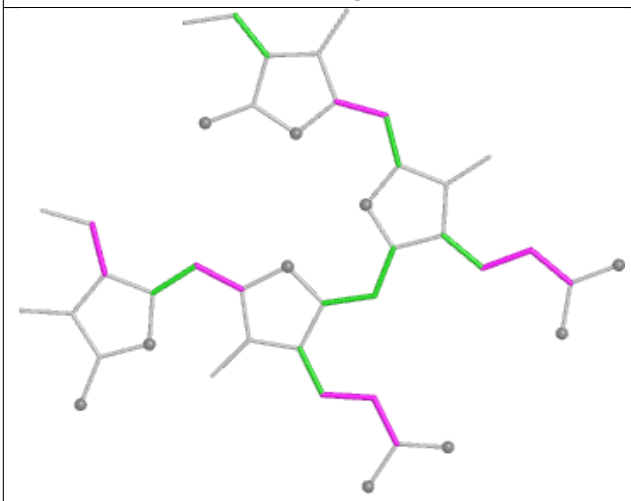


Bond angles



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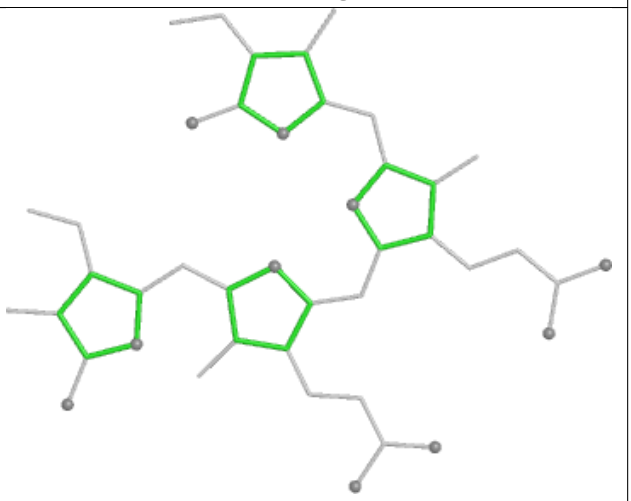
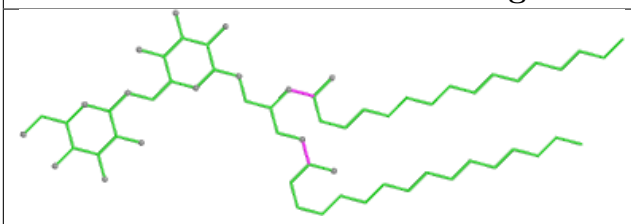
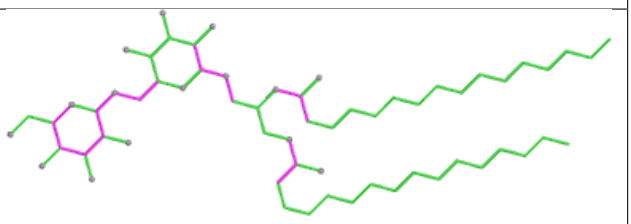


Rings

Ligand DGD AL 414



Bond lengths



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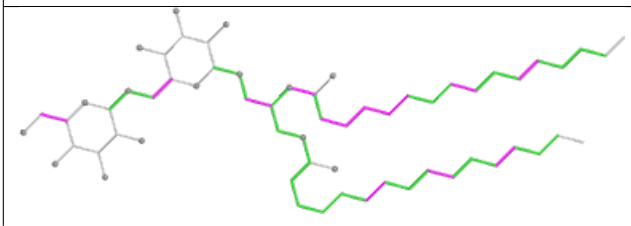
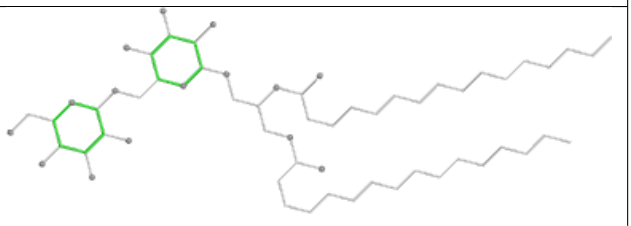
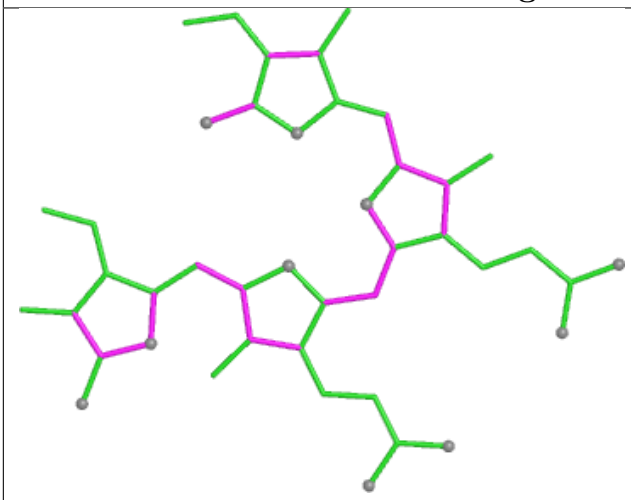


Torsions



Rings

Ligand PEB S9 201



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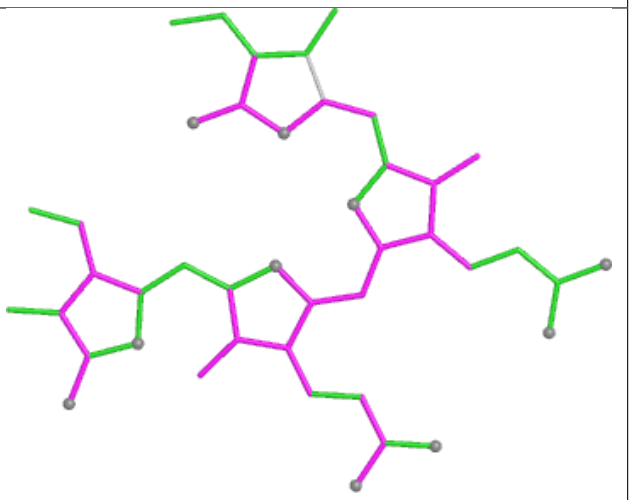

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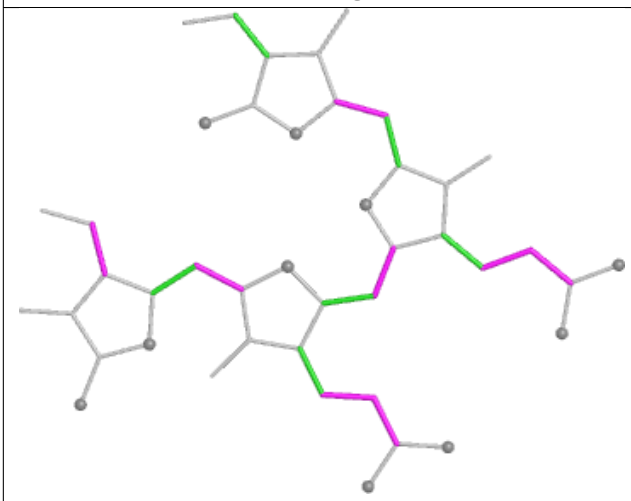

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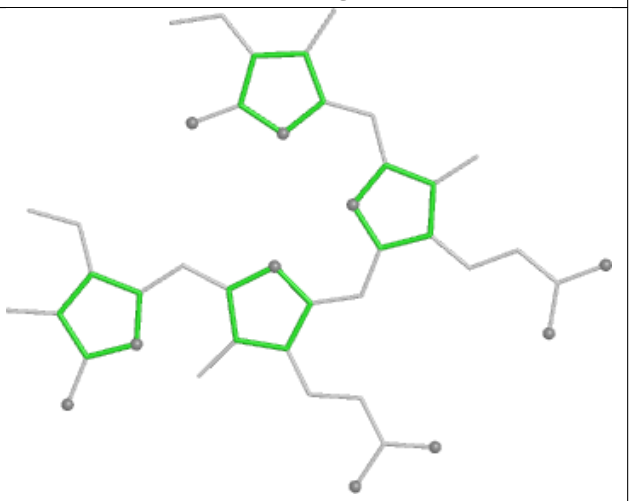
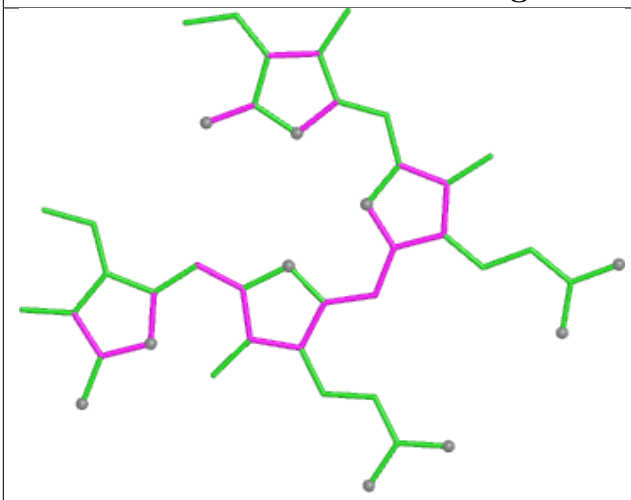


Rings

Ligand PEB OD 202



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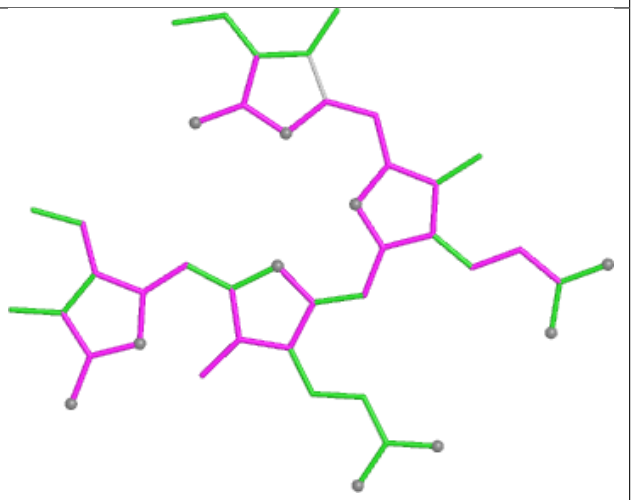

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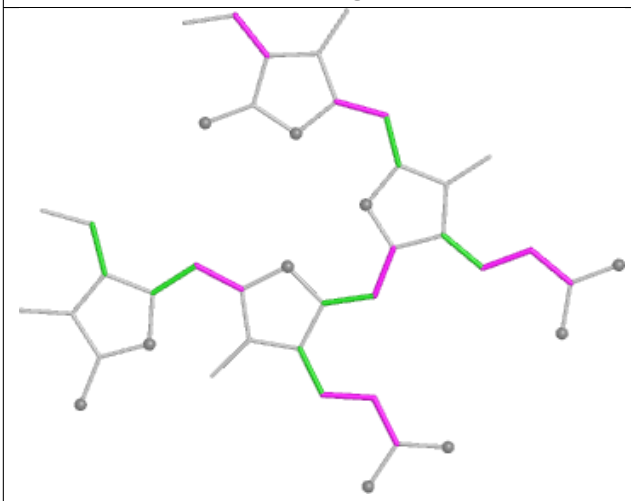

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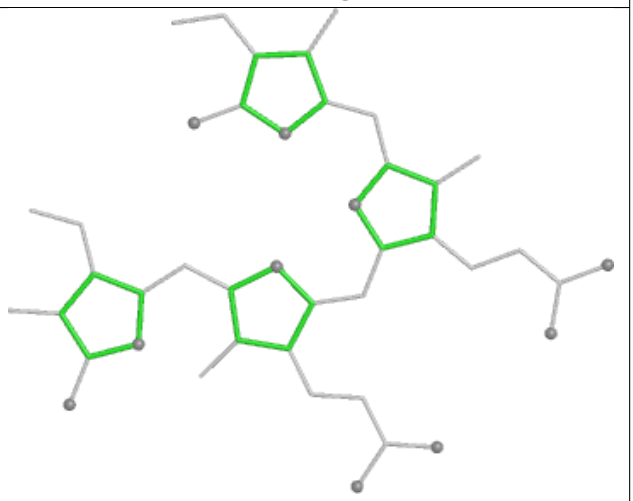
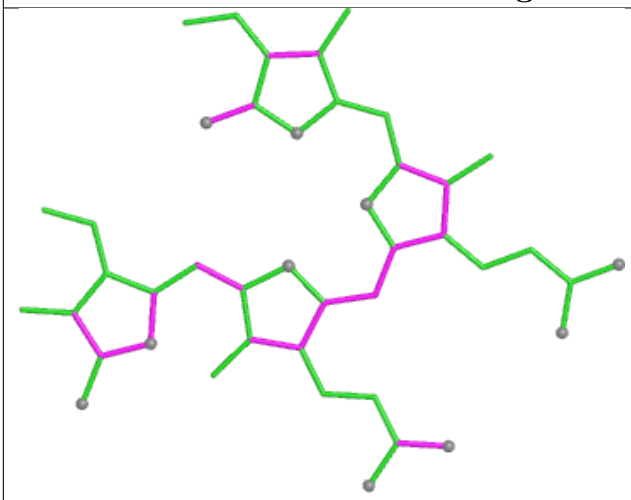


Rings

Ligand PEB aO 203



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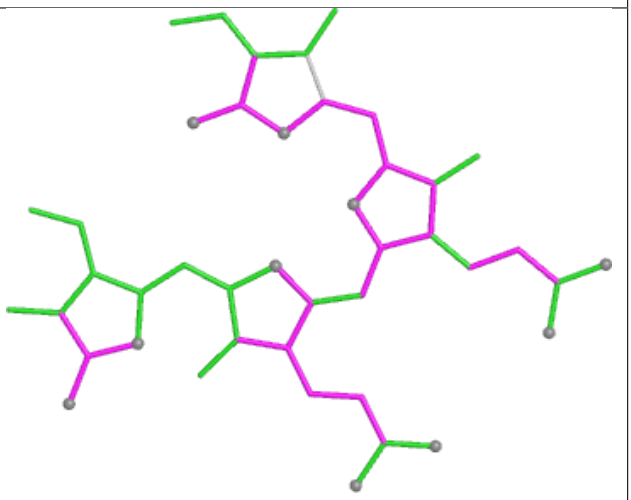

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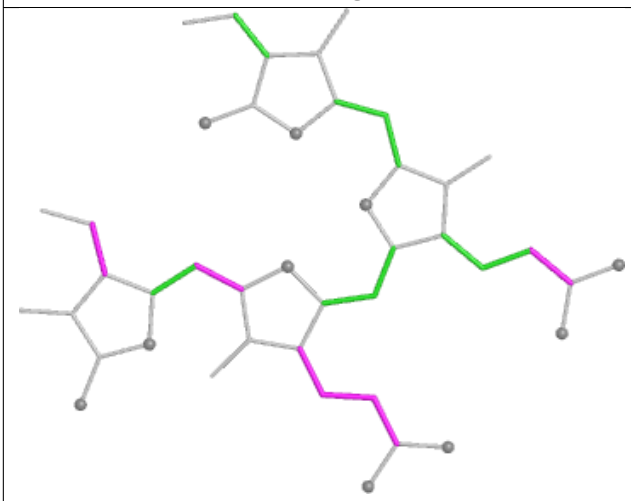

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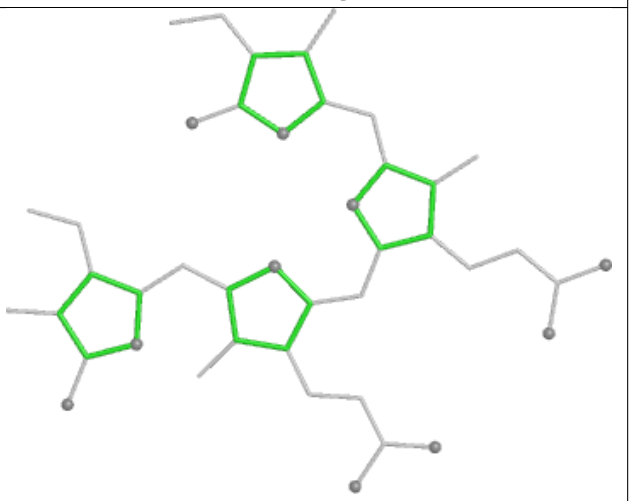
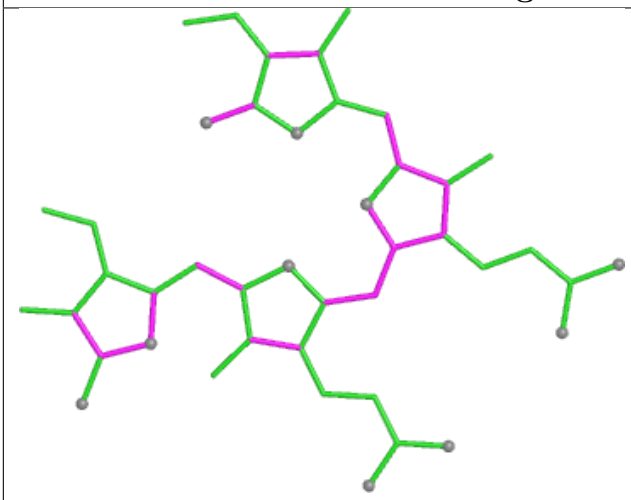


Rings

Ligand PEB bF 202



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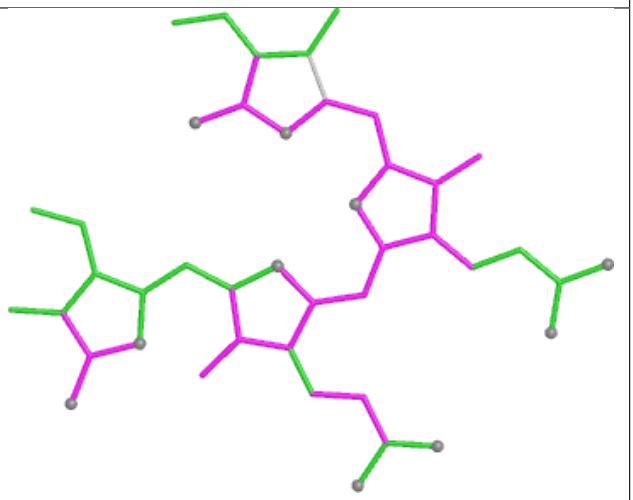
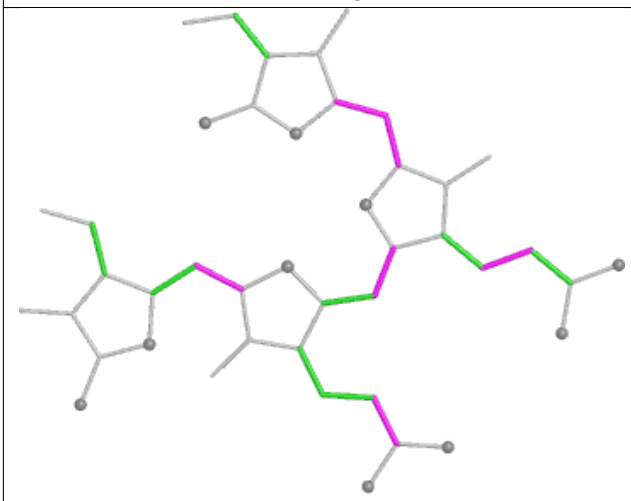


Bond angles



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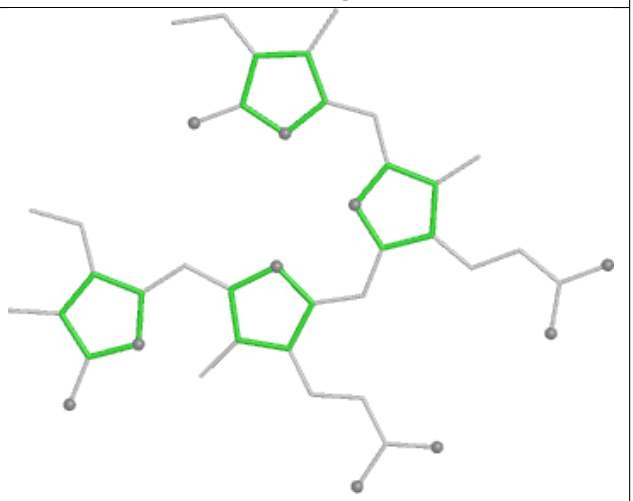
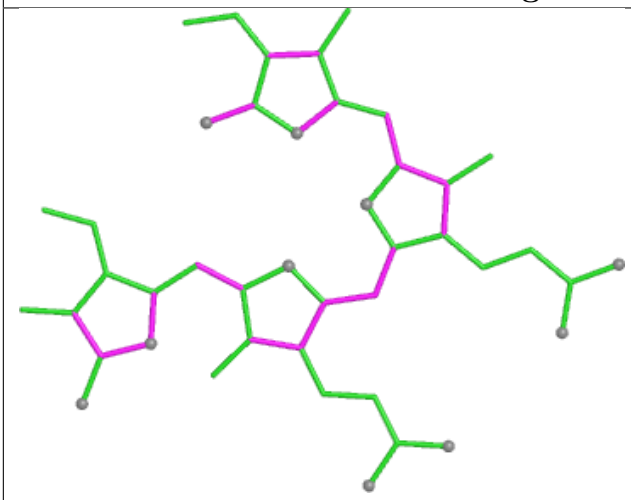


Rings

Ligand PEB I7 201



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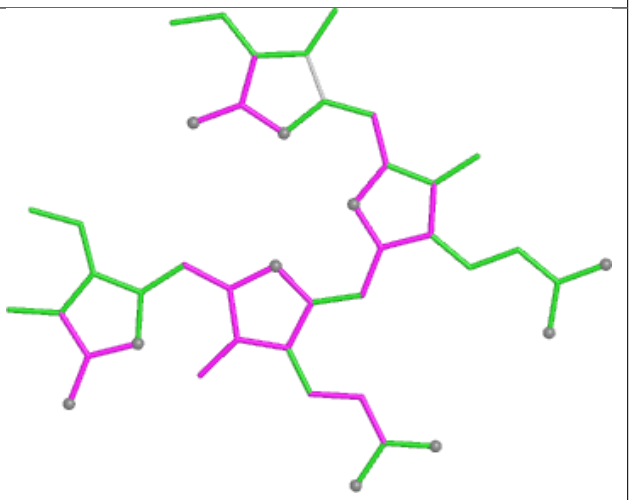

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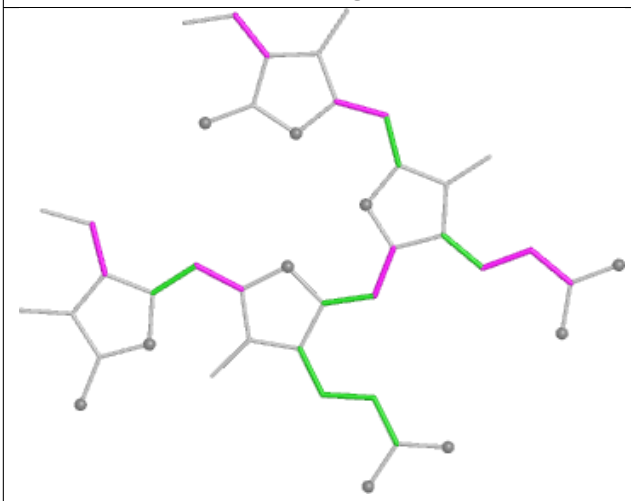

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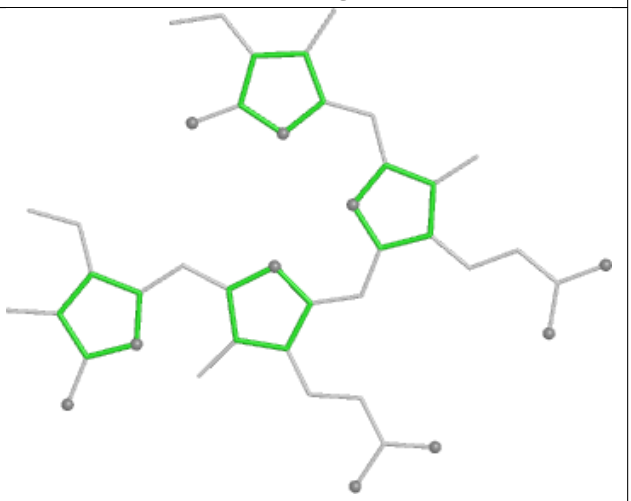
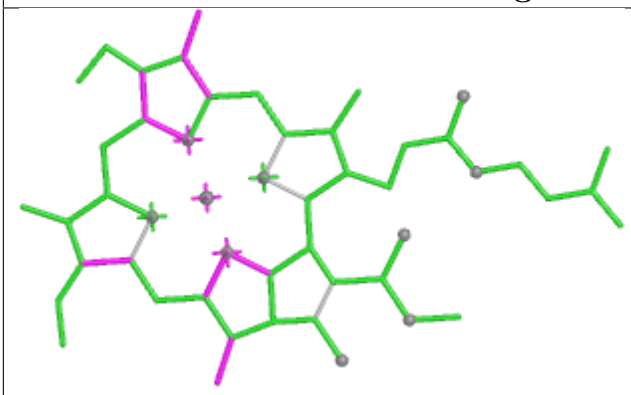


Rings

Ligand CLA 2N 309



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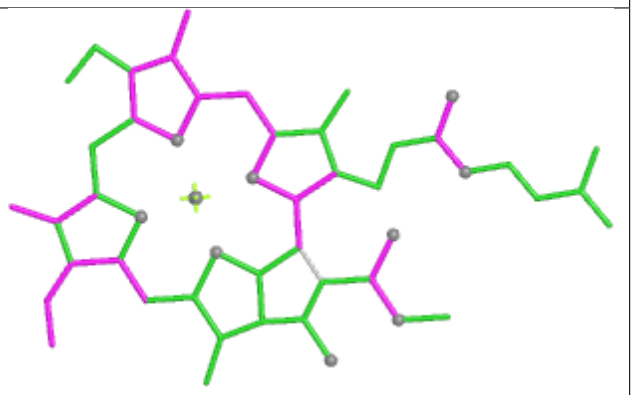

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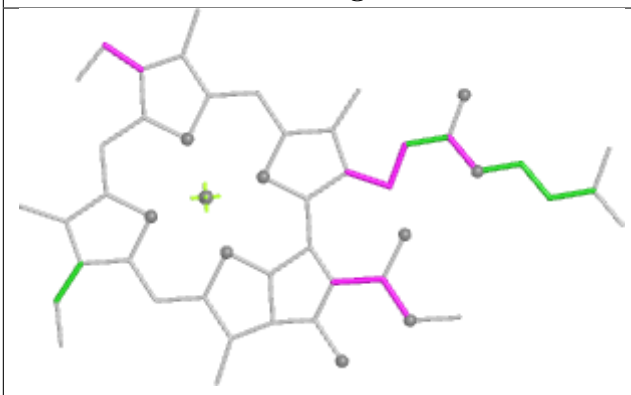

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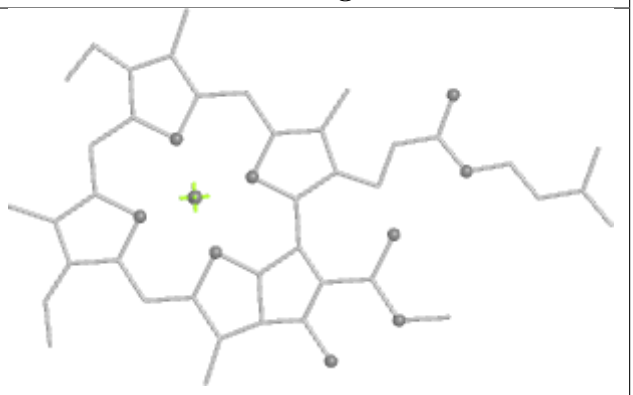
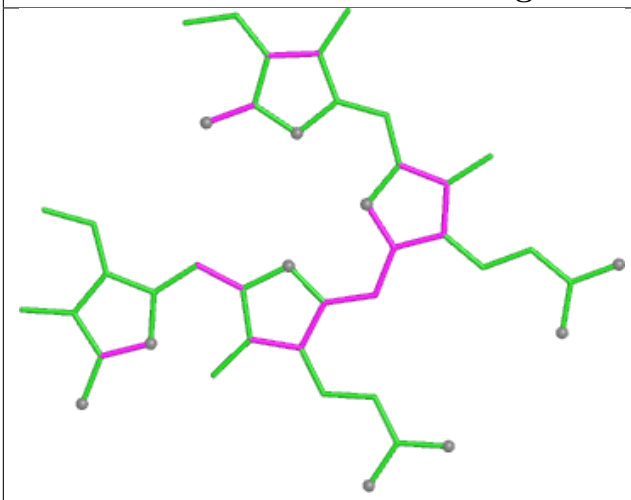


Rings

Ligand PEB xC 201



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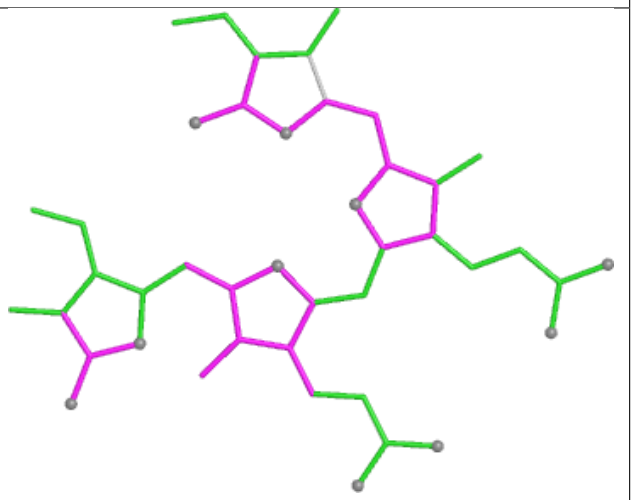

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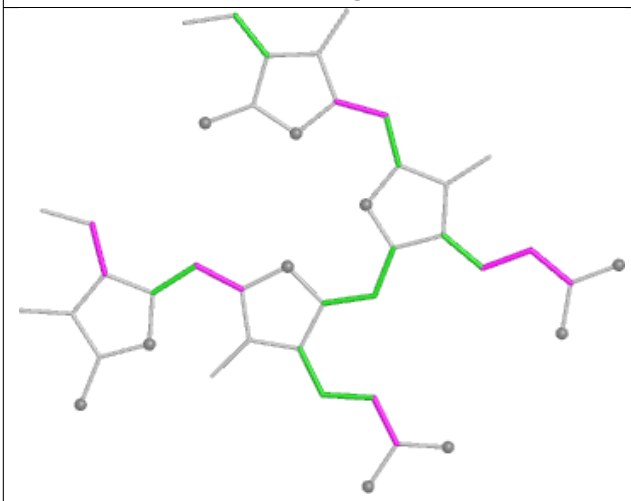

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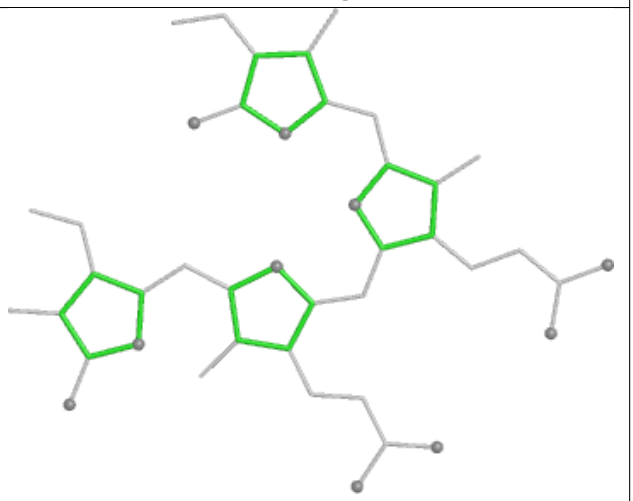
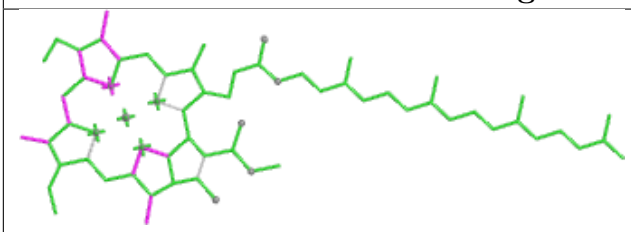


Rings

Ligand CLA aL 605



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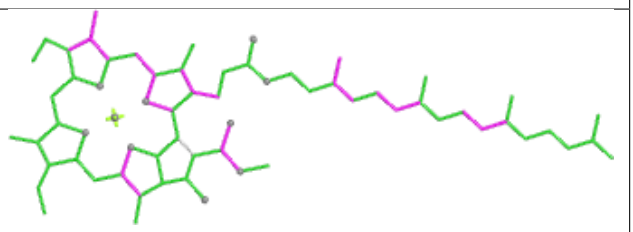

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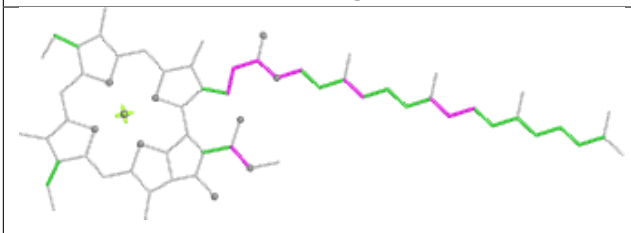

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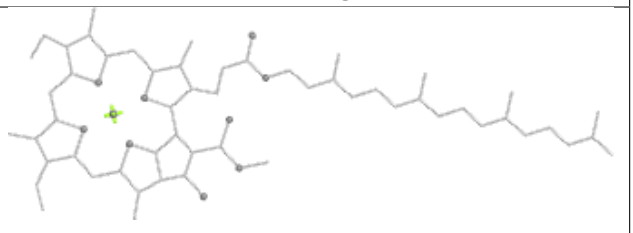
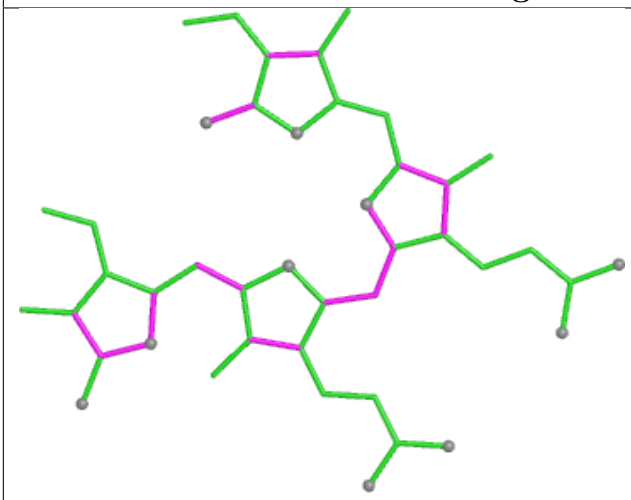


Rings

Ligand PEB HF 202



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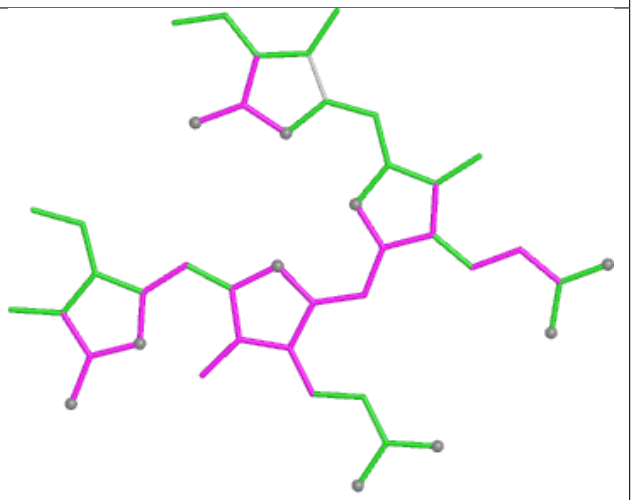
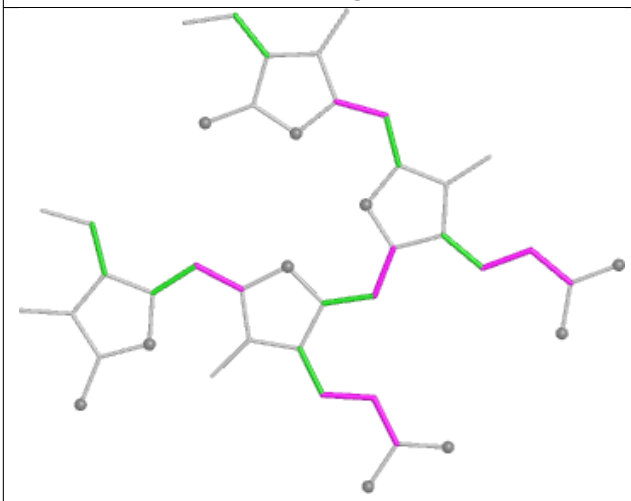


Bond angles



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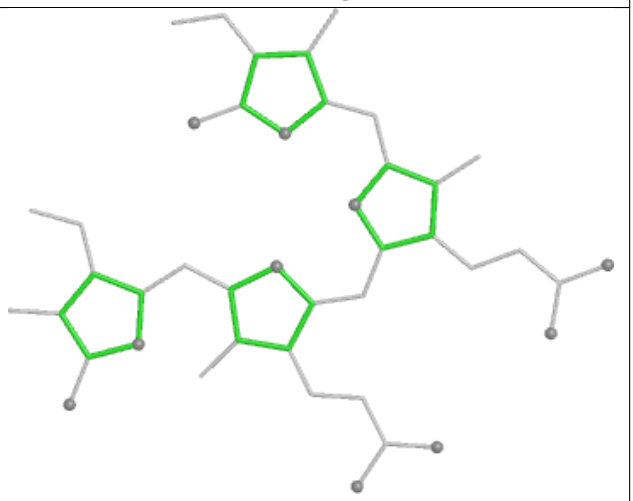
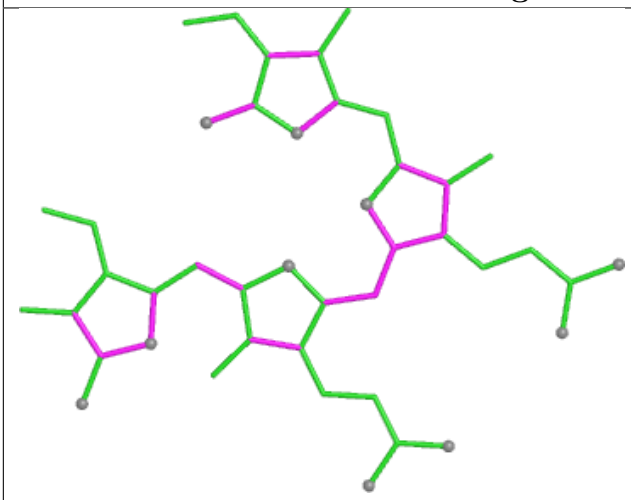


Rings

Ligand PEB AQ 303



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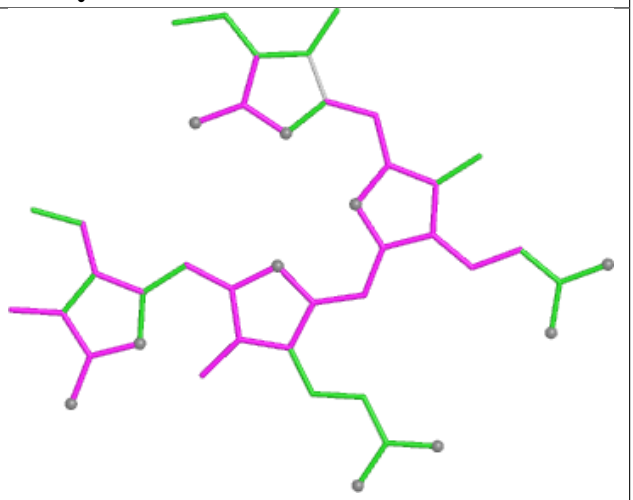

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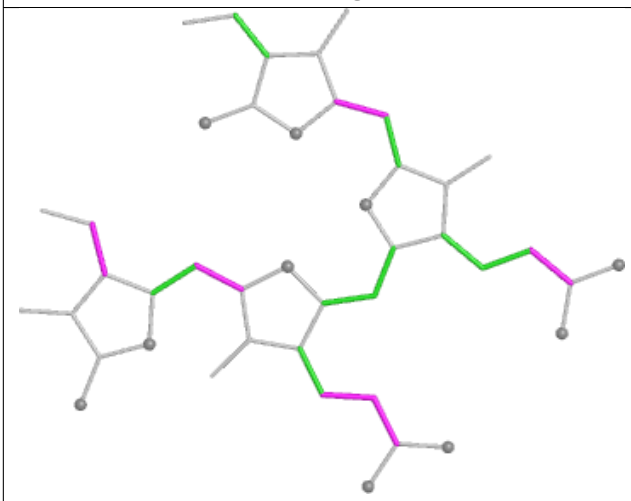

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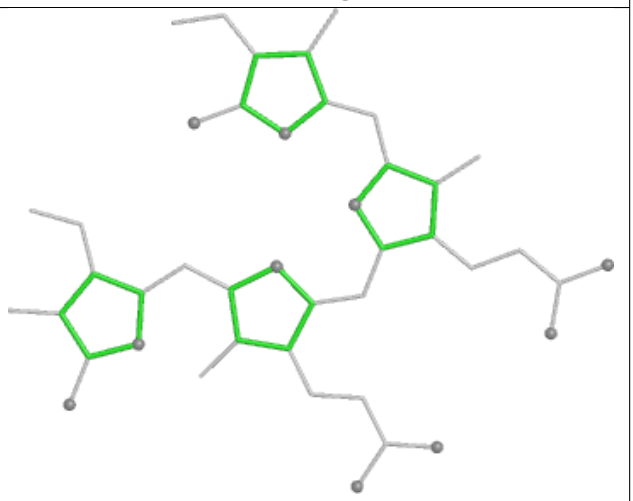
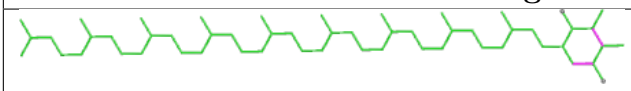


Rings

Ligand PL9 d6 408



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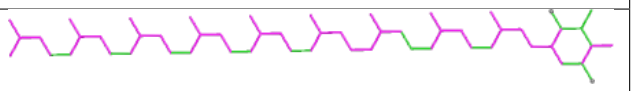
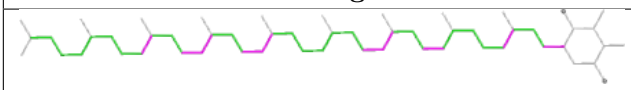


Bond angles



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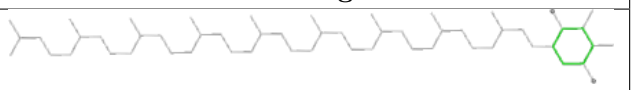
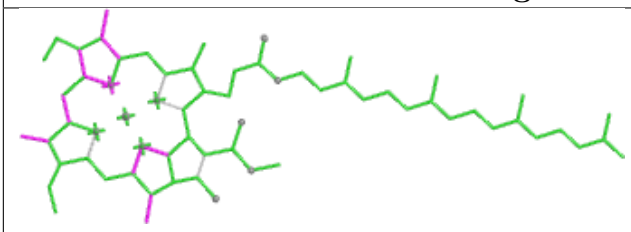


Rings

Ligand CLA CL 505



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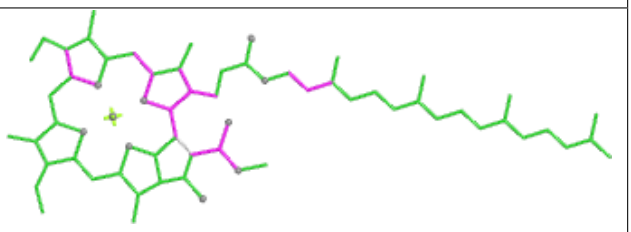
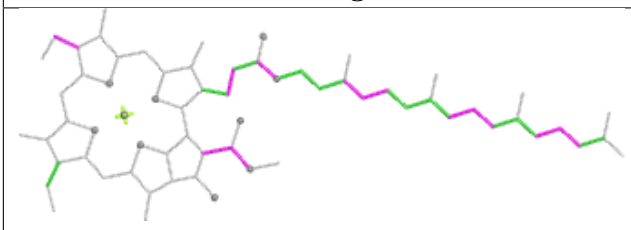


Bond angles



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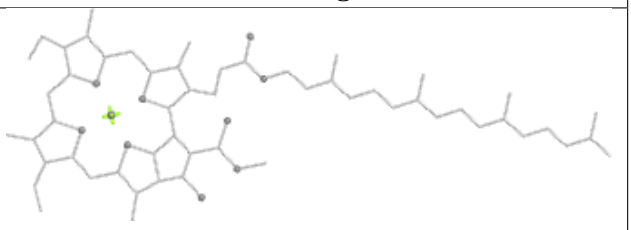
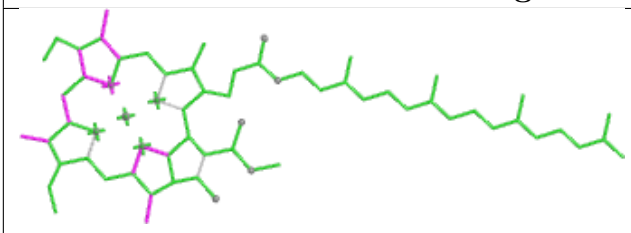


Rings

Ligand CLA H6 102



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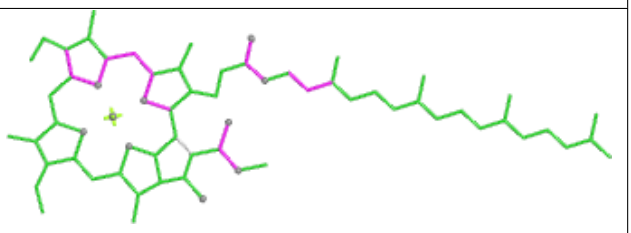
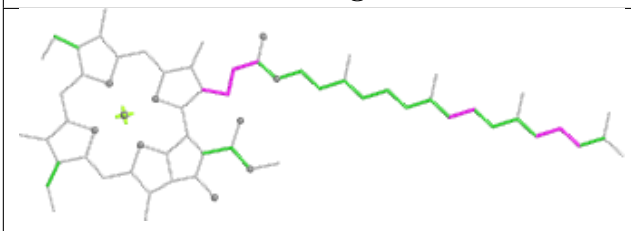


Bond angles



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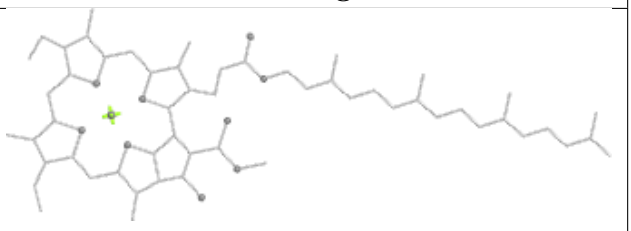
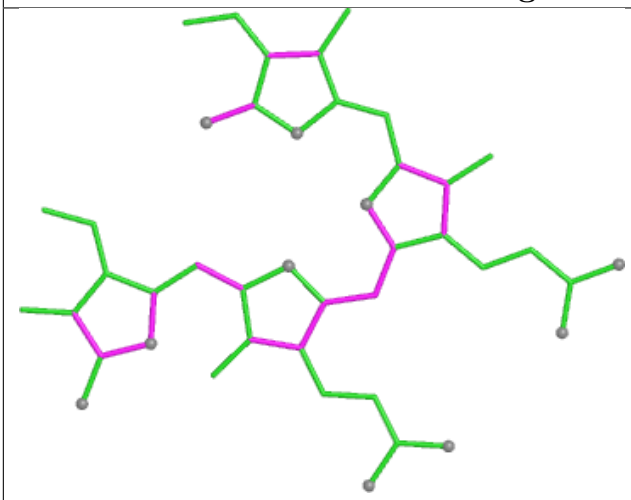
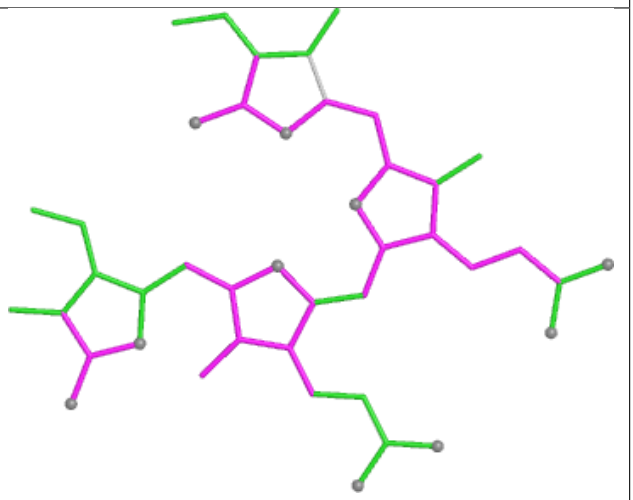


Rings

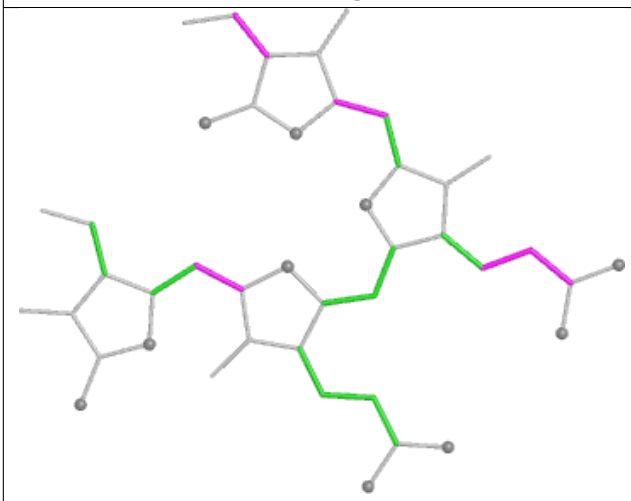
Ligand PEB IB 202



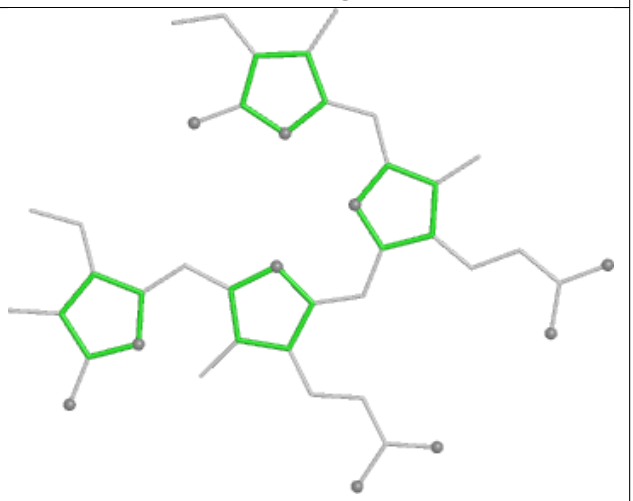
Bond lengths



Bond angles

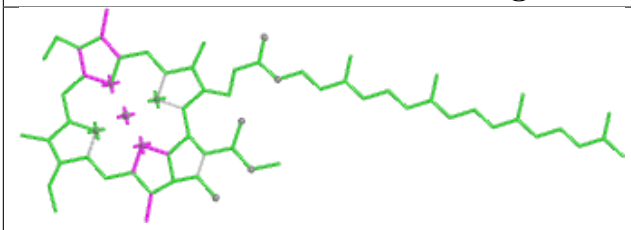


Torsions



Rings

Ligand CLA BN 819



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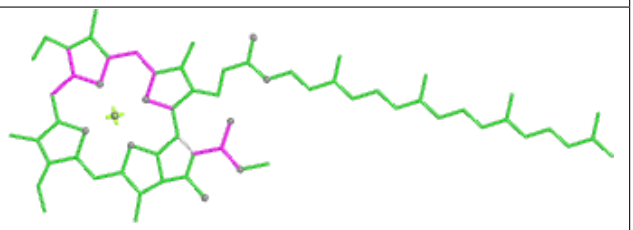
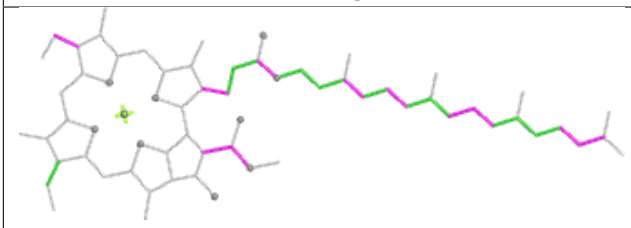


Bond angles



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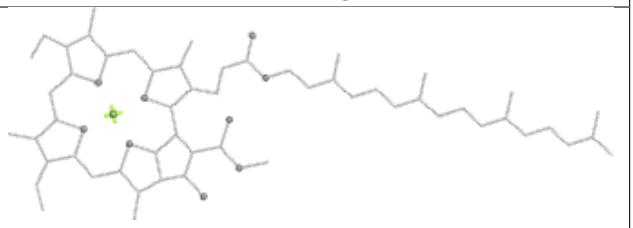
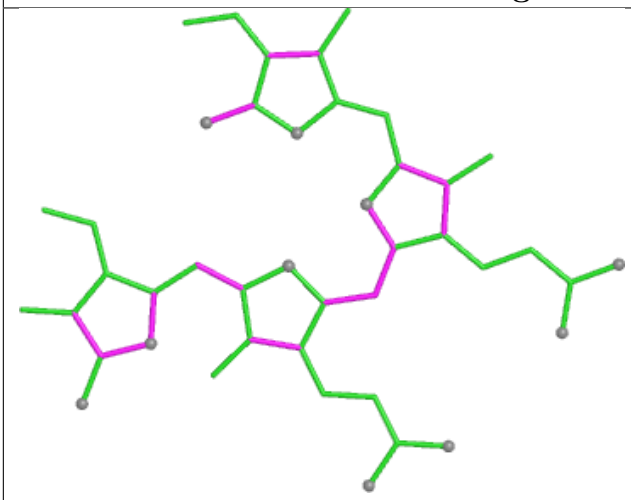


Rings

Ligand PEB PB 201



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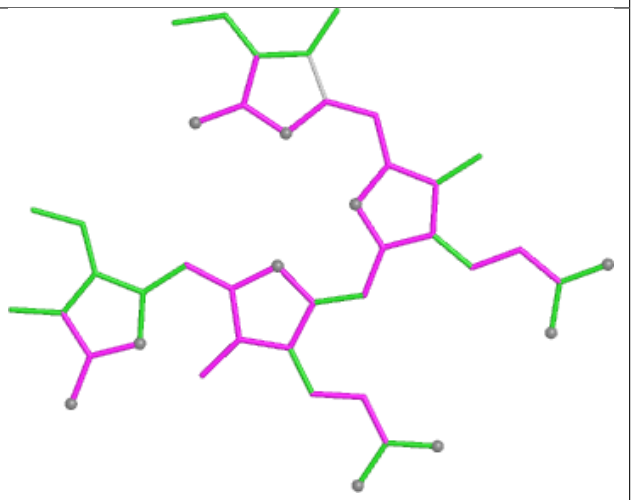

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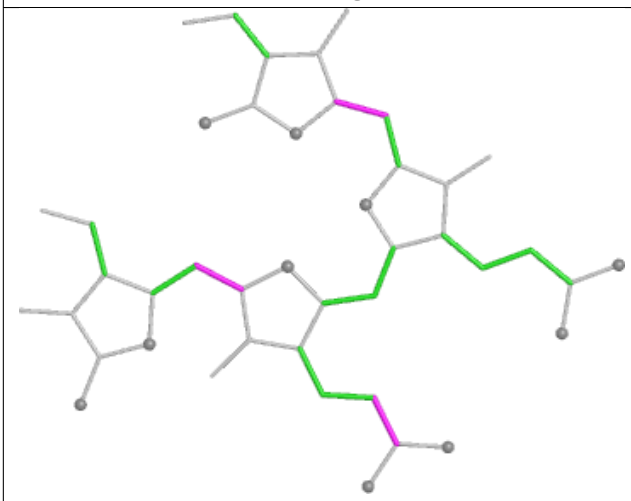

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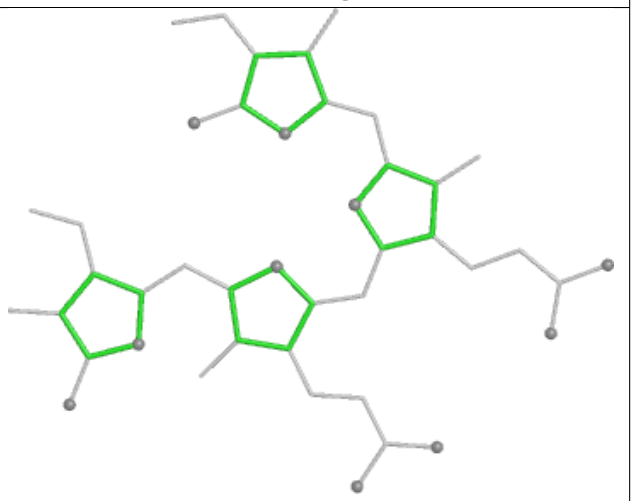
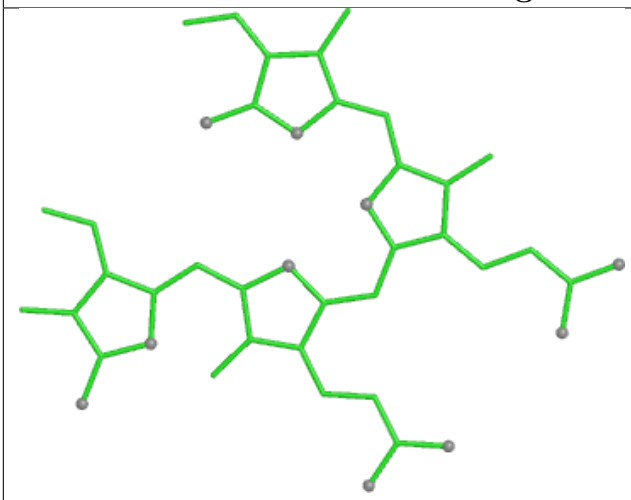


Rings

Ligand PEB Q4 202



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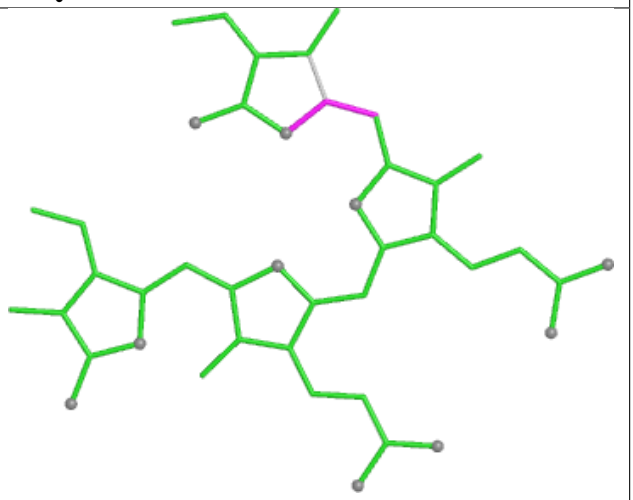

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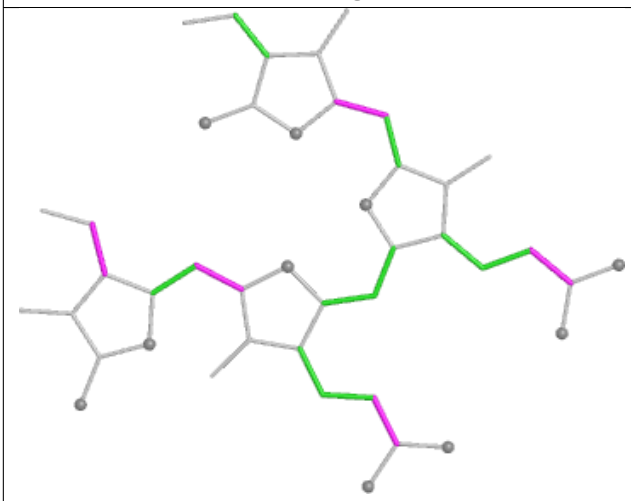

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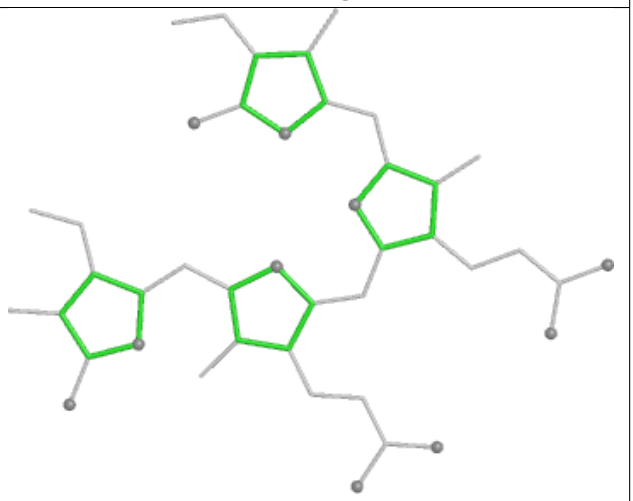
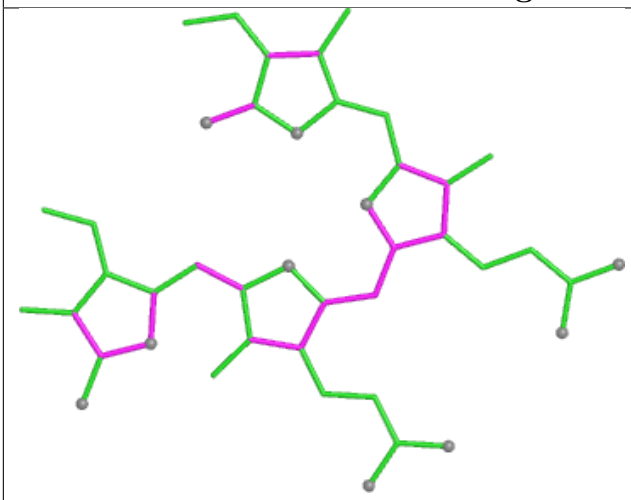


Rings

Ligand PEB R9 201



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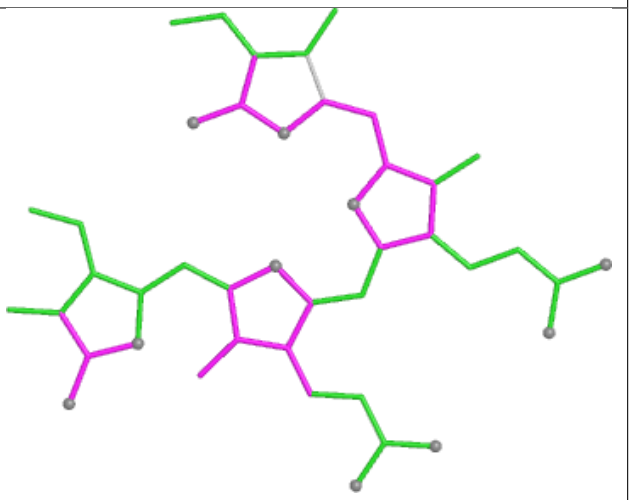

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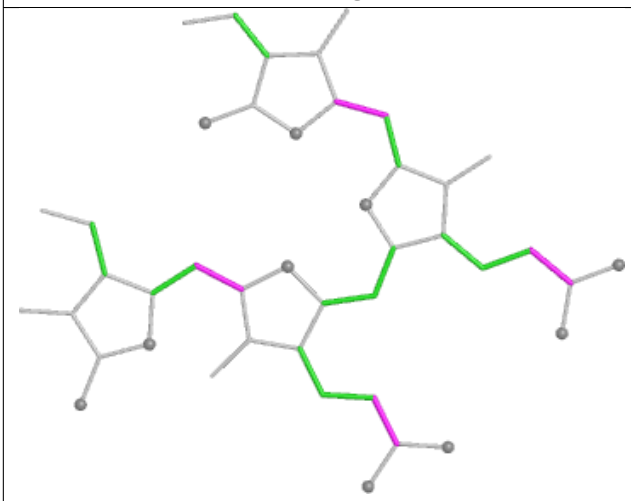

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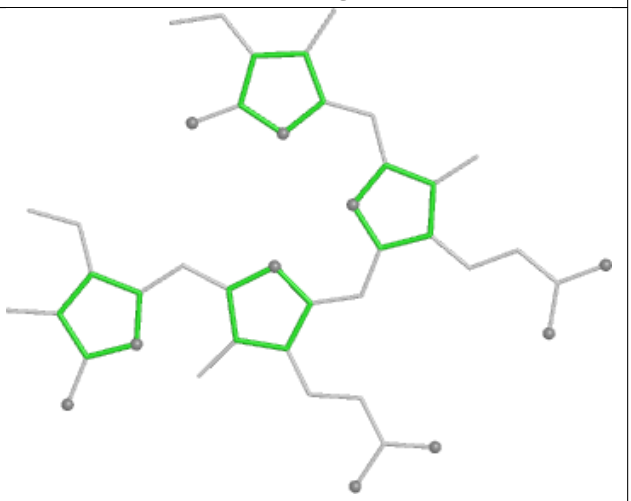
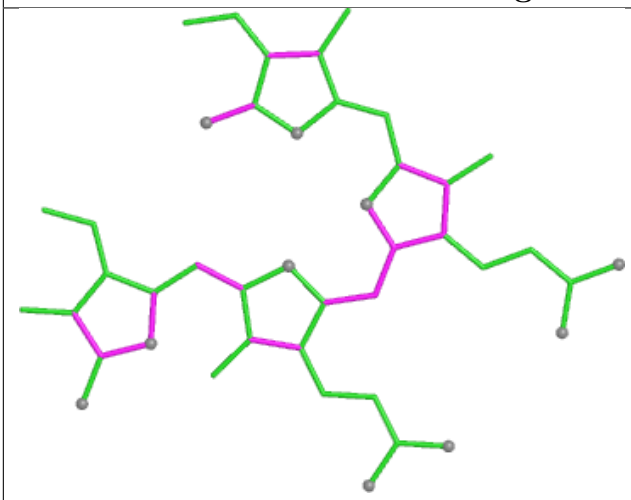


Rings

Ligand PEB N5 202



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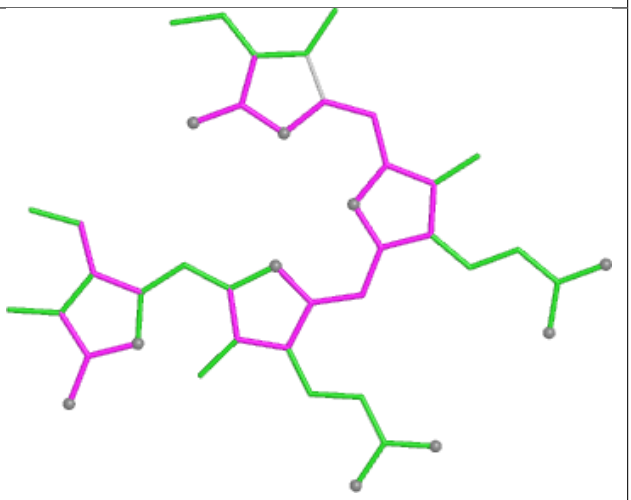

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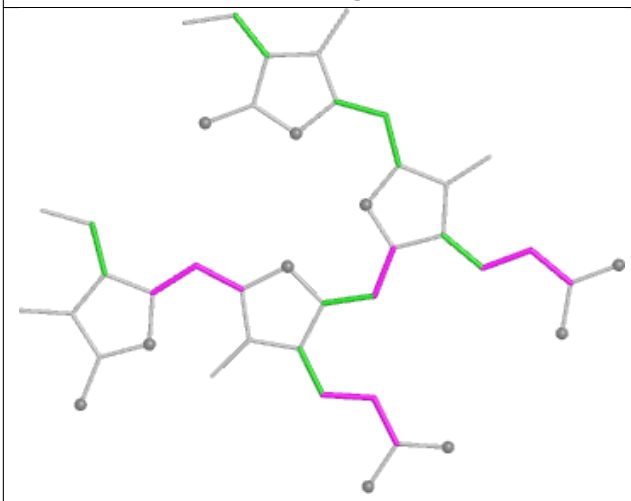

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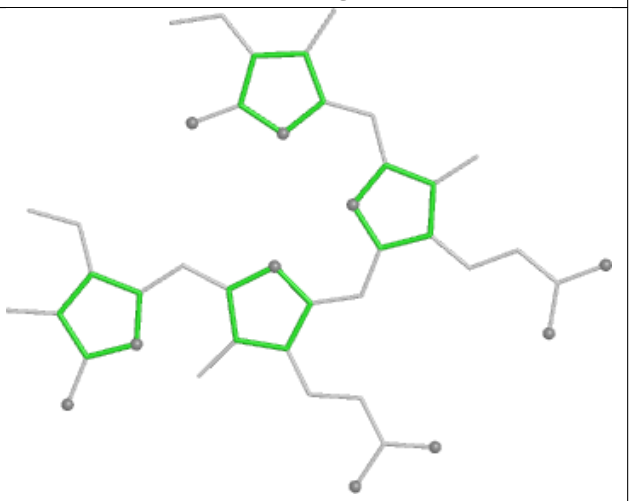
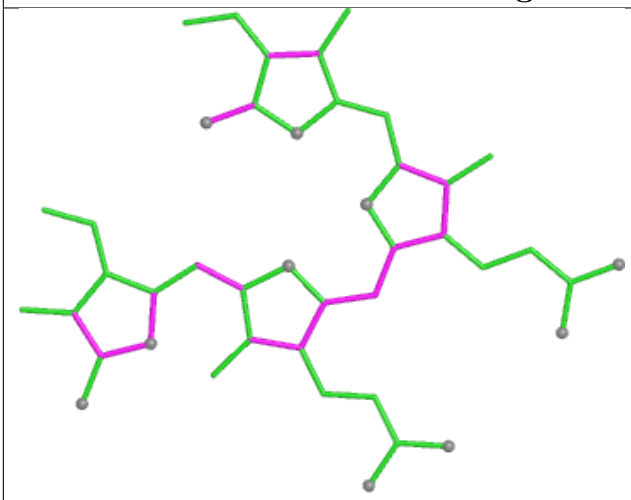


Rings

Ligand PEB iM 202



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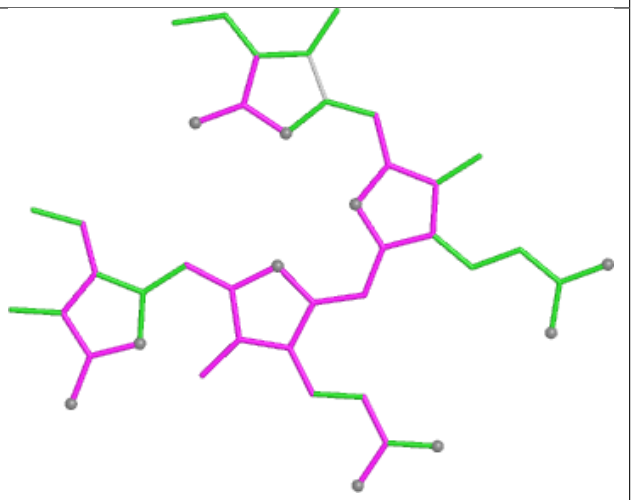

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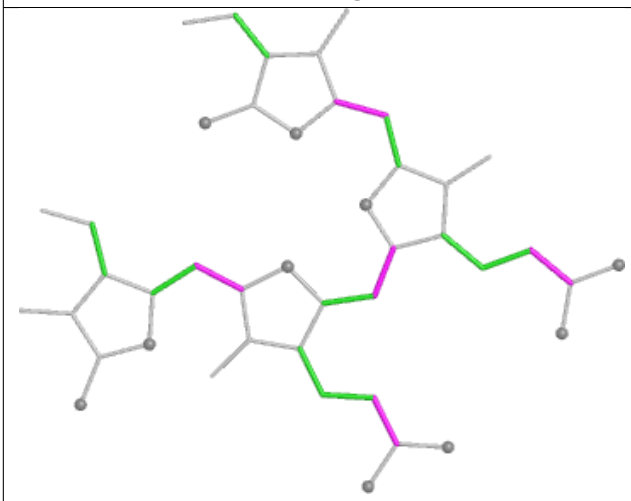

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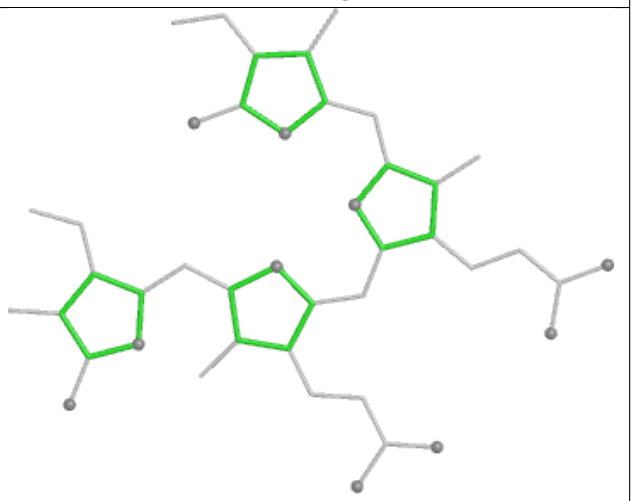
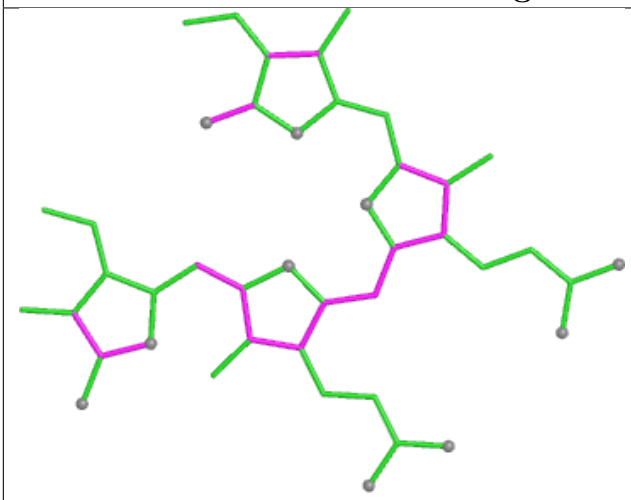


Rings

Ligand PEB uK 202



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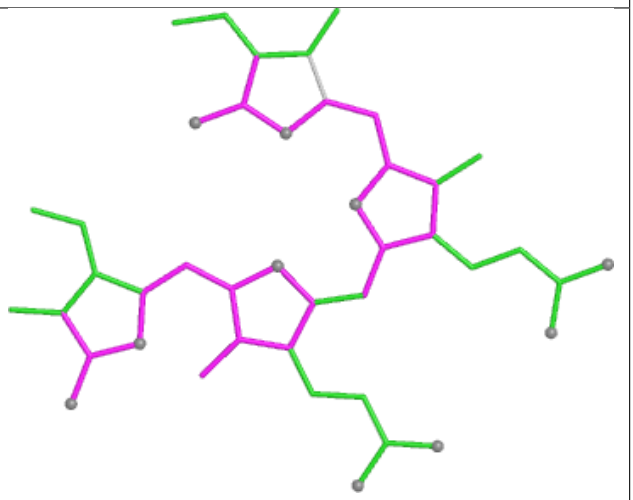

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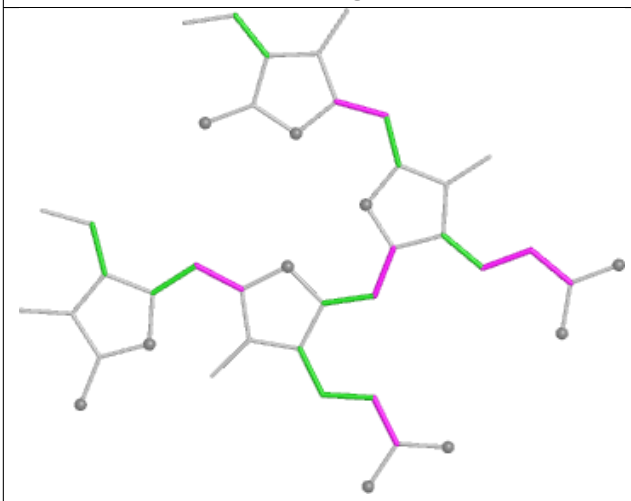

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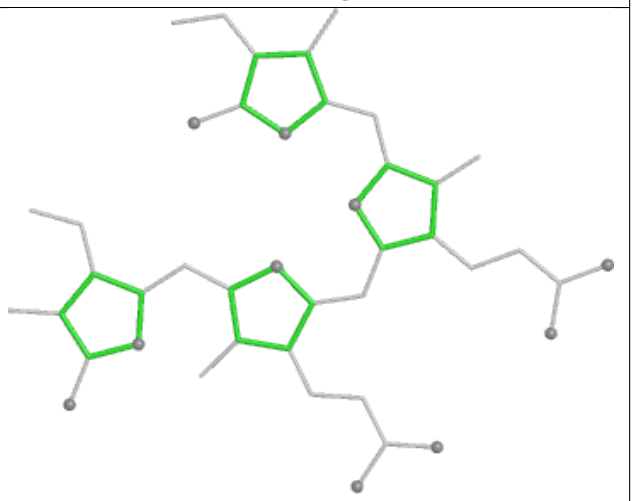
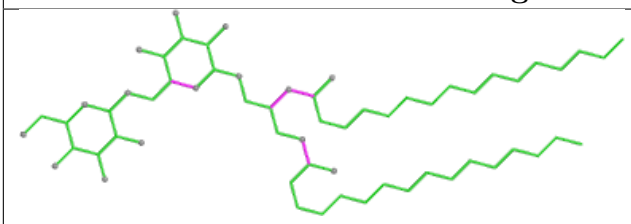


Rings

Ligand DGD C6 502



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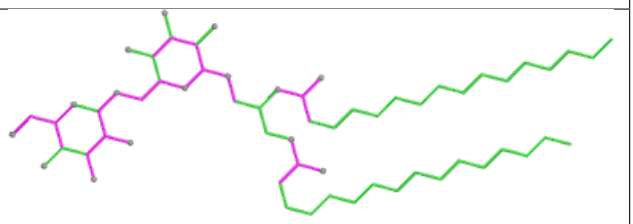

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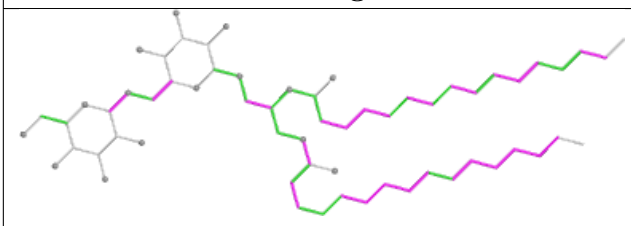

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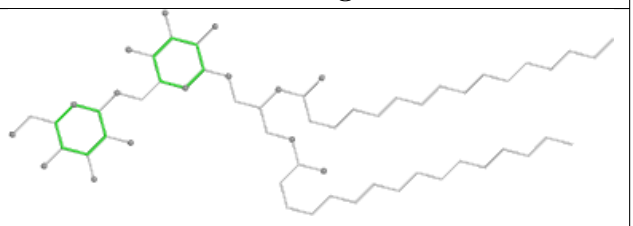
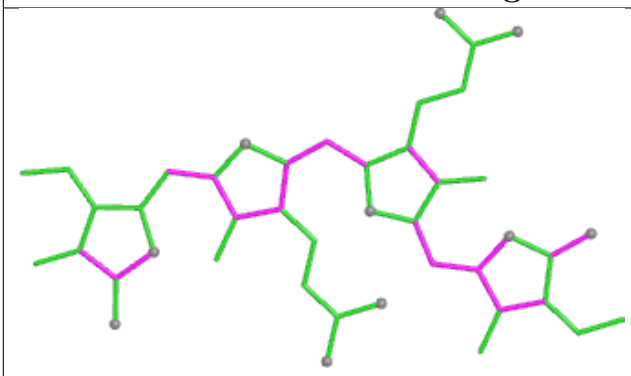


Rings

Ligand CYC D1 1001



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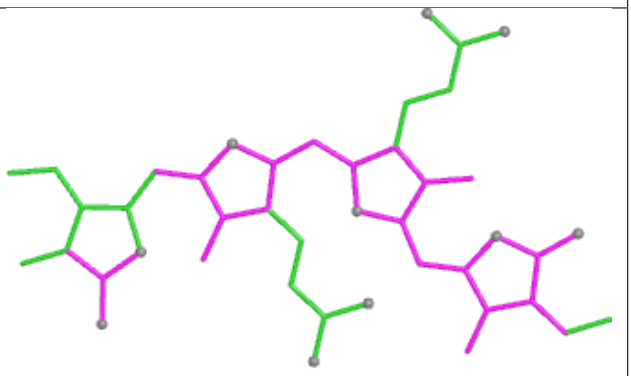

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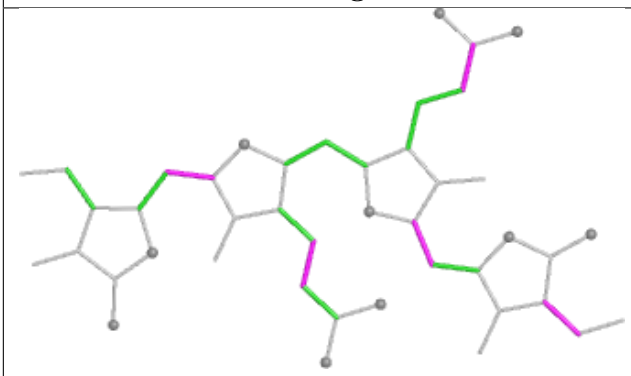

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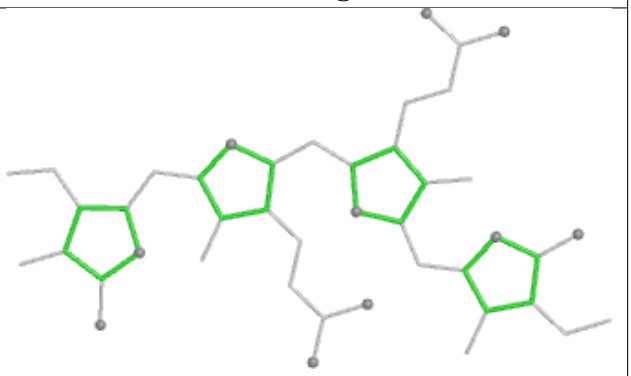
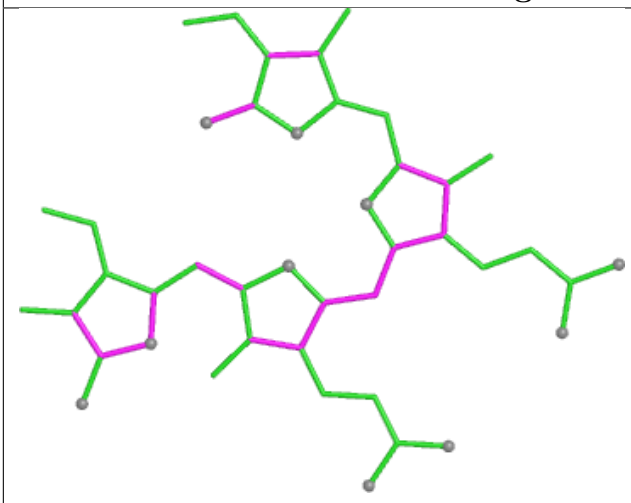


Rings

Ligand PEB uC 203



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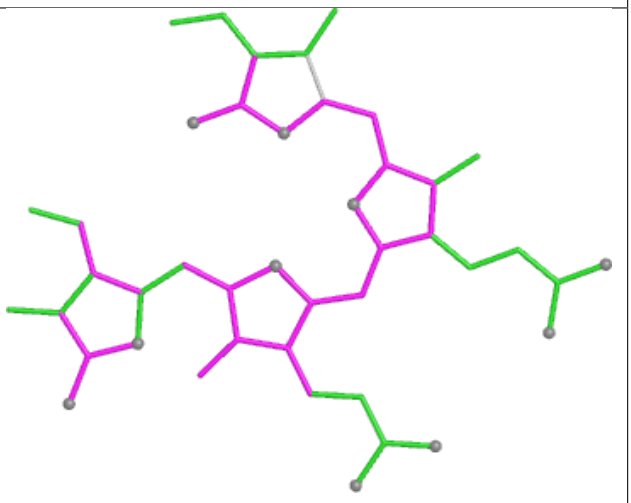

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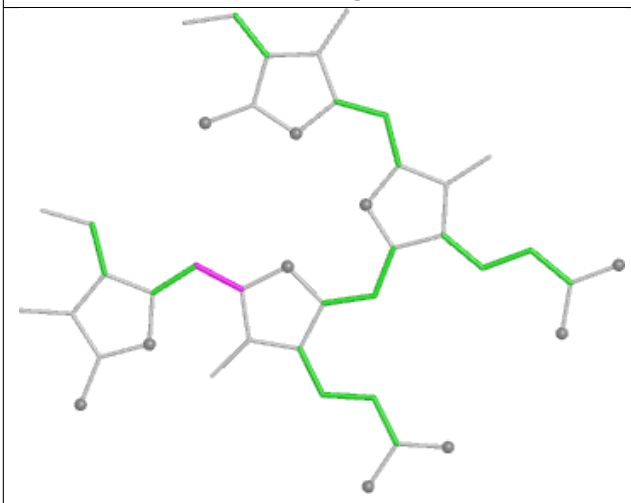

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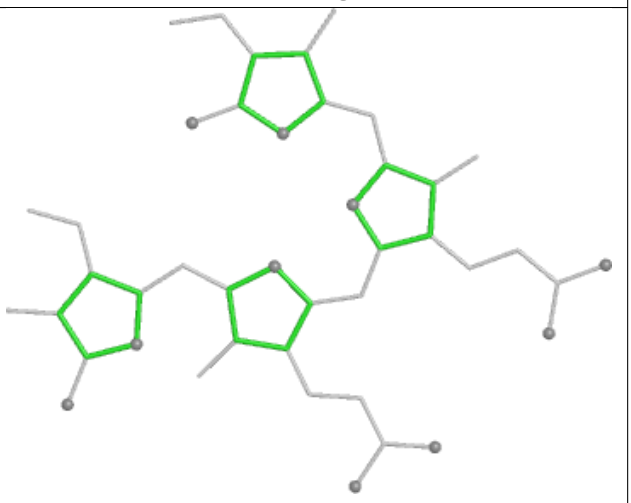
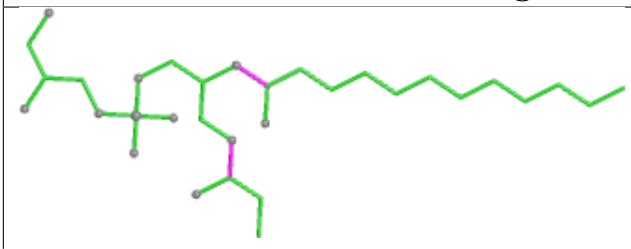


Rings

Ligand LHG C6 522



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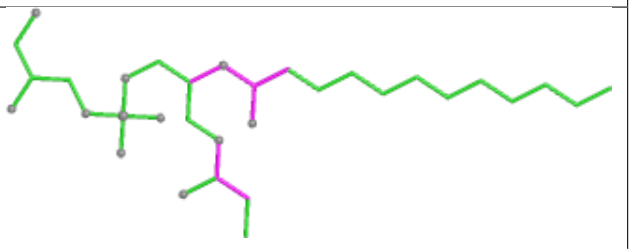

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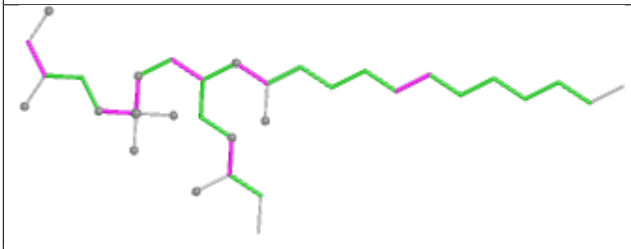

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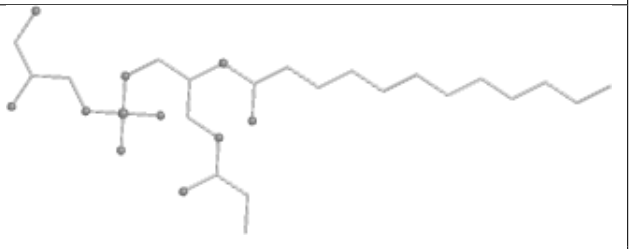
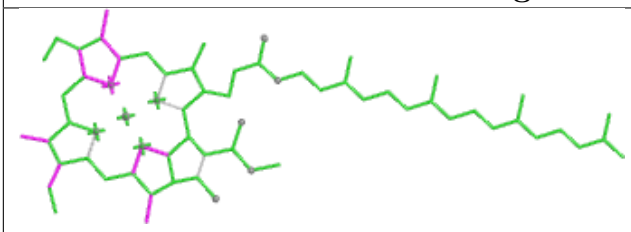


Rings

Ligand CLA CL 506



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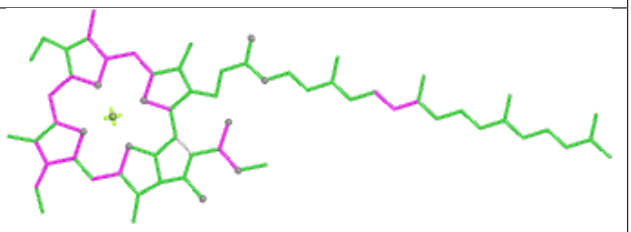

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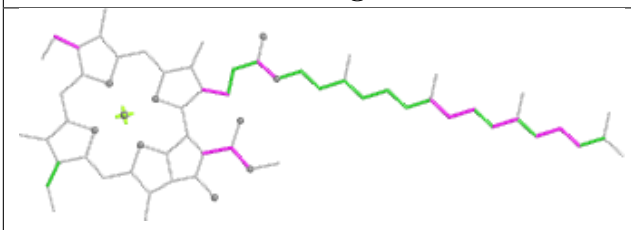

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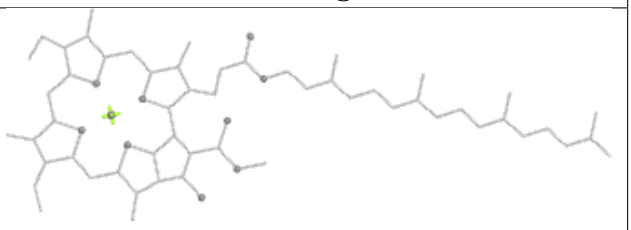
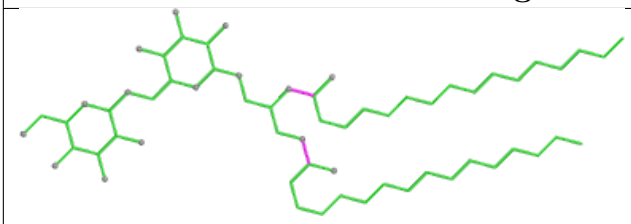
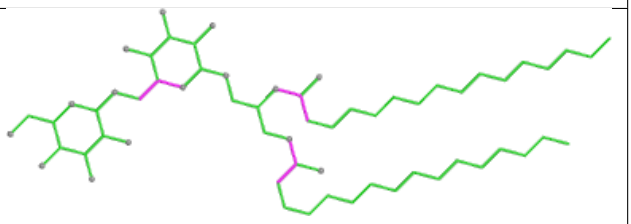


Rings

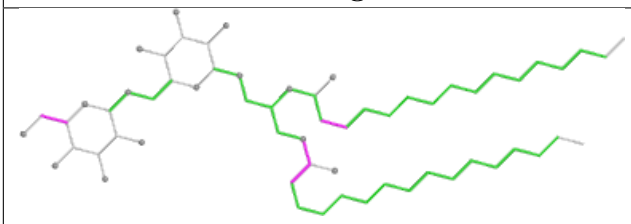
Ligand DGD cL 519



Bond lengths



Bond angles



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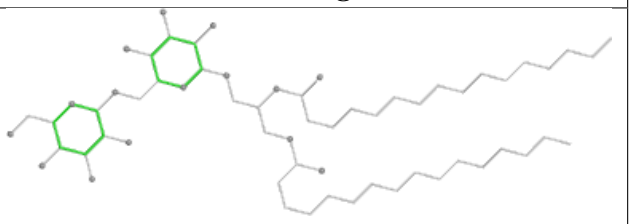
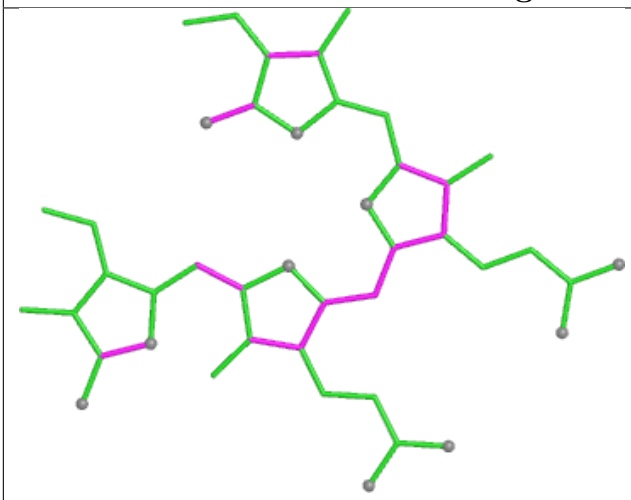


Rings

Ligand PEB R4 203



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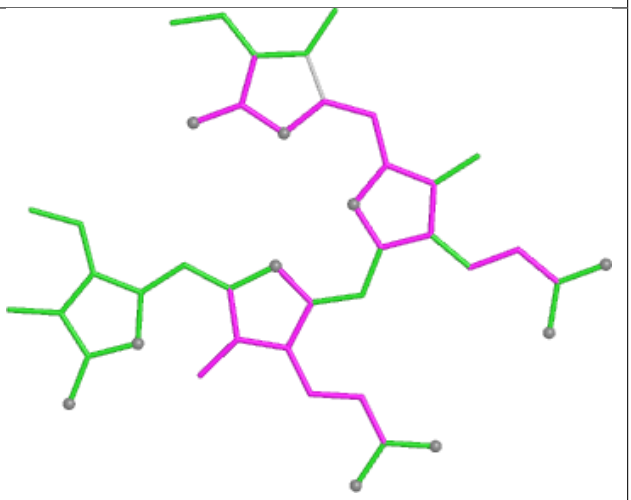
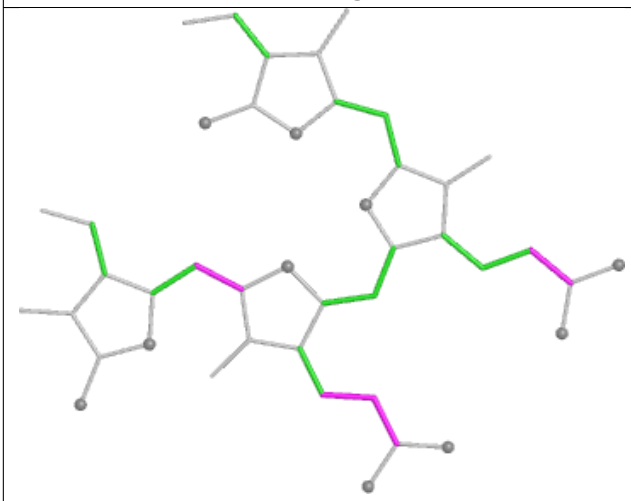


Bond angles



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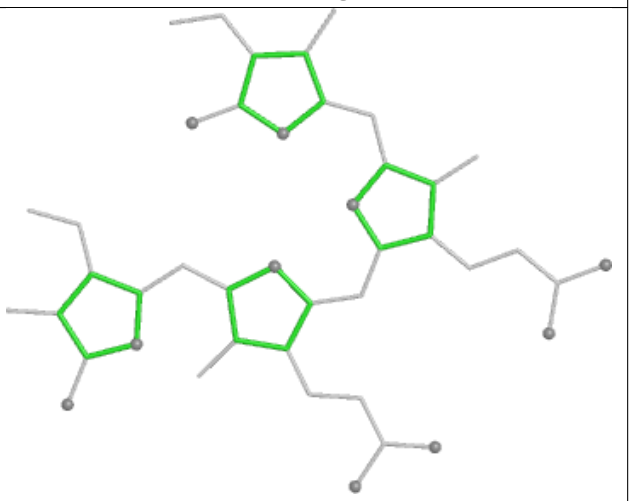
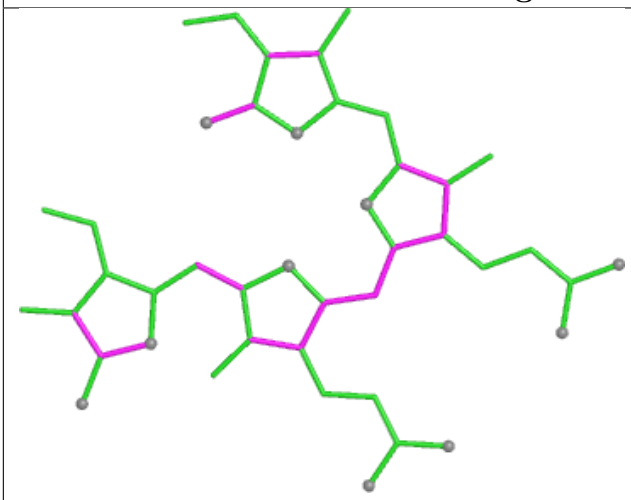
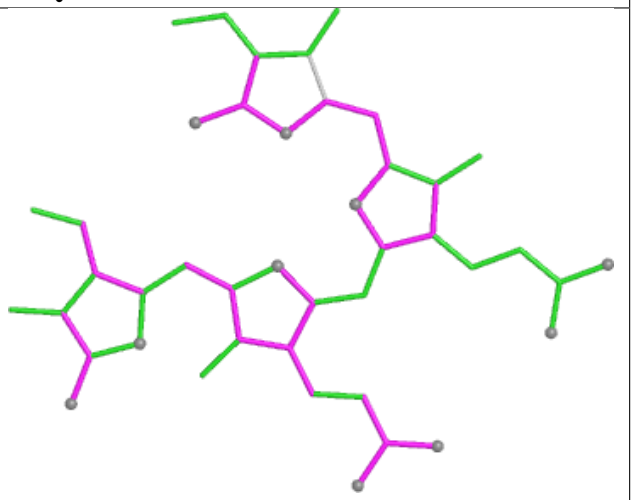


Rings

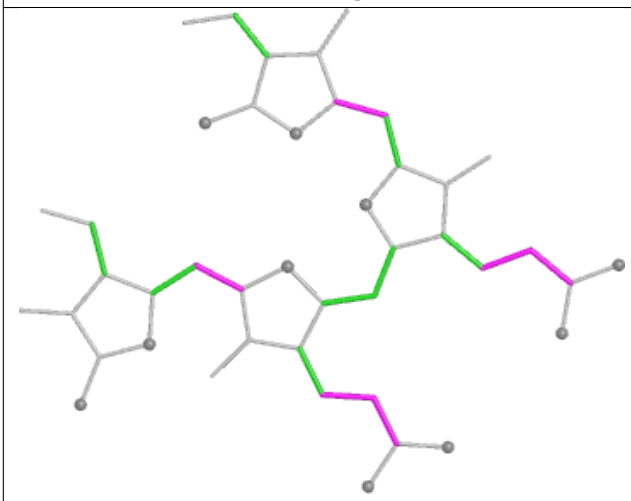
Ligand PEB Q9 201



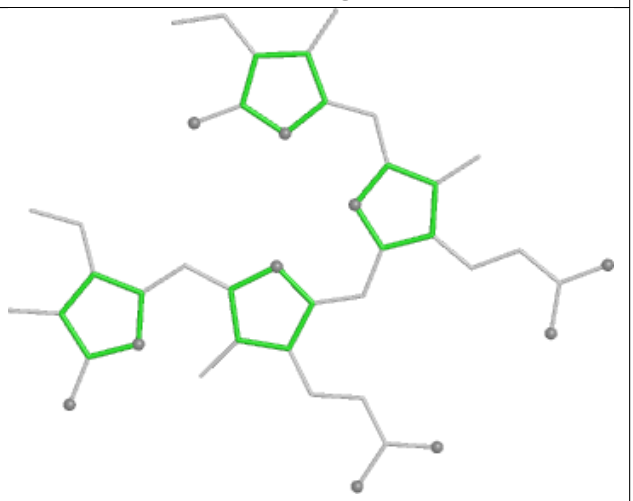
Bond lengths



Bond angles

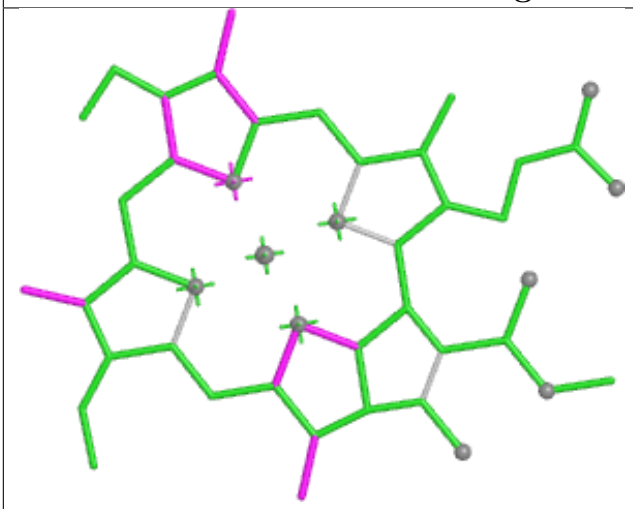


Torsions



Rings

Ligand CLA 5N 610



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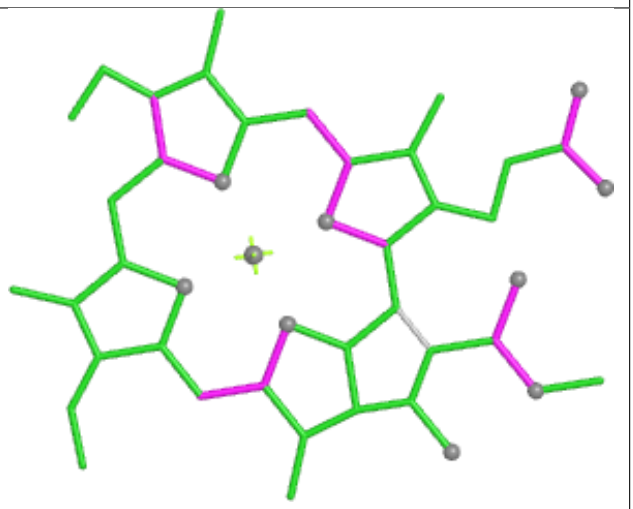

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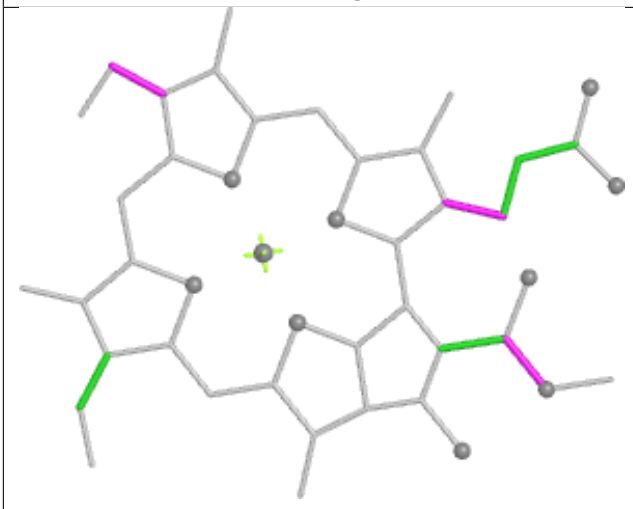
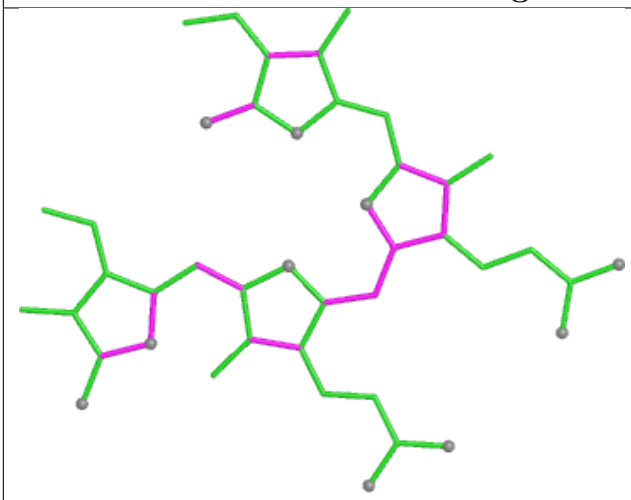


Torsions



Rings

Ligand PEB BA 203



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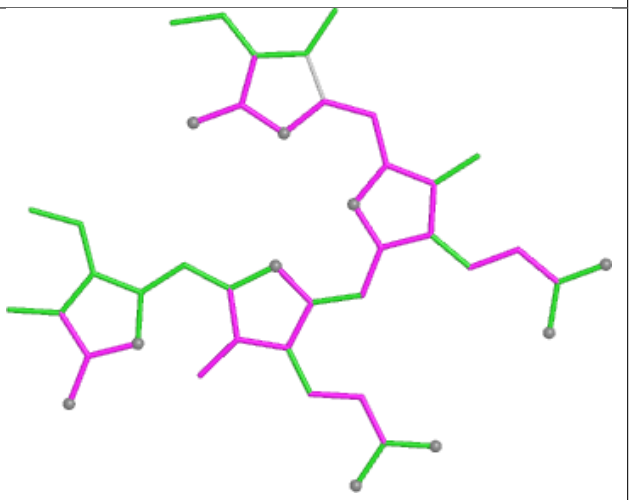

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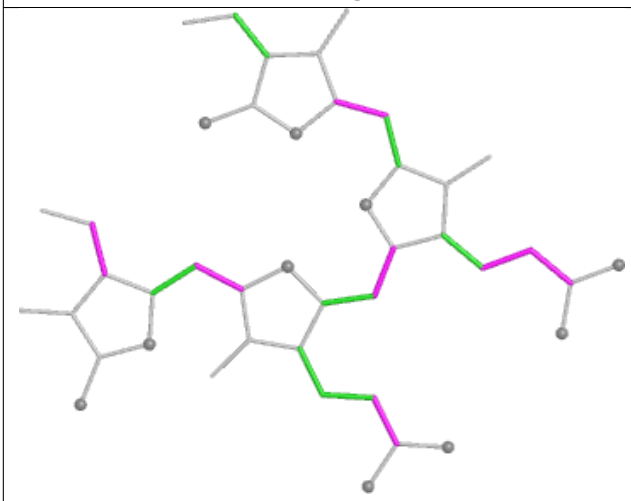

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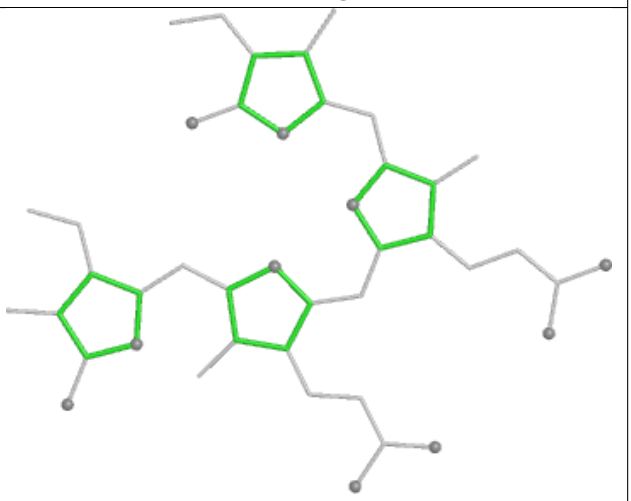
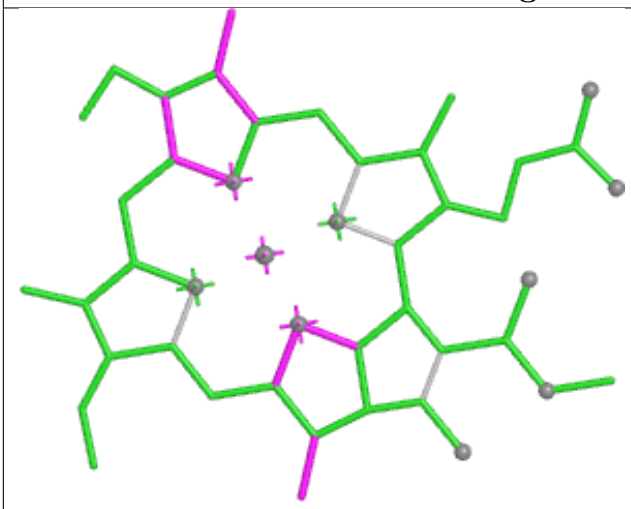


Rings

Ligand CLA 42 606



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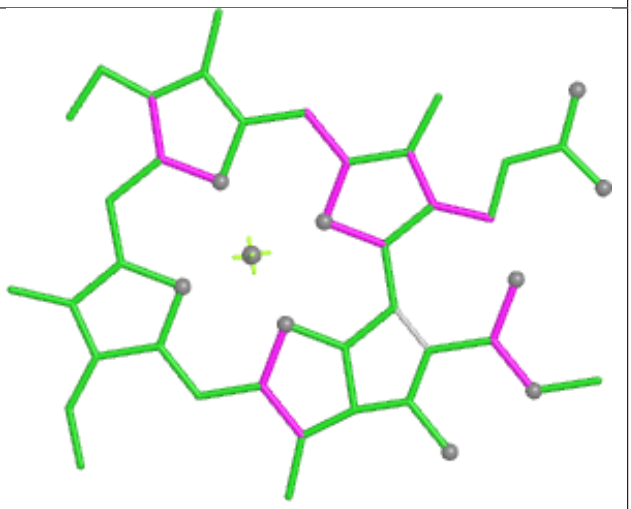

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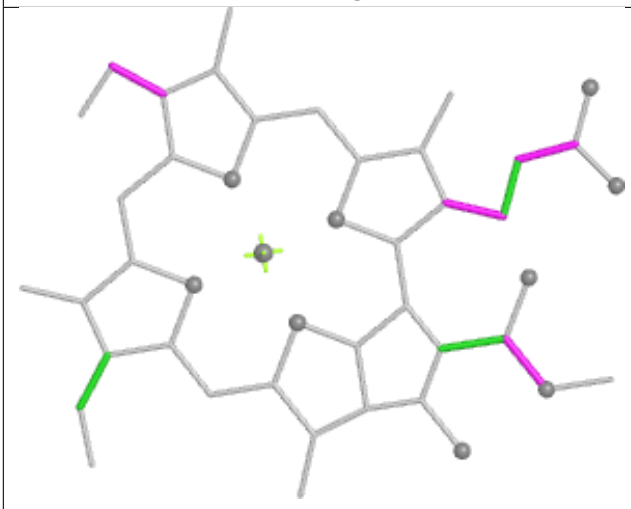
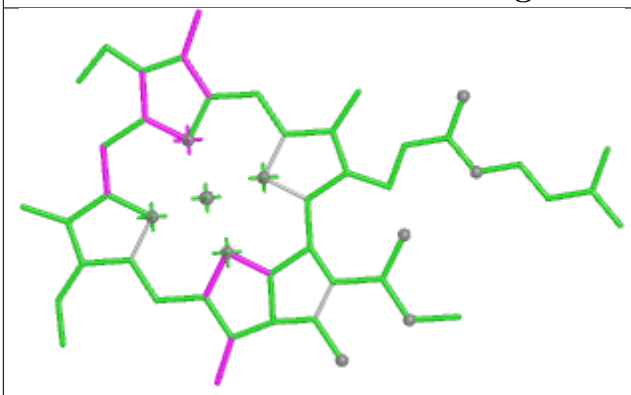


Torsions



Rings

Ligand CLA A6 404



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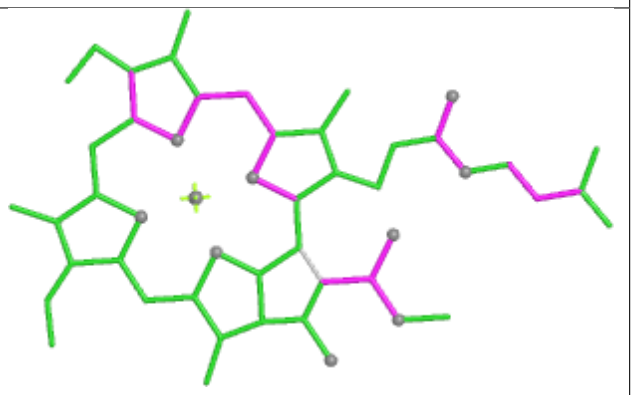

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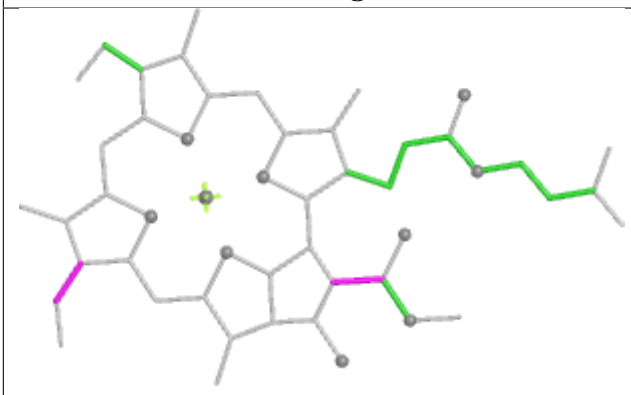

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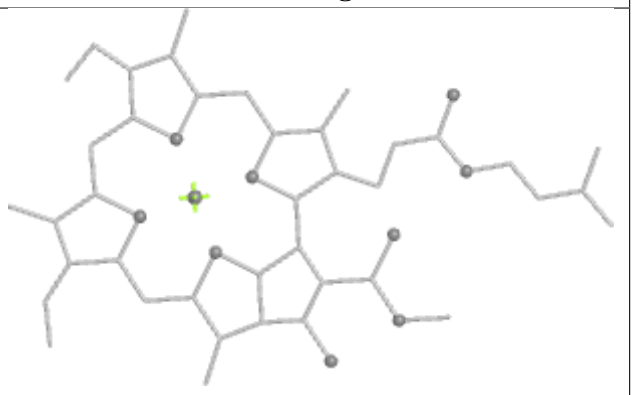
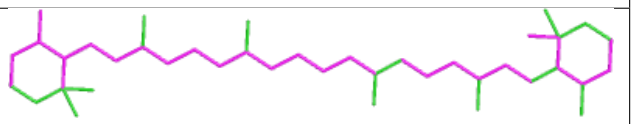


Rings

Ligand BCR AN 804



Bond lengths



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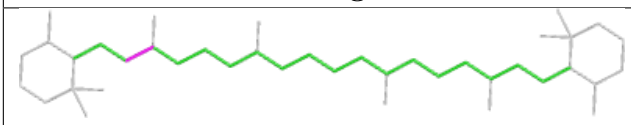

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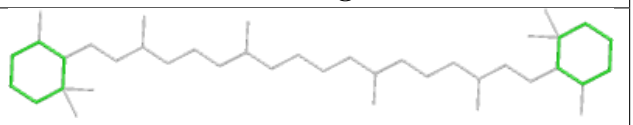
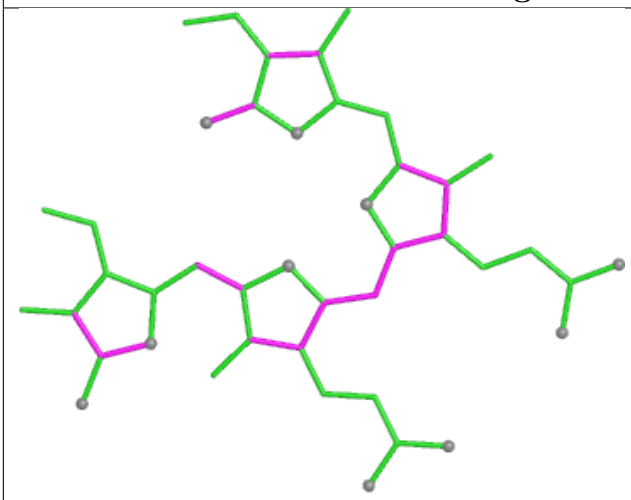


Rings

Ligand PEB SH 203



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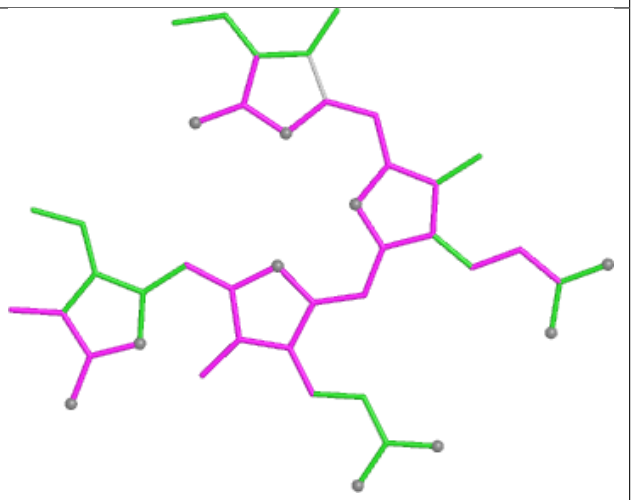

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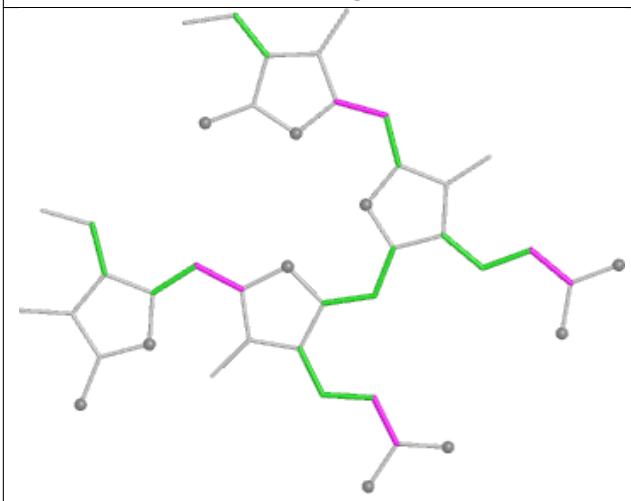

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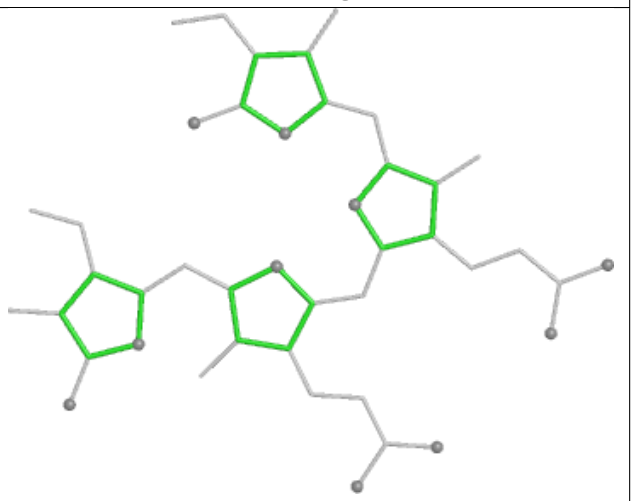

Rings

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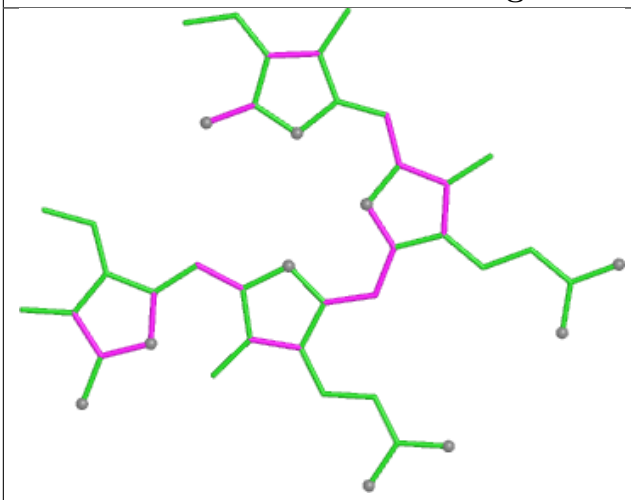

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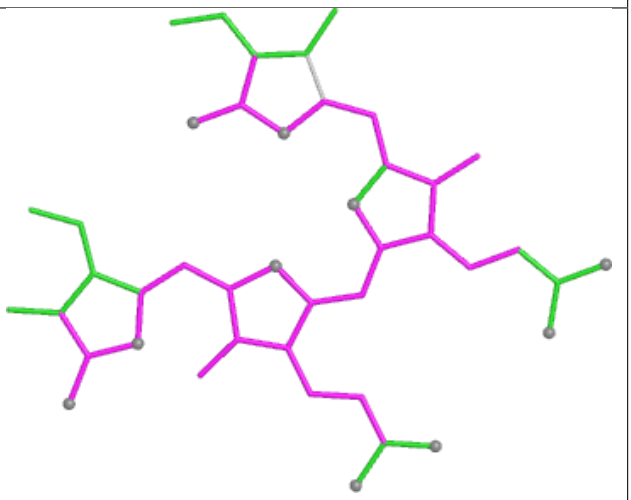

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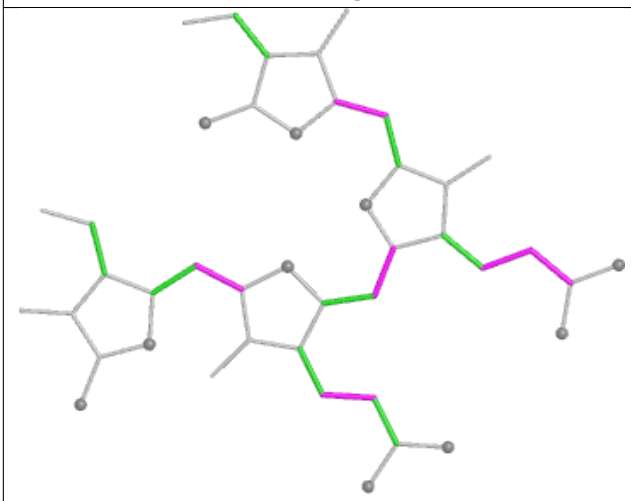

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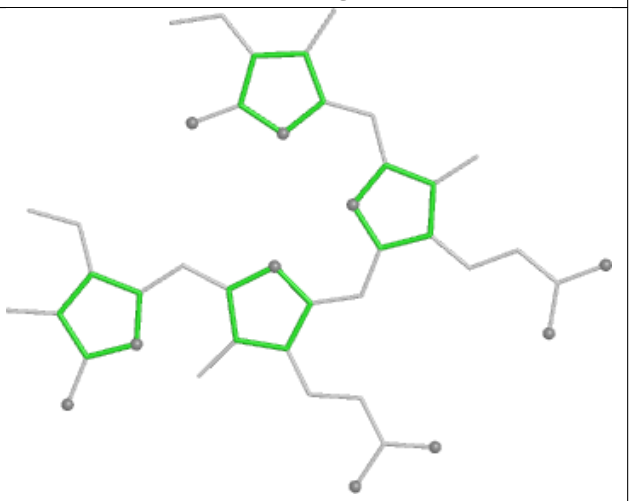
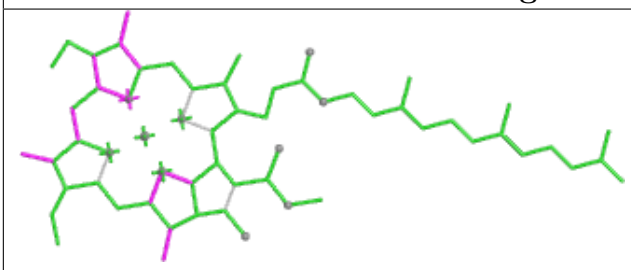


Rings

Ligand CLA a6 608



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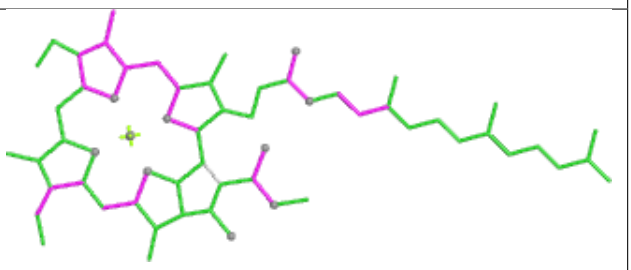

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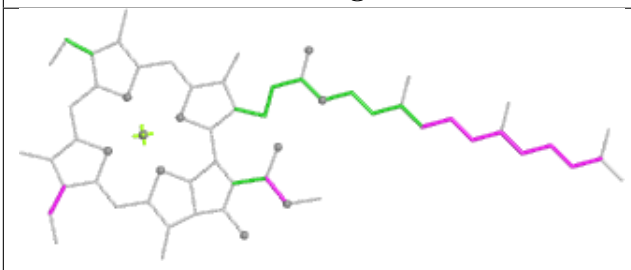

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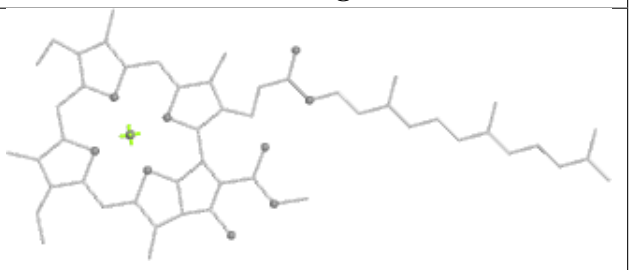
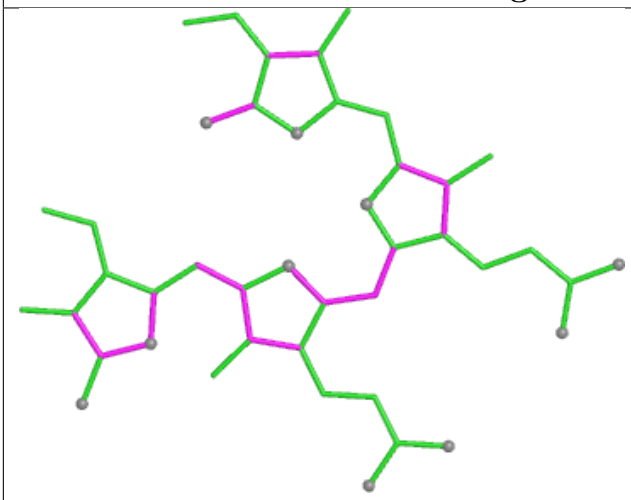


Rings

Ligand PEB DQ 202



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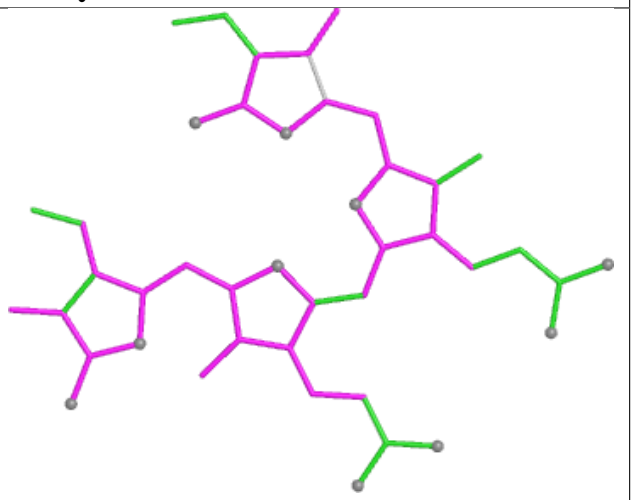
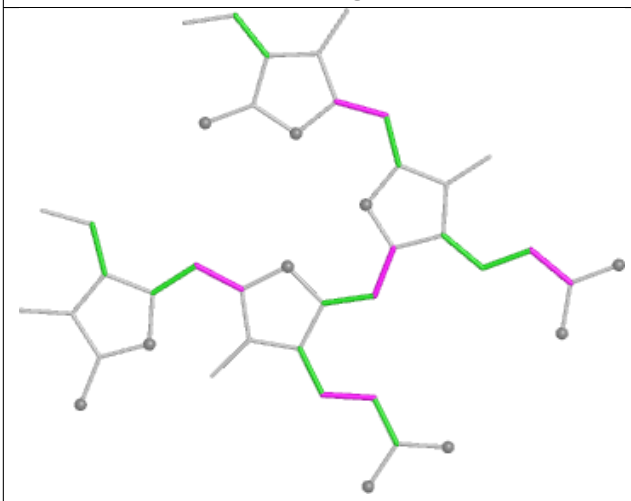


Bond angles



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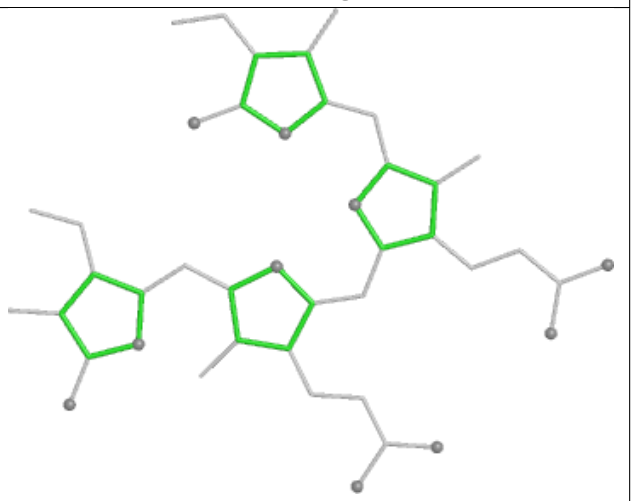
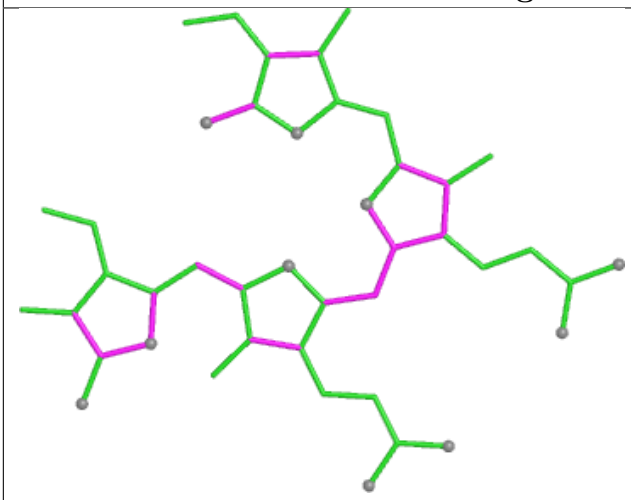


Rings

Ligand PEB bF 201



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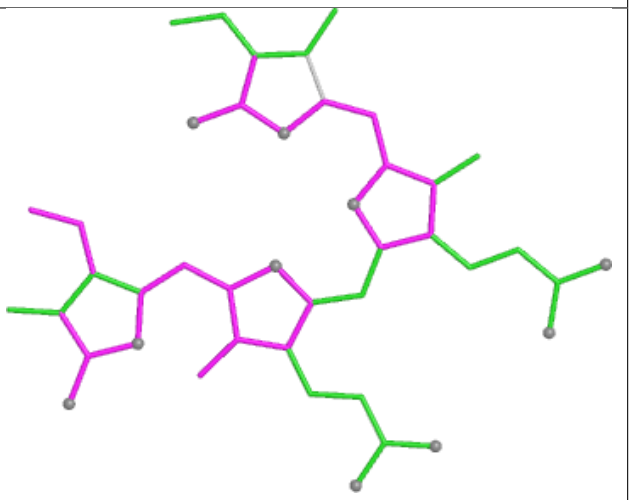

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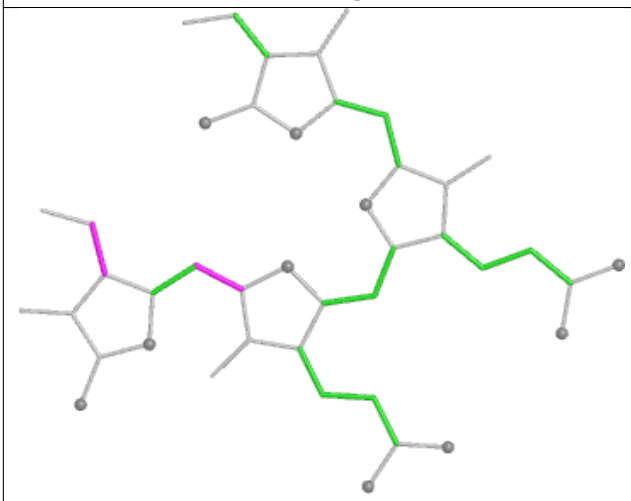

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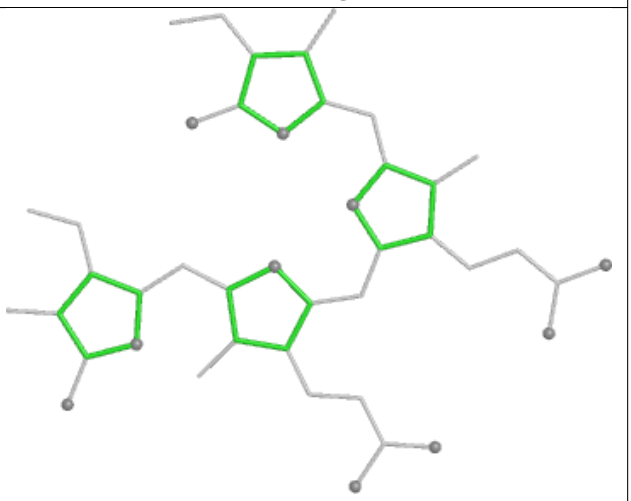
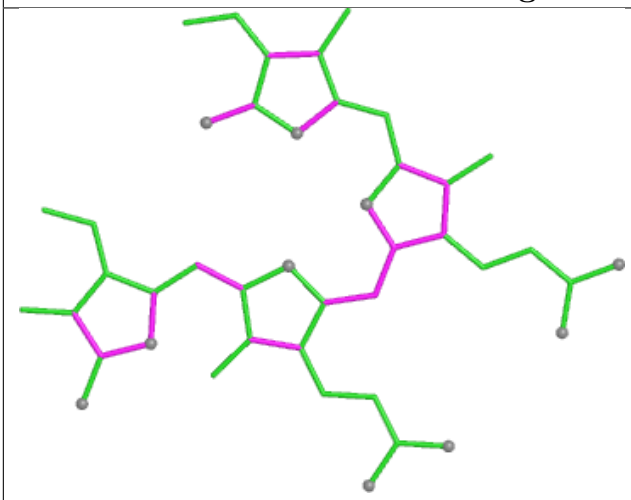


Rings

Ligand PEB lG 202



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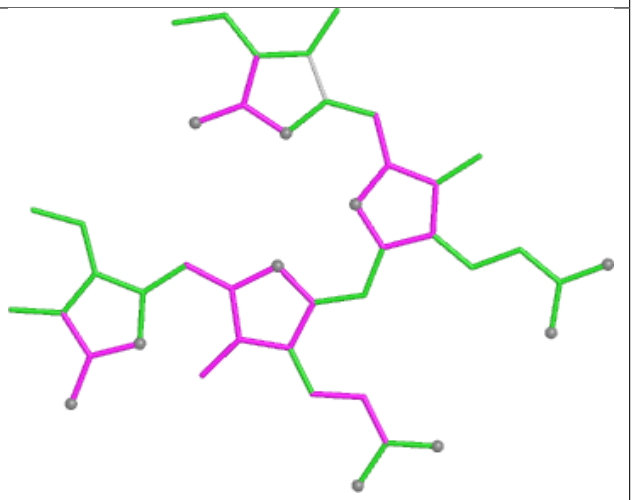

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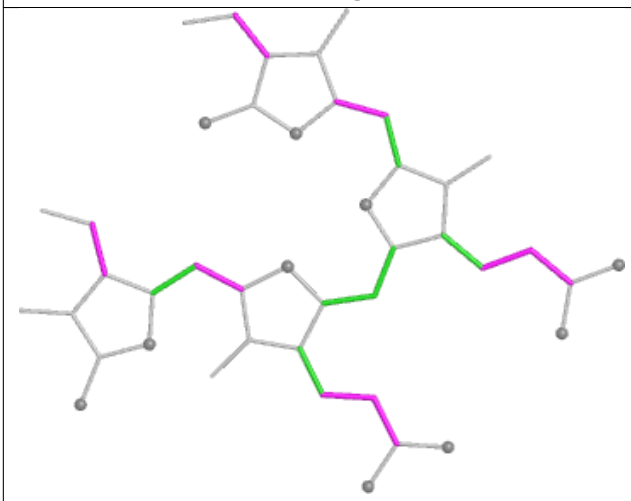

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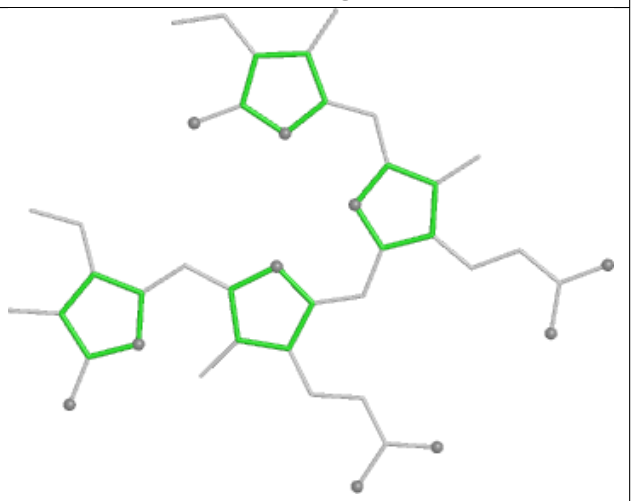
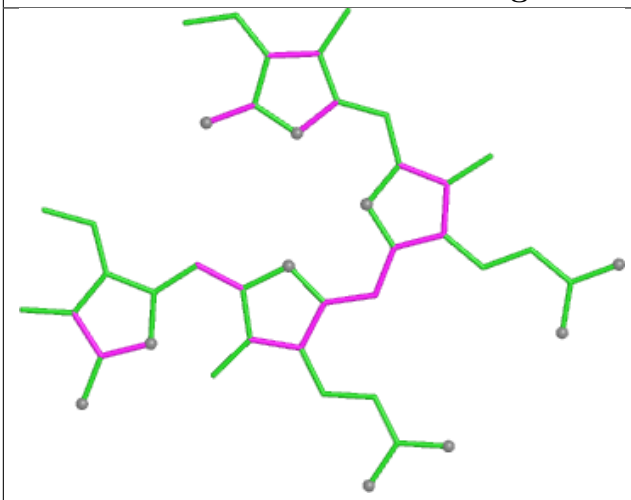


Rings

Ligand PEB RD 201



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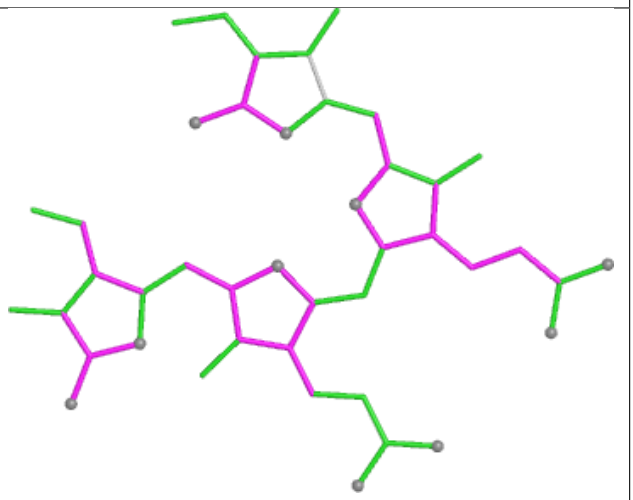

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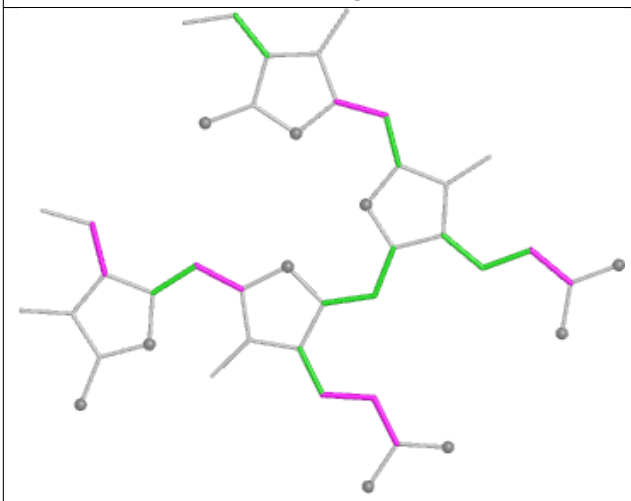

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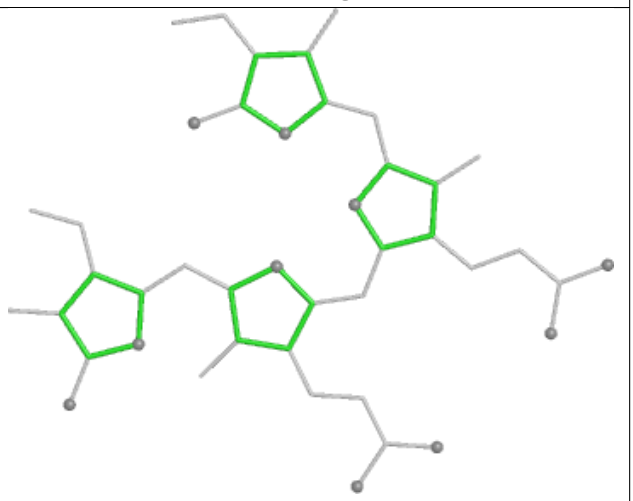
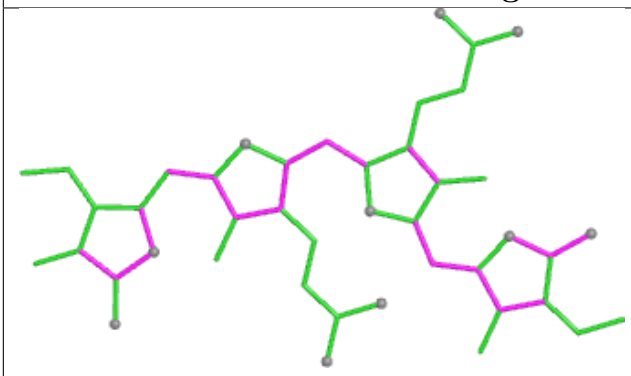


Rings

Ligand CYC m3 1001



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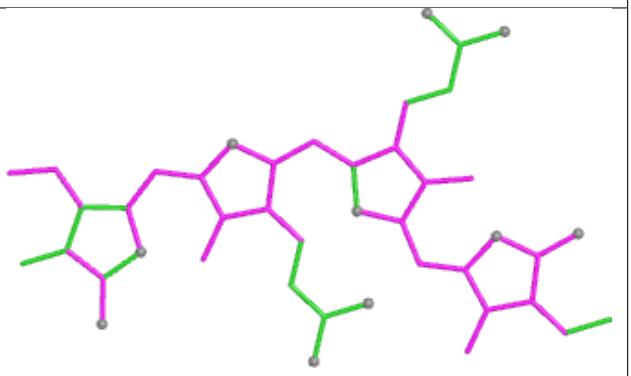
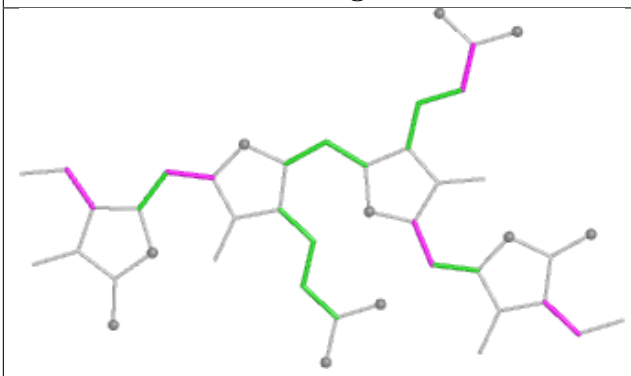


Bond angles



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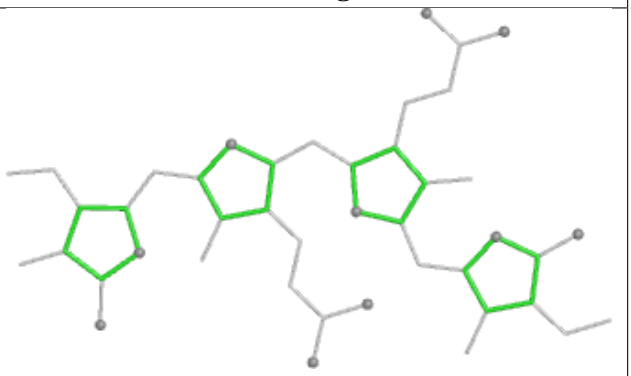
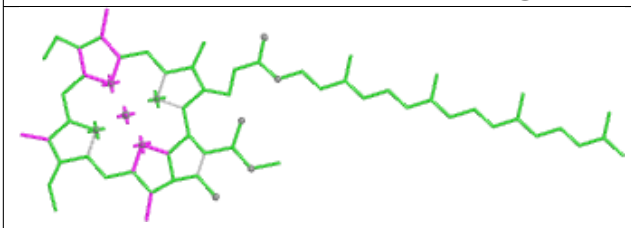


Rings

Ligand CLA bL 618



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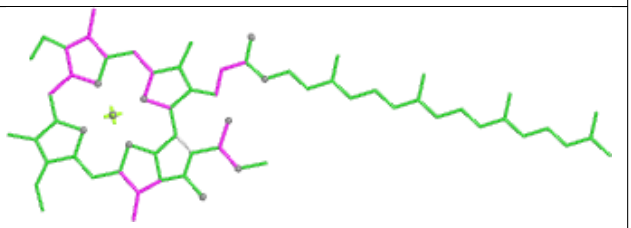
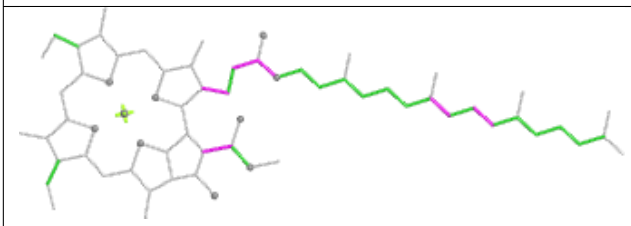


Bond angles



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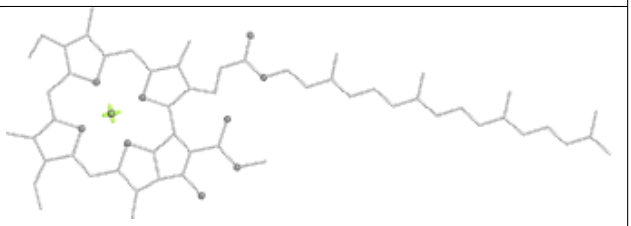
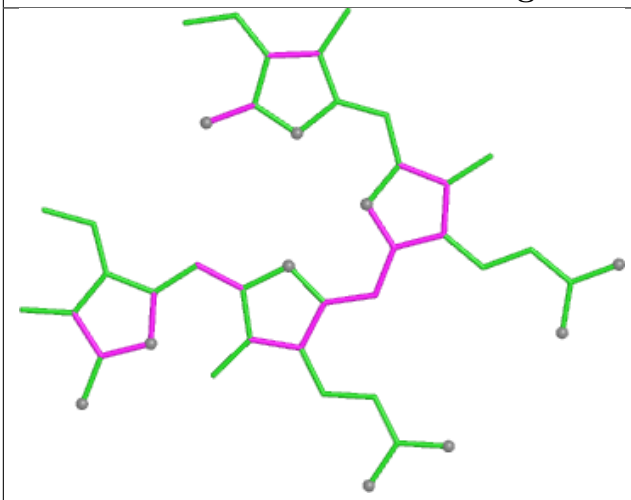


Rings

Ligand PEB ID 201



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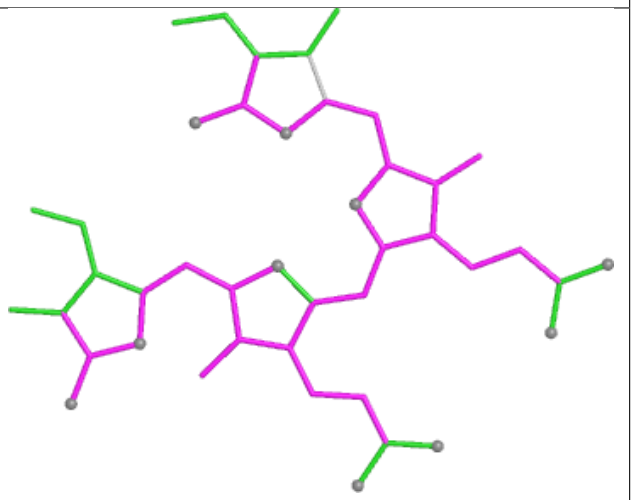
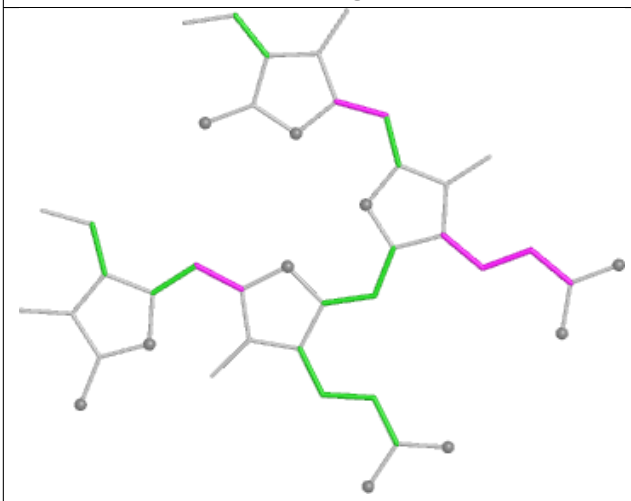


Bond angles



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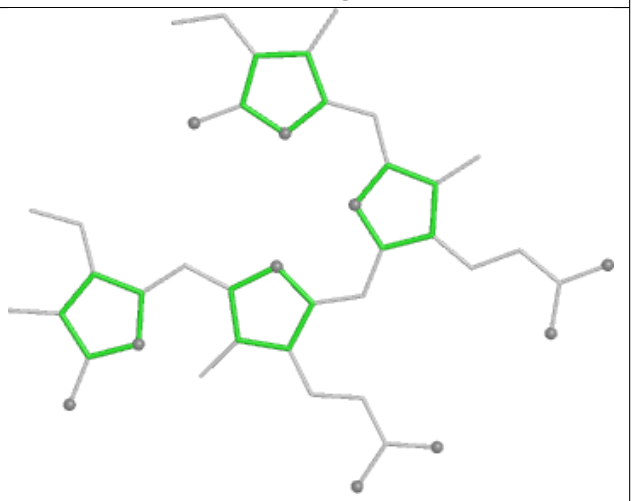
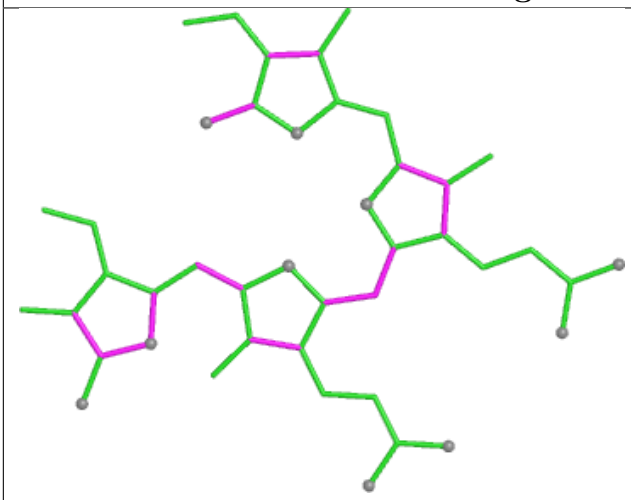


Rings

Ligand PEB KJ 201



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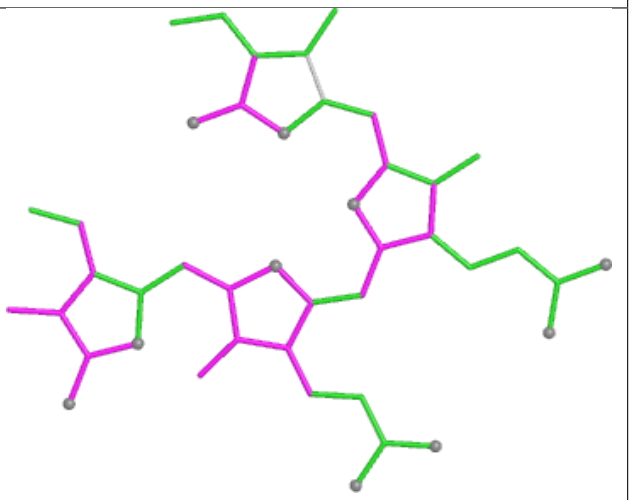

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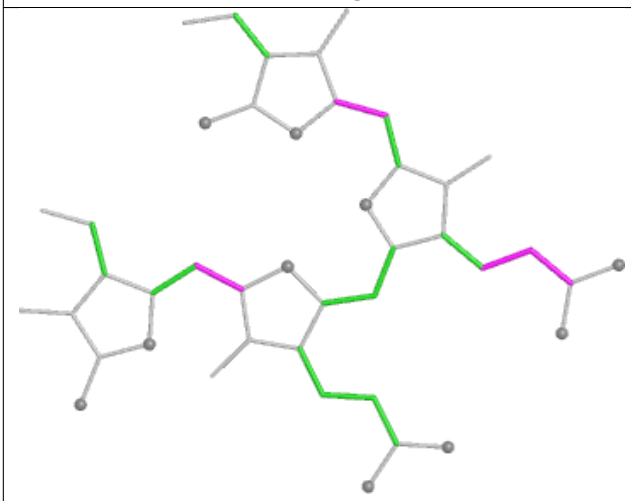

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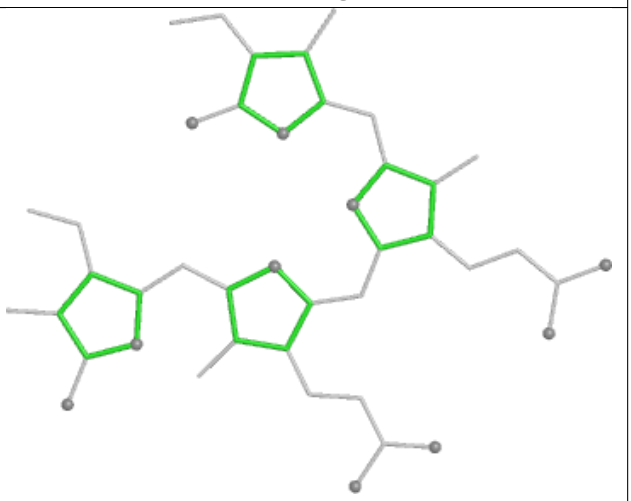
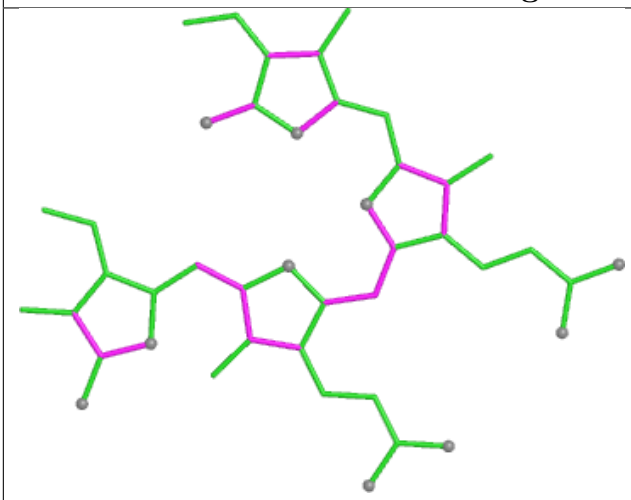


Rings

Ligand PEB r8 201



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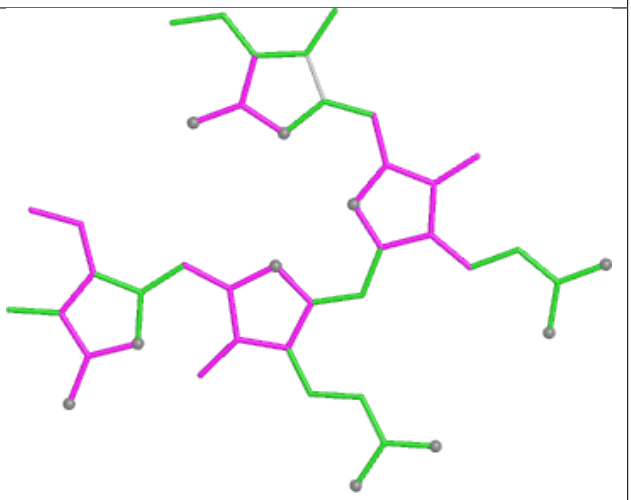

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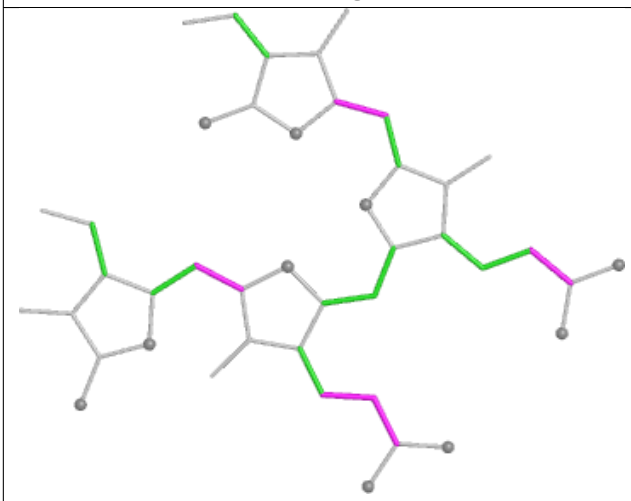

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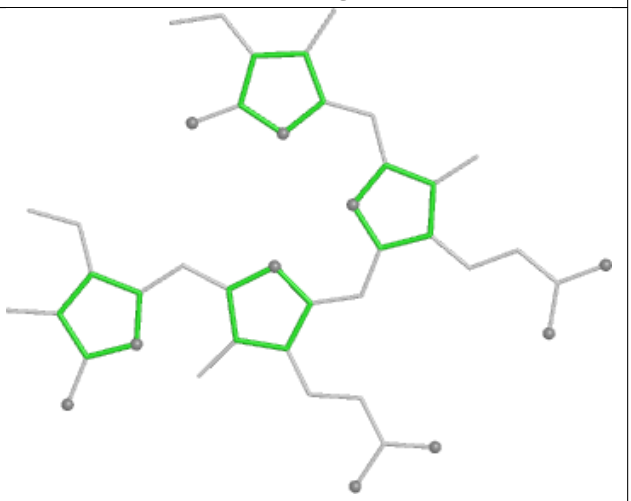
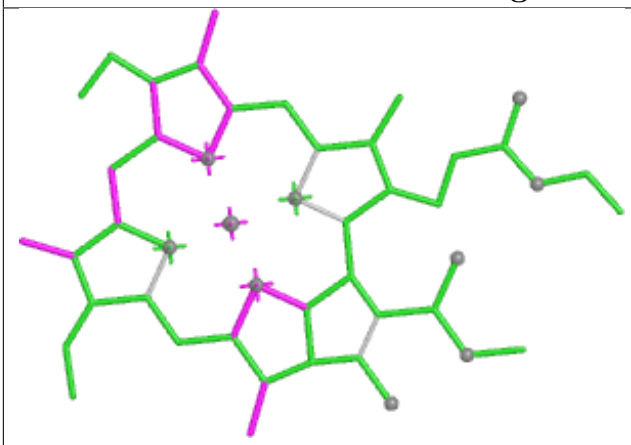


Rings

Ligand CLA BN 833



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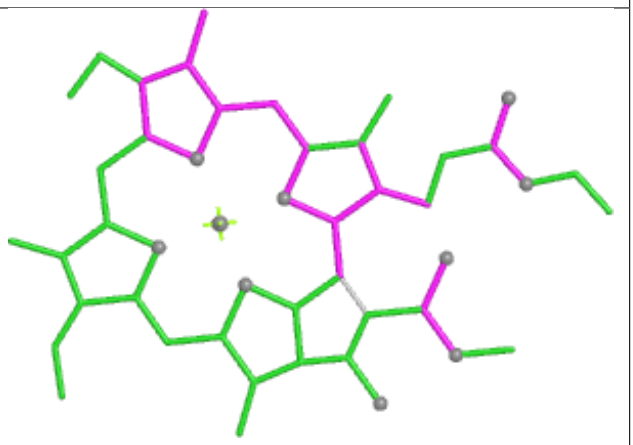

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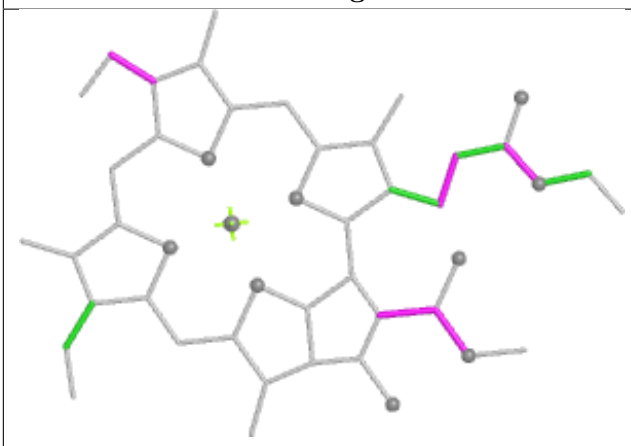

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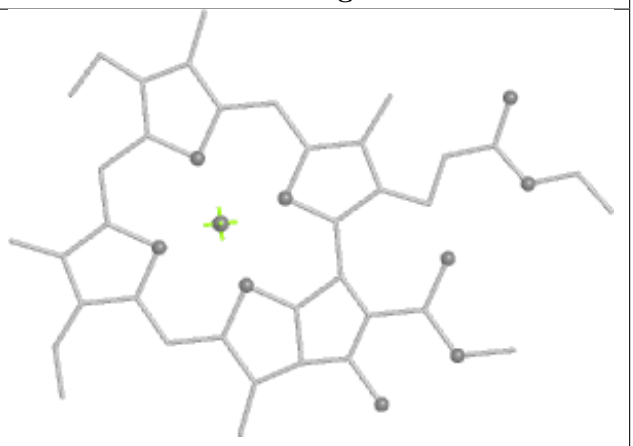
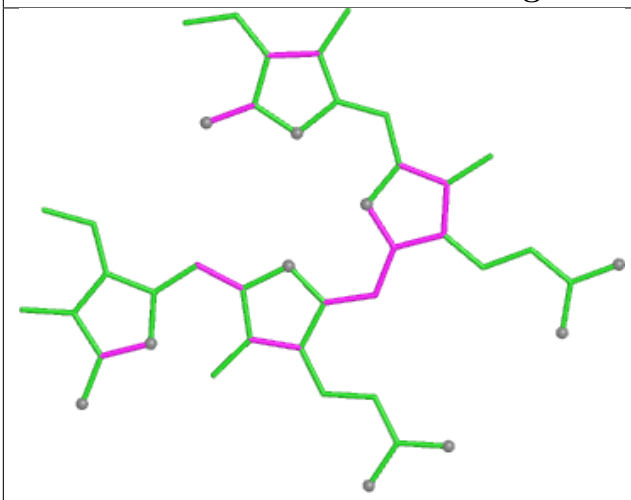


Rings

Ligand PEB jJ 202



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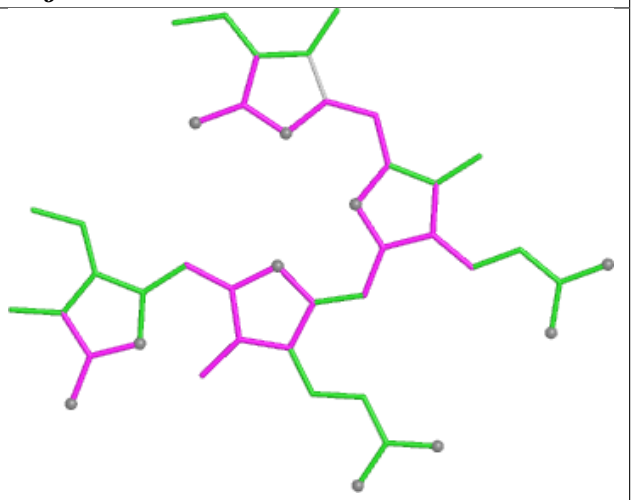

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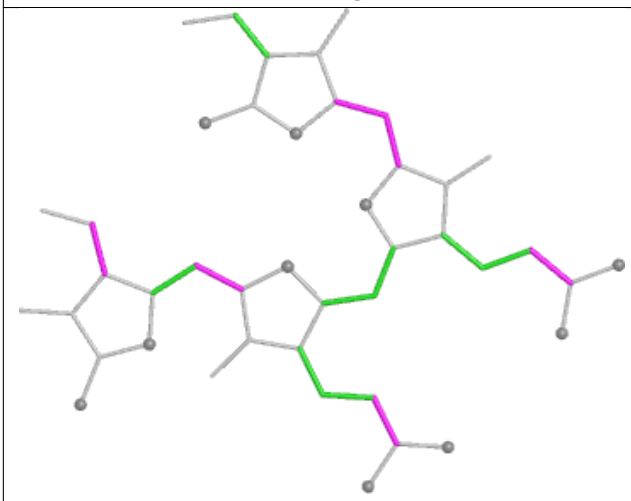

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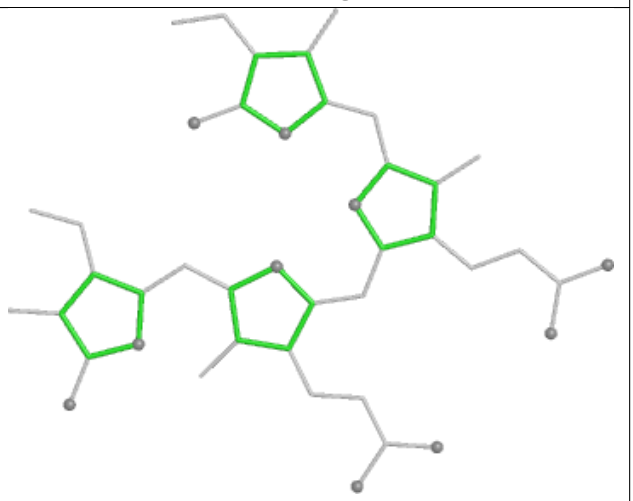
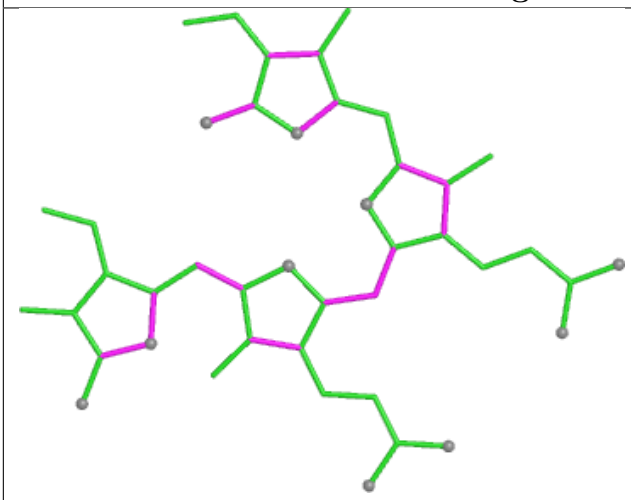


Rings

Ligand PEB M9 302



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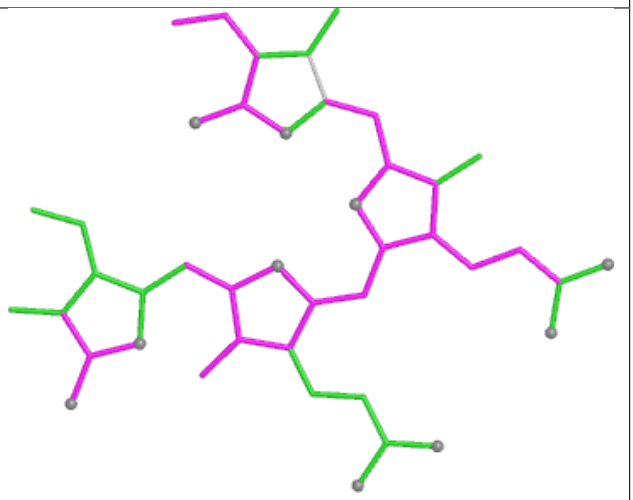

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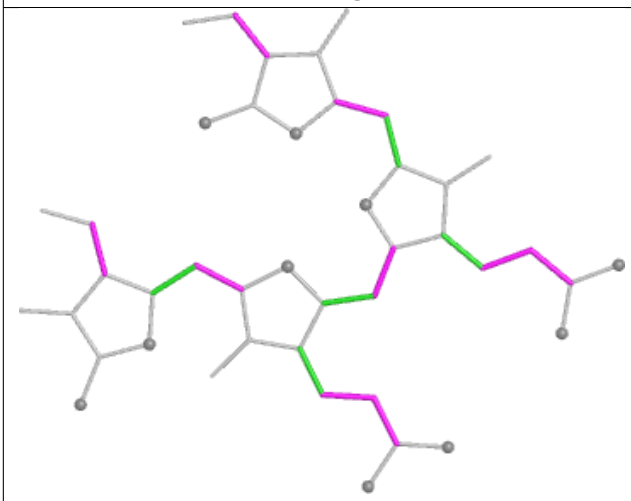

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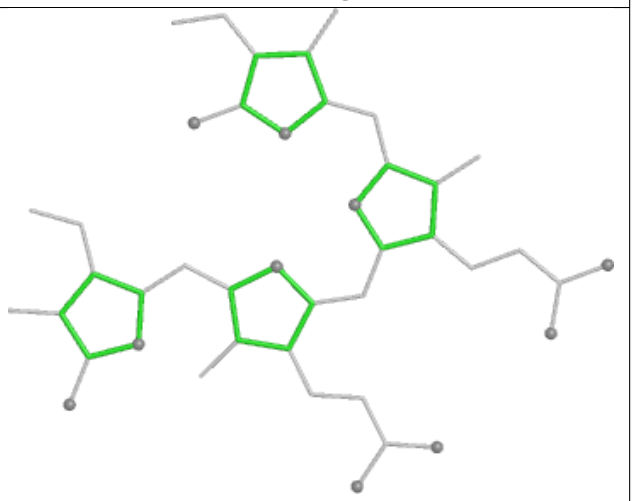

Rings

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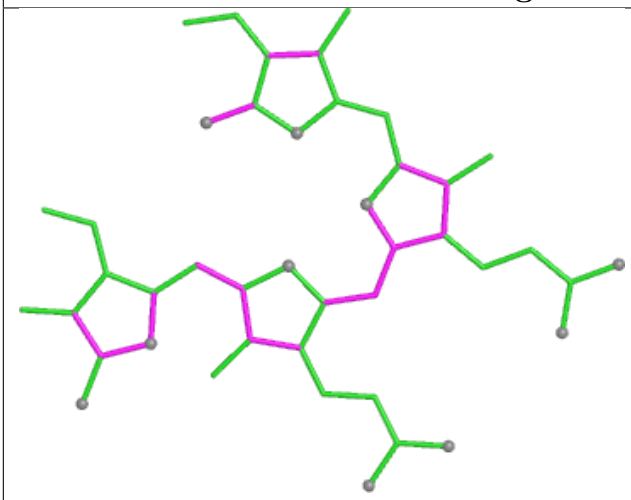

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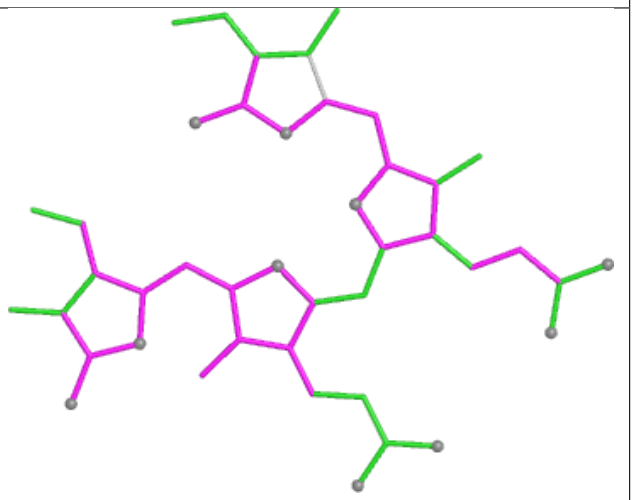

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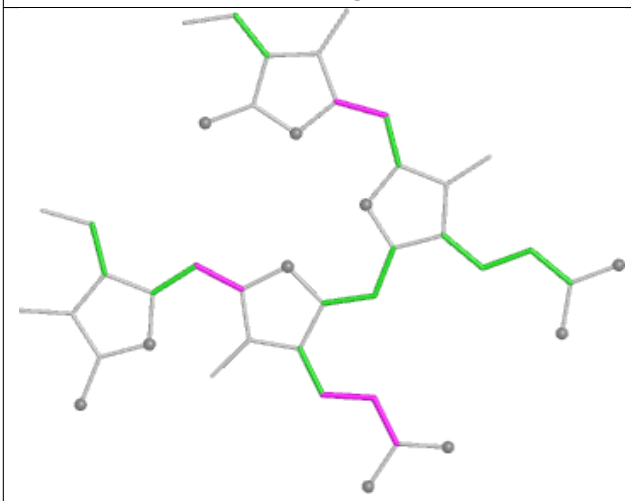

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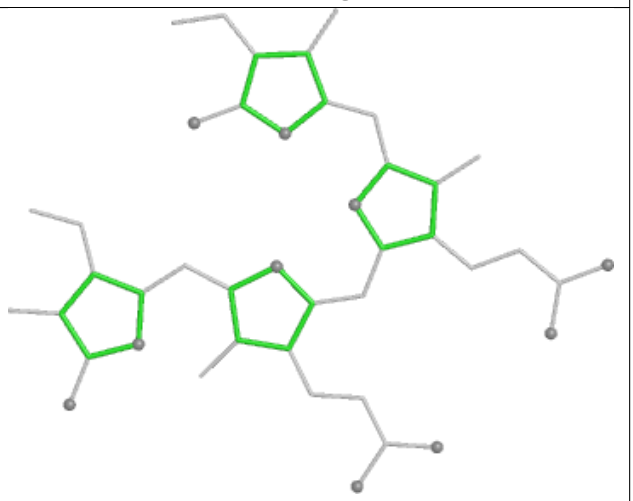
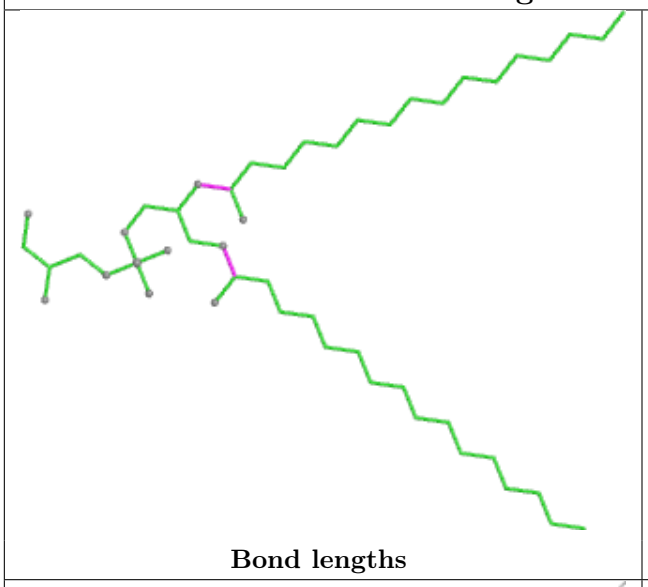


Rings

Ligand LHG bL 612



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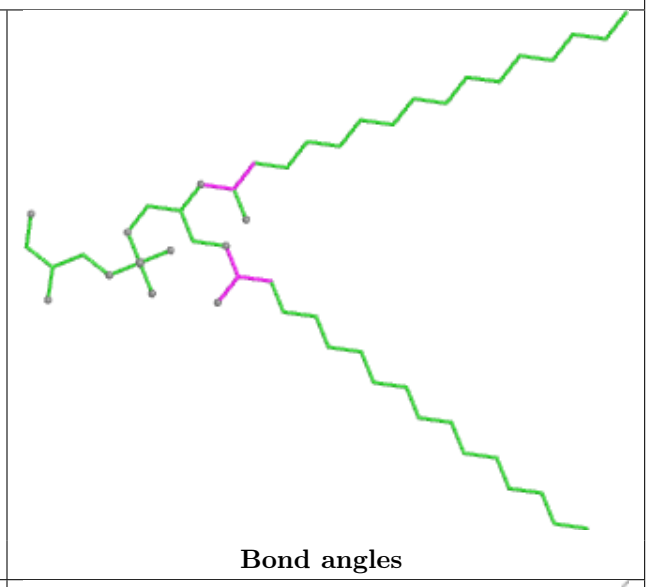

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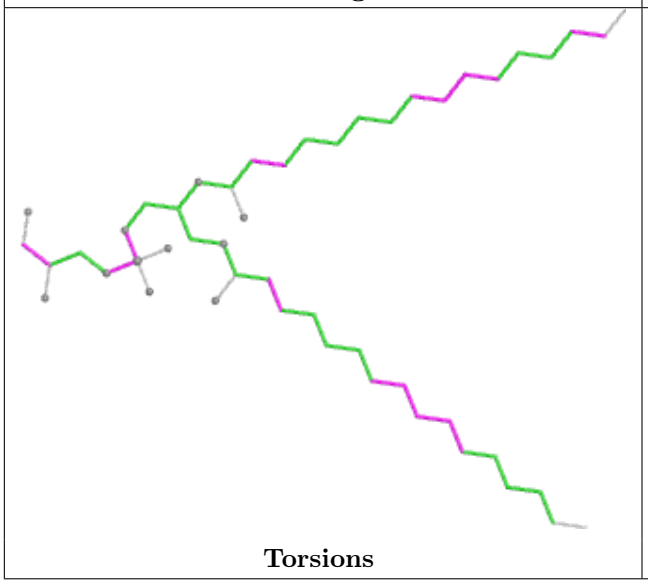

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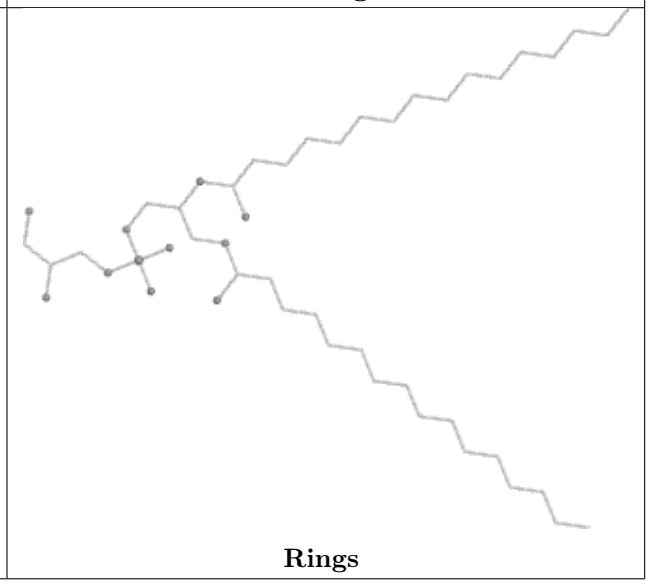
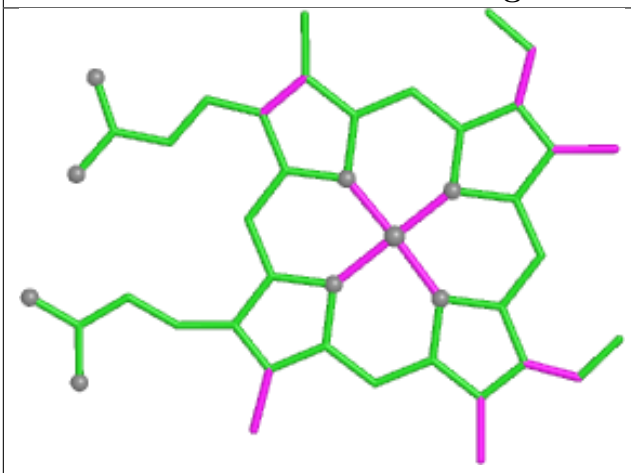


Rings

Ligand HEM GN 201



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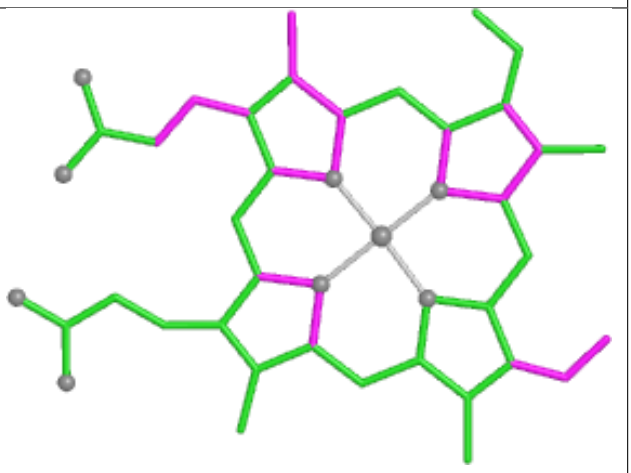

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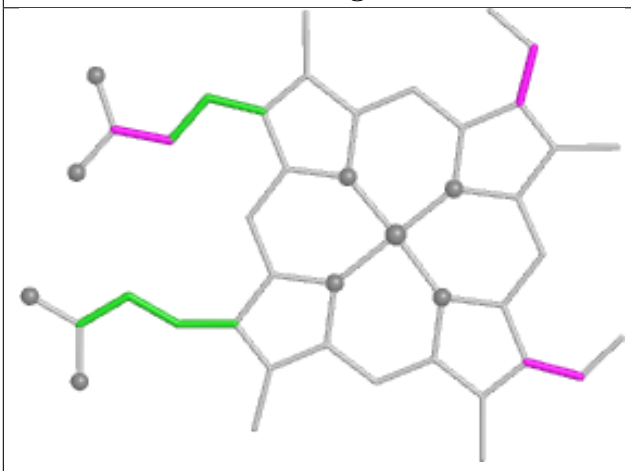

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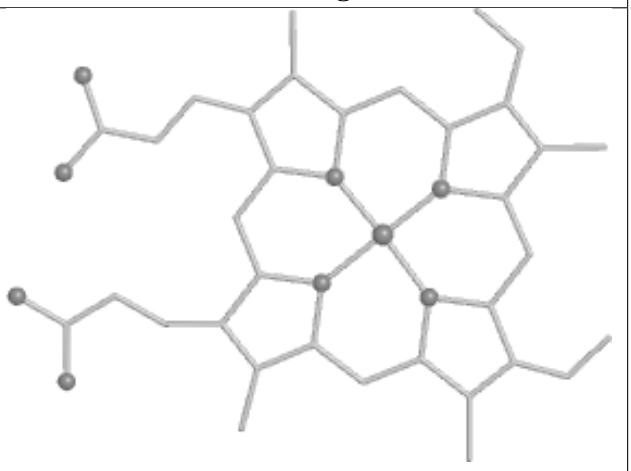
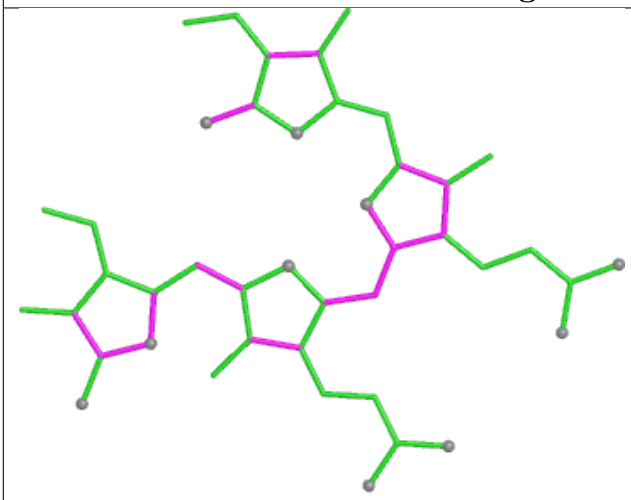


Rings

Ligand PEB iG 201



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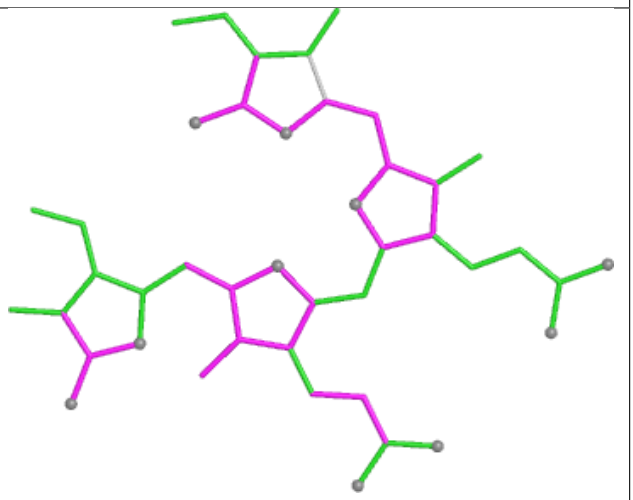

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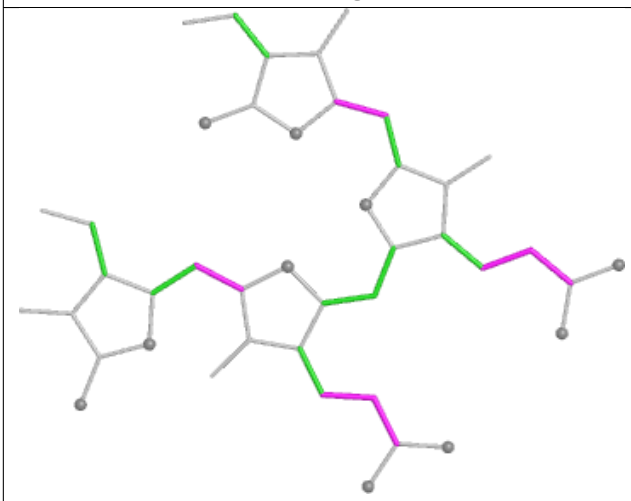

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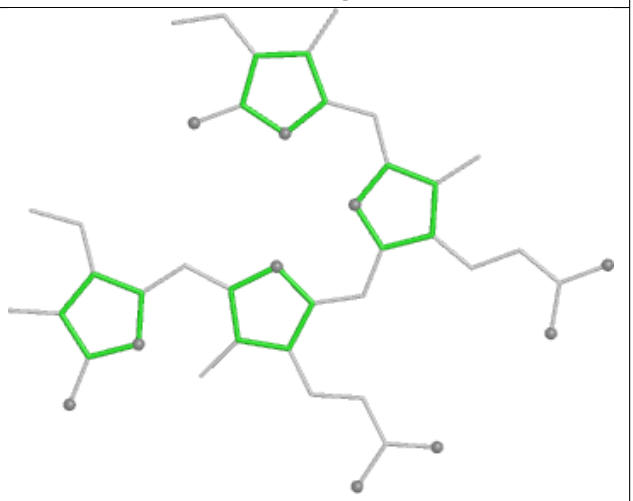
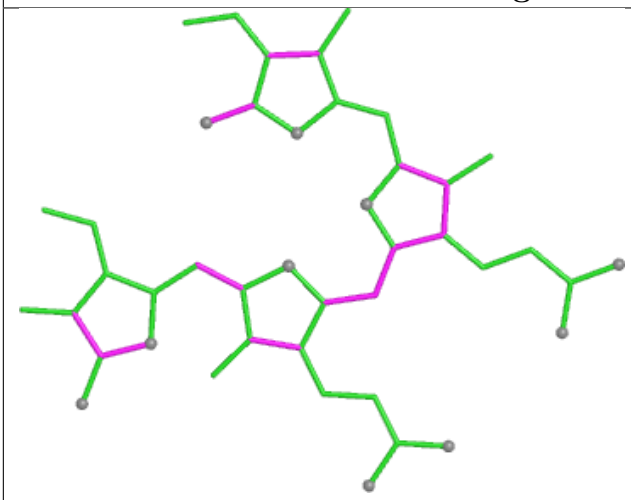


Rings

Ligand PEB VF 201



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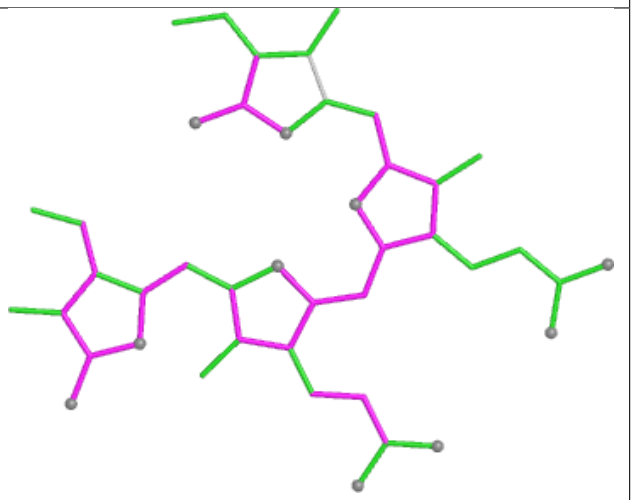

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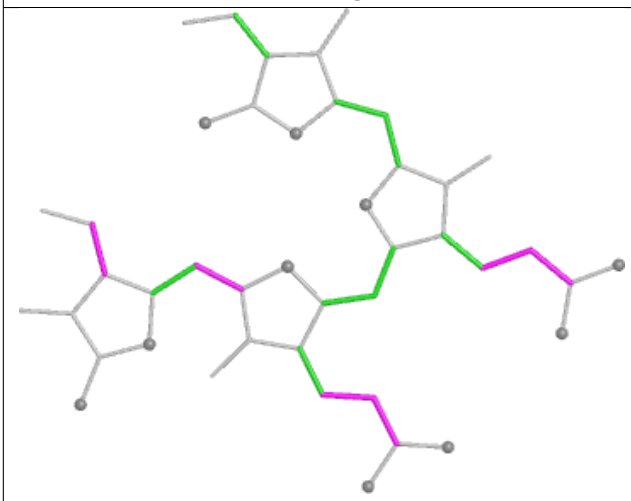

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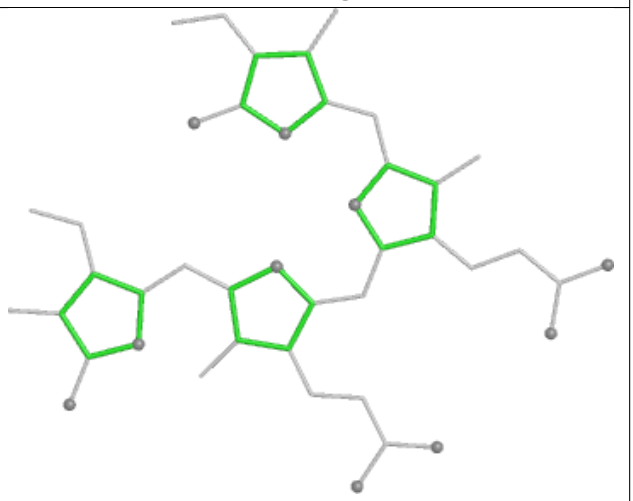
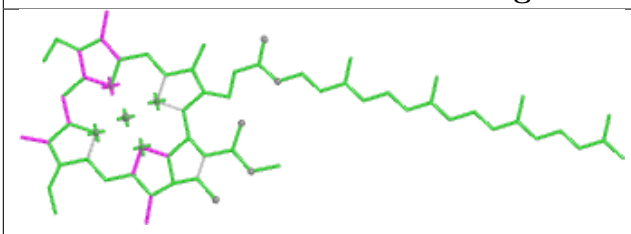


Rings

Ligand CLA BL 619



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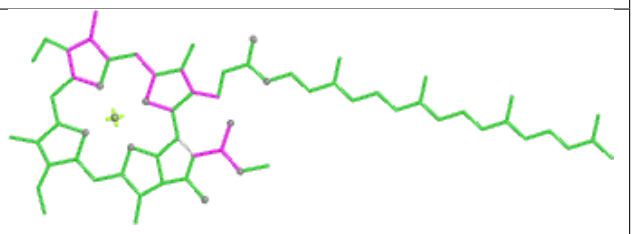

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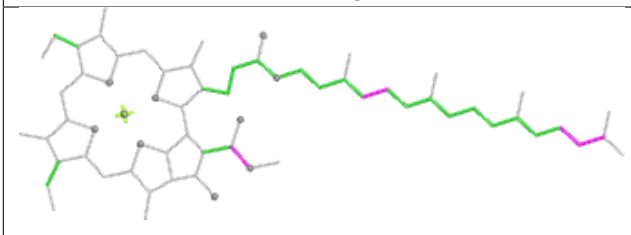

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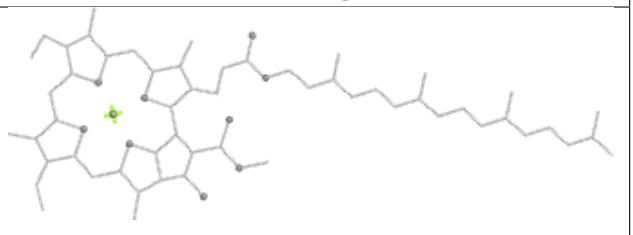
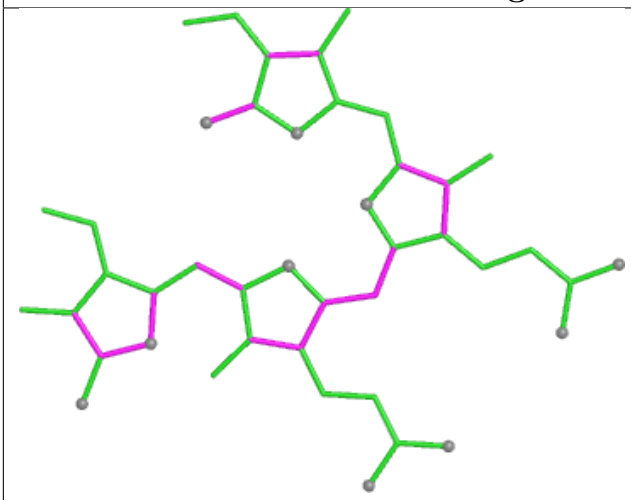


Rings

Ligand PEB WF 201



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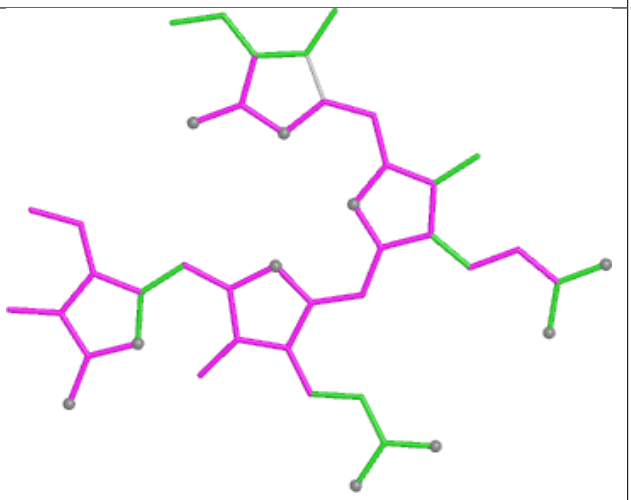

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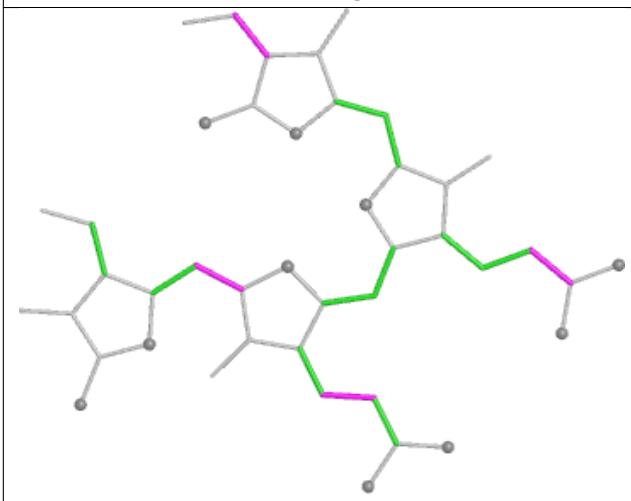

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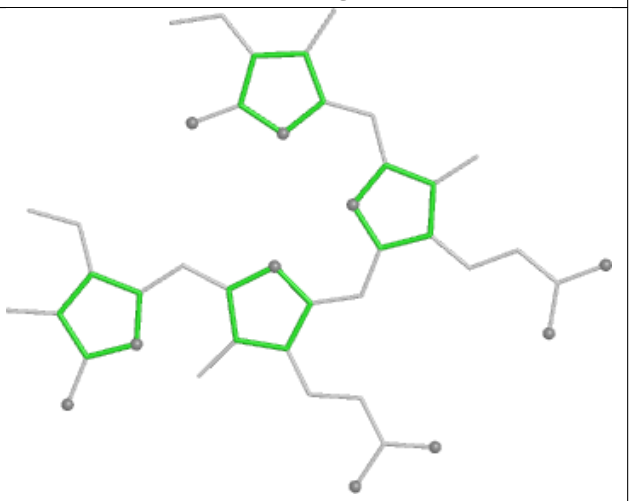
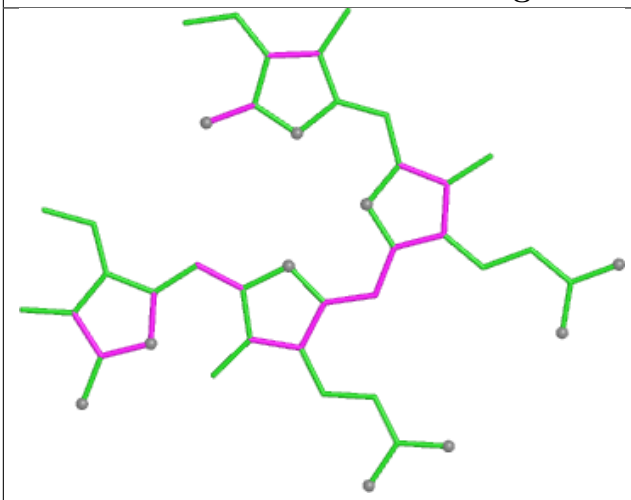


Rings

Ligand PEB FQ 202



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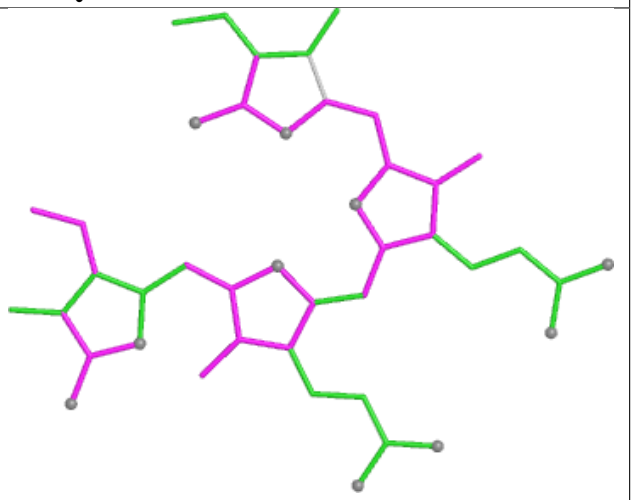
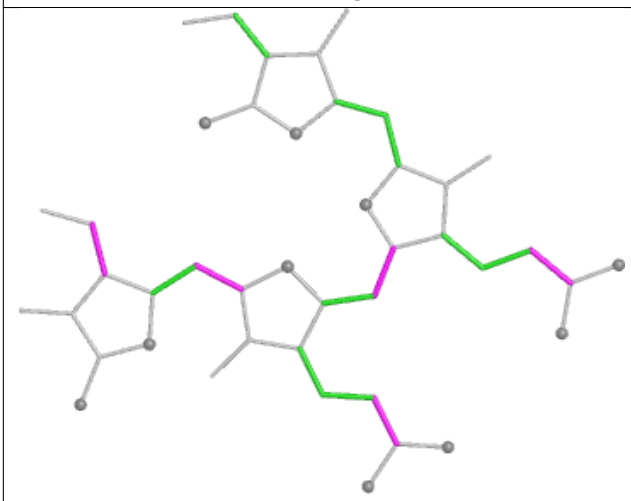


Bond angles



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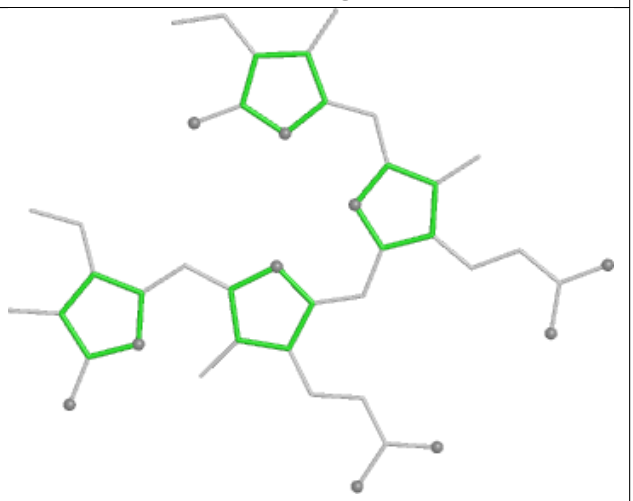
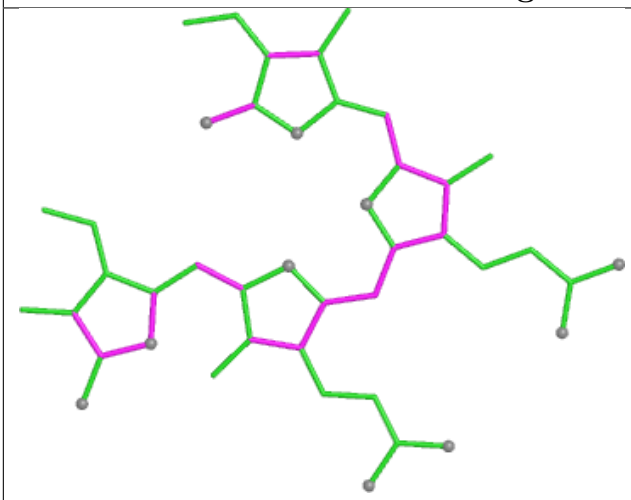


Rings

Ligand PEB E7 201



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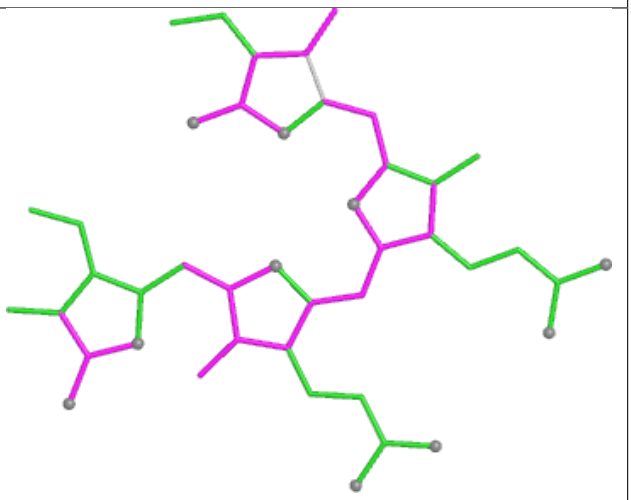
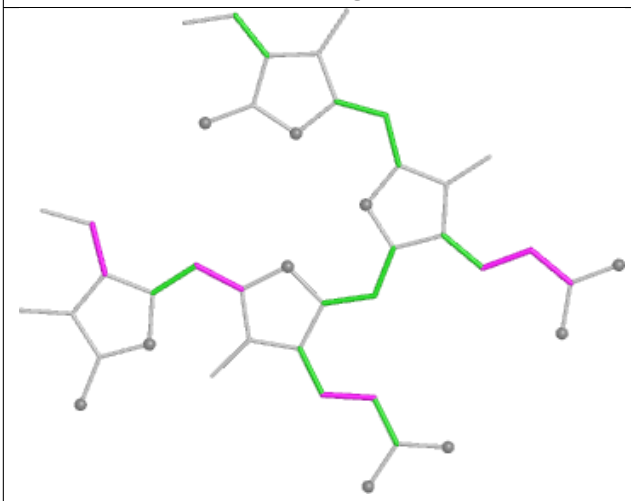


Bond angles



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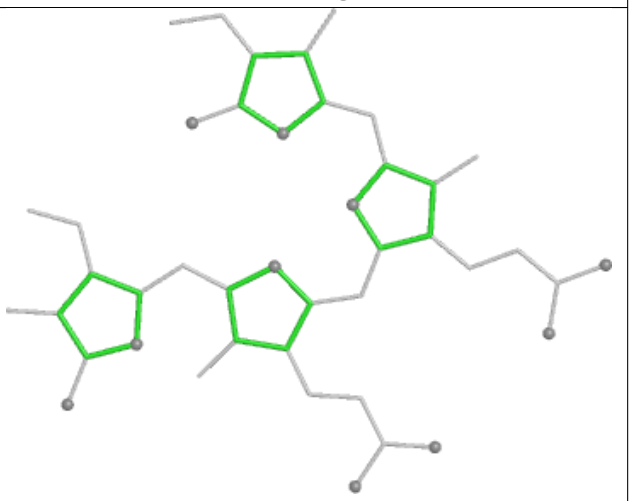
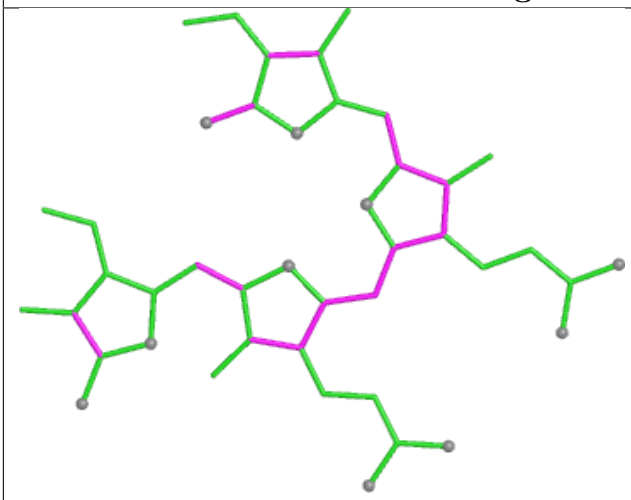


Rings

Ligand PEB vK 201



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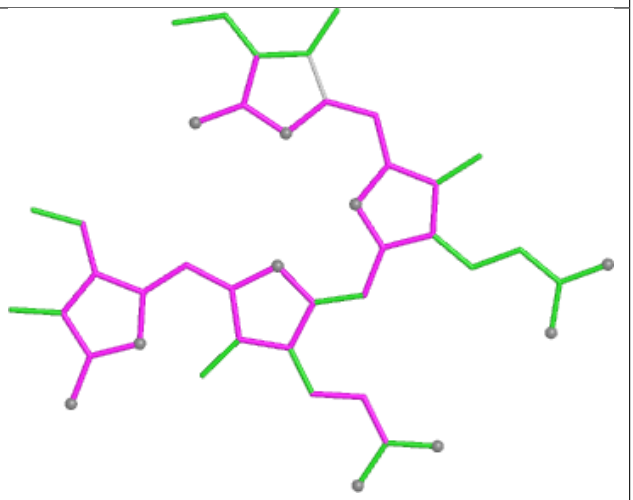

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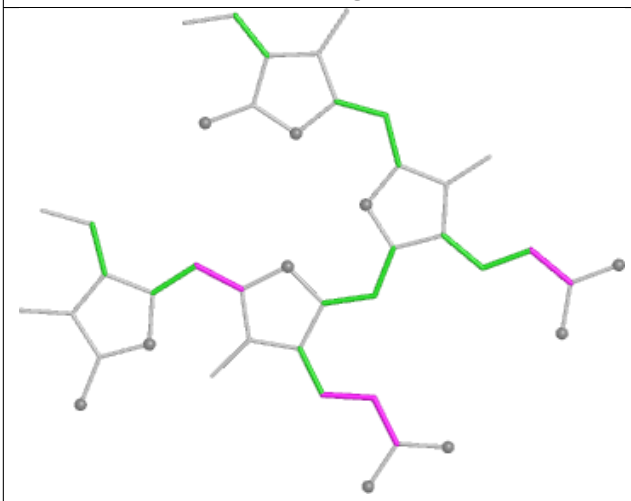
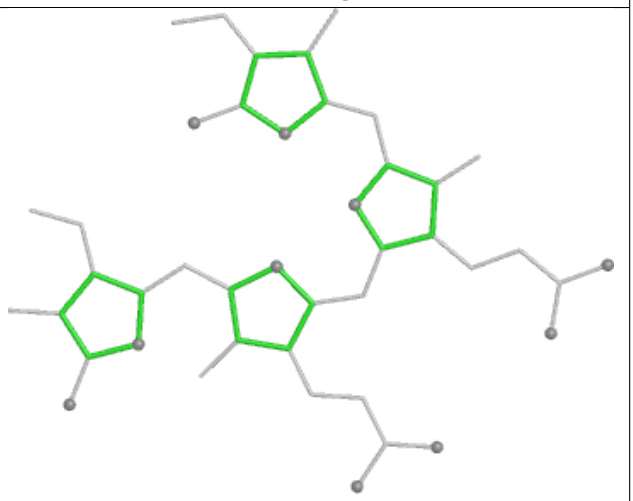
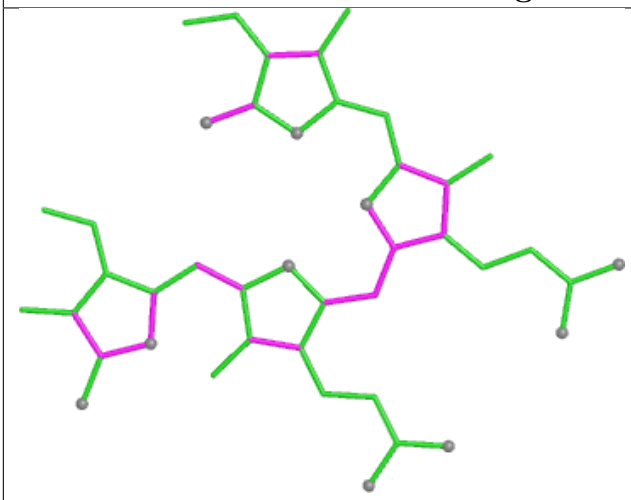


Torsions



Rings

Ligand PEB QJ 204



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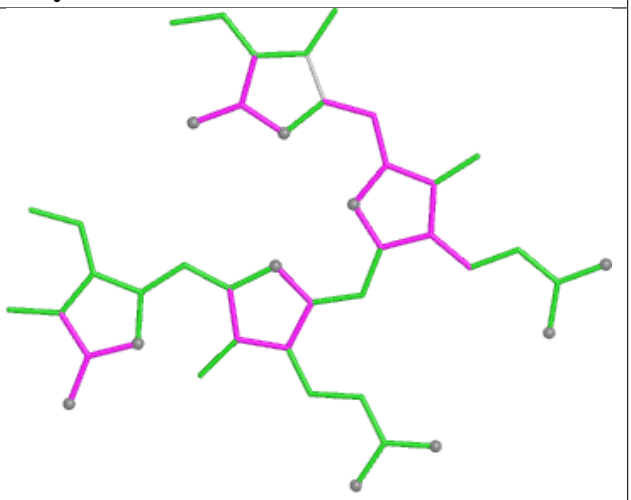

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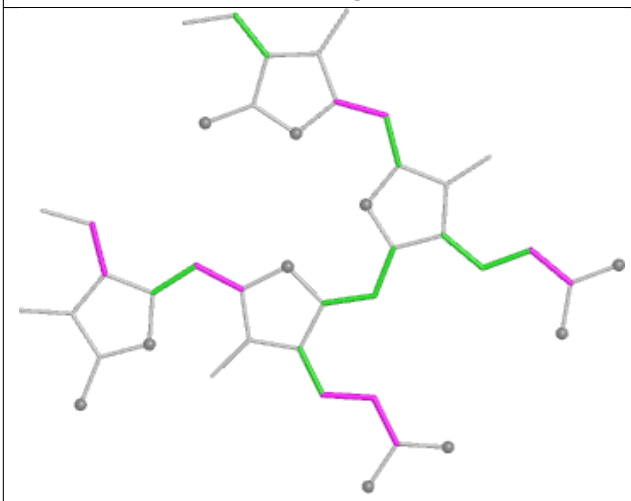

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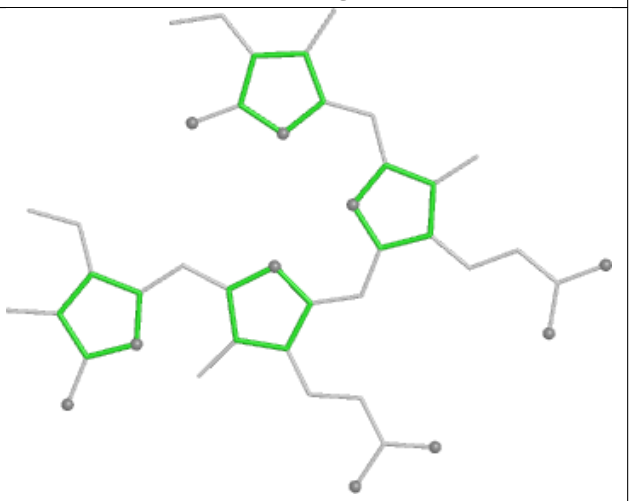
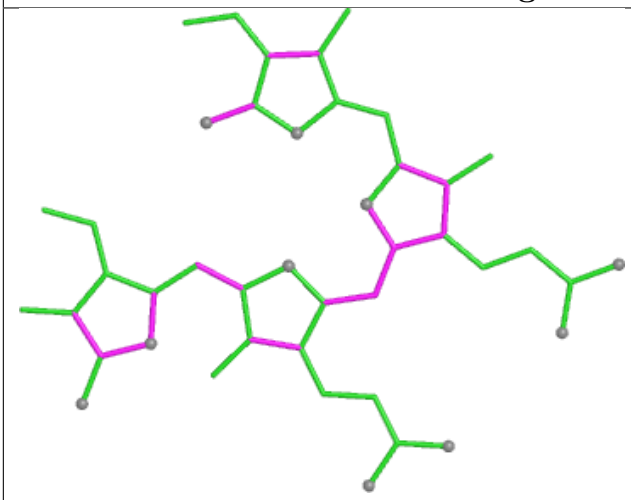


Rings

Ligand PEB jK 202



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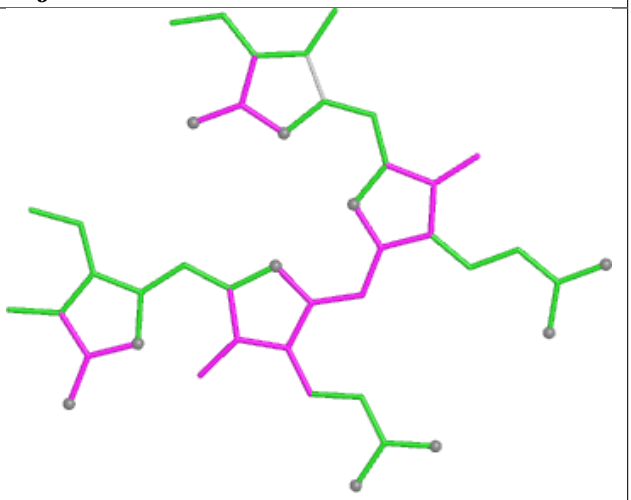

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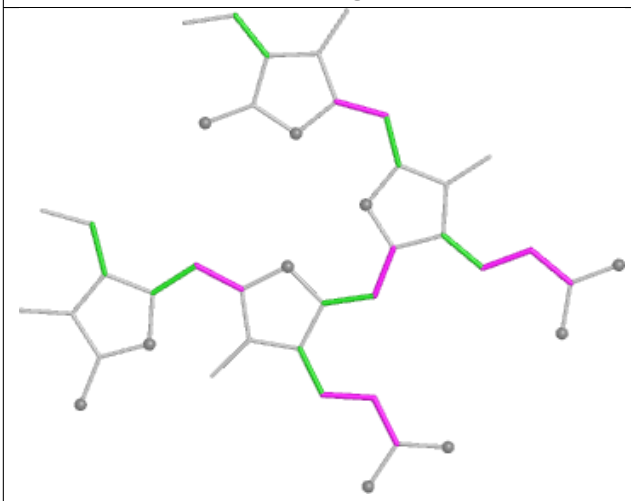

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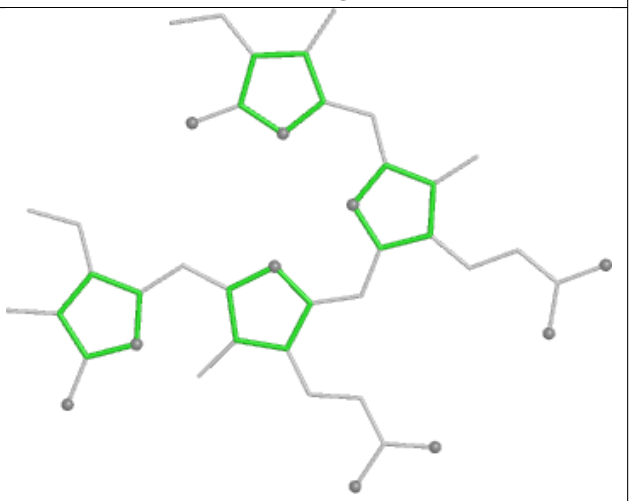
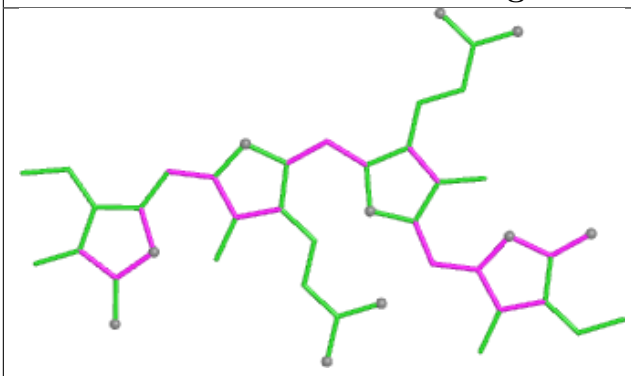


Rings

Ligand CYC KG 202



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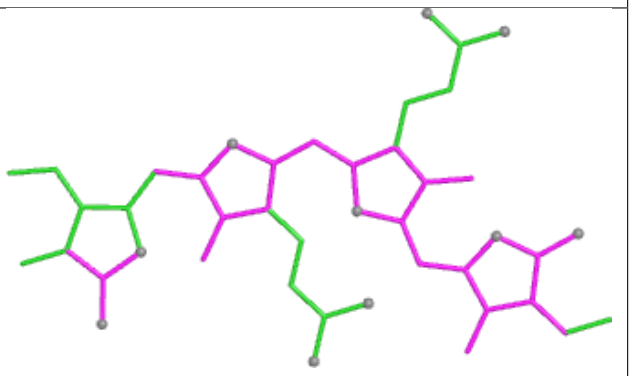

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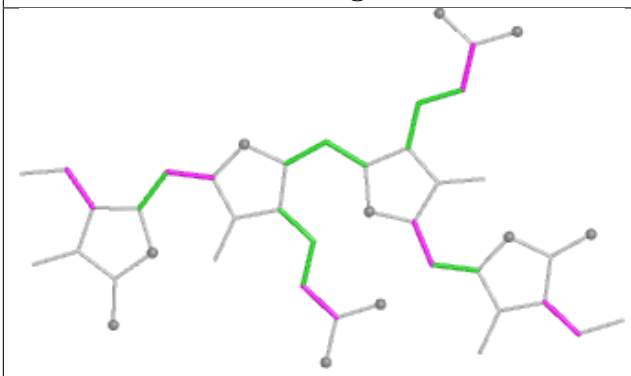

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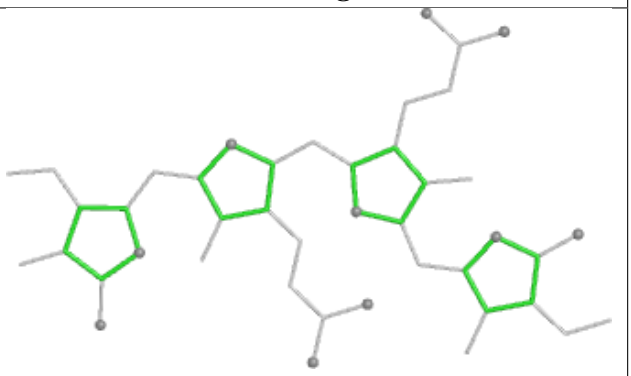
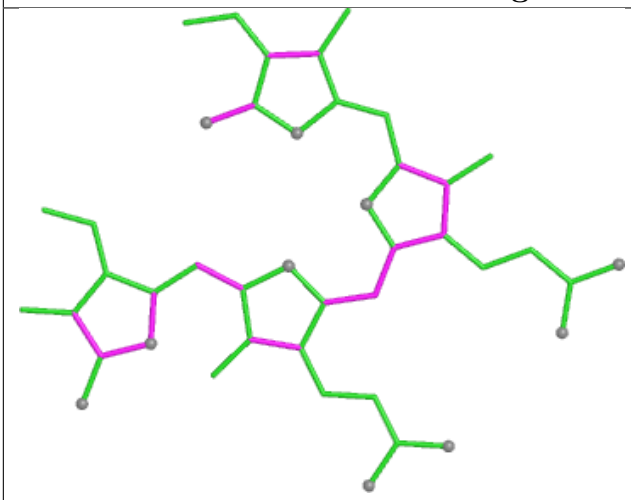


Rings

Ligand PEB mF 202



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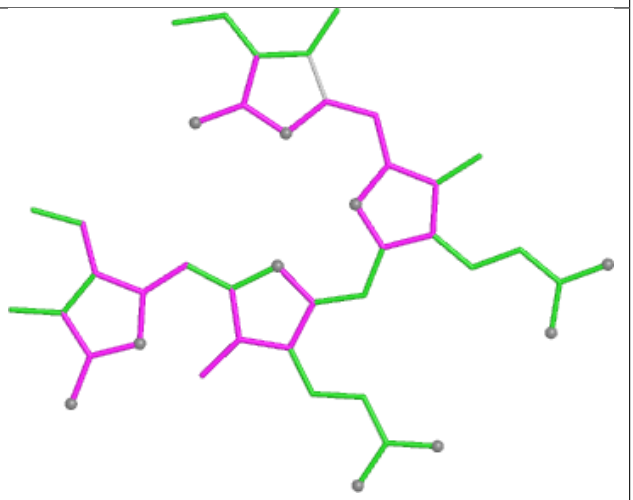

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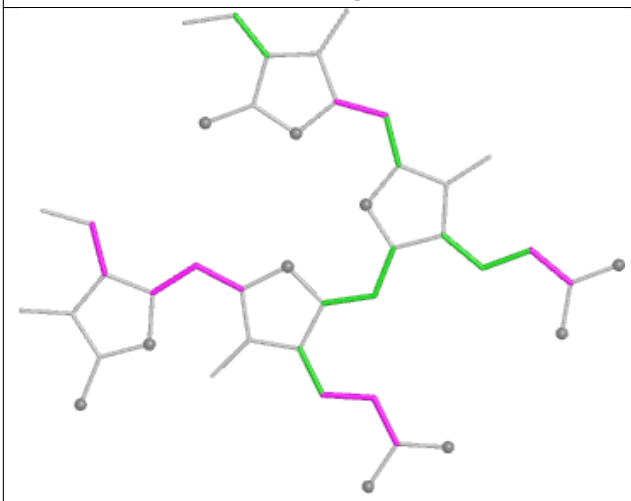

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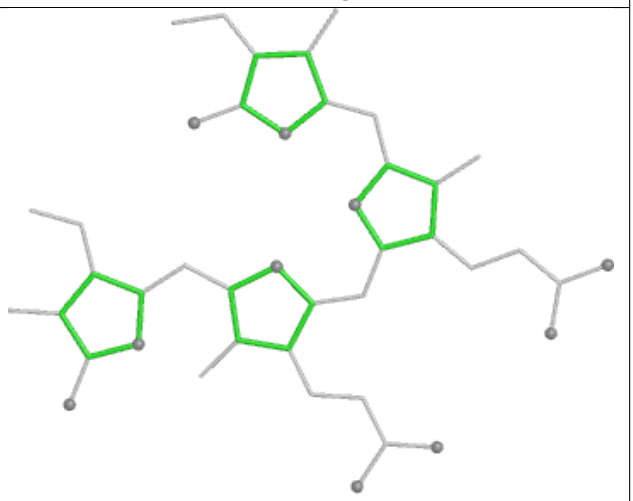
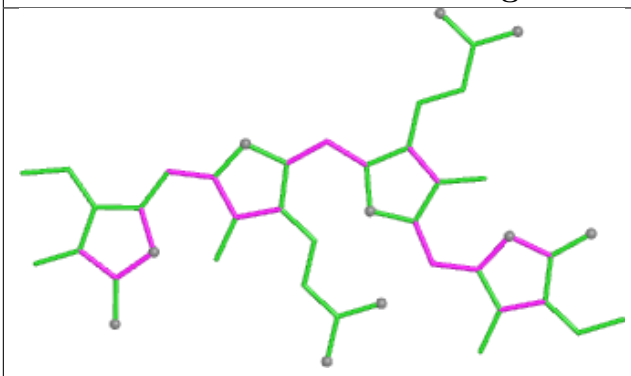


Rings

Ligand CYC LH 1001



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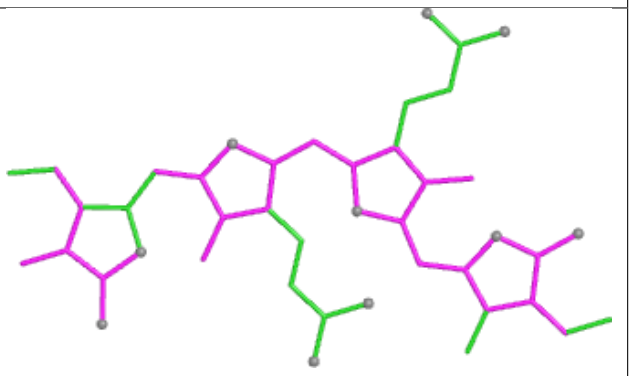

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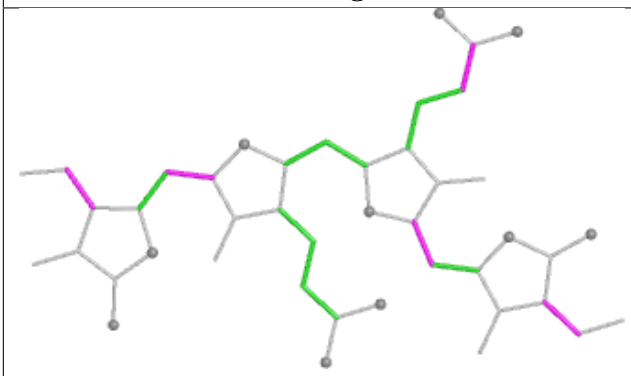

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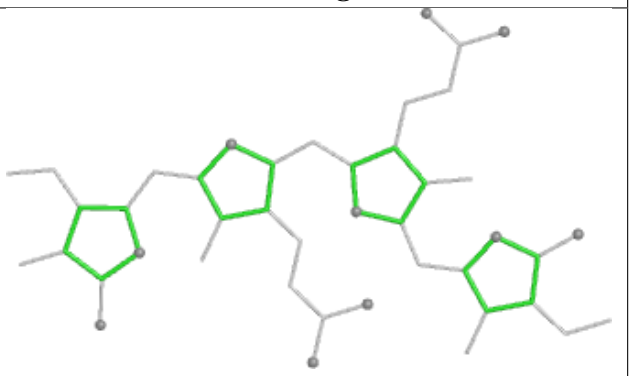
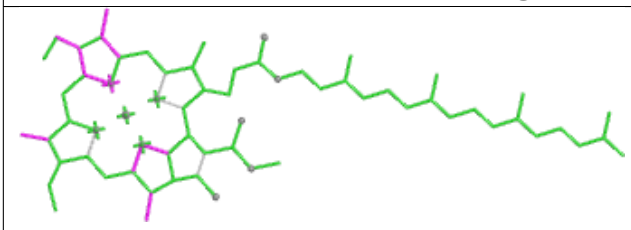


Rings

Ligand CLA A2 834



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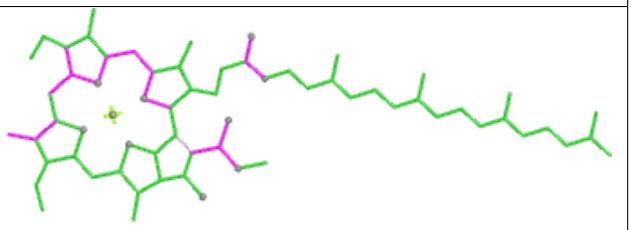

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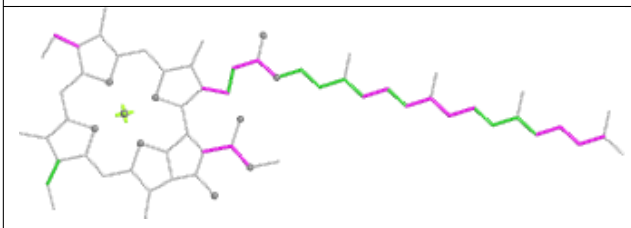

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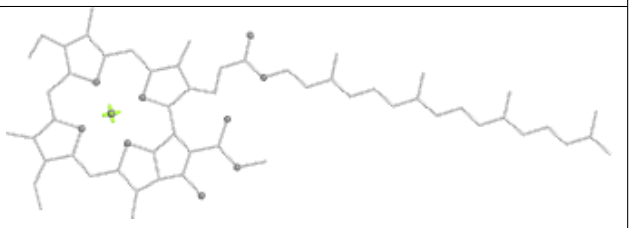
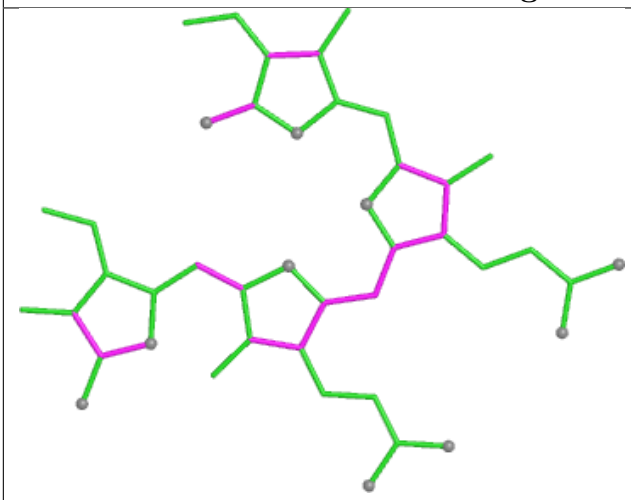


Rings

Ligand PEB cJ 202



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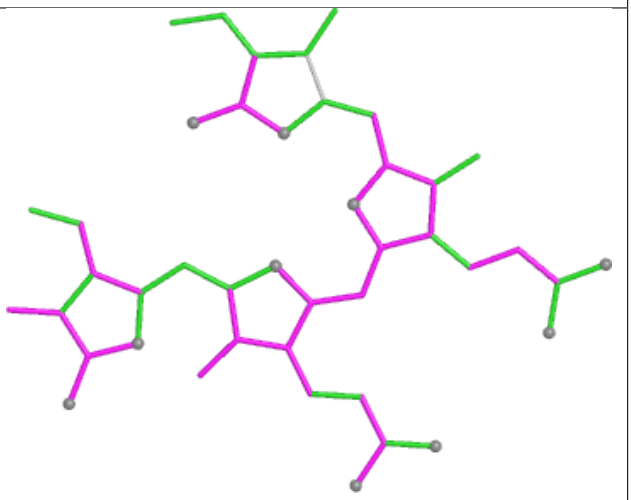

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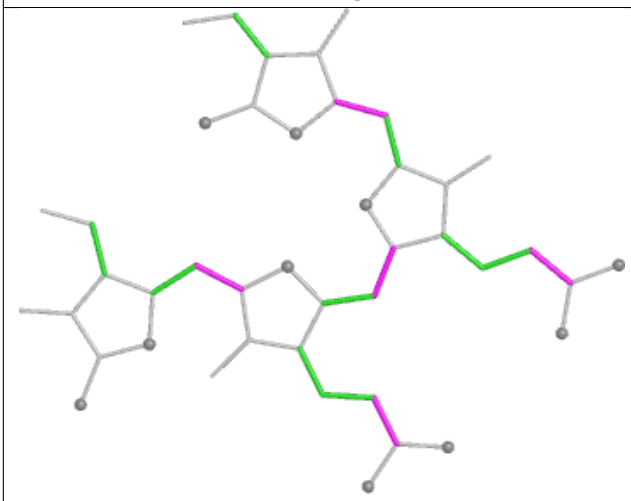

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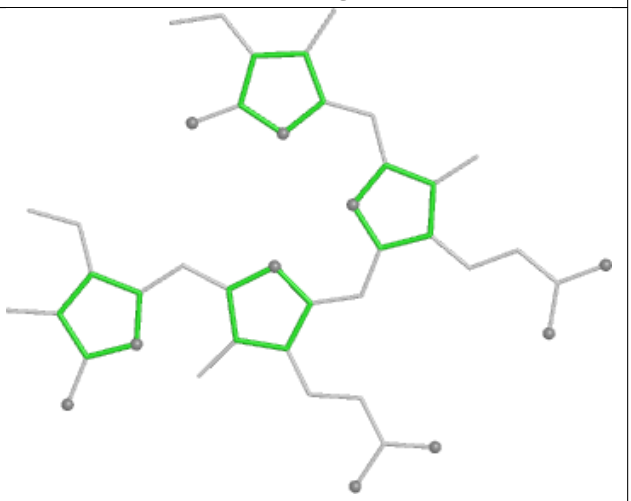
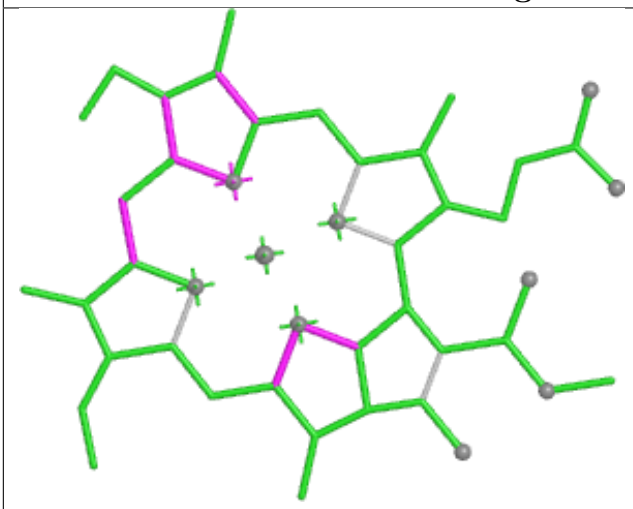


Rings

Ligand CLA 7N 601



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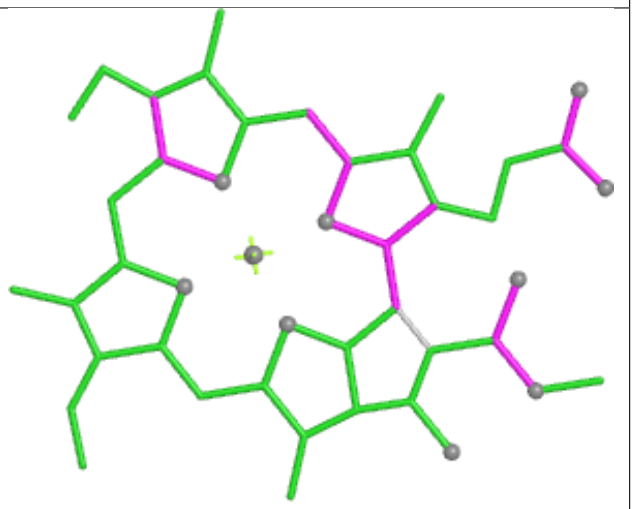

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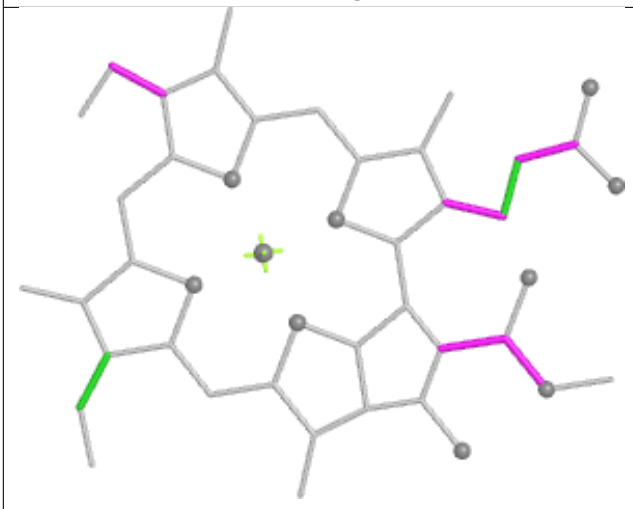
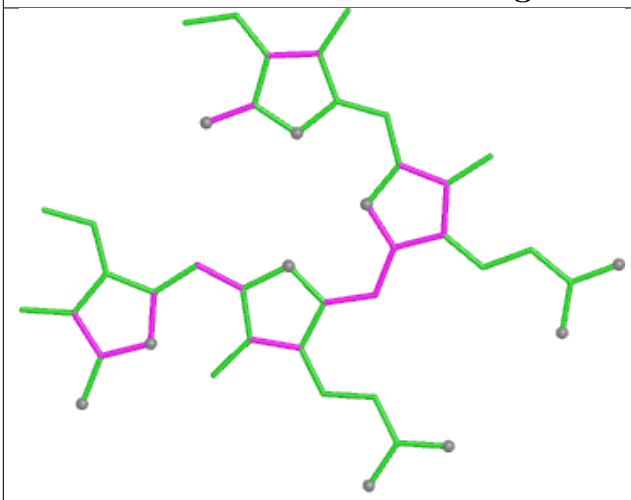


Torsions



Rings

Ligand PEB ZB 201



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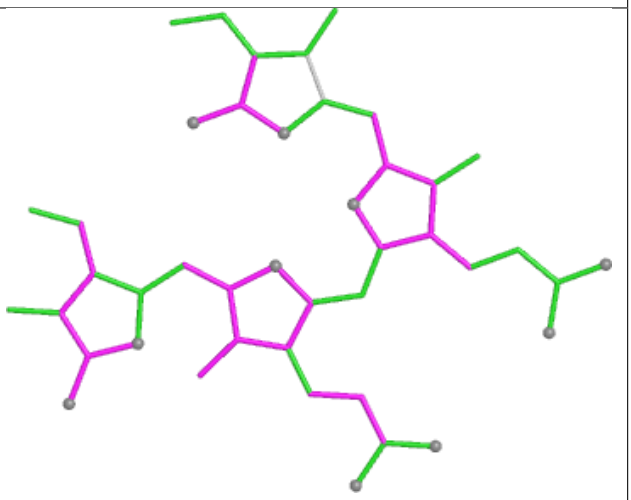

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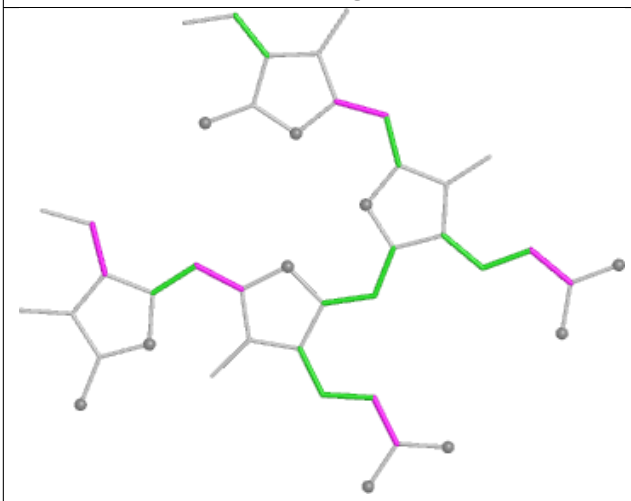

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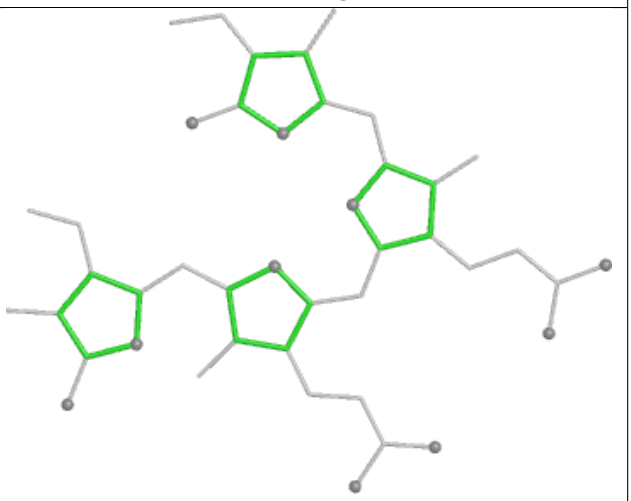
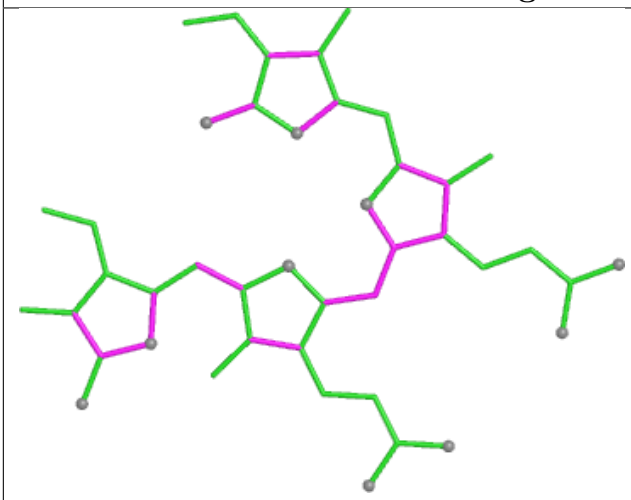


Rings

Ligand PEB jO 202



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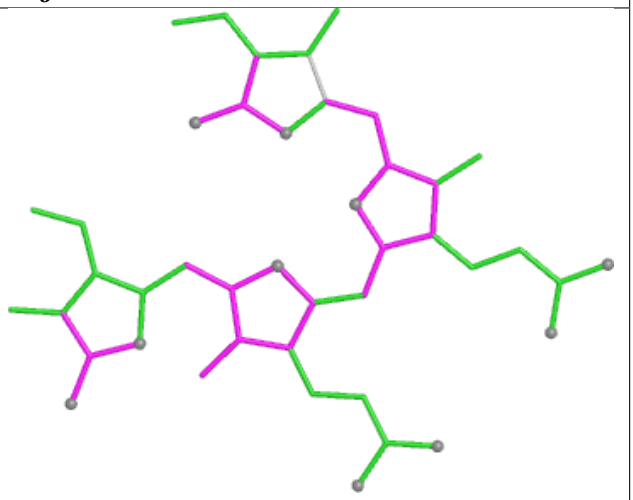

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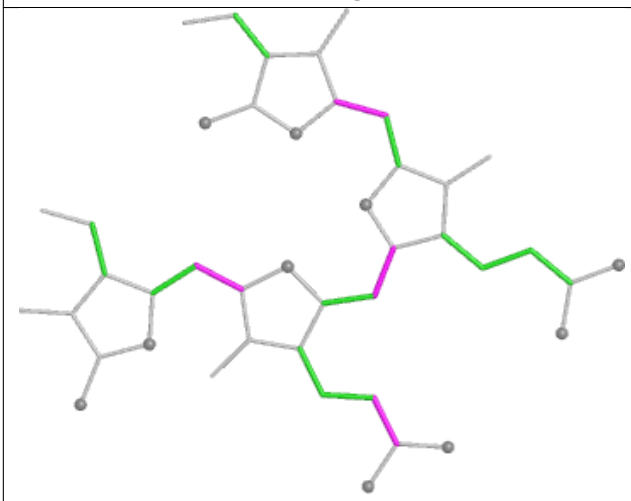

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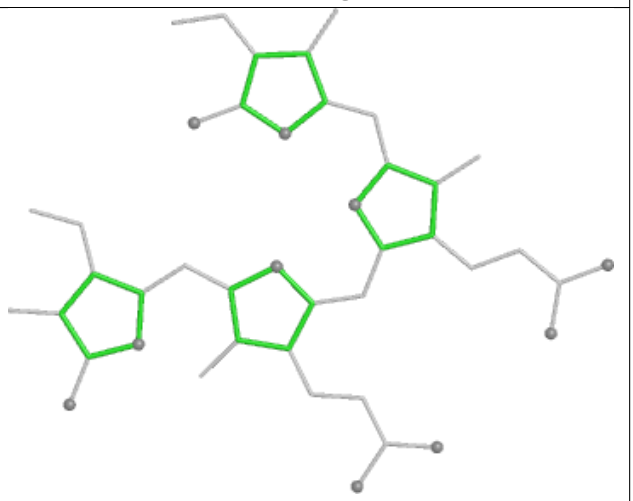
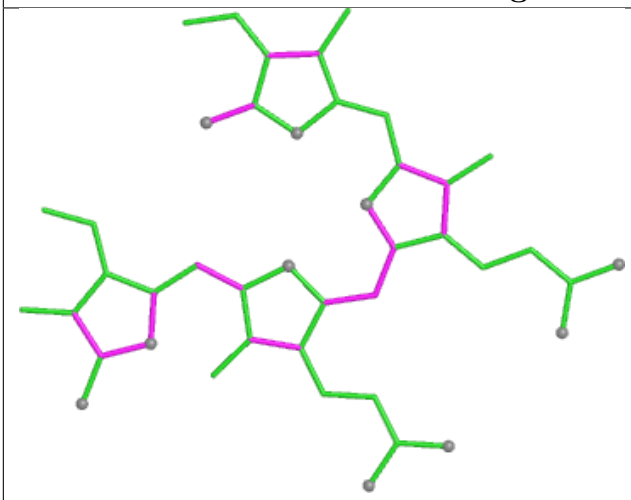


Rings

Ligand PEB OG 202



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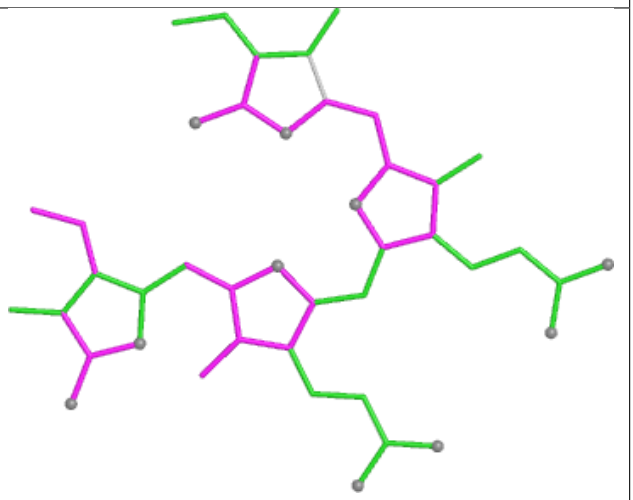

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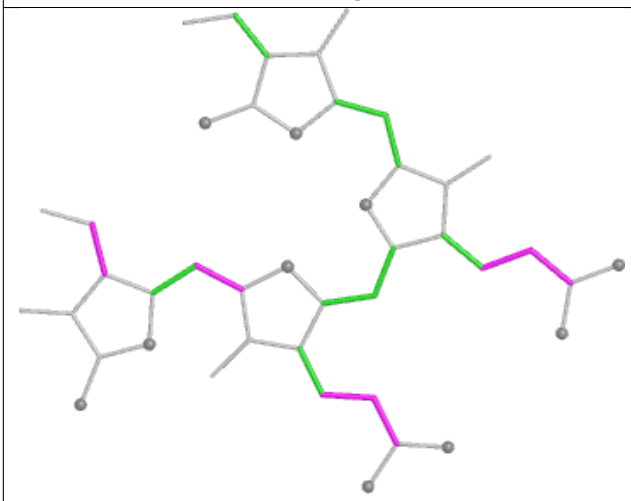

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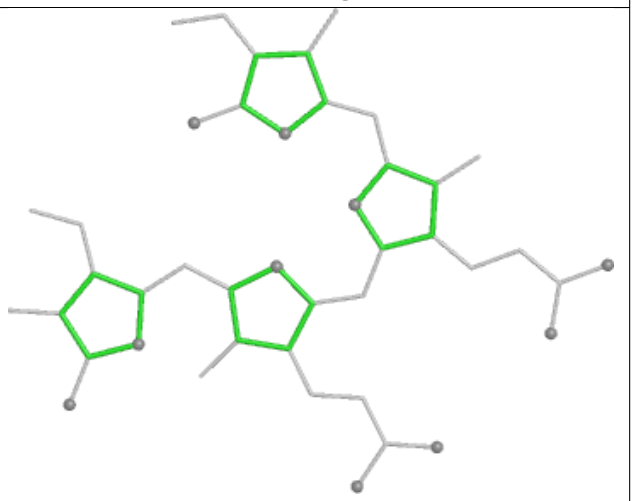
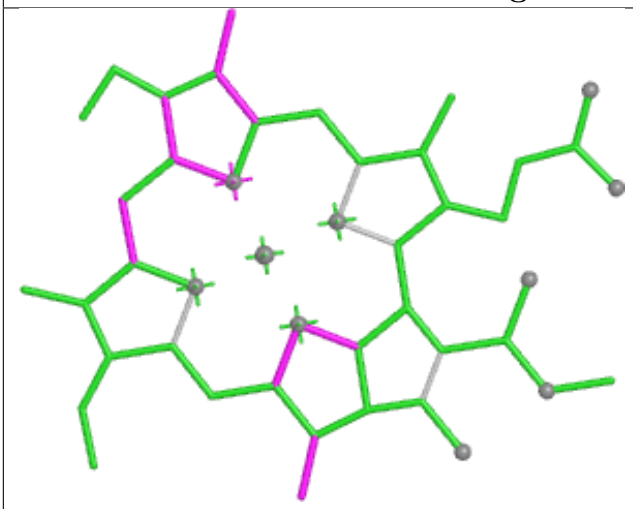


Rings

Ligand CLA RN 204



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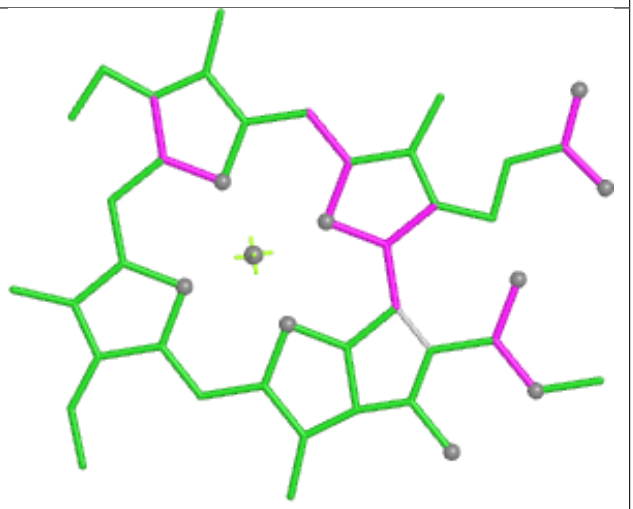
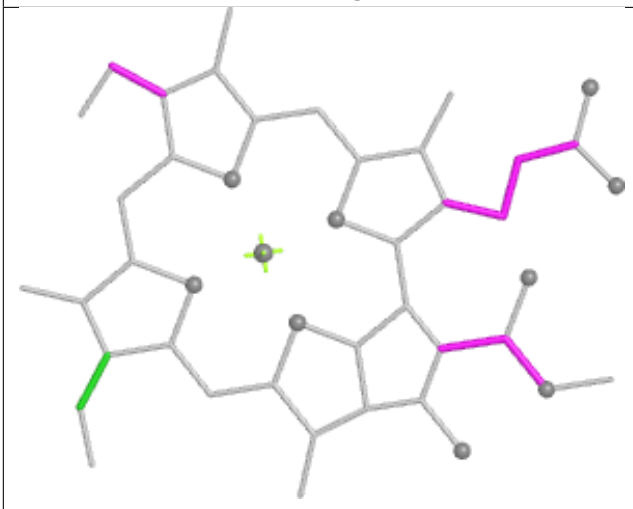


Bond angles

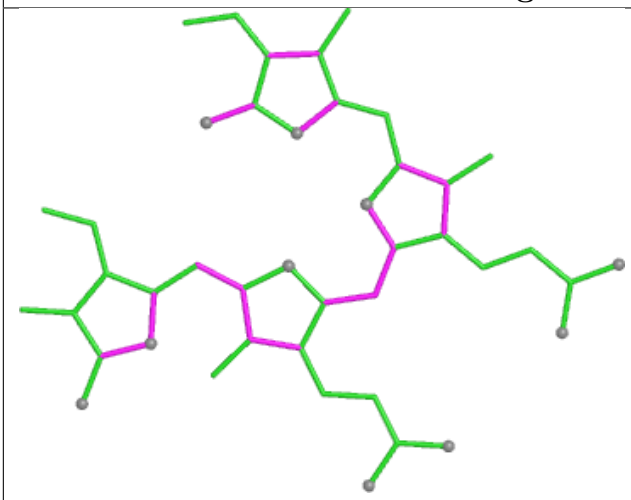


Torsions



Rings

Ligand PEB sK 201



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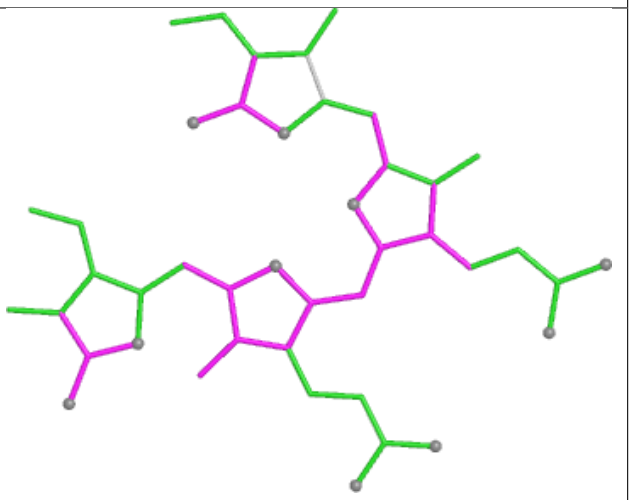
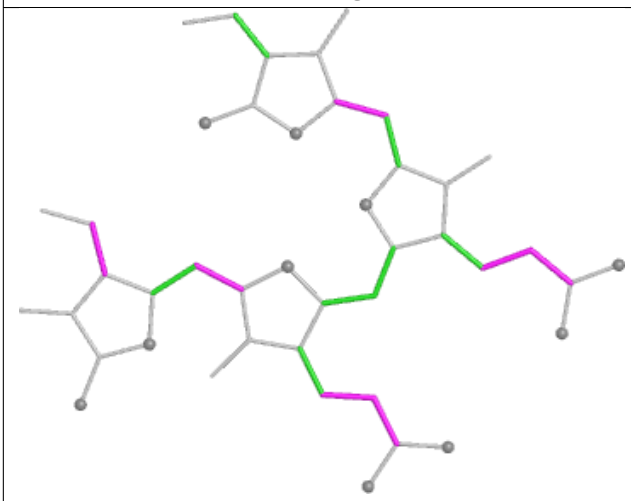


Bond angles



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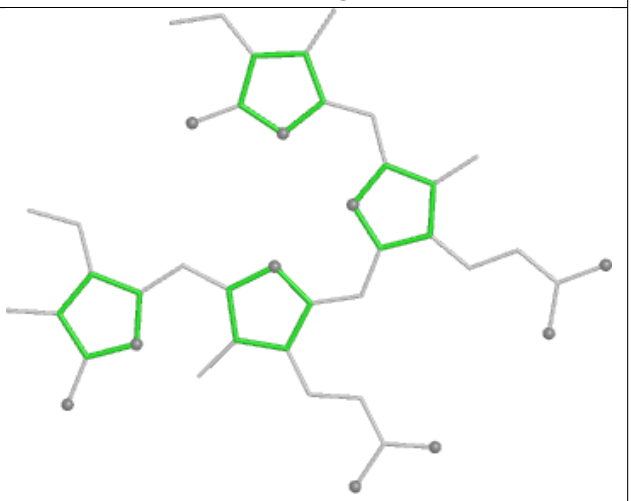
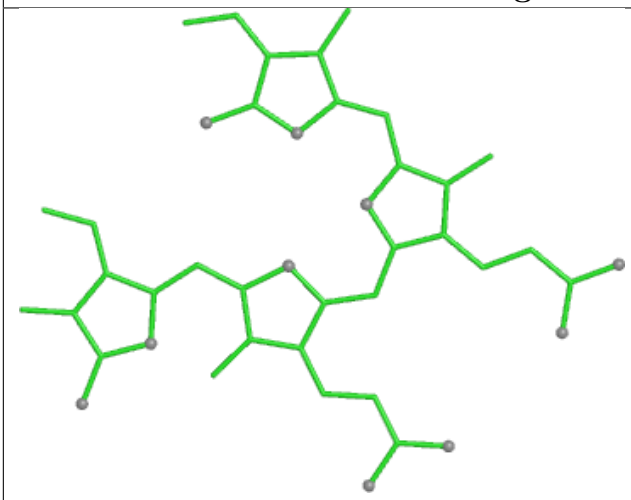


Rings

Ligand PEB MI 401



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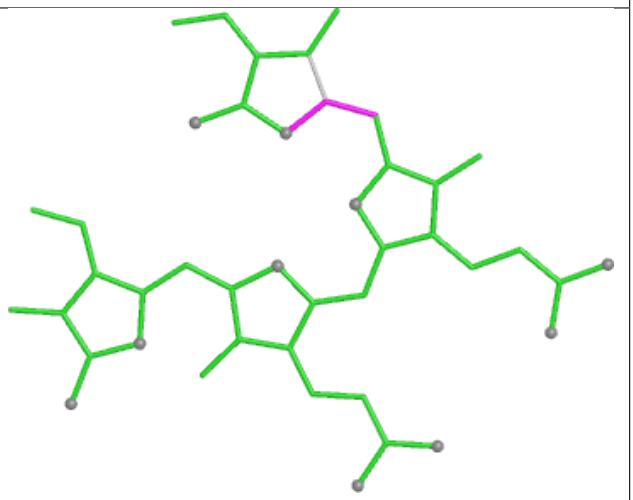
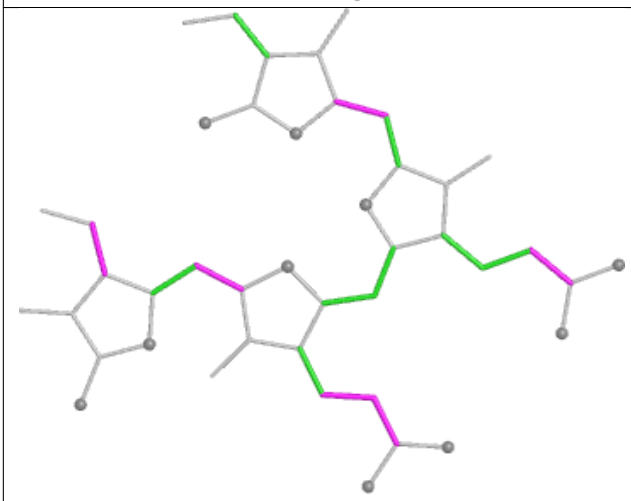


Bond angles



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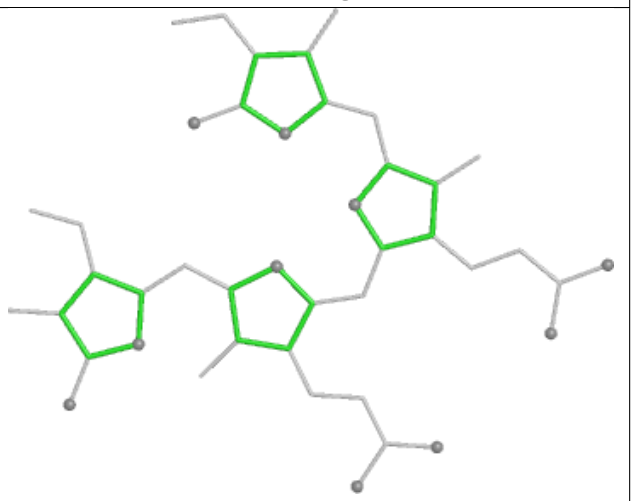

Rings

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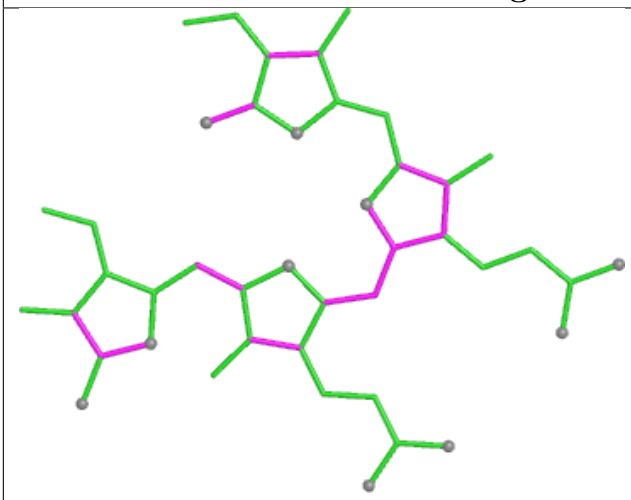
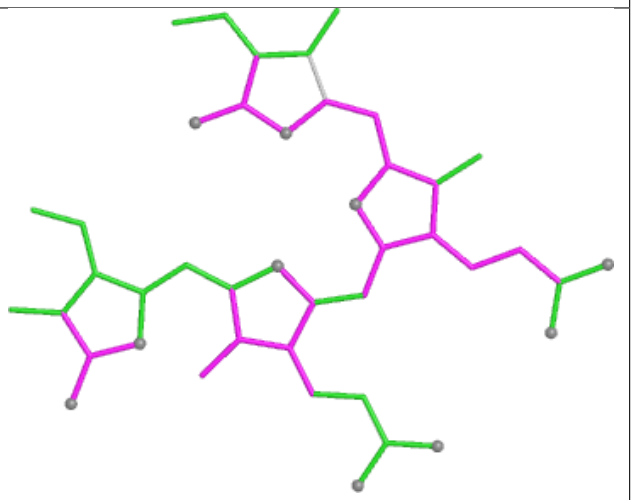
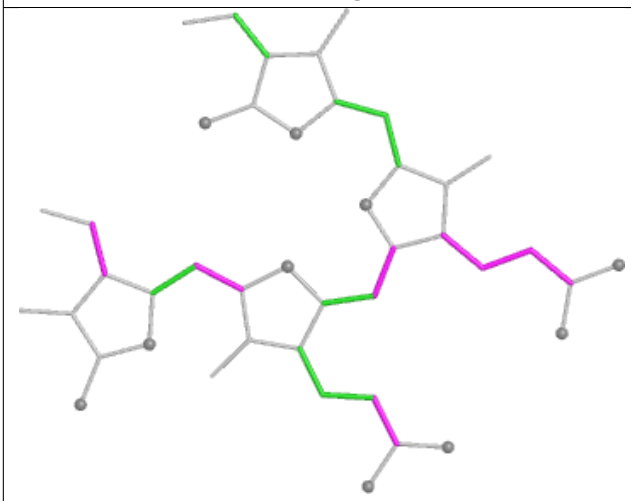


Bond lengths



Bond angles



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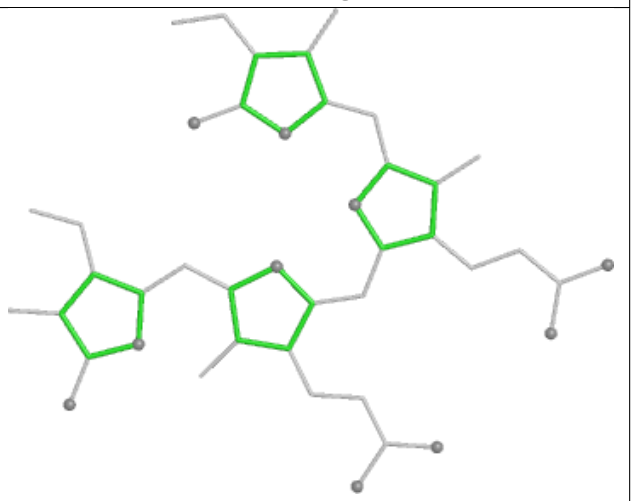
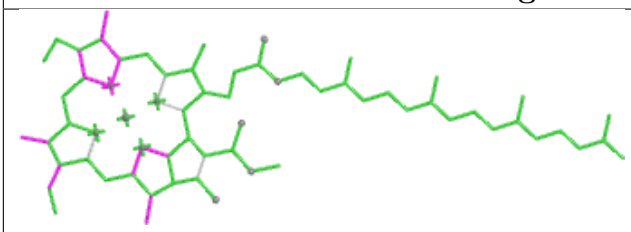


Rings

Ligand CLA cL 508



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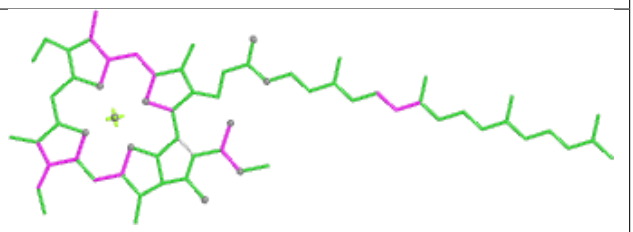

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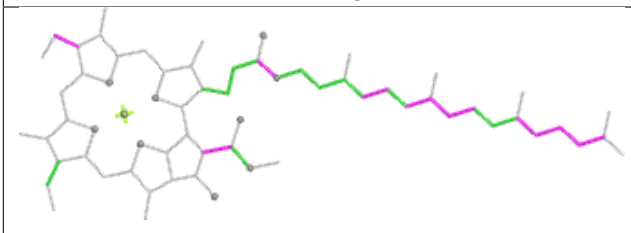

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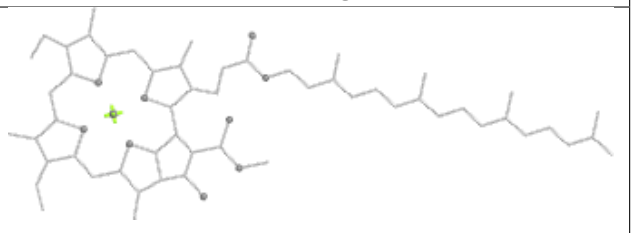
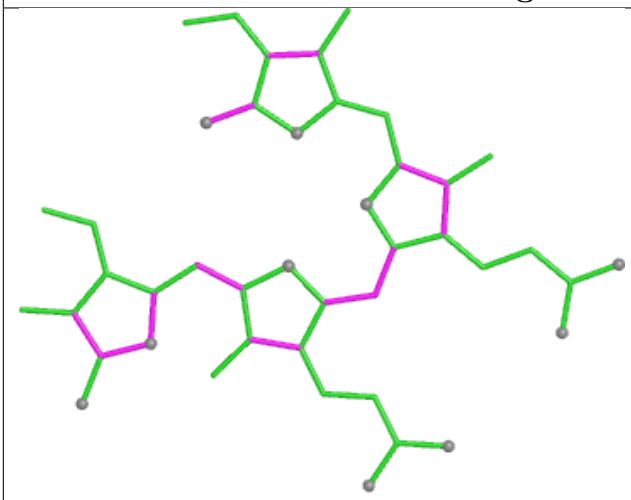


Rings

Ligand PEB cO 201



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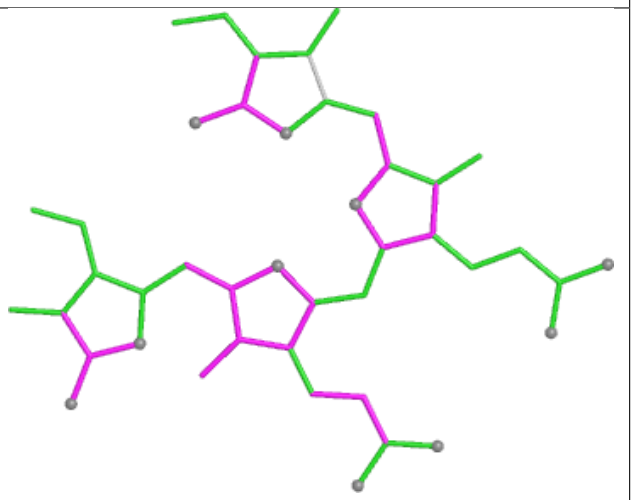

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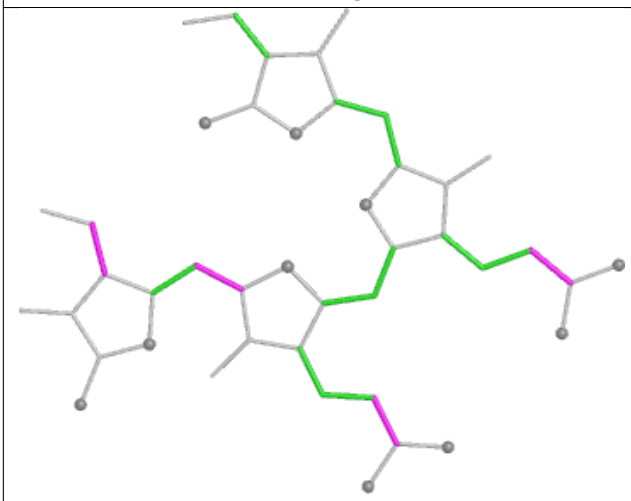

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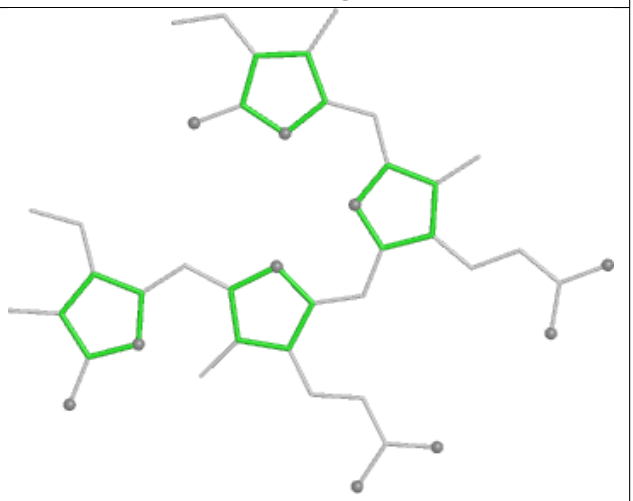
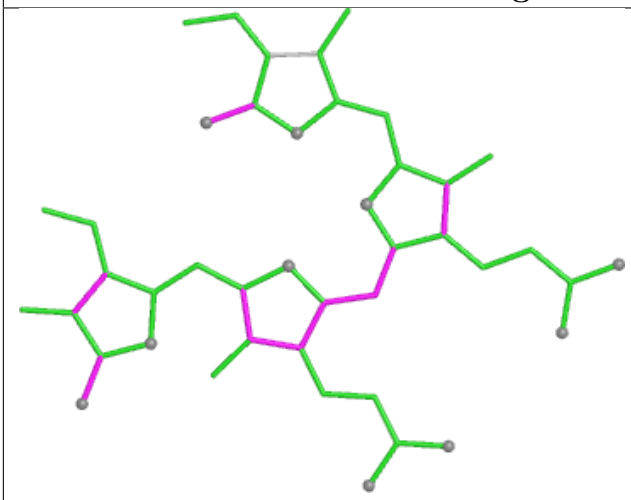


Rings

Ligand PUB xK 305



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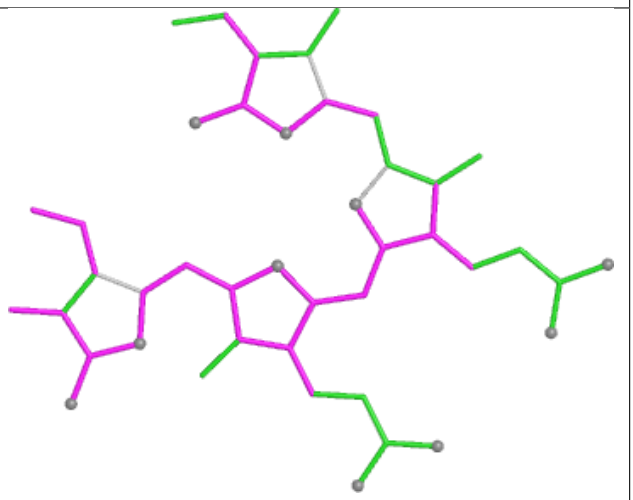

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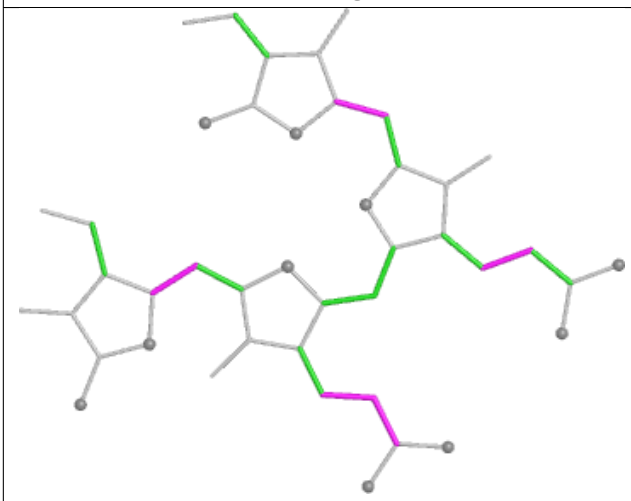

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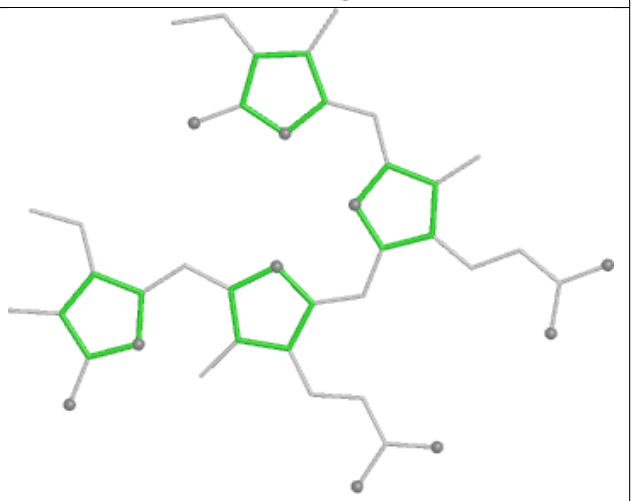
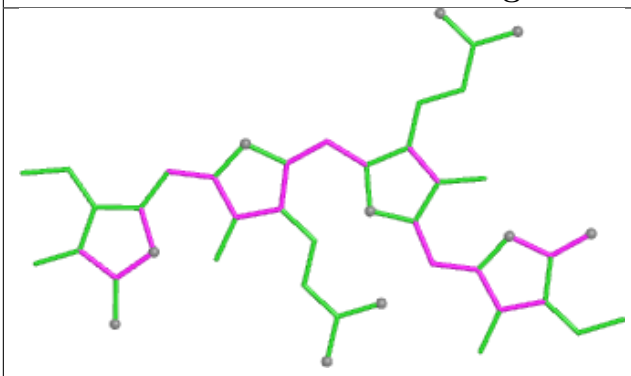


Rings

Ligand CYC N3 1001



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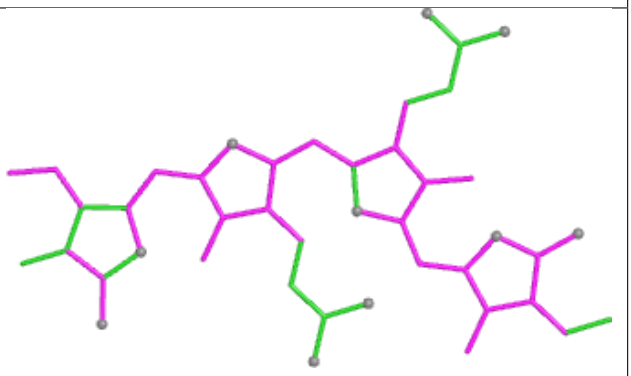

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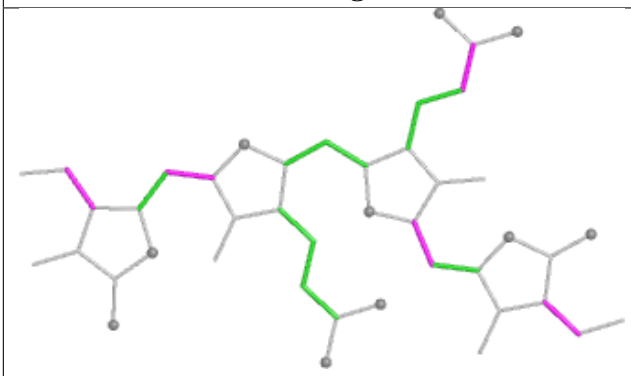

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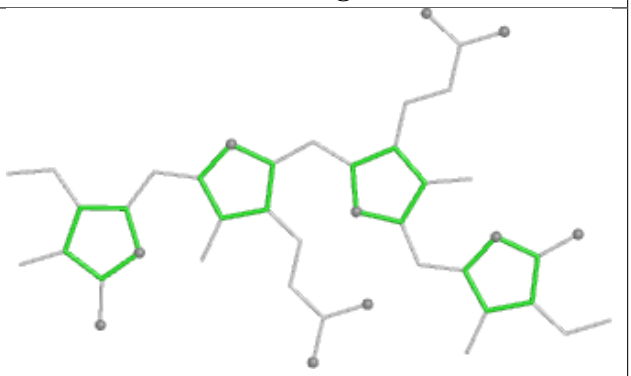
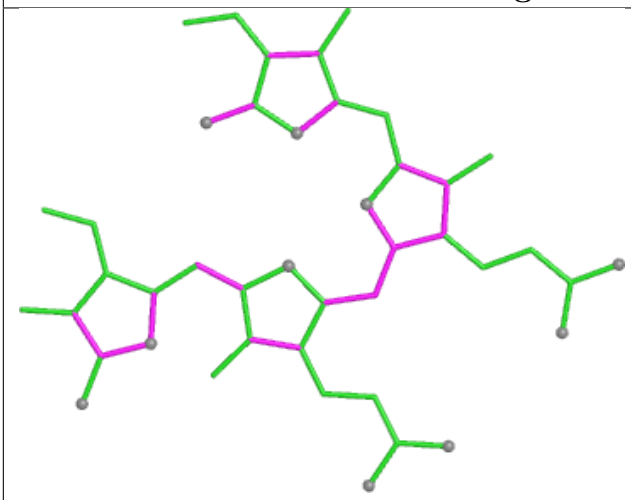


Rings

Ligand PEB SO 202



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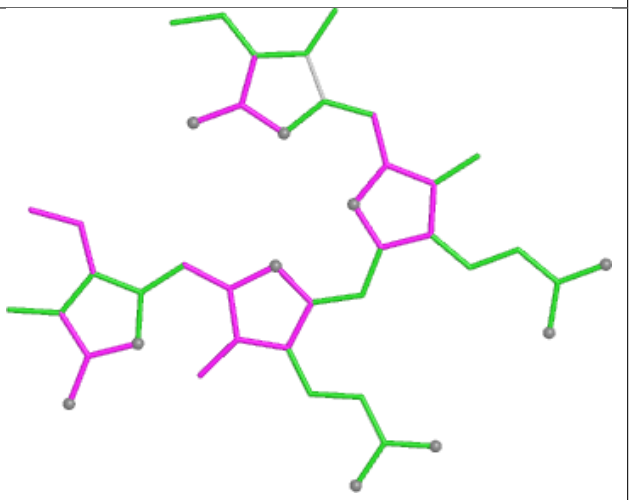

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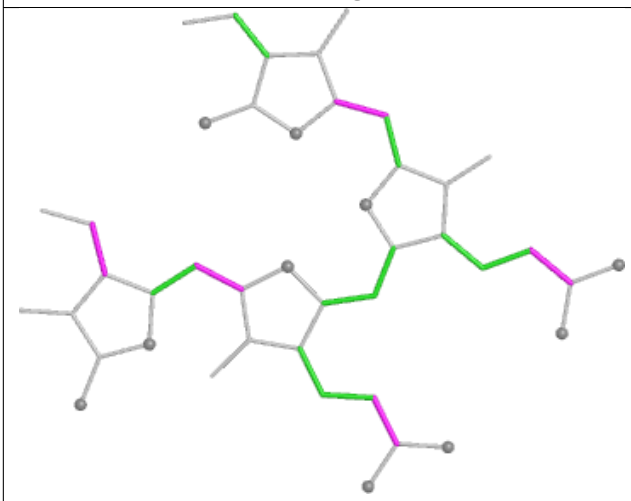

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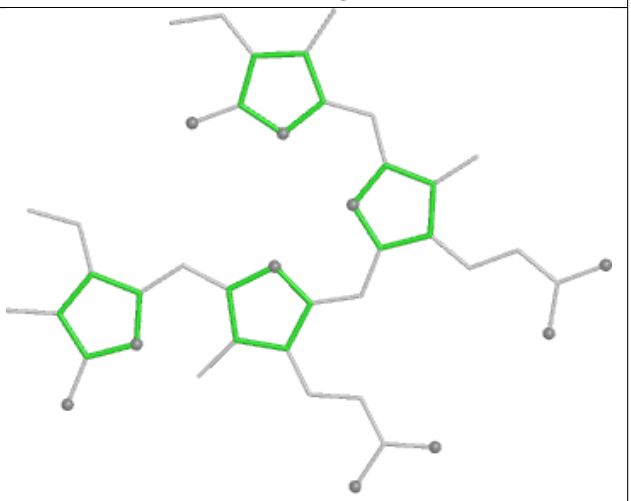
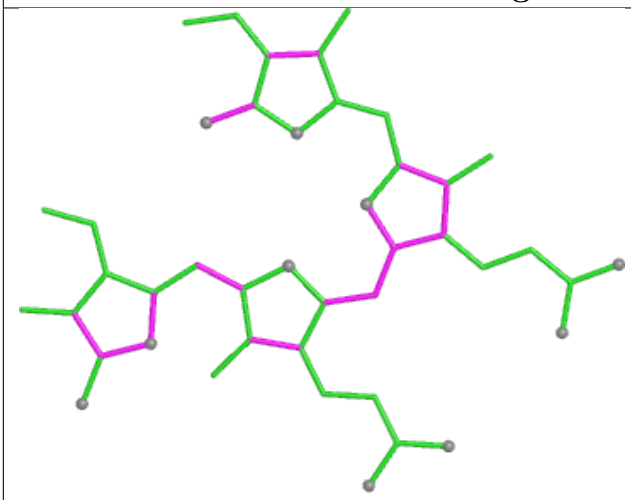


Rings

Ligand PEB QE 202



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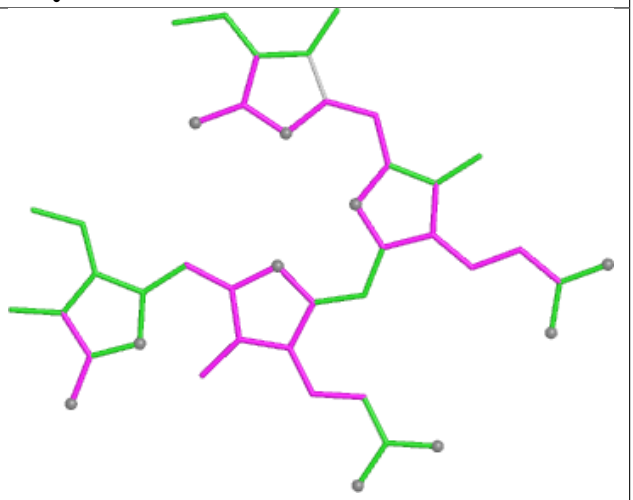

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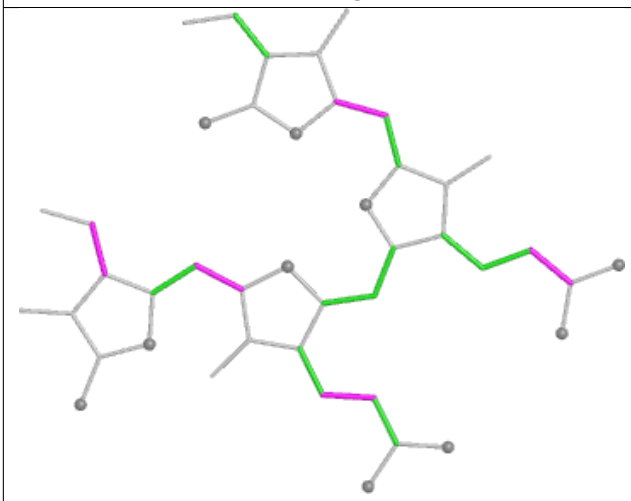

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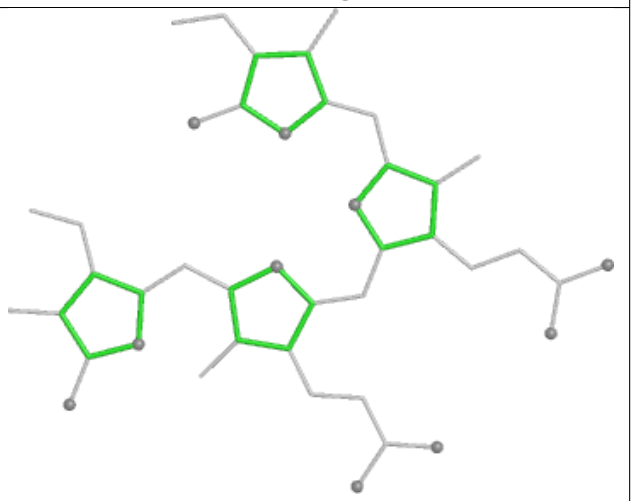
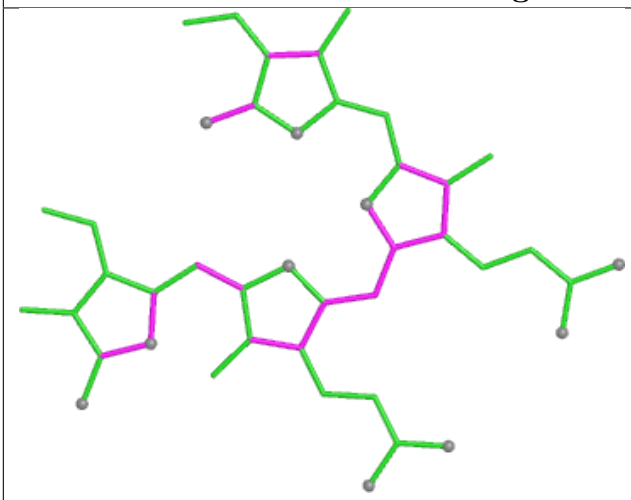


Rings

Ligand PEB YA 303



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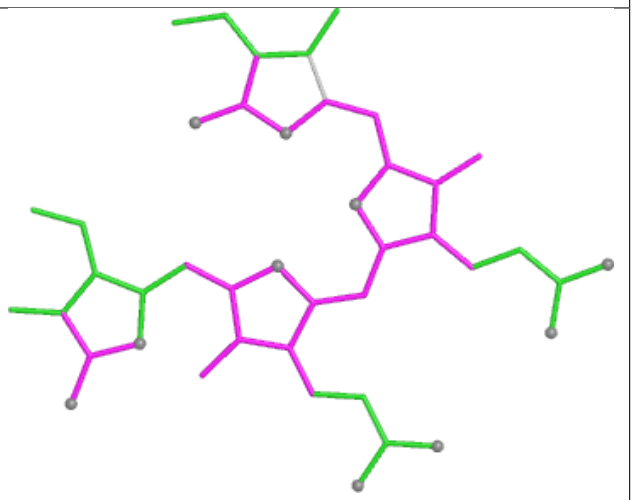

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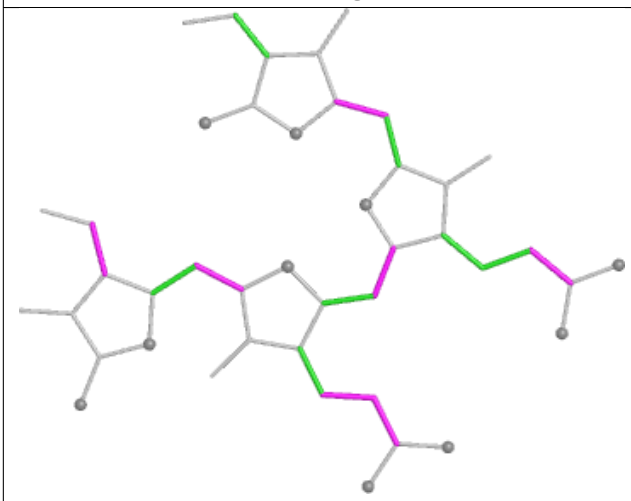

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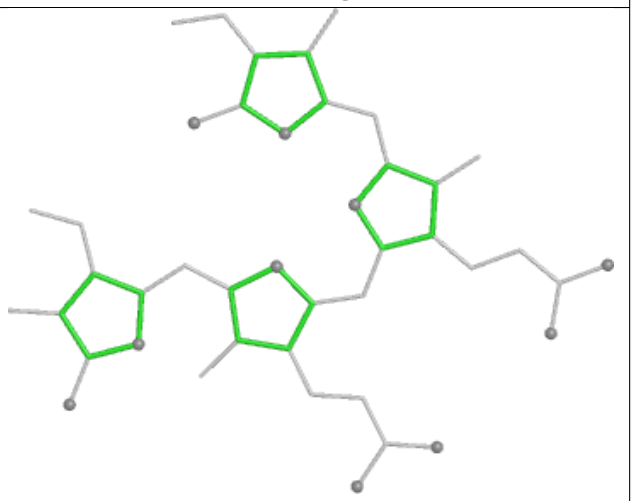
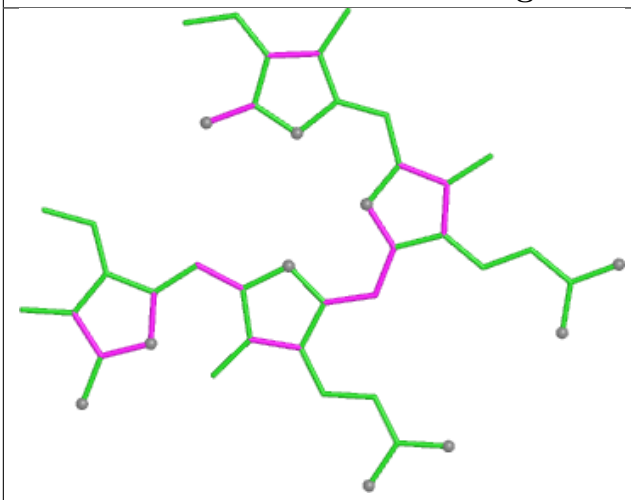


Rings

Ligand PEB aB 202



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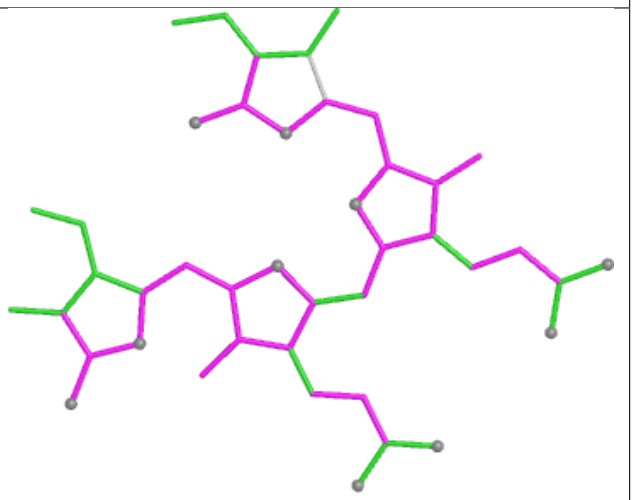

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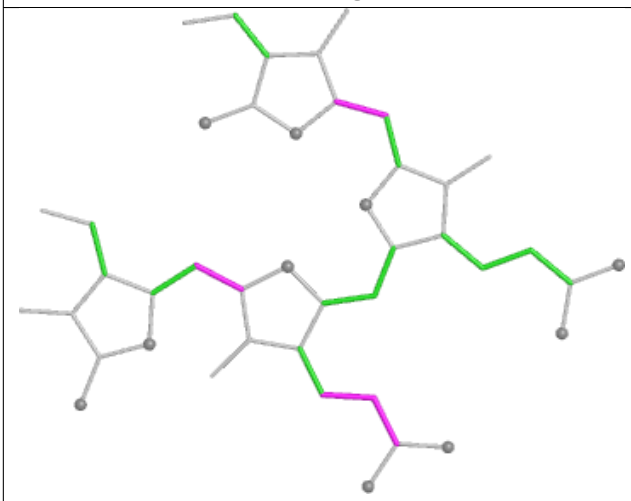

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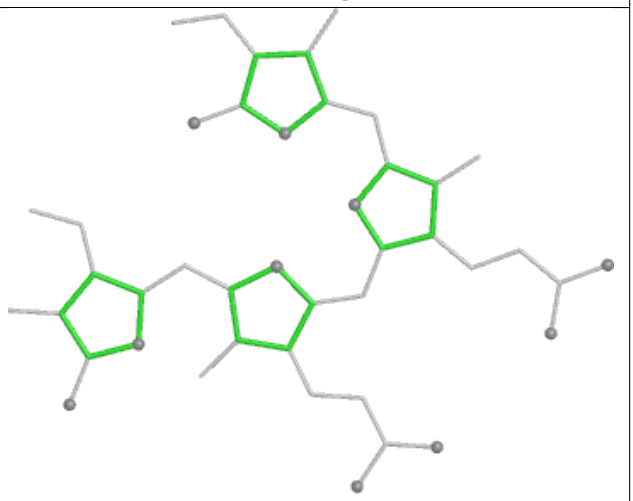
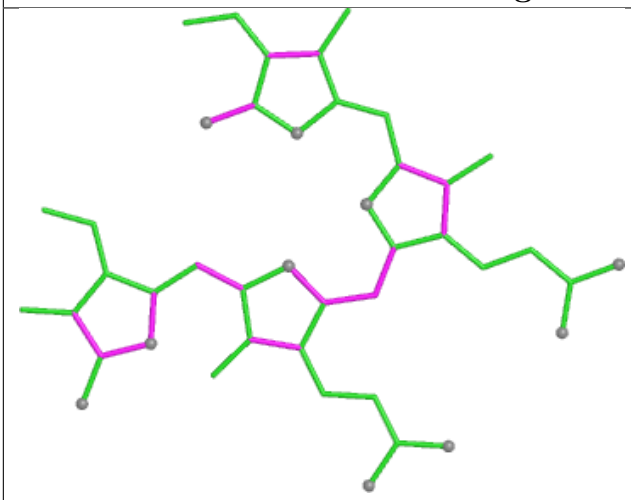


Rings

Ligand PEB KJ 203



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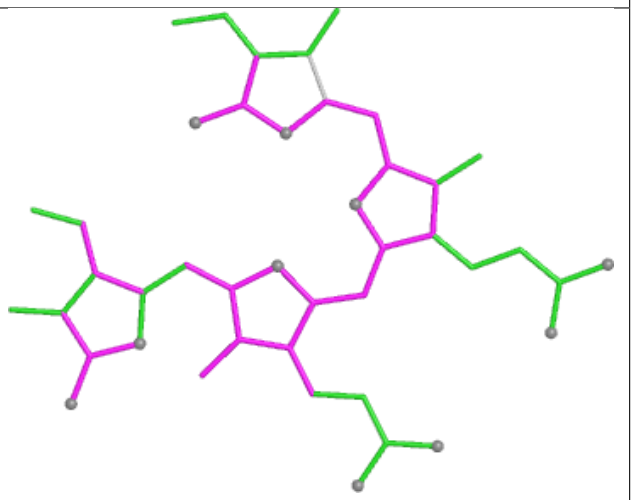

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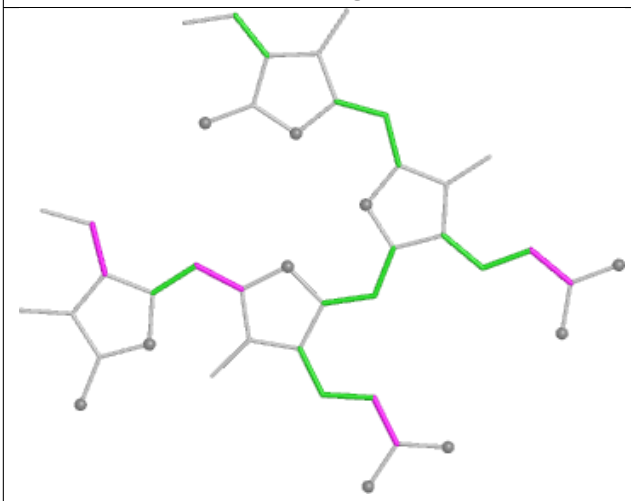

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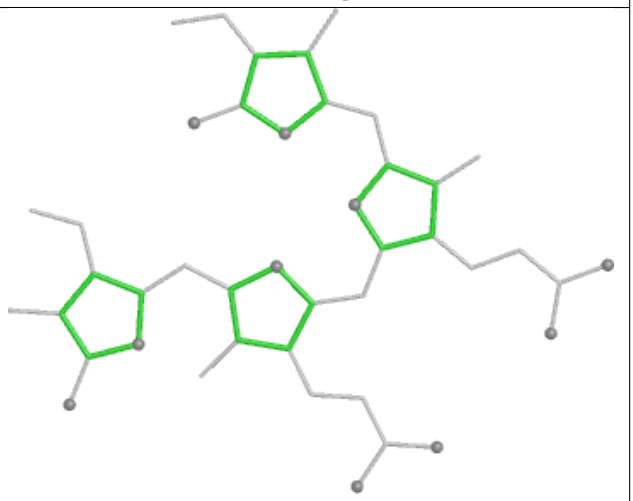
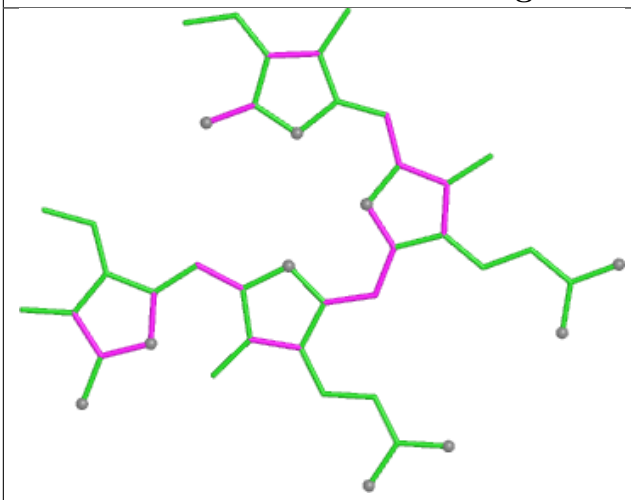


Rings

Ligand PEB SP 201



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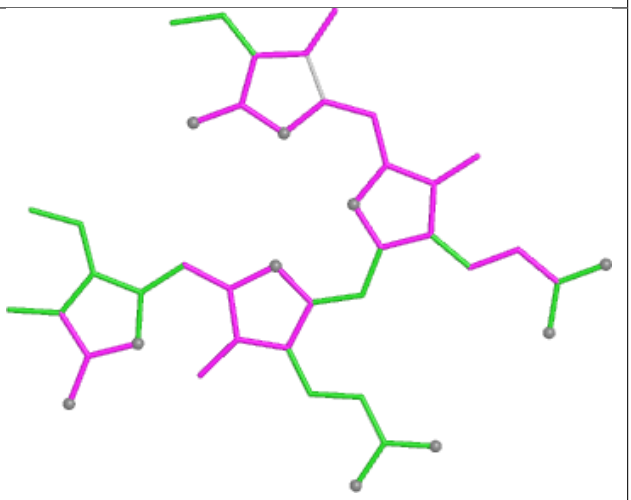
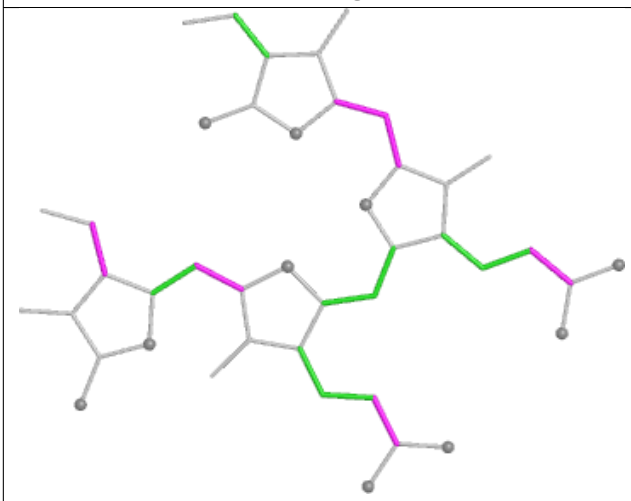


Bond angles



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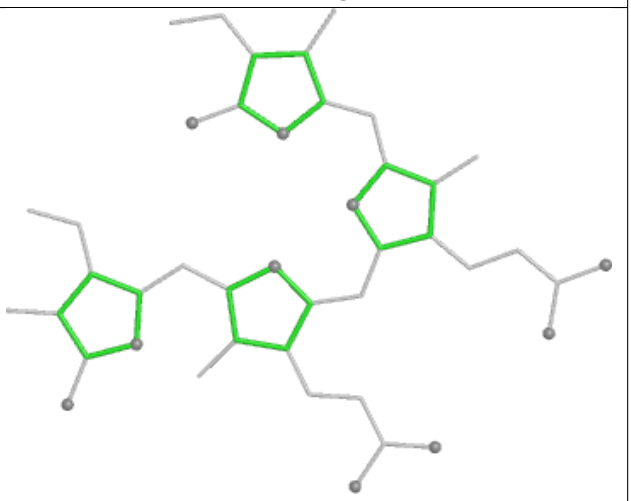
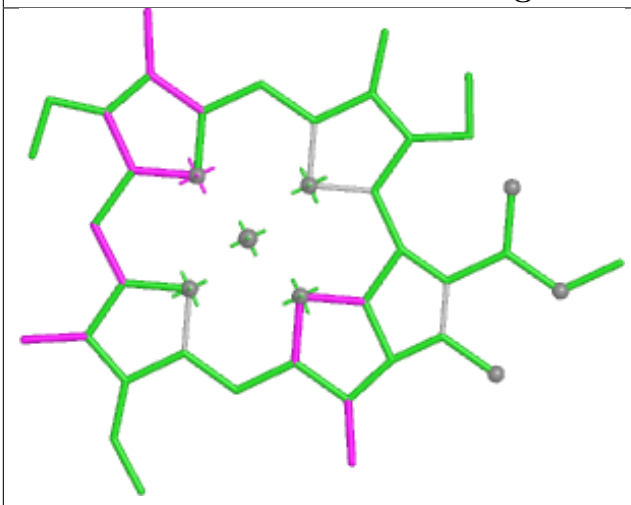


Rings

Ligand CLA 1N 604



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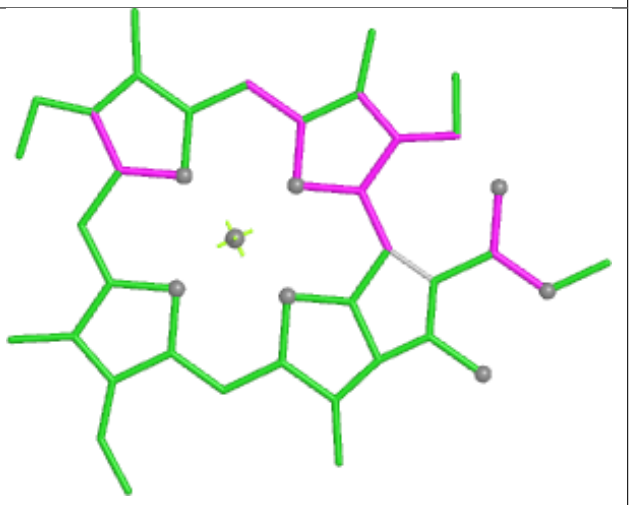
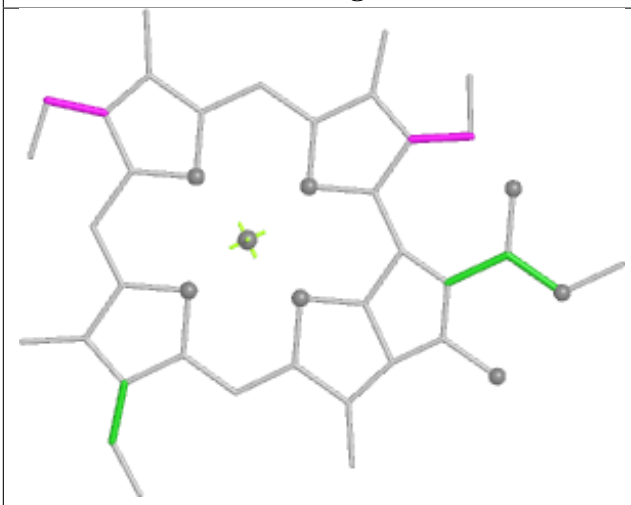


Bond angles

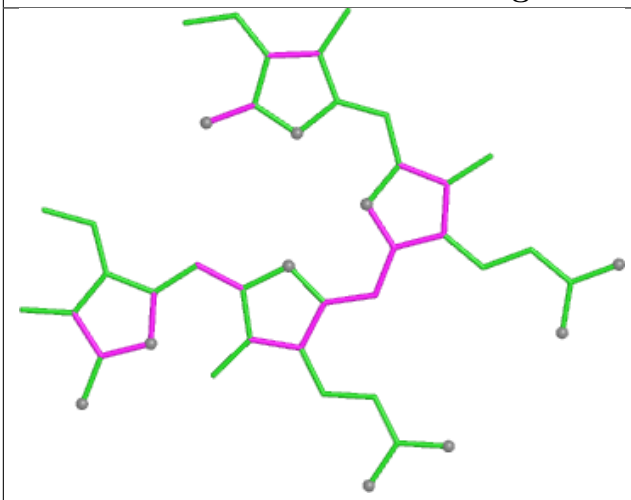


Torsions



Rings

Ligand PEB AP 202



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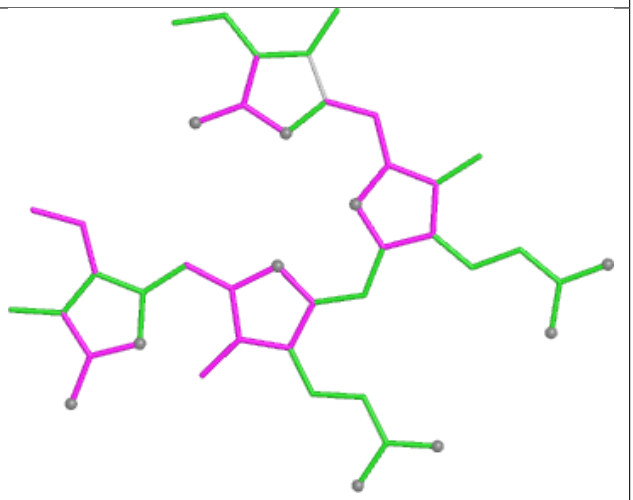
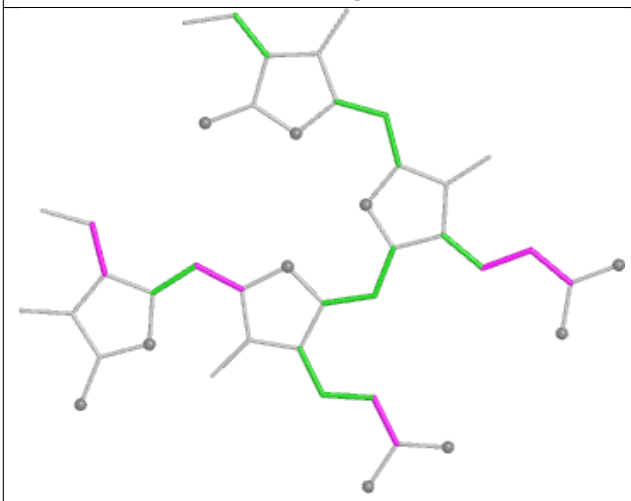


Bond angles



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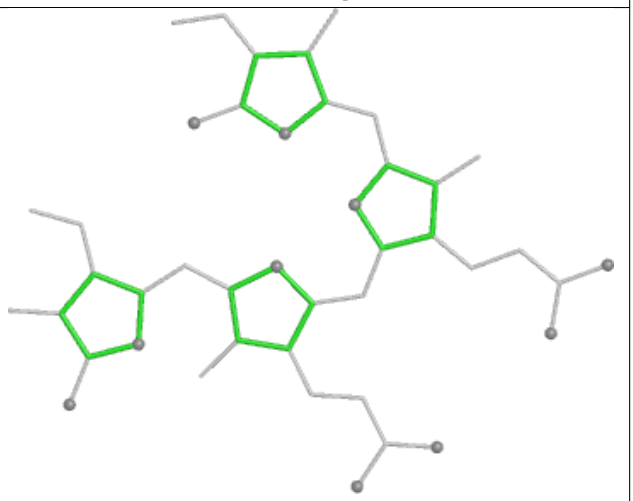
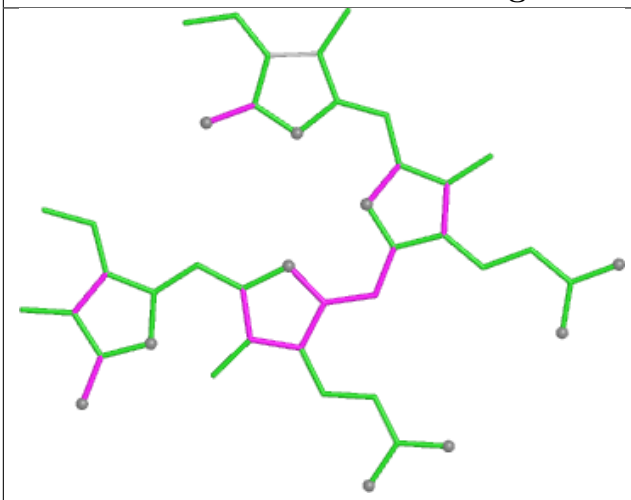


Rings

Ligand PUB wK 304



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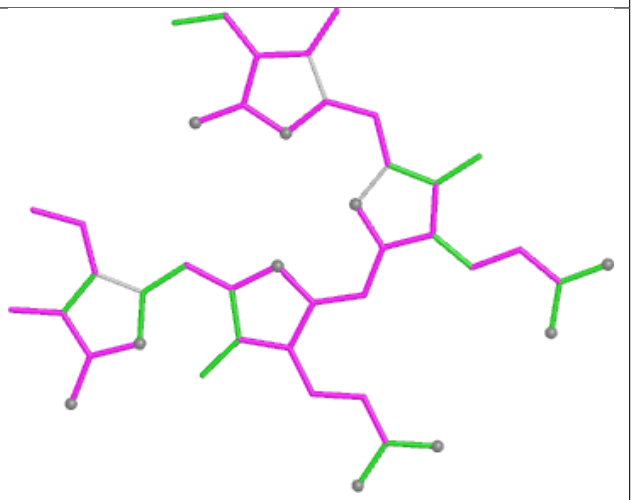
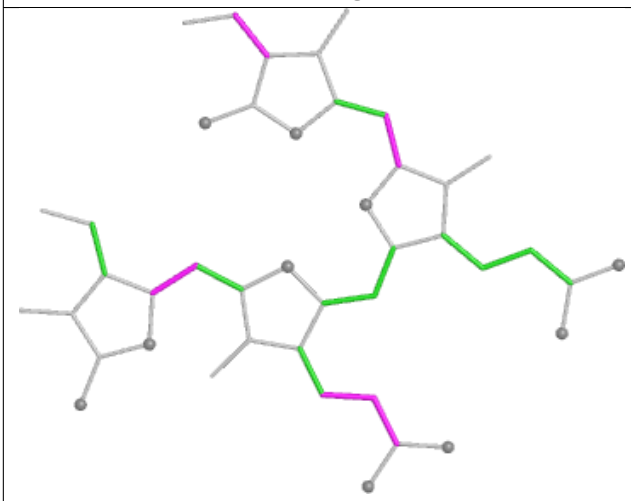


Bond angles



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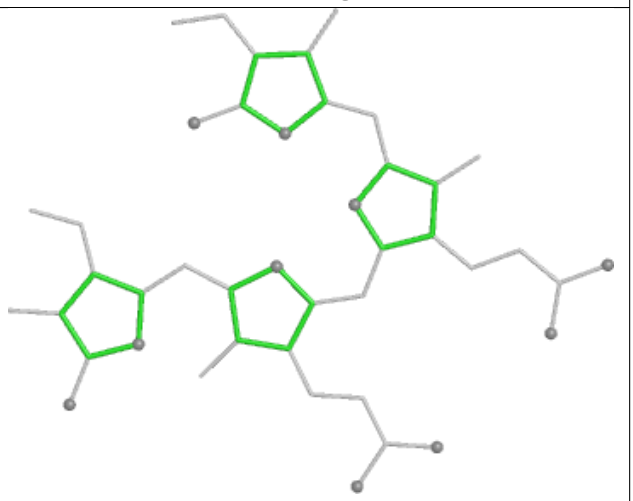
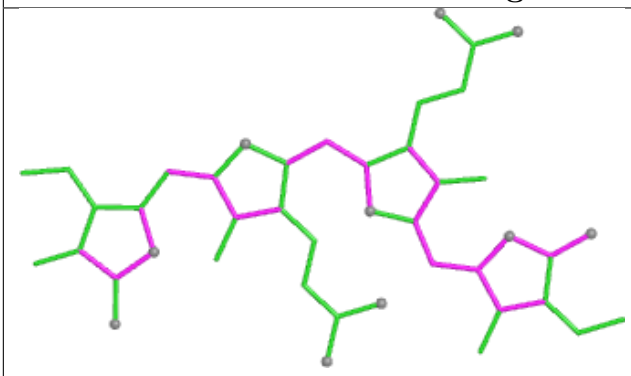


Rings

Ligand CYC L4 1001



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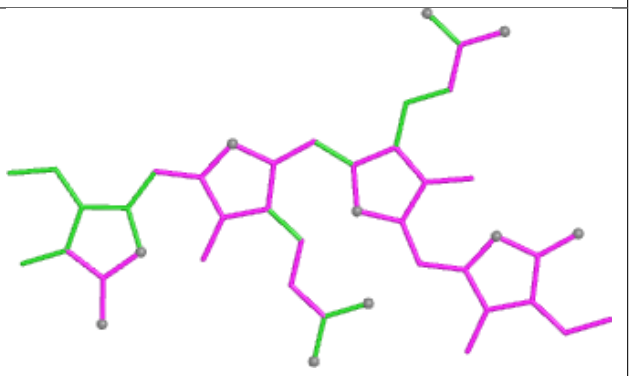
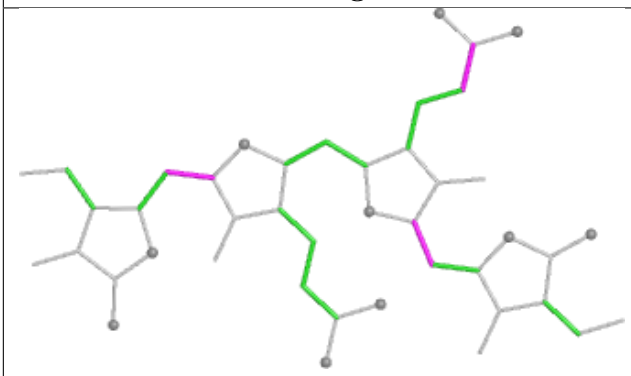


Bond angles



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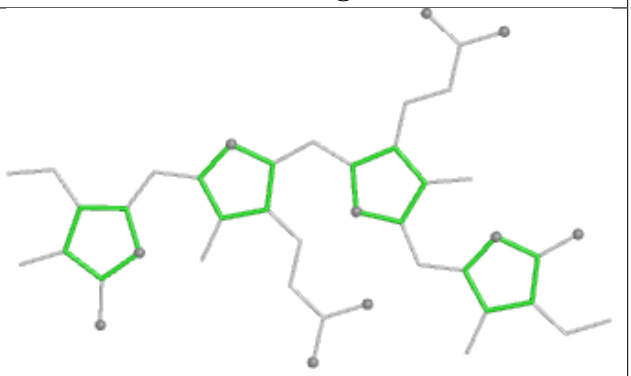
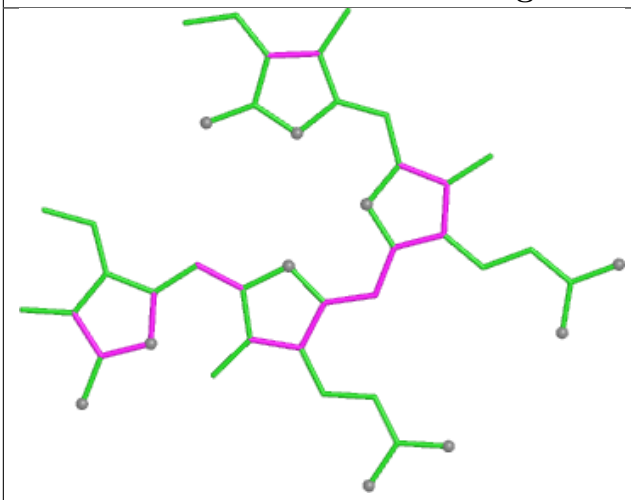


Rings

Ligand PEB T7 201



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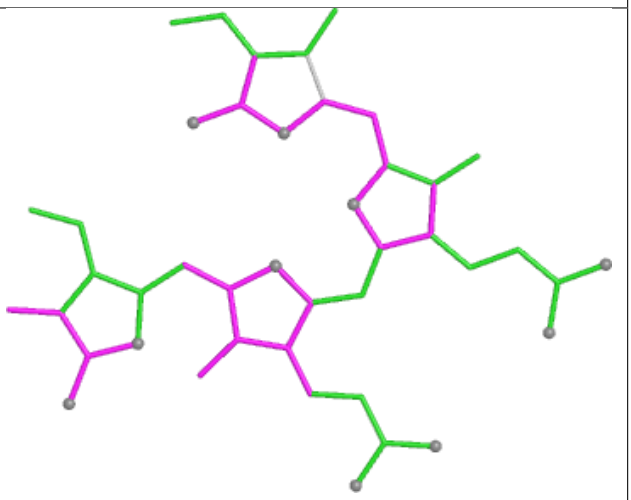

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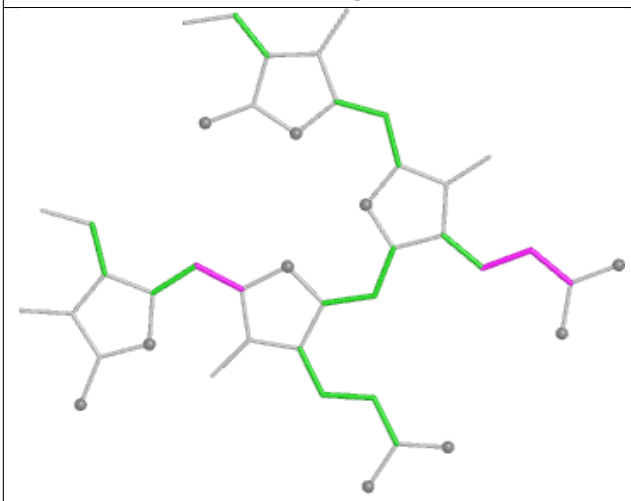
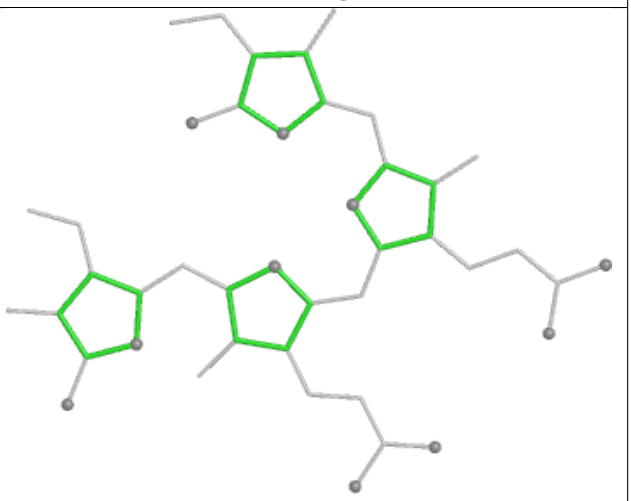
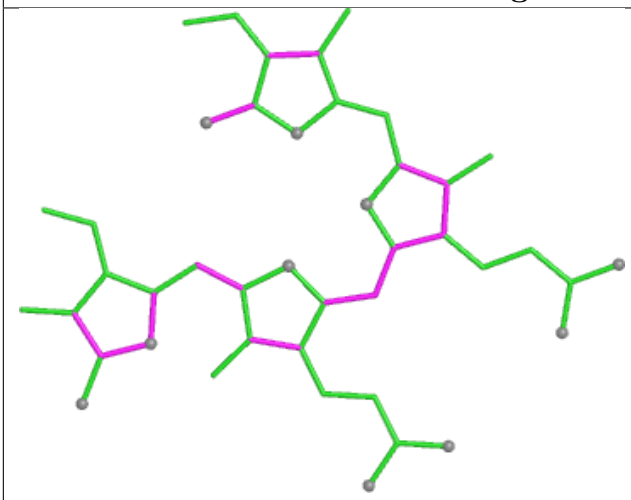


Torsions



Rings

Ligand PEB SM 201



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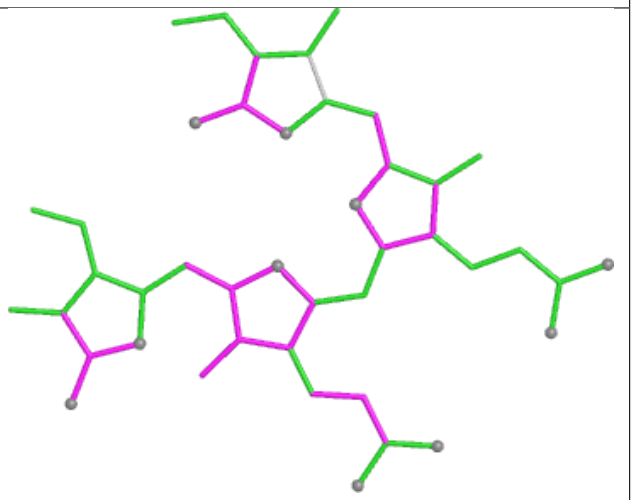

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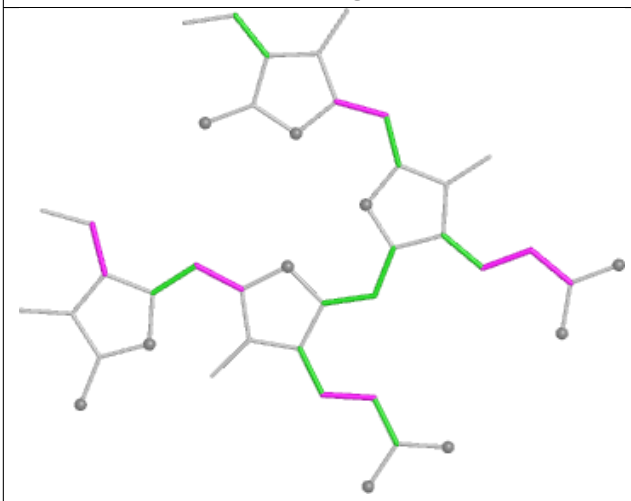

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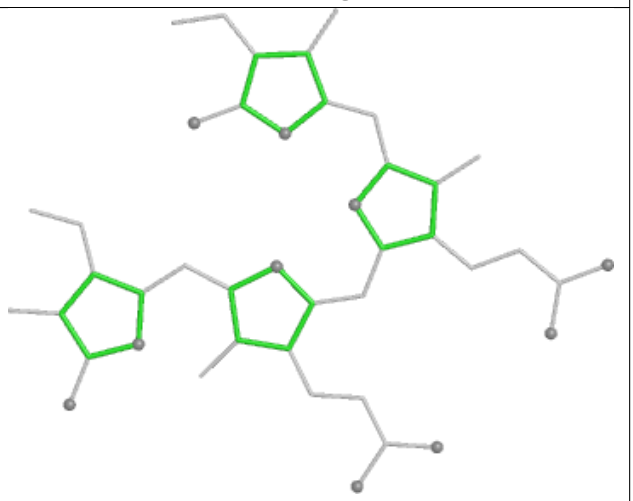
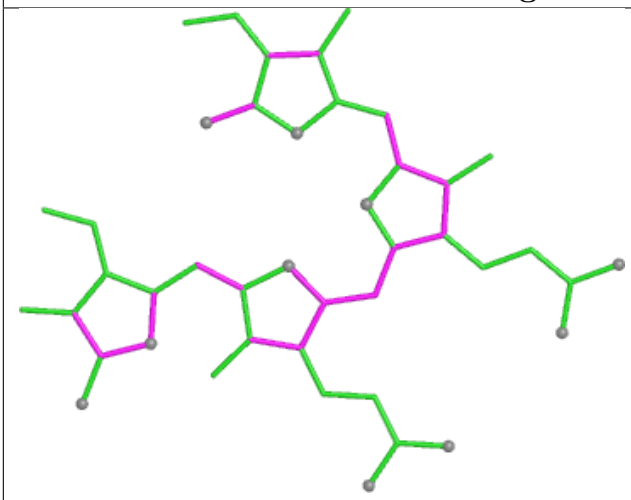


Rings

Ligand PEB sF 203



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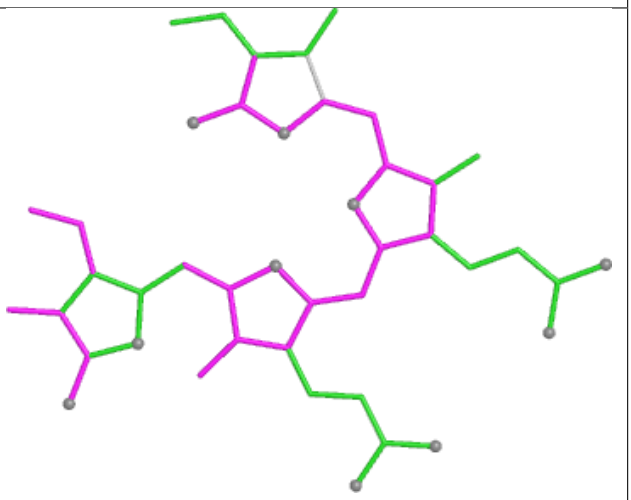

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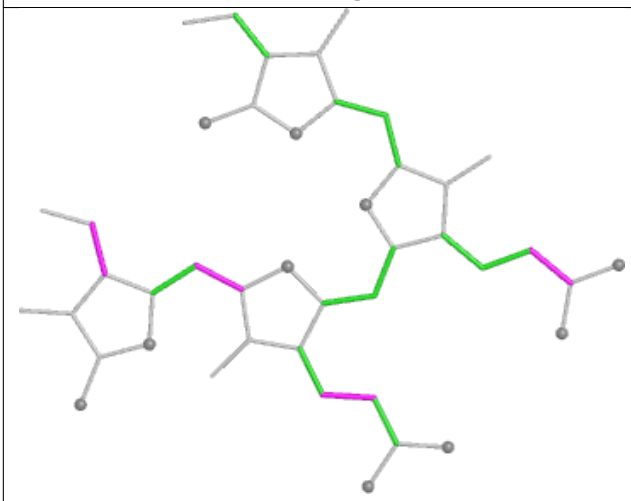

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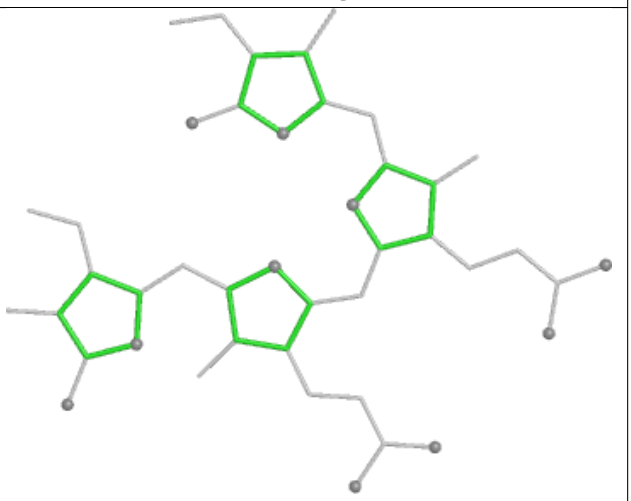
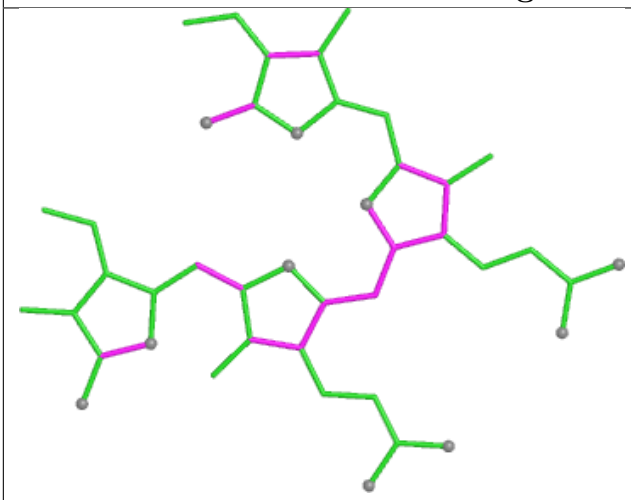


Rings

Ligand PEB zC 202



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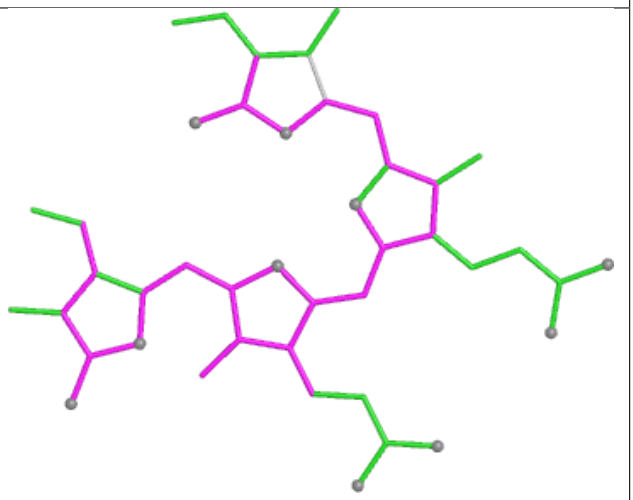

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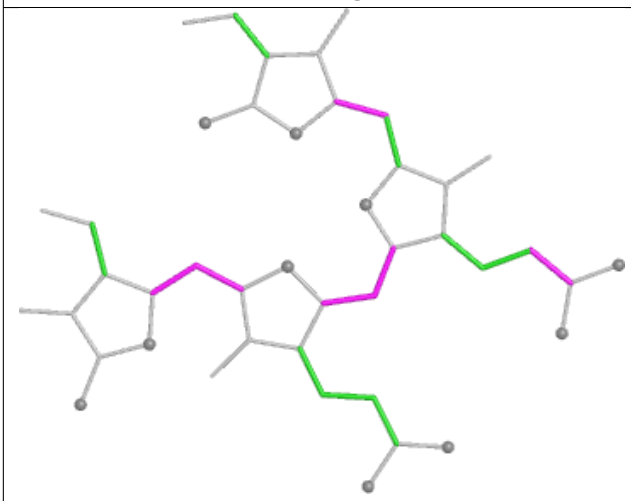

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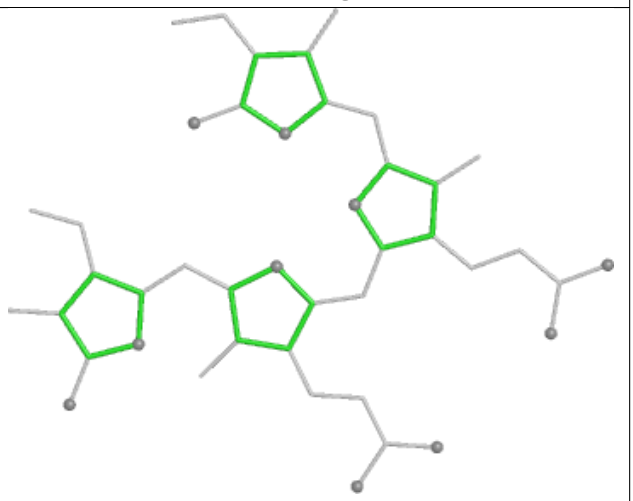

Rings

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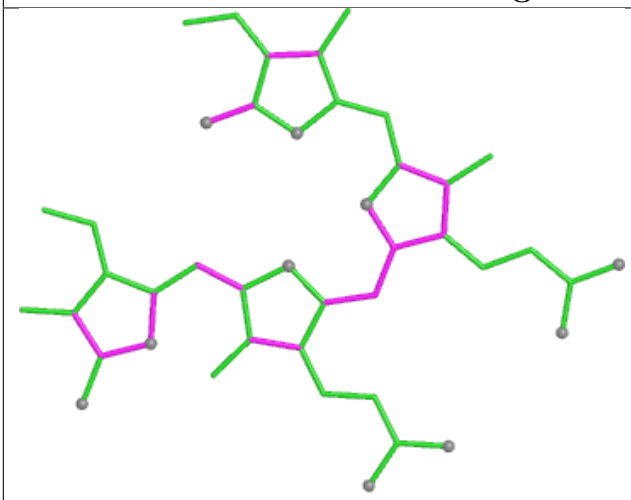

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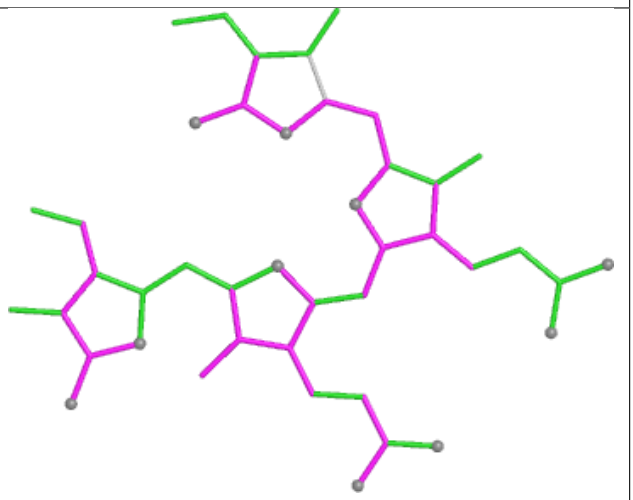

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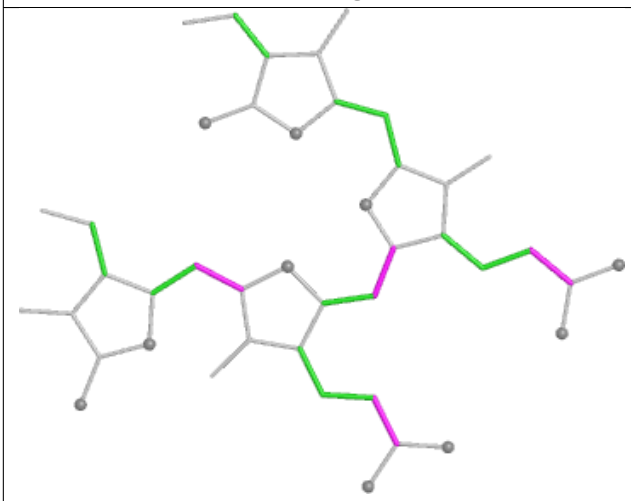

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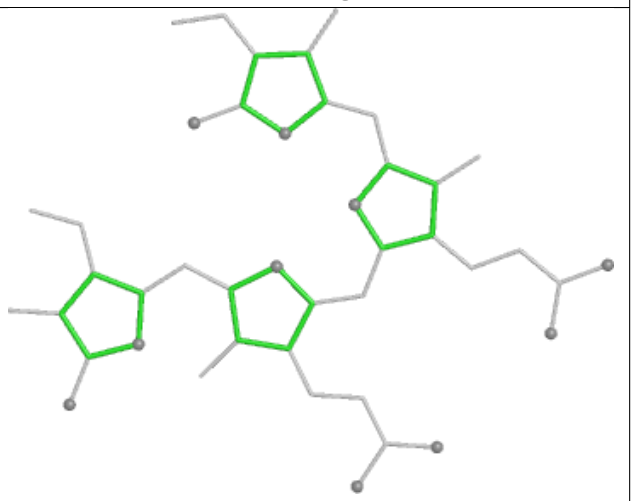
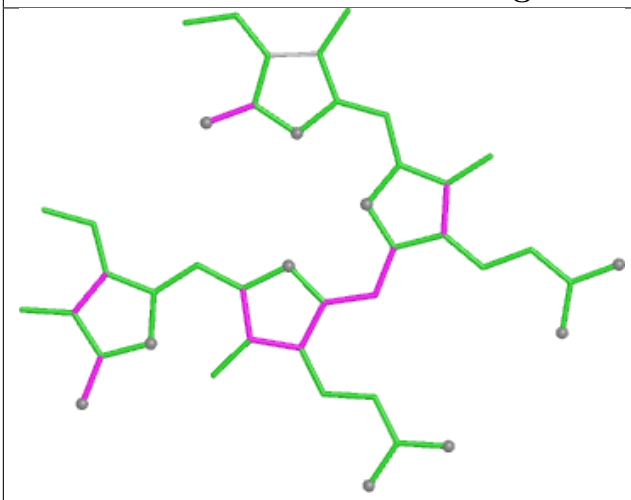


Rings

Ligand PUB A4 303



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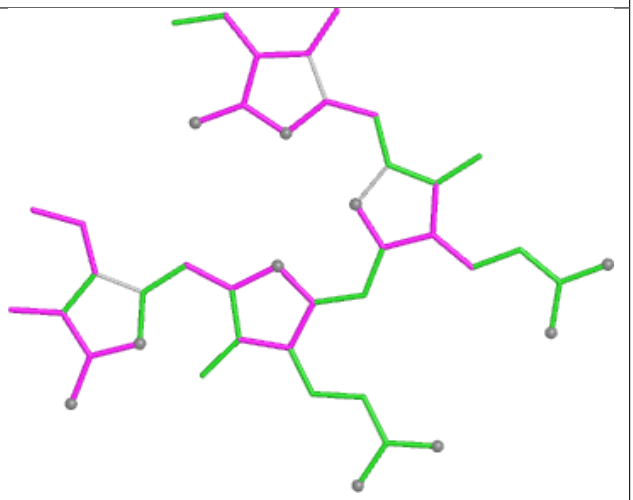

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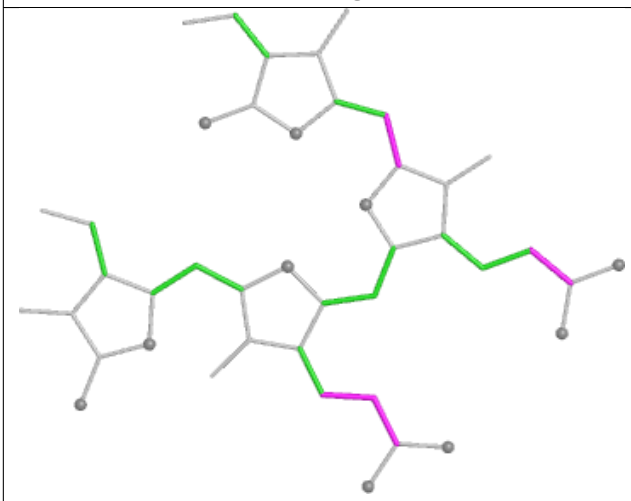

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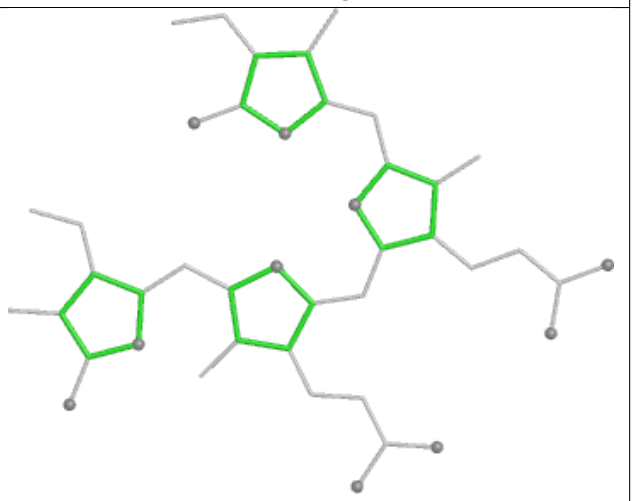
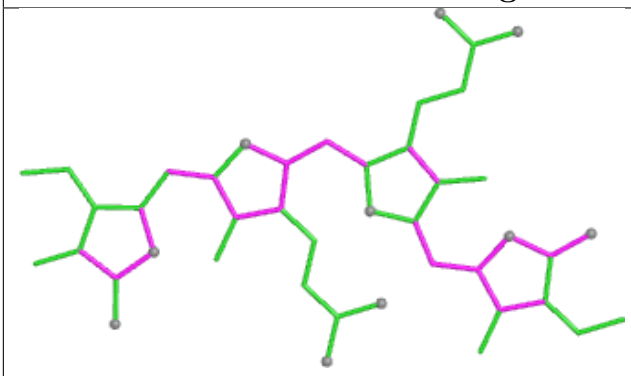


Rings

Ligand CYC BG 1001



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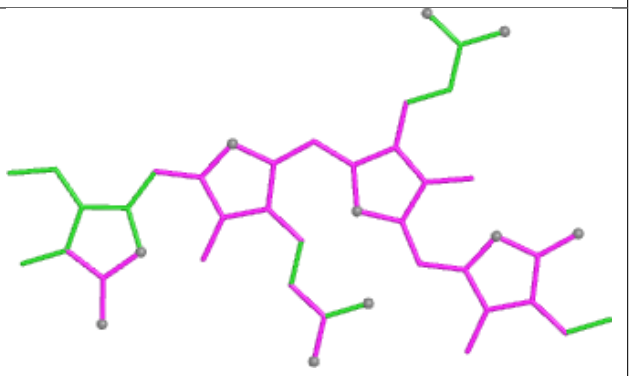

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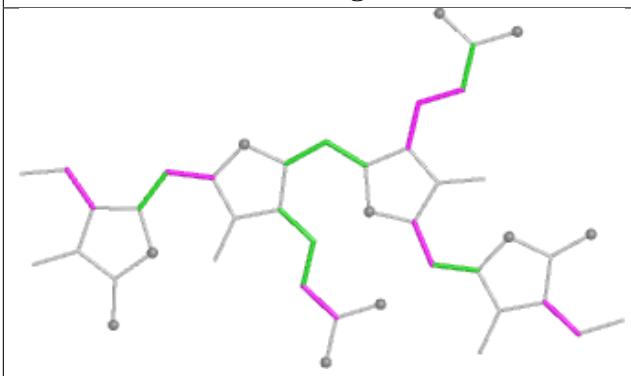

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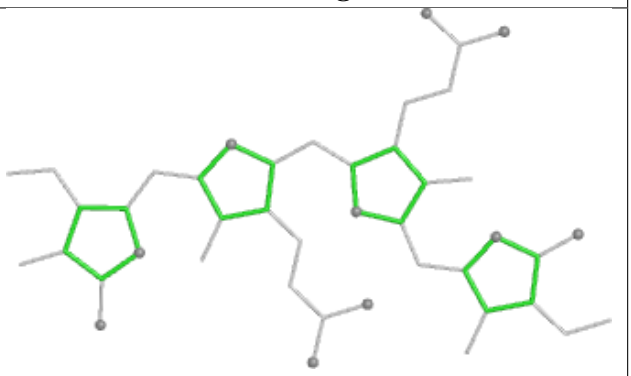
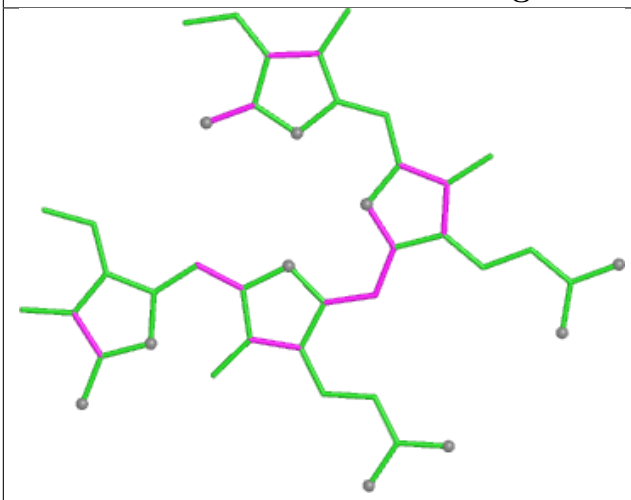


Rings

Ligand PEB DF 201



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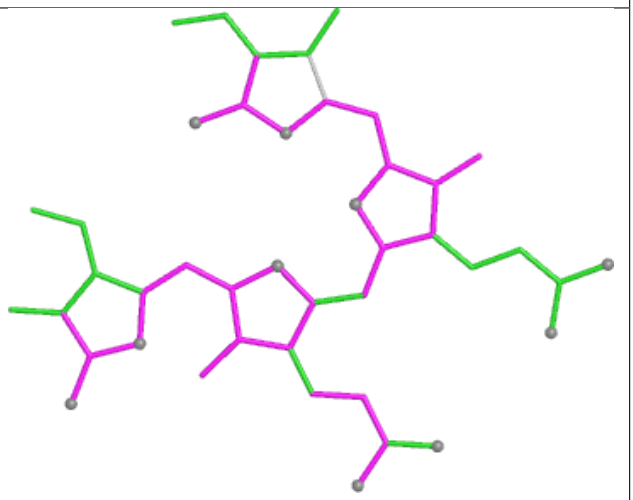

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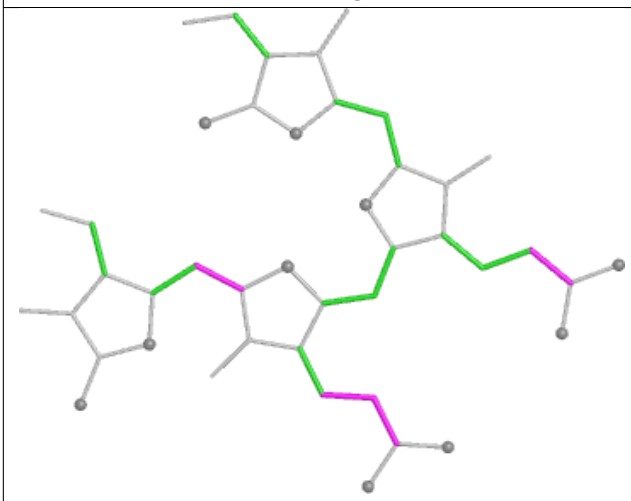

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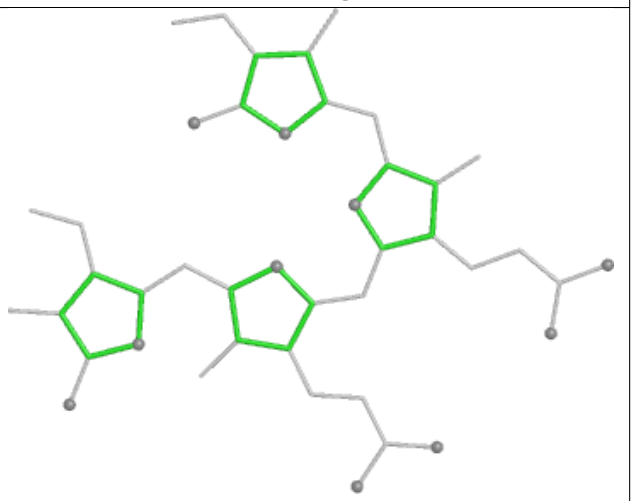

Rings

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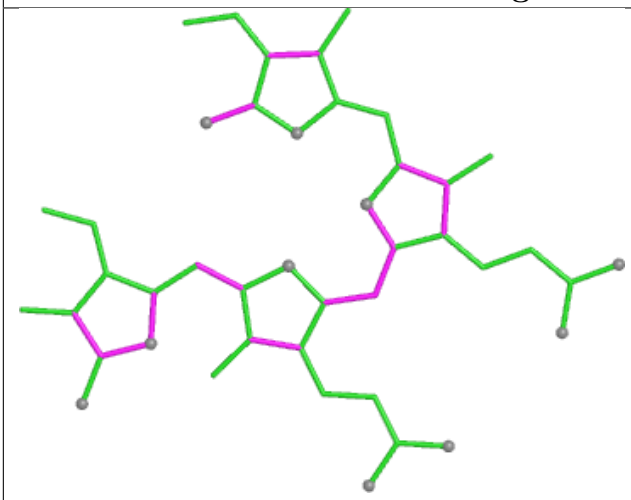

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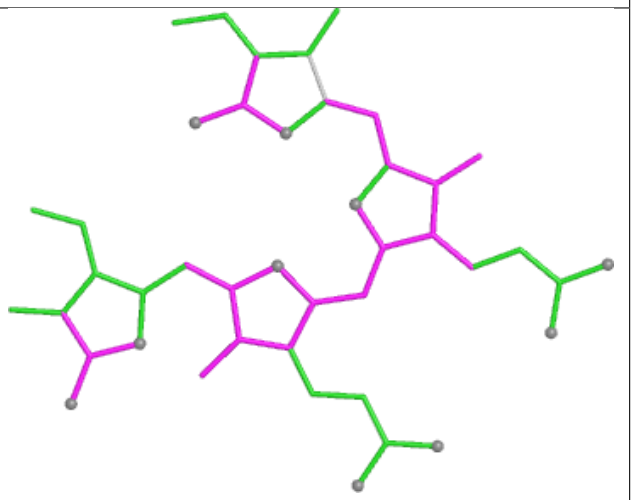

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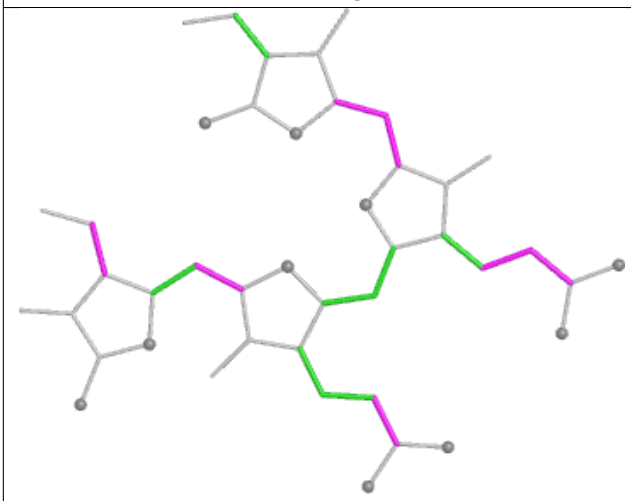

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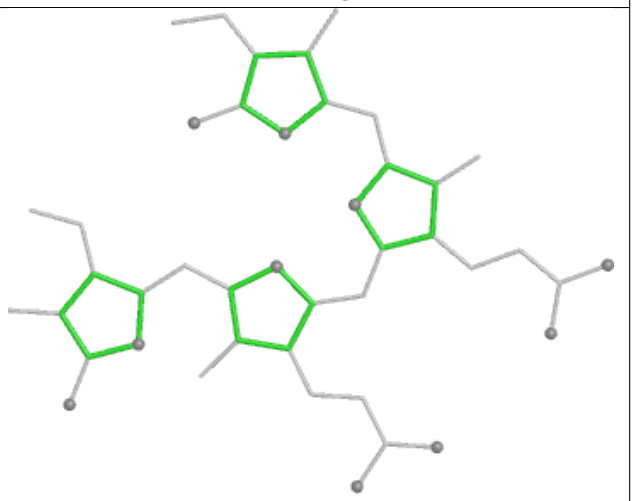
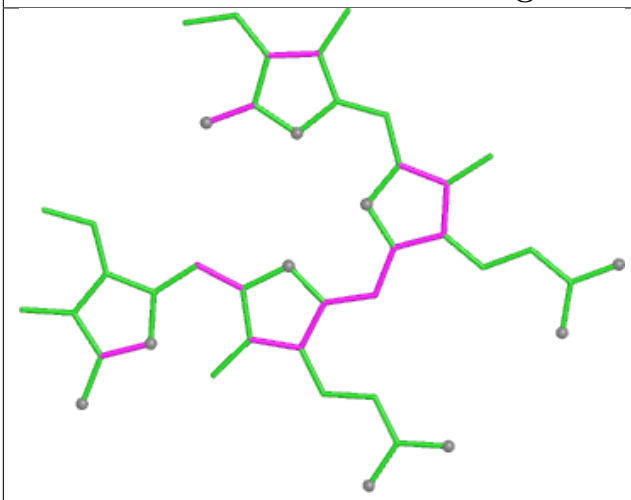


Rings

Ligand PEB T4 203



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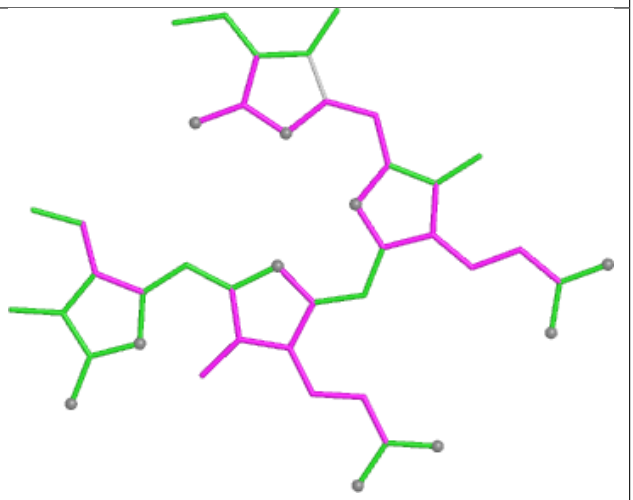

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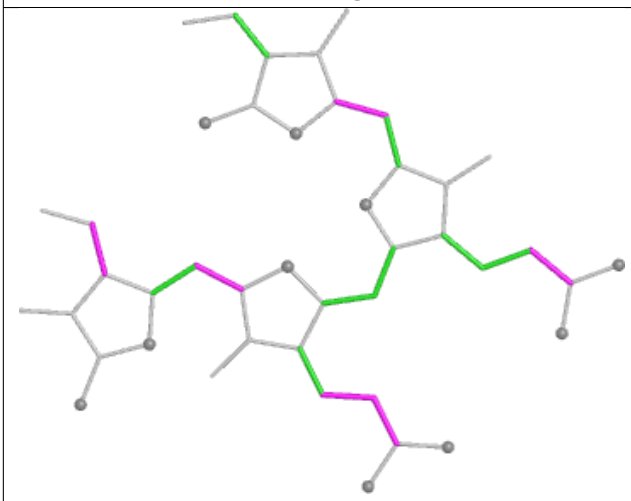

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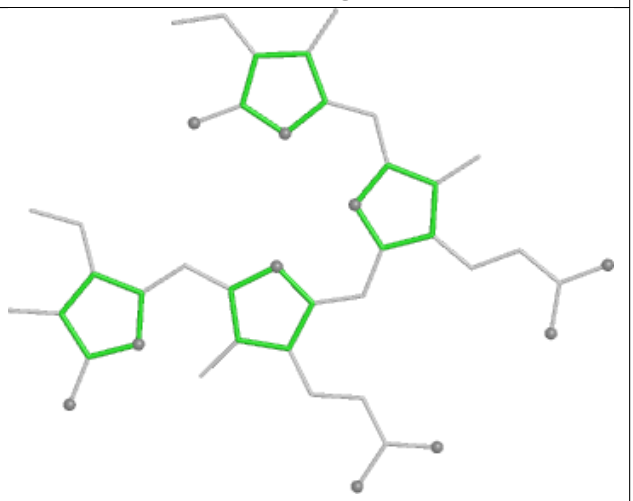
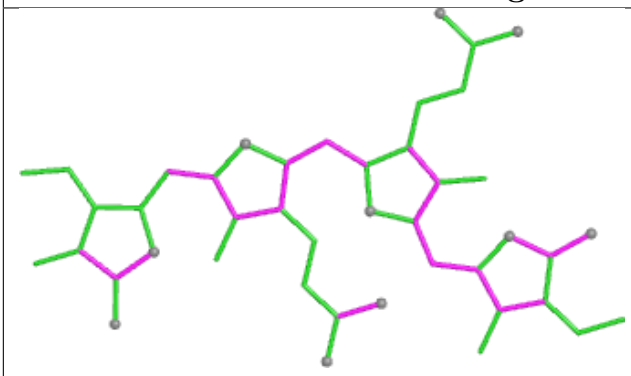


Rings

Ligand CYC q3 1001



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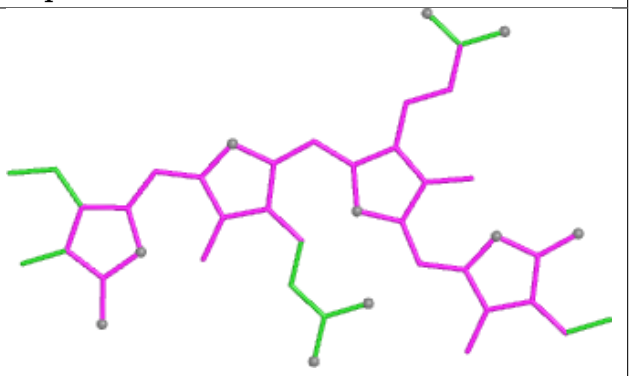

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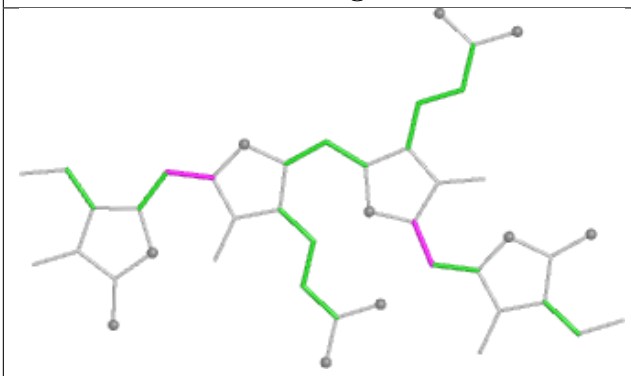

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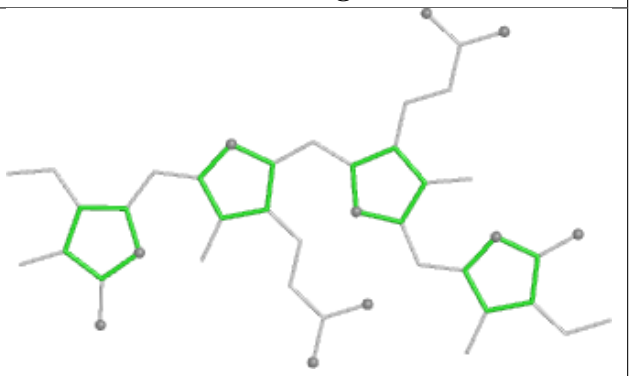
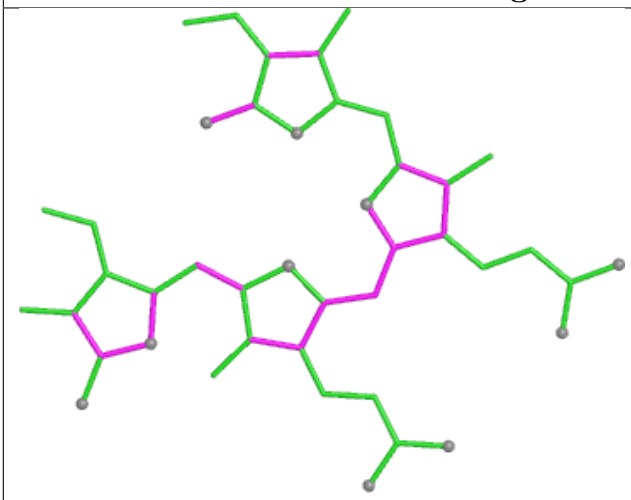


Rings

Ligand PEB W9 201



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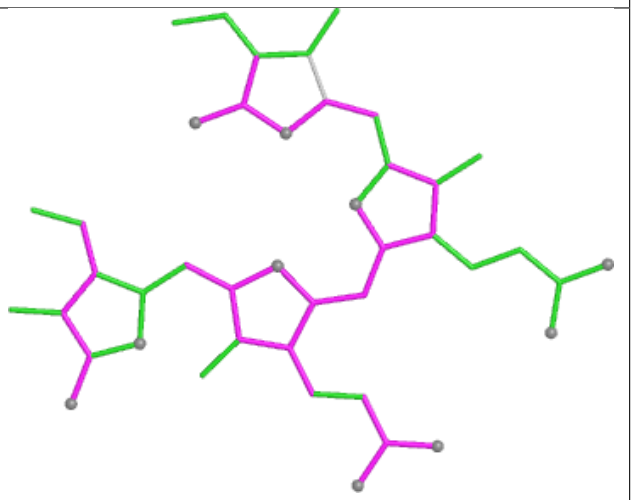

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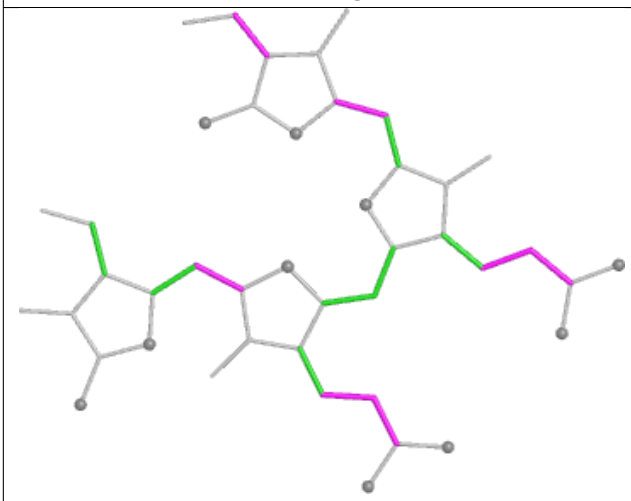

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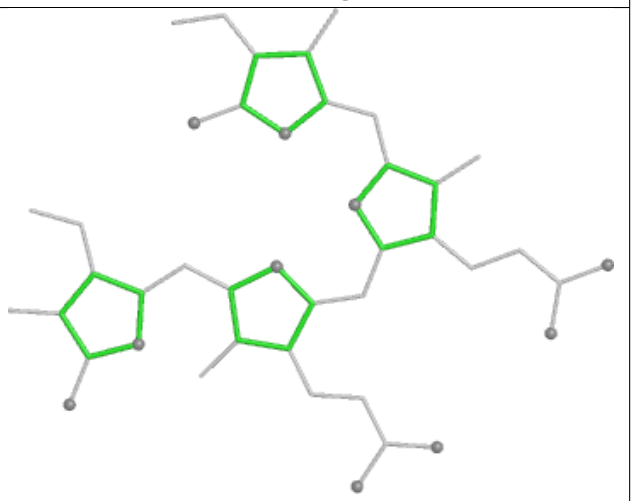
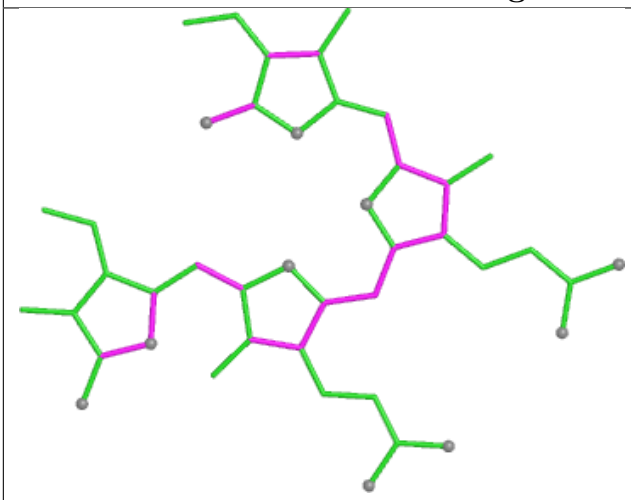


Rings

Ligand PEB WF 203



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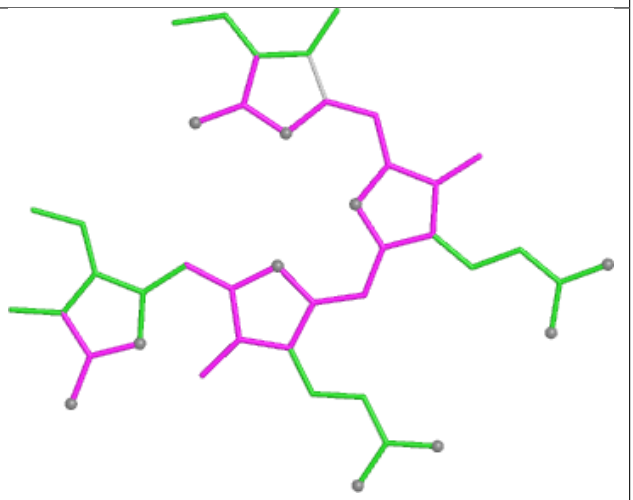
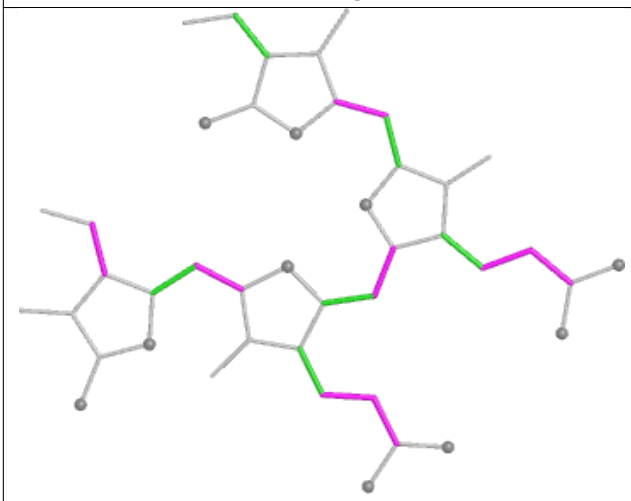


Bond angles



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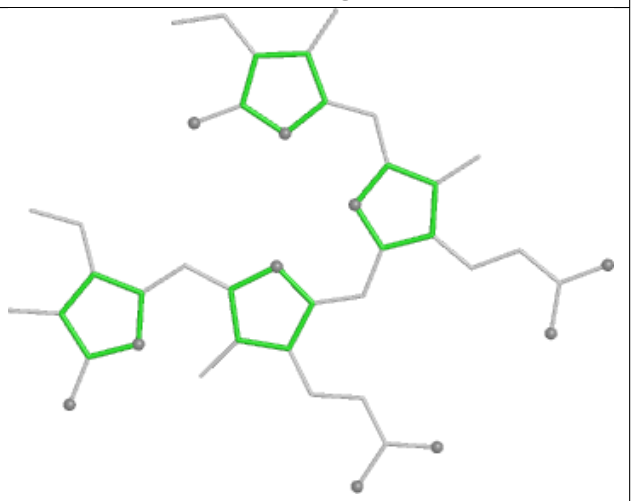
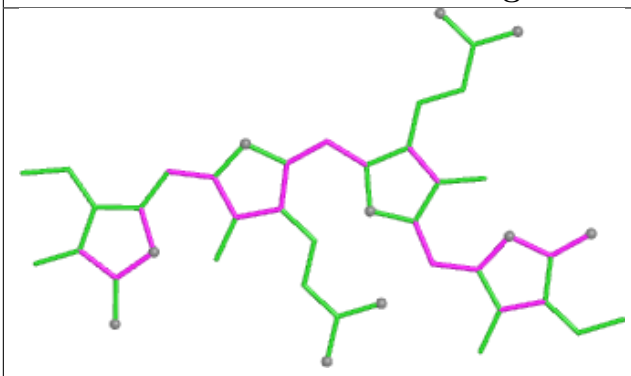


Rings

Ligand CYC G4 1001



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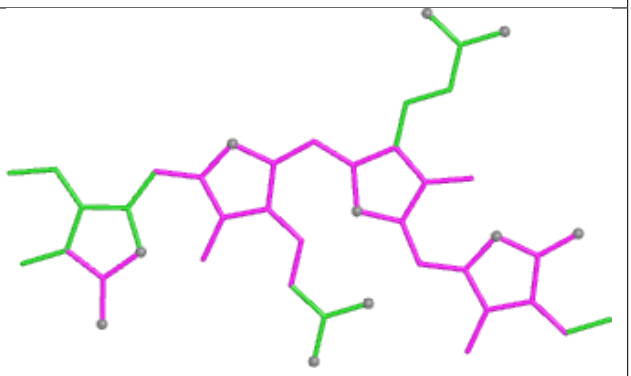
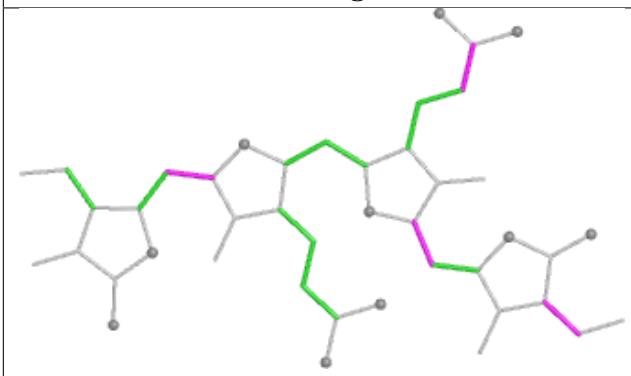


Bond angles



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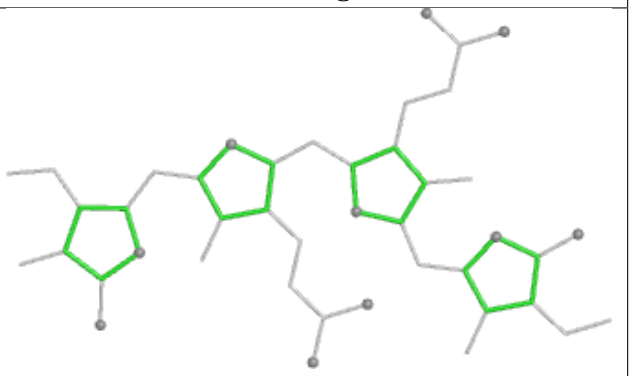
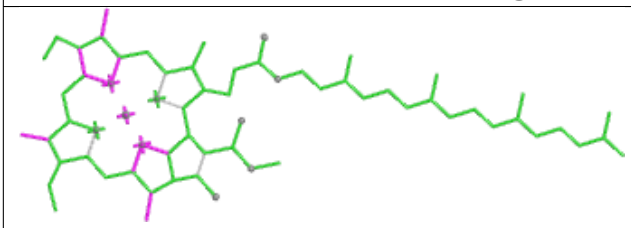


Rings

Ligand CLA BN 827



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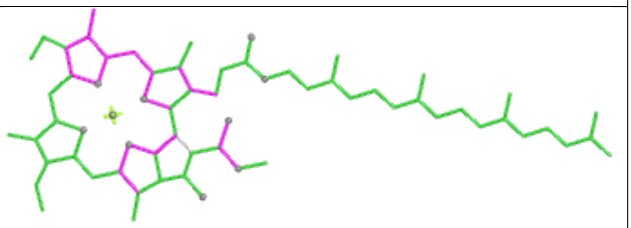
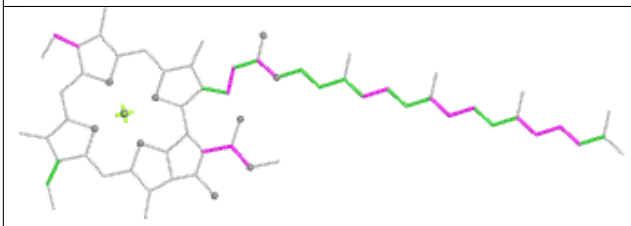
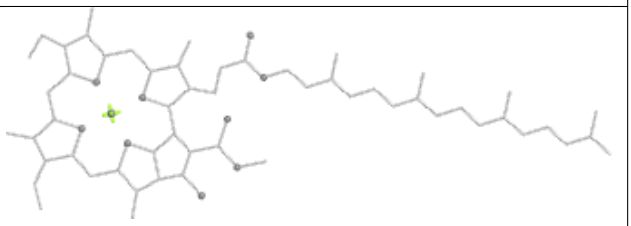


Bond angles

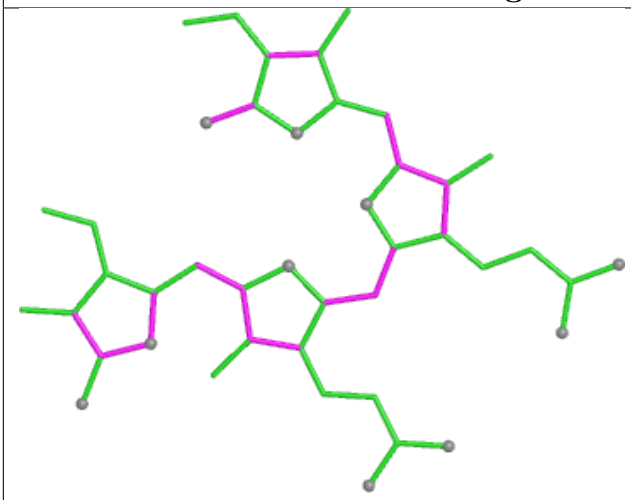


Torsions



Rings

Ligand PEB WK 202



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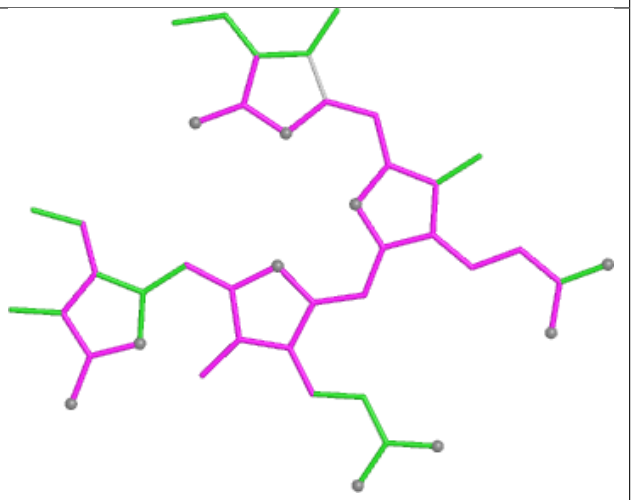
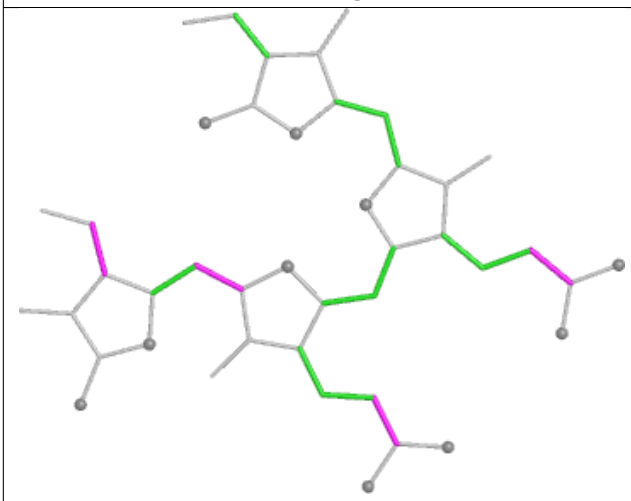


Bond angles



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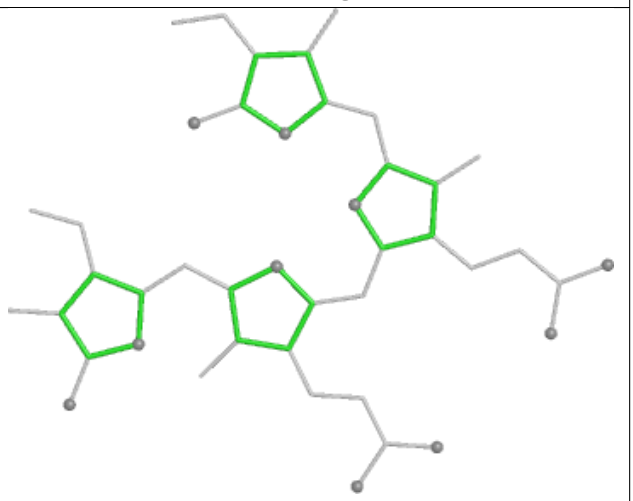
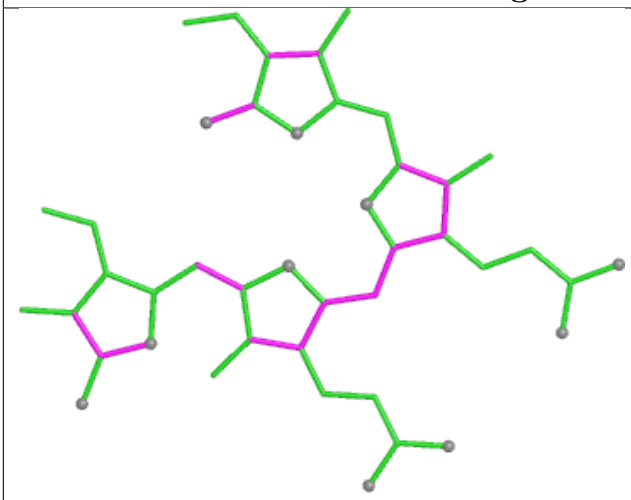


Rings

Ligand PEB YO 203



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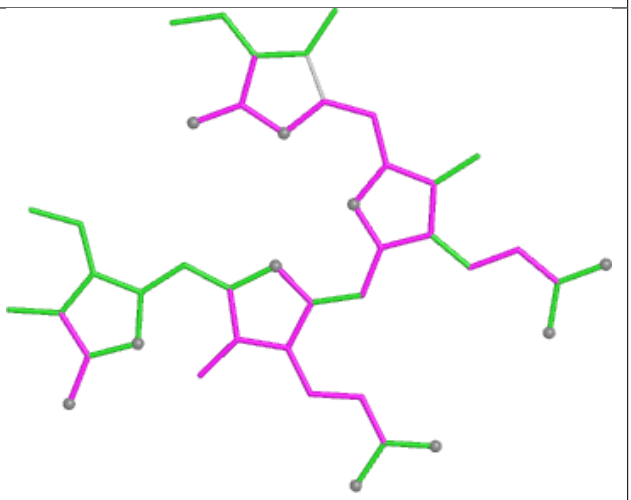

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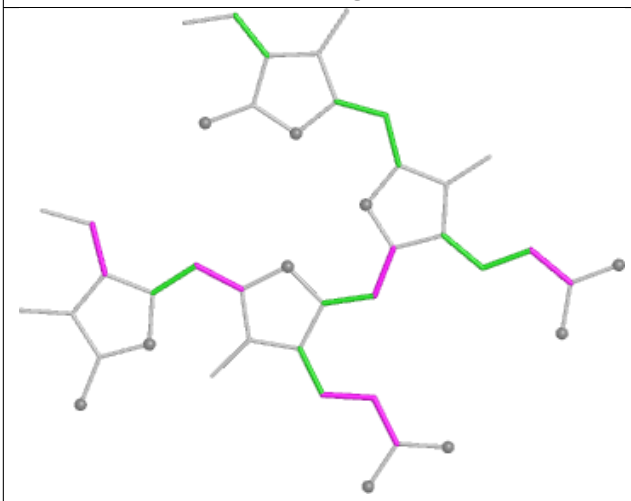

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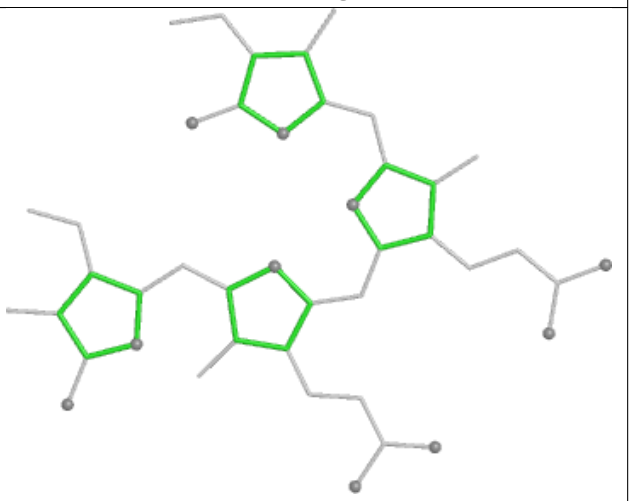
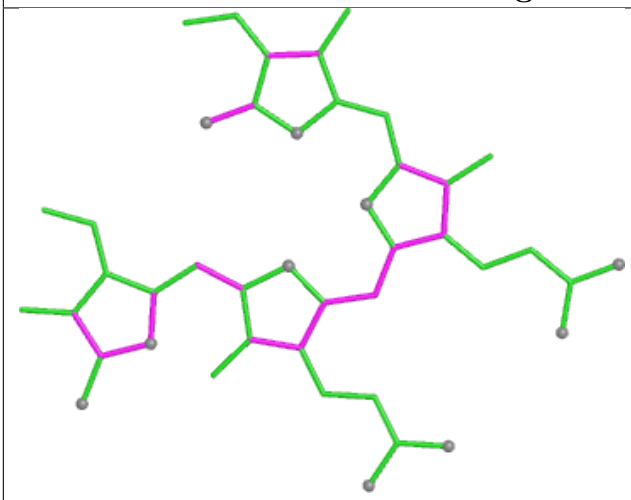


Rings

Ligand PEB qC 202



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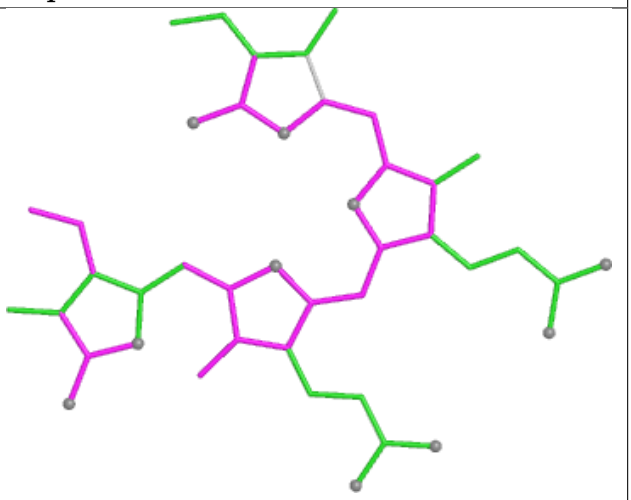

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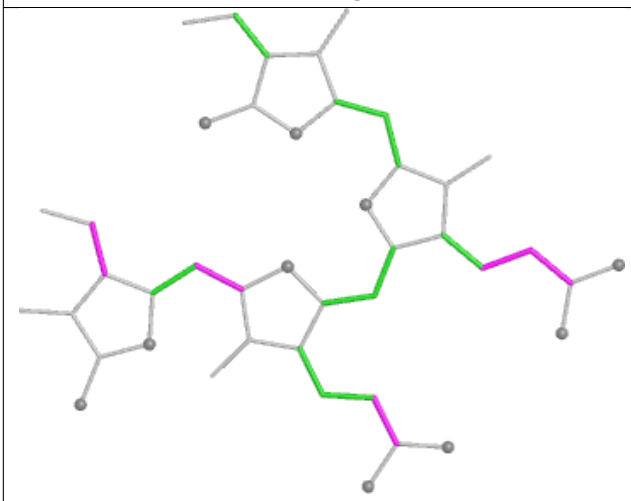

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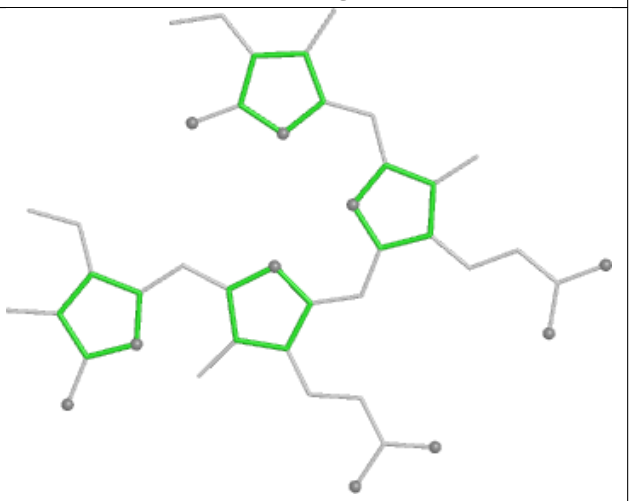
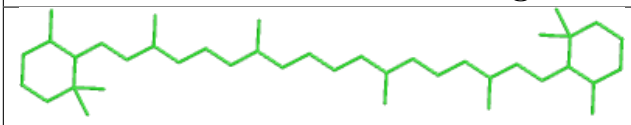


Rings

Ligand BCR BL 617



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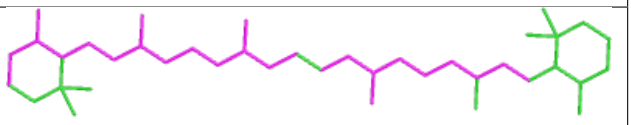

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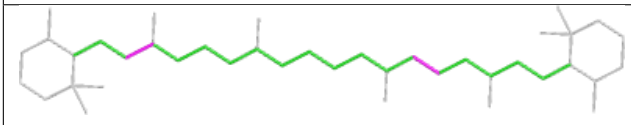

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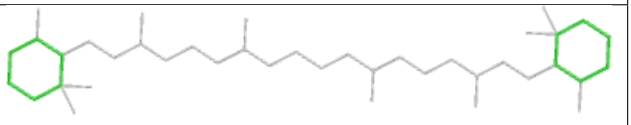
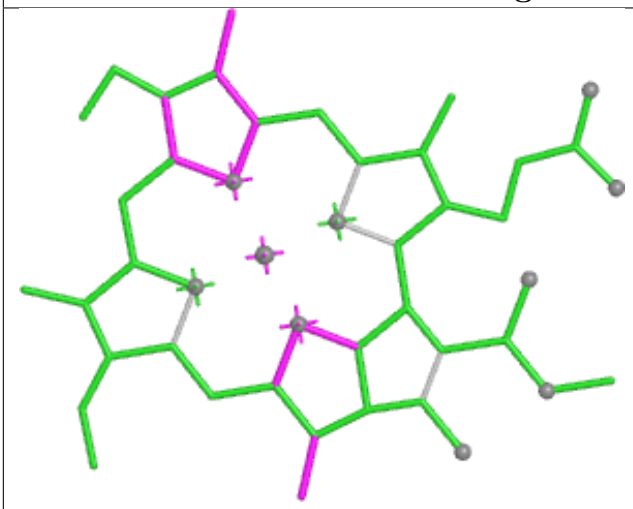


Rings

Ligand CLA A2 822



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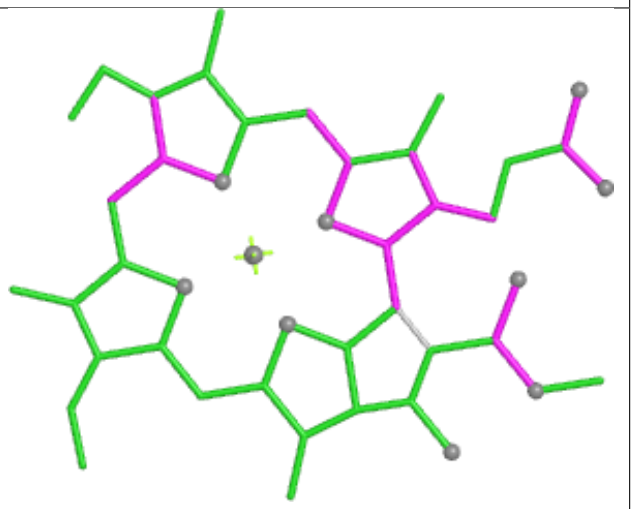

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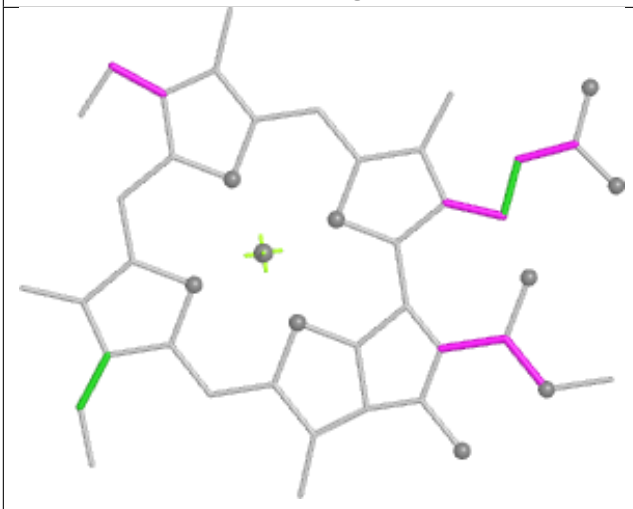
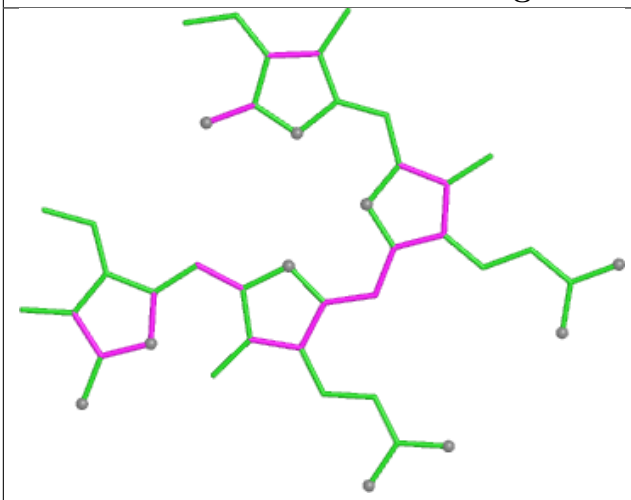


Torsions



Rings

Ligand PEB m4 202



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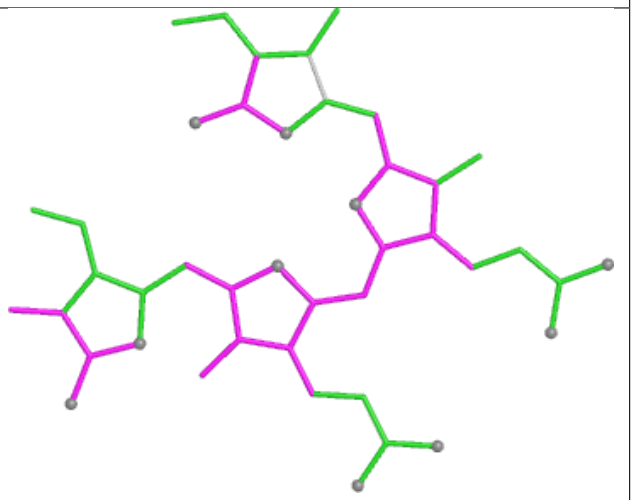

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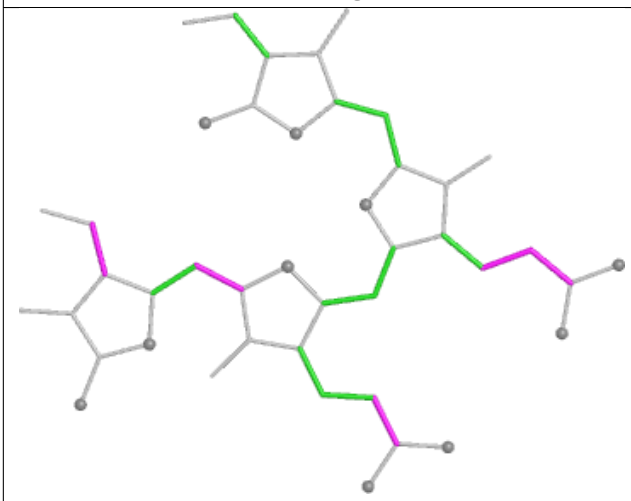

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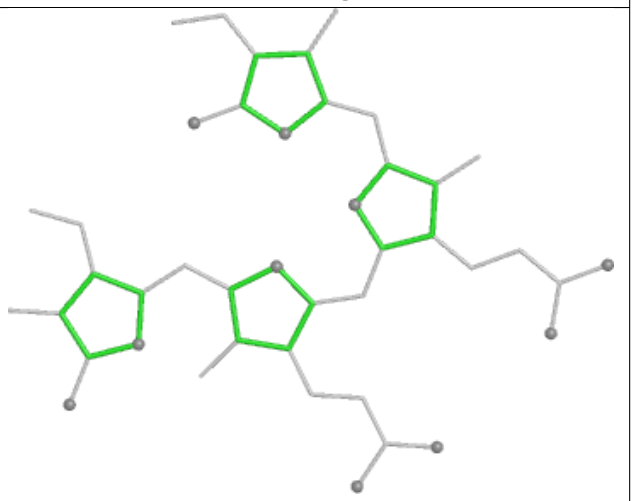
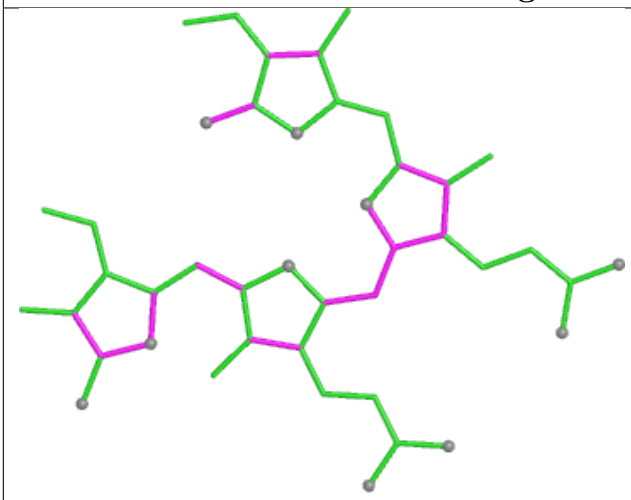


Rings

Ligand PEB CI 202



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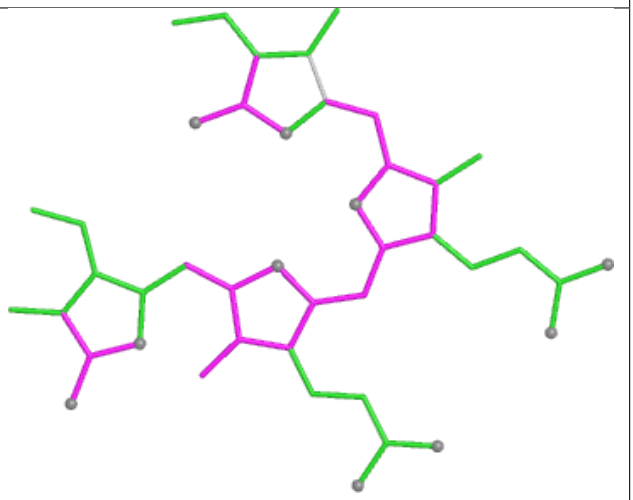

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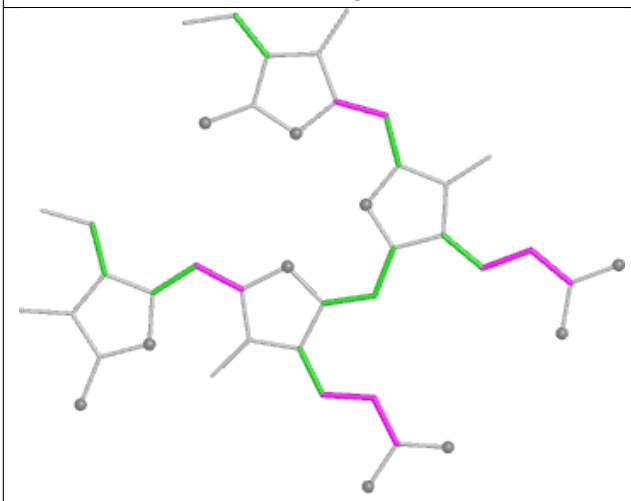

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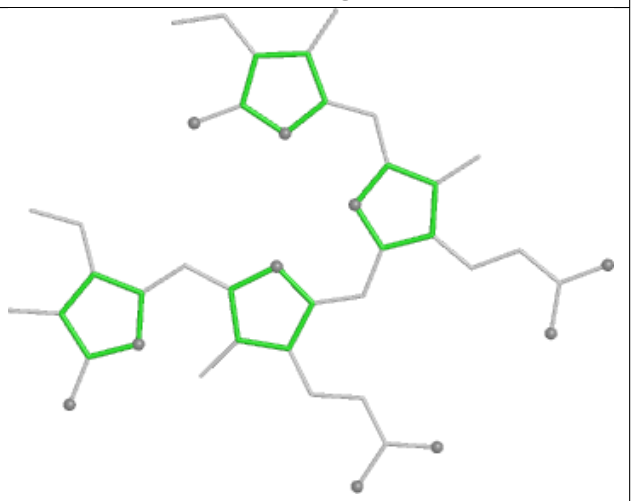
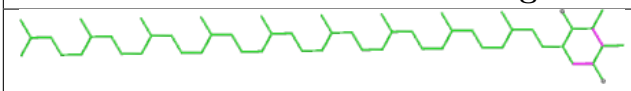


Rings

Ligand PL9 D6 408



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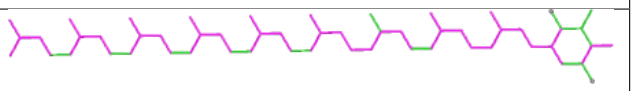
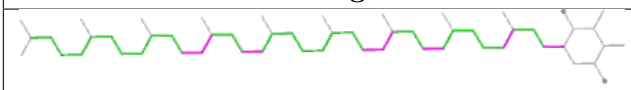


Bond angles



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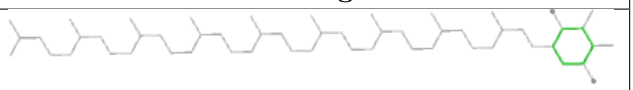
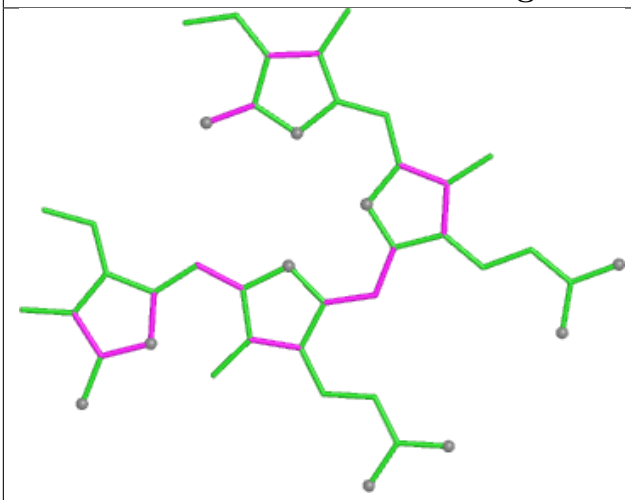


Rings

Ligand PEB cB 402



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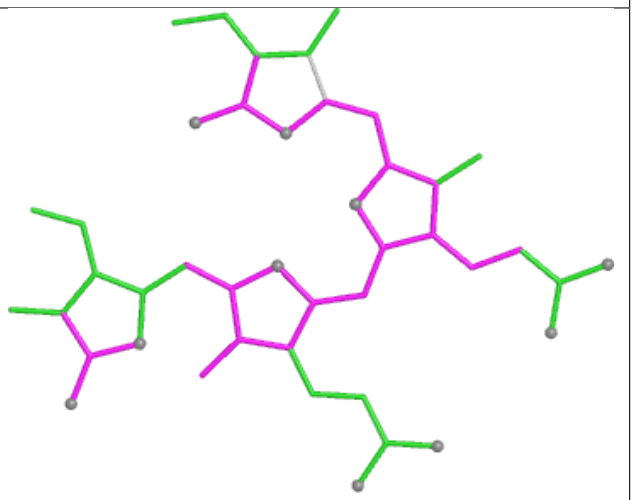

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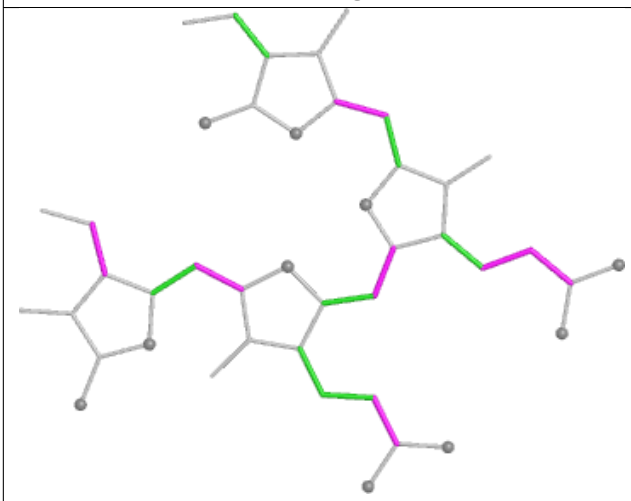

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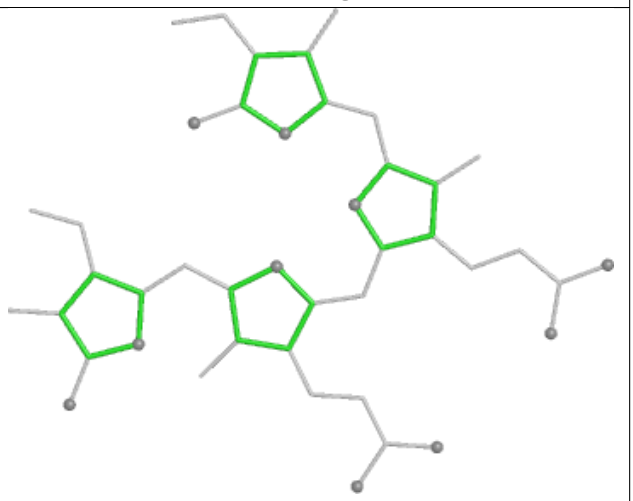
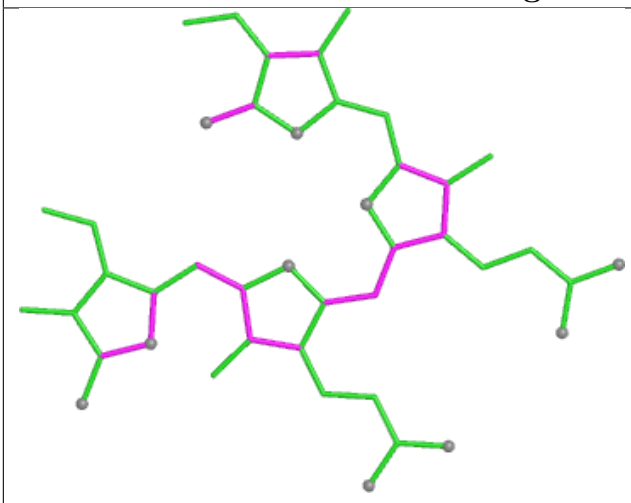


Rings

Ligand PEB j1 201



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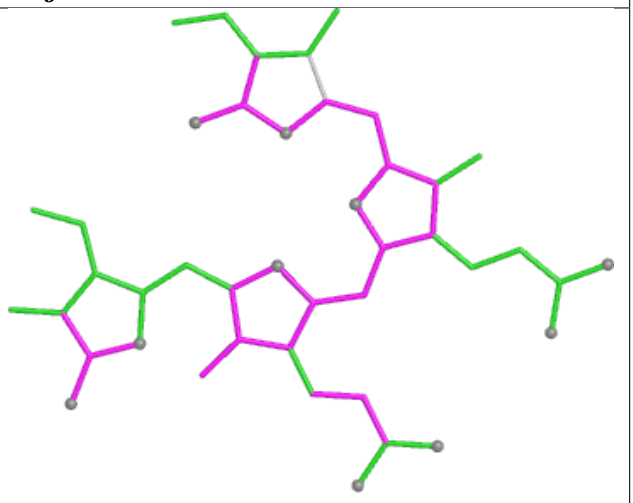

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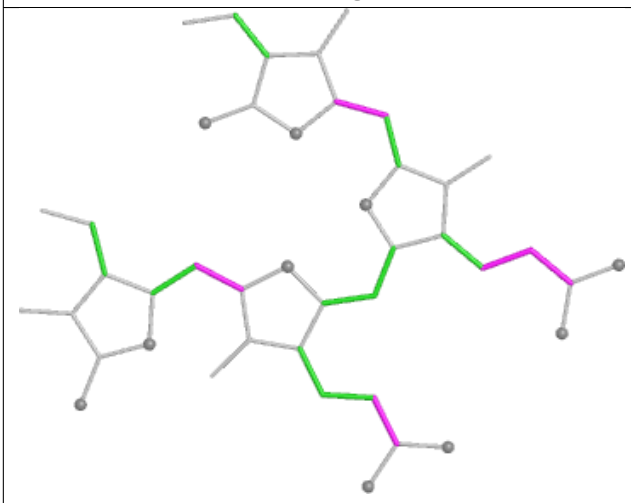

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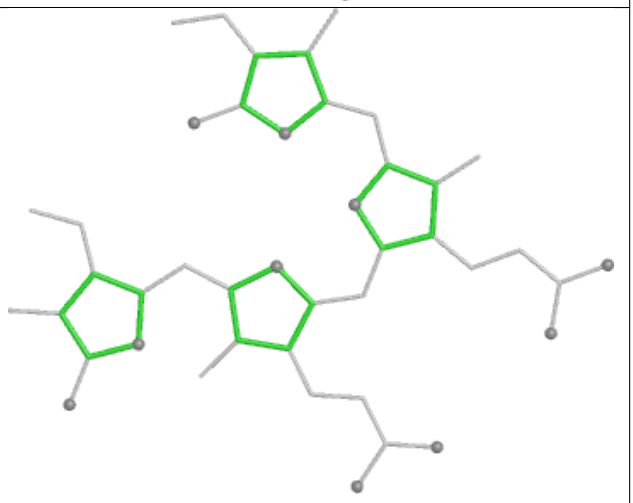
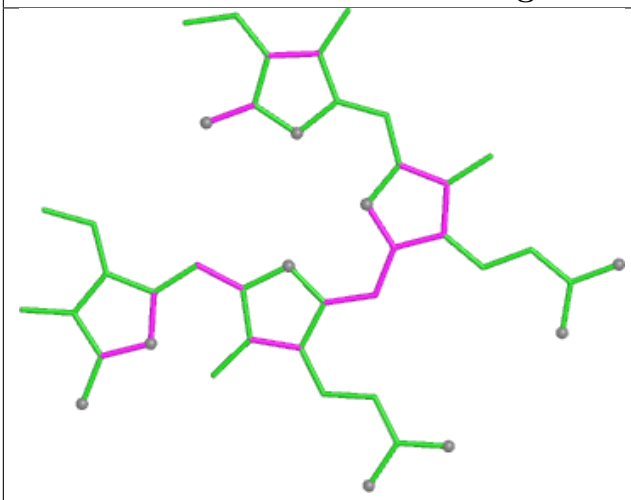


Rings

Ligand PEB GI 202



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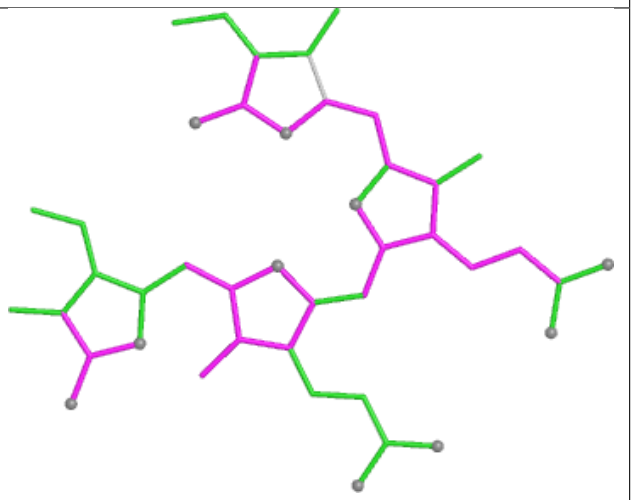

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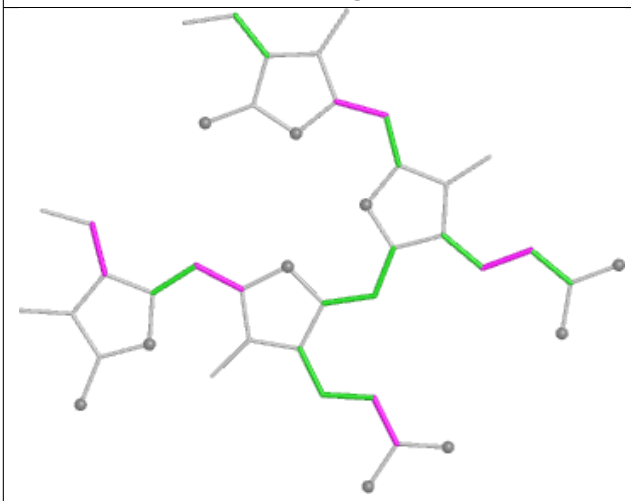

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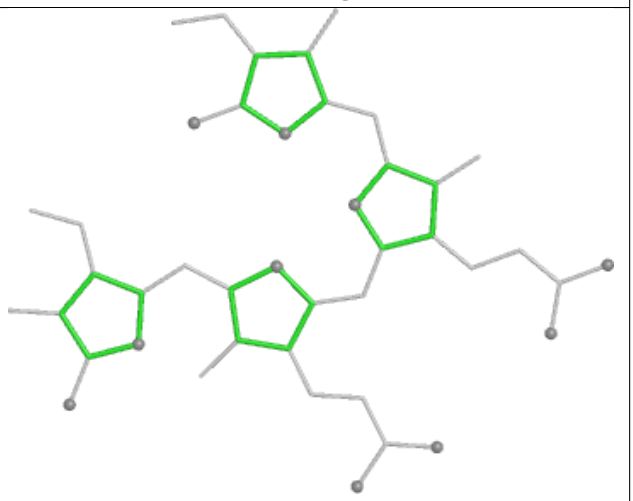
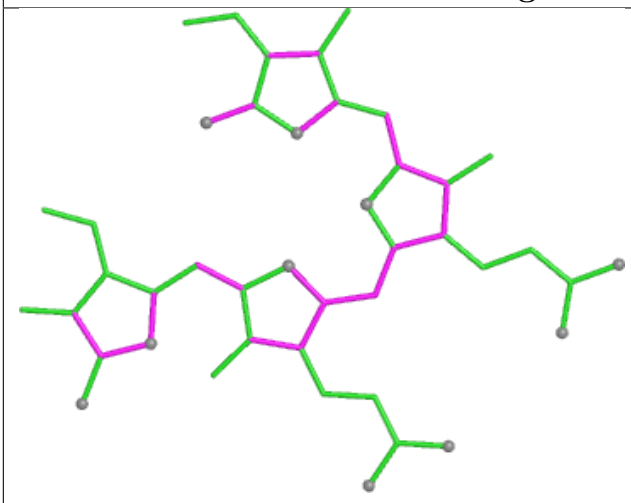


Rings

Ligand PEB jH 203



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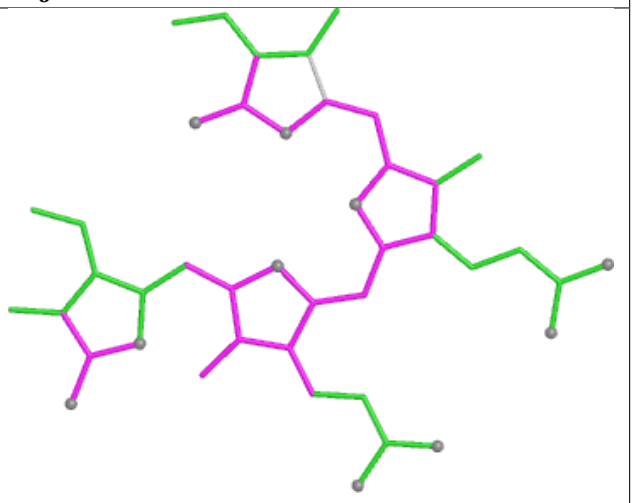
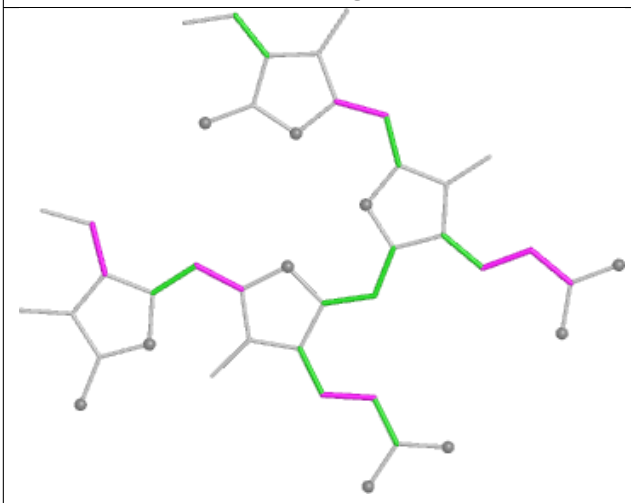


Bond angles



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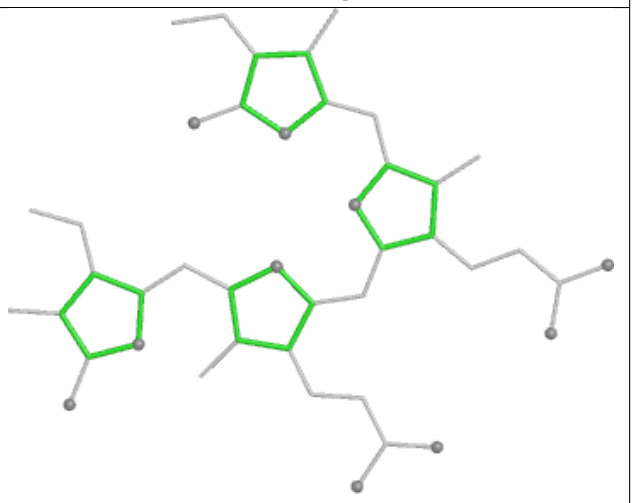
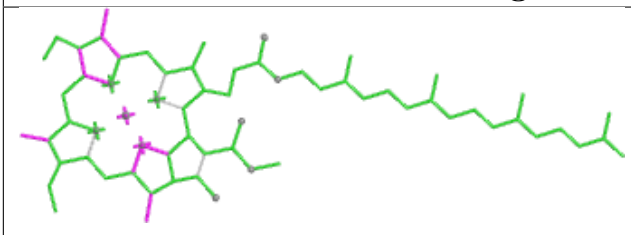


Rings

Ligand CLA AN 828



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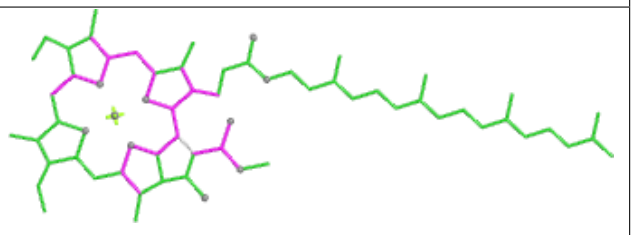
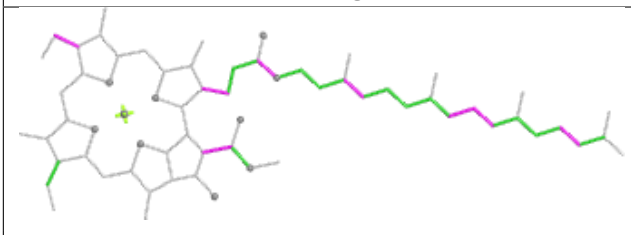


Bond angles



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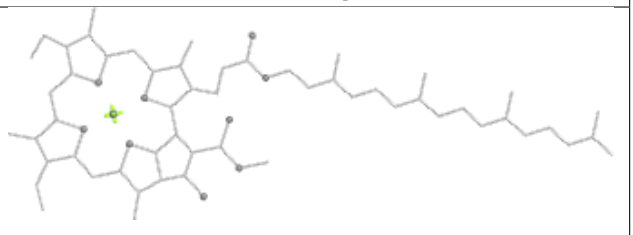
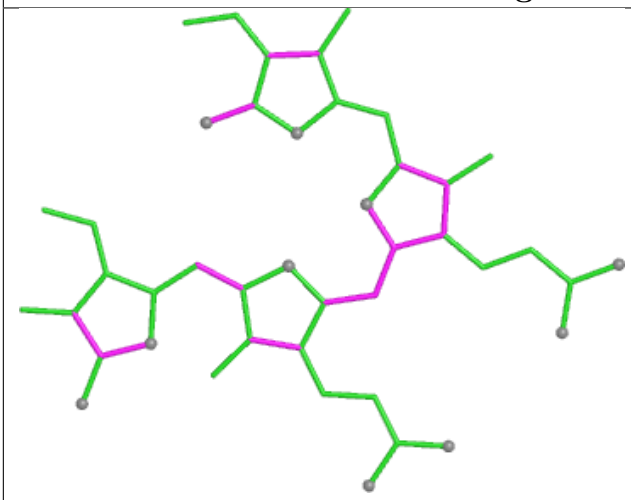


Rings

Ligand PEB Y9 203



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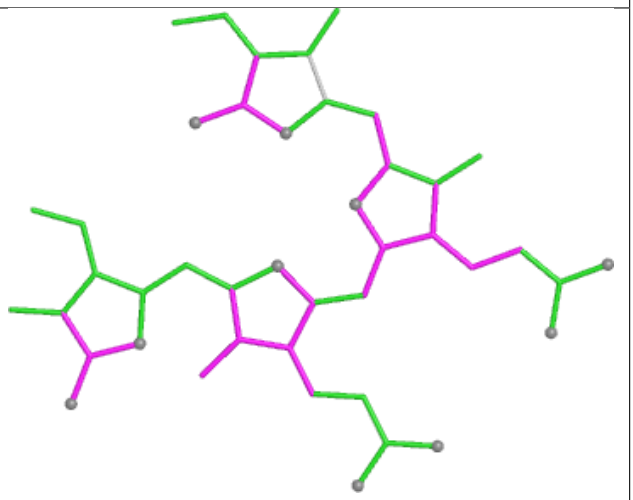
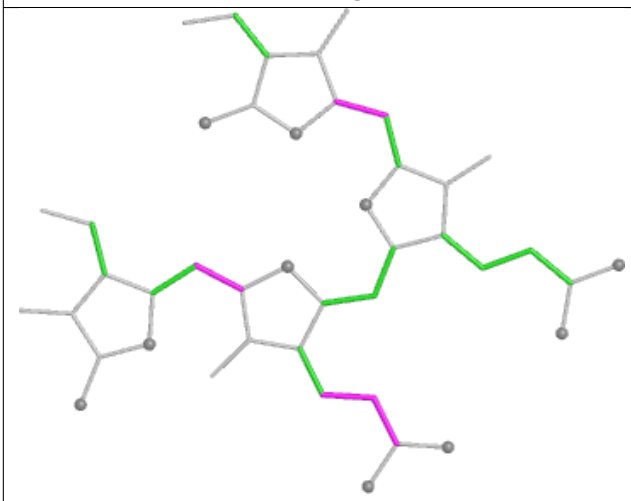


Bond angles



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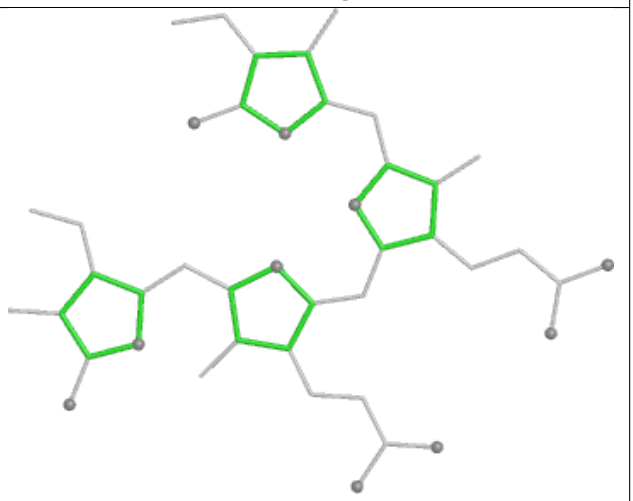
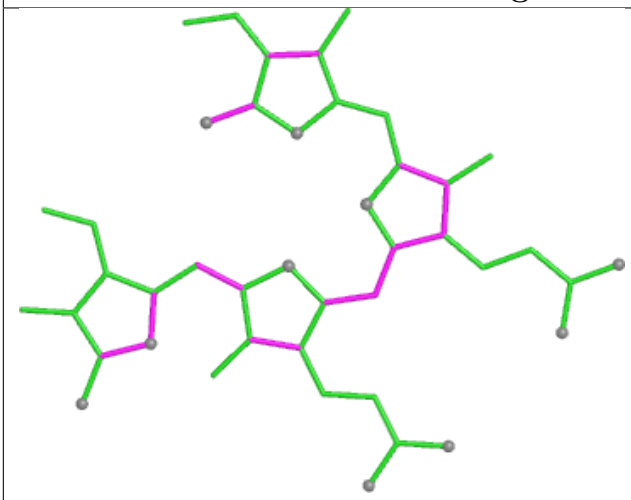
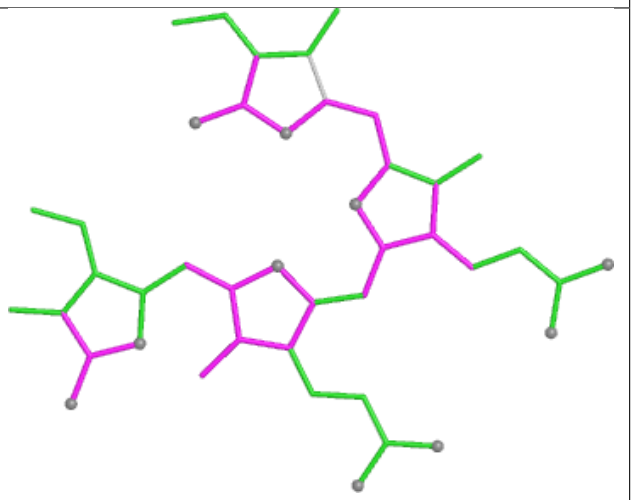


Rings

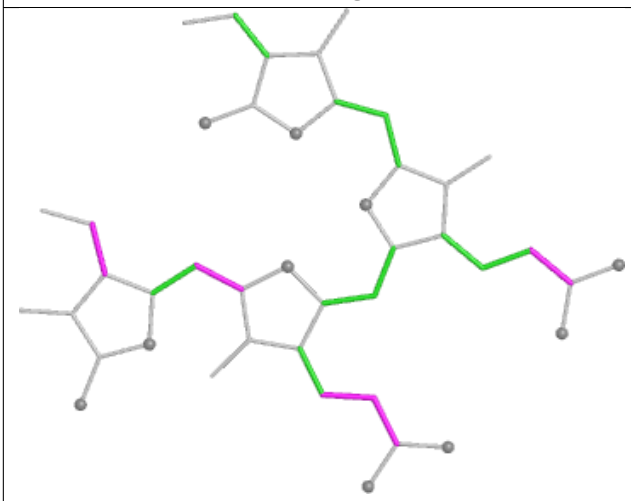
Ligand PEB AO 304



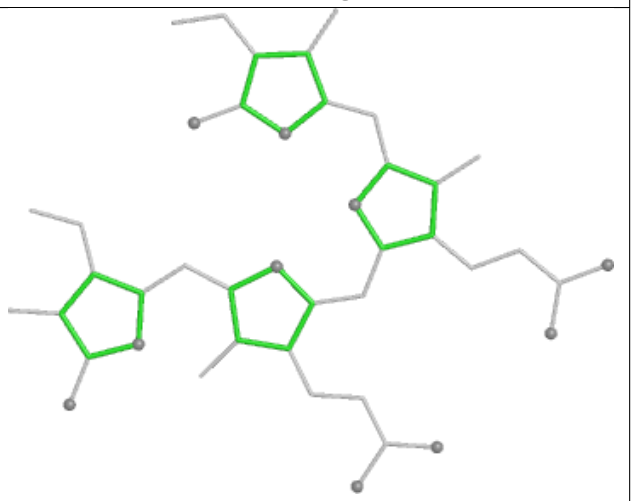
Bond lengths



Bond angles

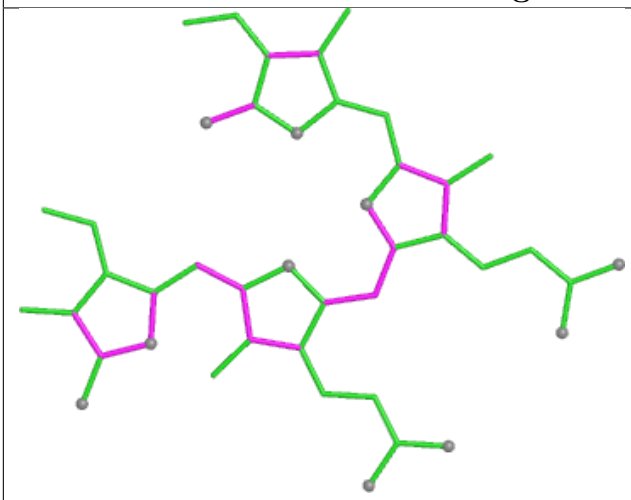


Torsions



Rings

Ligand PEB ZG 203



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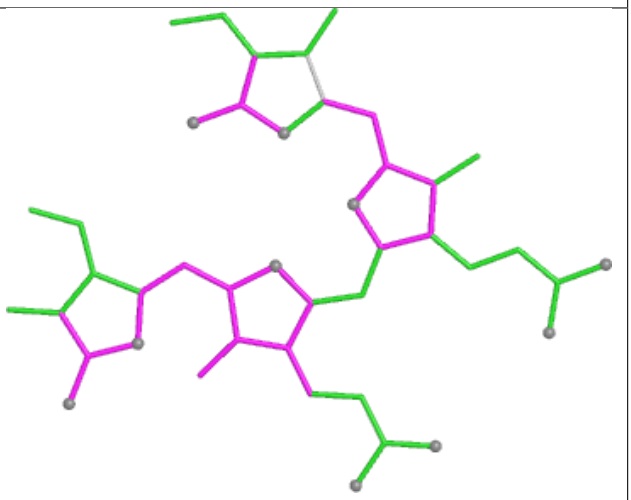

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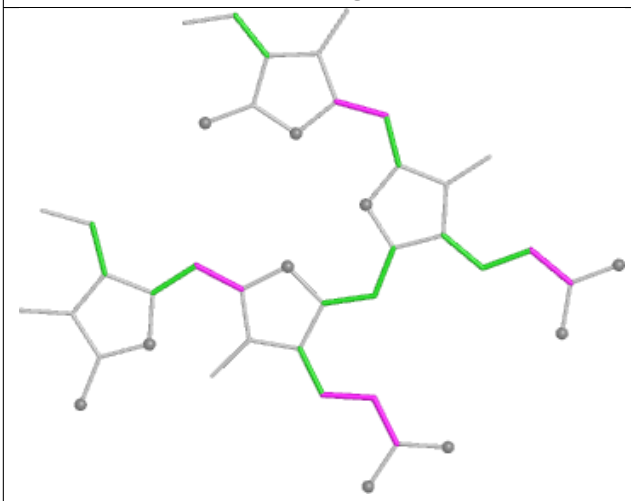

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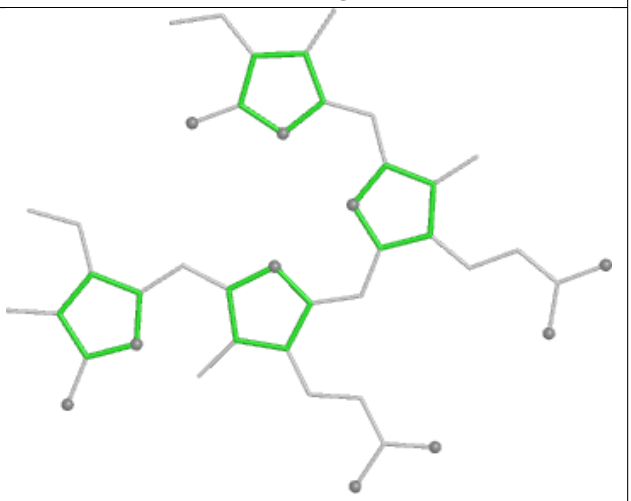
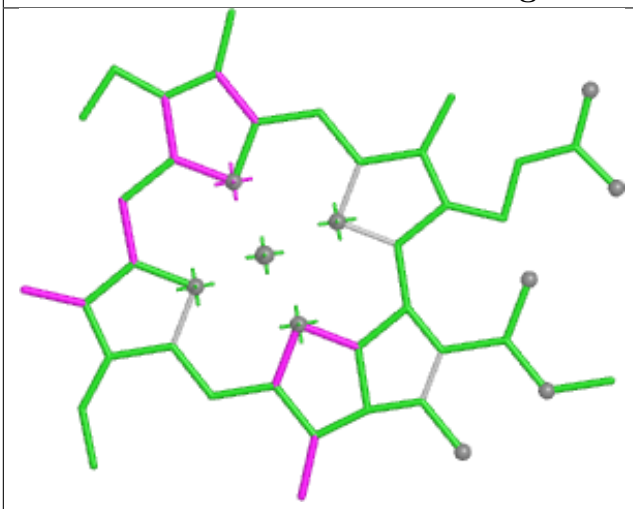


Rings

Ligand CLA 42 611



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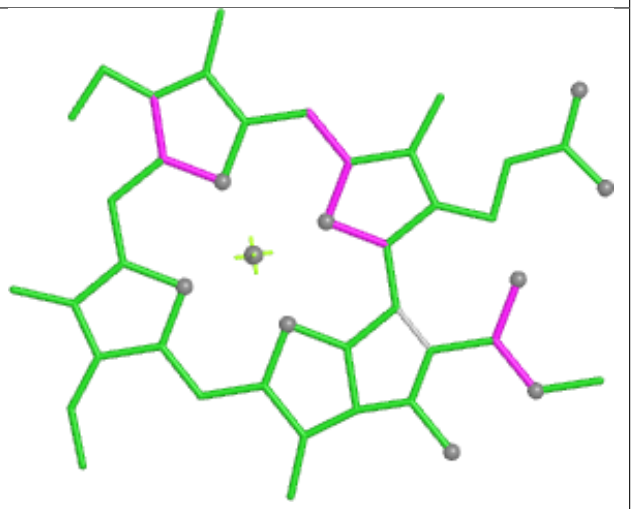
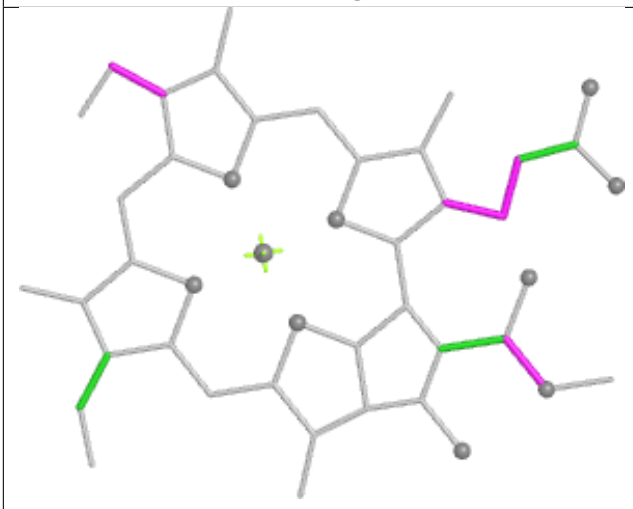


Bond angles

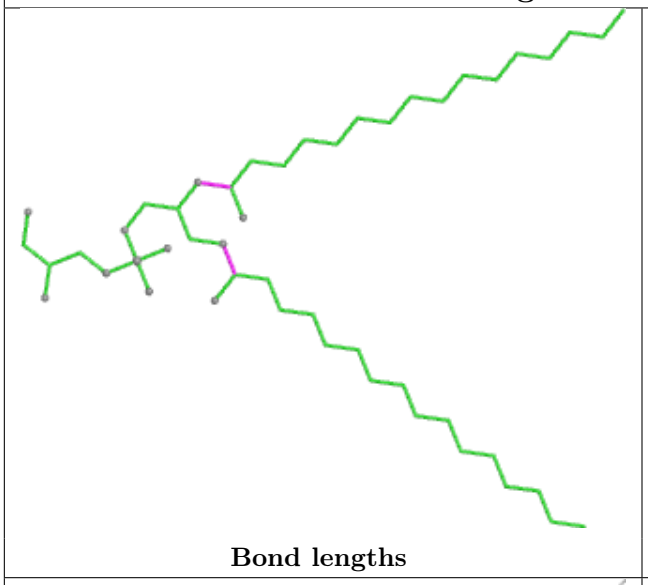


Torsions



Rings

Ligand LHG L6 101



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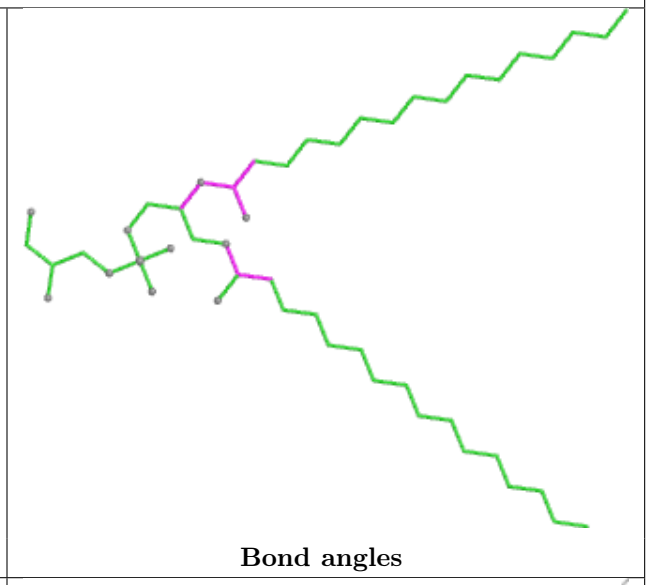

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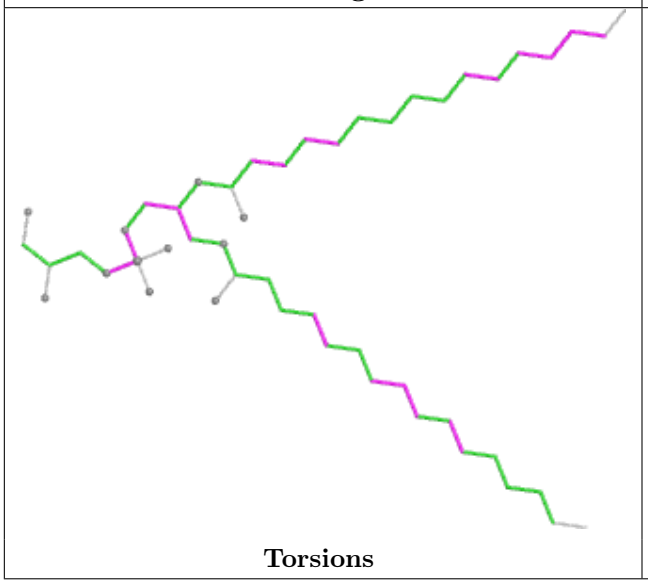

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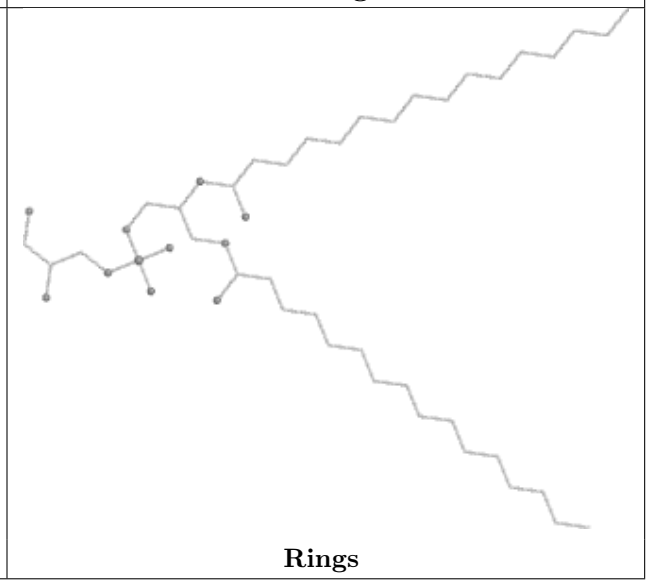
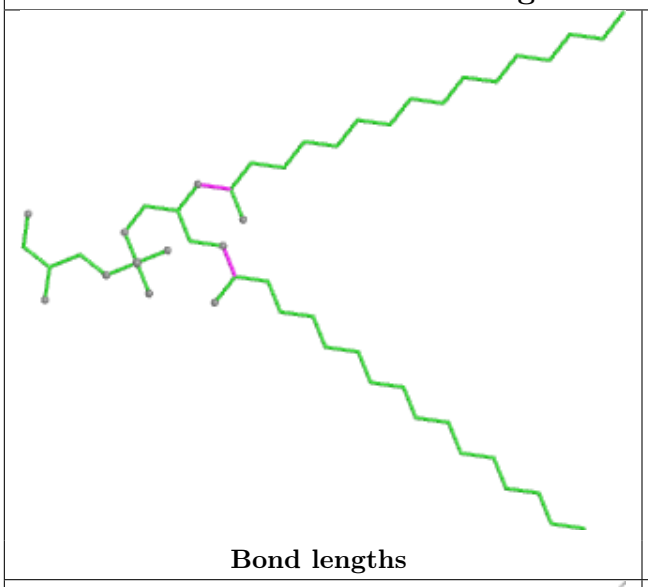


Rings

Ligand LHG d6 407



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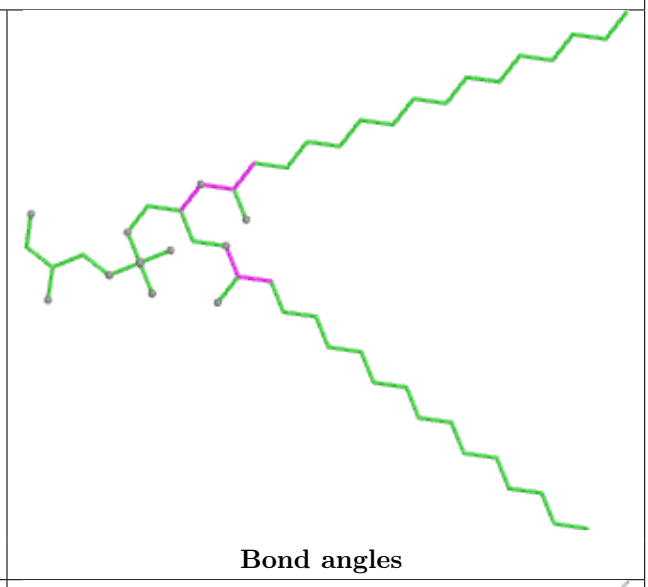
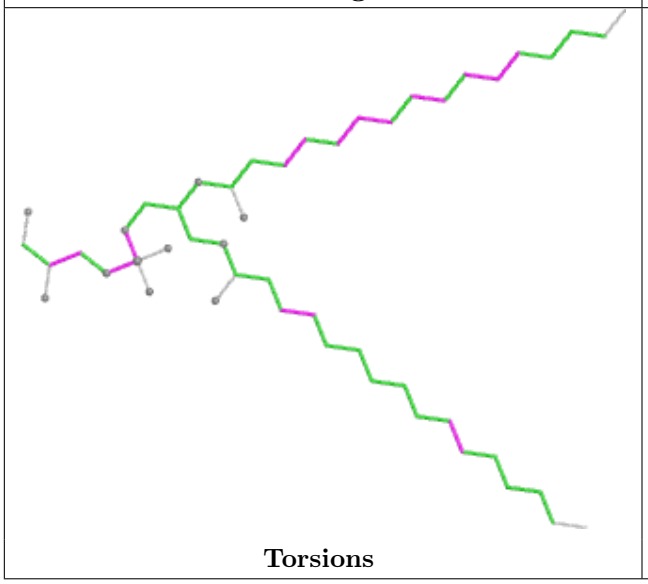


Bond angles



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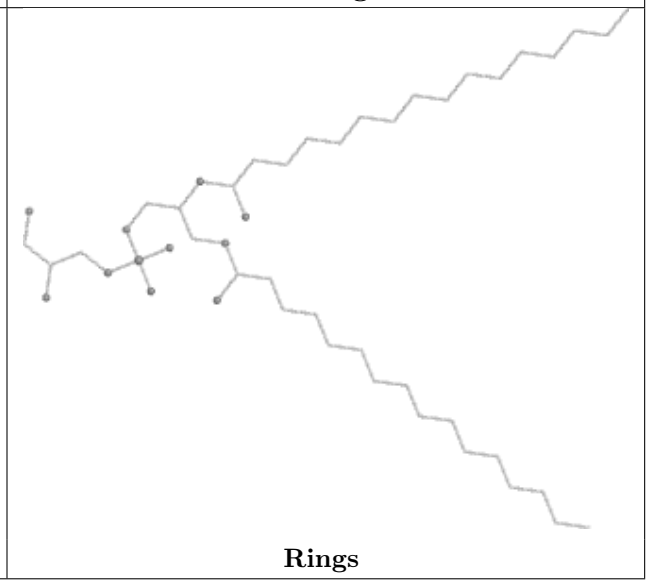
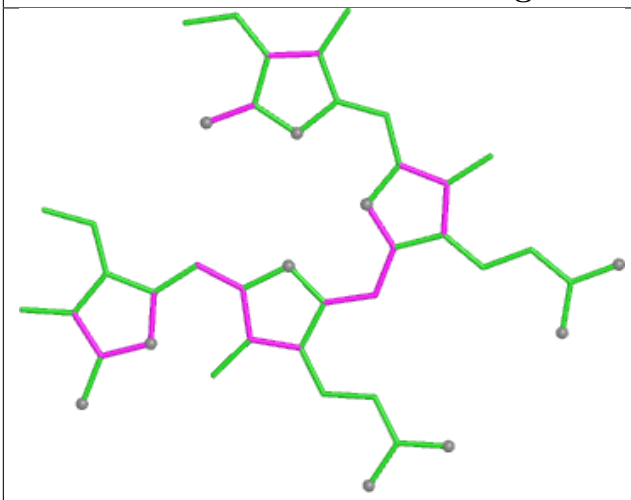


Rings

Ligand PEB gK 201



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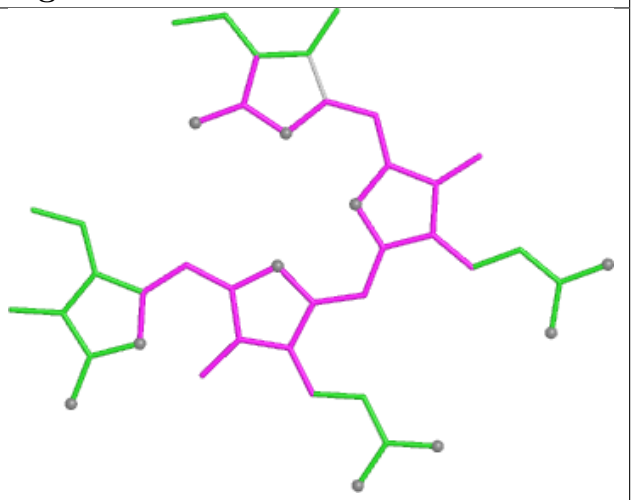

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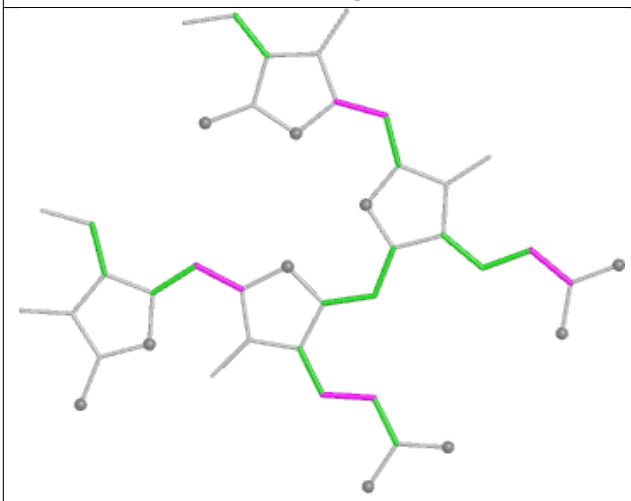

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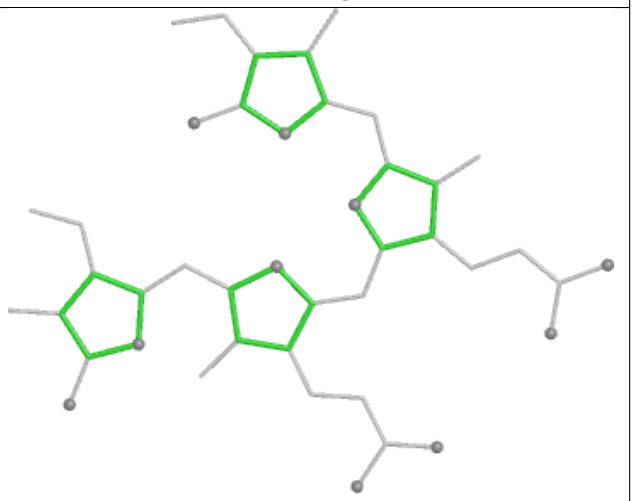
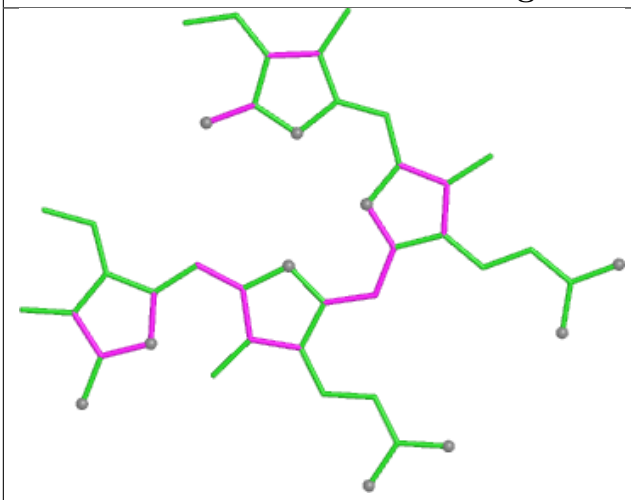


Rings

Ligand PEB gF 201



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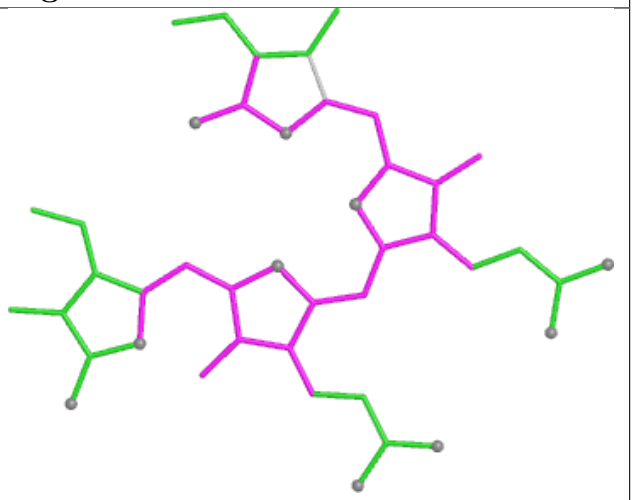
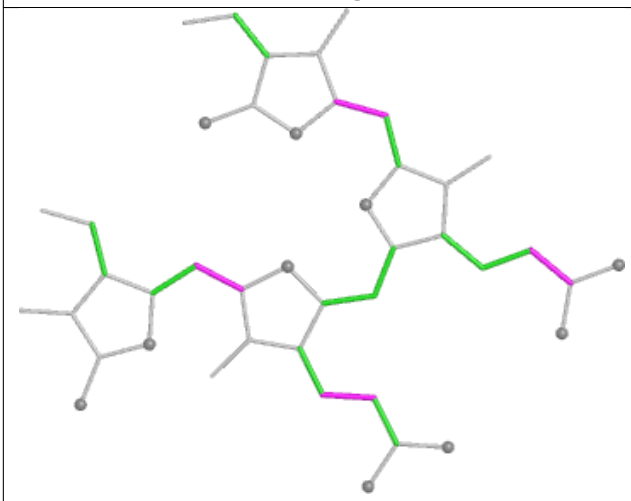


Bond angles



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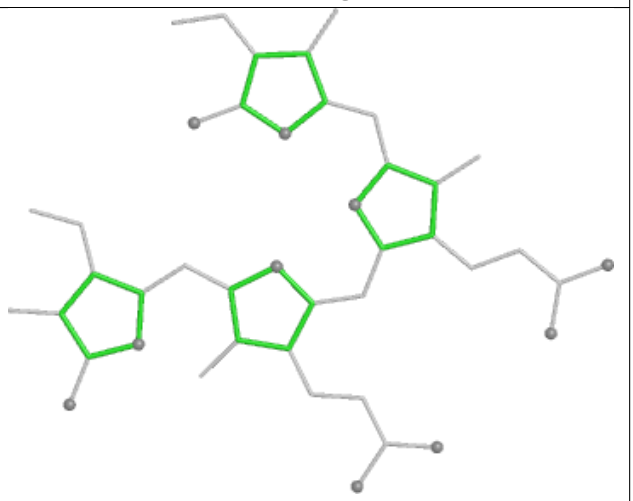
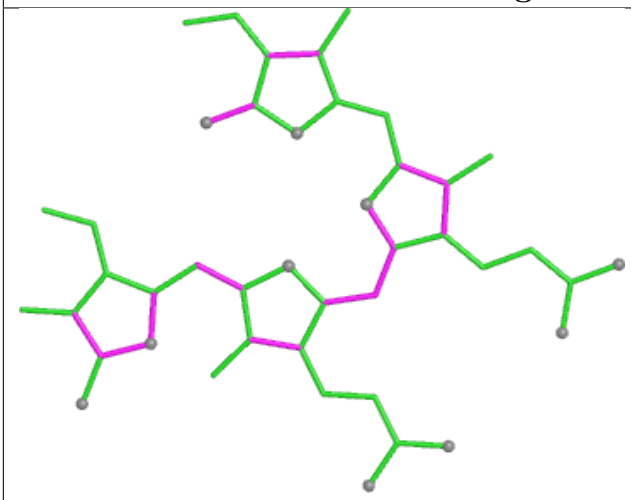


Rings

Ligand PEB UJ 202



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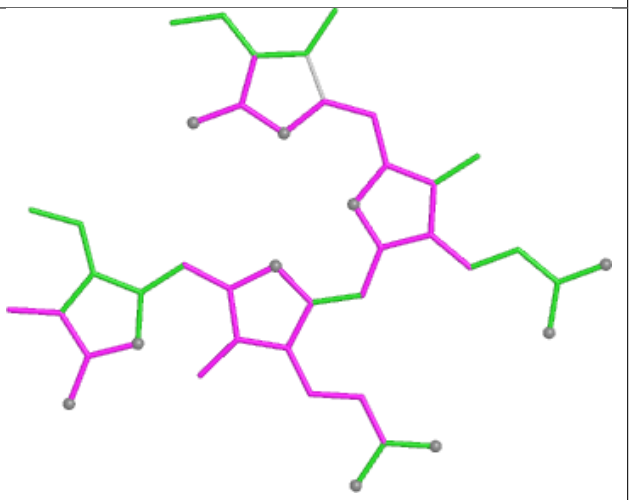
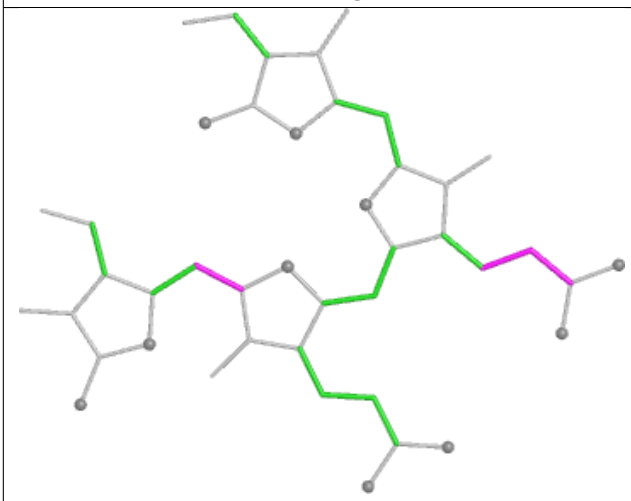


Bond angles



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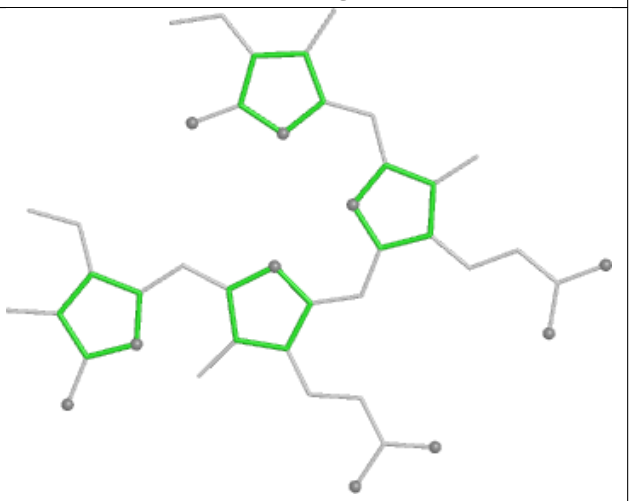
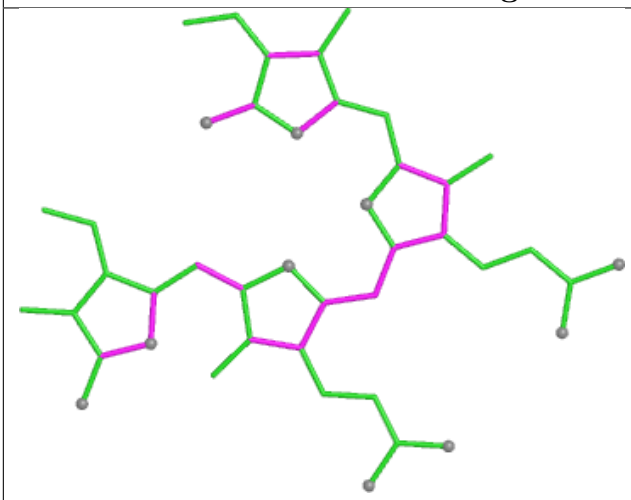


Rings

Ligand PEB NH 1002



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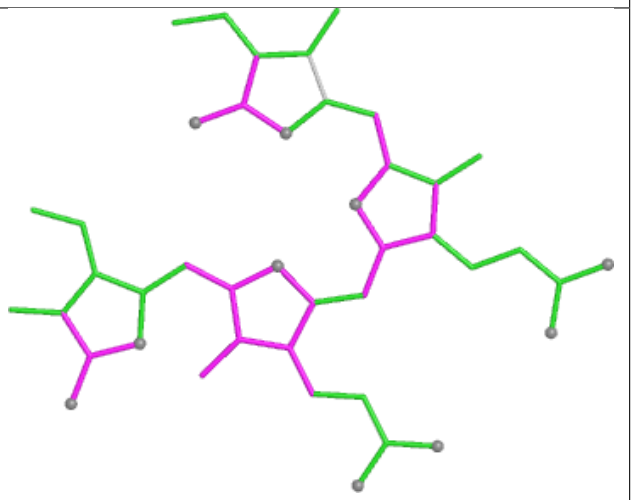

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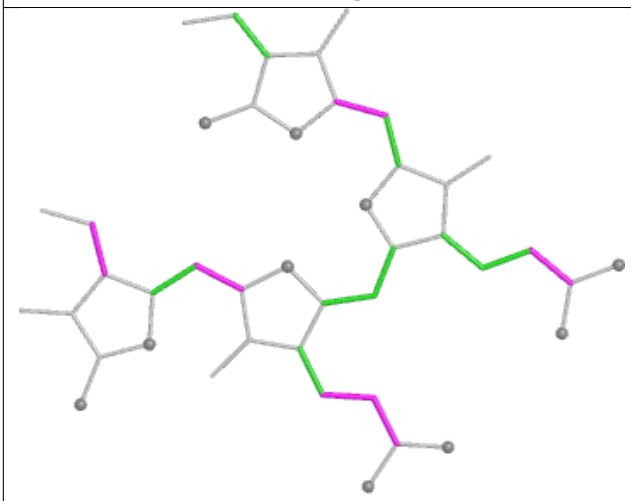

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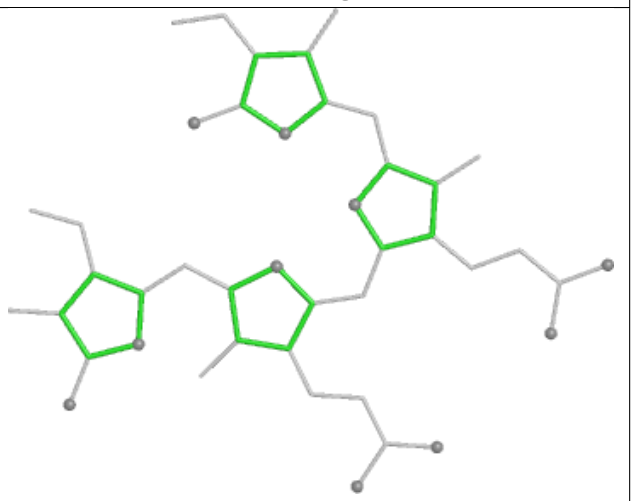
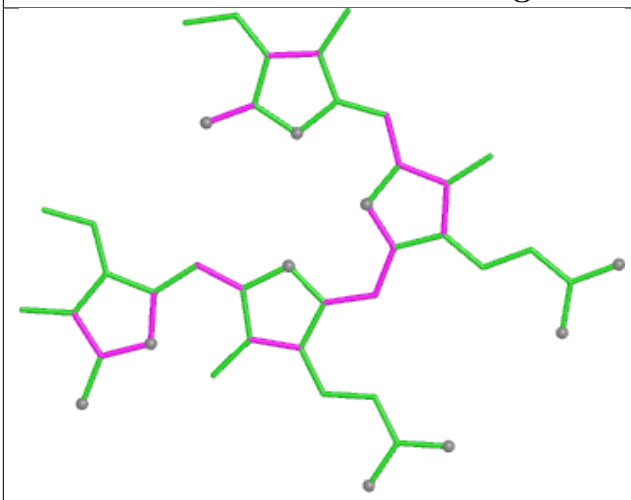


Rings

Ligand PEB mJ 201



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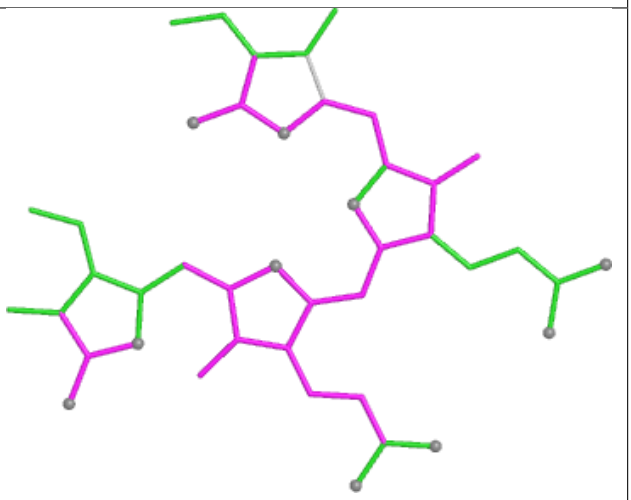
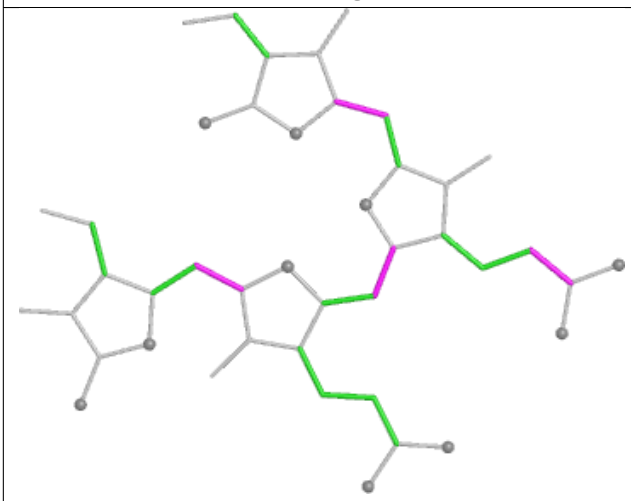


Bond angles



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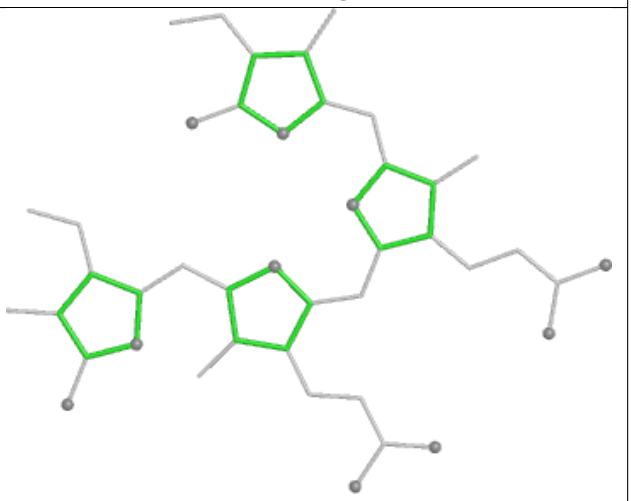
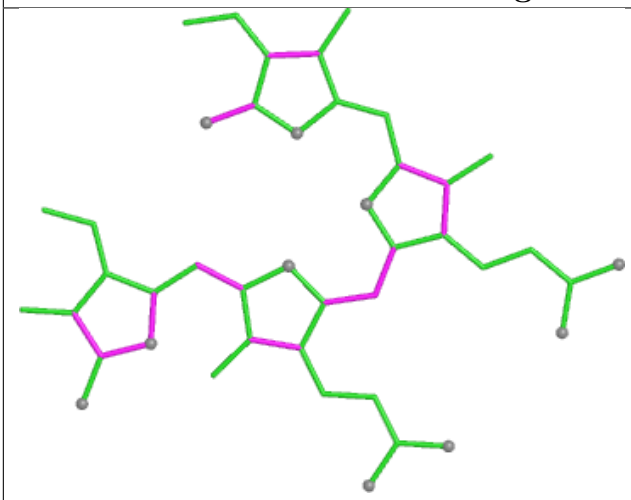


Rings

Ligand PEB bO 201



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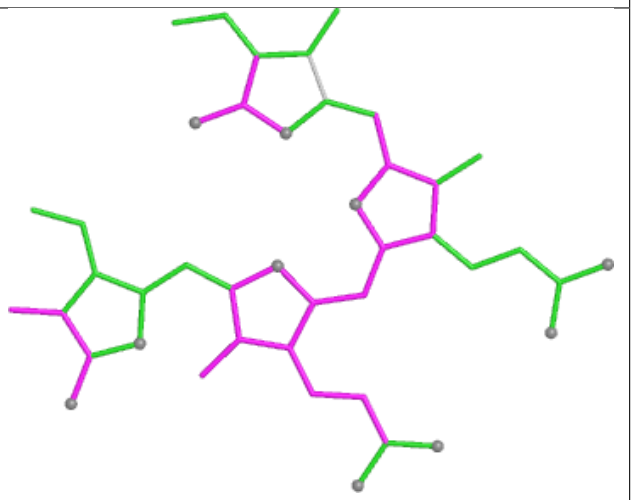

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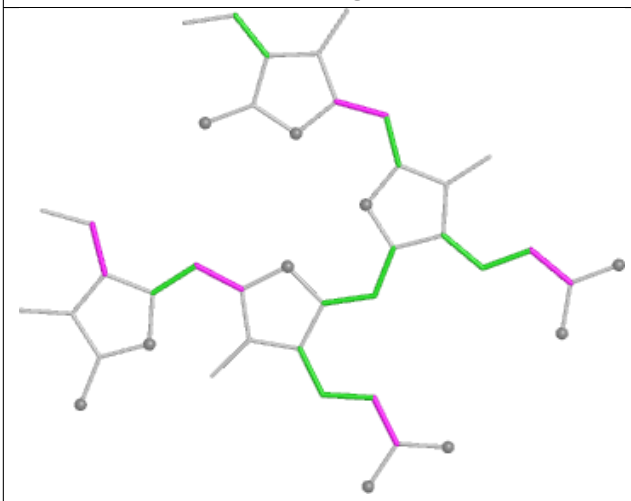

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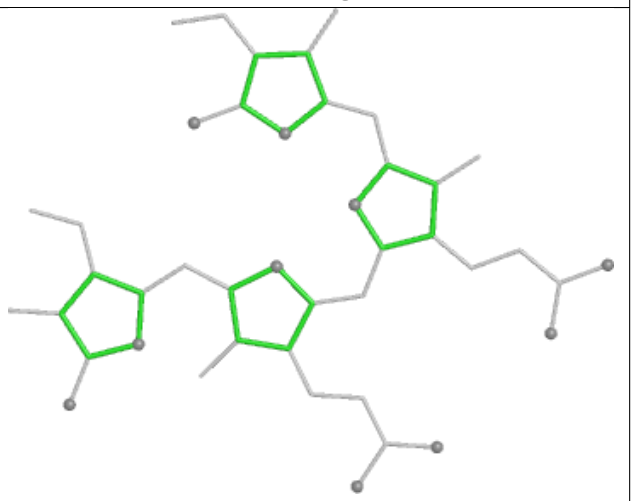
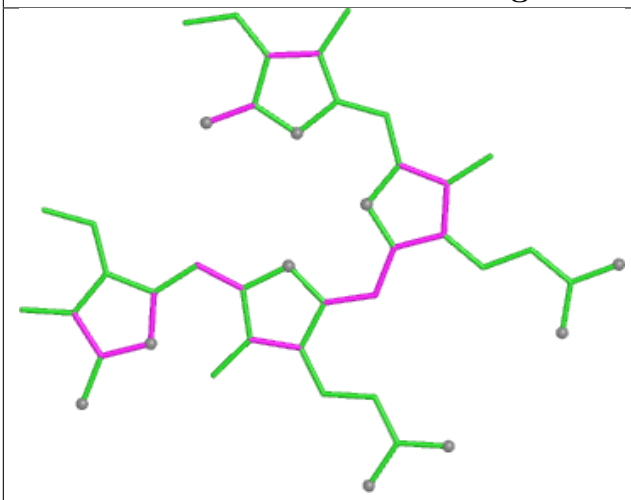


Rings

Ligand PEB CD 202



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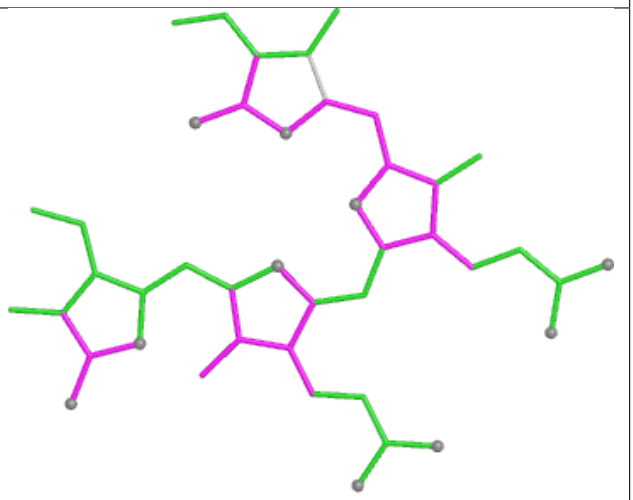
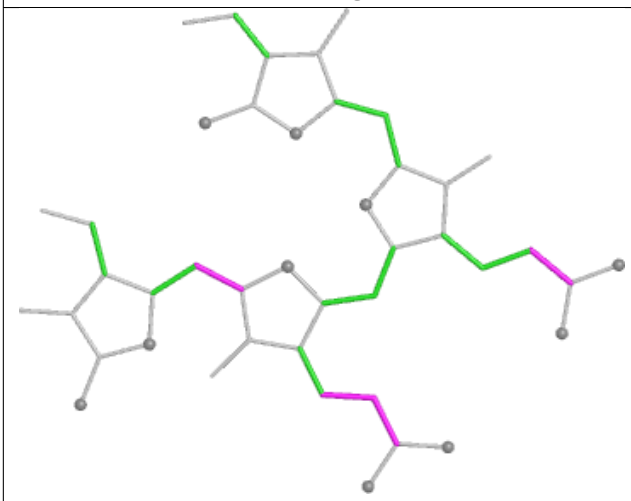


Bond angles



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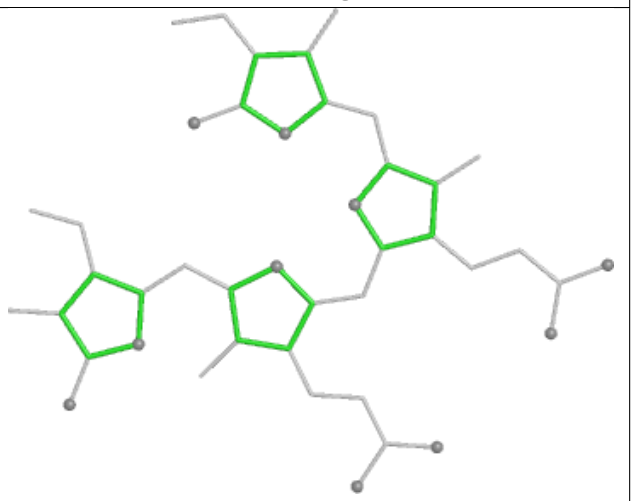
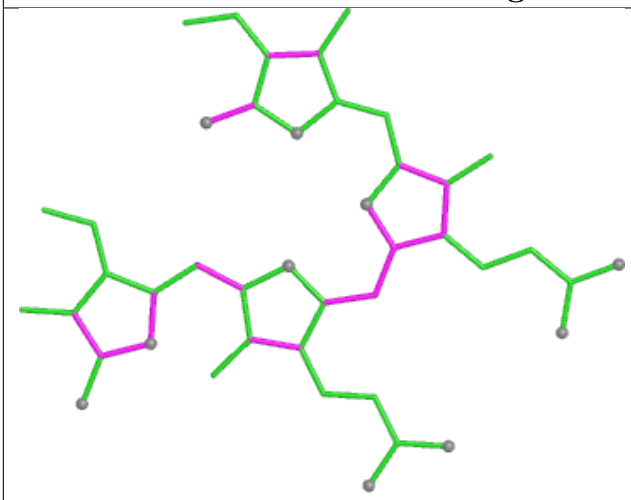


Rings

Ligand PEB WE 202



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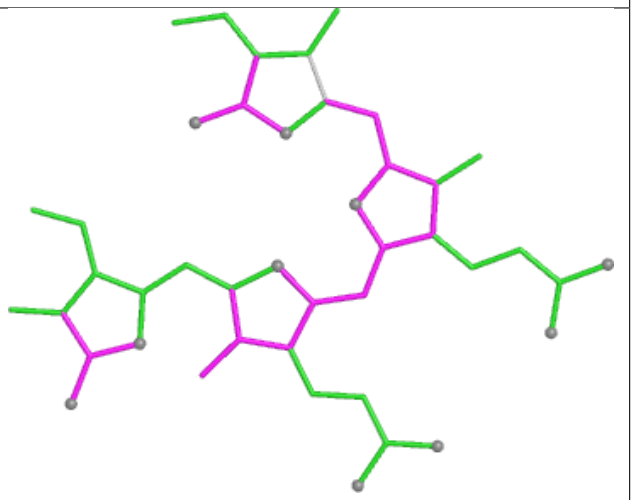
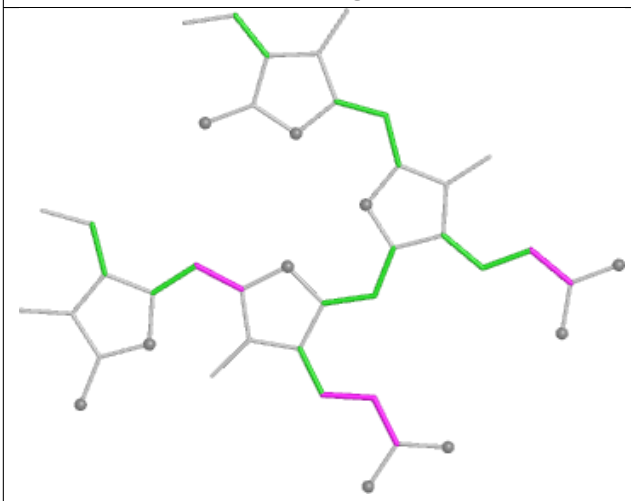


Bond angles



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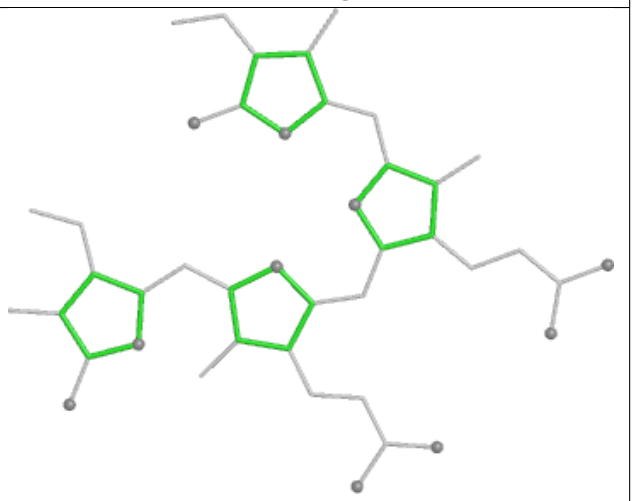
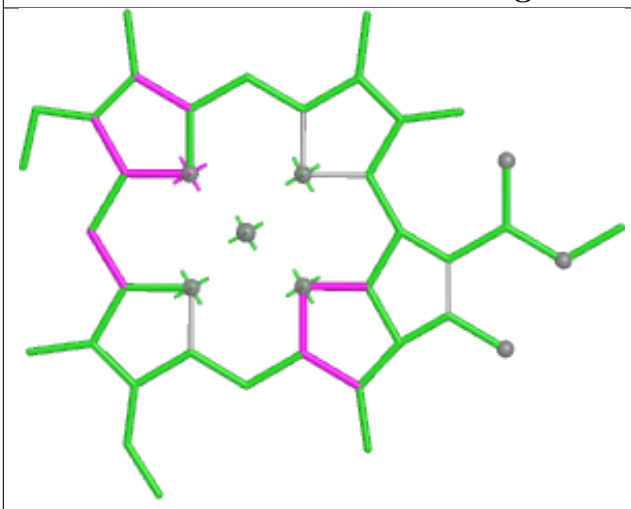


Rings

Ligand CLA 1N 608



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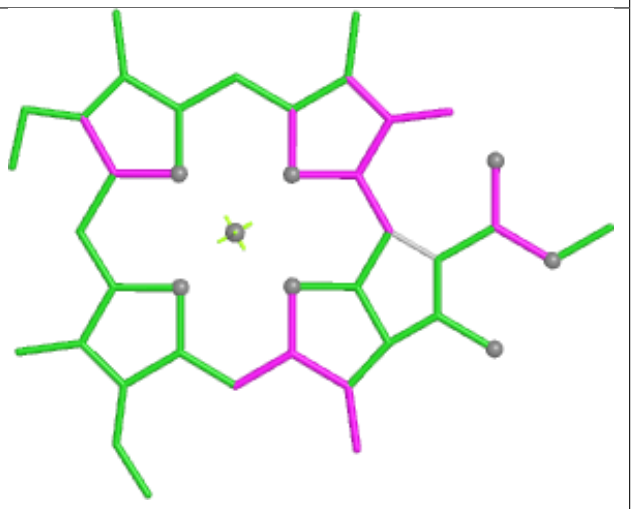
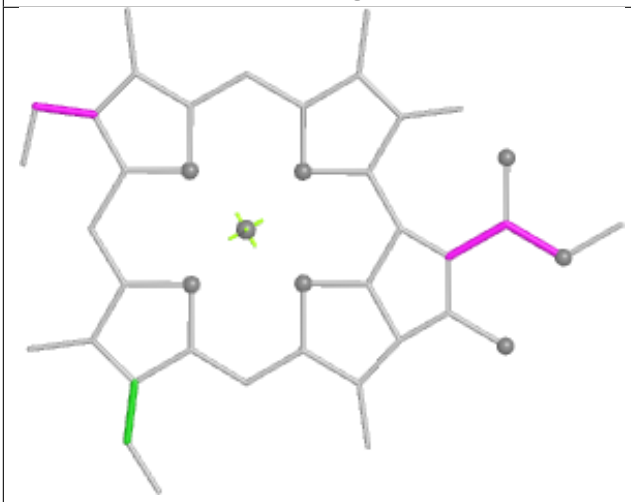


Bond angles



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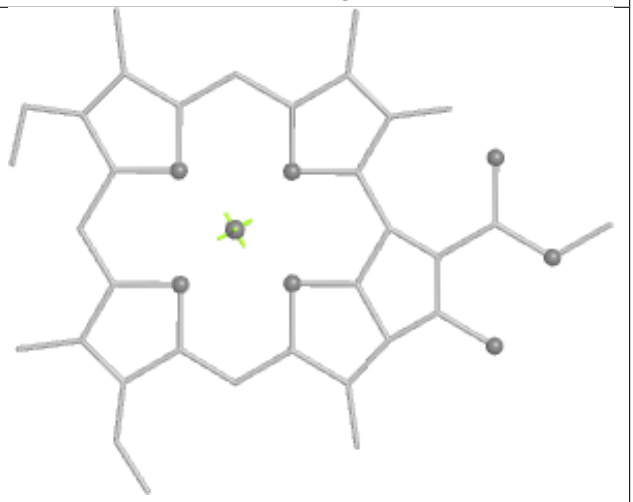
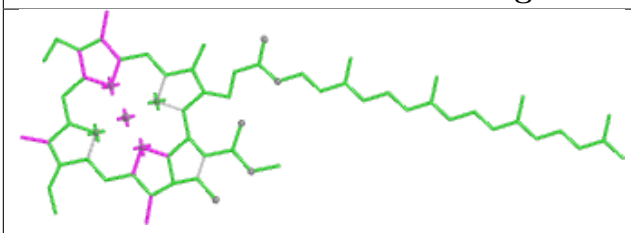


Rings

Ligand CLA A2 841



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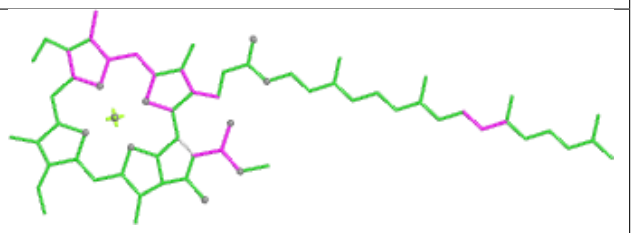
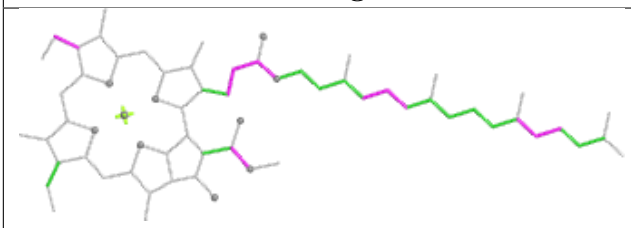


Bond angles



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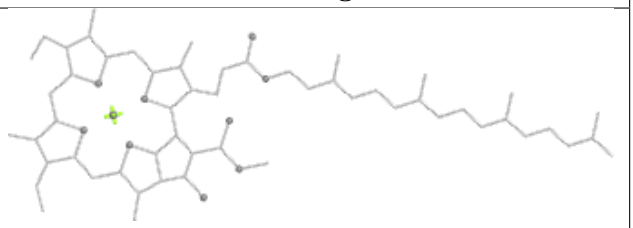
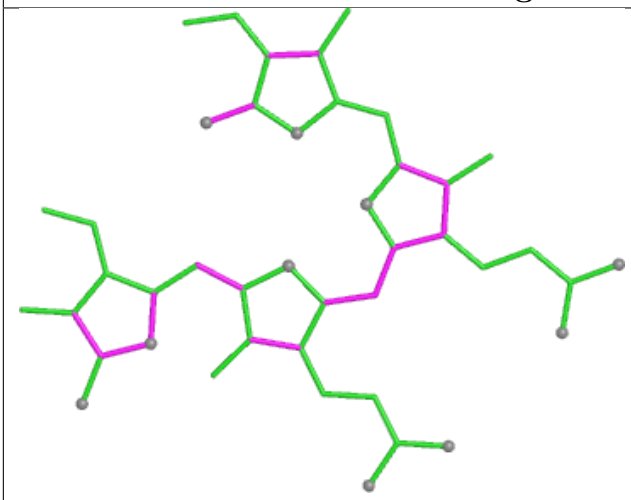
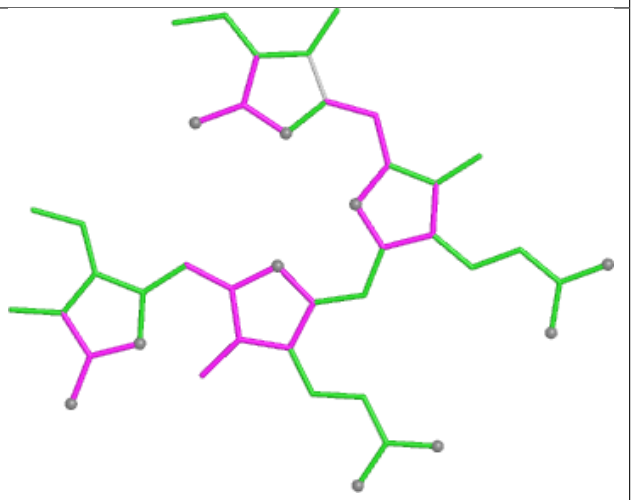


Rings

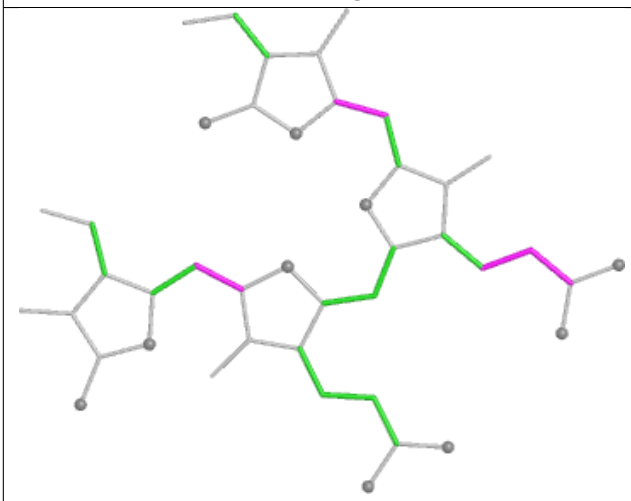
Ligand PEB fM 201



Bond lengths



Bond angles



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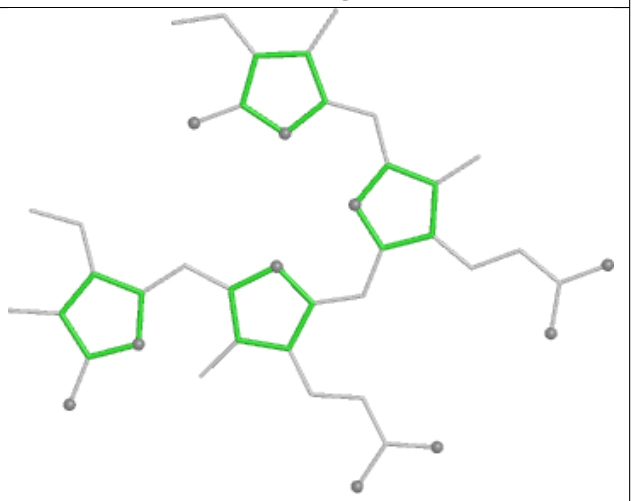
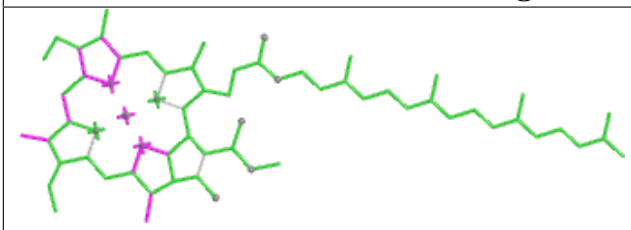


Rings

Ligand CLA B2 823



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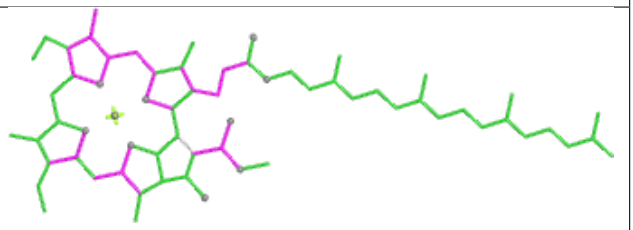

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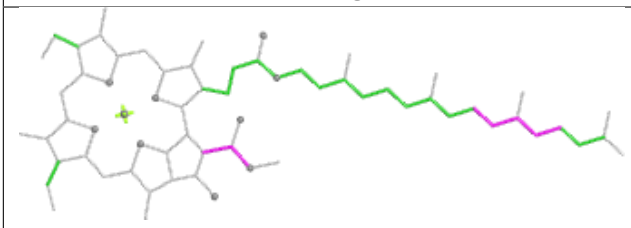

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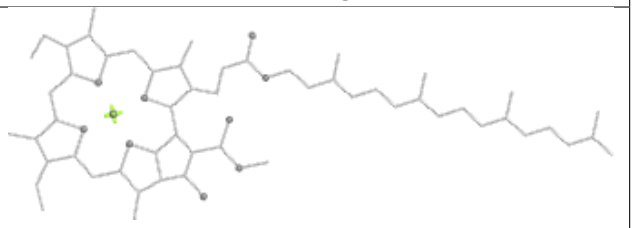
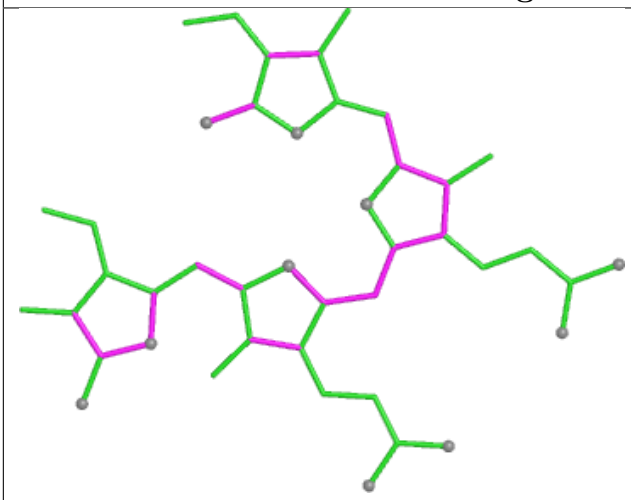


Rings

Ligand PEB T4 202



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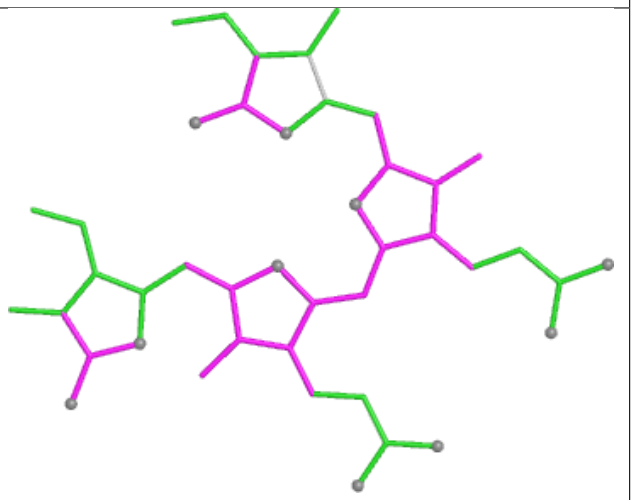

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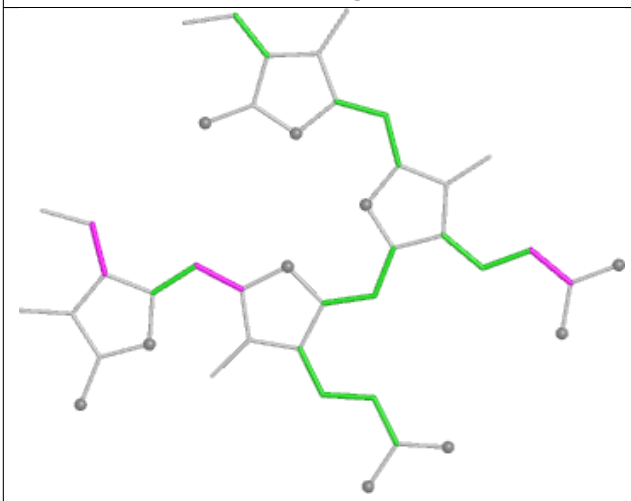

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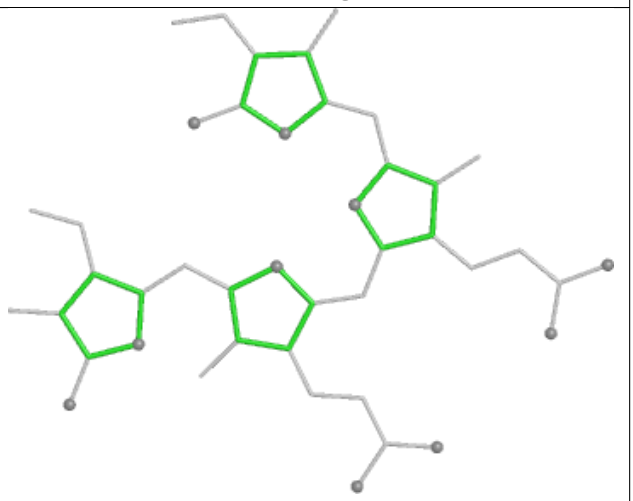
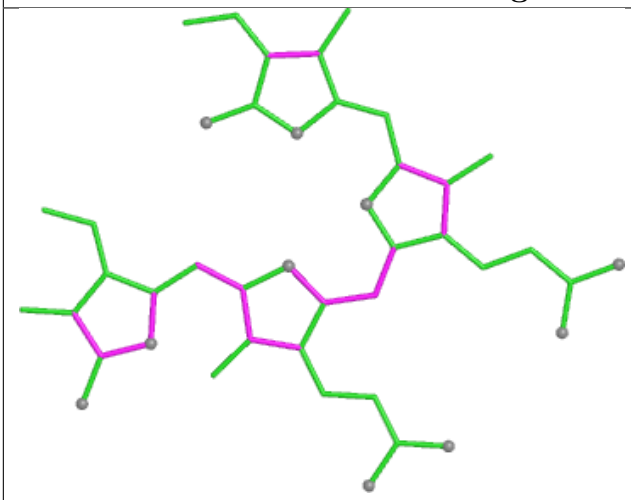


Rings

Ligand PEB QA 201



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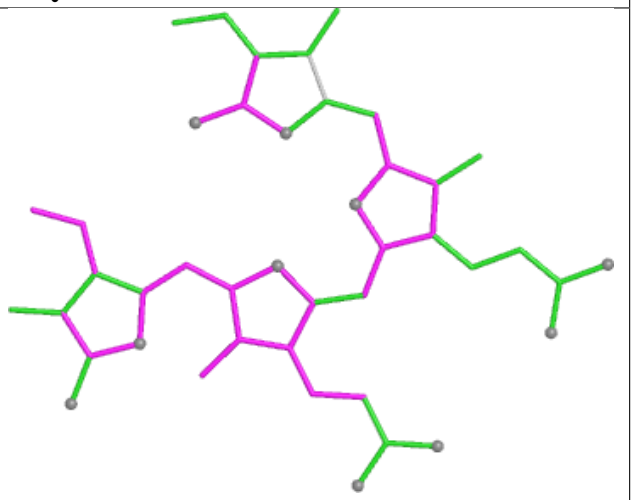
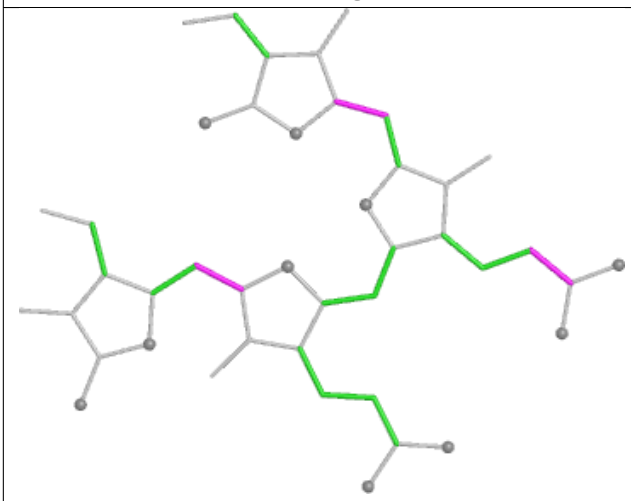


Bond angles



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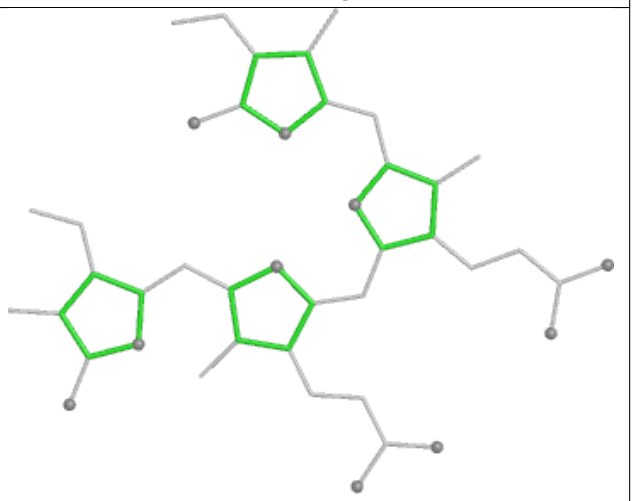
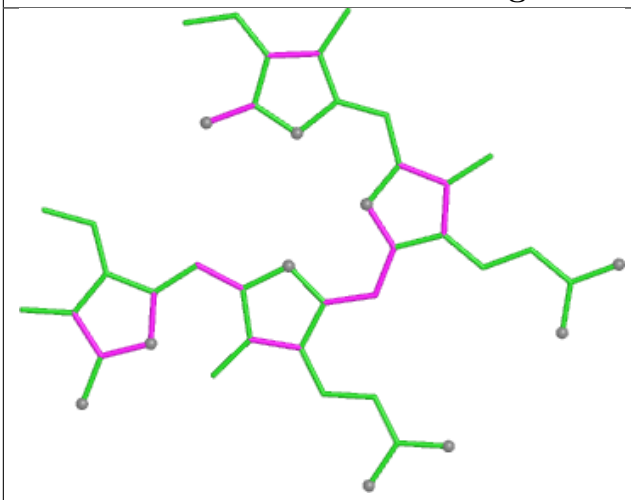


Rings

Ligand PEB F4 1002



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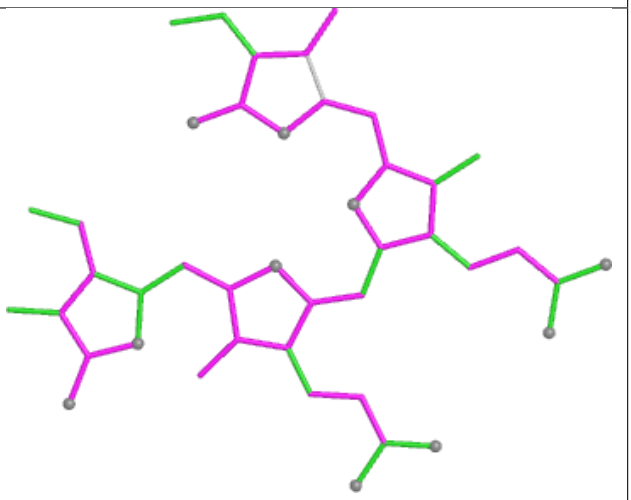

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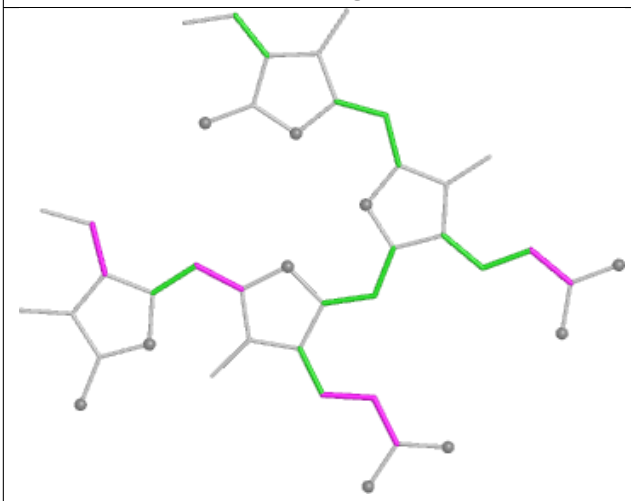

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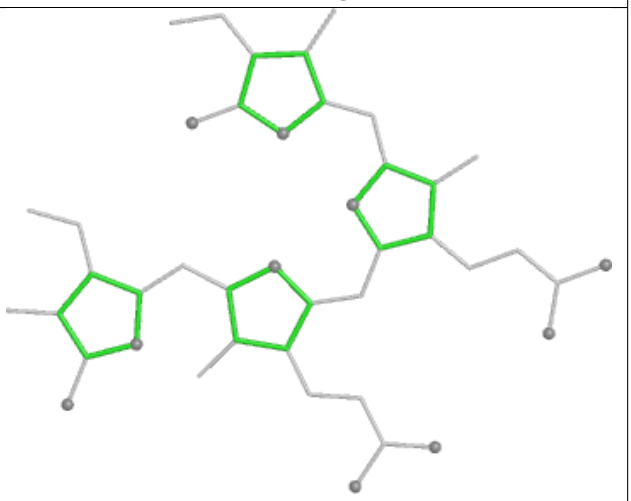
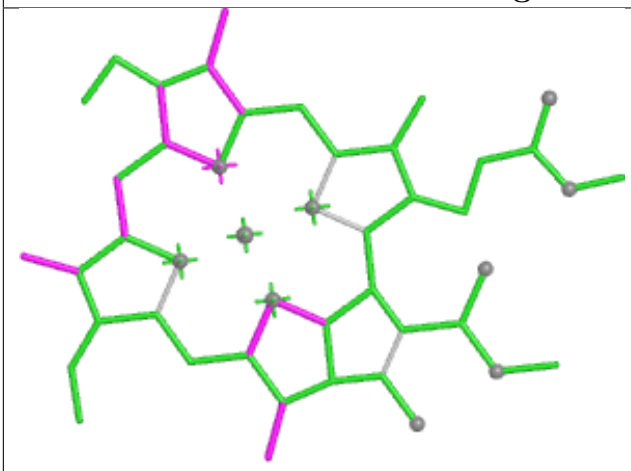


Rings

Ligand CLA CL 518



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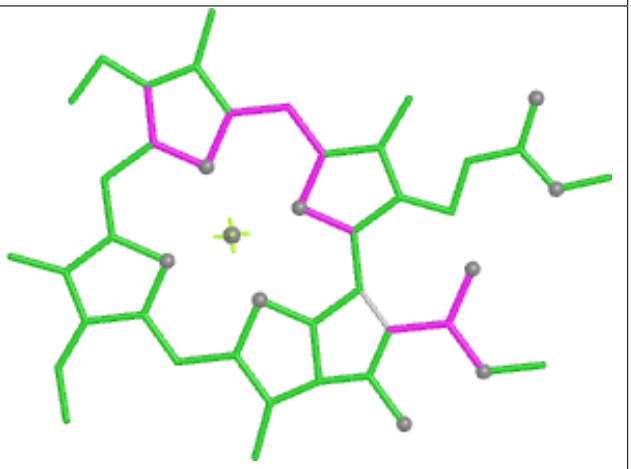

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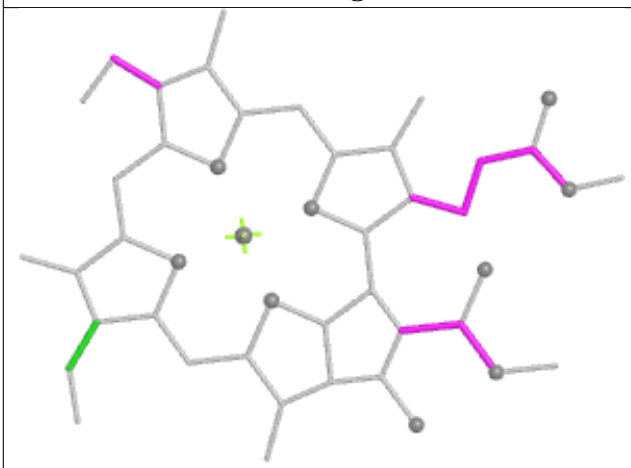

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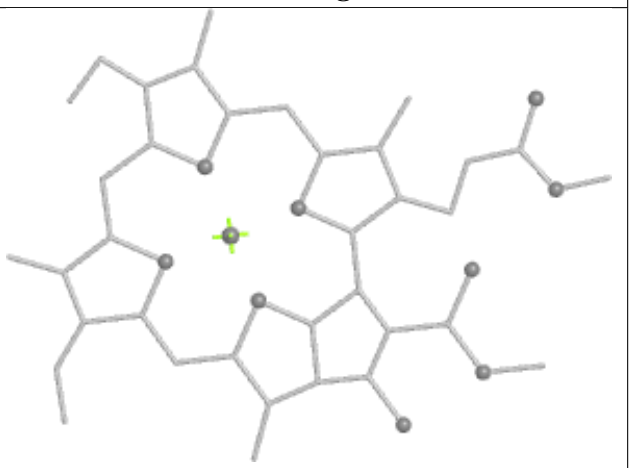
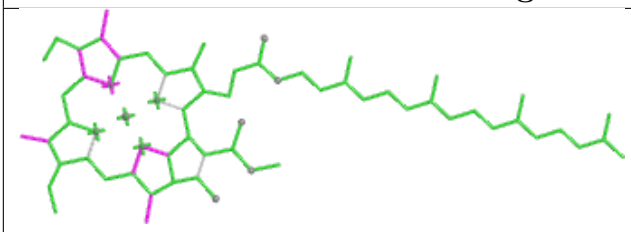


Rings

Ligand CLA IN 103



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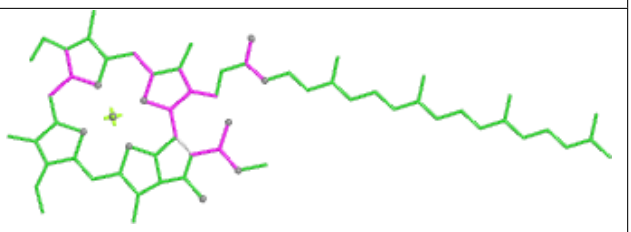
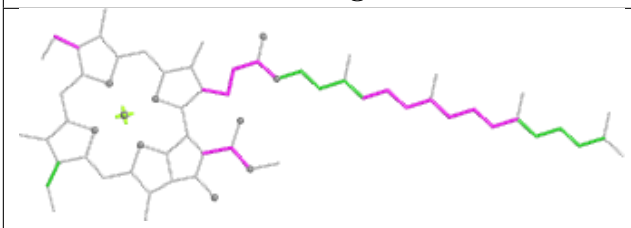


Bond angles



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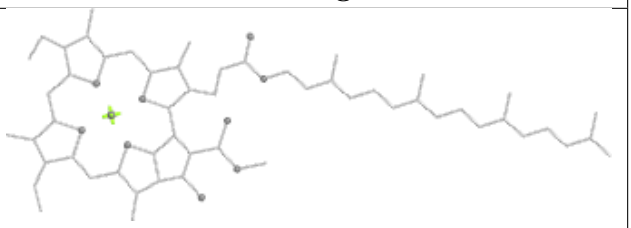
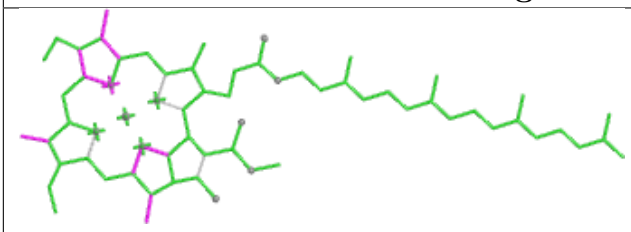


Rings

Ligand CLA B6 611



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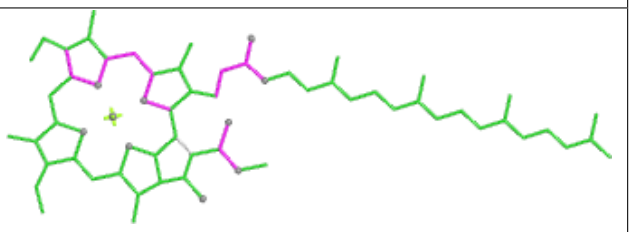

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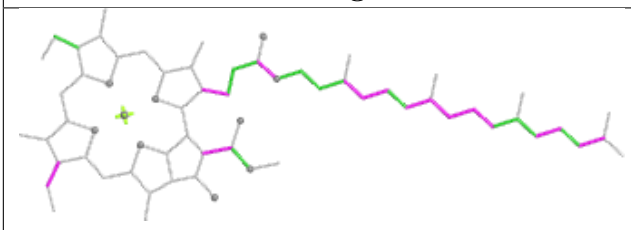

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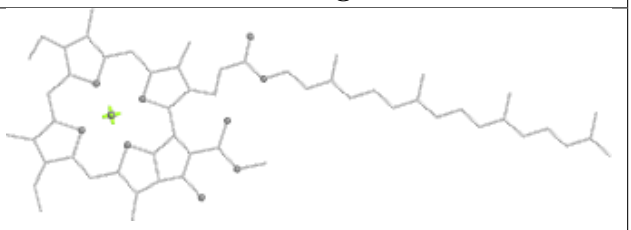
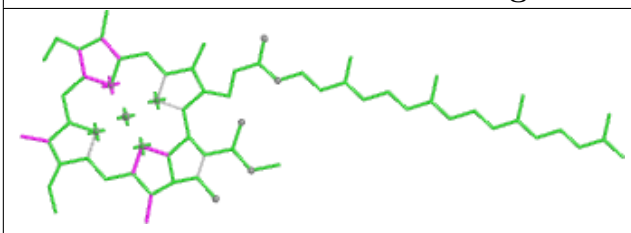


Rings

Ligand CLA AN 839



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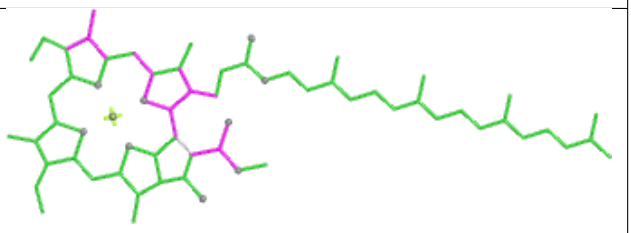

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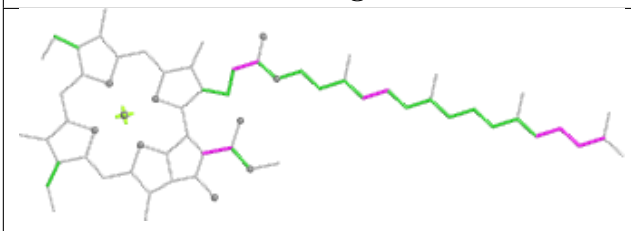

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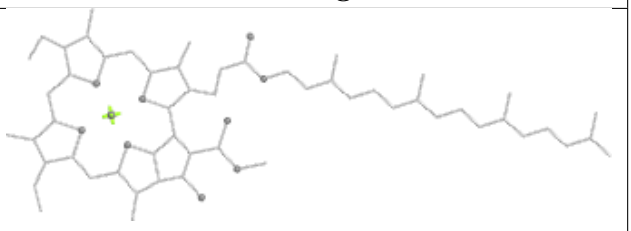
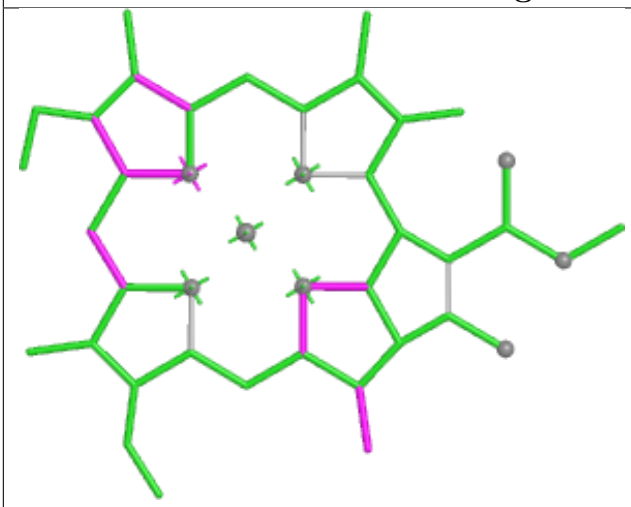


Rings

Ligand CLA O2 201



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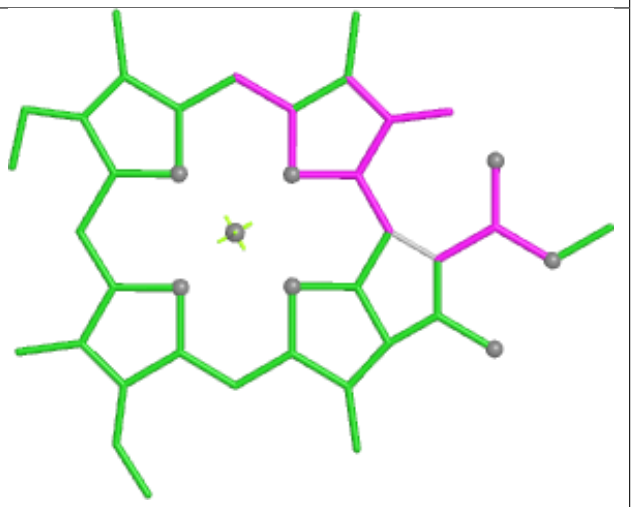
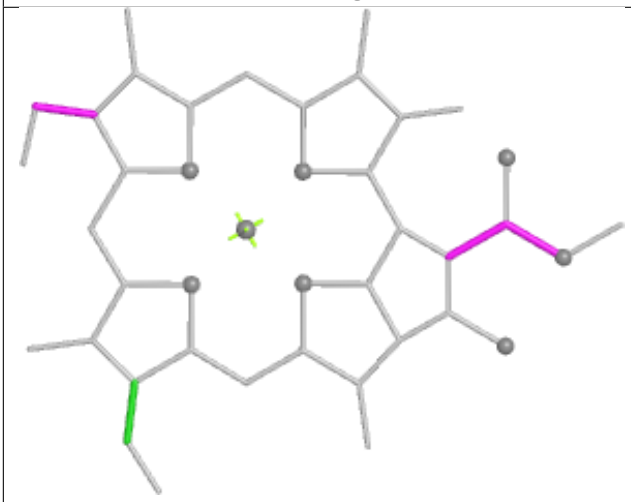


Bond angles



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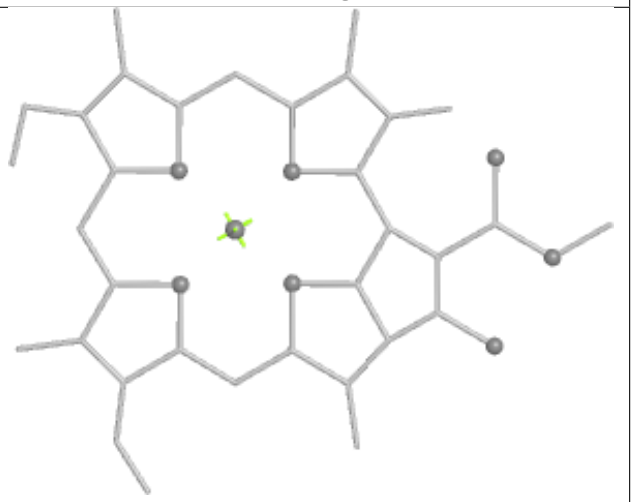
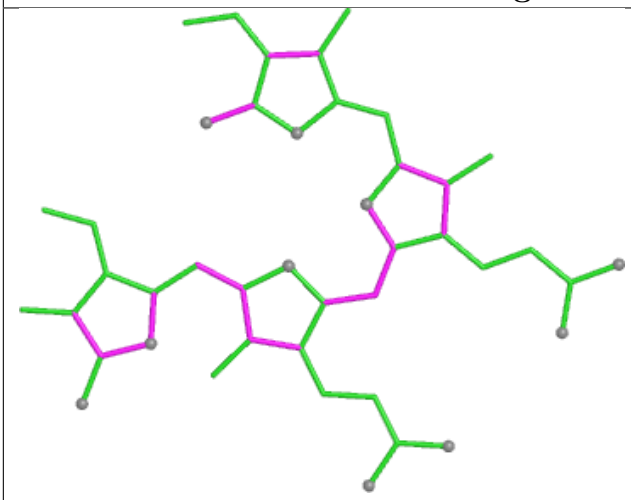


Rings

Ligand PEB m4 201



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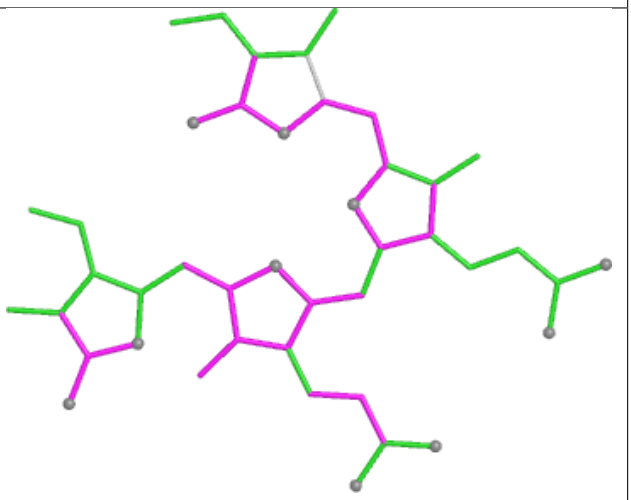

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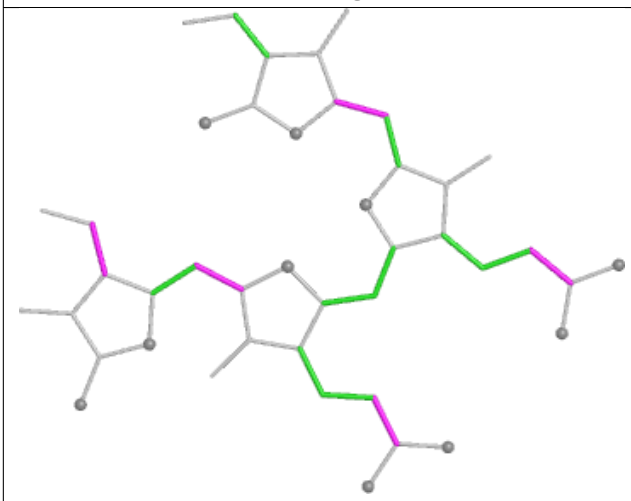

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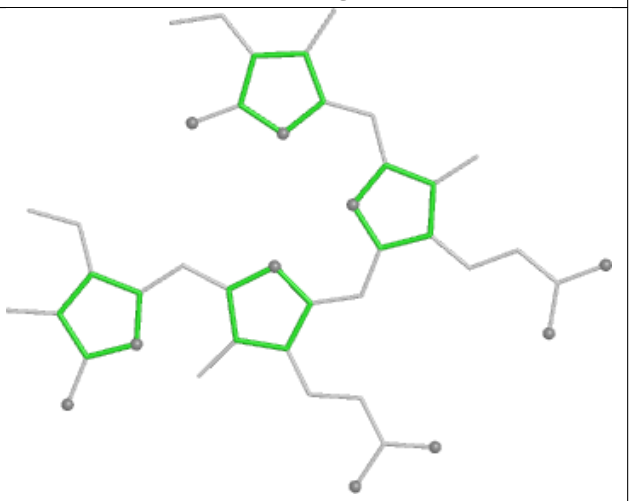
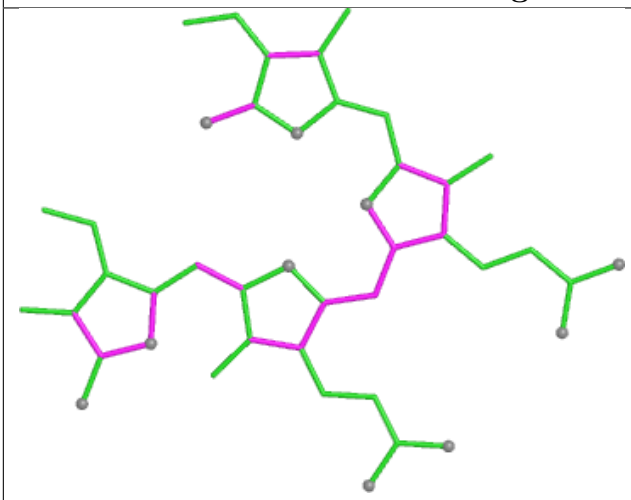


Rings

Ligand PEB mE 203



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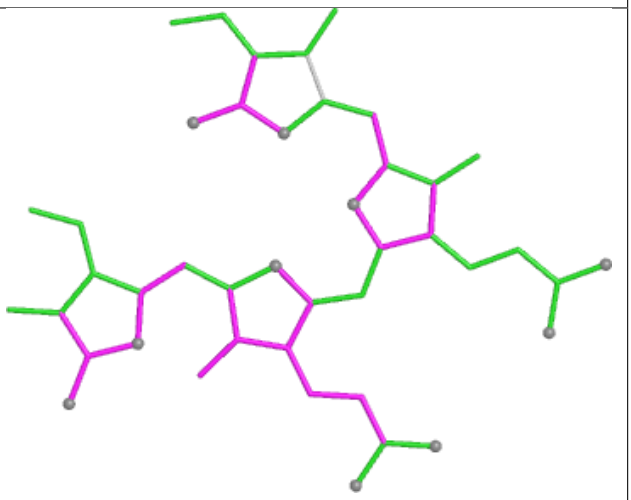

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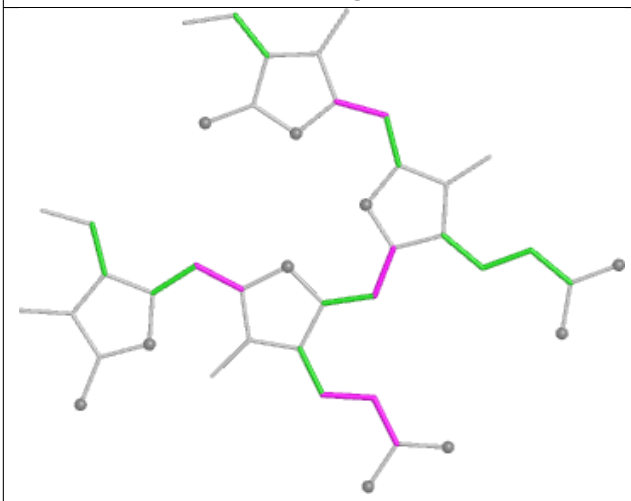

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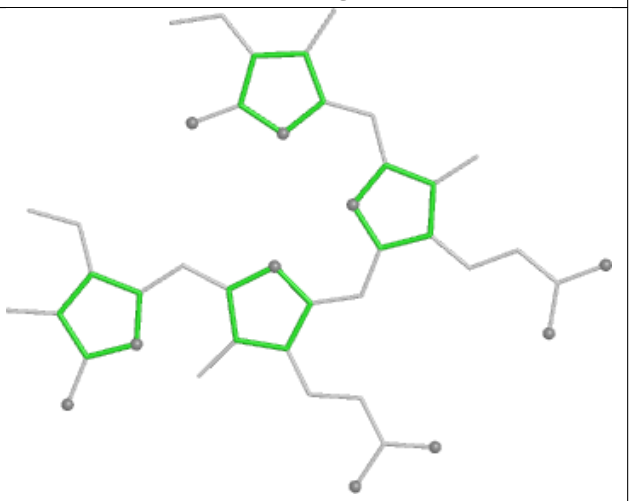
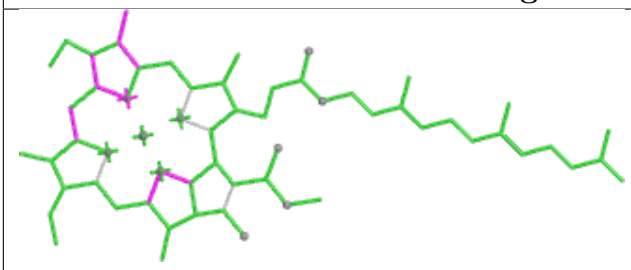


Rings

Ligand CLA c6 614



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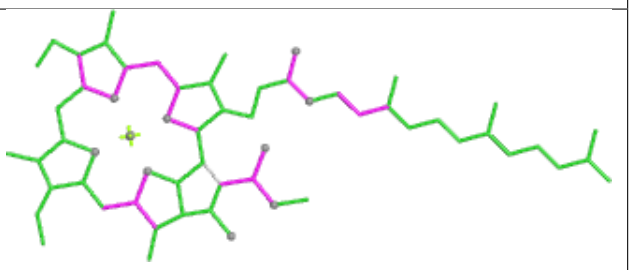
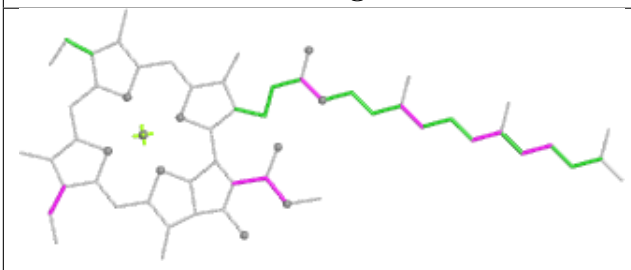


Bond angles



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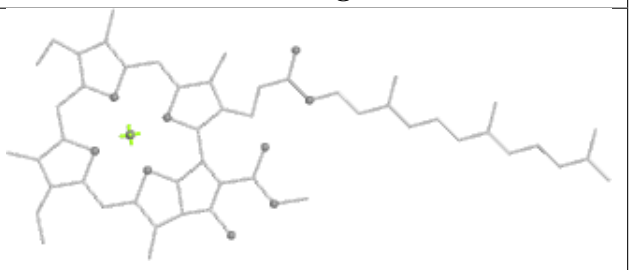
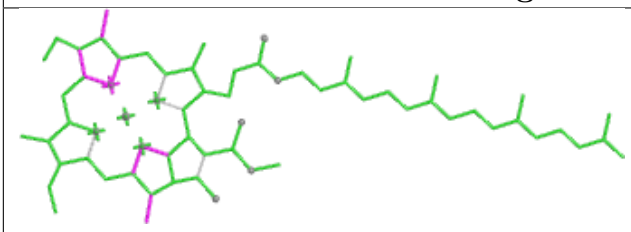


Rings

Ligand CLA bL 614



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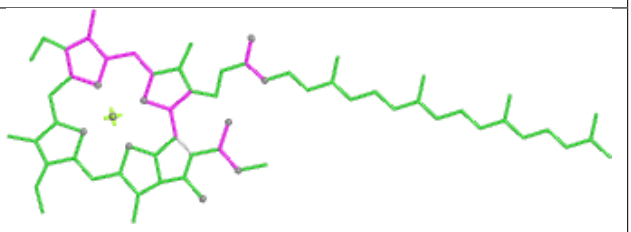
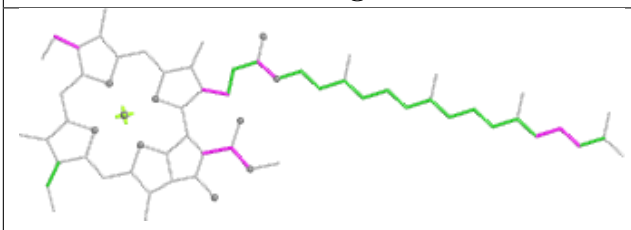


Bond angles



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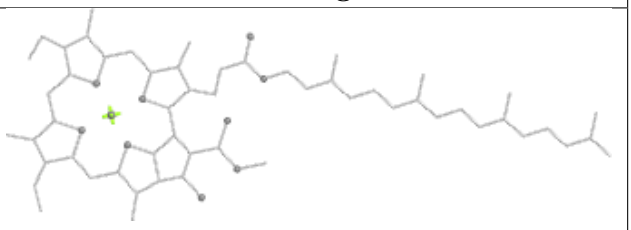
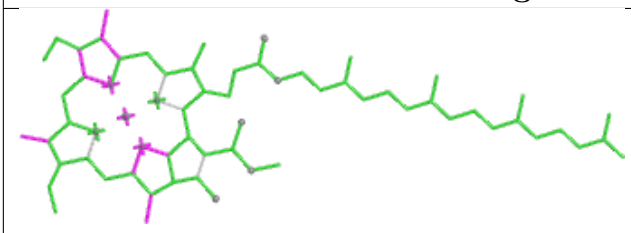


Rings

Ligand CLA CL 509



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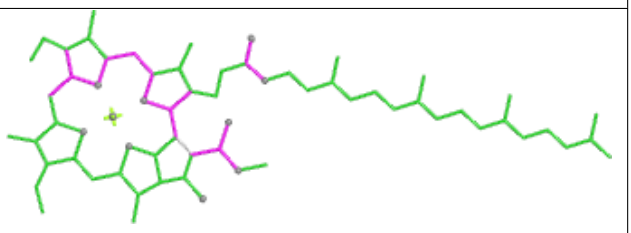
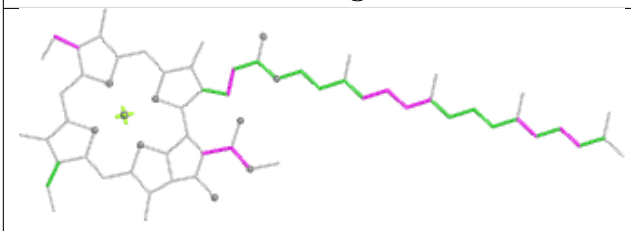


Bond angles



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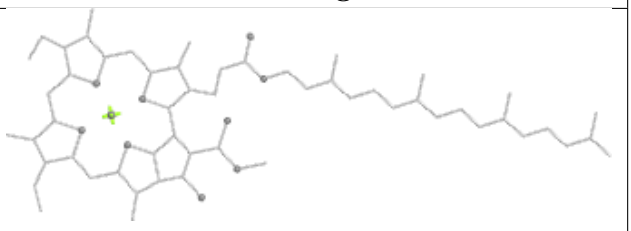
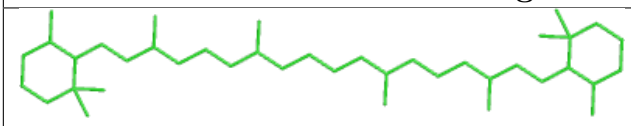


Rings

Ligand BCR aL 604



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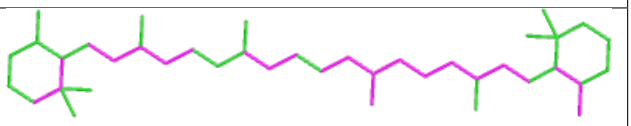
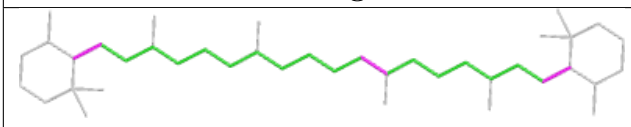
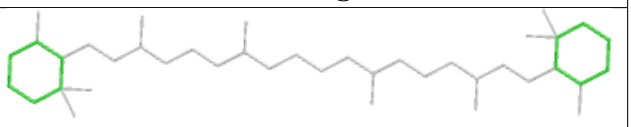


Bond angles

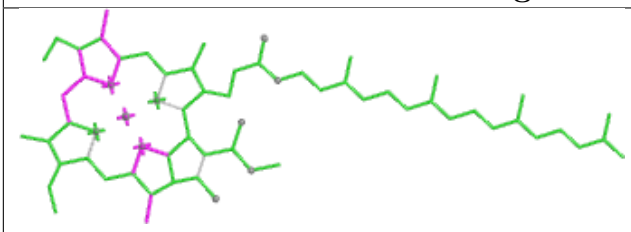


Torsions



Rings

Ligand CLA BL 620



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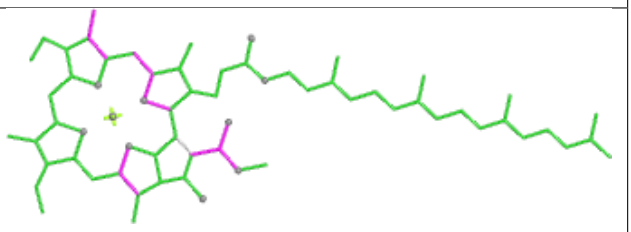

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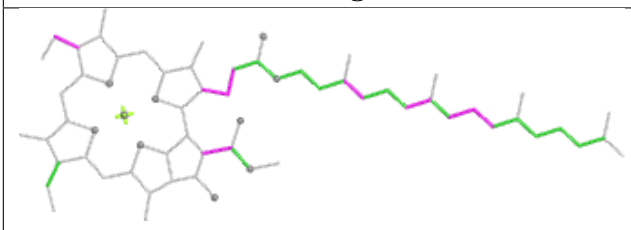

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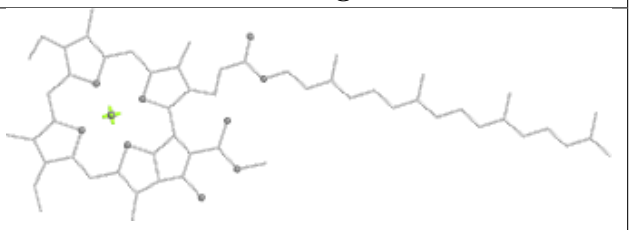
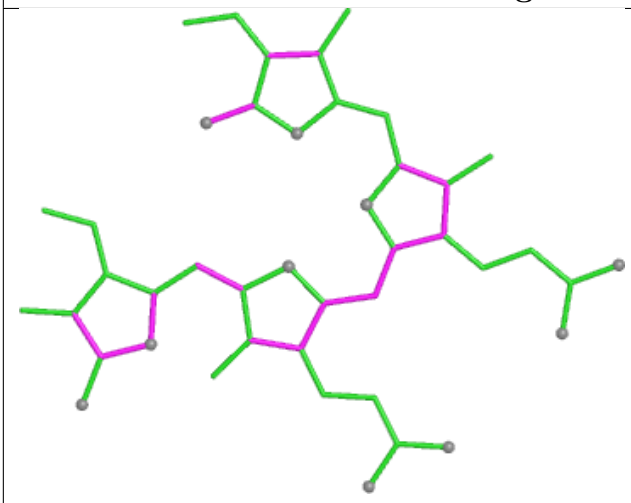


Rings

Ligand PEB jM 203



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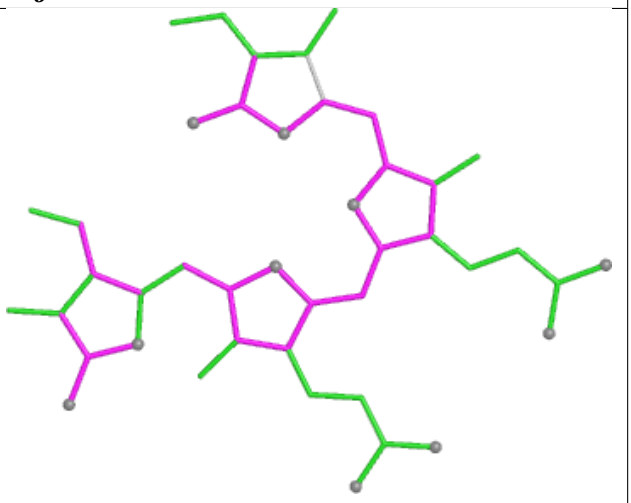

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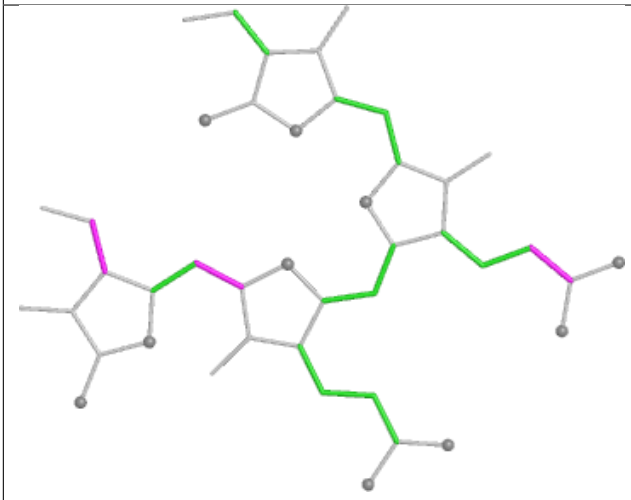

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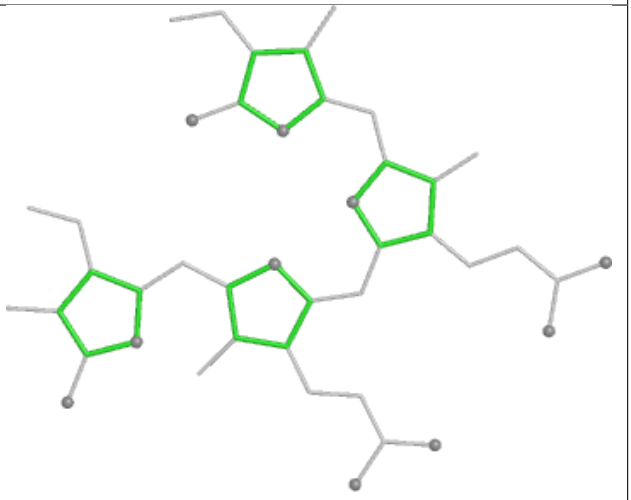
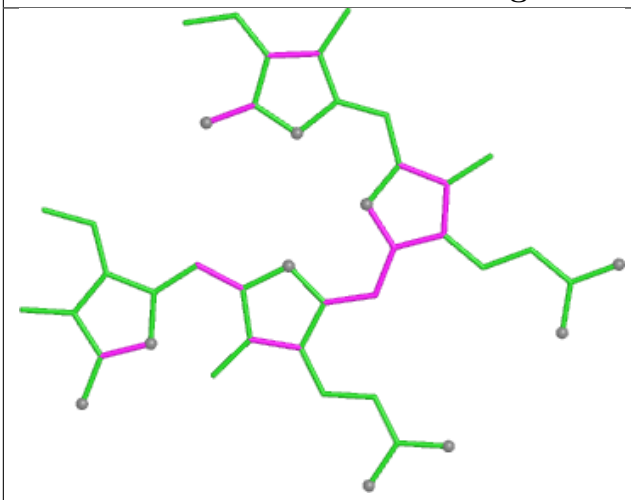


Rings

Ligand PEB AH 301



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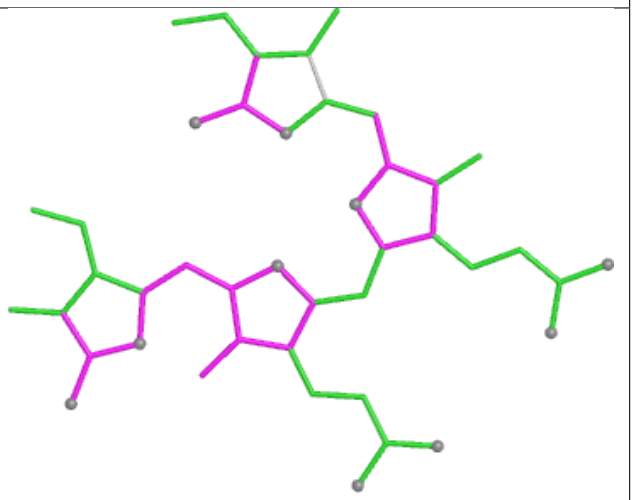

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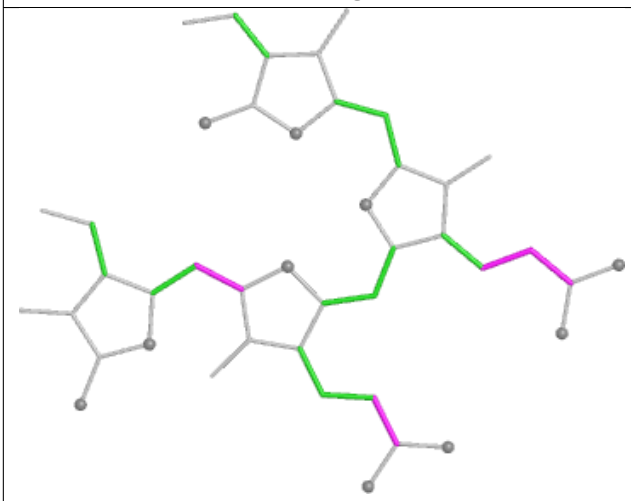

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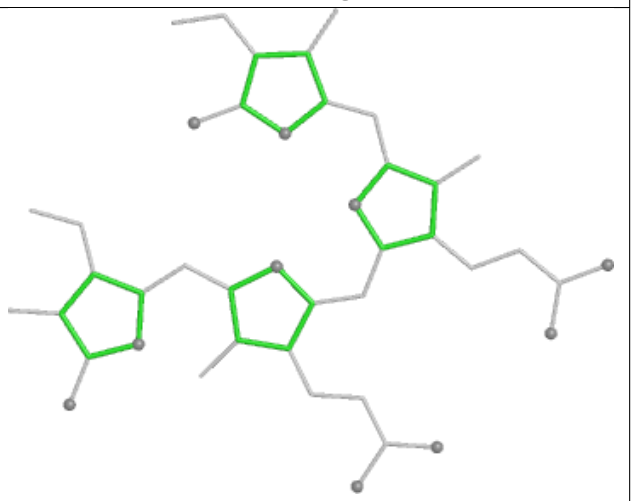
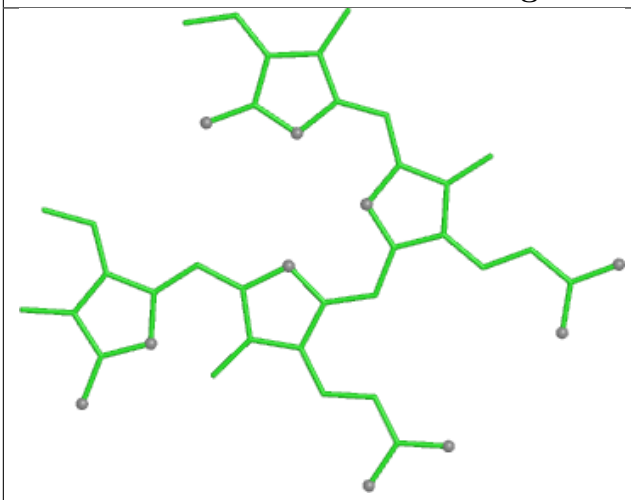


Rings

Ligand PEB e7 301



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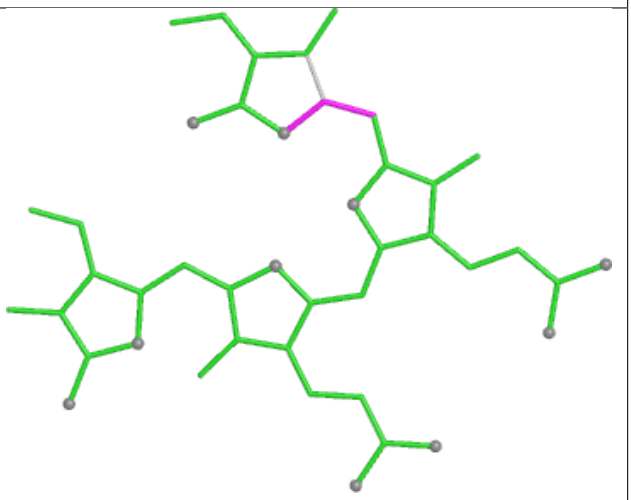
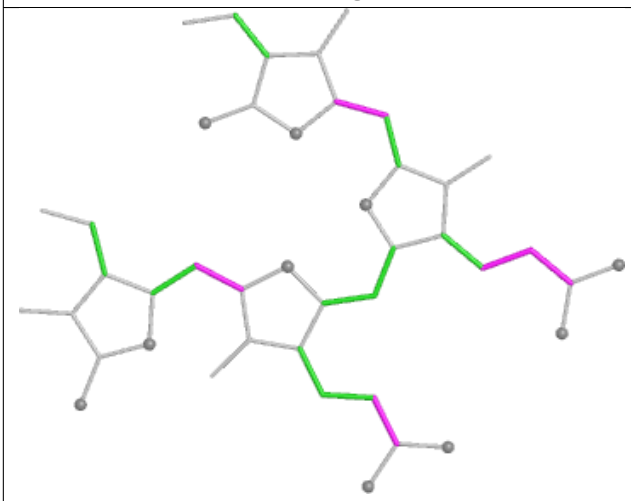


Bond angles



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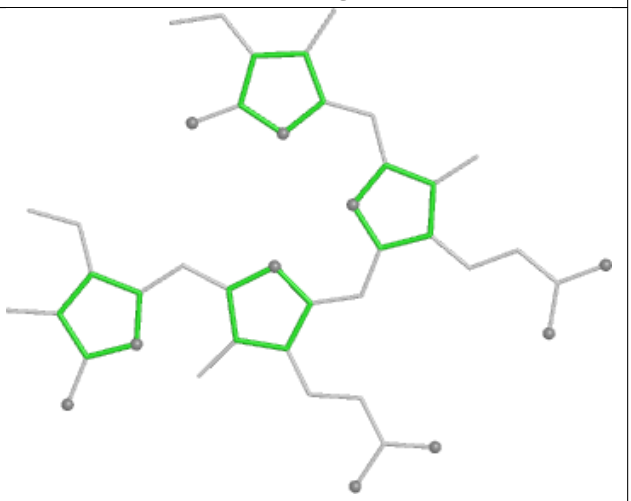
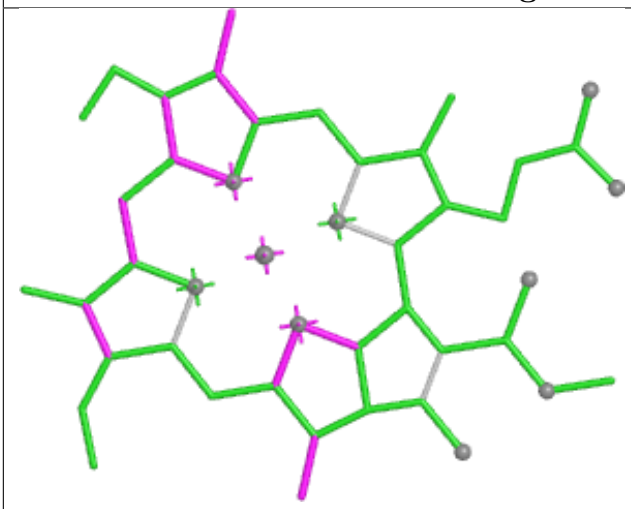


Rings

Ligand CLA 82 308



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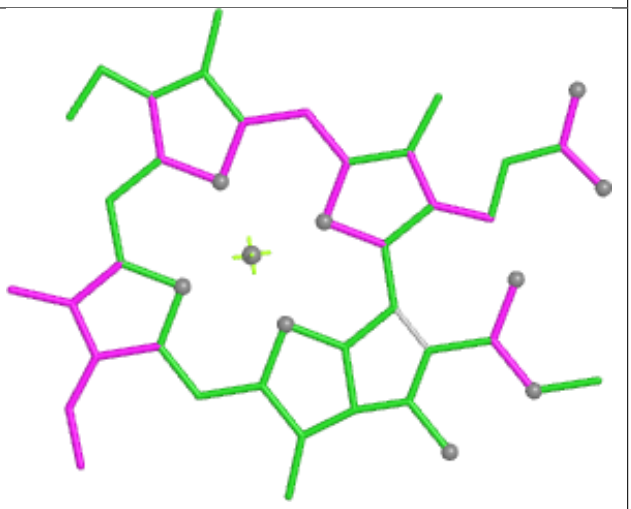

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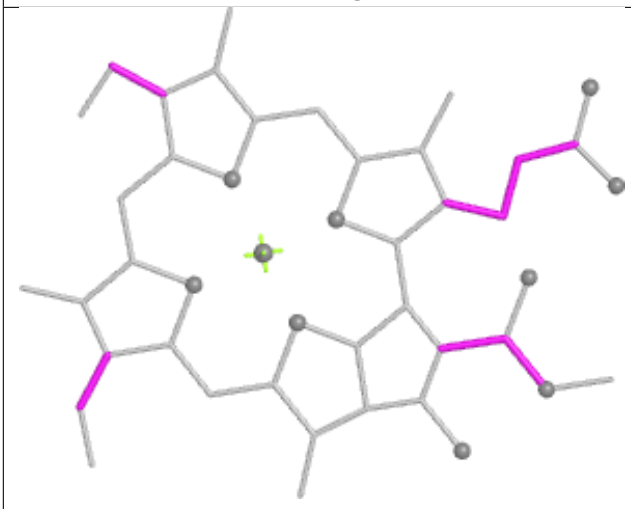
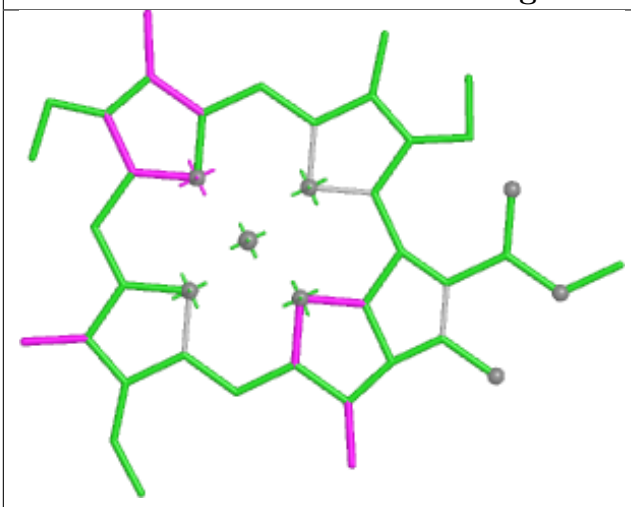


Torsions



Rings

Ligand CLA 12 609



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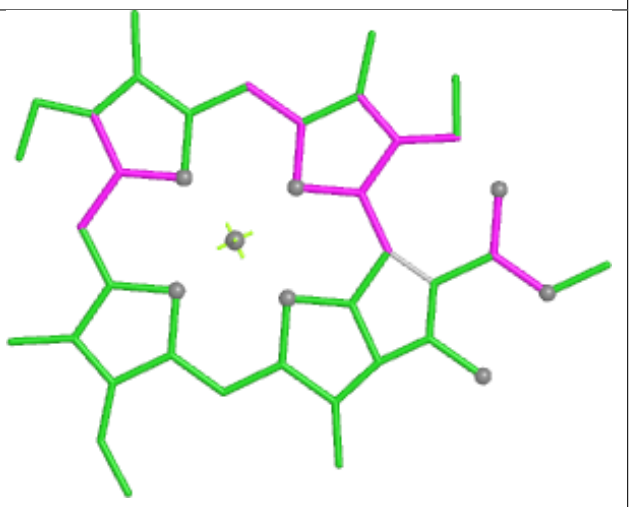

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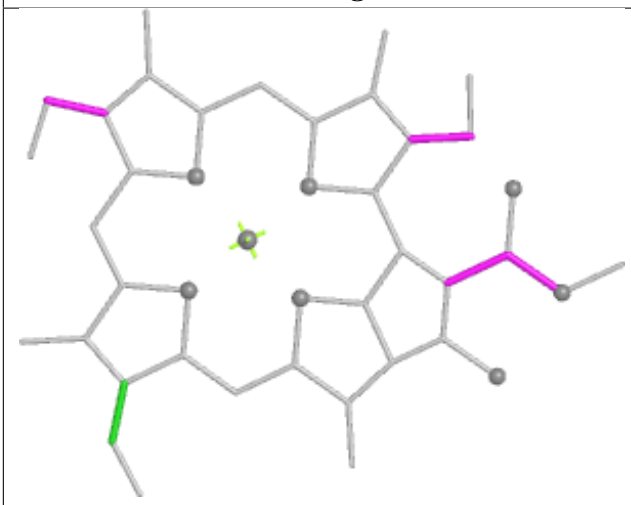
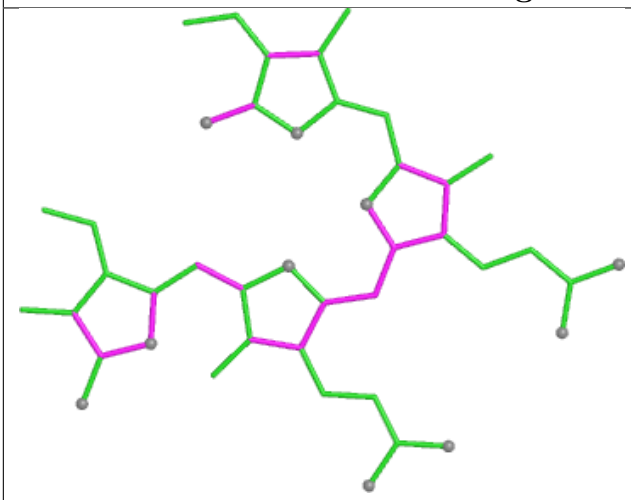


Torsions



Rings

Ligand PEB X7 203



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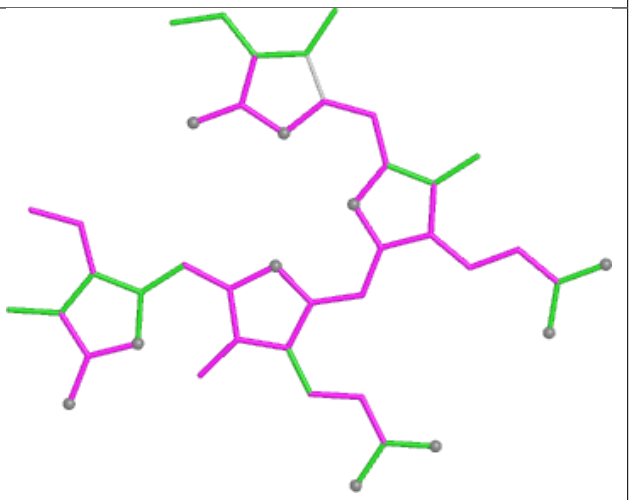

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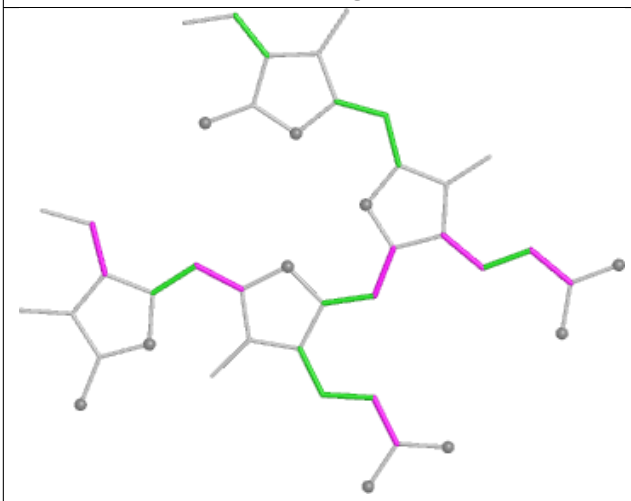

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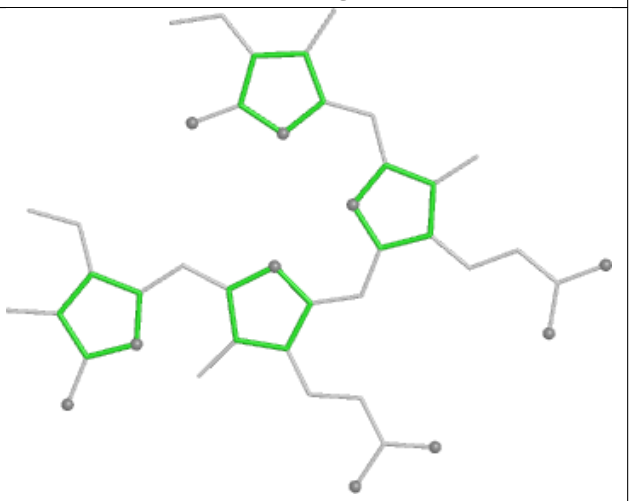
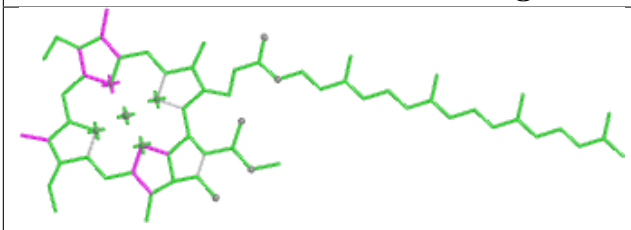


Rings

Ligand CLA A2 801



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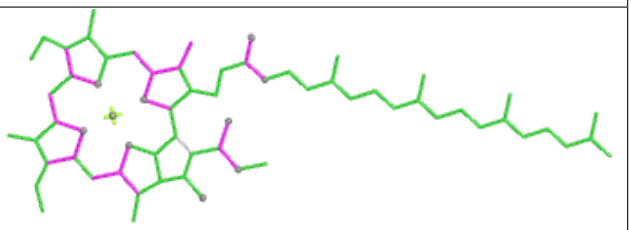

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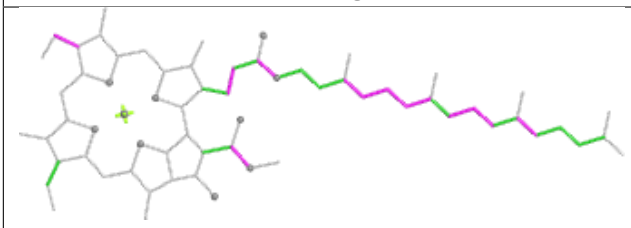

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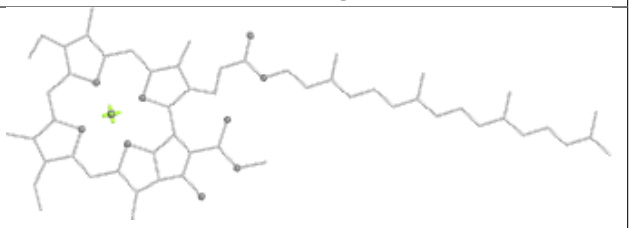
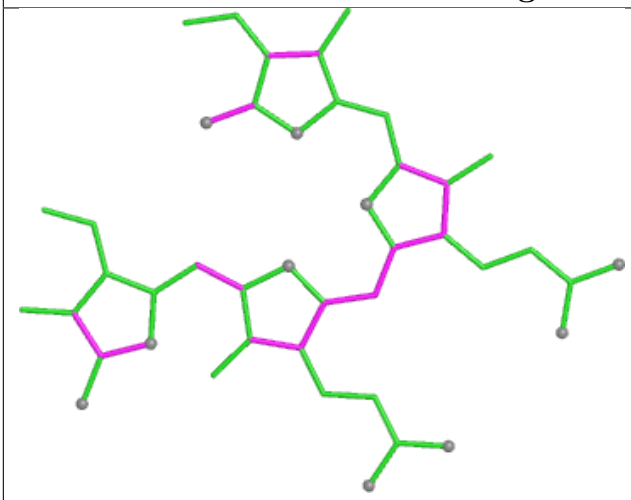


Rings

Ligand PEB L9 203



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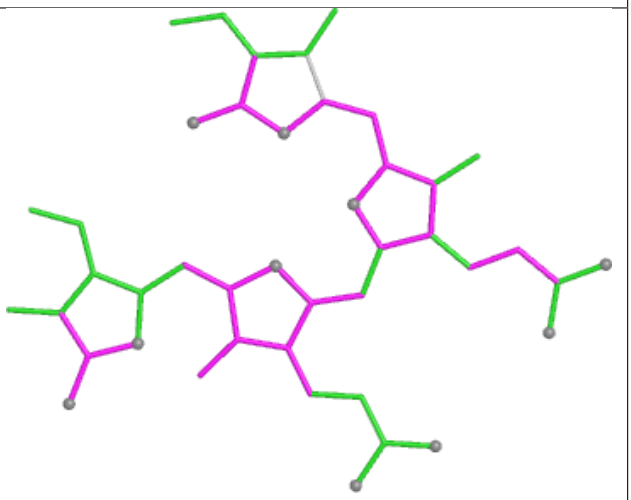

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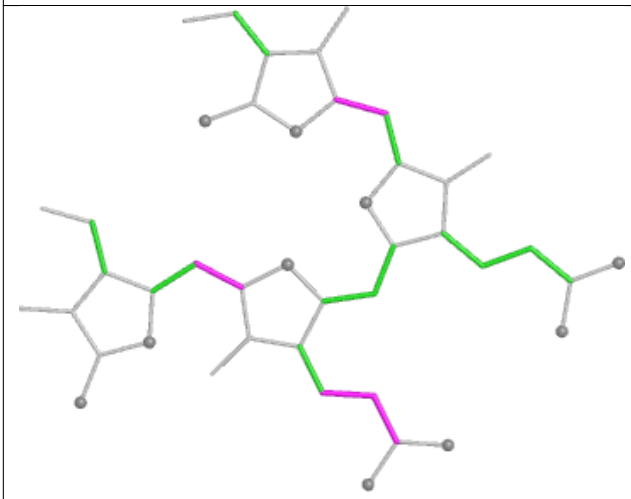

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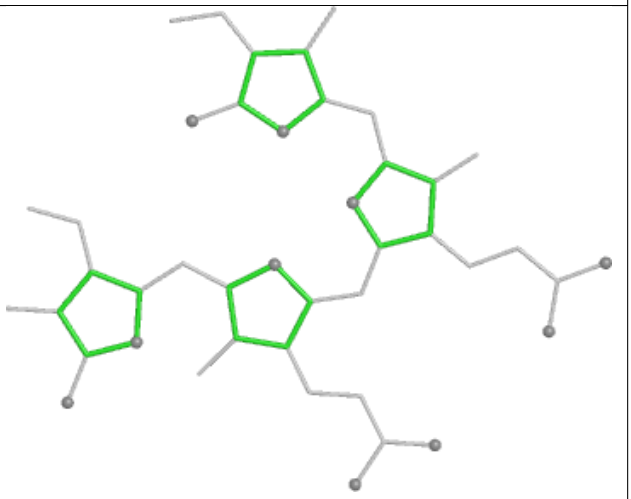
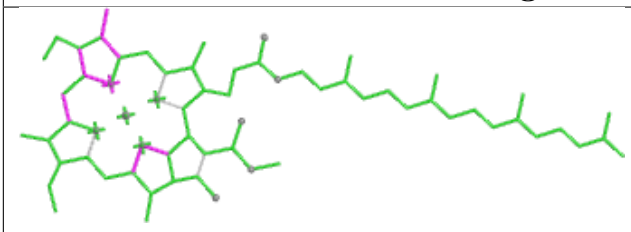


Rings

Ligand CLA 62 303



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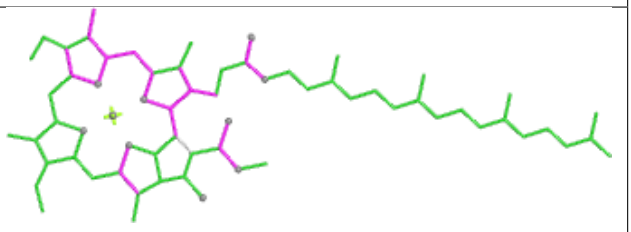

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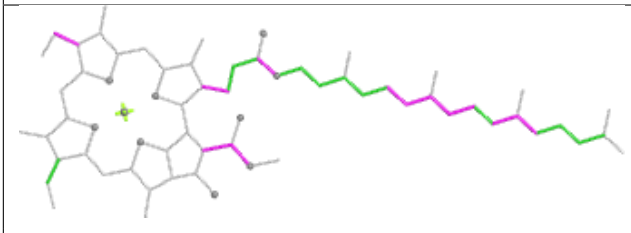

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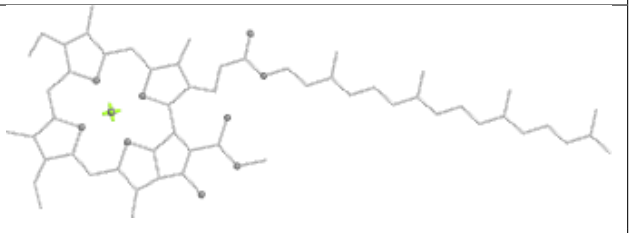
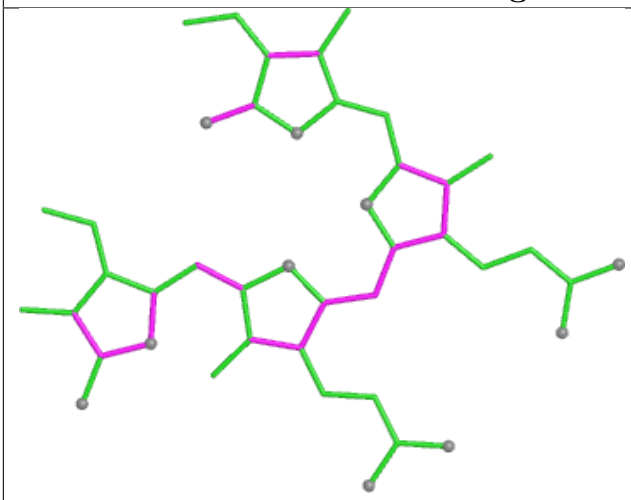


Rings

Ligand PEB MF 202



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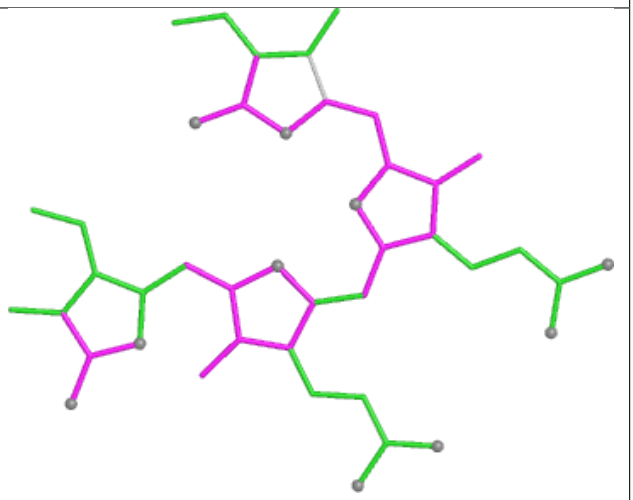

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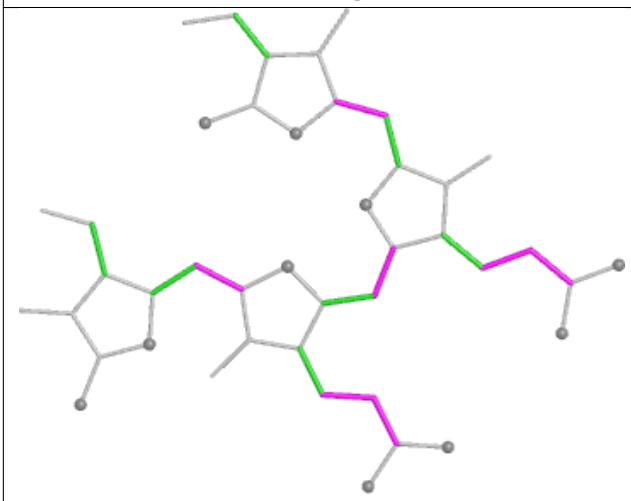

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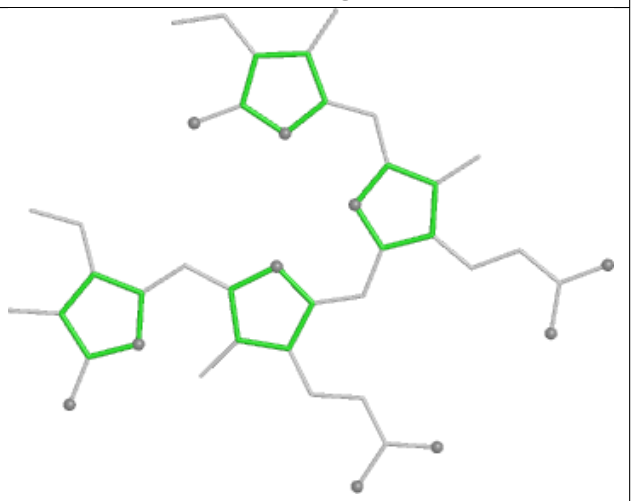
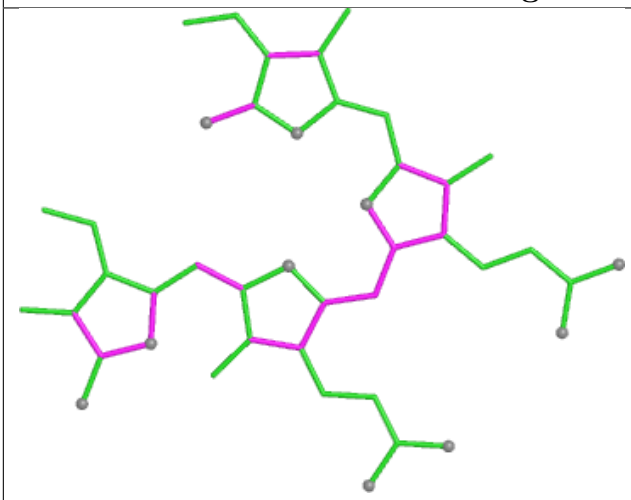


Rings

Ligand PEB IJ 203



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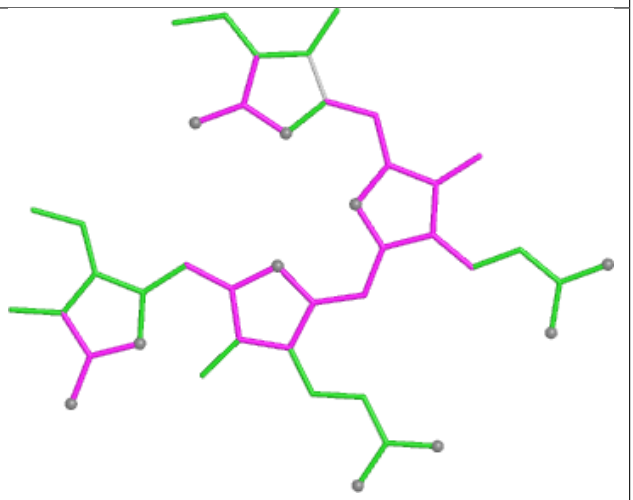

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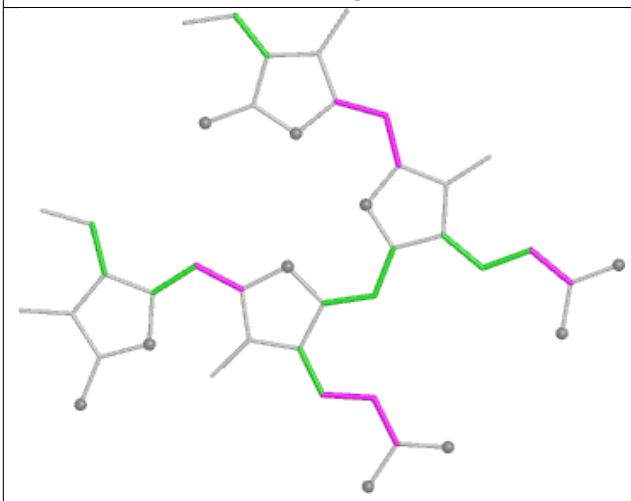

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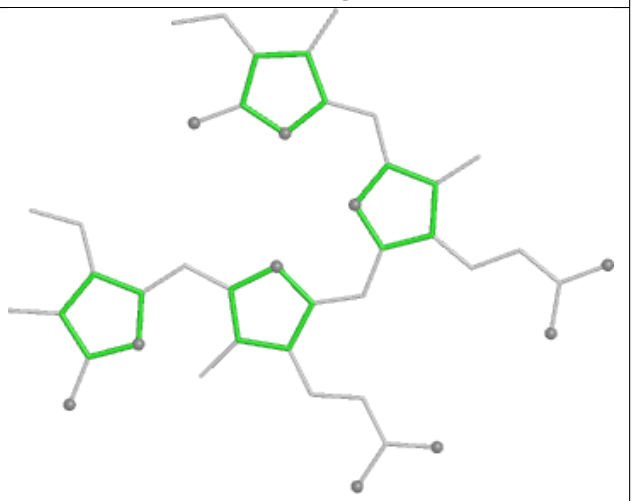
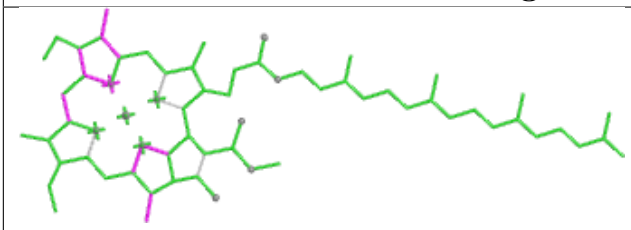


Rings

Ligand CLA c6 604



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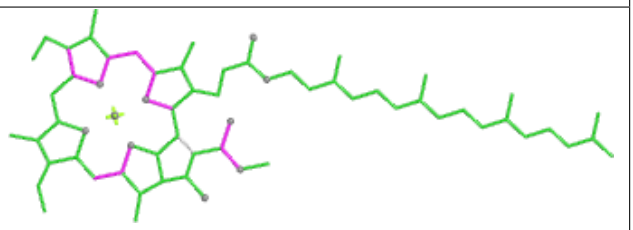
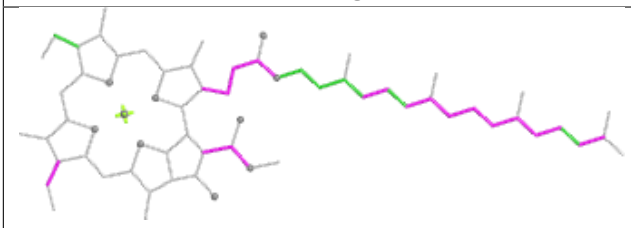


Bond angles



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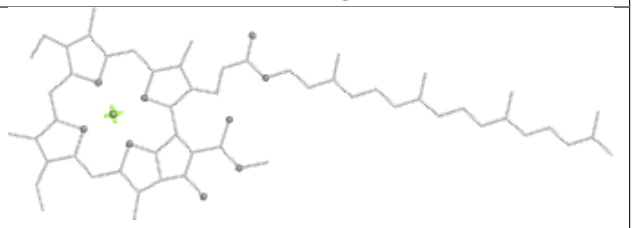
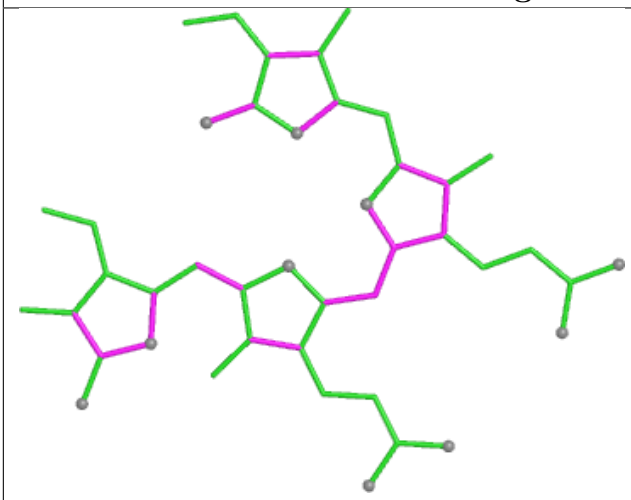


Rings

Ligand PEB dO 202



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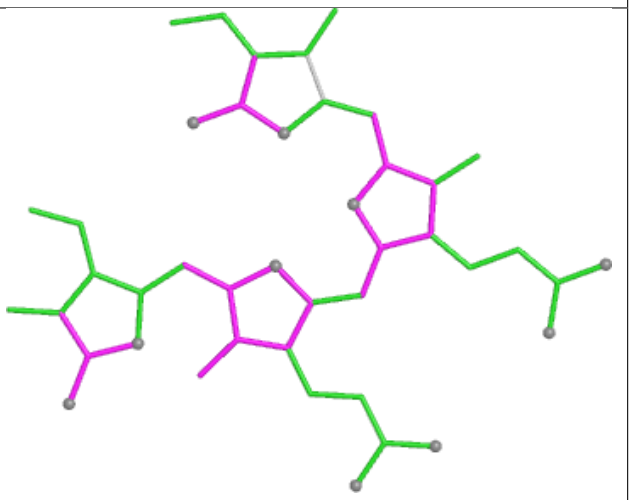

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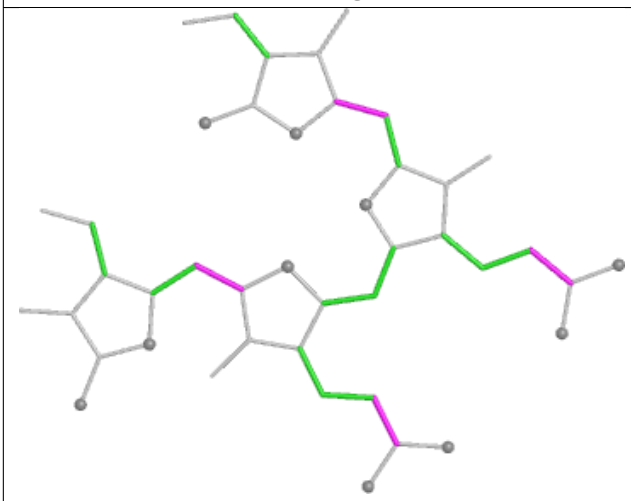

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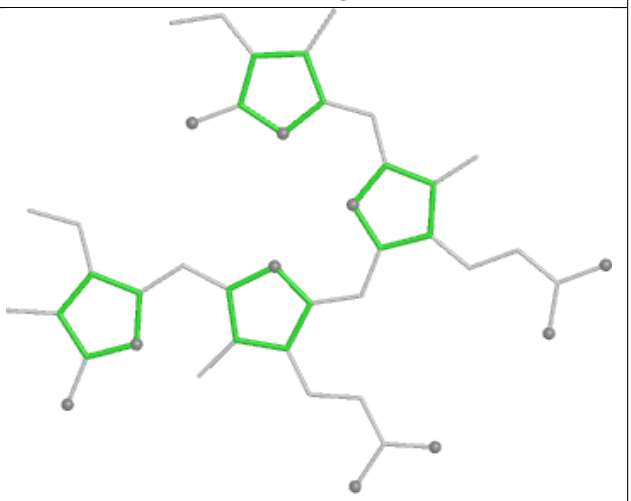
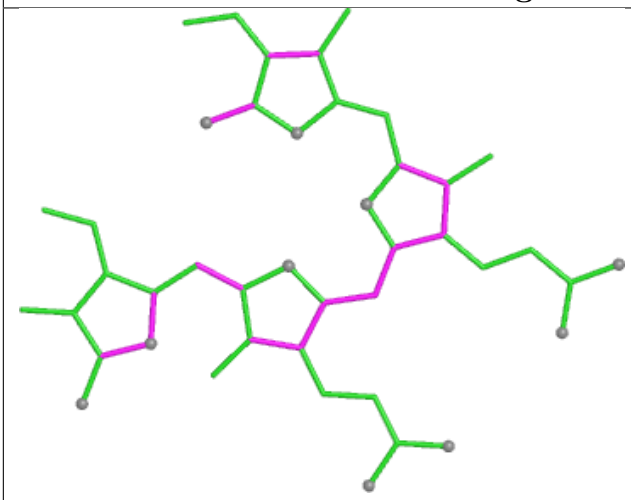


Rings

Ligand PEB fM 203



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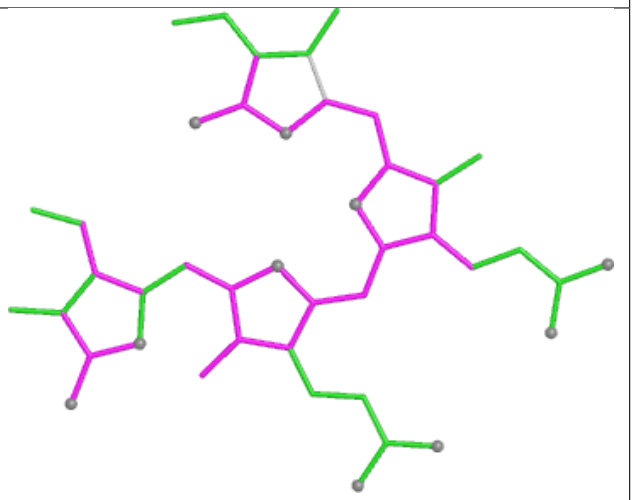

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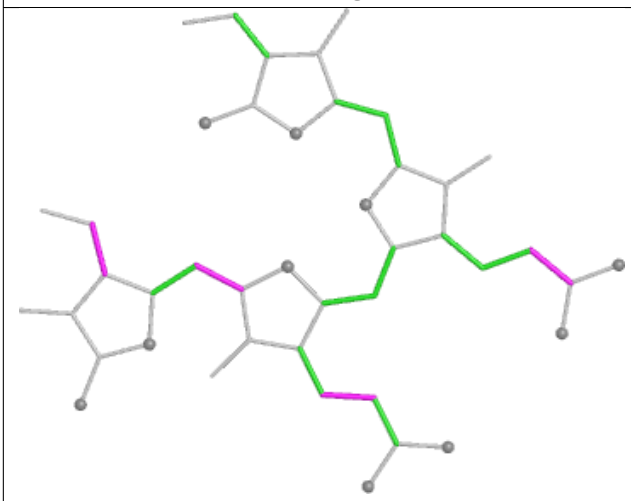
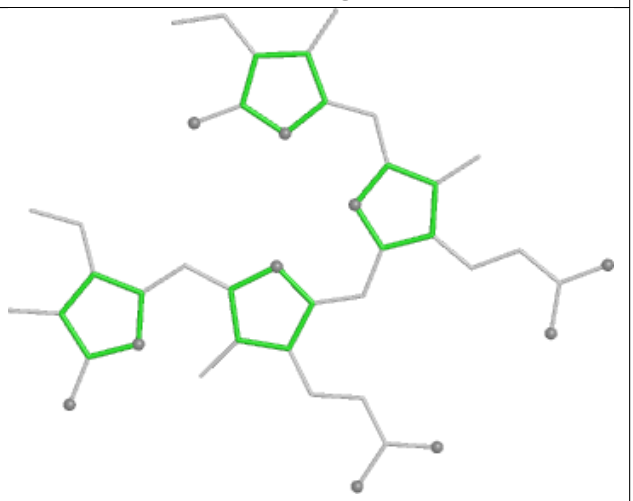
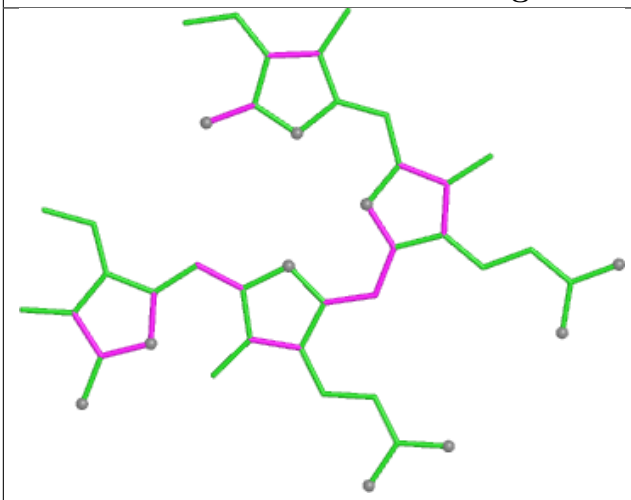


Torsions



Rings

Ligand PEB RB 201



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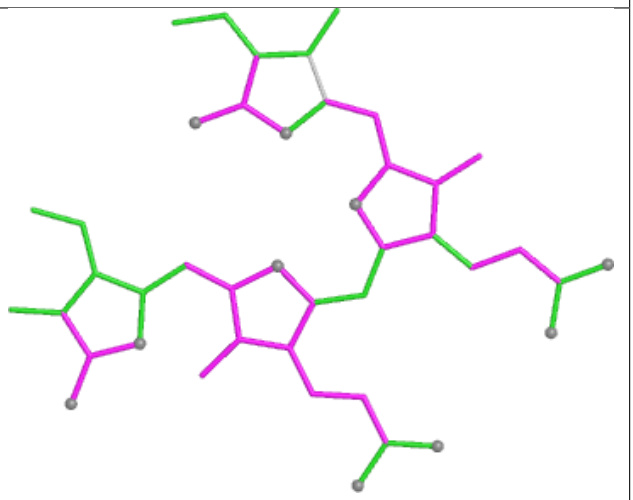

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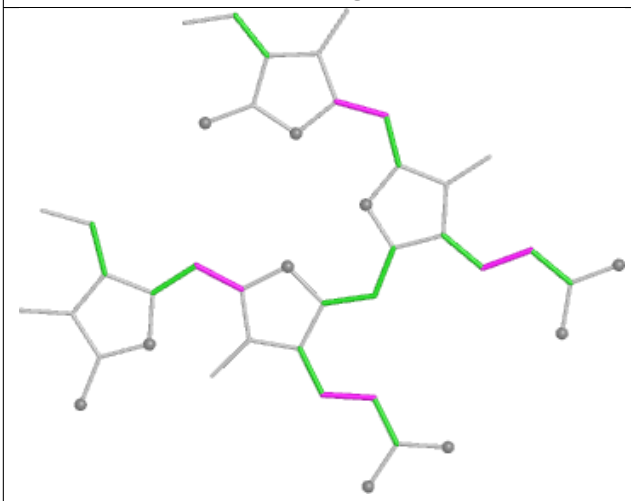

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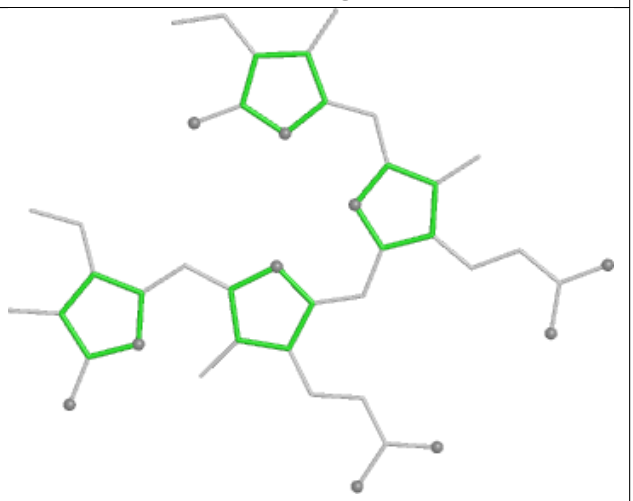
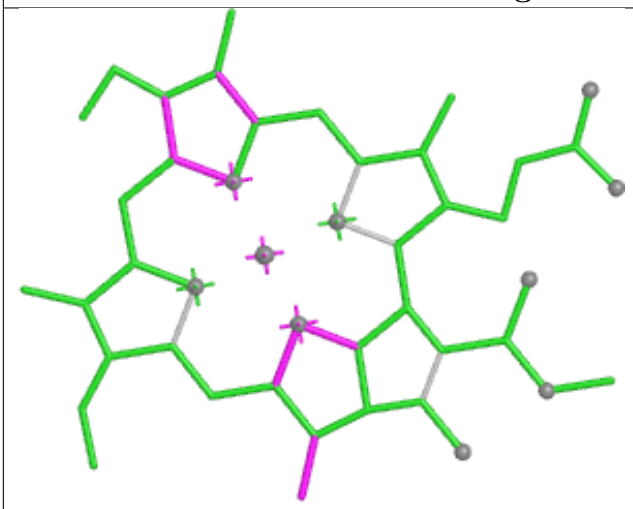


Rings

Ligand CLA 2N 307



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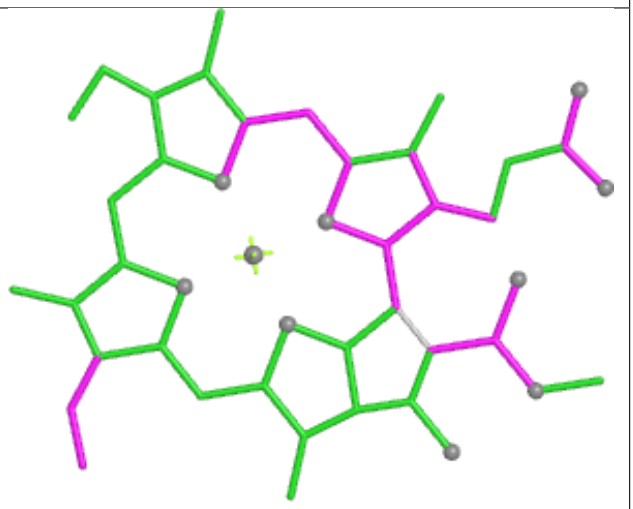

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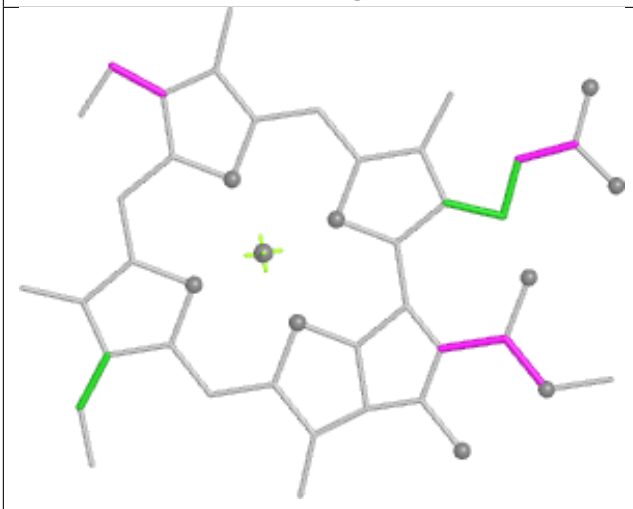
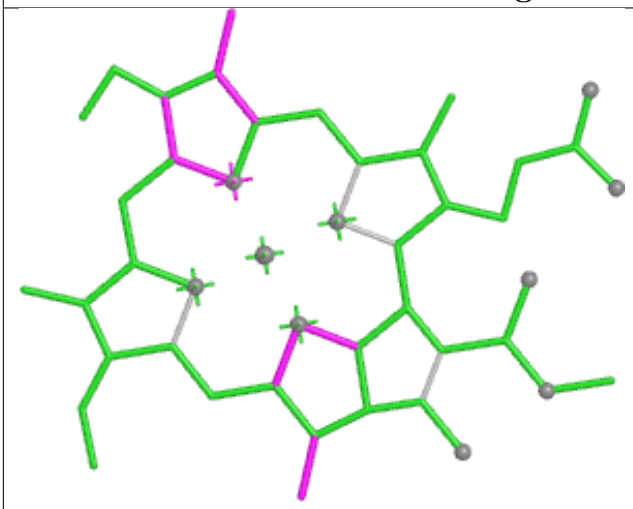


Torsions



Rings

Ligand CLA R2 202



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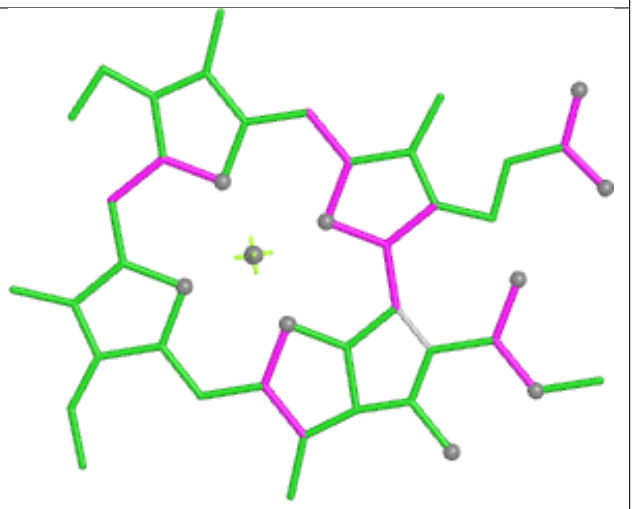

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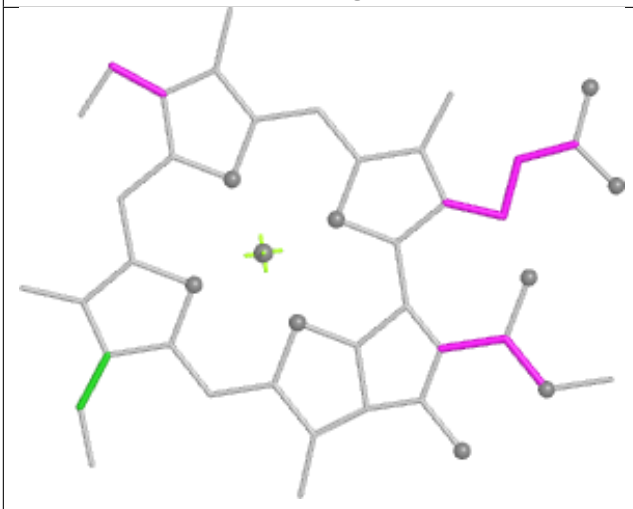
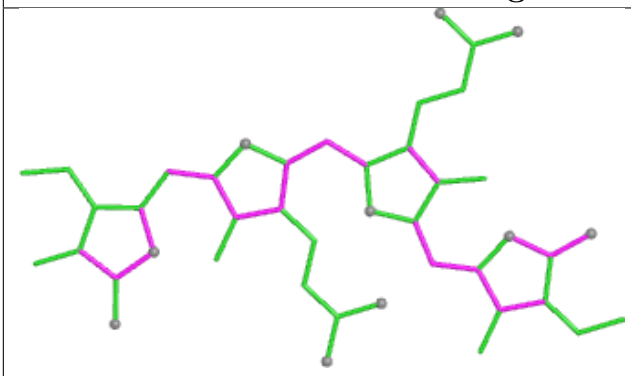


Torsions



Rings

Ligand CYC v3 1001



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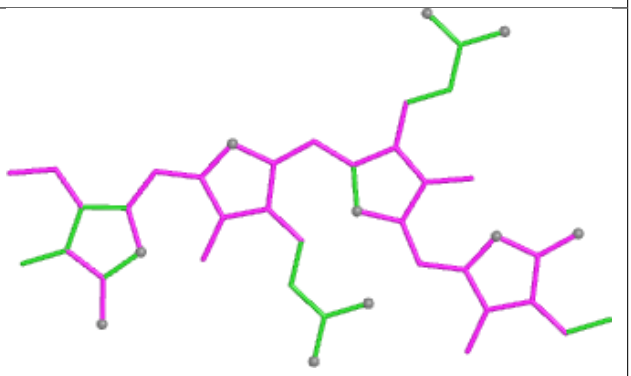

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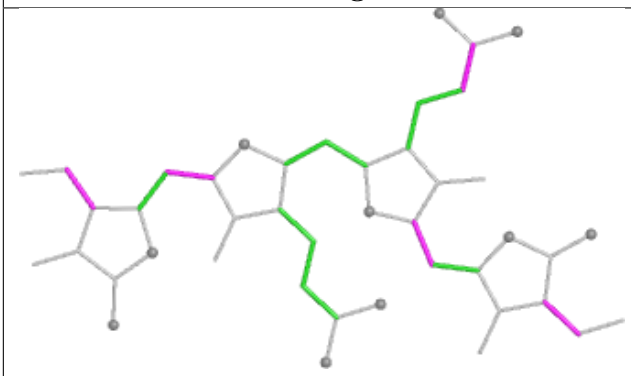

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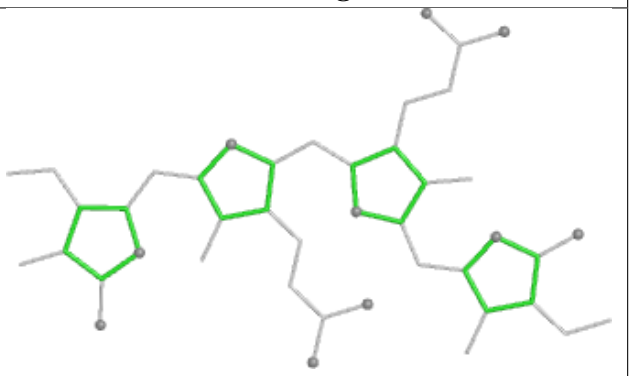
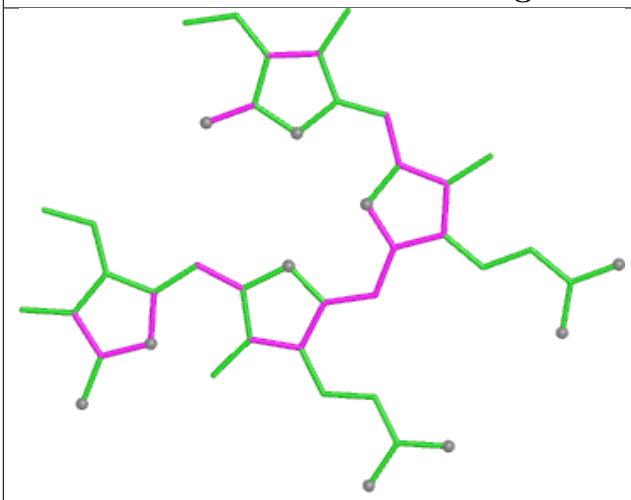


Rings

Ligand PEB PF 202



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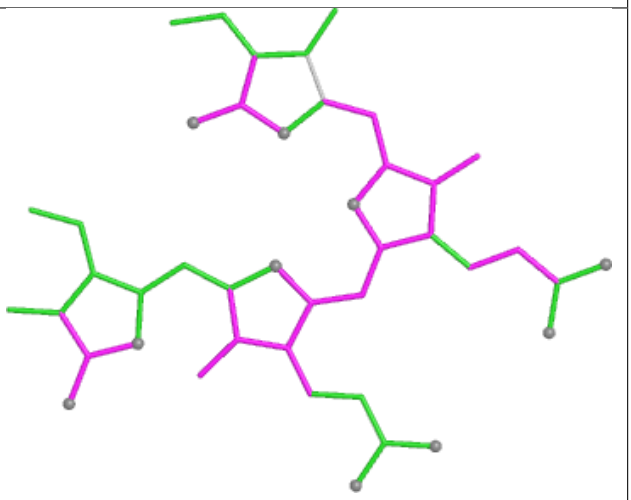

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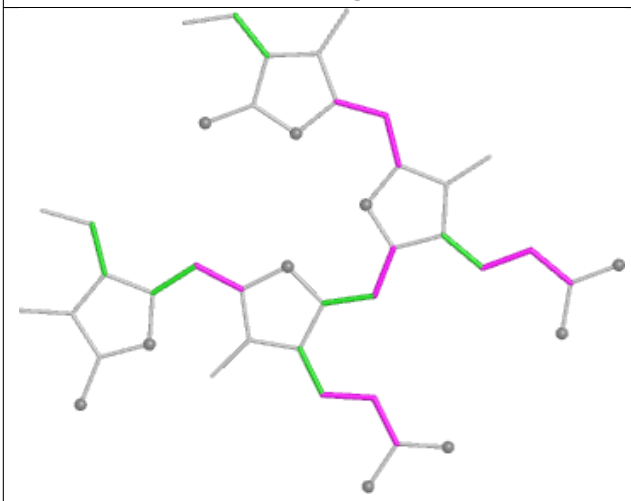

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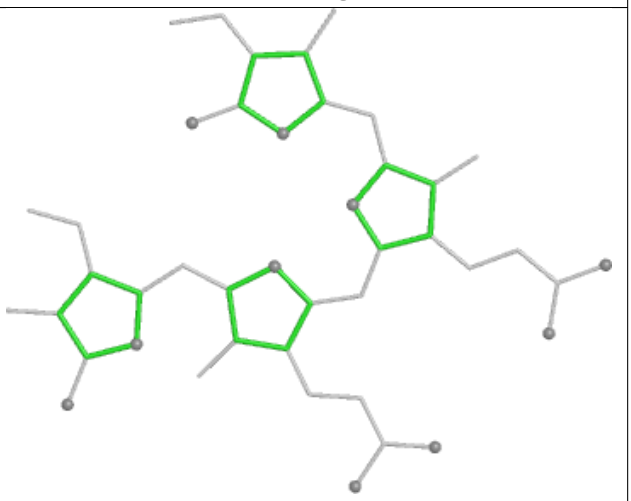

Rings

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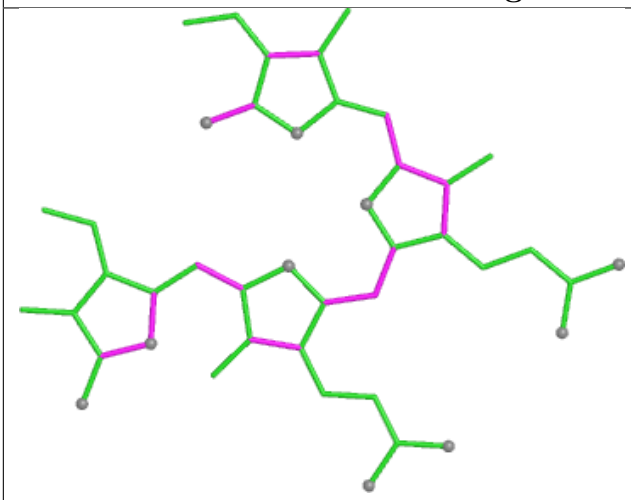

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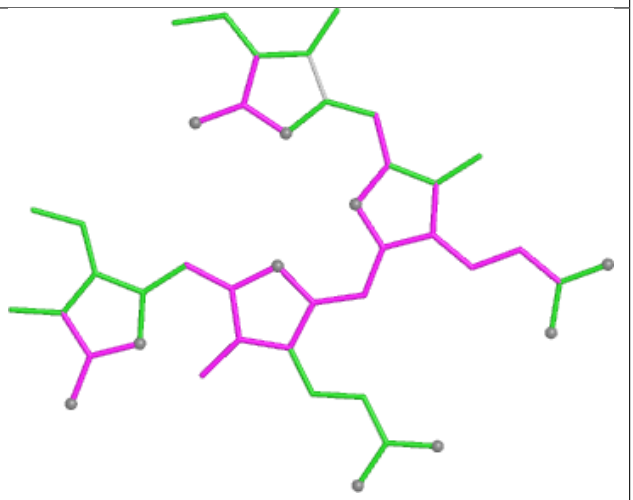

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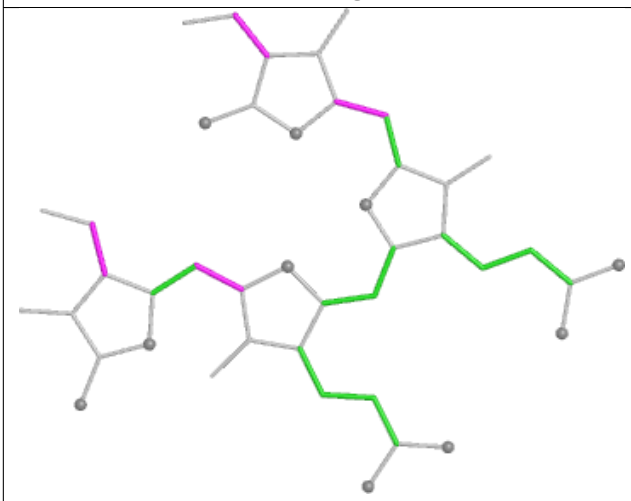

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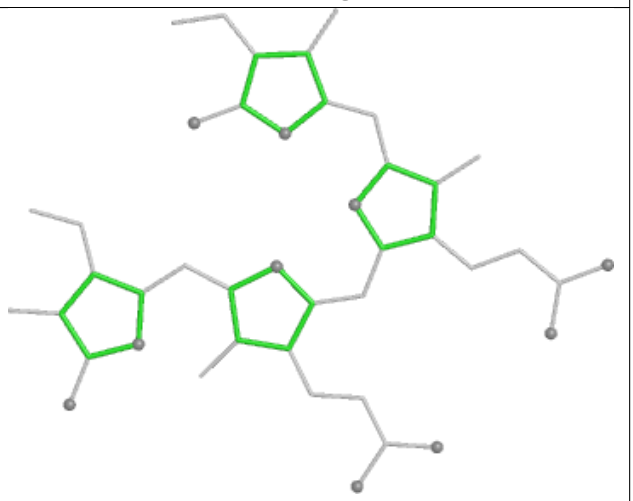
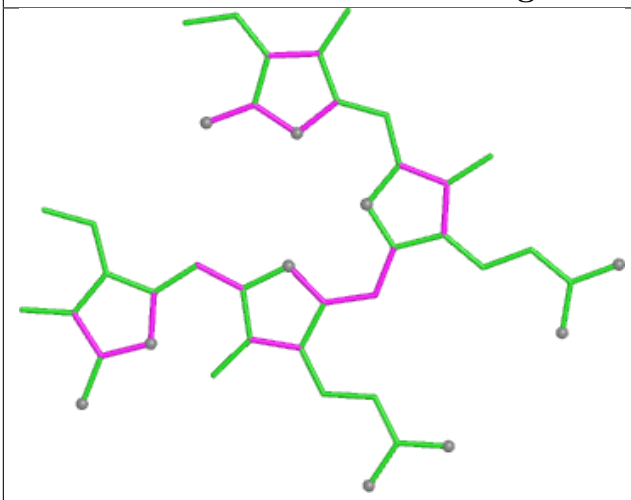


Rings

Ligand PEB AI 203



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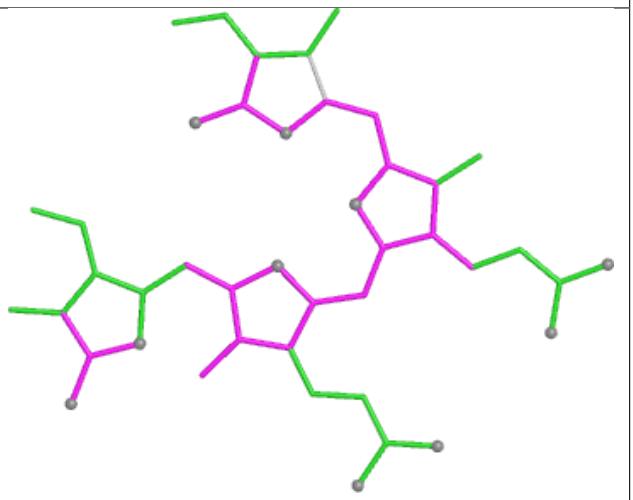

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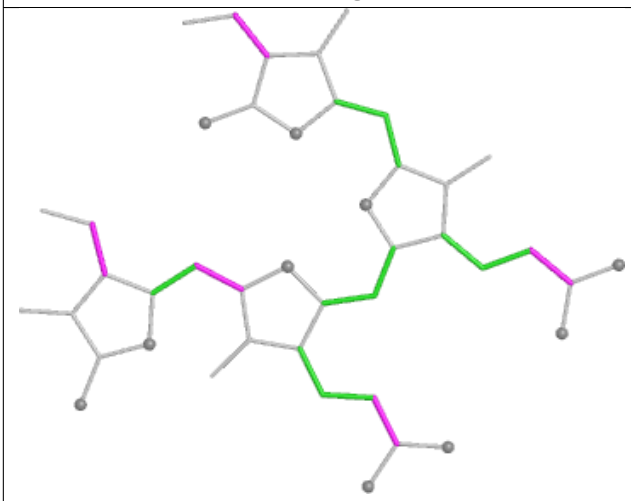

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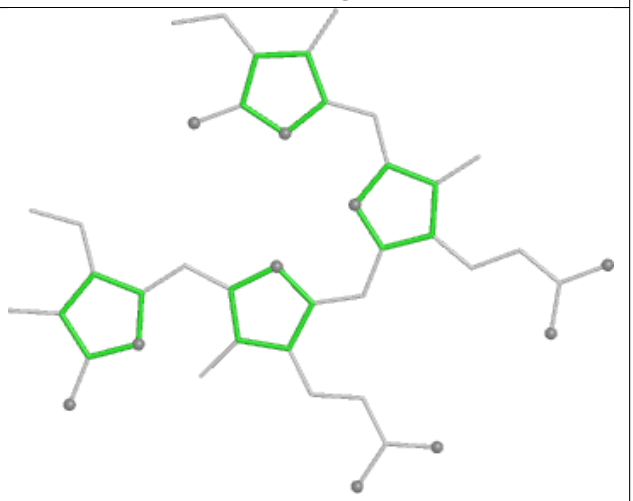
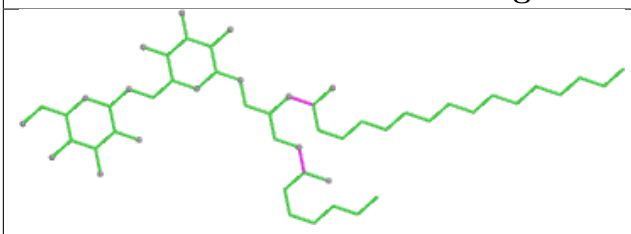


Rings

Ligand DGD aL 603



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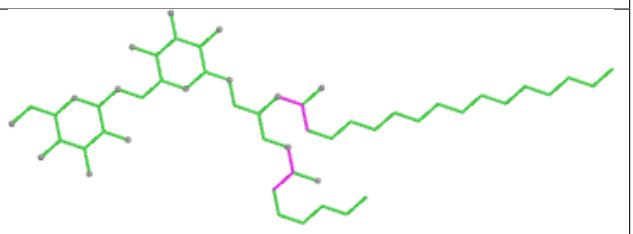

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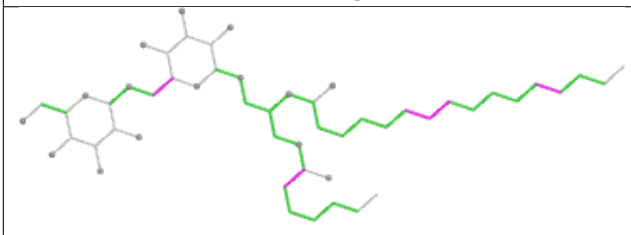

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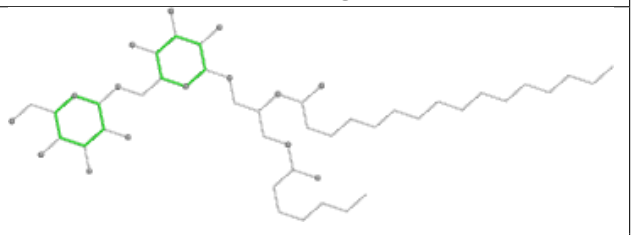
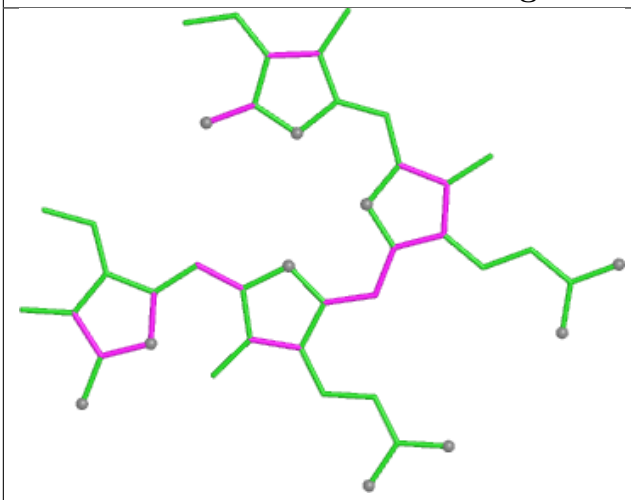


Rings

Ligand PEB aJ 204



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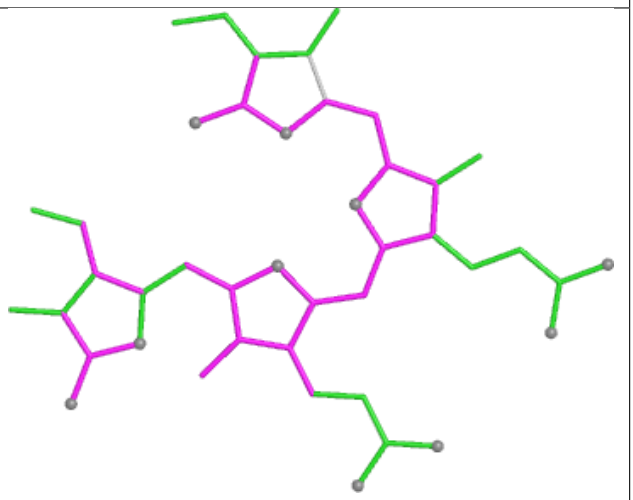

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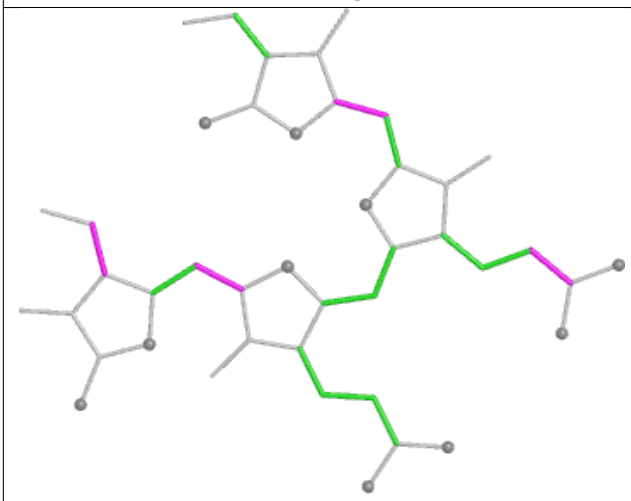

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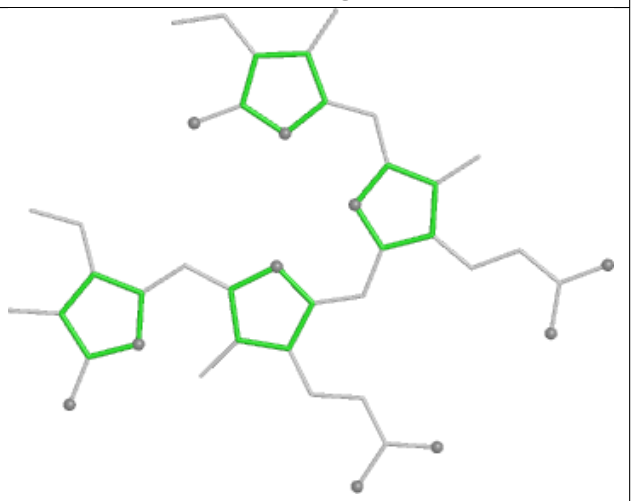

Rings

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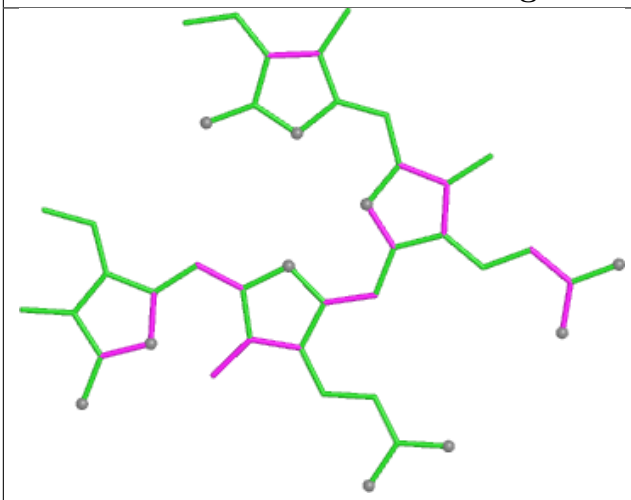

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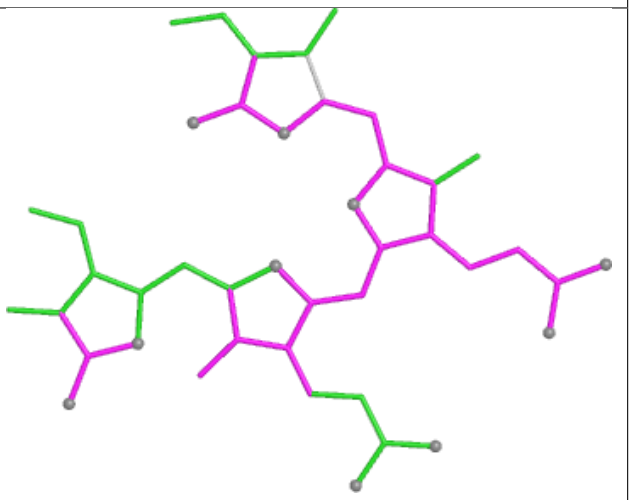

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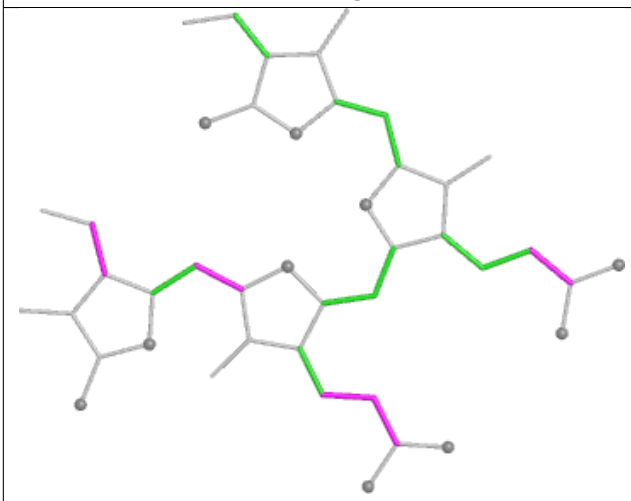

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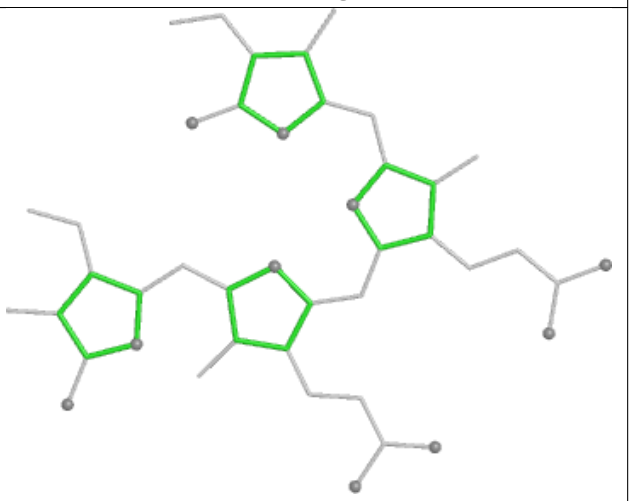
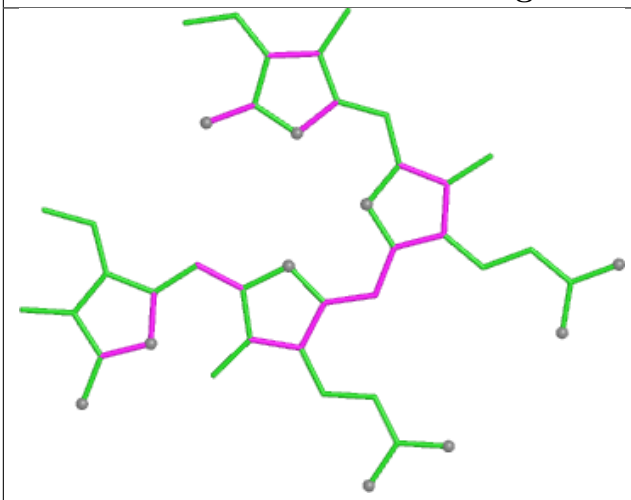


Rings

Ligand PEB 1C 201



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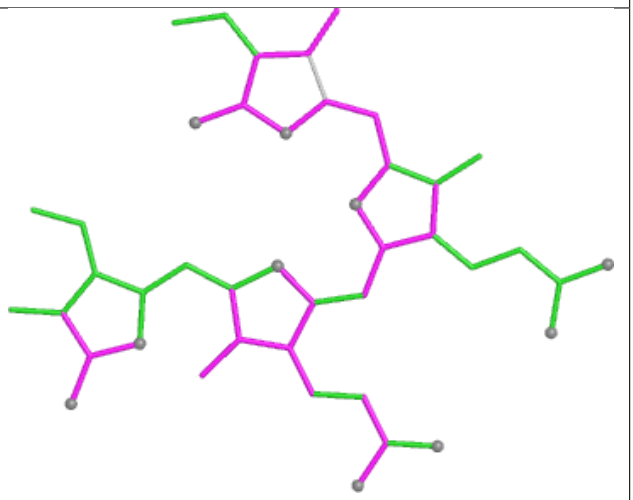

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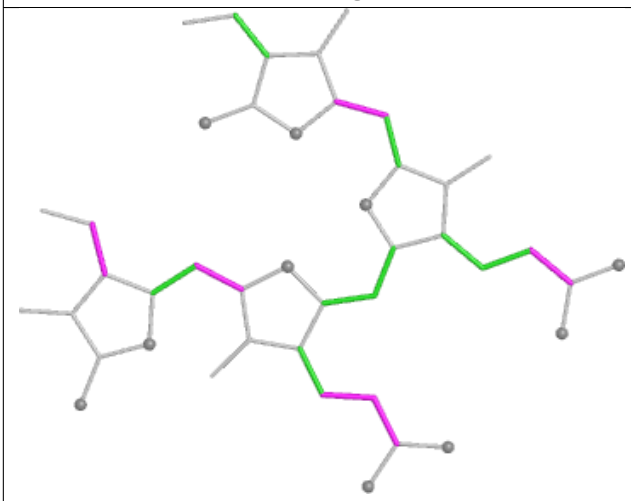

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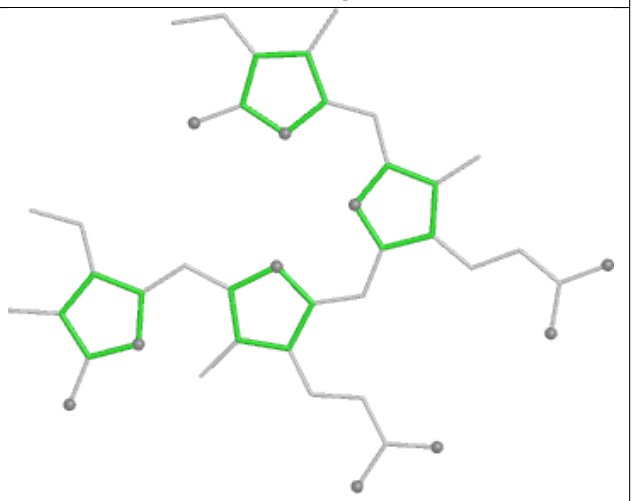
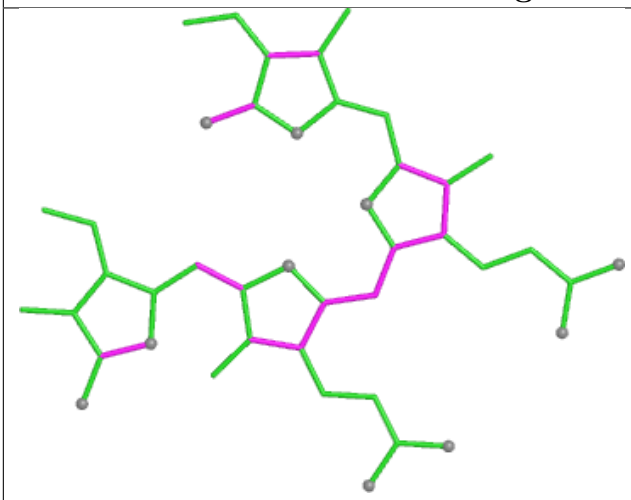


Rings

Ligand PEB U9 203



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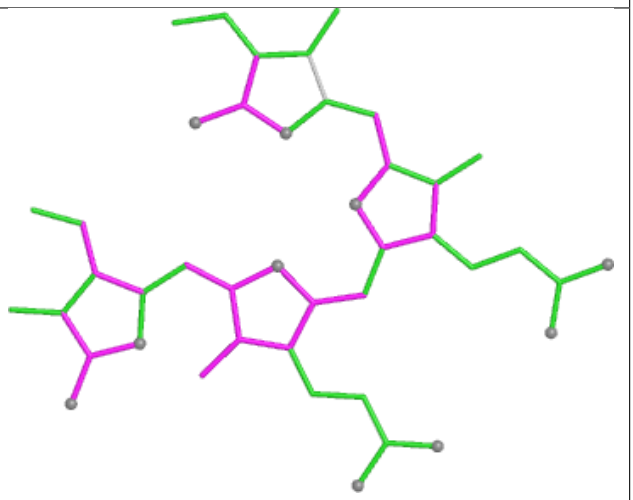
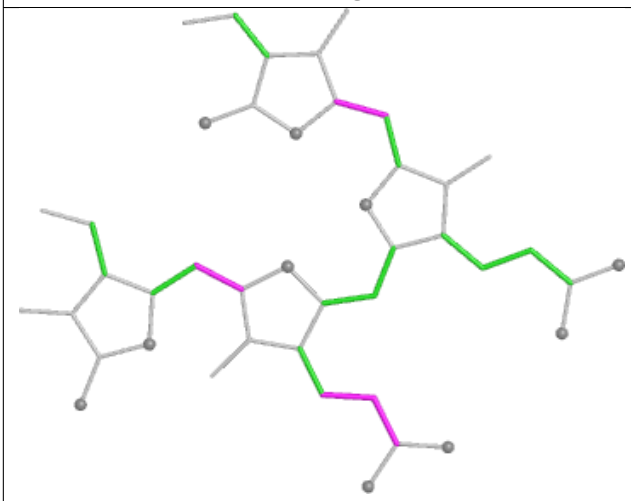


Bond angles



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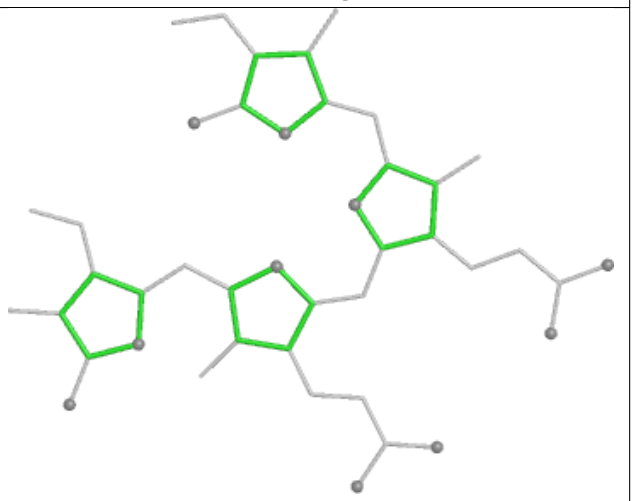
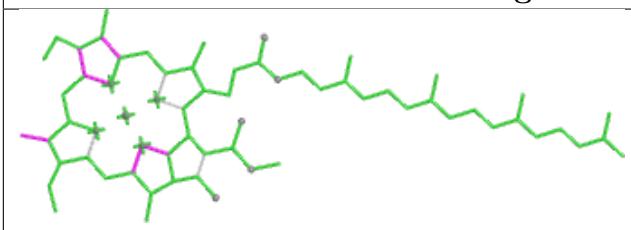


Rings

Ligand CLA 1N 602



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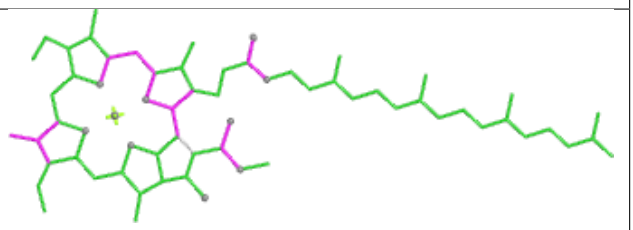

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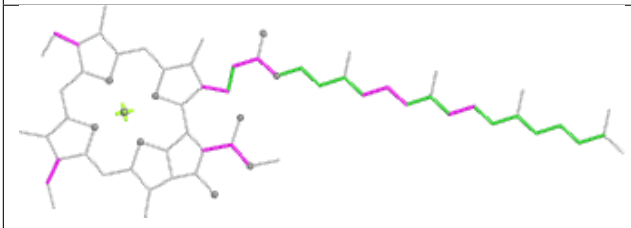

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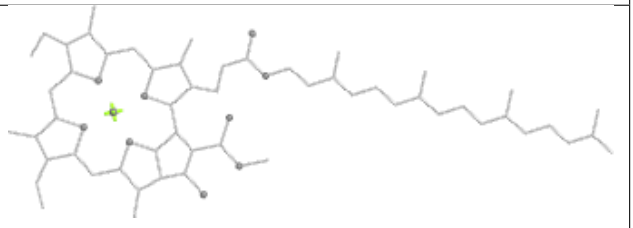
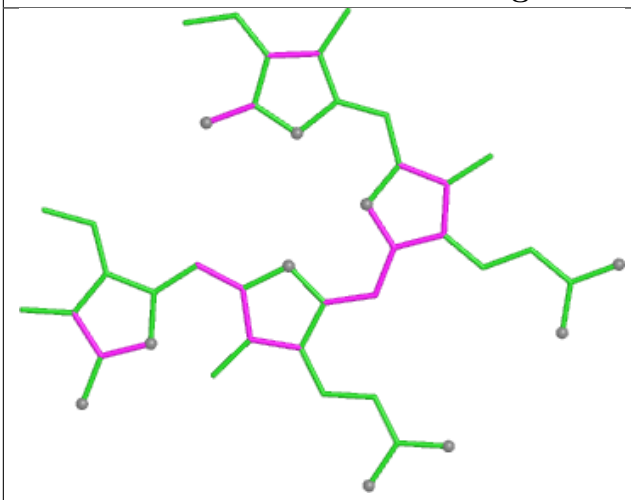


Rings

Ligand PEB M9 304



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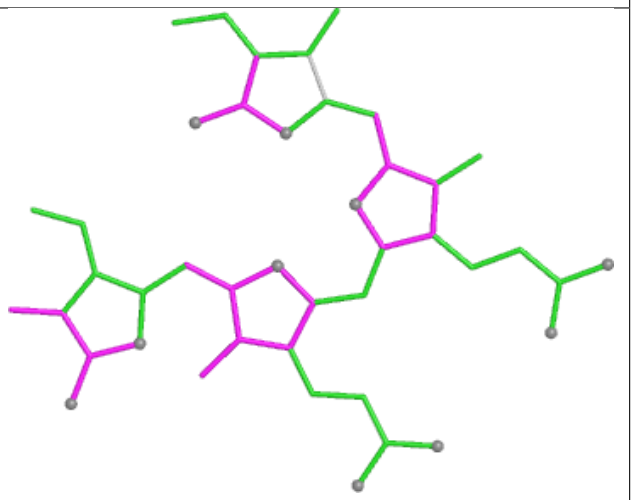
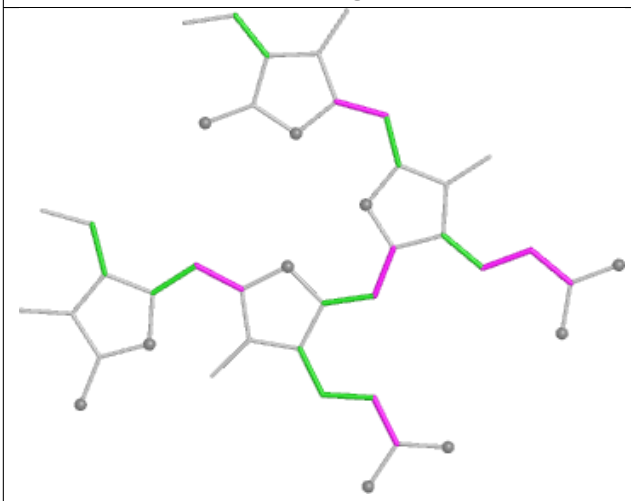


Bond angles



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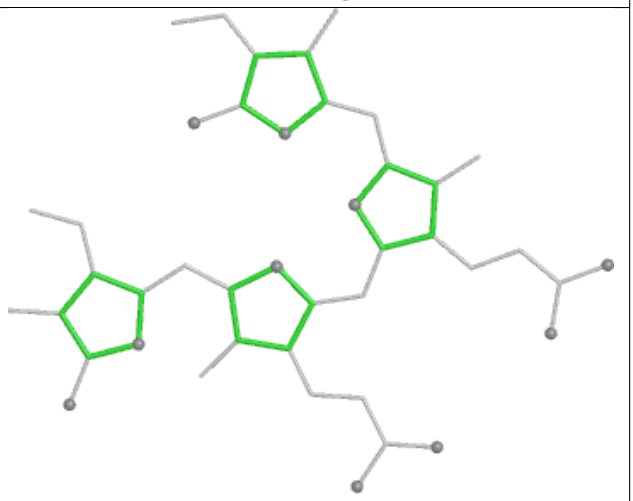
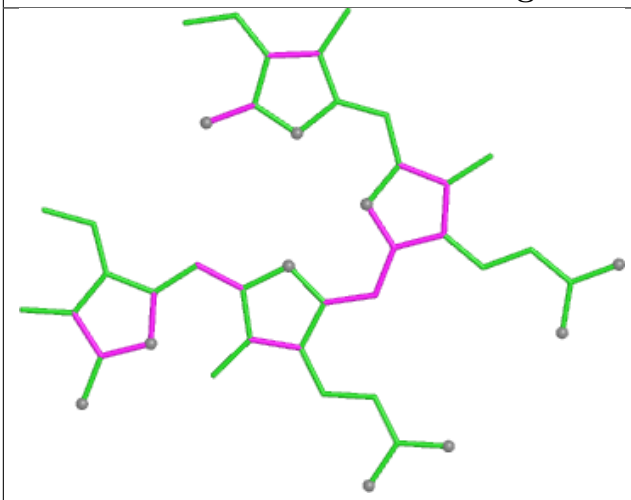
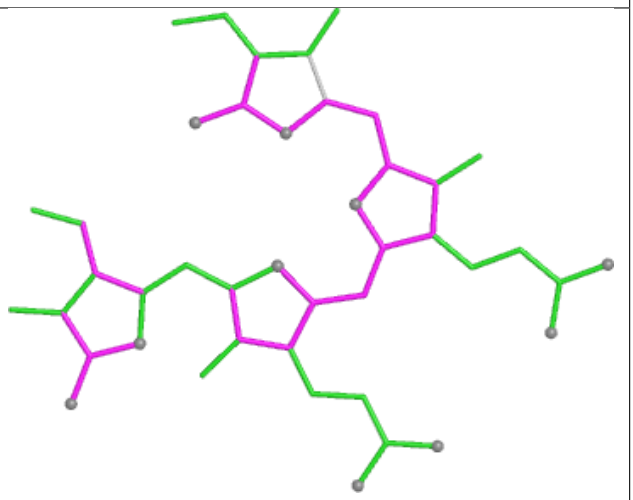


Rings

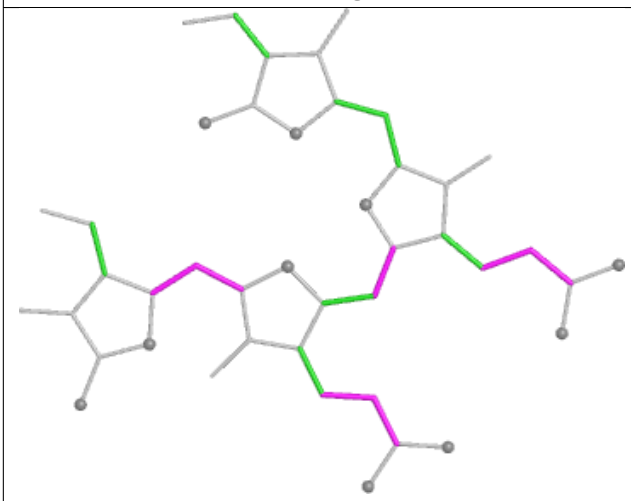
Ligand PEB E5 202



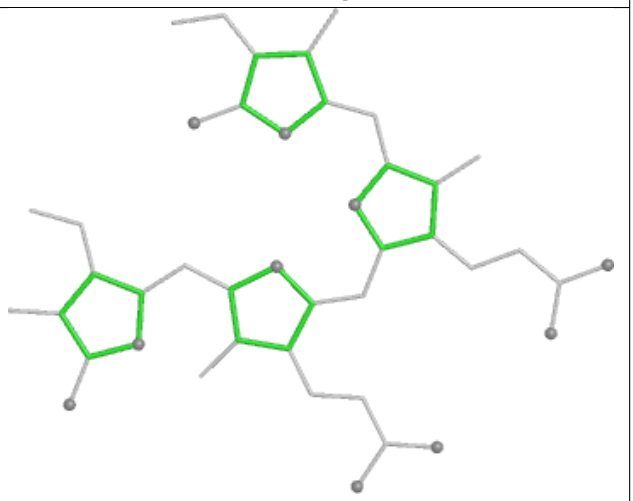
Bond lengths



Bond angles

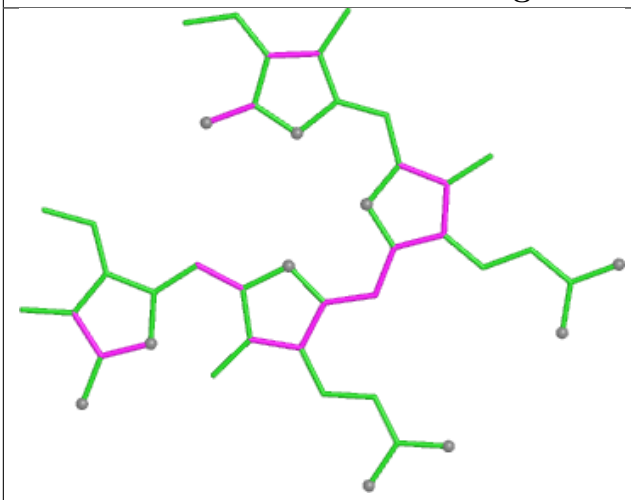


Torsions



Rings

Ligand PEB LA 202



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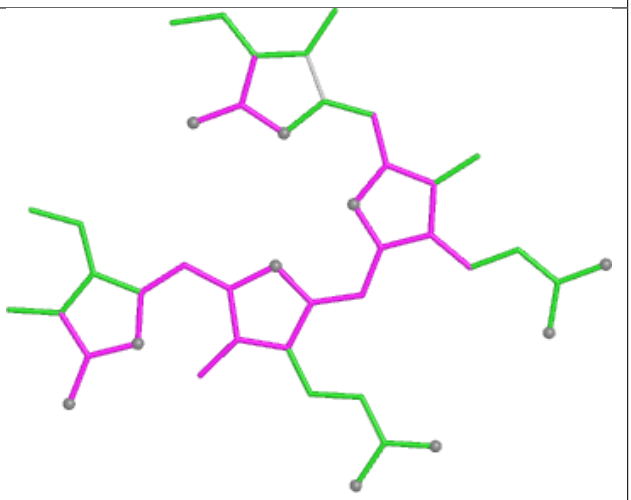
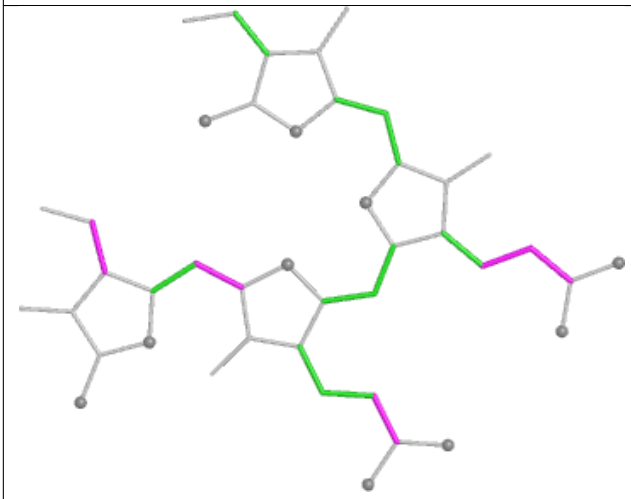


Bond angles



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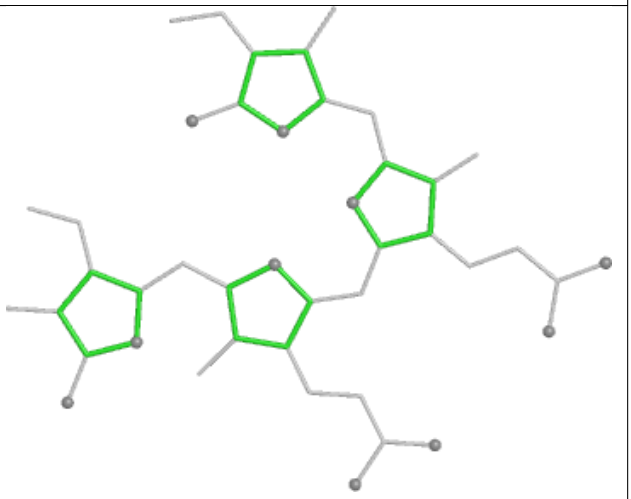
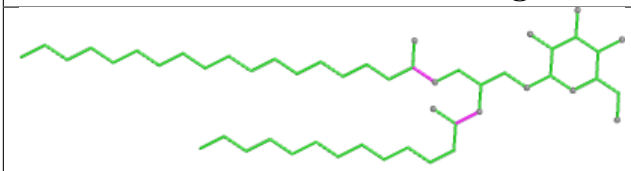


Rings

Ligand LMG B6 622



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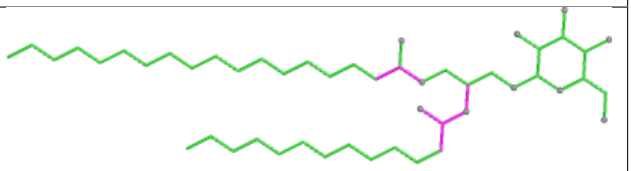

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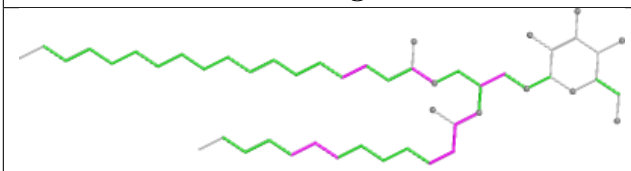

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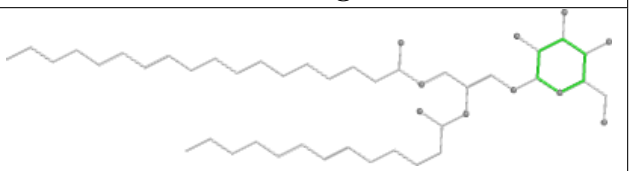
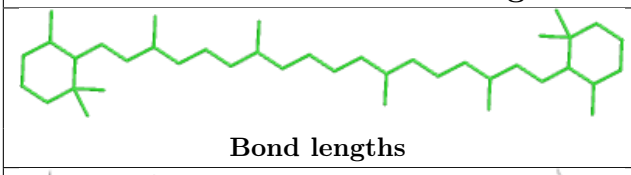


Rings

Ligand BCR KN 104



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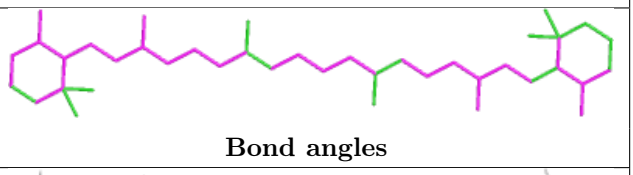
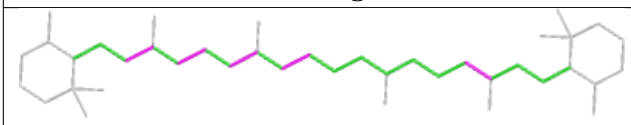


Bond angles



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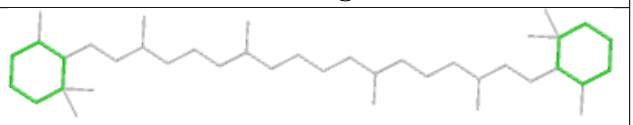
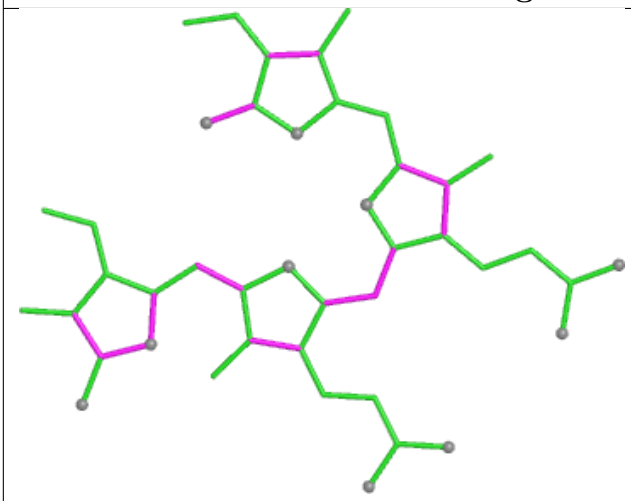


Rings

Ligand PEB lM 202



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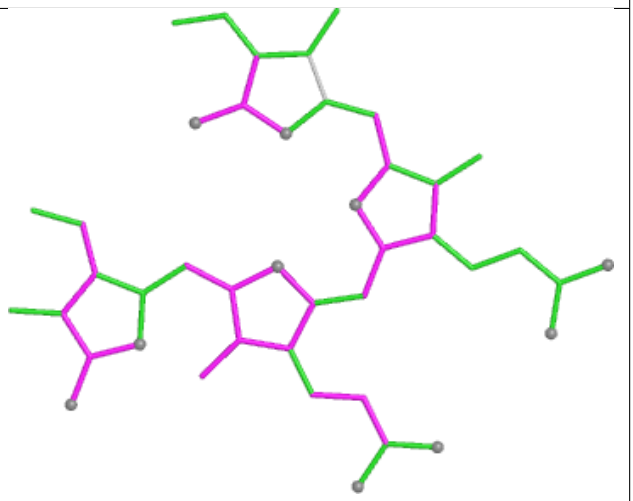
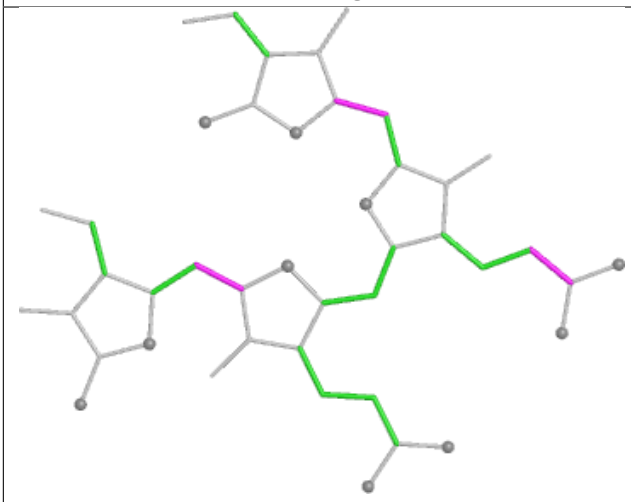


Bond angles



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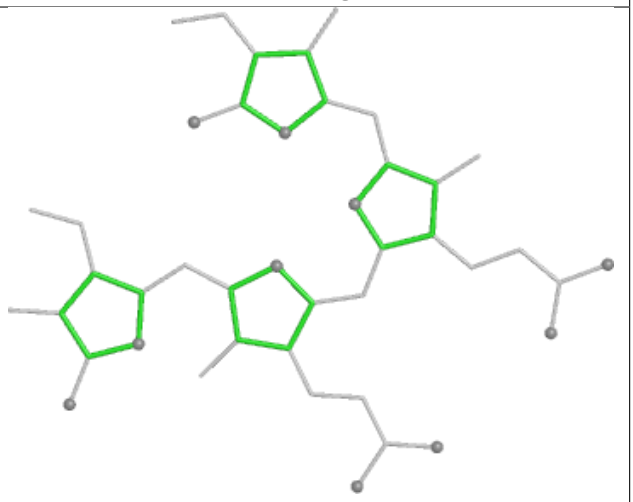
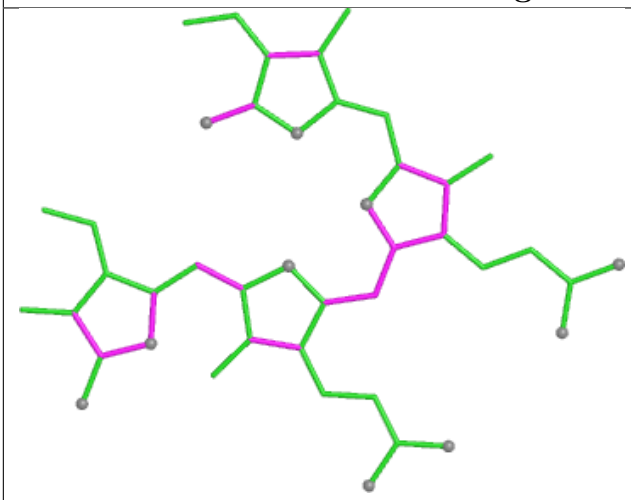


Rings

Ligand PEB SQ 201



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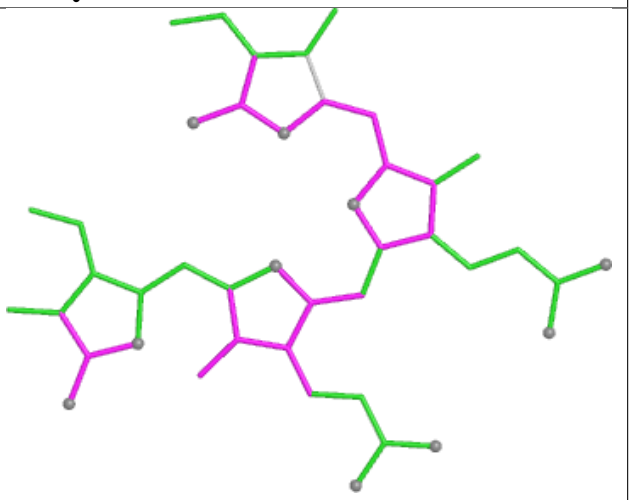
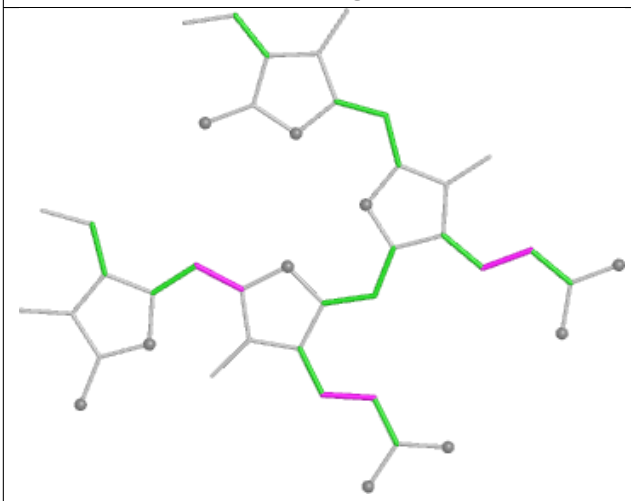


Bond angles



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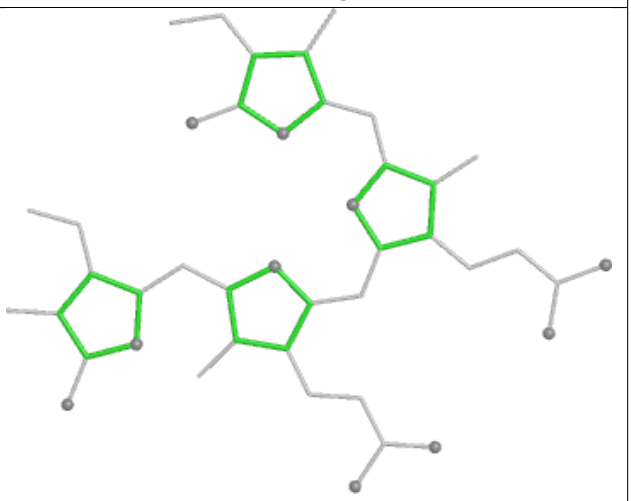
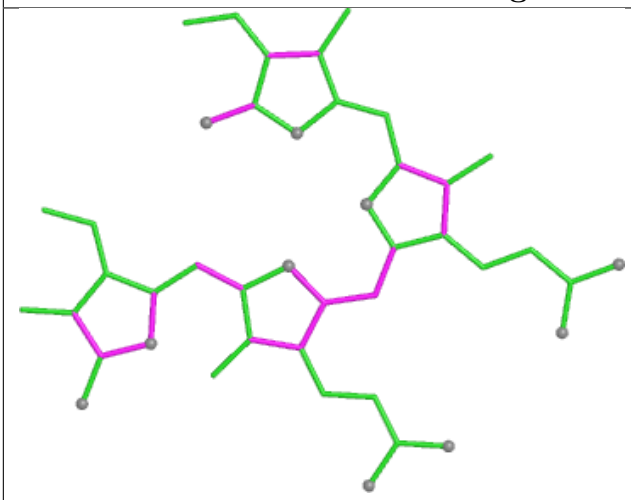


Rings

Ligand PEB HK 201



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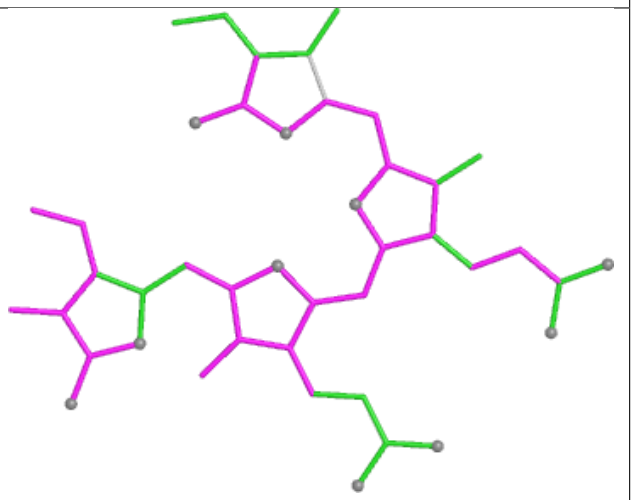
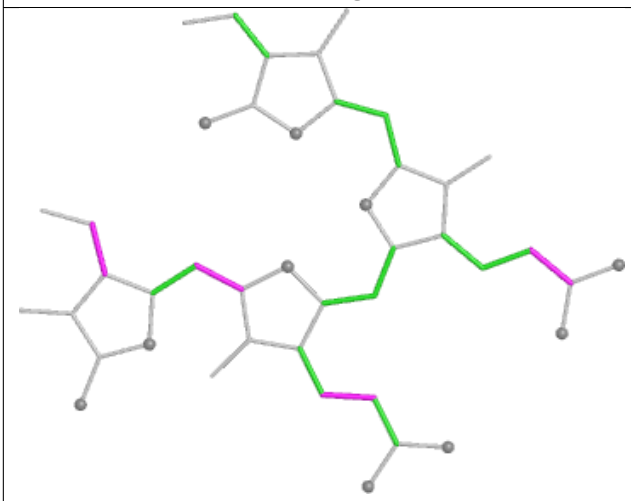


Bond angles



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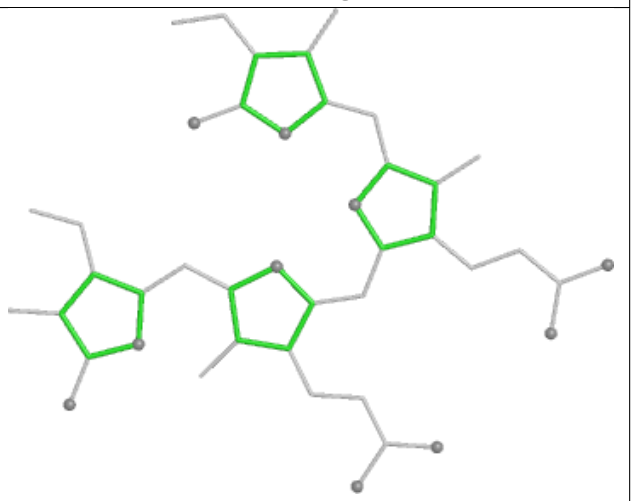
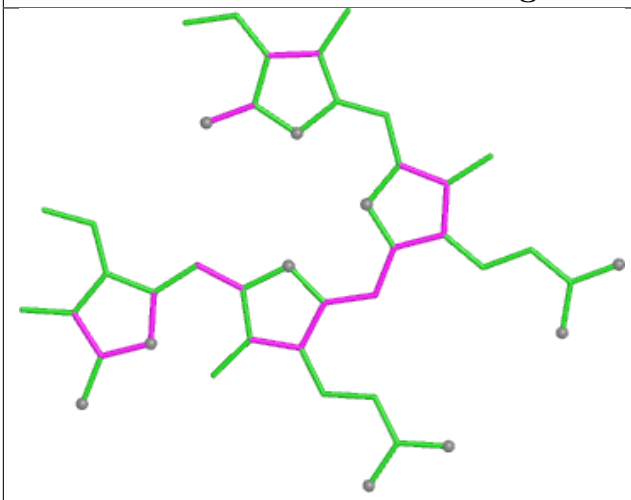


Rings

Ligand PEB q8 201



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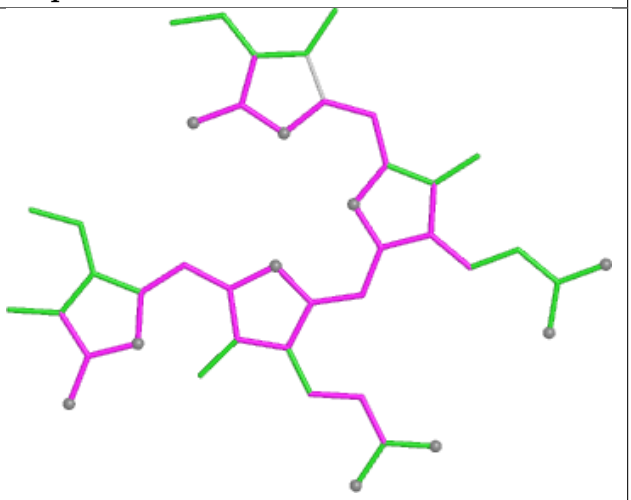
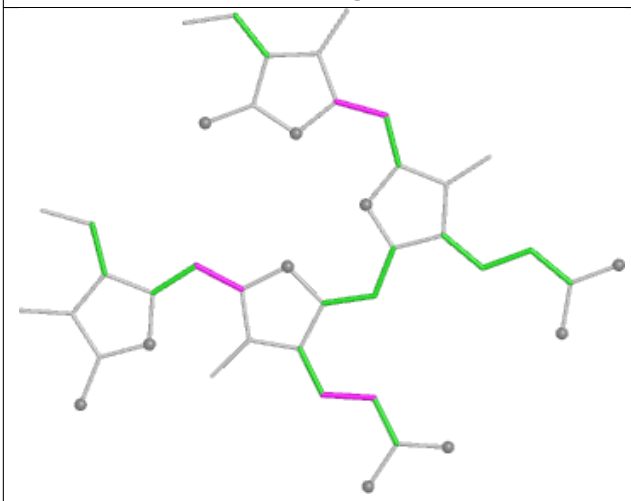


Bond angles



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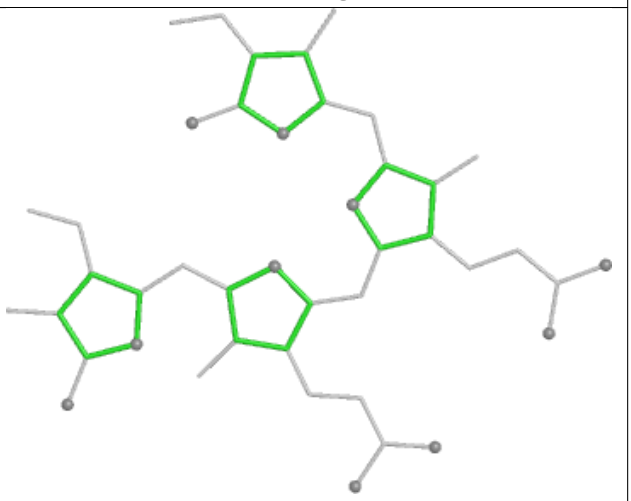
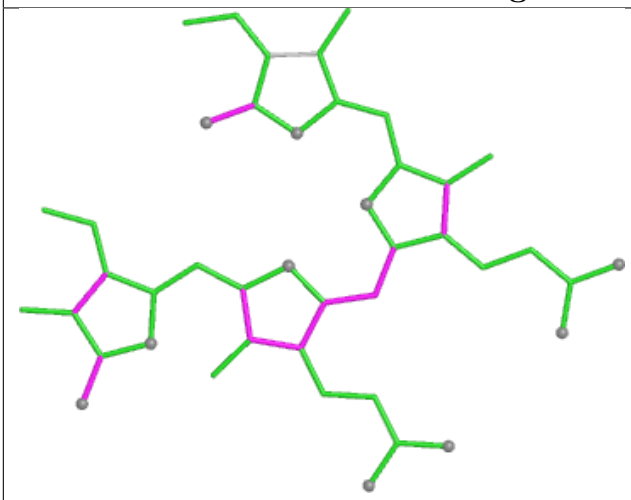


Rings

Ligand PUB AQ 302



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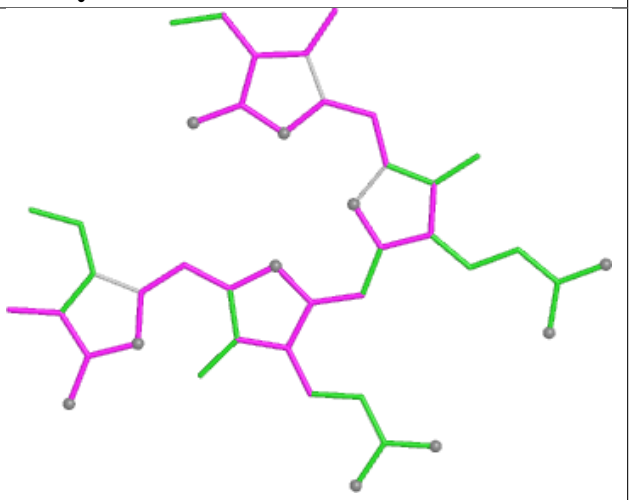
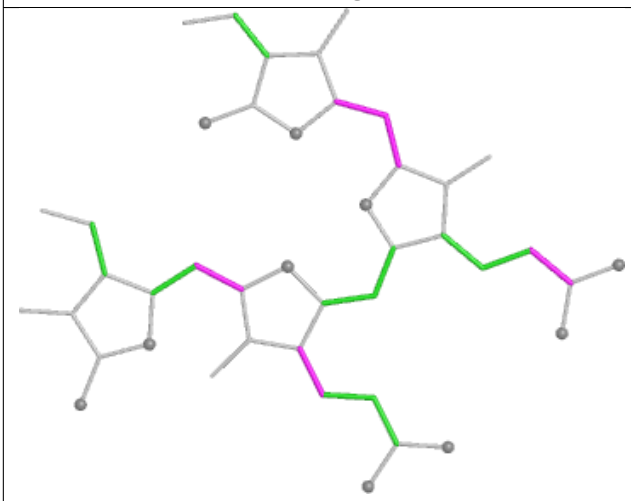


Bond angles



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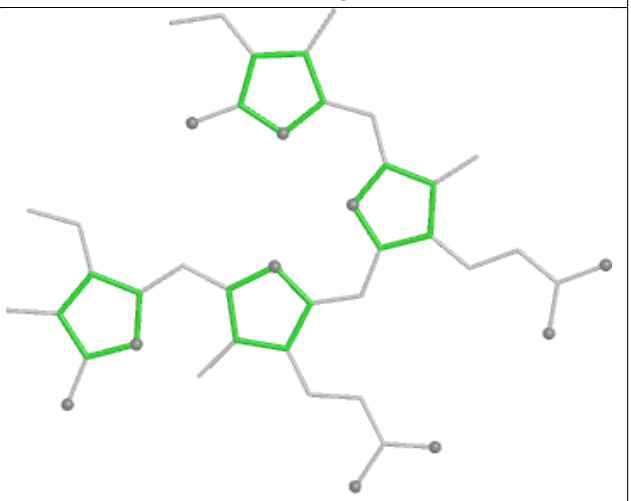
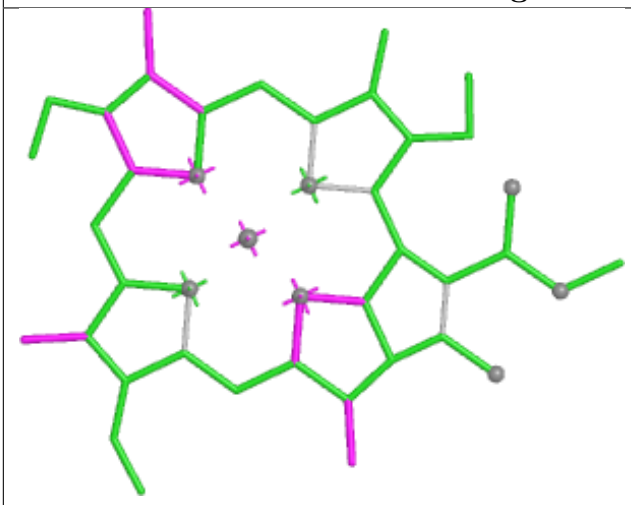


Rings

Ligand CLA BN 815



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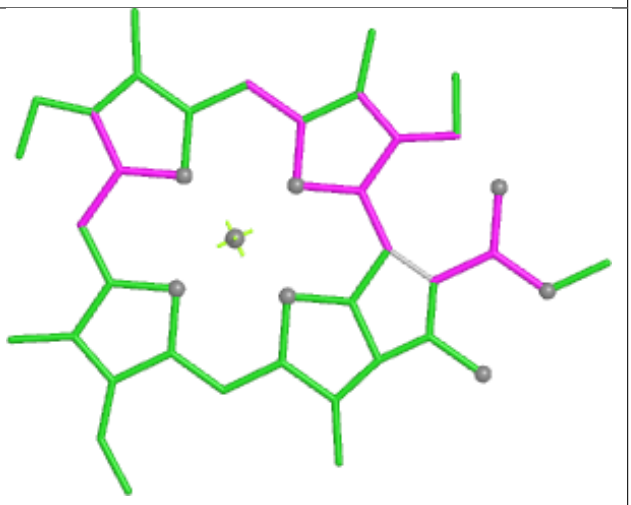
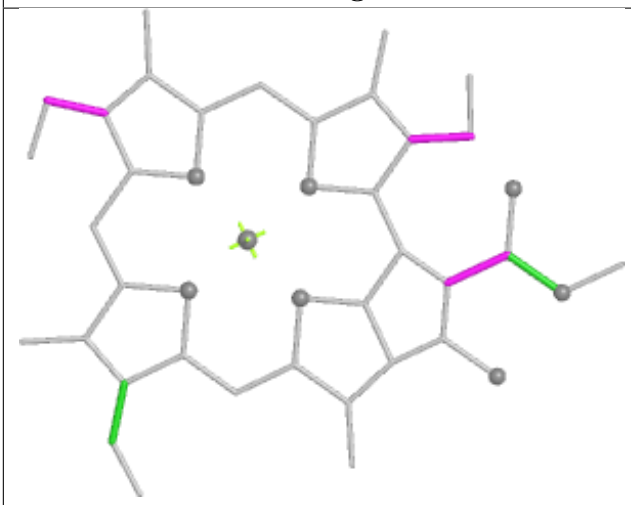


Bond angles

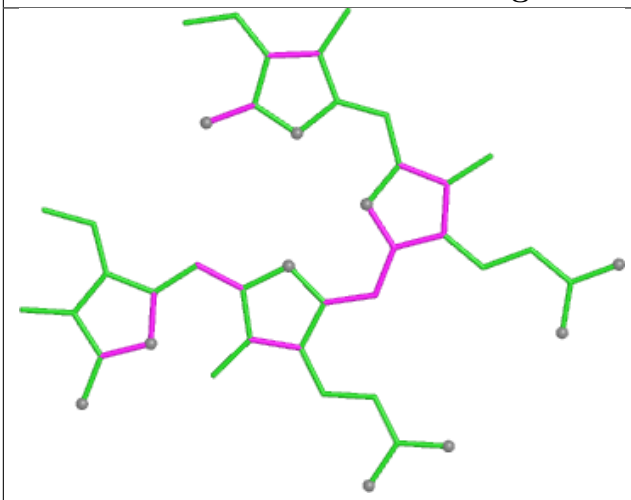


Torsions



Rings

Ligand PEB PD 203



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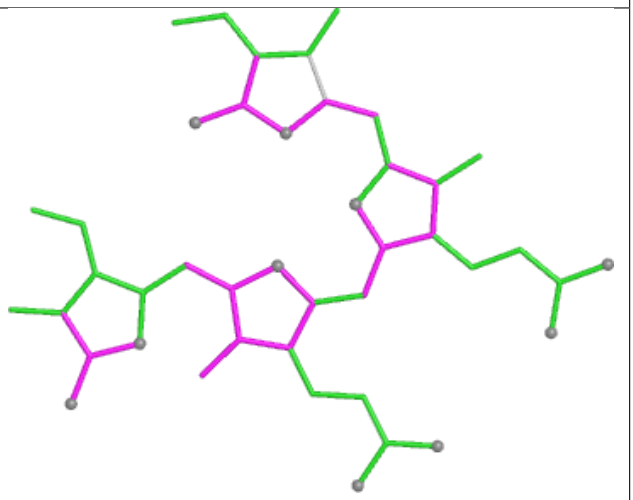
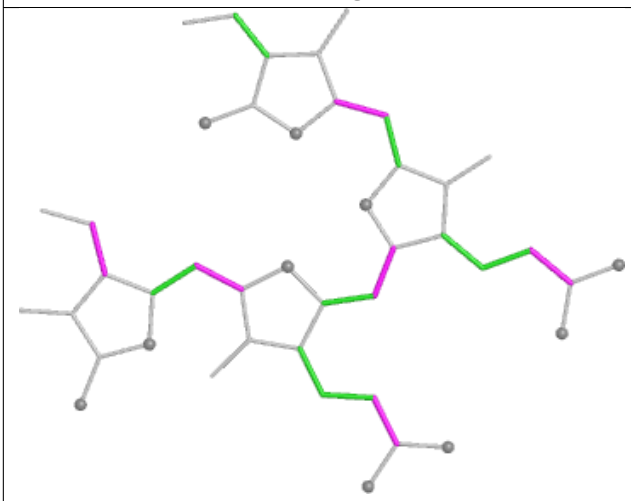


Bond angles



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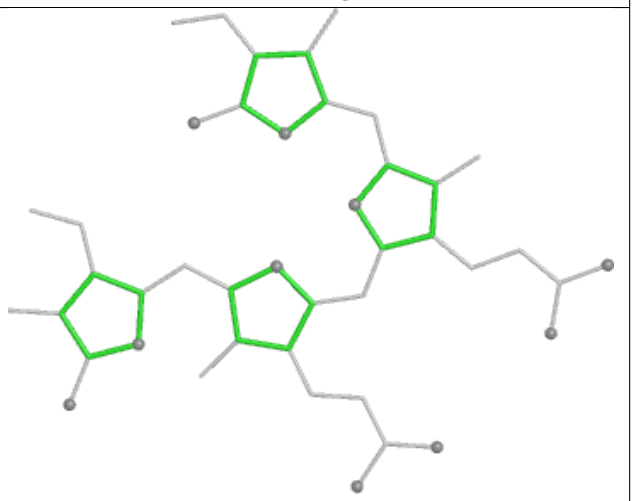
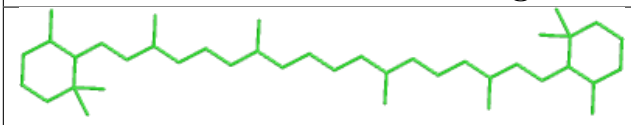


Rings

Ligand BCR JN 102



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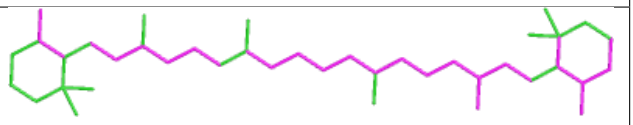
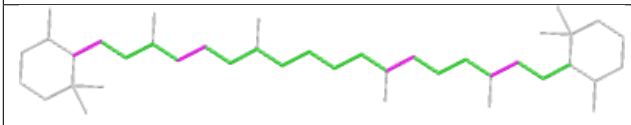


Bond angles



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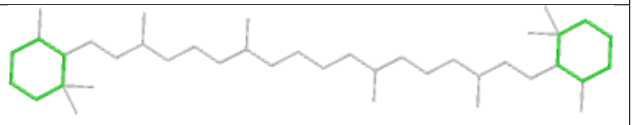
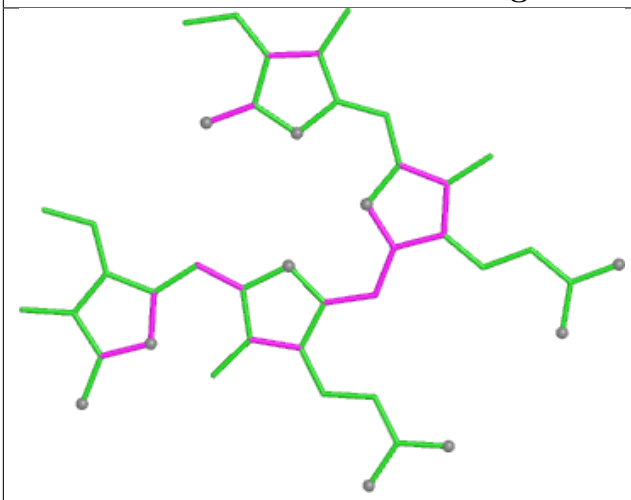


Rings

Ligand PEB AD 301



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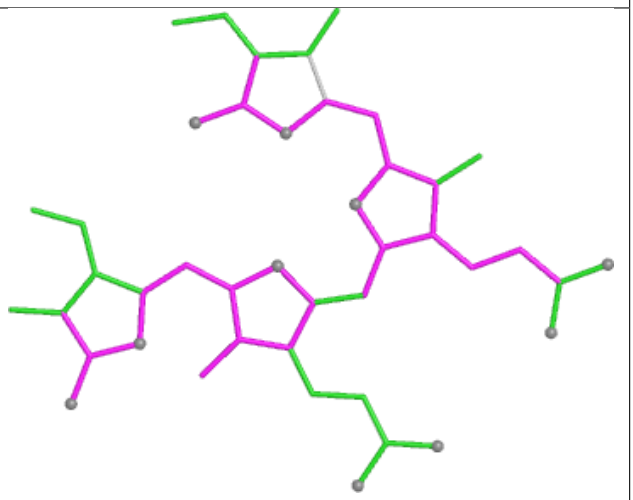
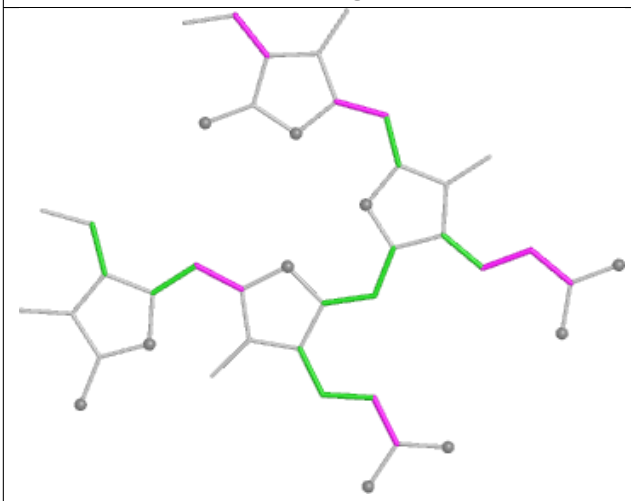


Bond angles



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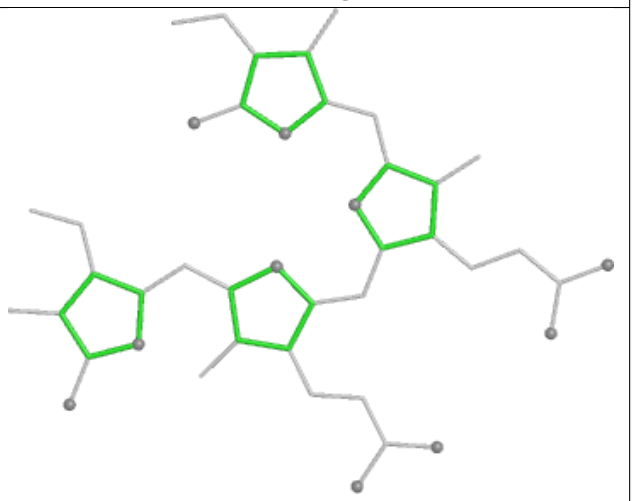
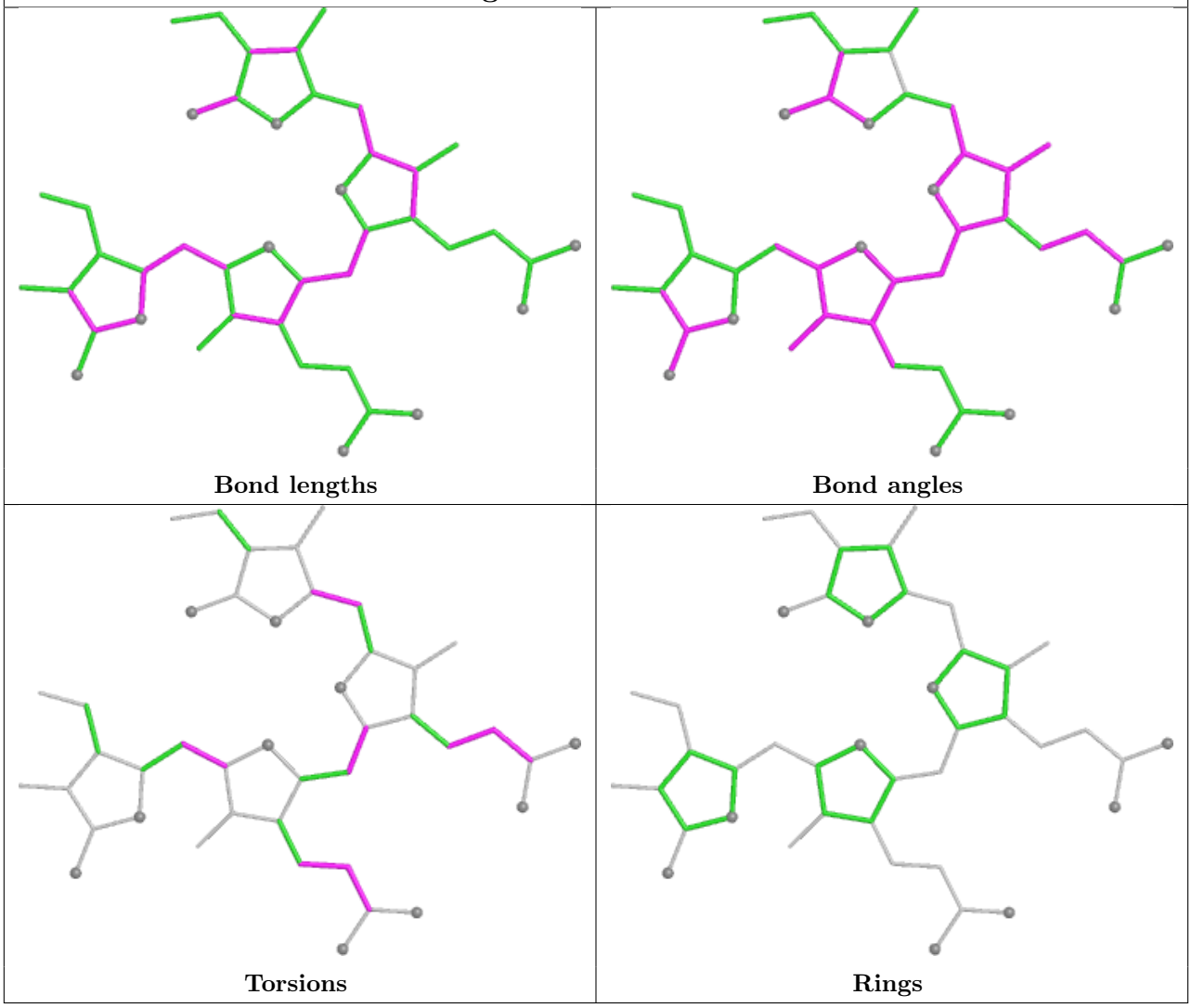
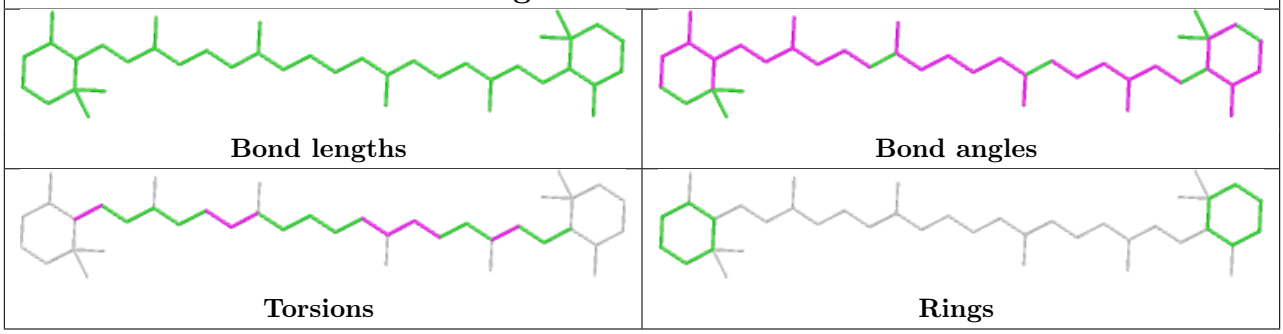


Rings

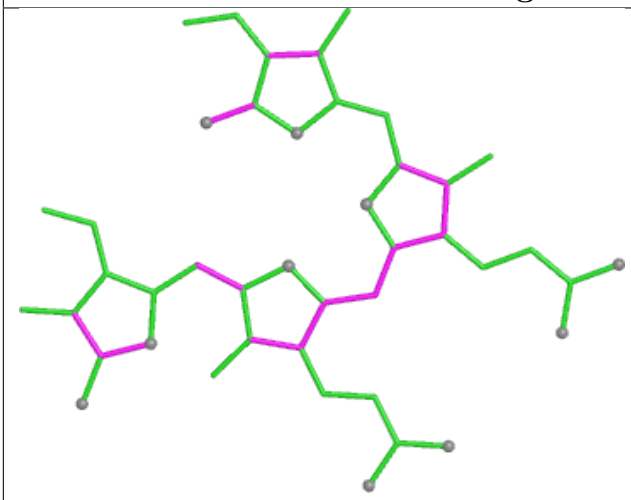
Ligand PEB eF 201



Ligand BCR K6 102



Ligand PEB P1 202



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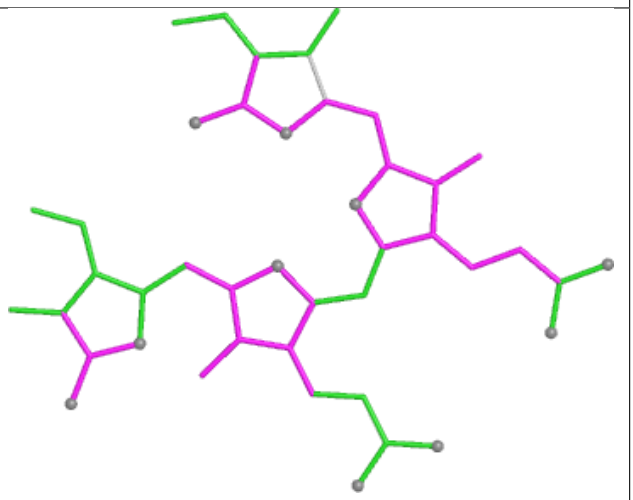
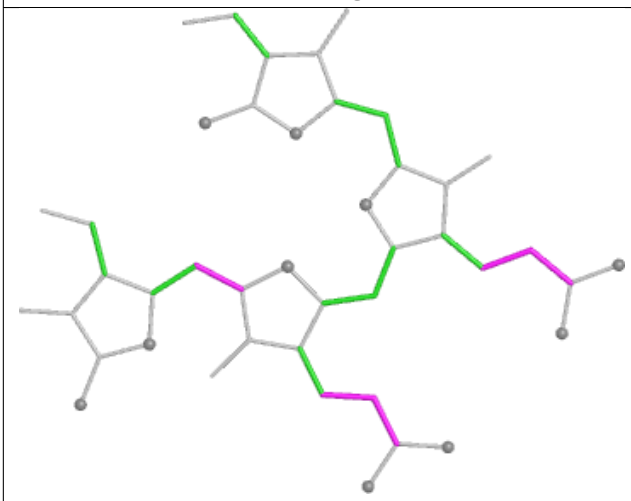


Bond angles



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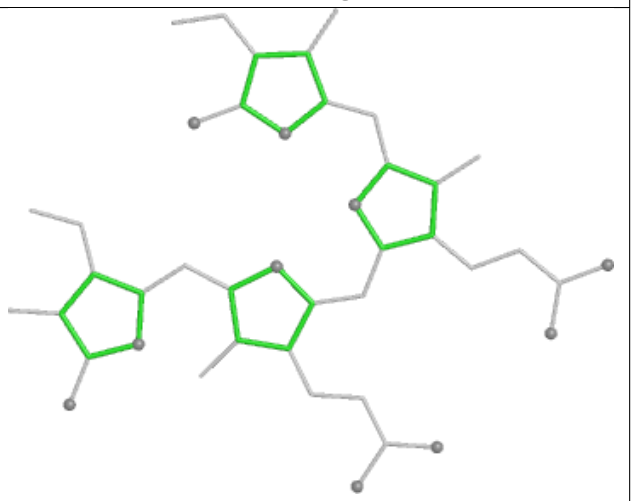
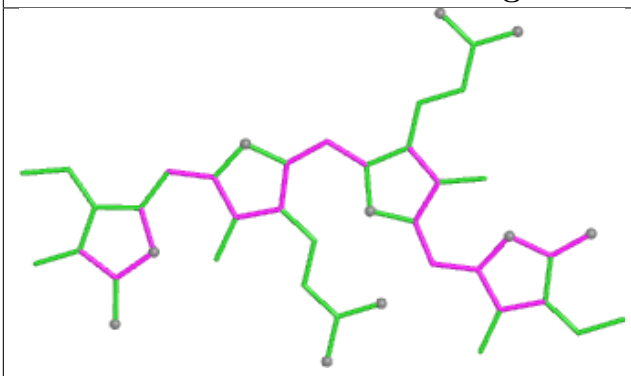
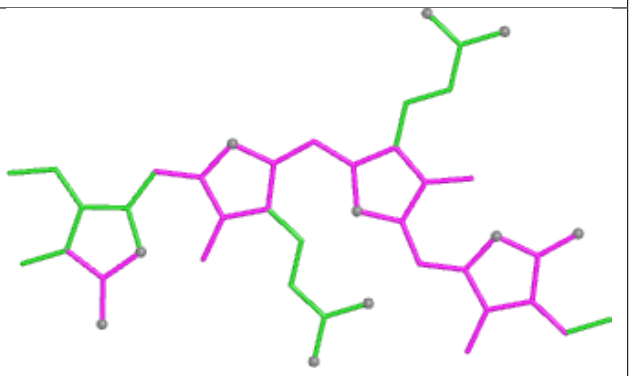


Rings

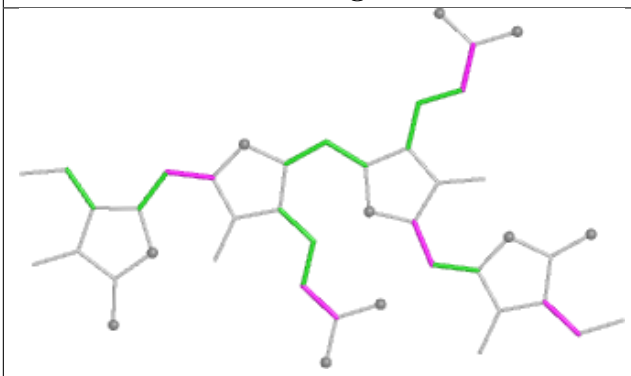
Ligand CYC FE 1001



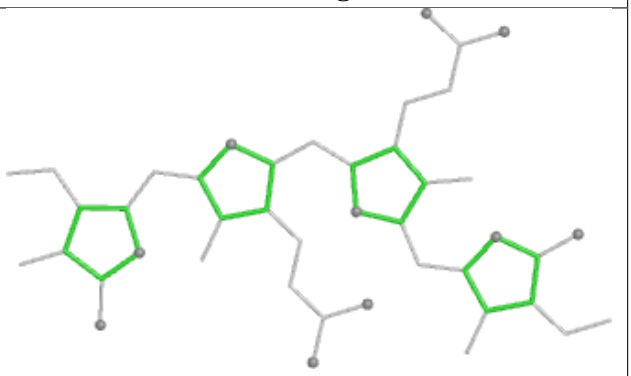
Bond lengths



Bond angles

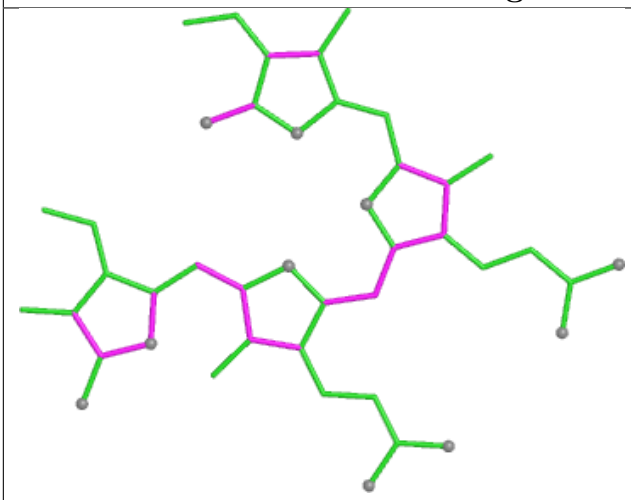


Torsions



Rings

Ligand PEB D1 1002



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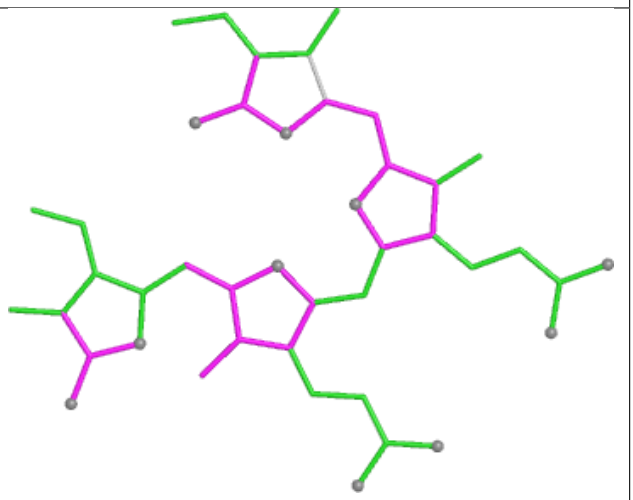

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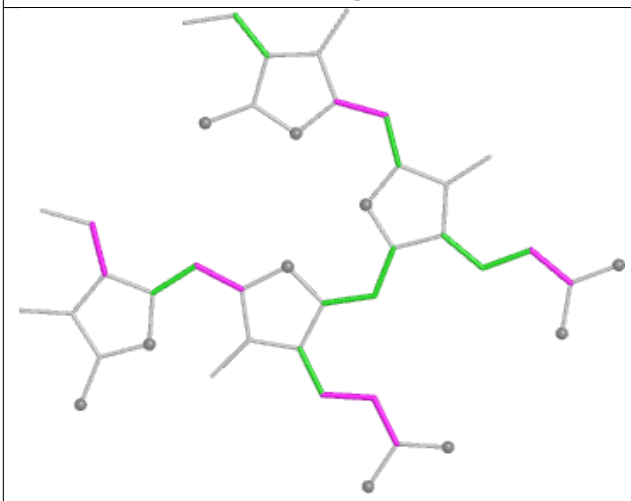

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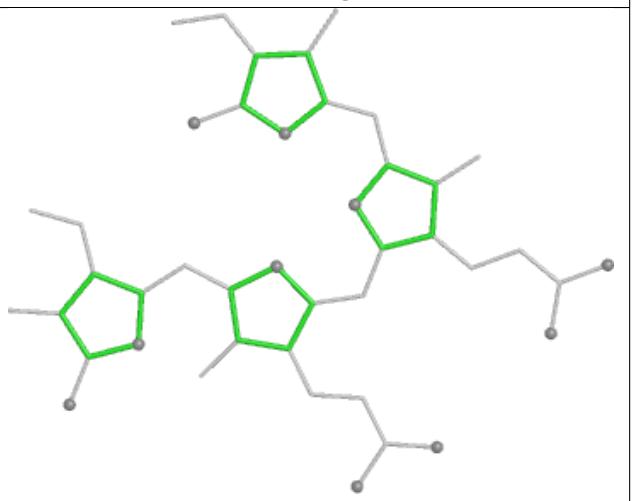
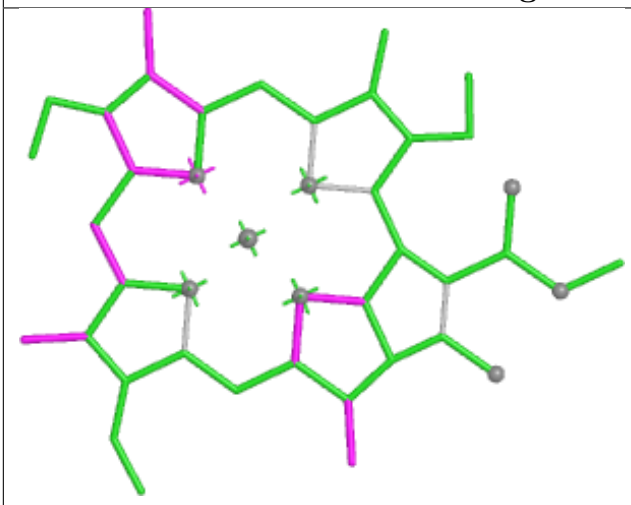


Rings

Ligand CLA 12 604



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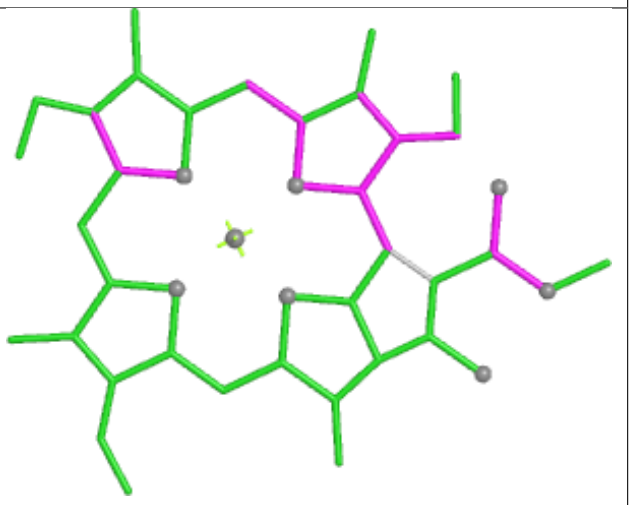

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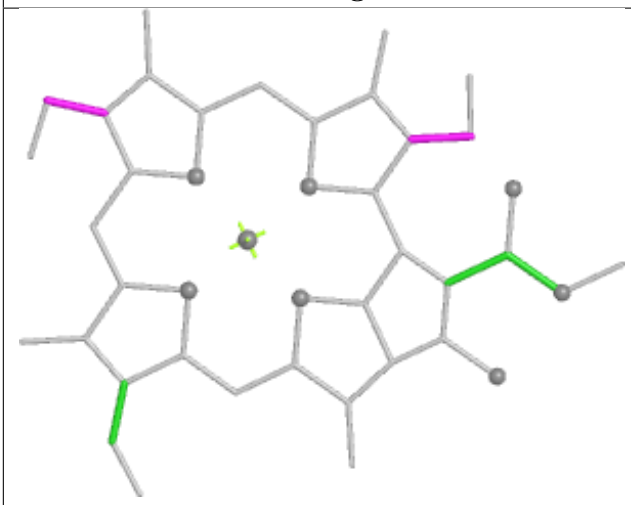
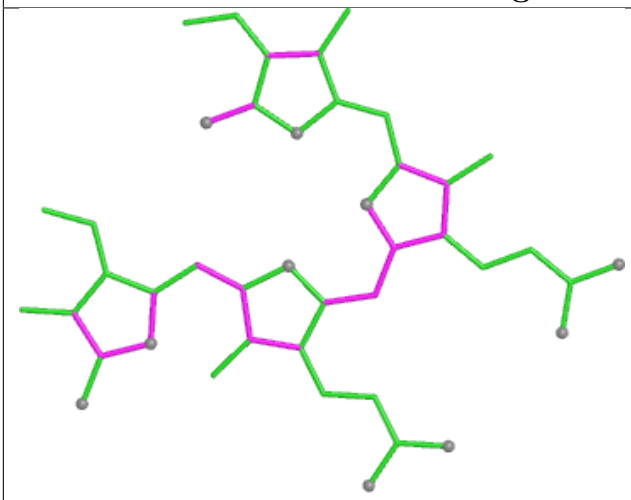


Torsions



Rings

Ligand PEB ED 201



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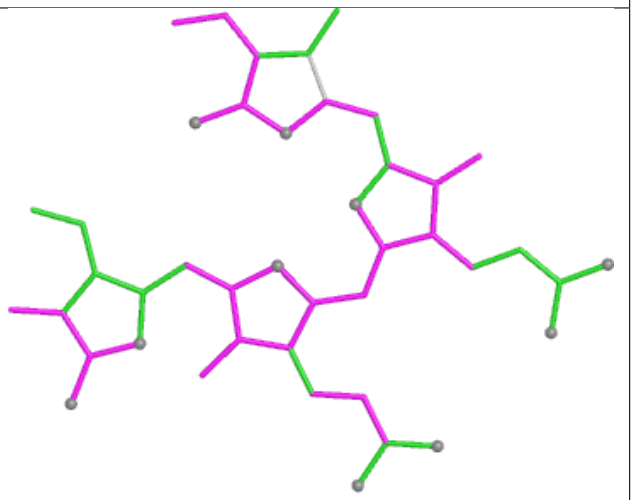

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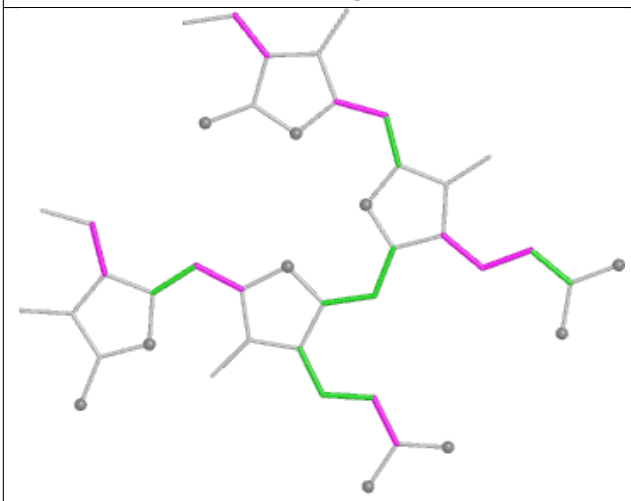

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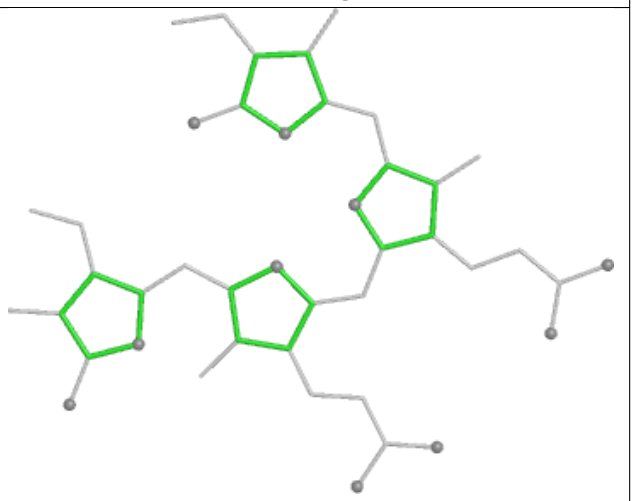
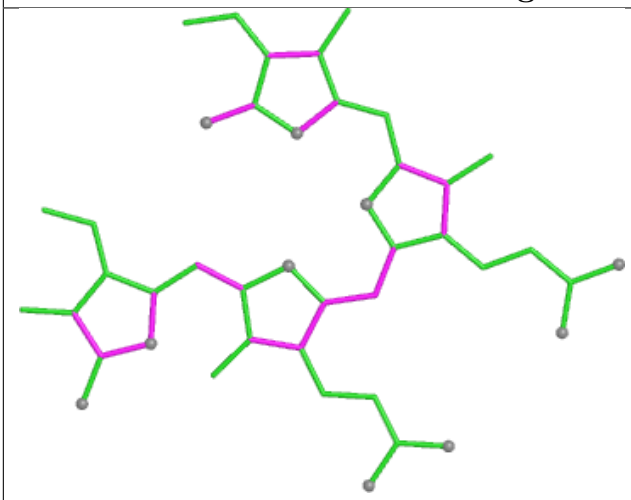


Rings

Ligand PEB IA 201



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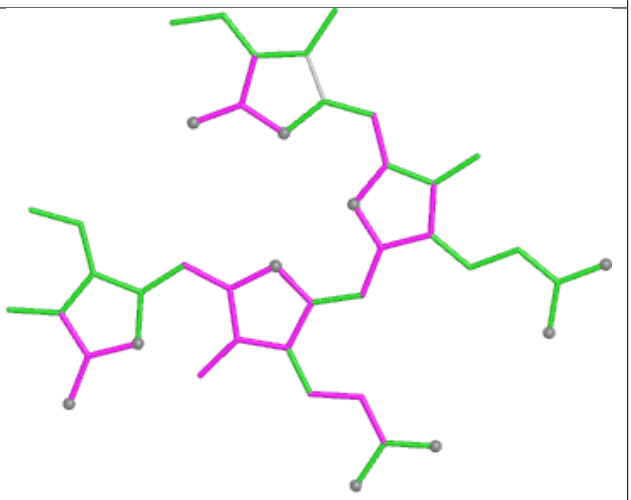
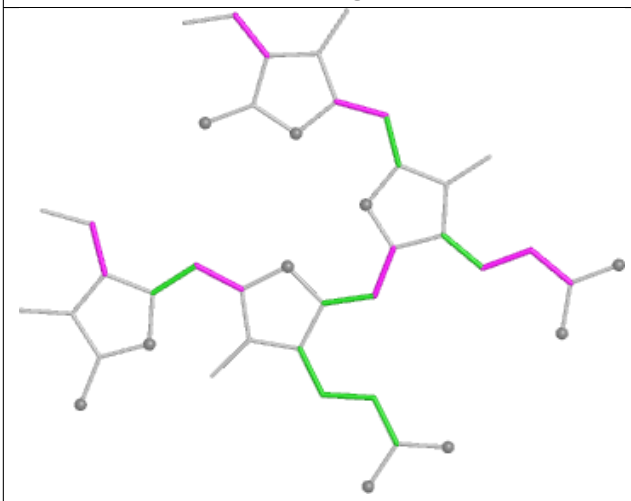


Bond angles



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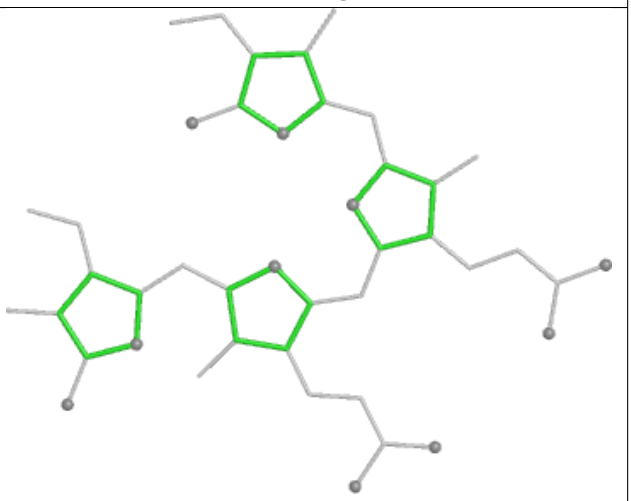
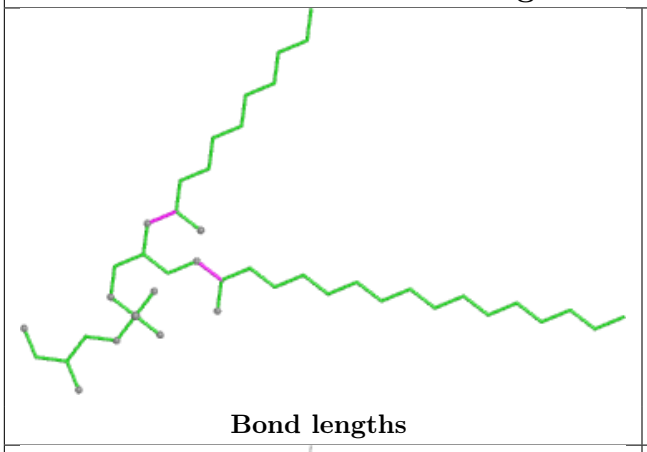


Rings

Ligand LHG aL 607



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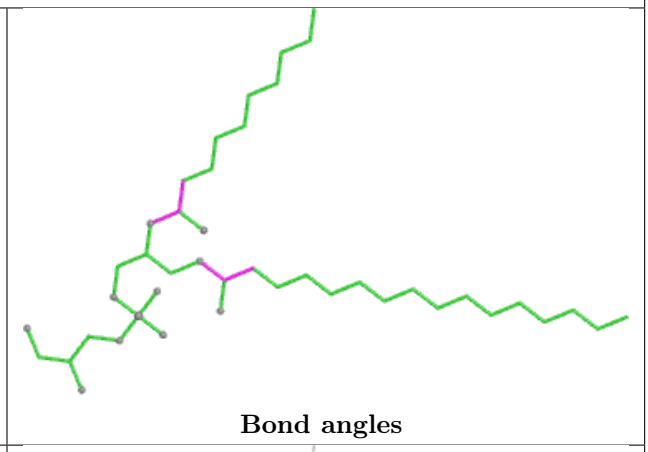

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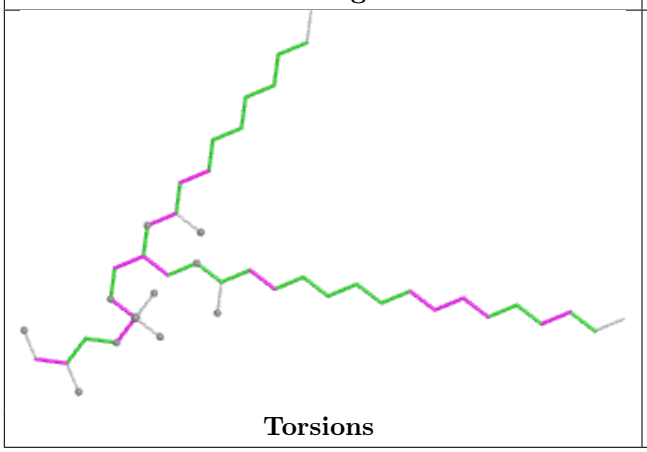

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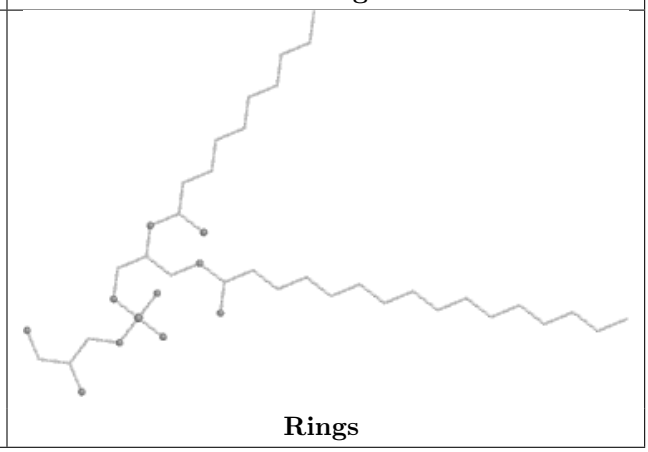
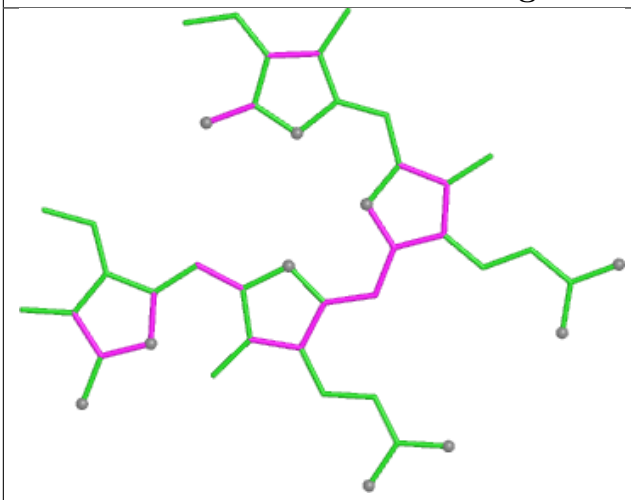


Rings

Ligand PEB PI 202



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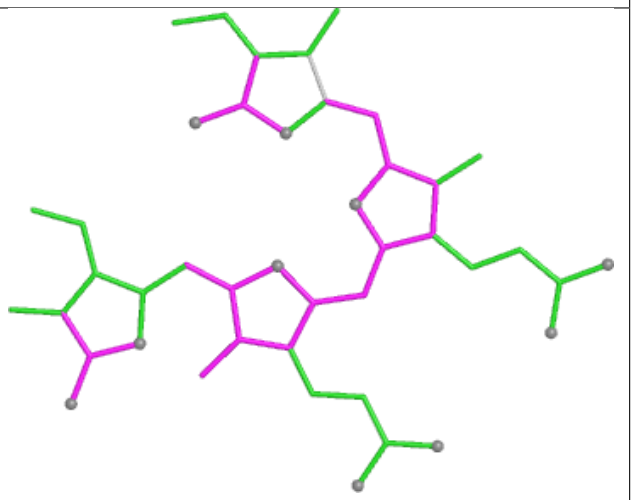
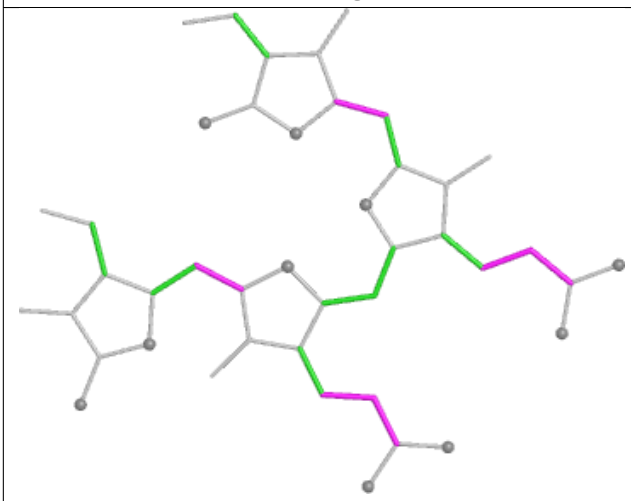


Bond angles



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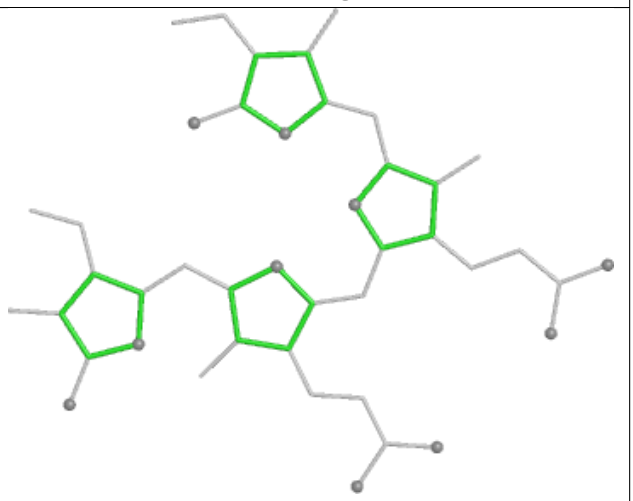
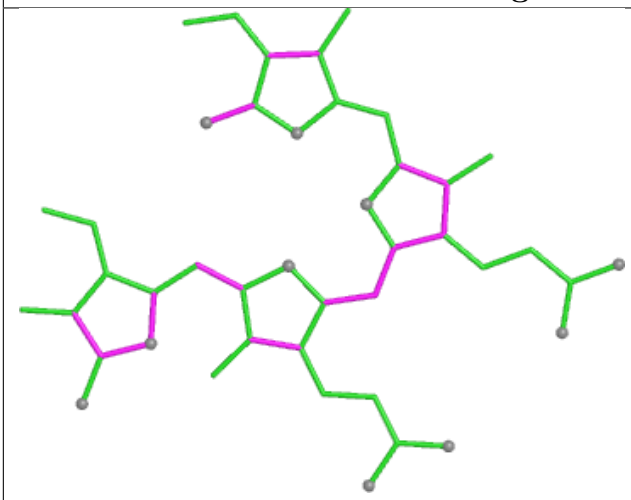


Rings

Ligand PEB CQ 202



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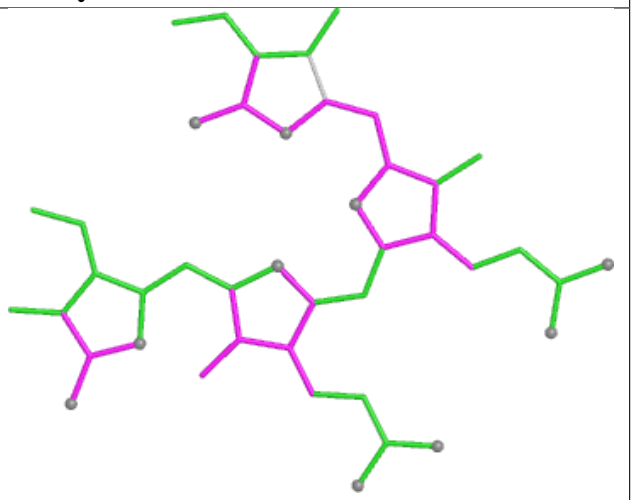

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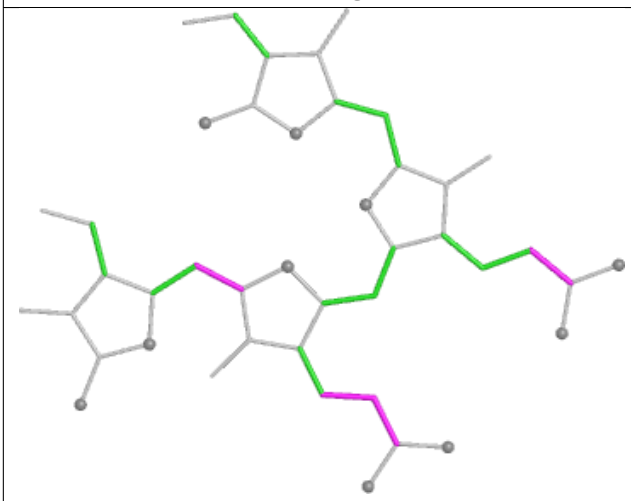

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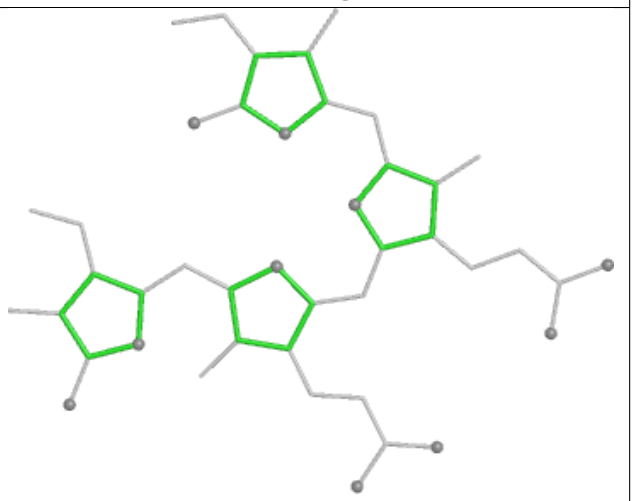
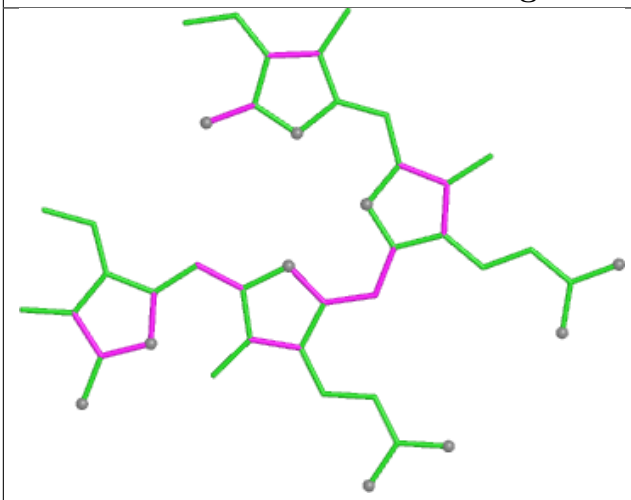


Rings

Ligand PEB IF 203



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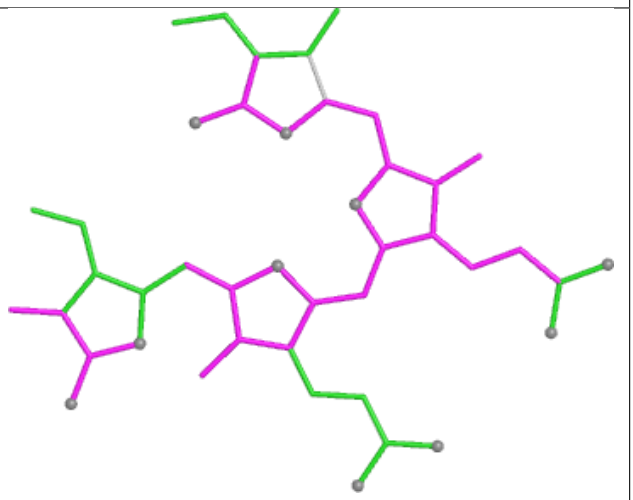

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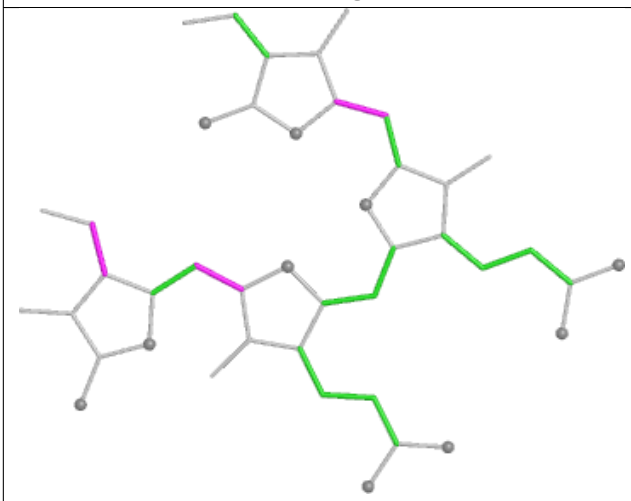

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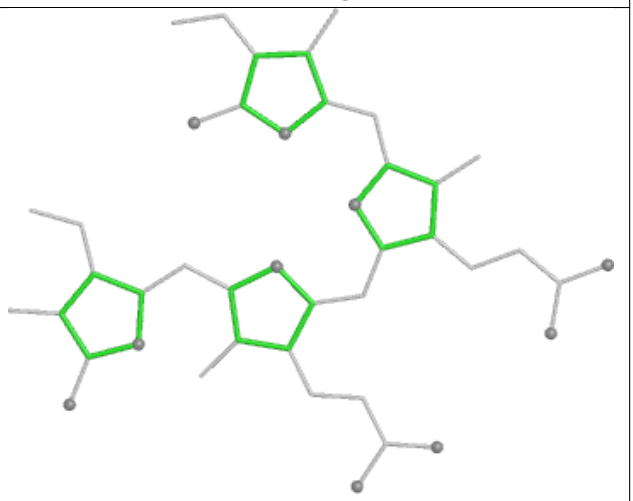
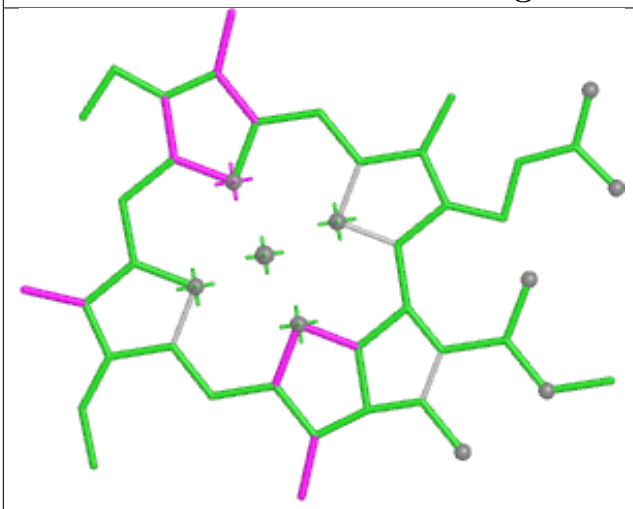


Rings

Ligand CLA A2 836



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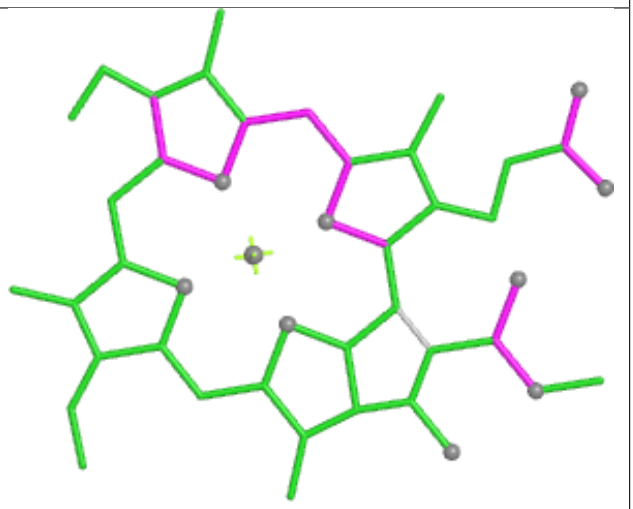
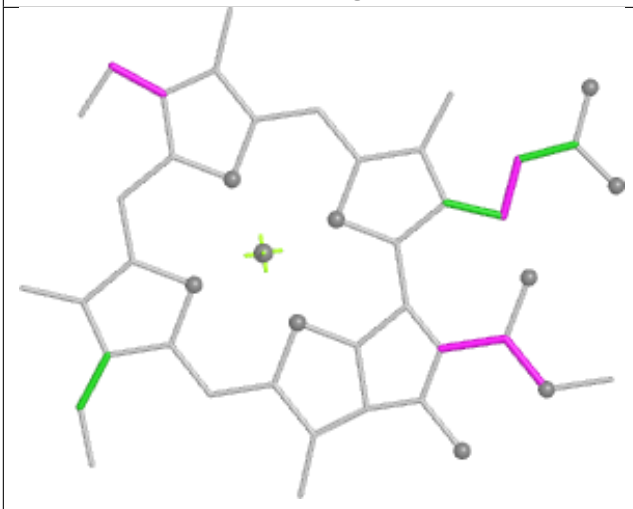


Bond angles

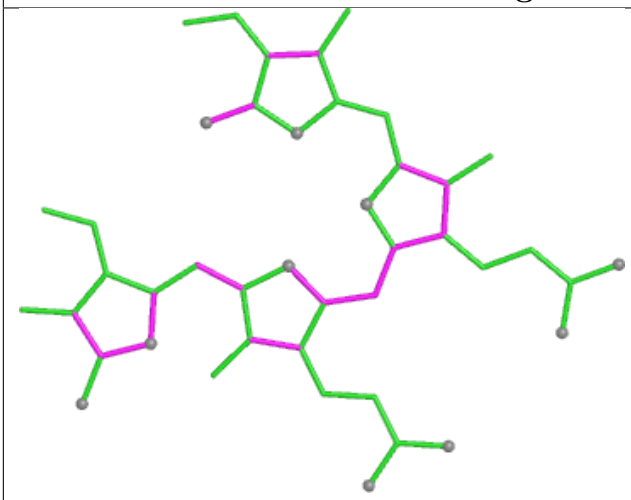


Torsions



Rings

Ligand PEB aO 202



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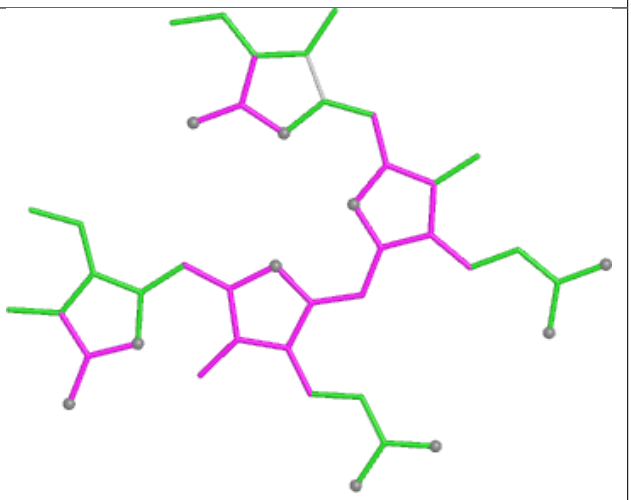

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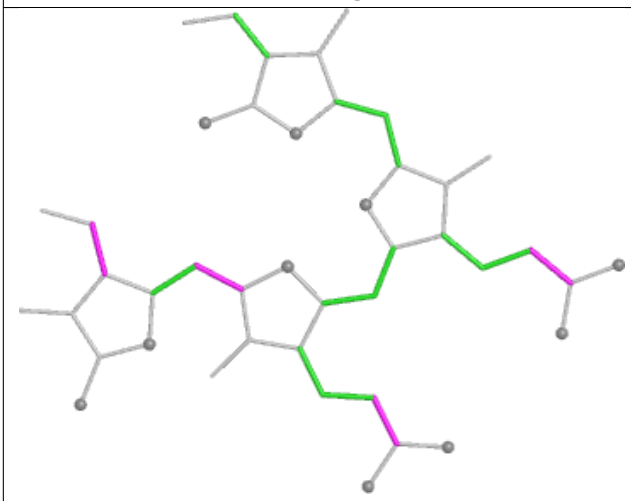

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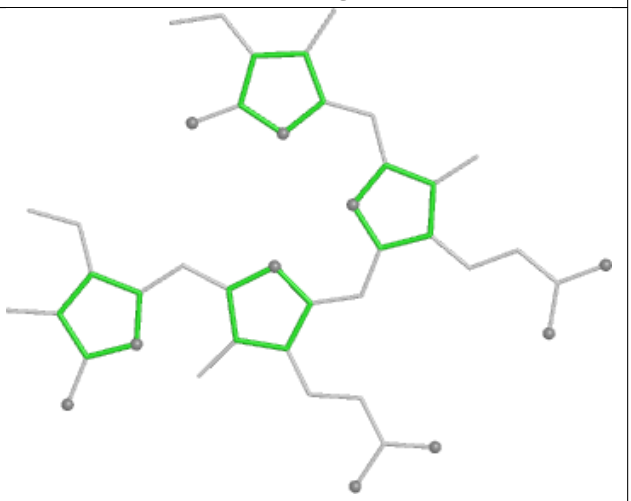
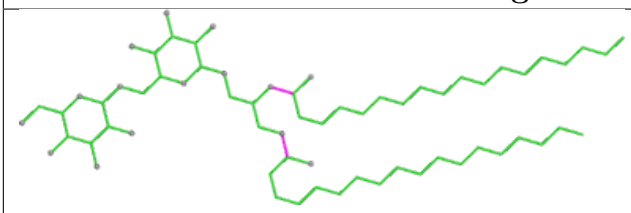


Rings

Ligand DGD B2 844



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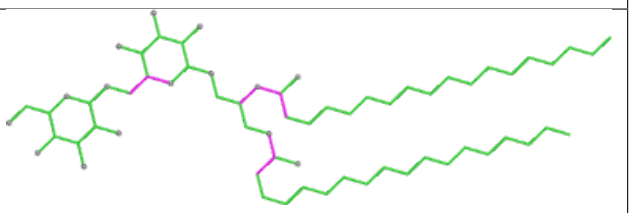
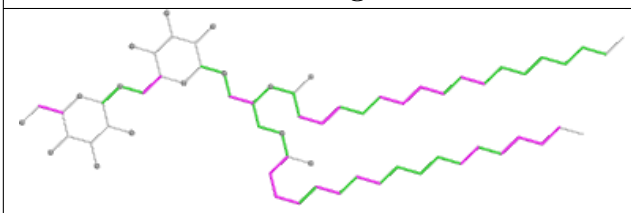


Bond angles



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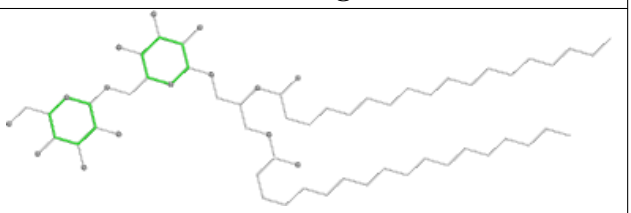
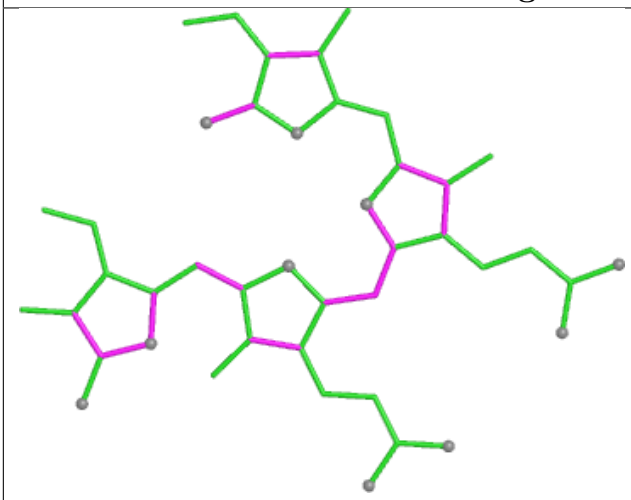


Rings

Ligand PEB eF 203



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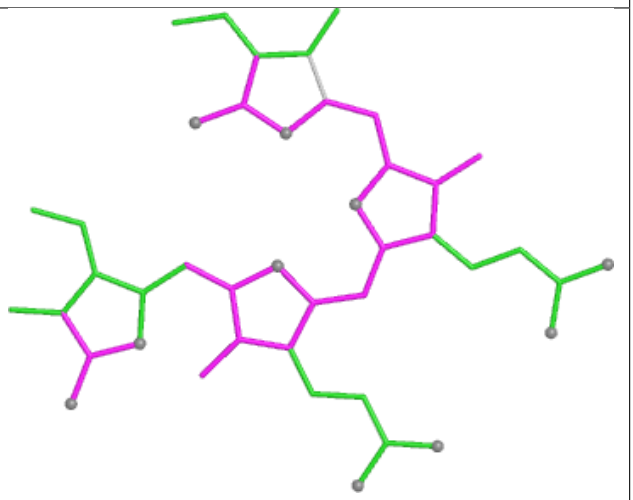

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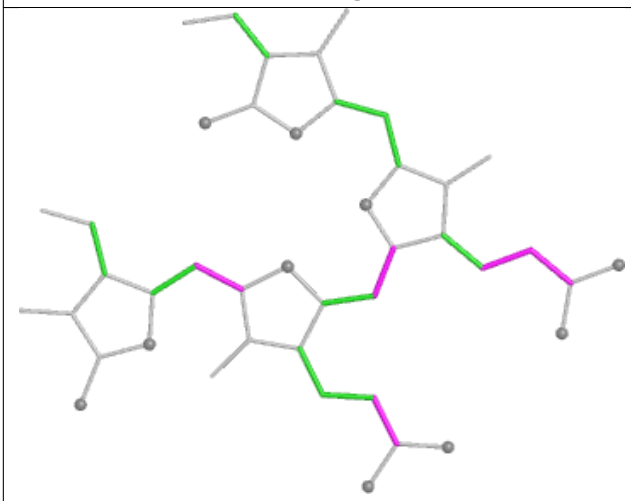

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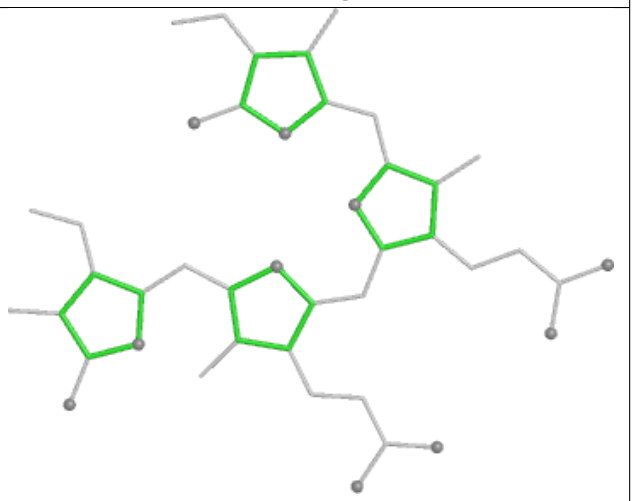
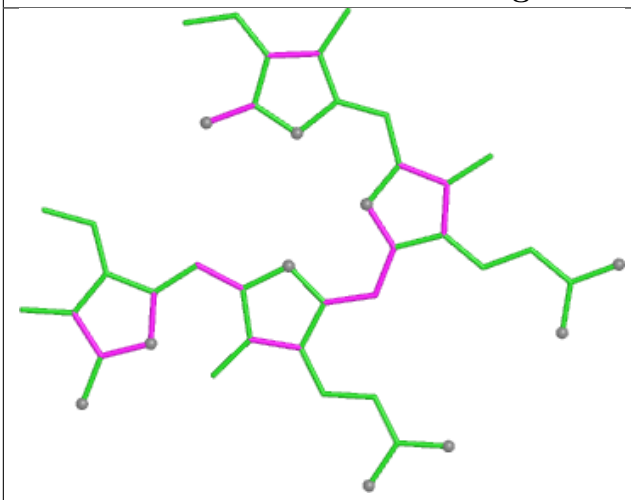


Rings

Ligand PEB OE 202



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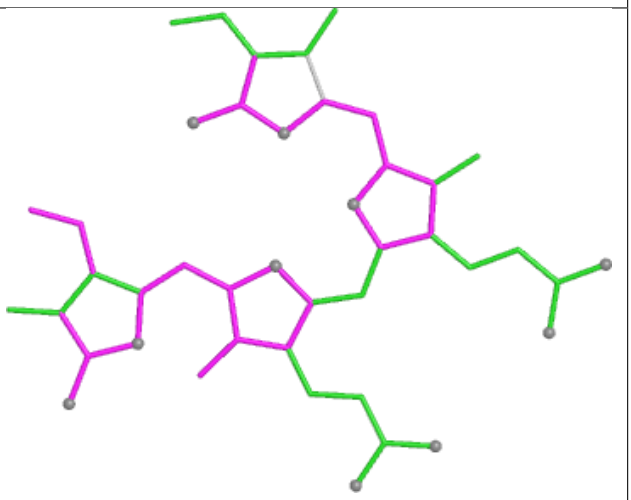
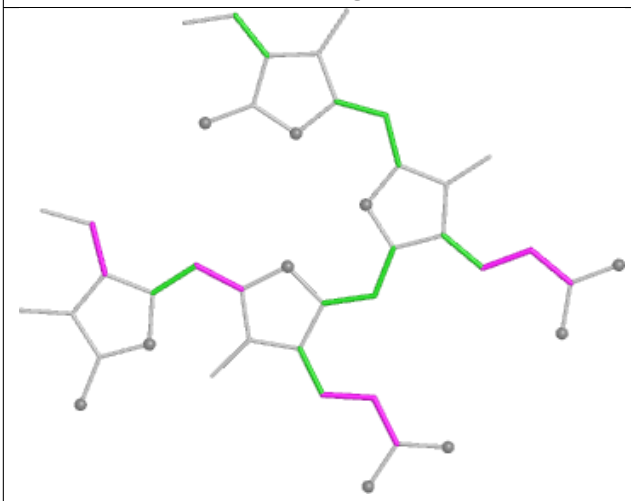


Bond angles



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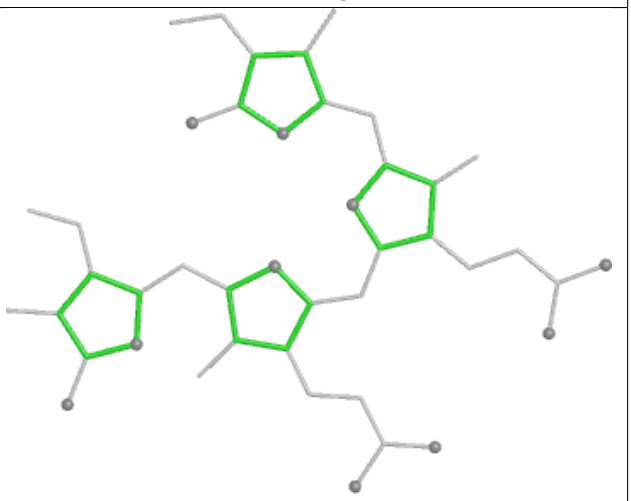
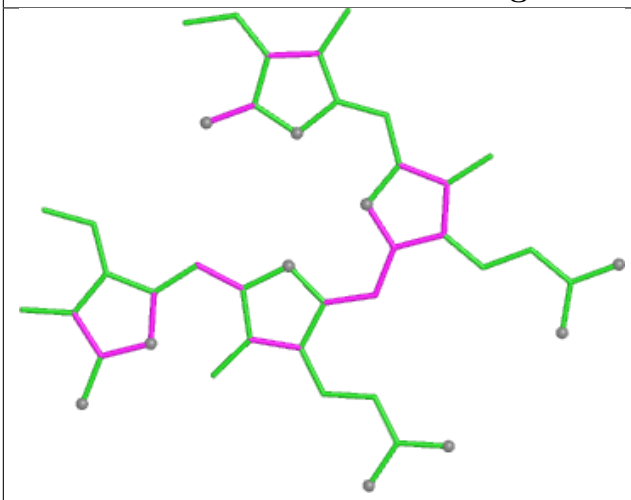


Rings

Ligand PEB WJ 202



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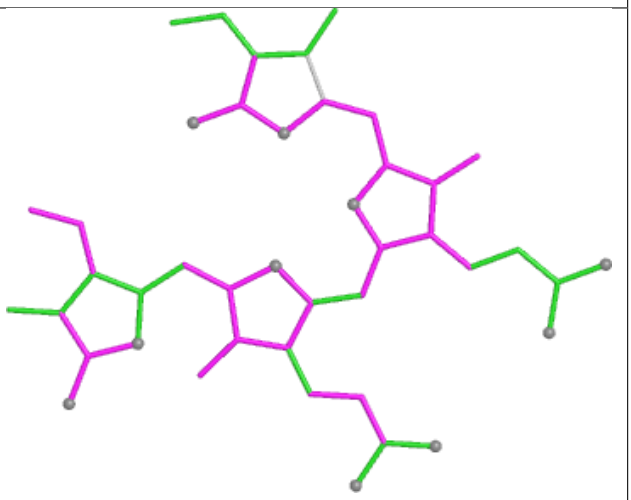
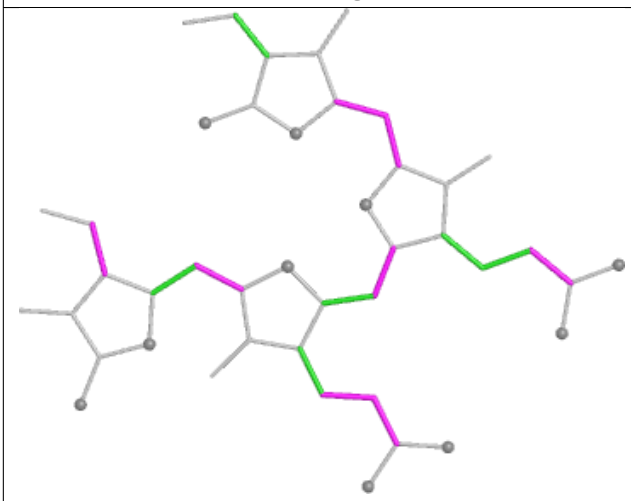


Bond angles



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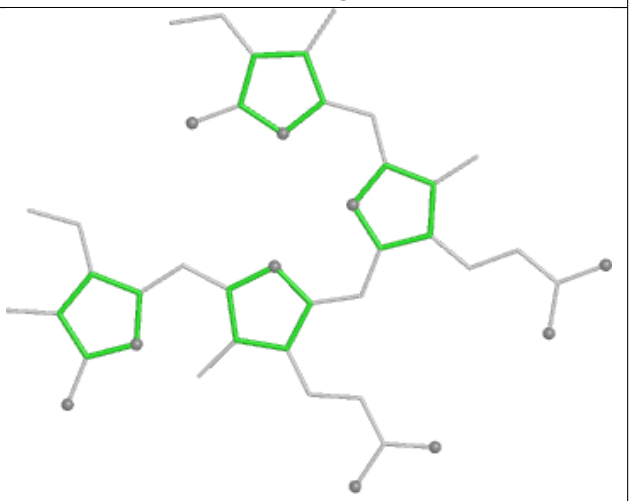
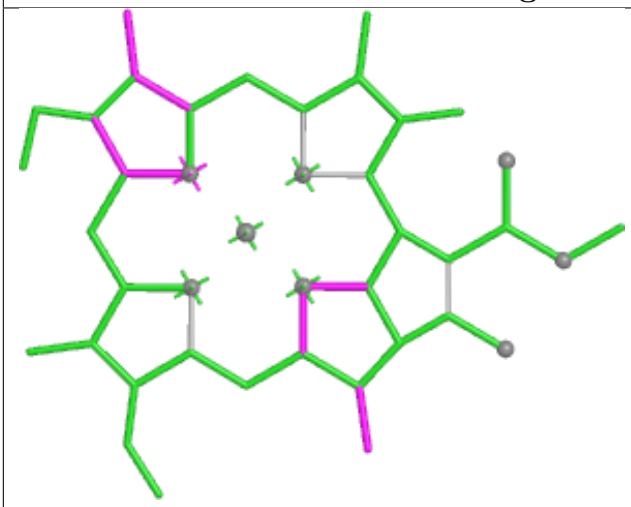


Rings

Ligand CLA 62 310



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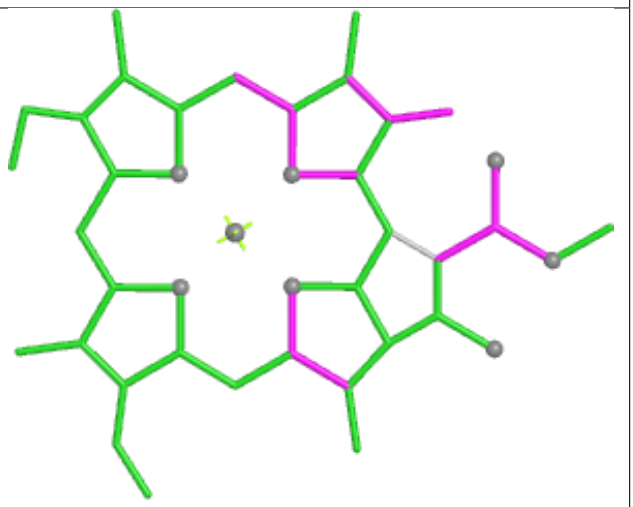
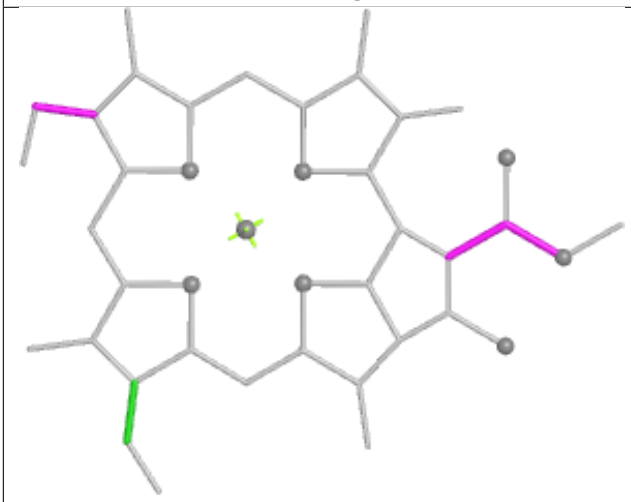


Bond angles



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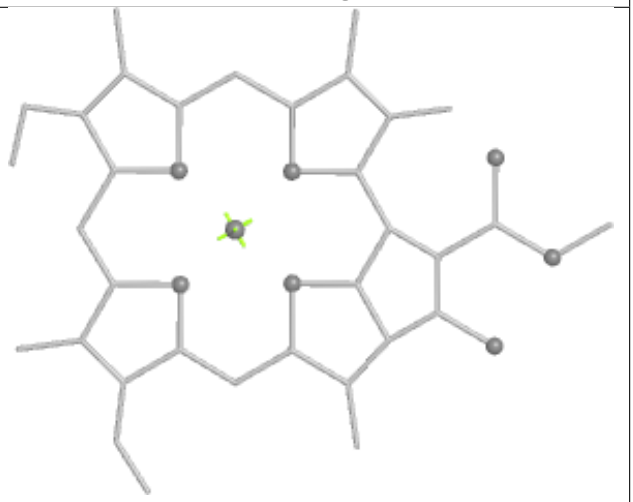
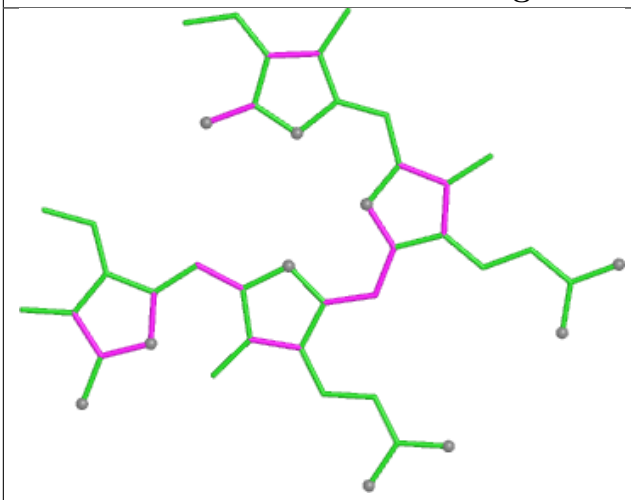


Rings

Ligand PEB AF 201



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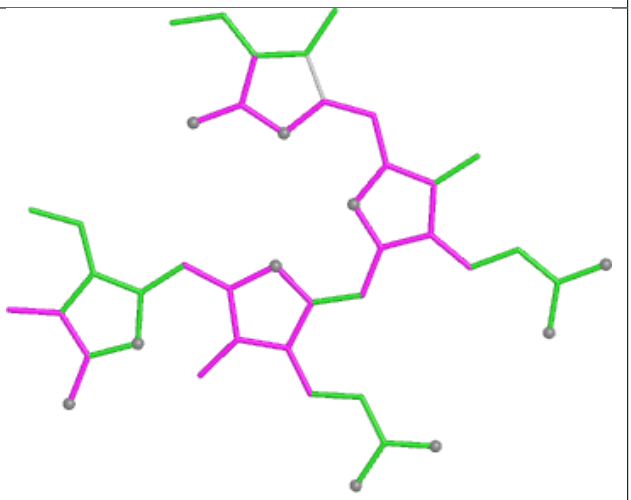

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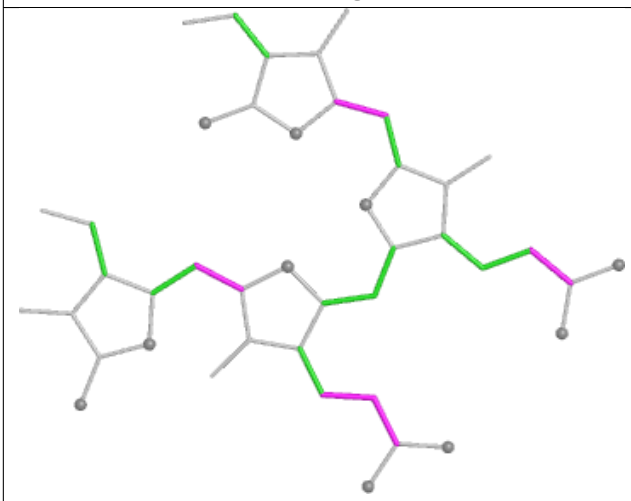

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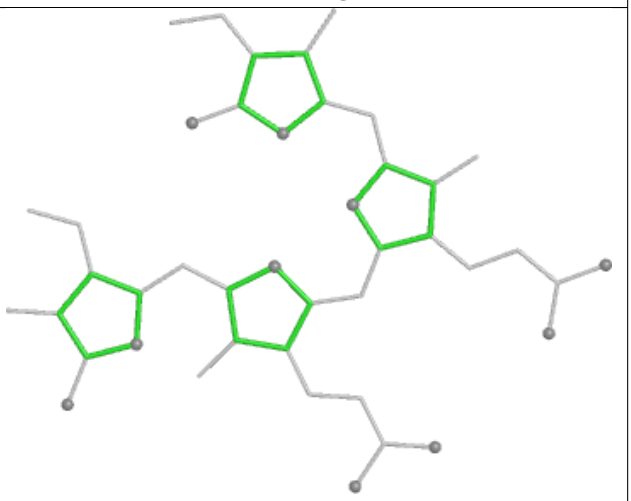
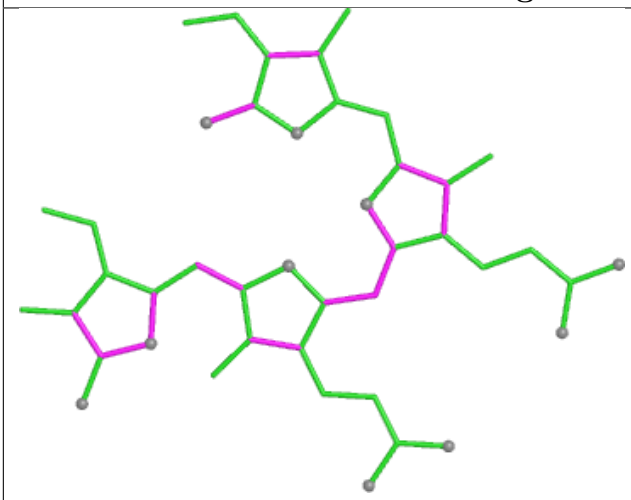


Rings

Ligand PEB T7 203



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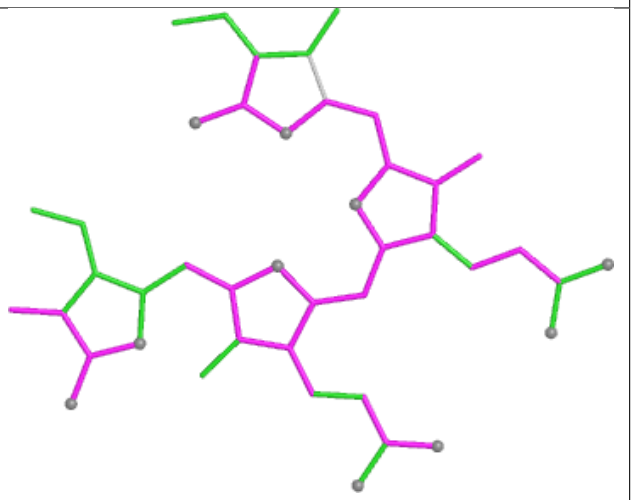

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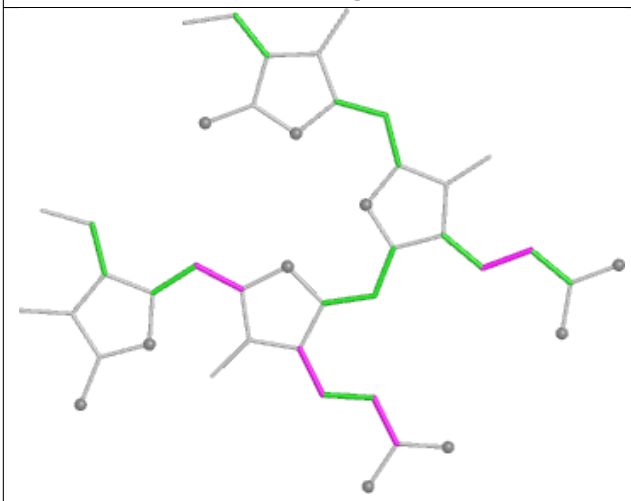

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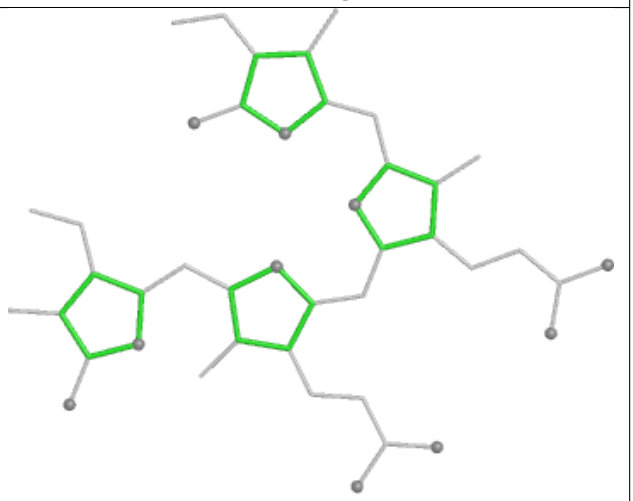
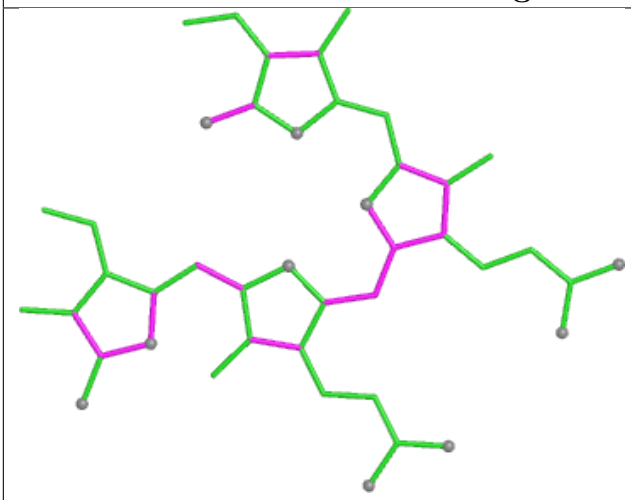


Rings

Ligand PEB LA 201



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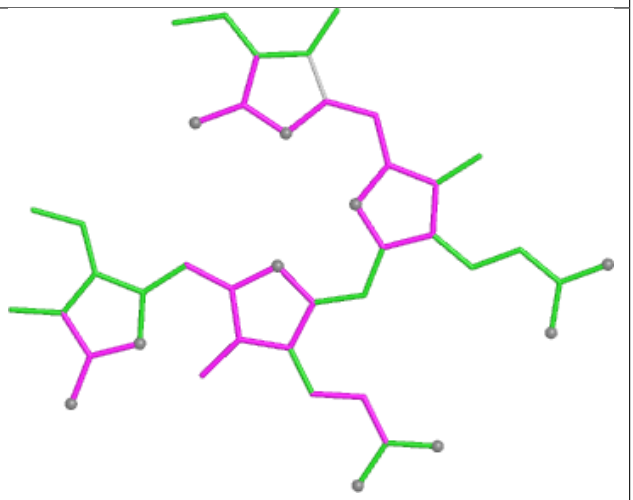

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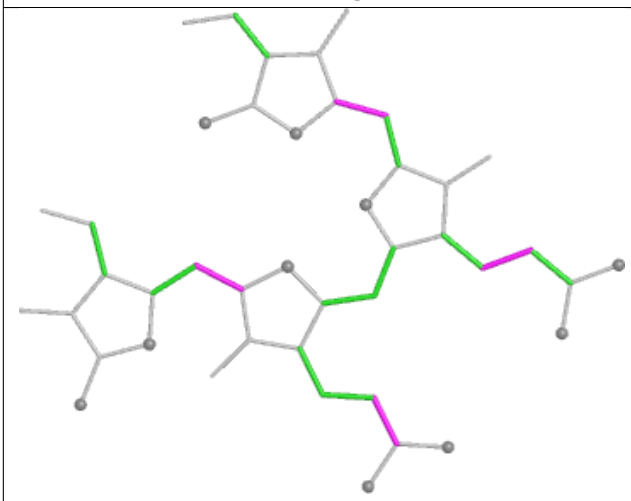

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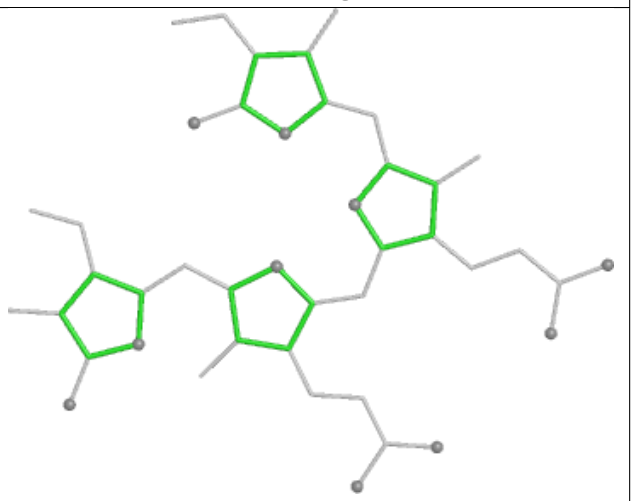
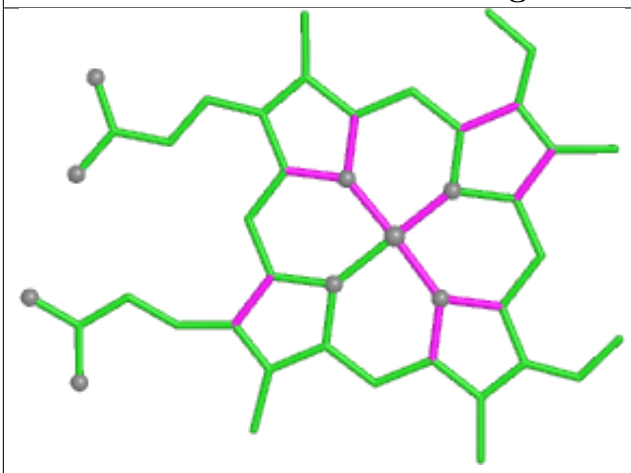


Rings

Ligand HEM V6 201



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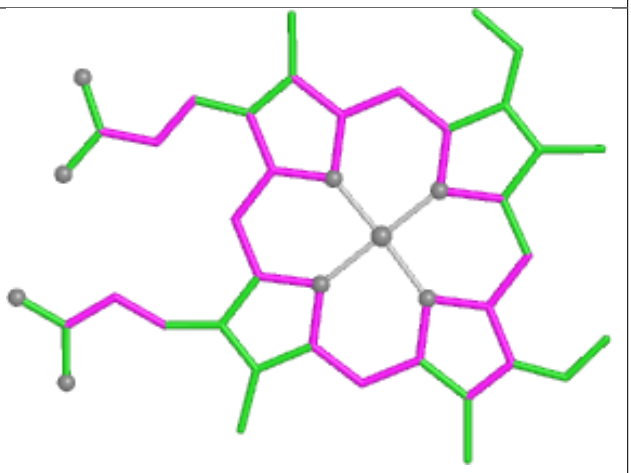

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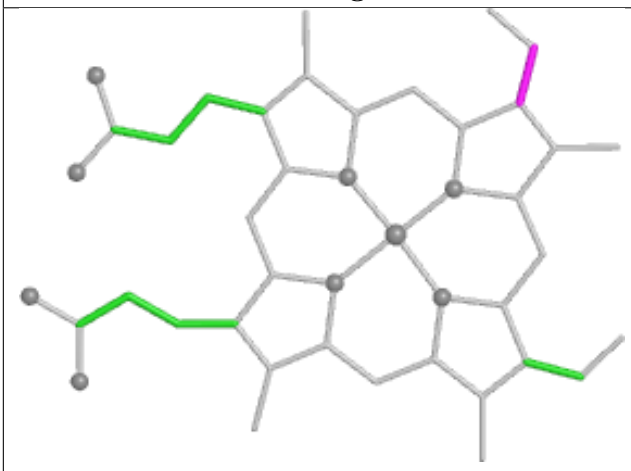

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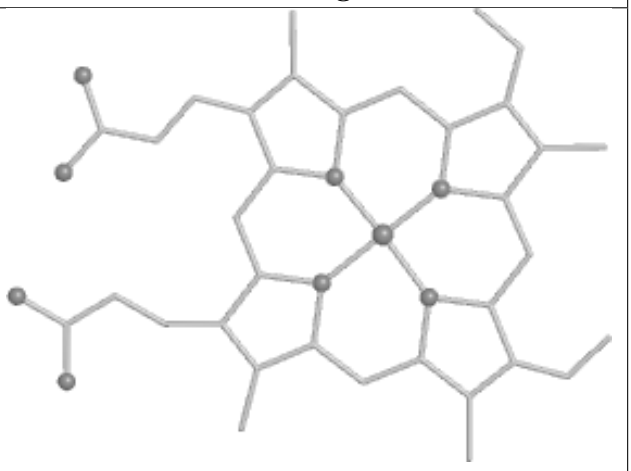
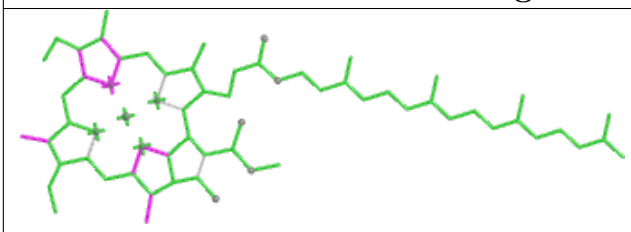


Rings

Ligand CLA A2 839



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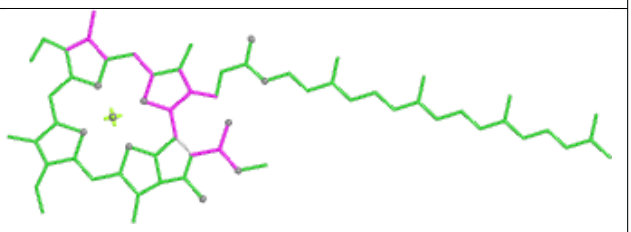

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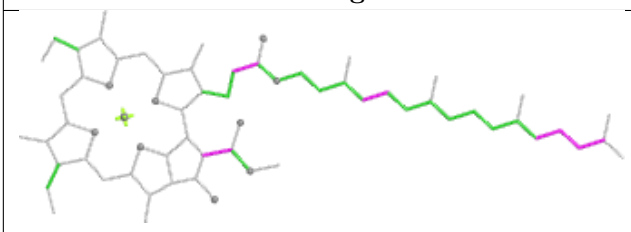

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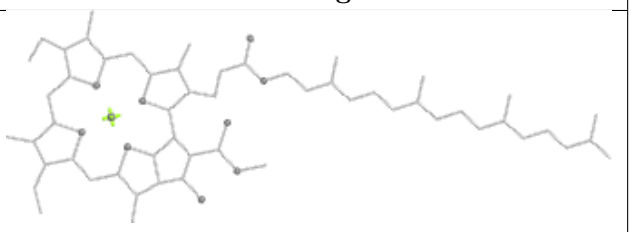
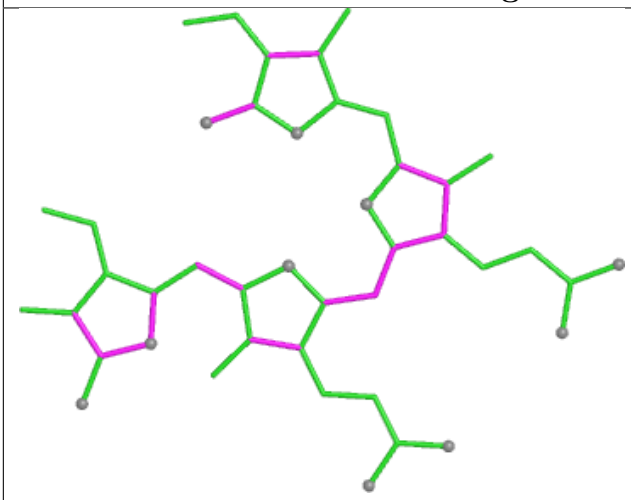


Rings

Ligand PEB DO 1002



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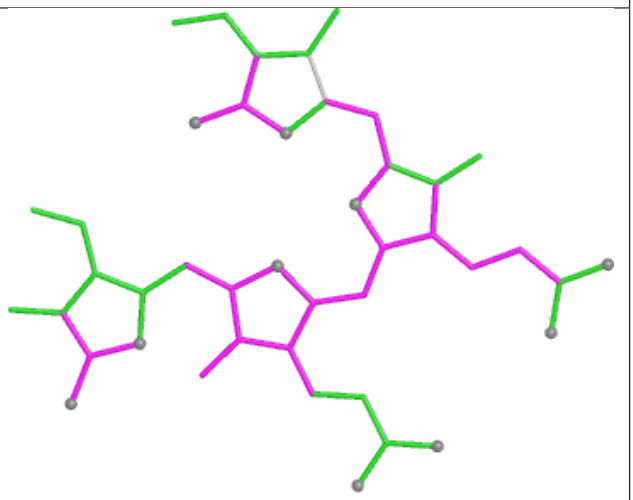

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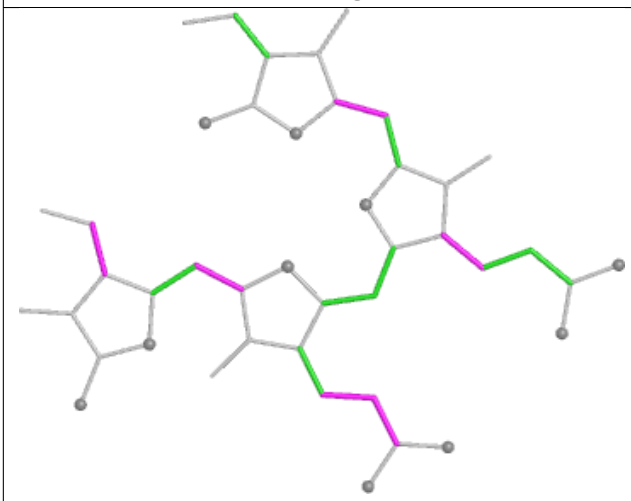

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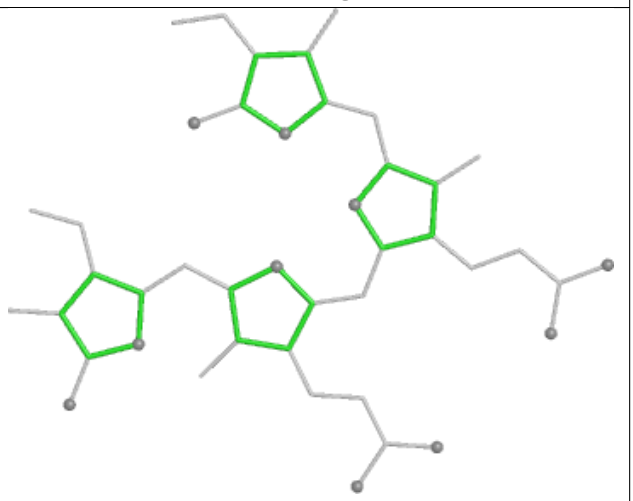
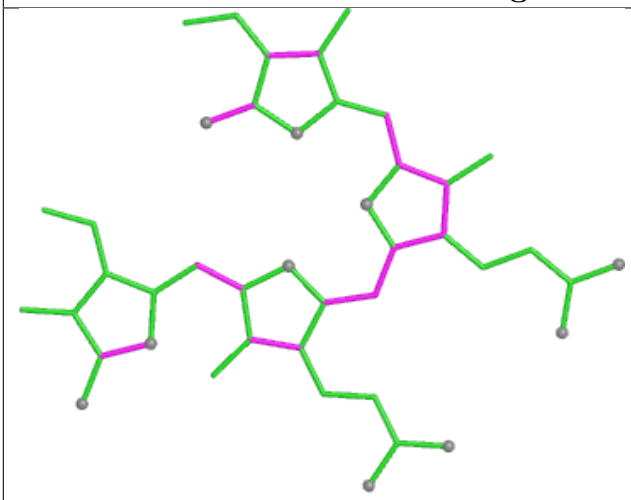


Rings

Ligand PEB ND 204



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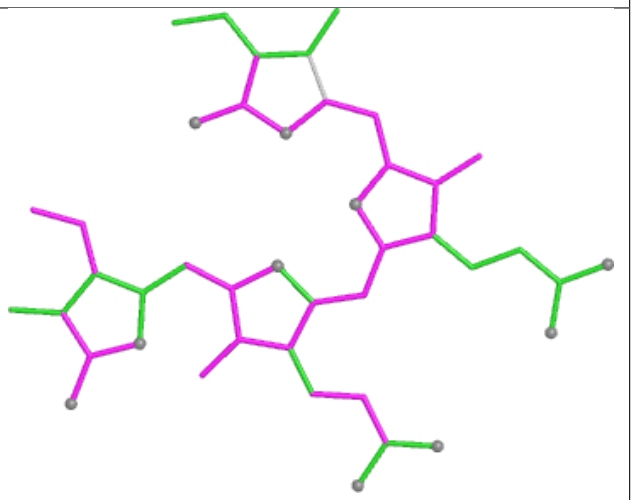

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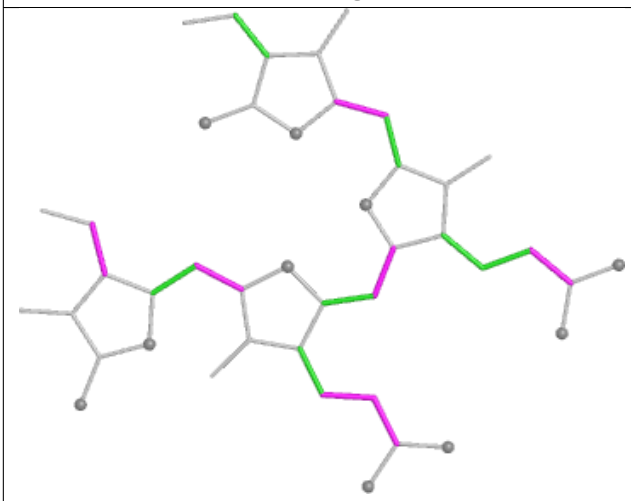

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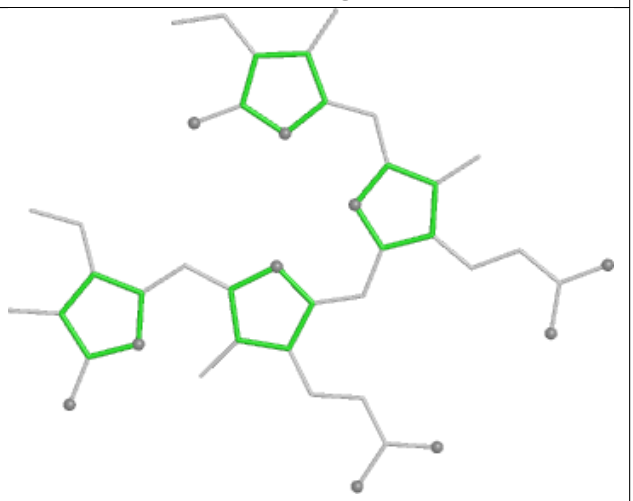
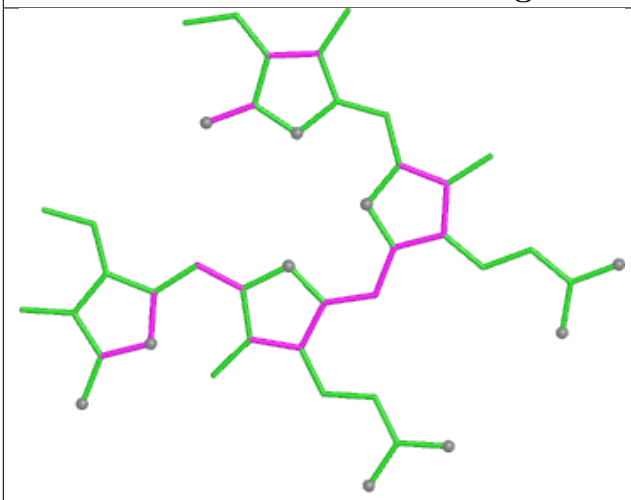


Rings

Ligand PEB G7 202



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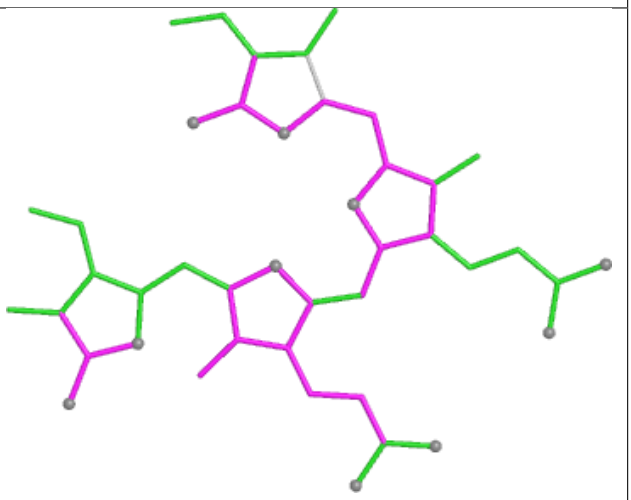

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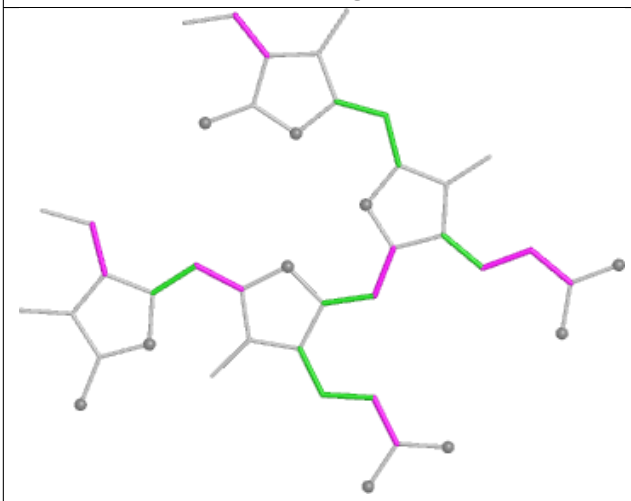

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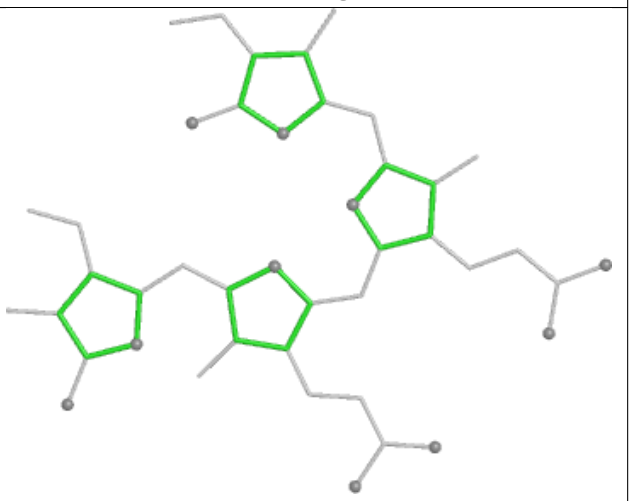
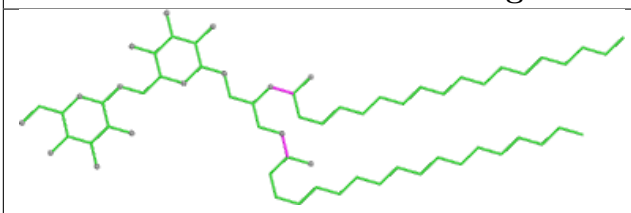


Rings

Ligand DGD BN 844



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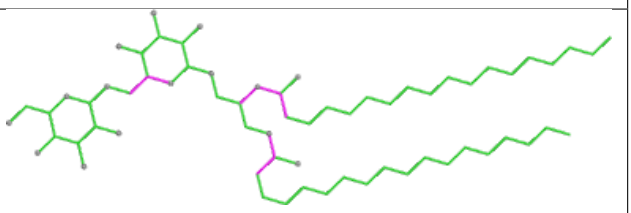

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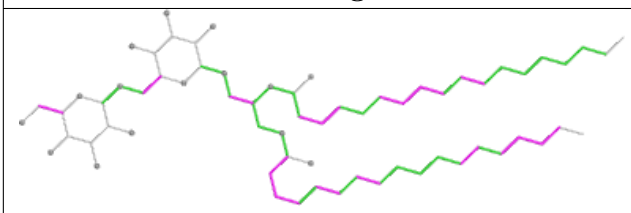

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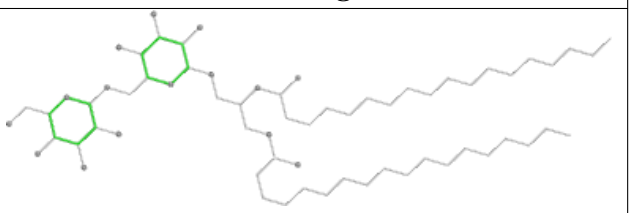
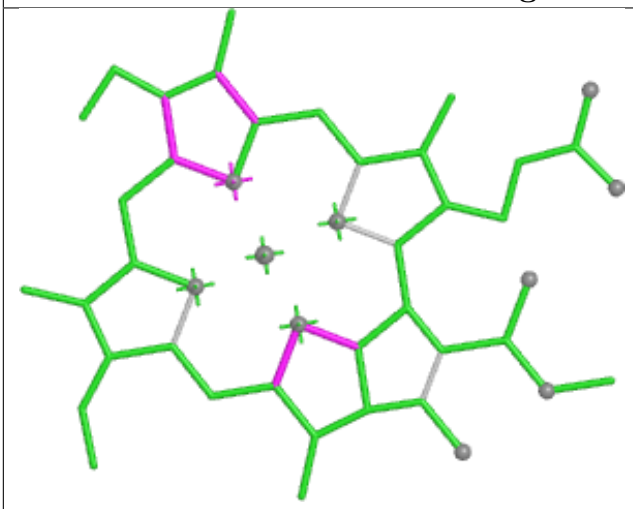


Rings

Ligand CLA 22 601



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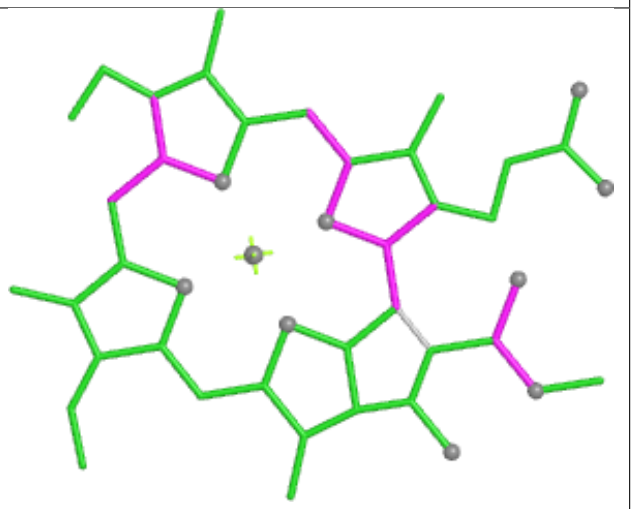

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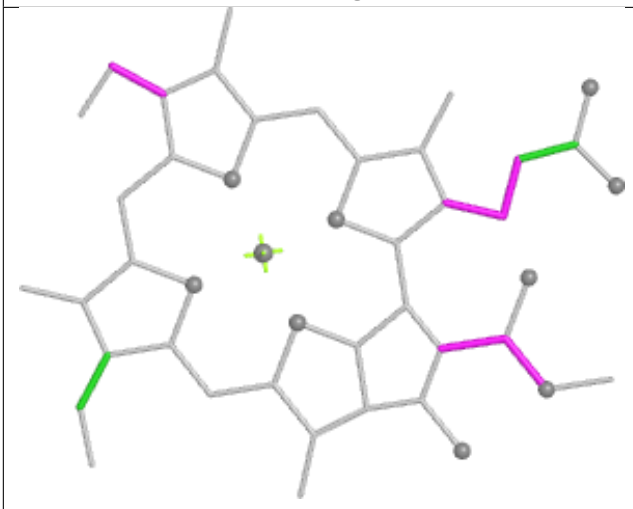
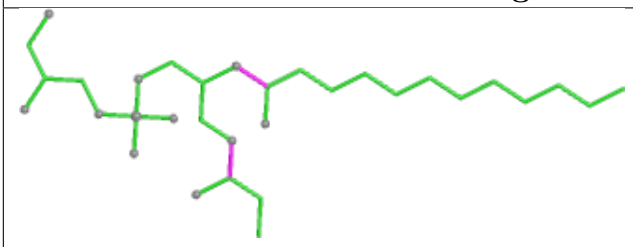


Torsions



Rings

Ligand LHG CL 522



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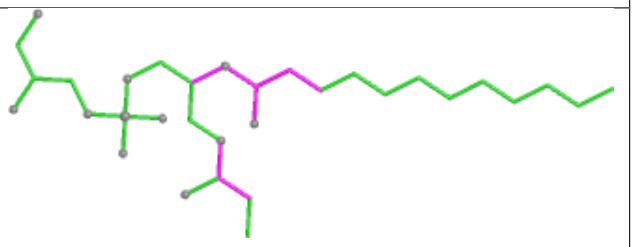
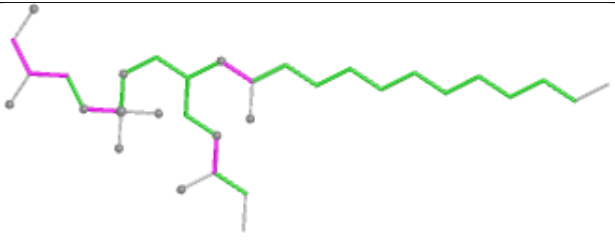


Bond angles



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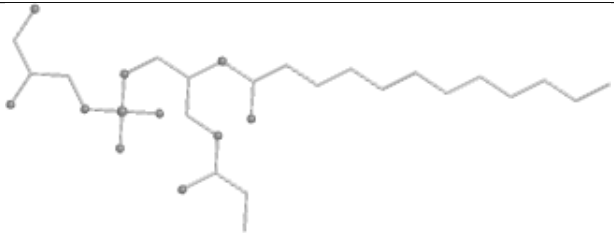
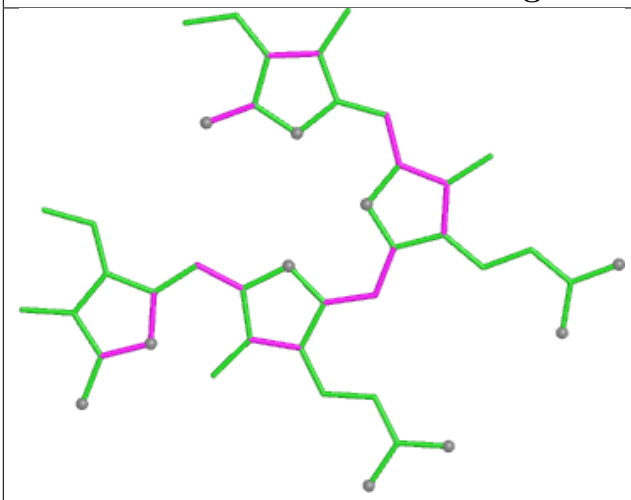


Rings

Ligand PEB f1 202



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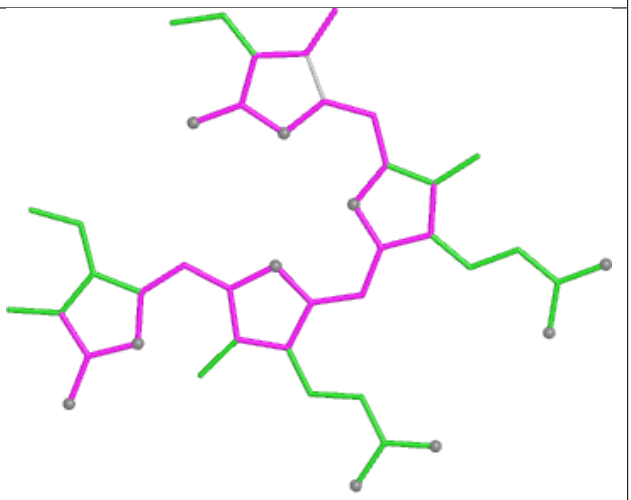
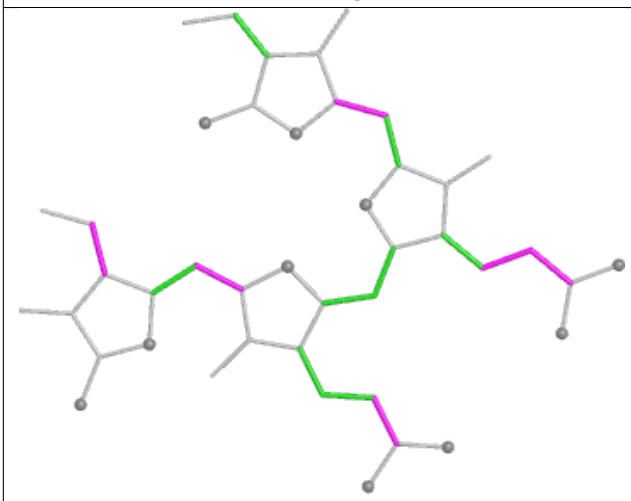


Bond angles



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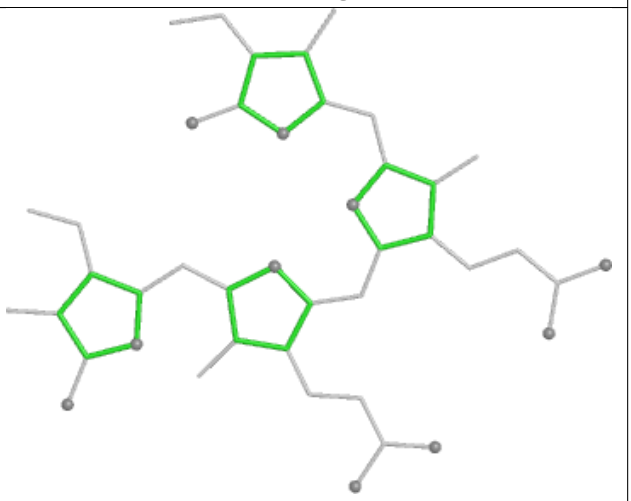
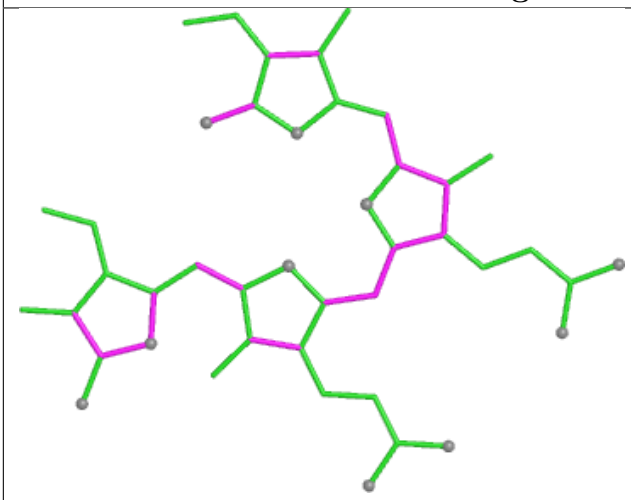


Rings

Ligand PEB TO 202



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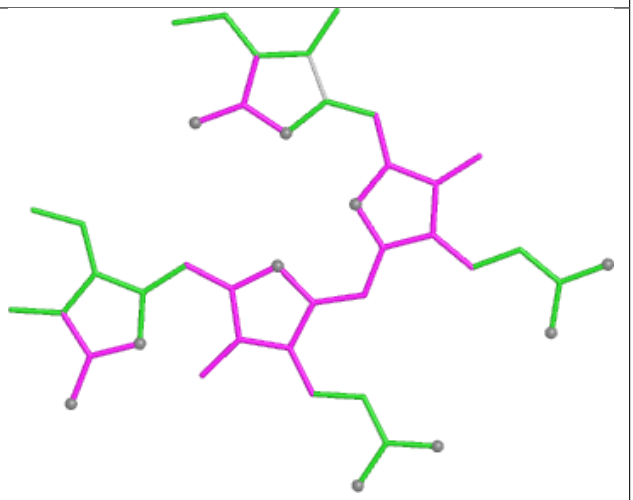
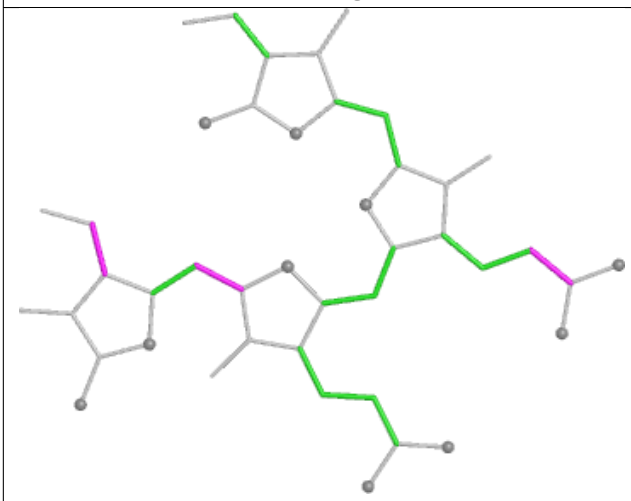


Bond angles



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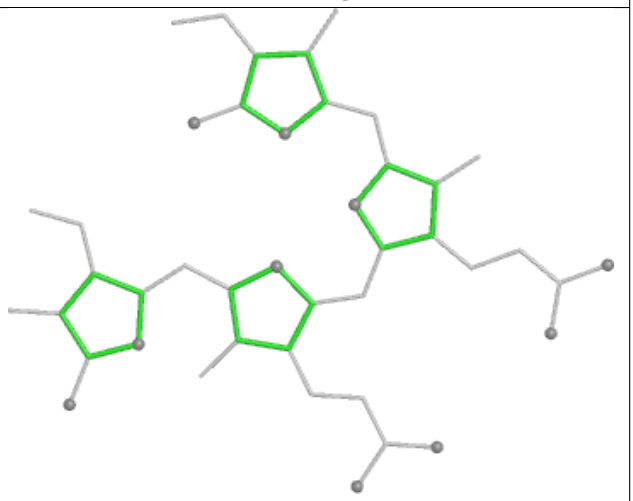
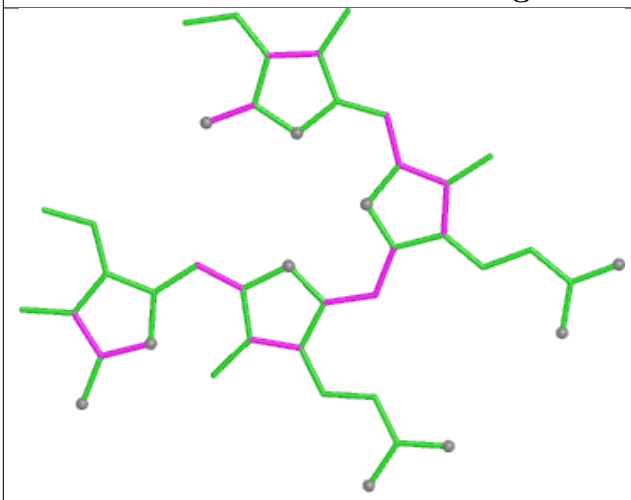


Rings

Ligand PEB ZH 201



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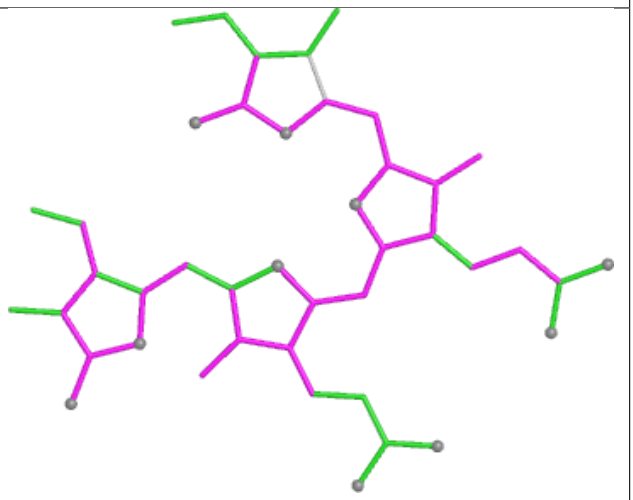
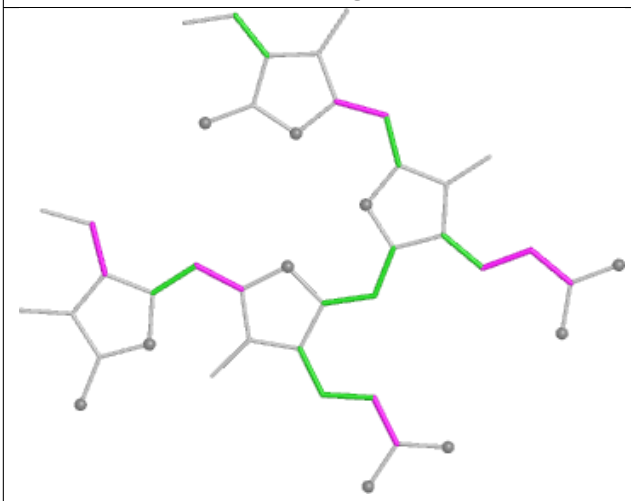


Bond angles



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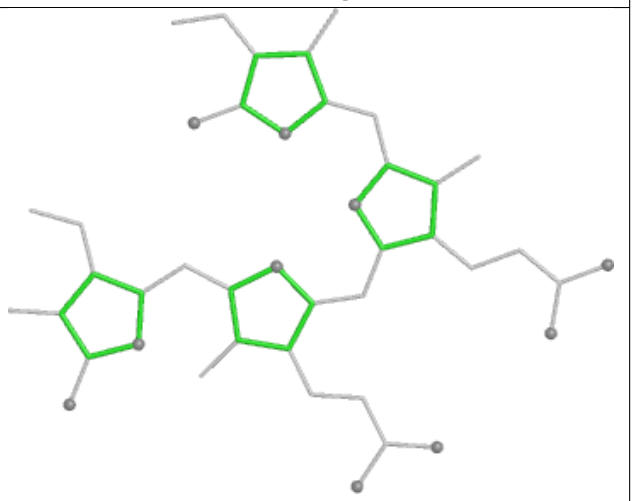
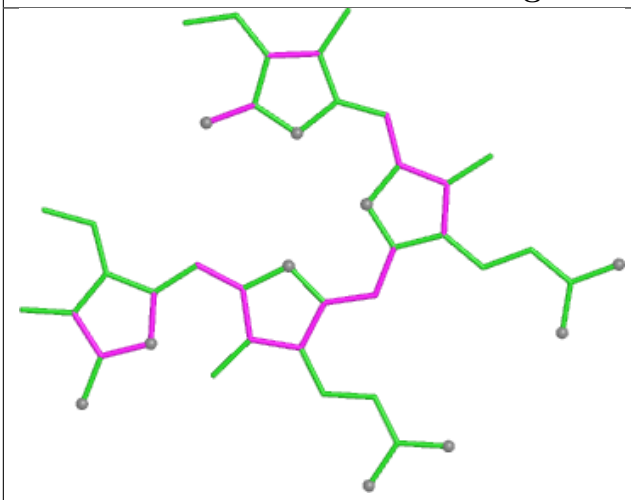
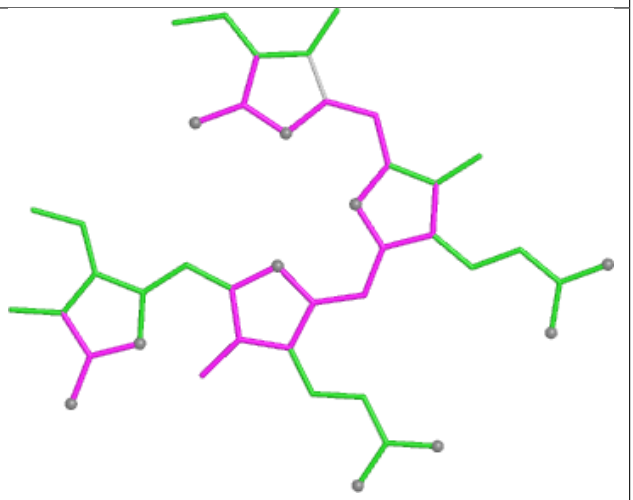


Rings

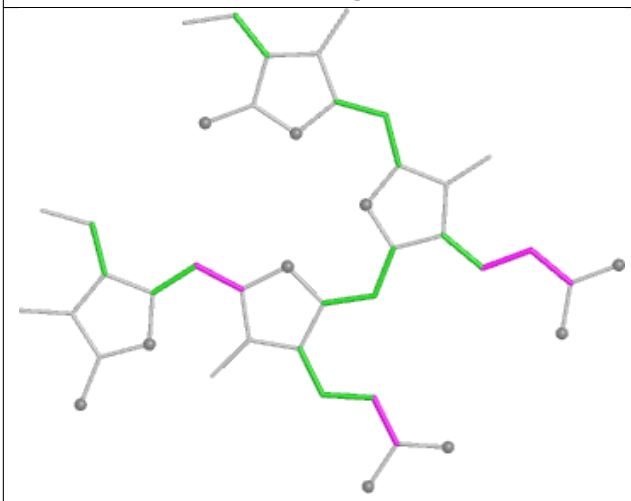
Ligand PEB i1 201



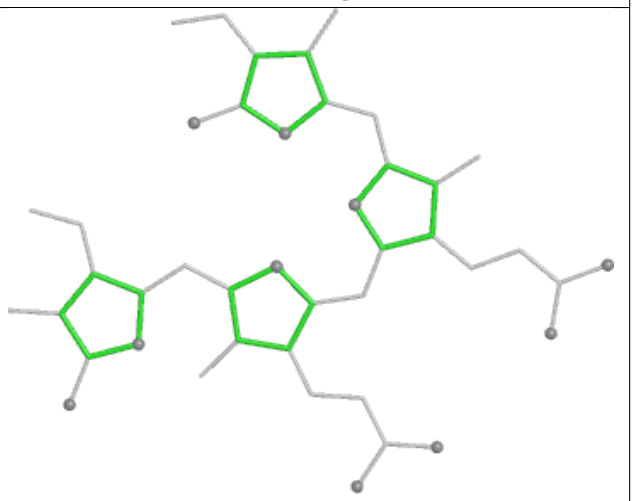
Bond lengths



Bond angles

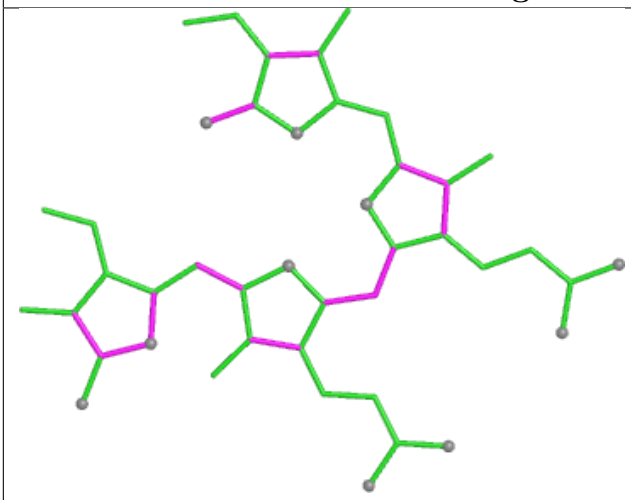


Torsions



Rings

Ligand PEB RP 202



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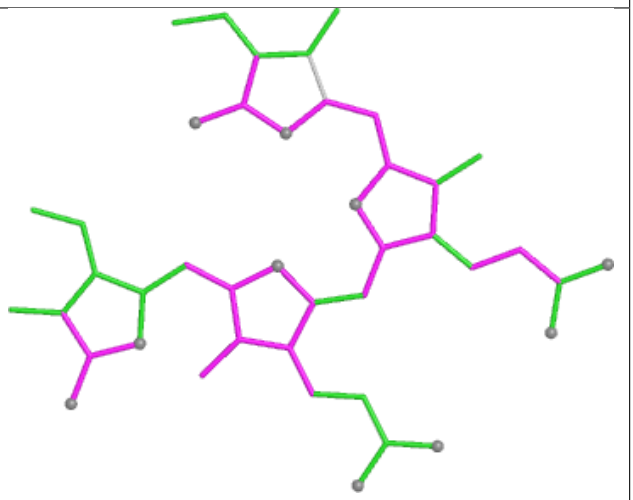

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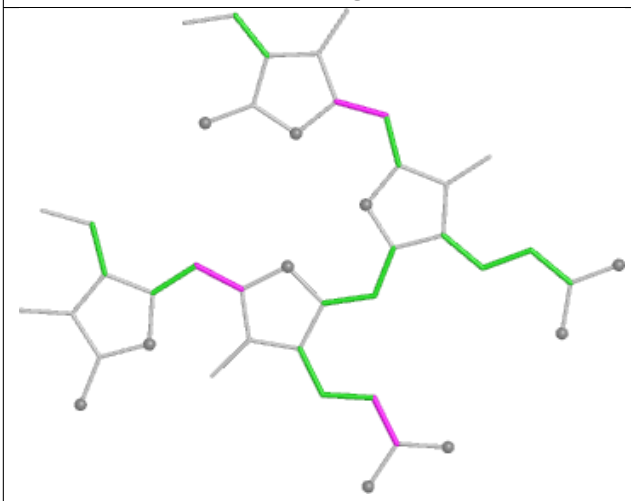

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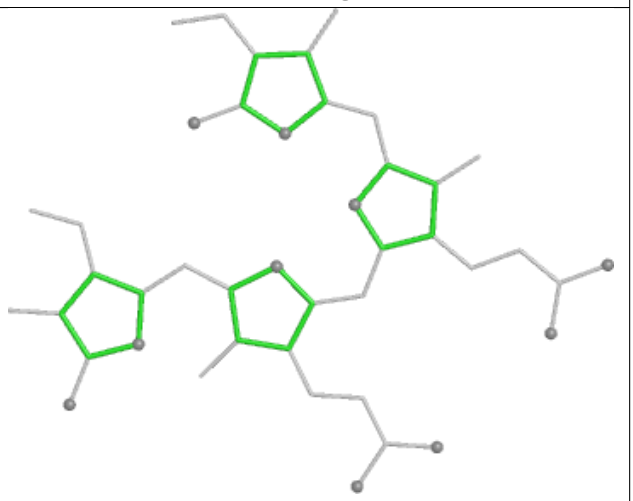
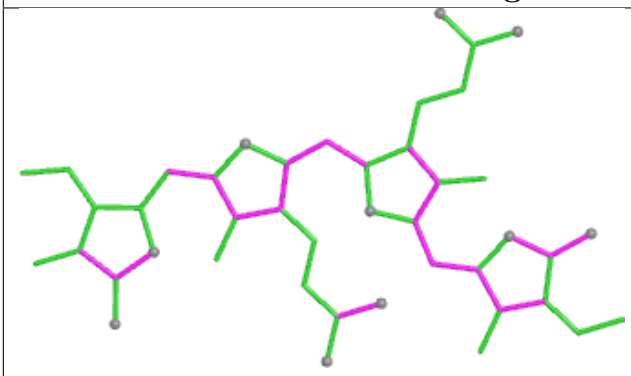


Rings

Ligand CYC O3 1001



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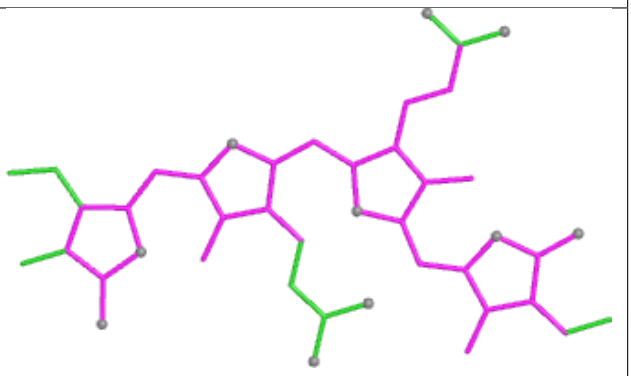

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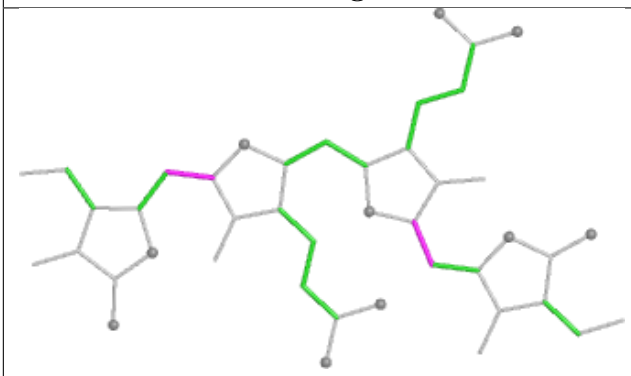

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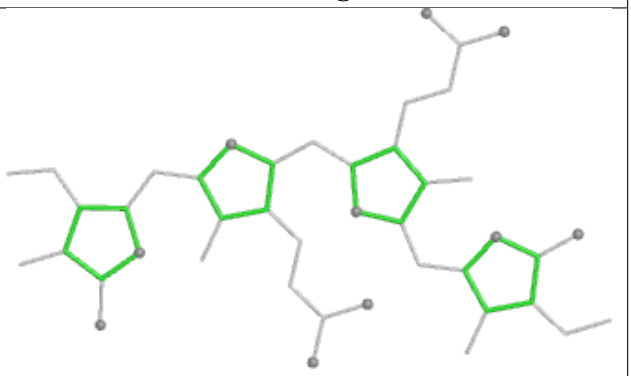
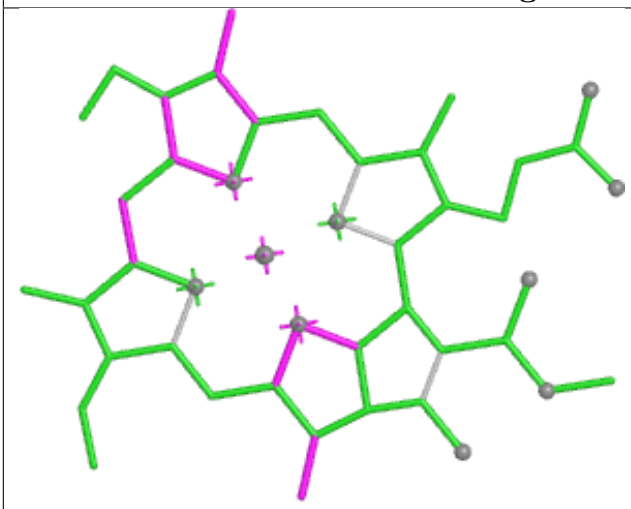


Rings

Ligand CLA 72 606



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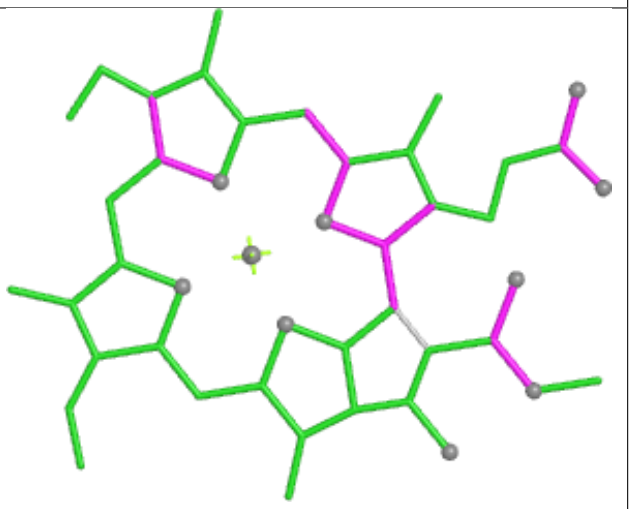

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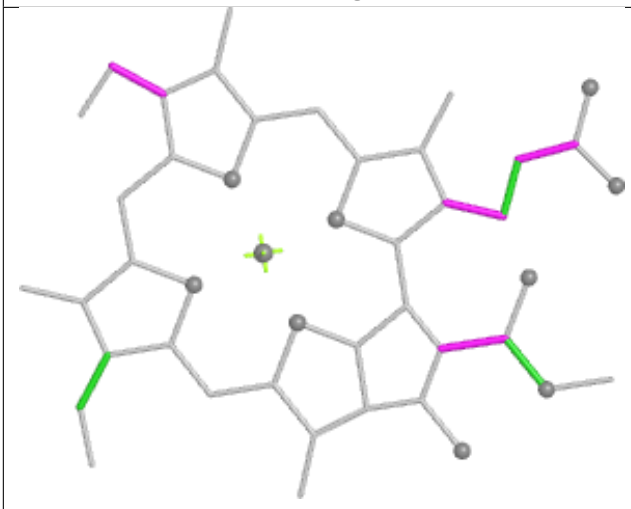
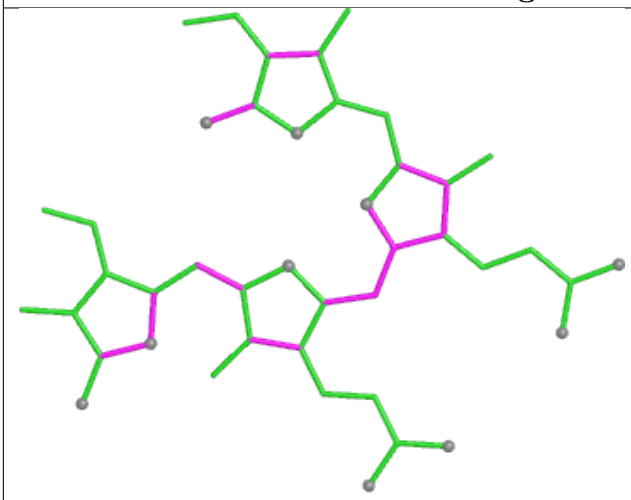


Torsions



Rings

Ligand PEB L7 203



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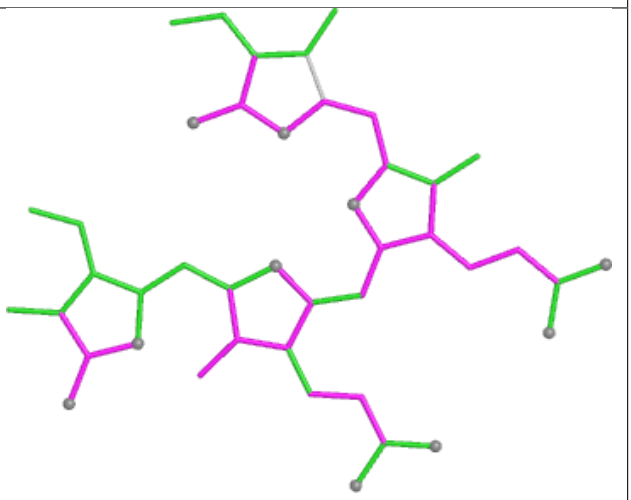
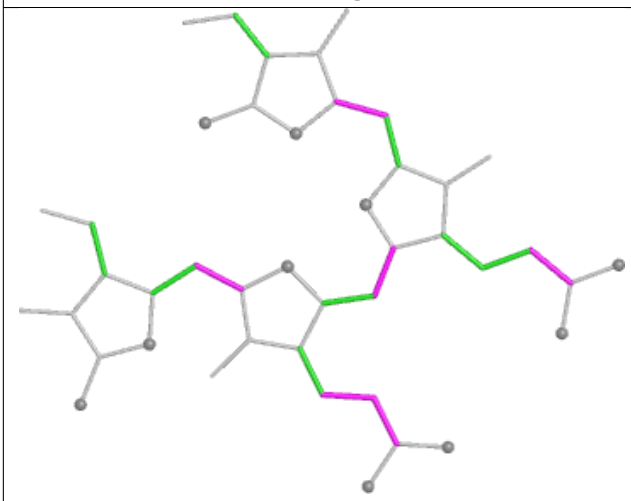


Bond angles



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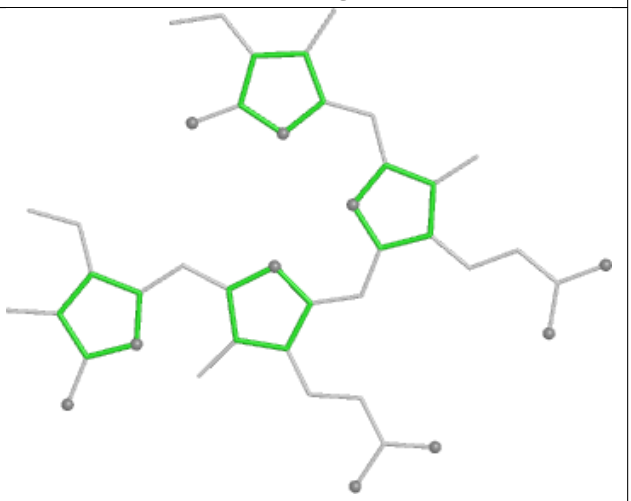
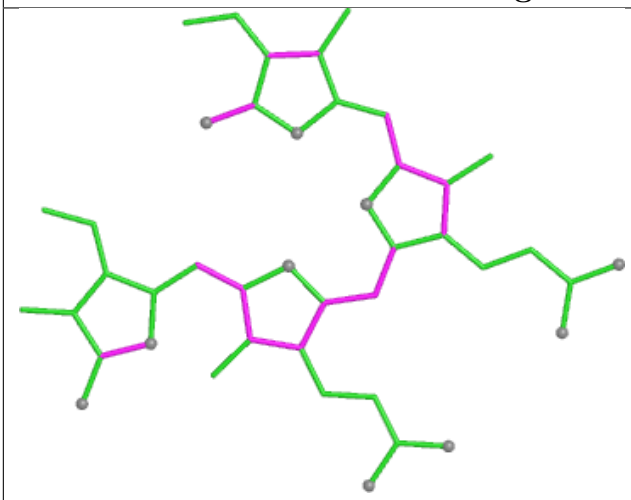


Rings

Ligand PEB oK 201



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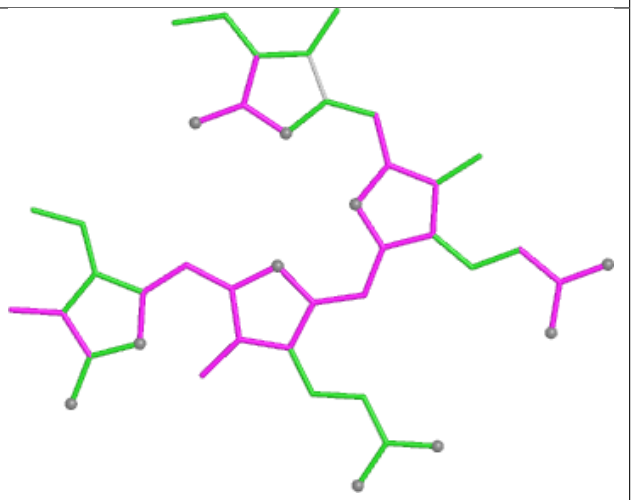

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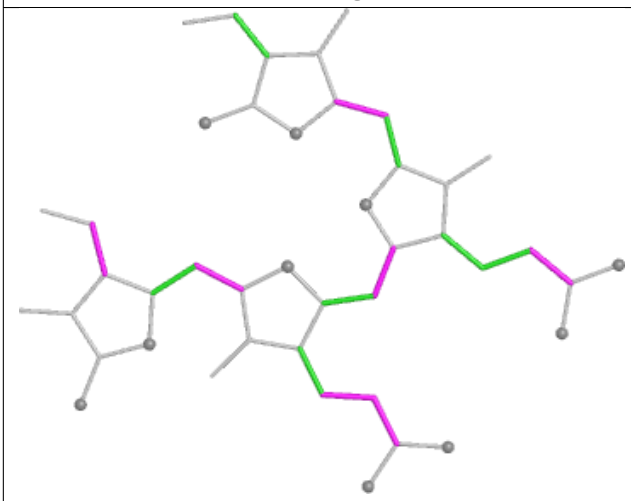

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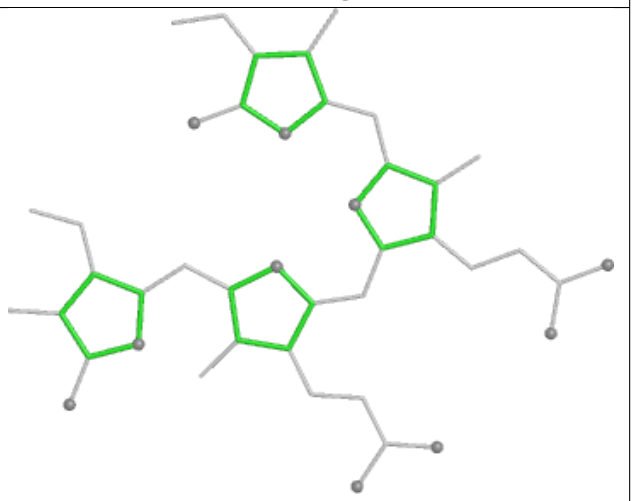
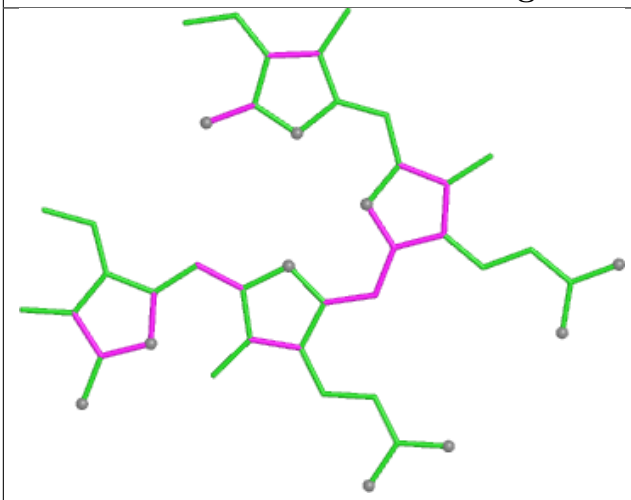


Rings

Ligand PEB LJ 202



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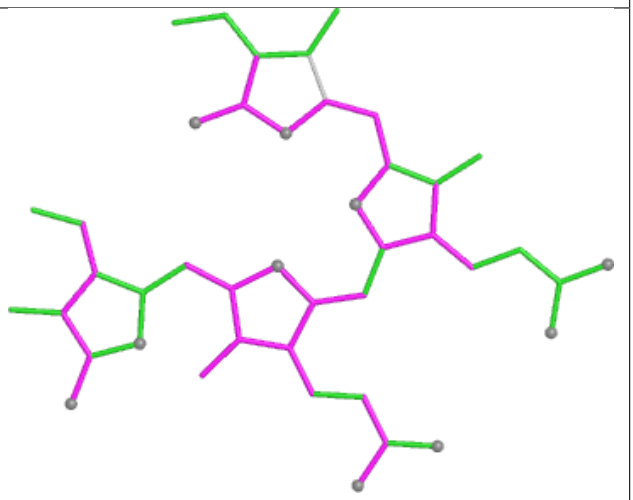

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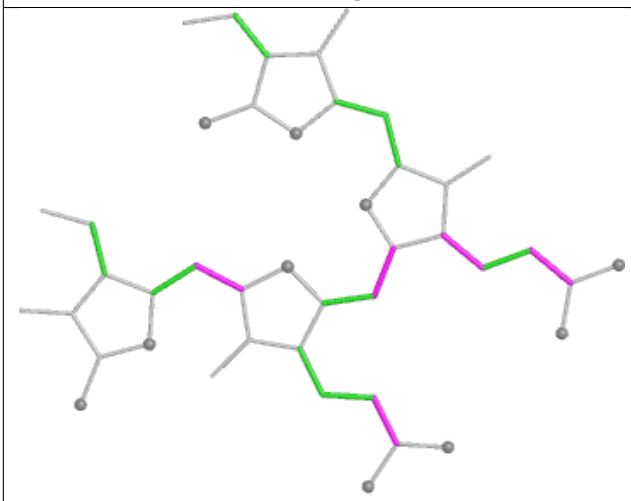

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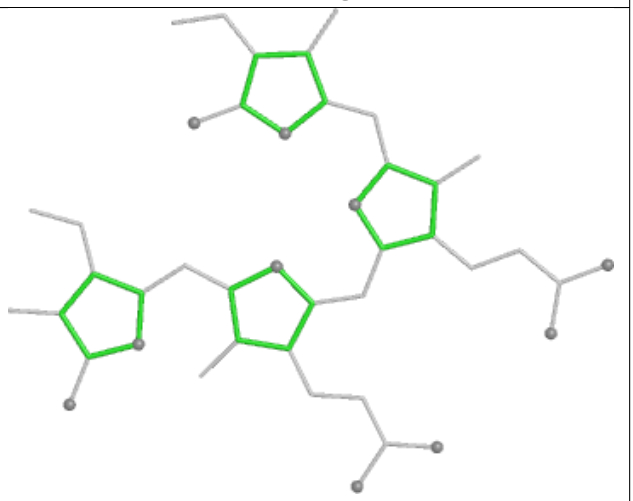
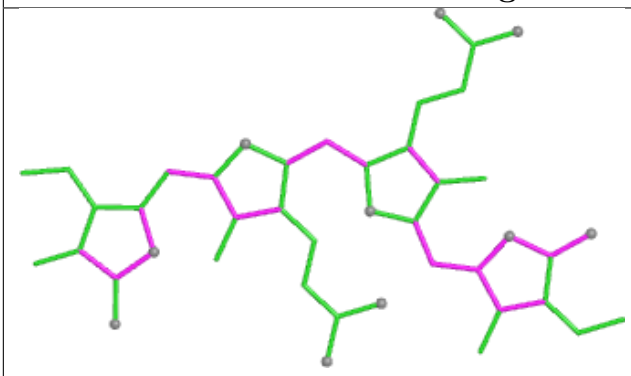


Rings

Ligand CYC KO 1001



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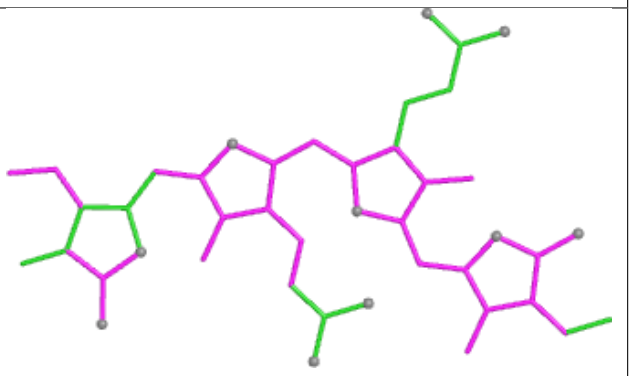

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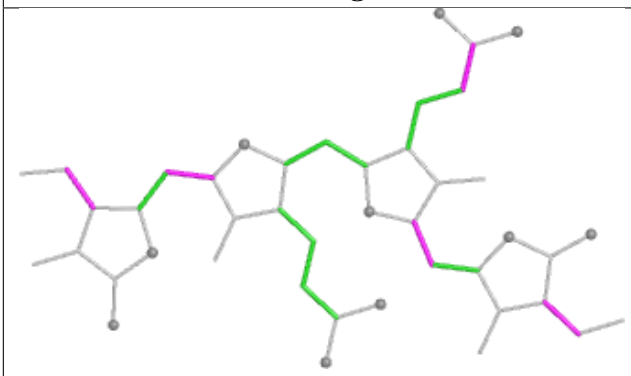

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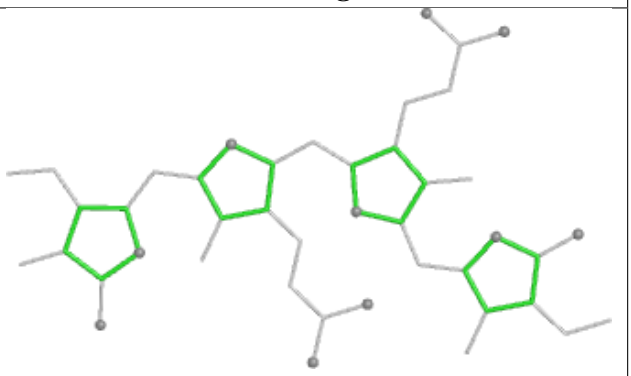
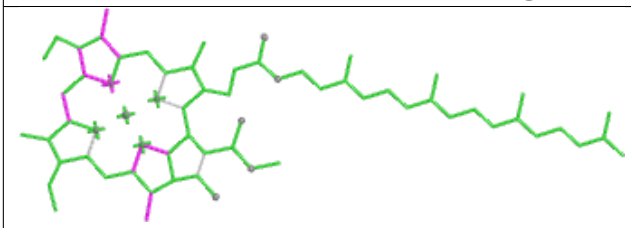


Rings

Ligand CLA c6 616



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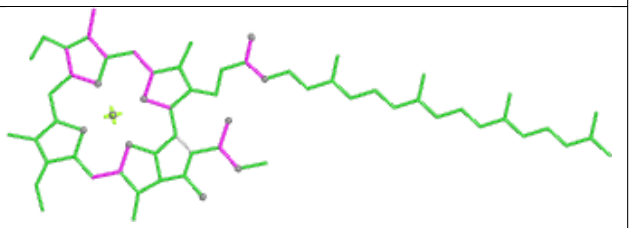
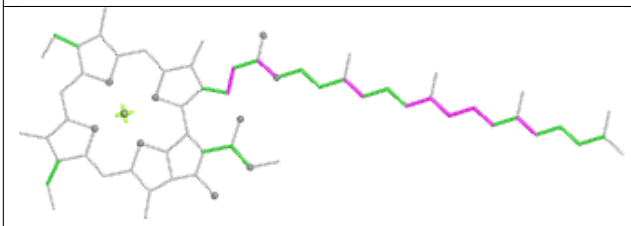


Bond angles



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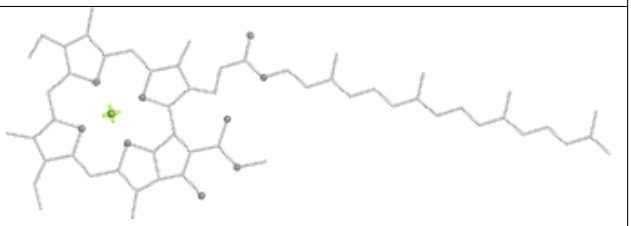
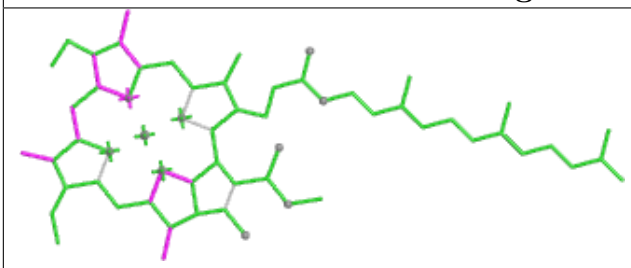
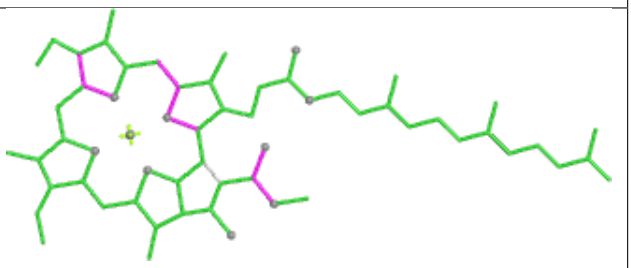
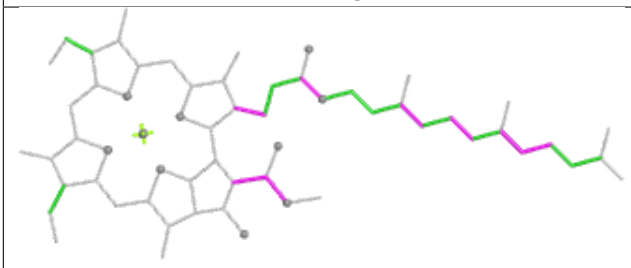
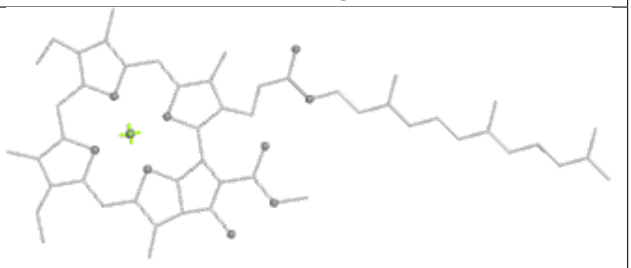


Rings

Ligand CLA C6 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

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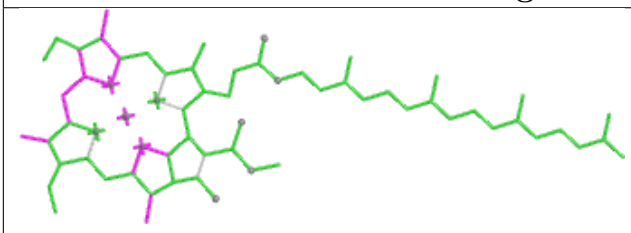	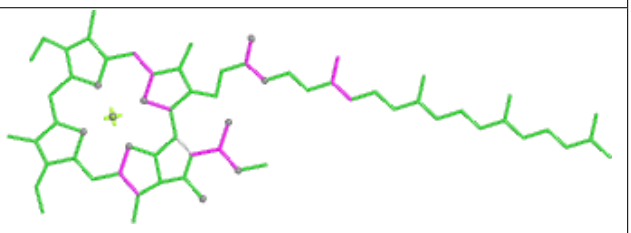
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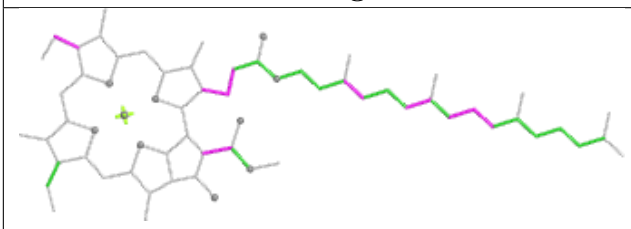
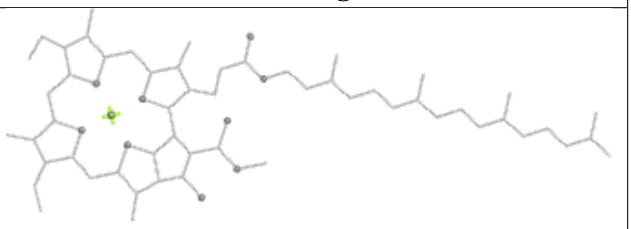
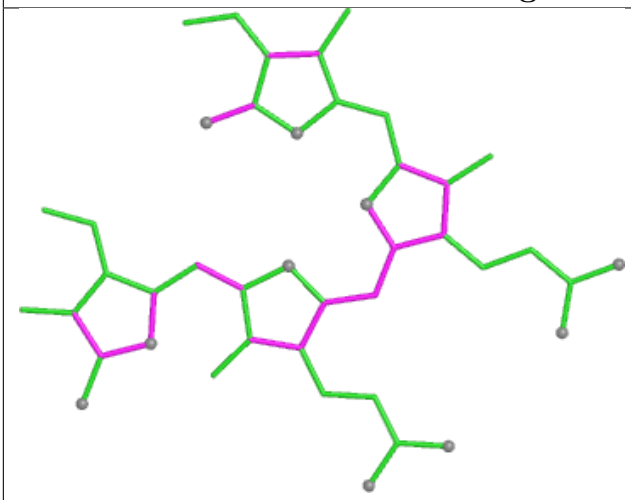
	
Torsions	Rings

Ligand PEB k4 201



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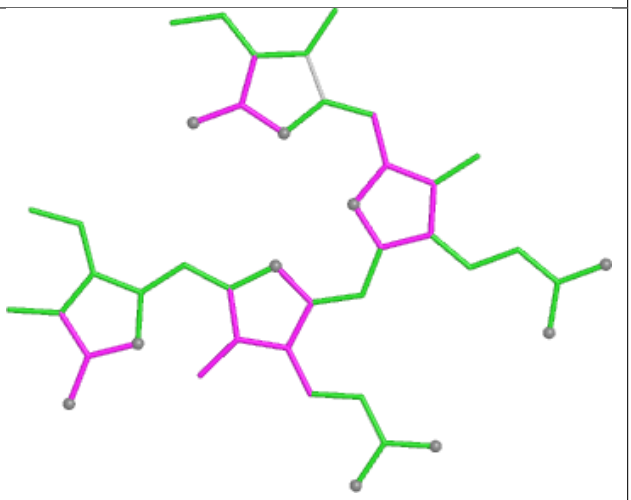
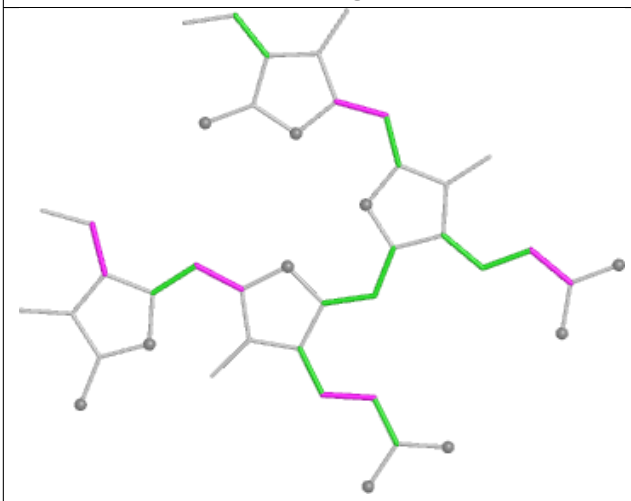


Bond angles



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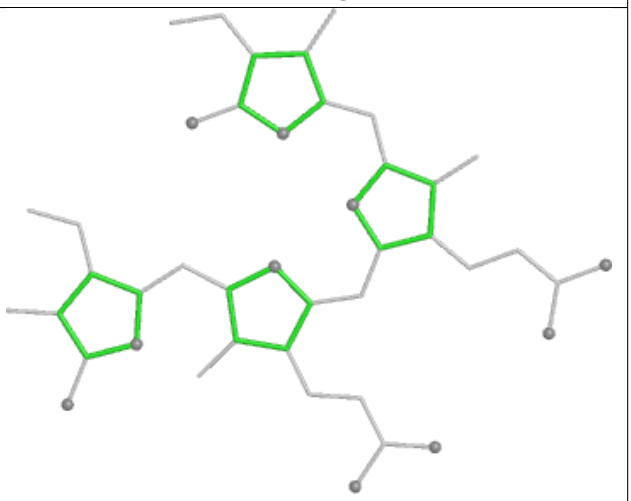
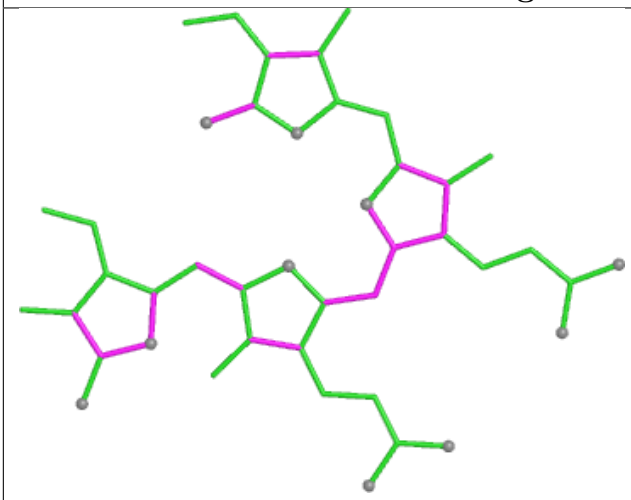


Rings

Ligand PEB NI 201



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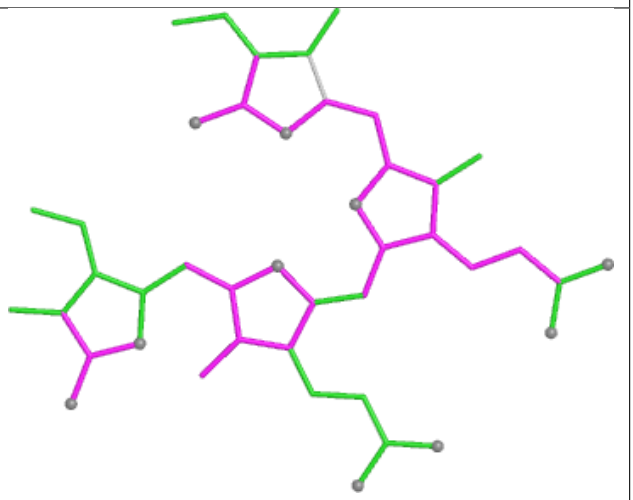
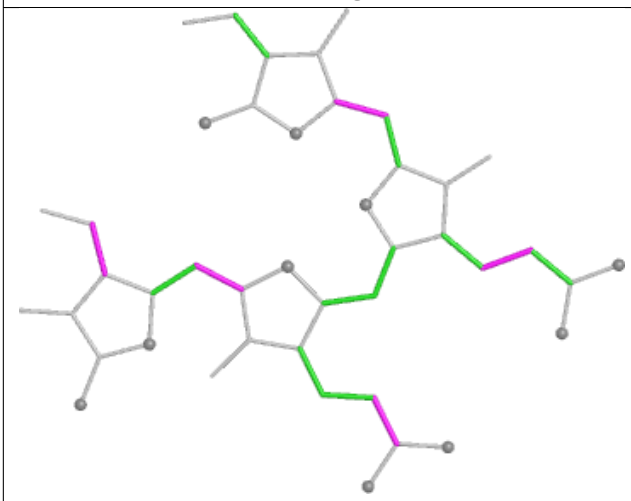


Bond angles



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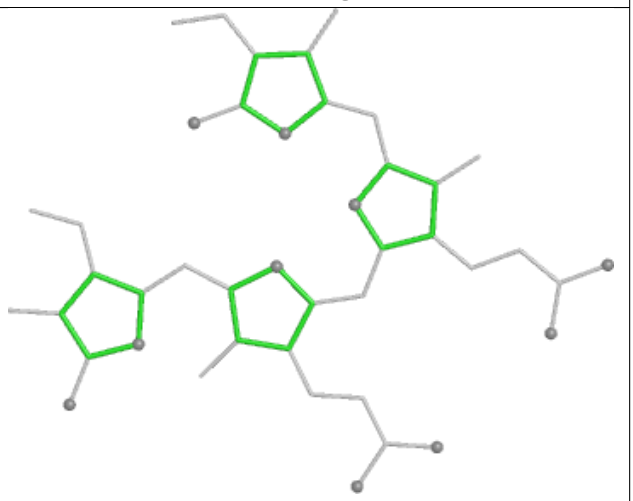
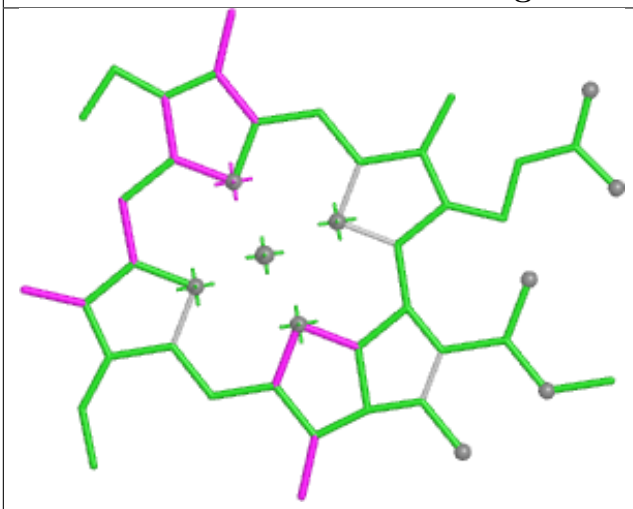
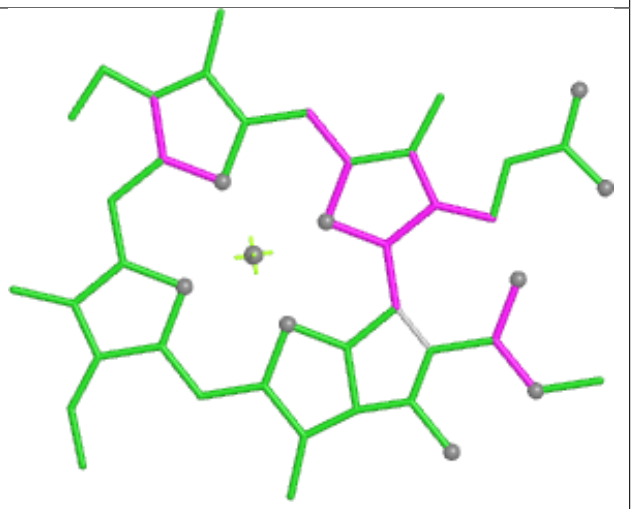


Rings

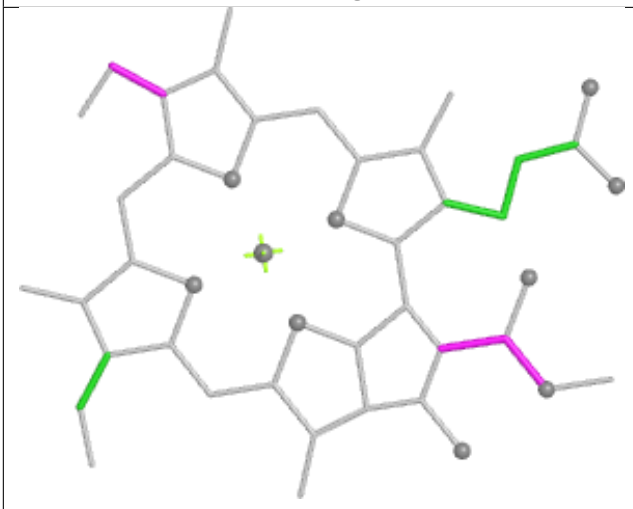
Ligand CLA 7N 610



Bond lengths



Bond angles

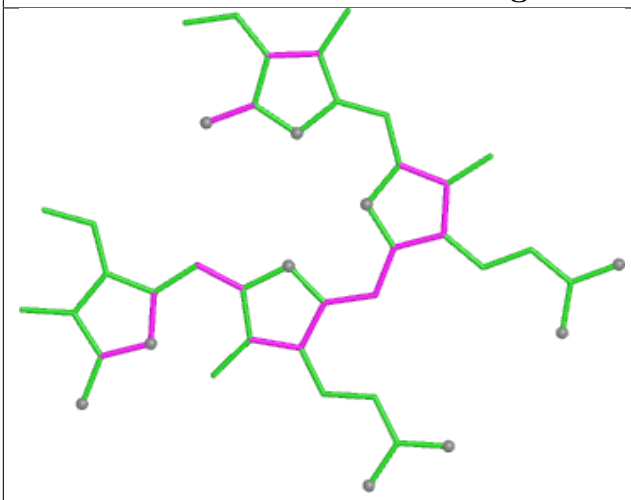


Torsions



Rings

Ligand PEB OH 202



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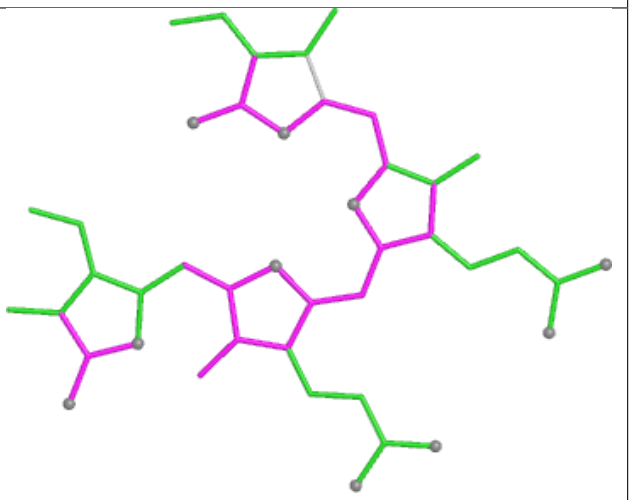
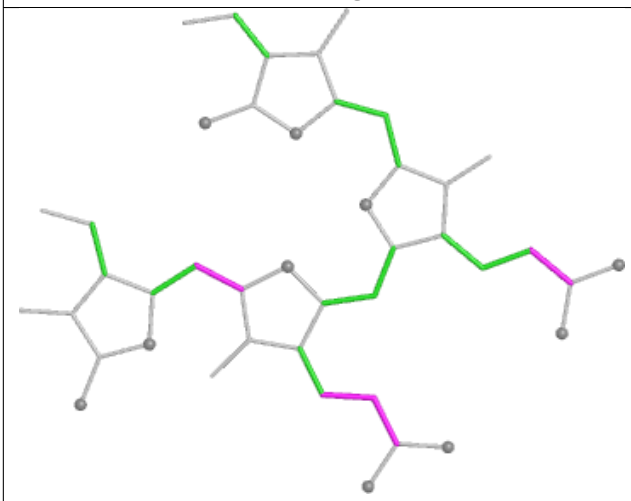
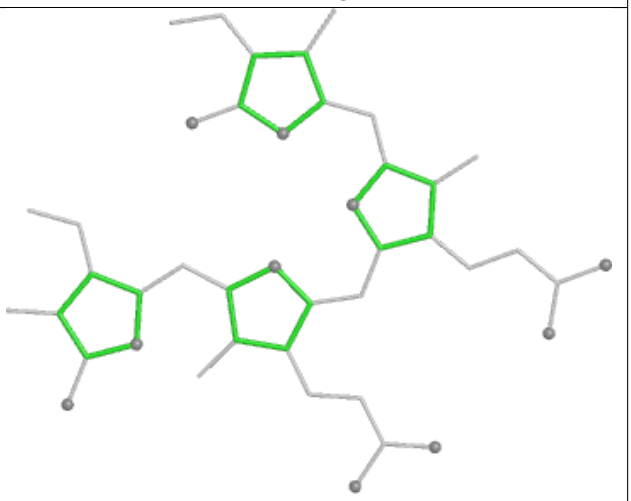


Bond angles

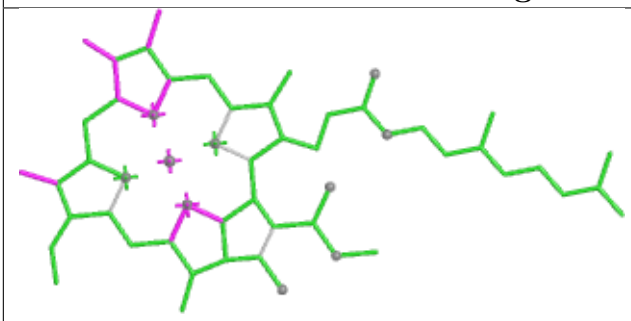


Torsions

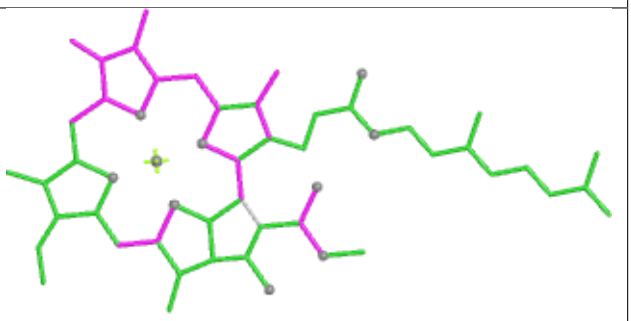


Rings

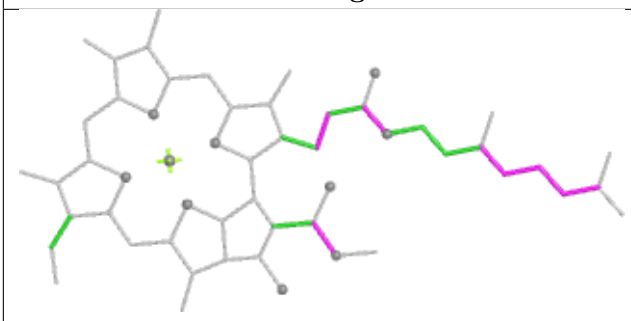
Ligand CLA 2N 301



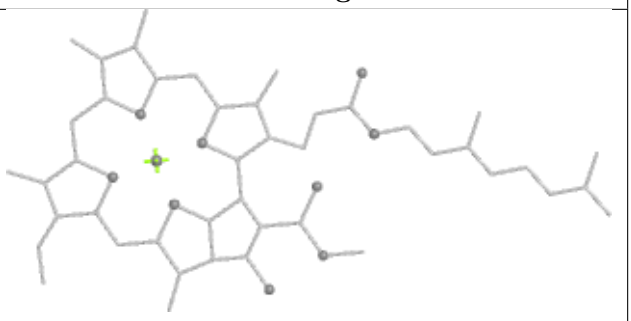
Bond lengths



Bond angles

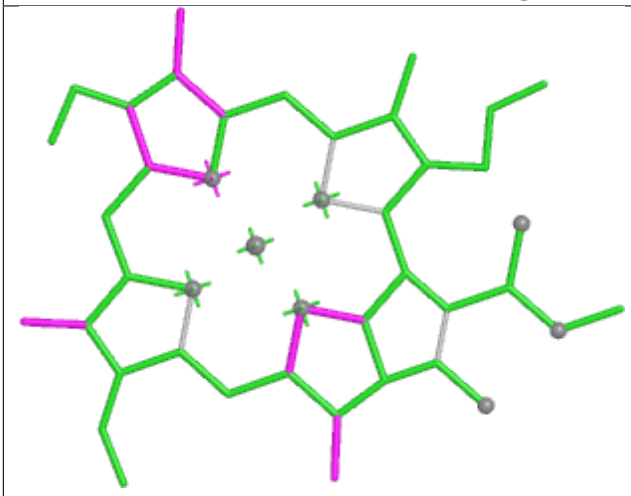


Torsions



Rings

Ligand CLA B2 829



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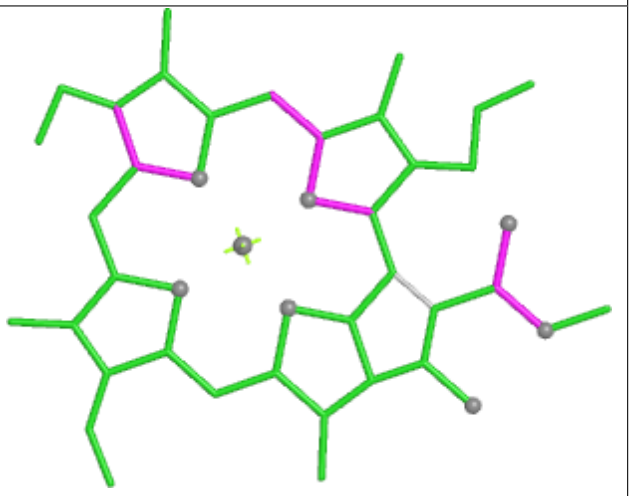

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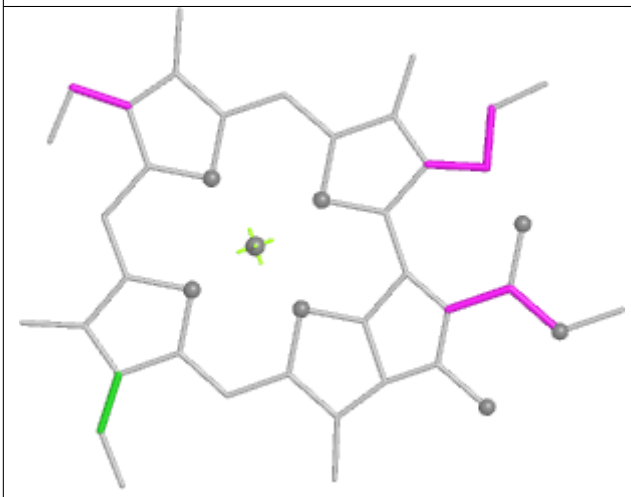

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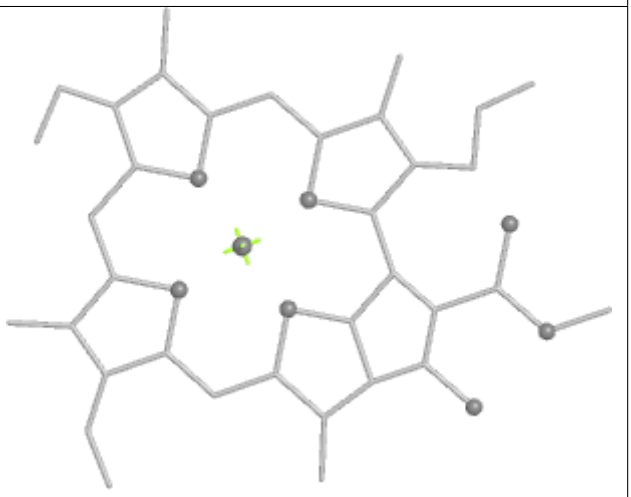
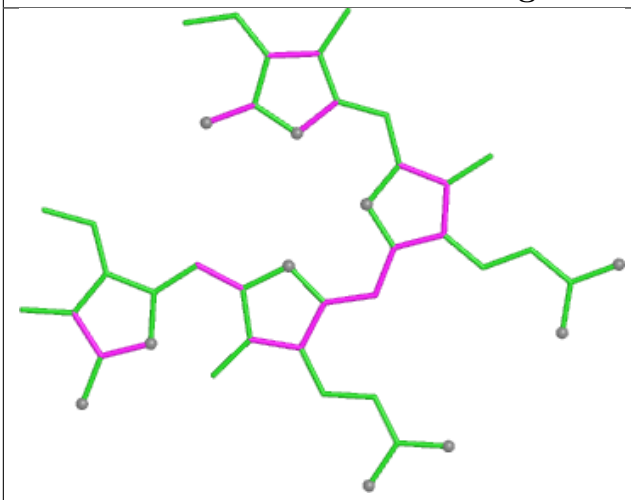


Rings

Ligand PEB jH 202



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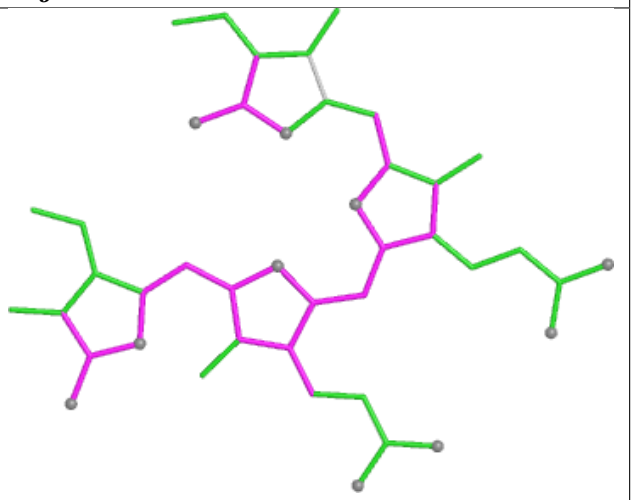

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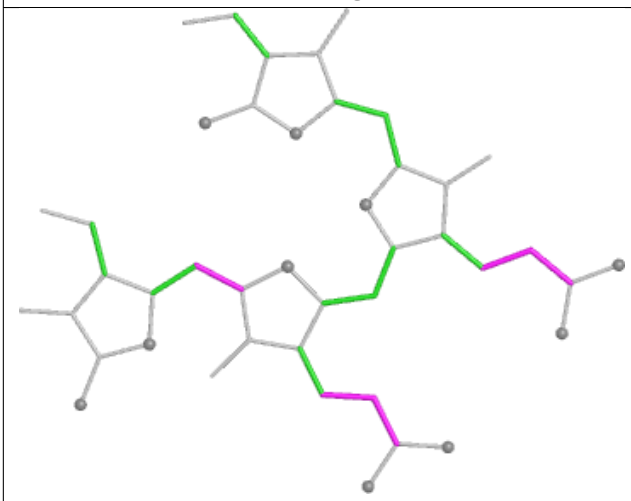

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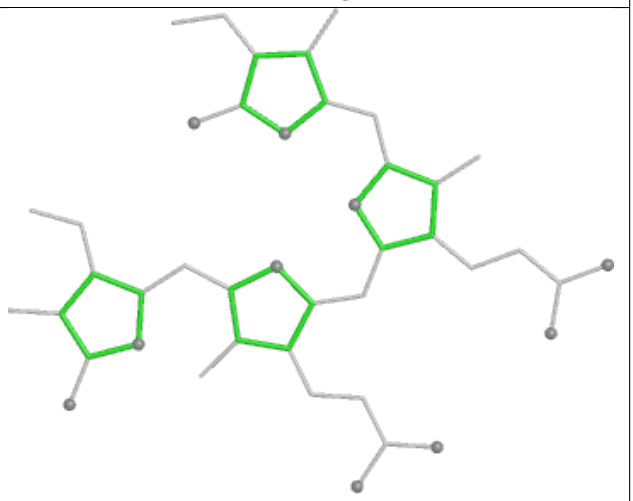
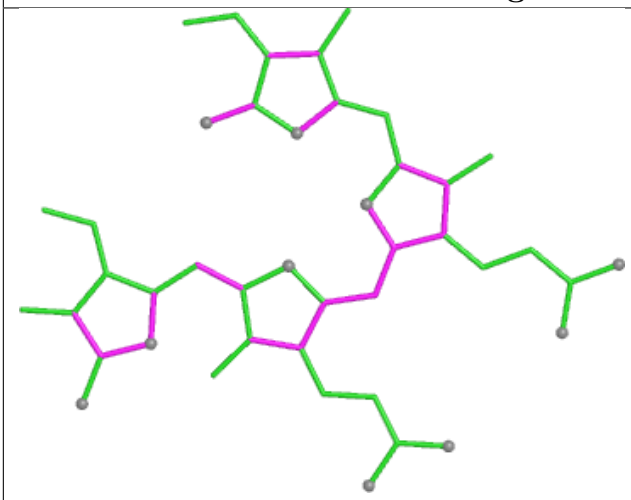


Rings

Ligand PEB OM 202



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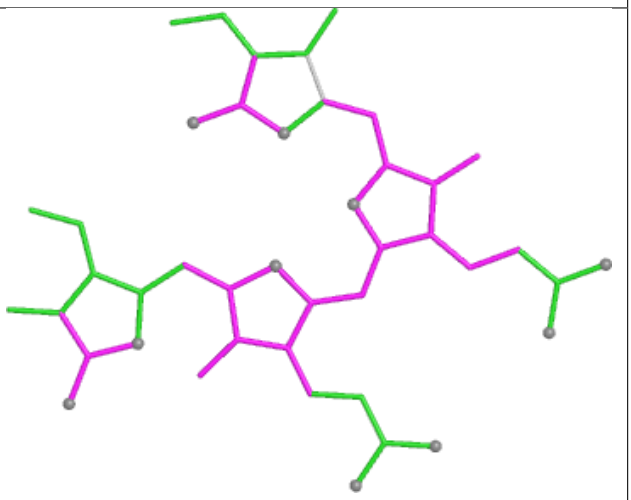

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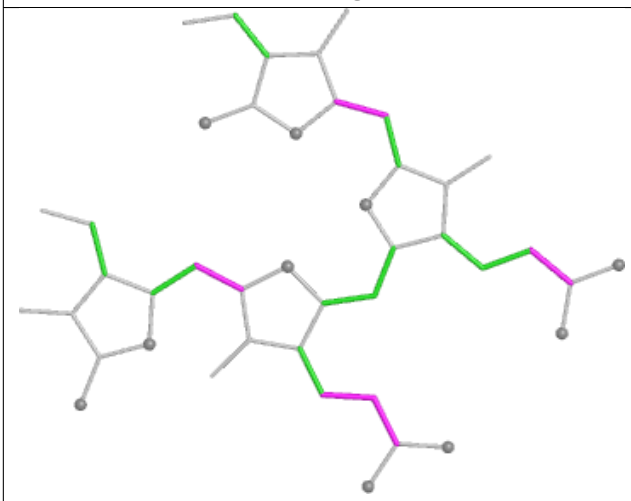

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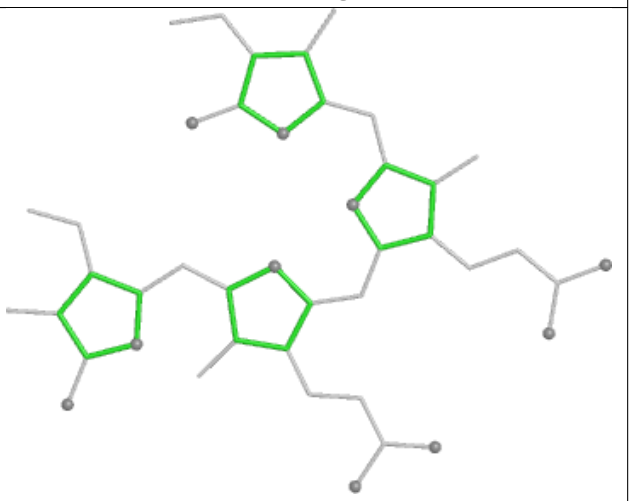
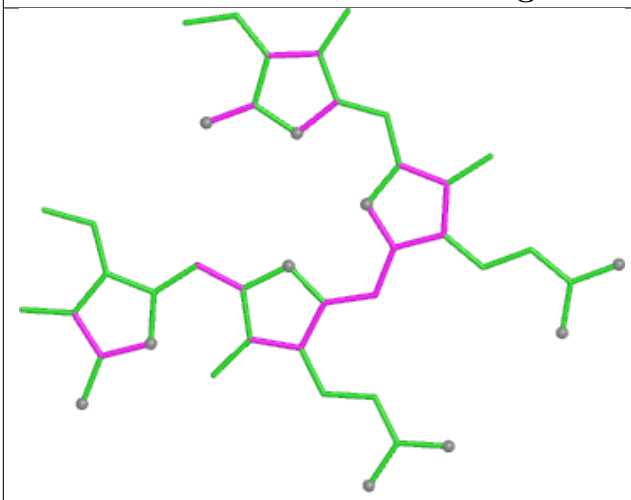


Rings

Ligand PEB rC 202



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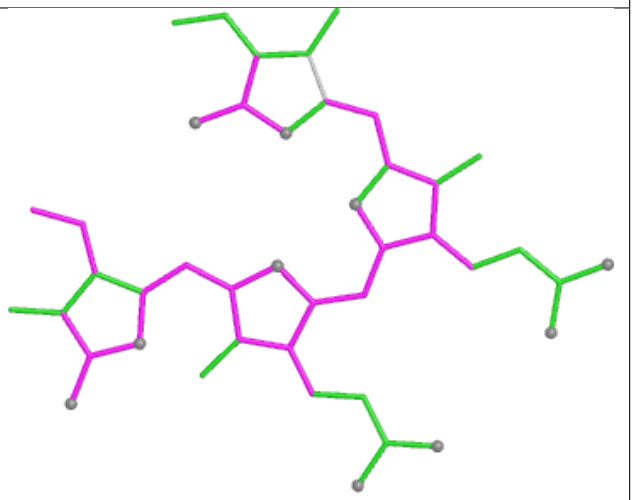

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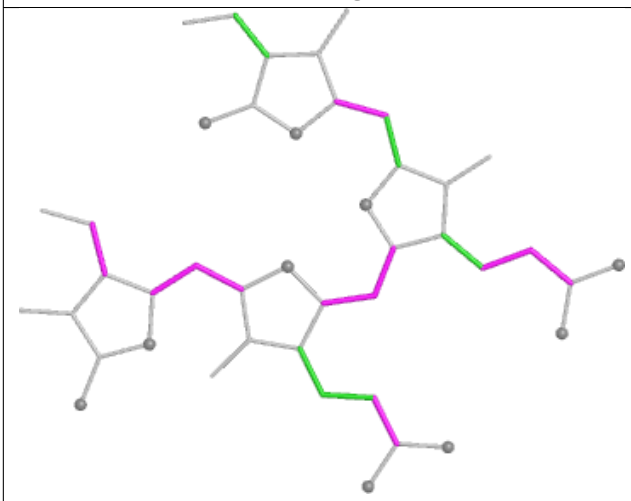

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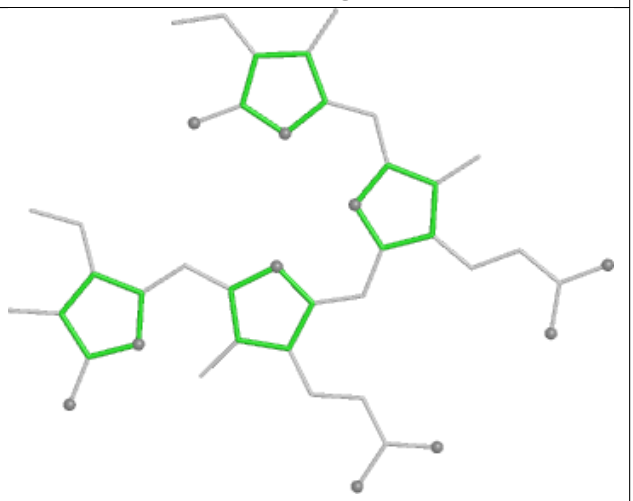
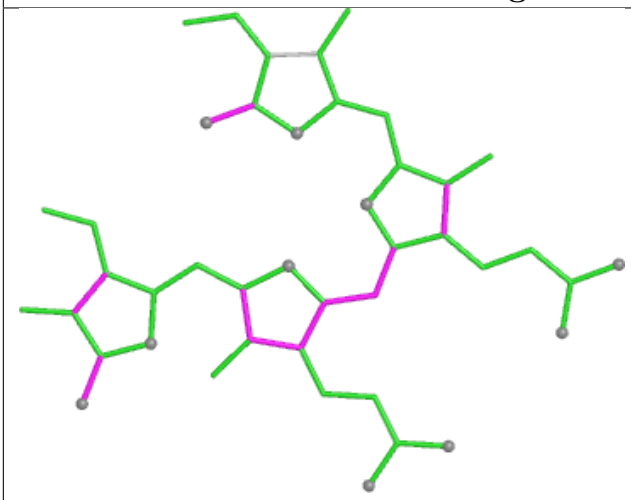


Rings

Ligand PUB AG 303



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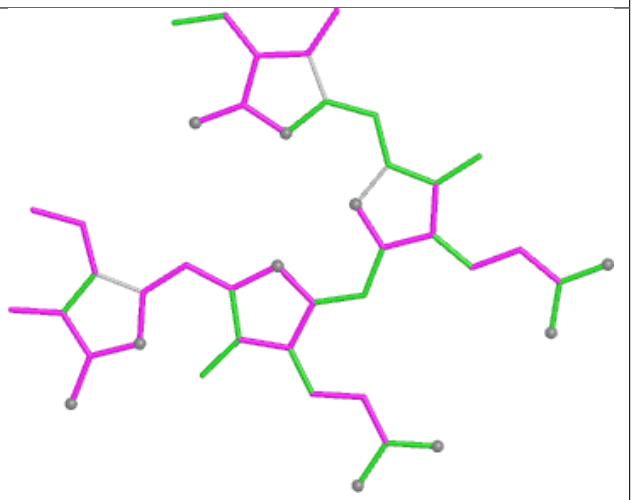

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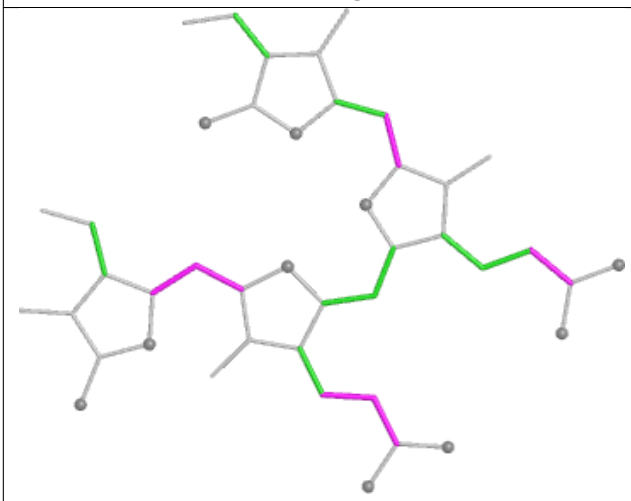

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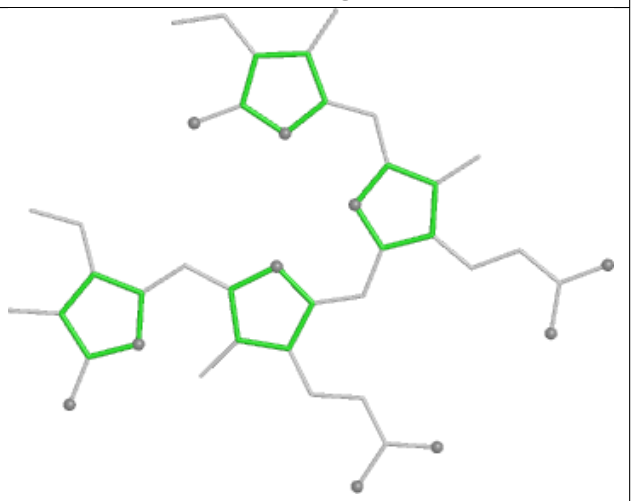
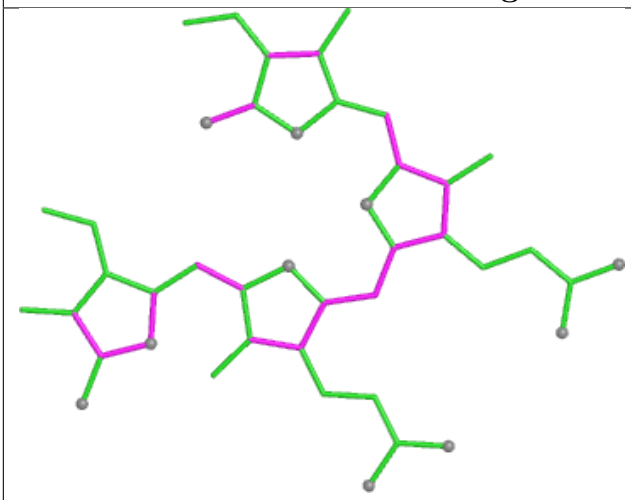


Rings

Ligand PEB DG 1002



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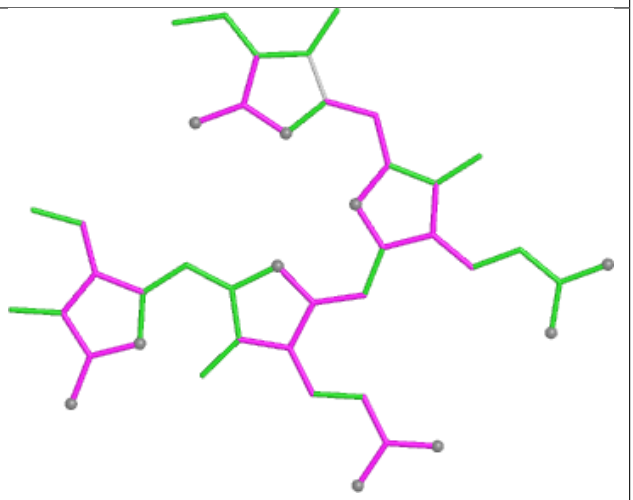
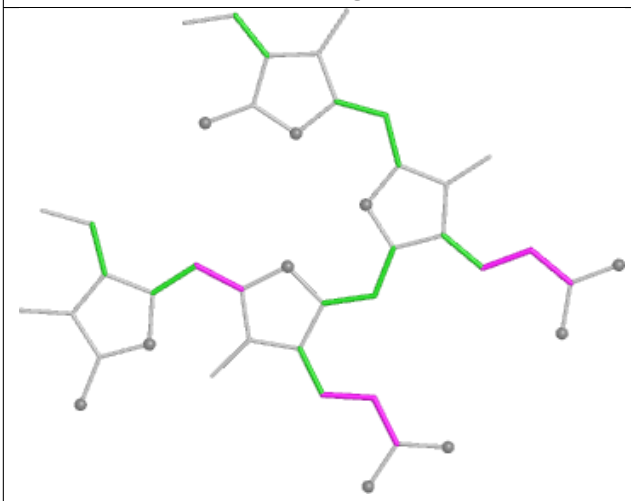


Bond angles



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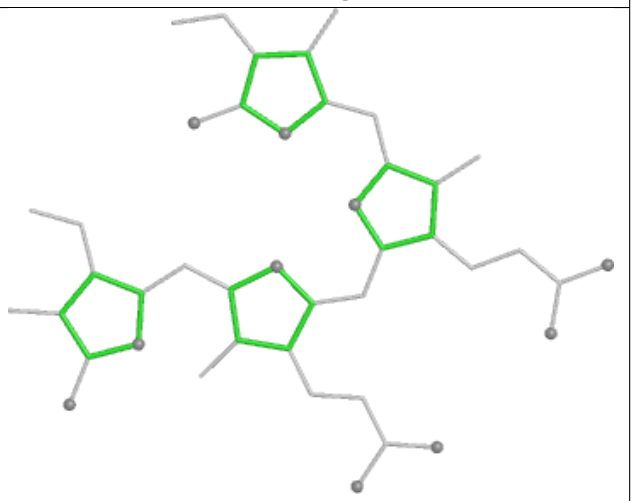
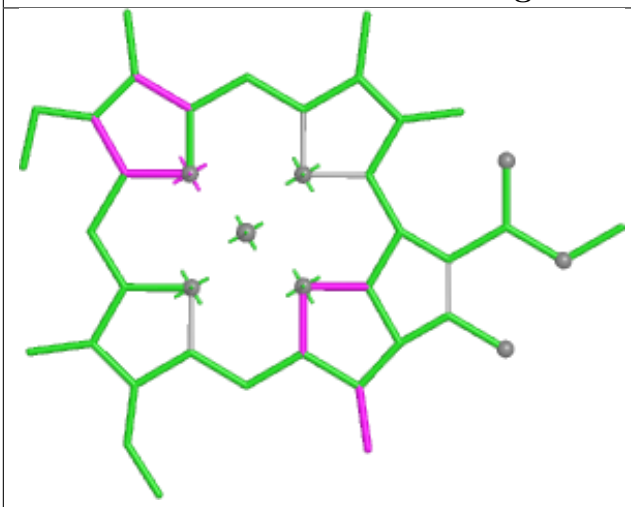


Rings

Ligand CLA 6N 609



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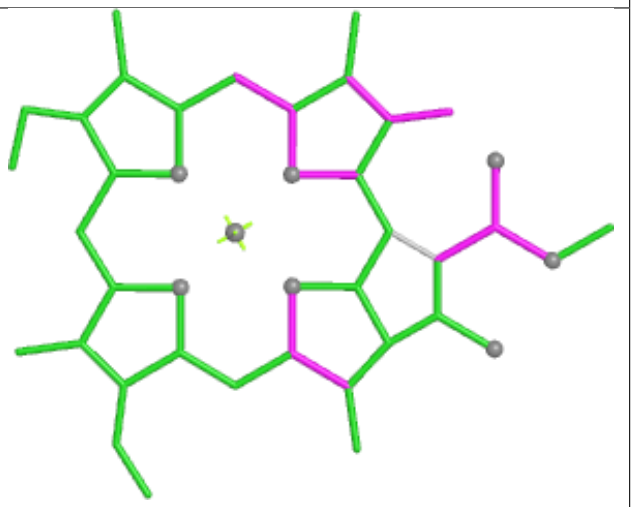

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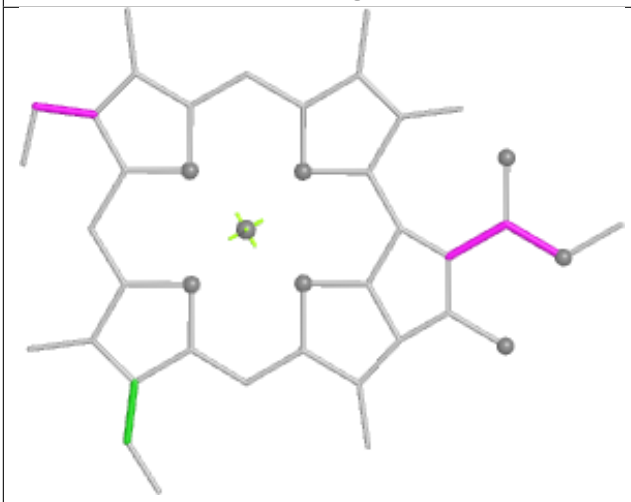

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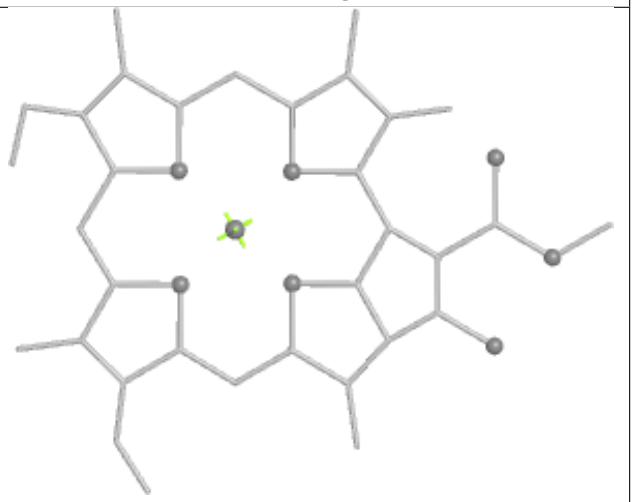
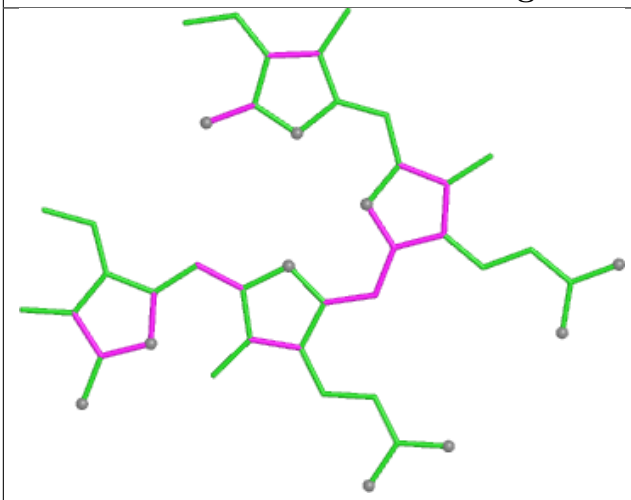


Rings

Ligand PEB YI 201



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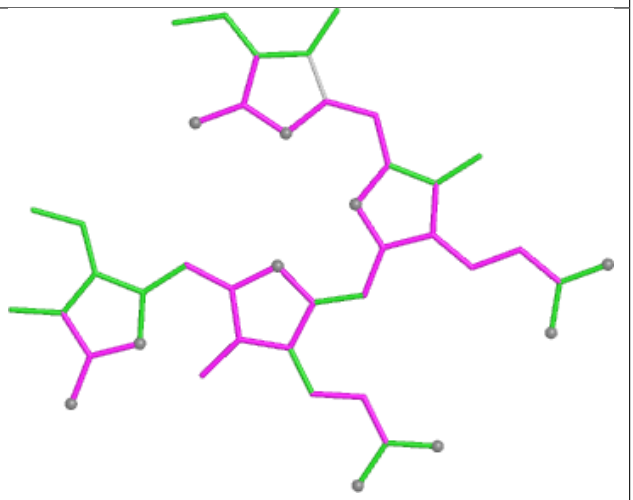
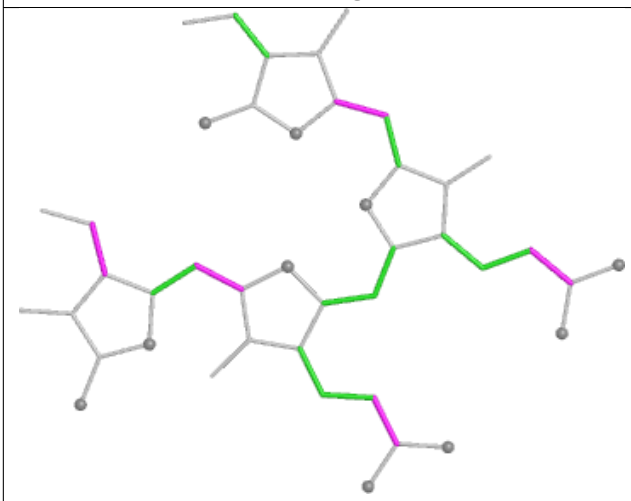


Bond angles



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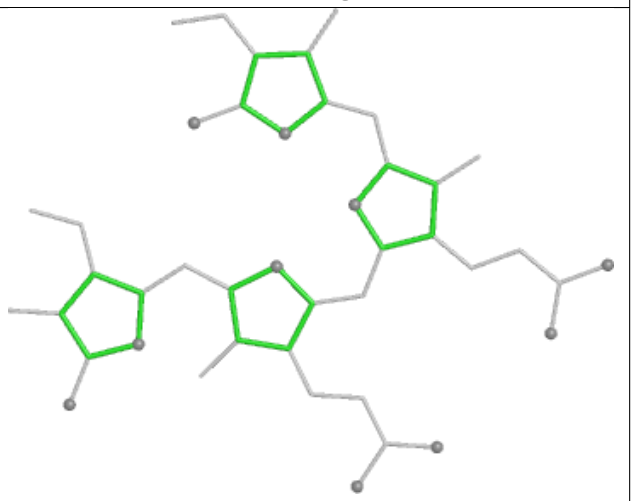
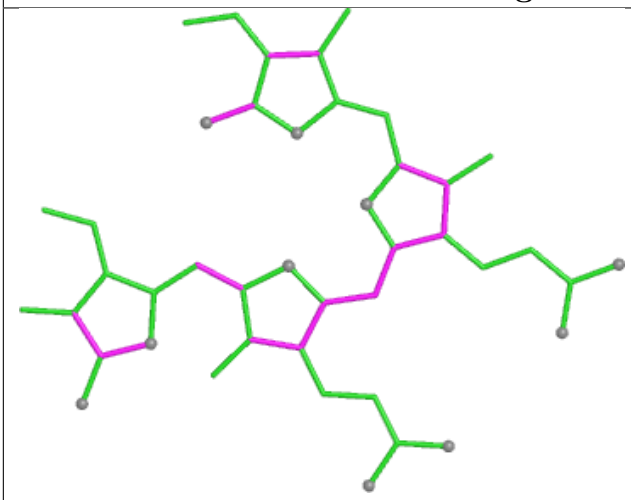


Rings

Ligand PEB V7 202



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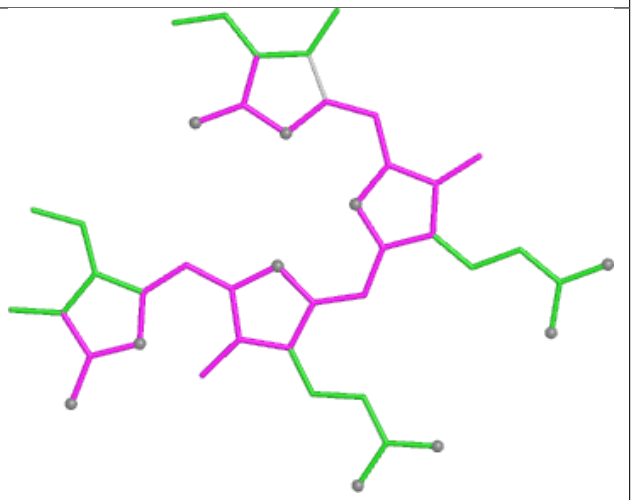
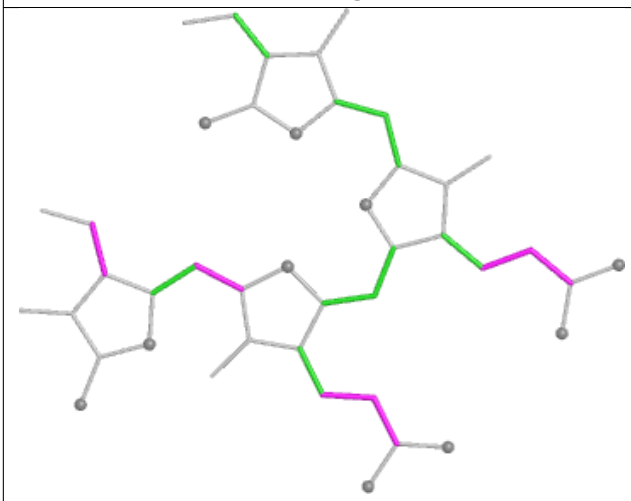


Bond angles



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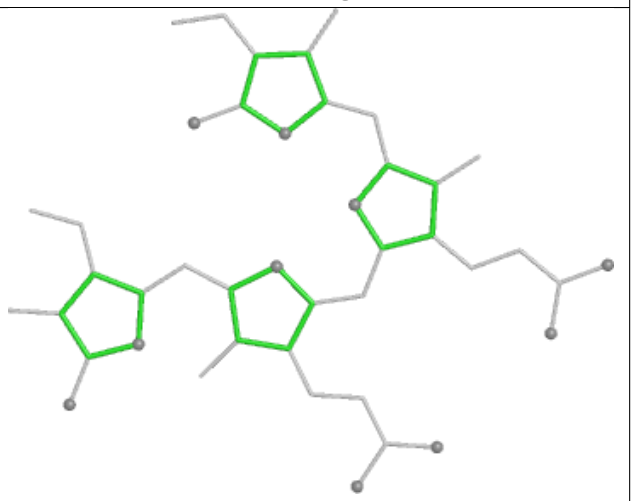
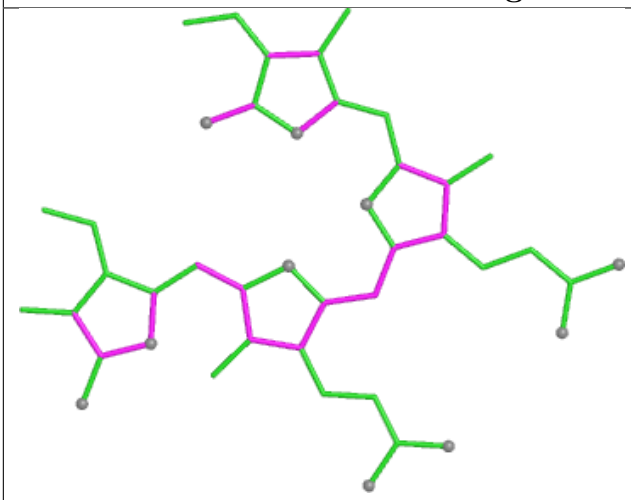


Rings

Ligand PEB WD 202



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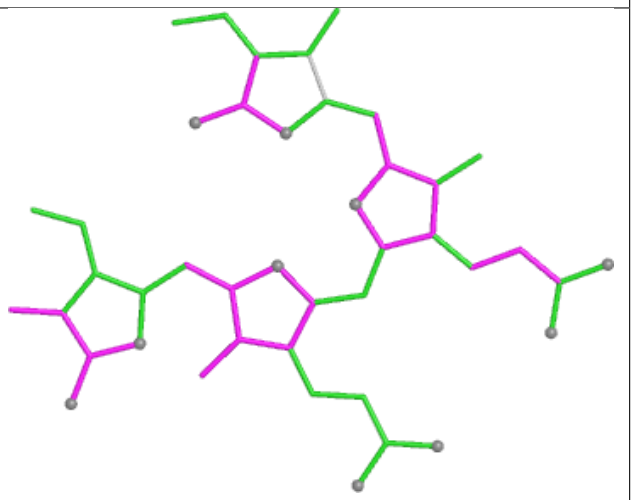

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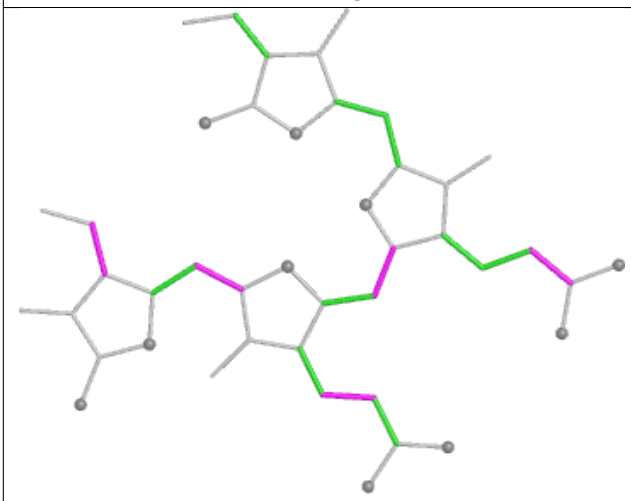

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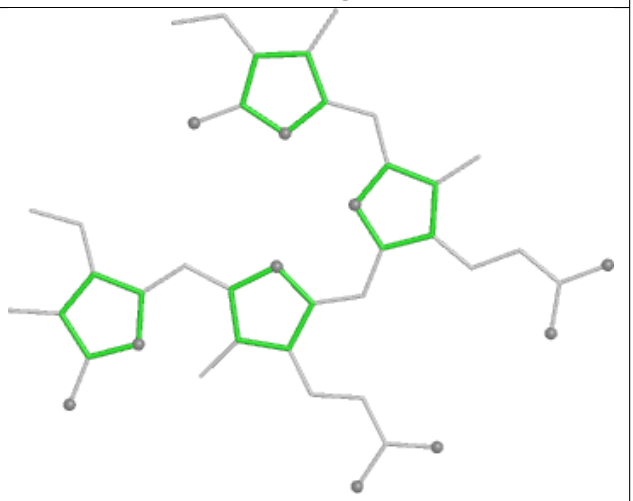
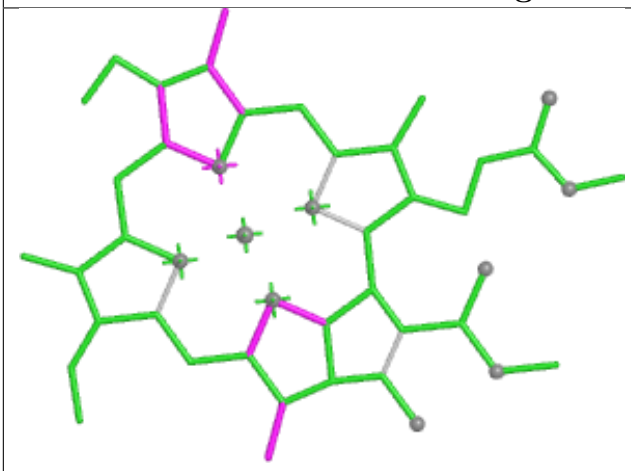


Rings

Ligand CLA R2 203



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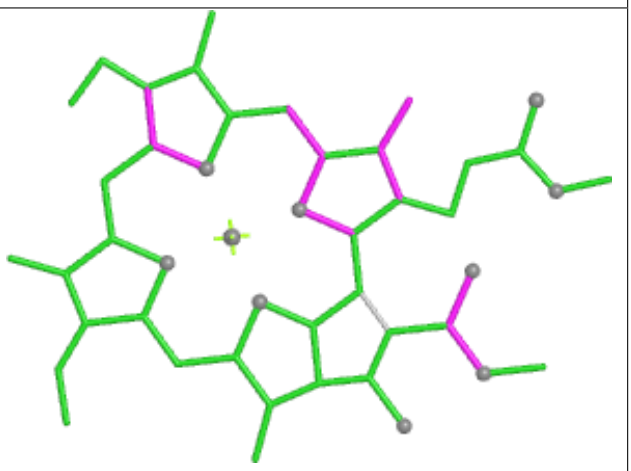
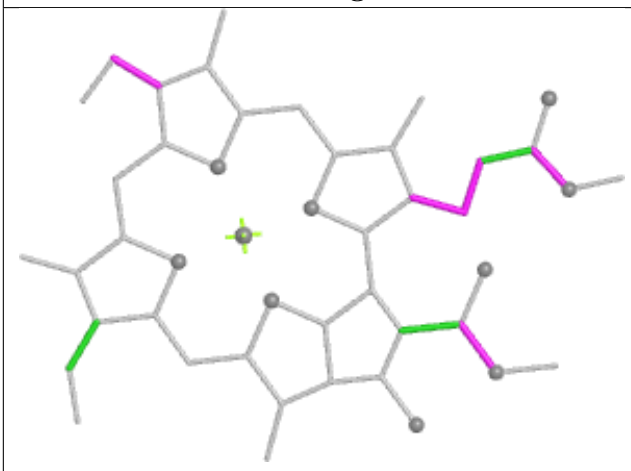


Bond angles



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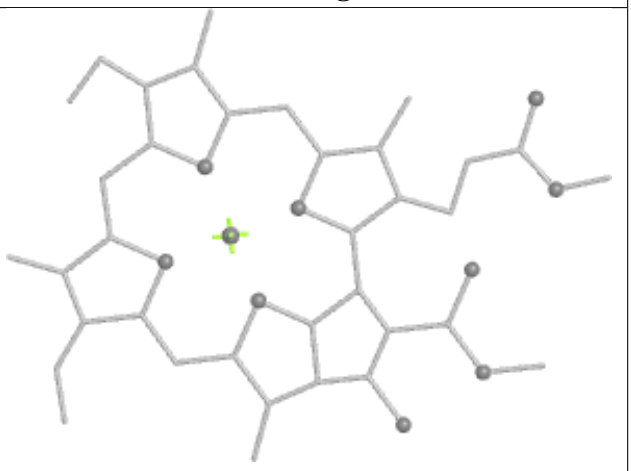
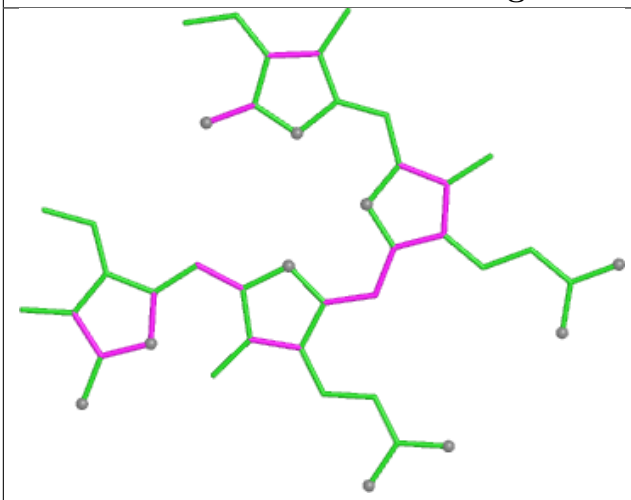


Rings

Ligand PEB CM 203



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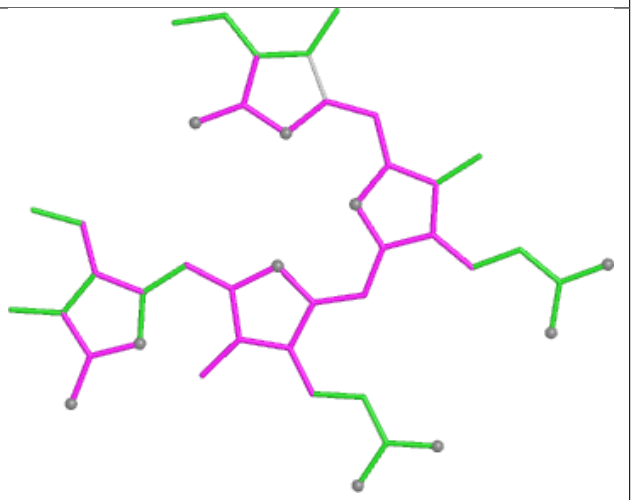
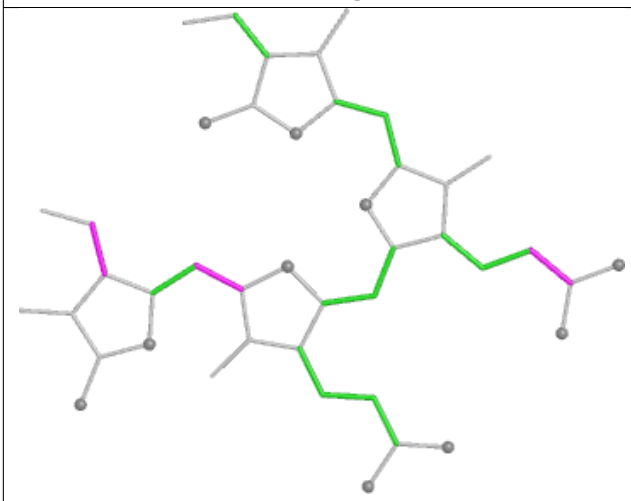


Bond angles



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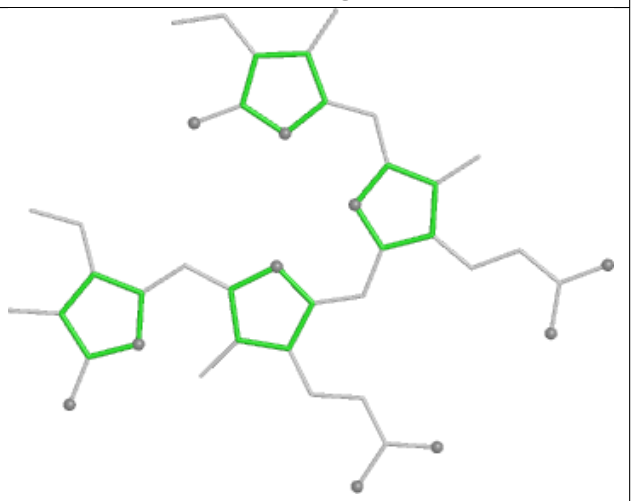
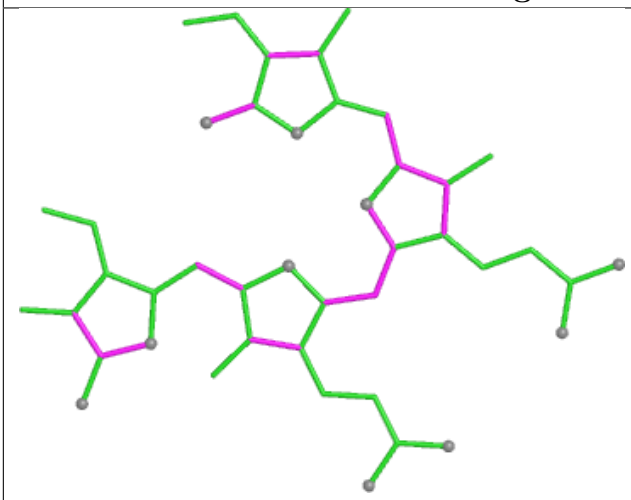


Rings

Ligand PEB bK 202



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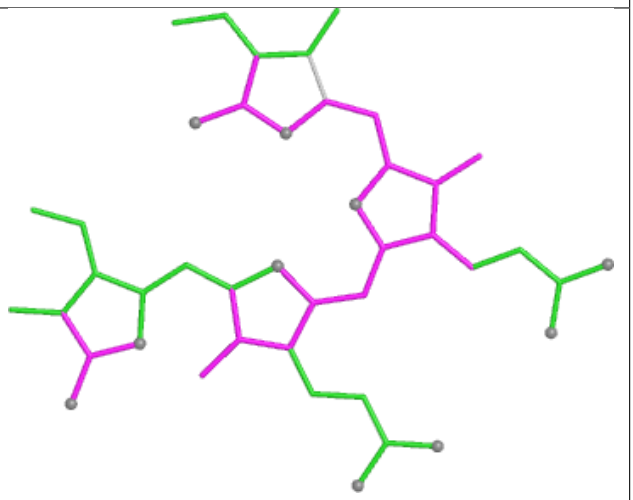
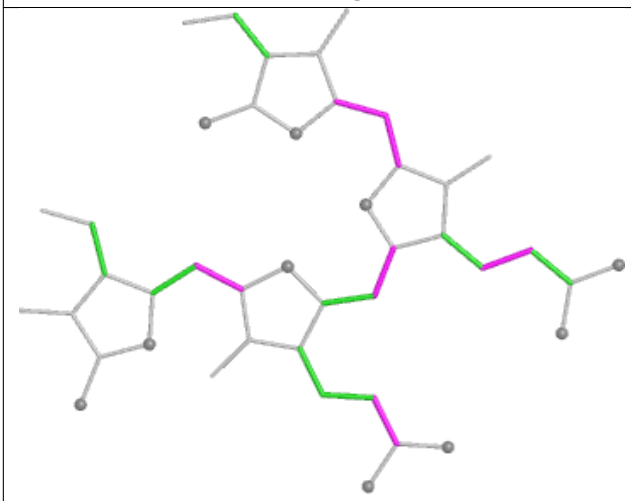


Bond angles



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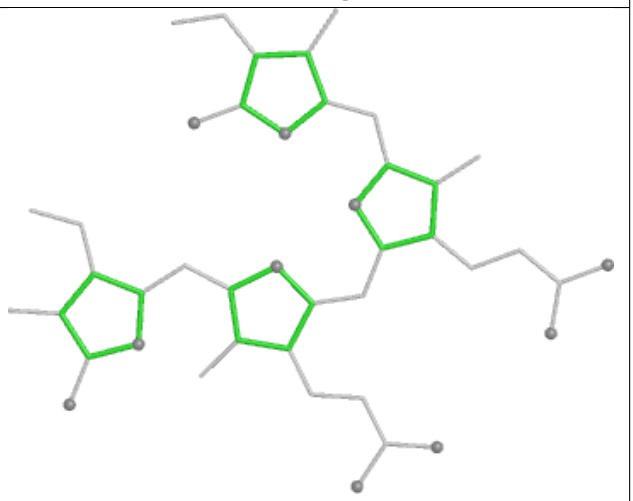
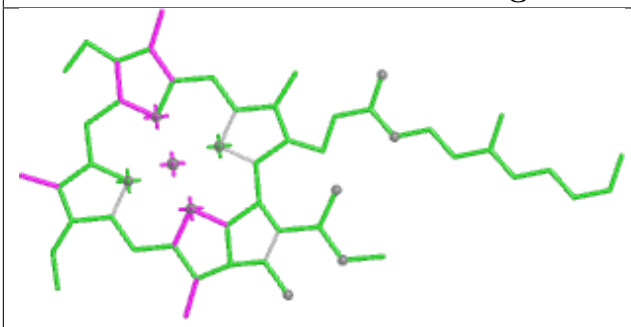
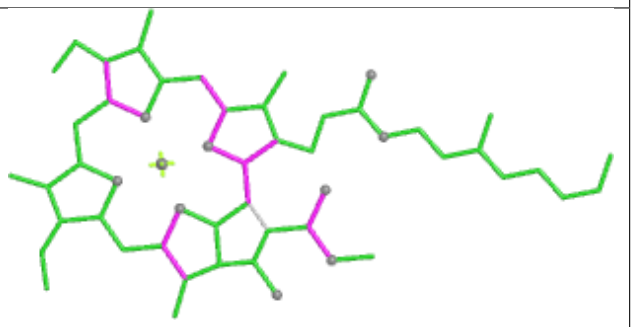


Rings

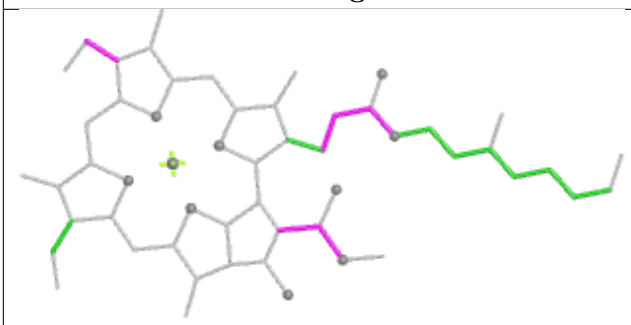
Ligand CLA AN 814



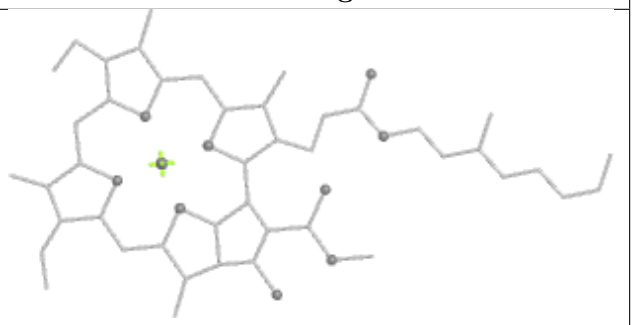
Bond lengths



Bond angles

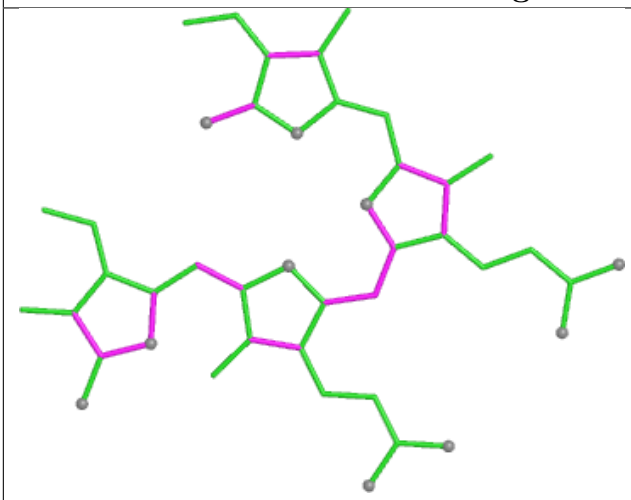


Torsions



Rings

Ligand PEB BB 203



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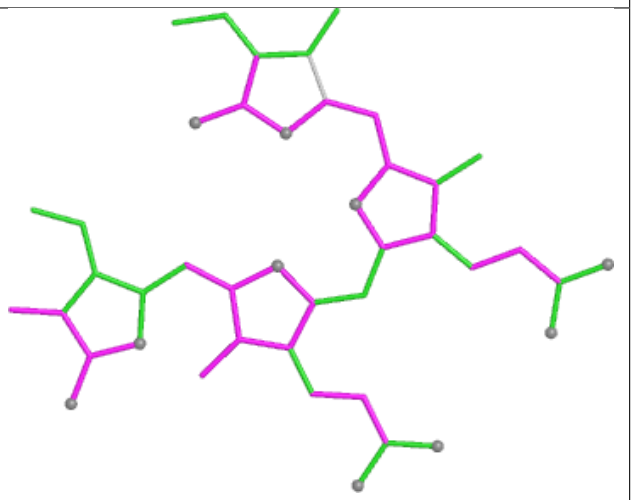
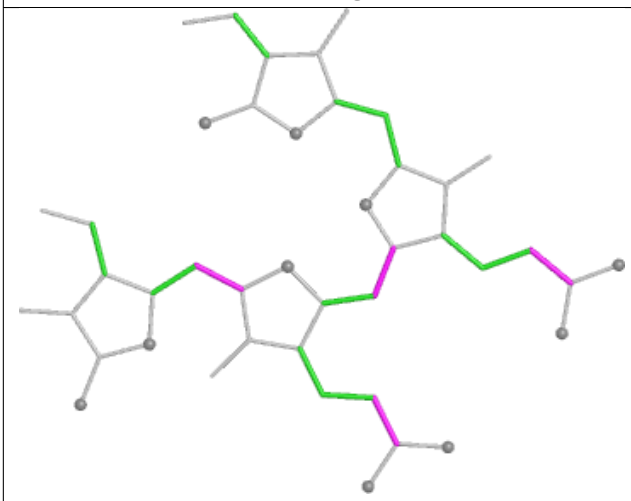


Bond angles



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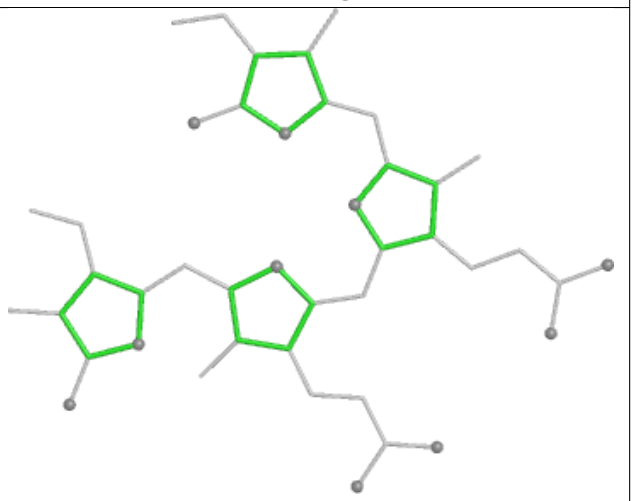
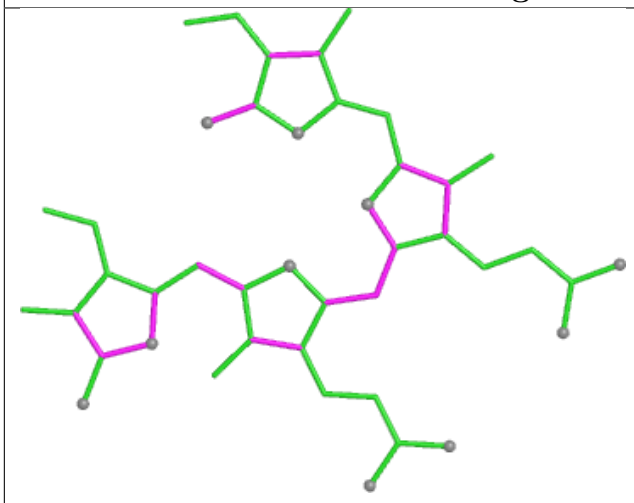


Rings

Ligand PEB HB 203



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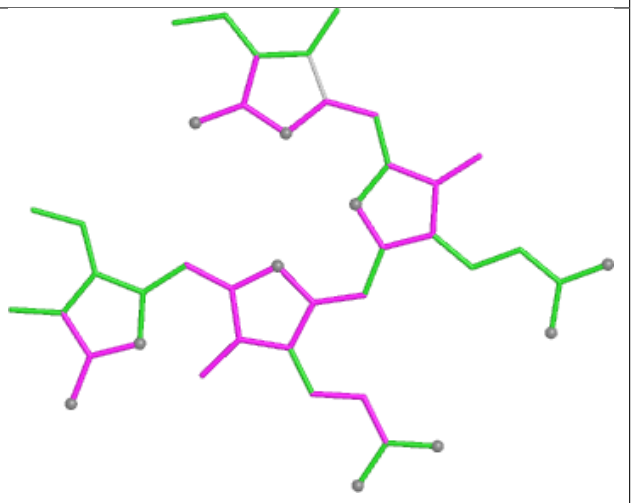

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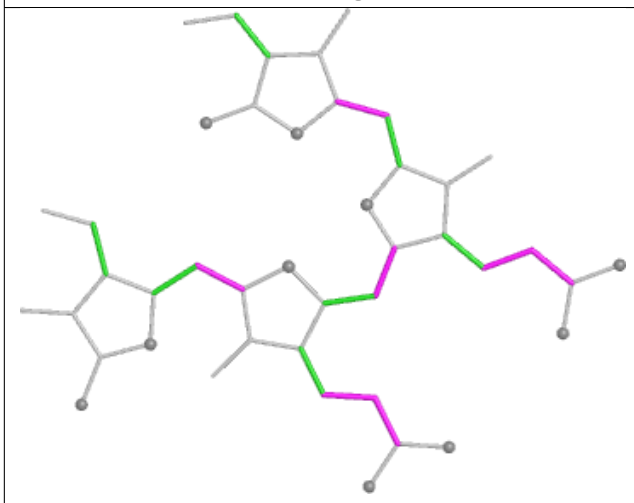

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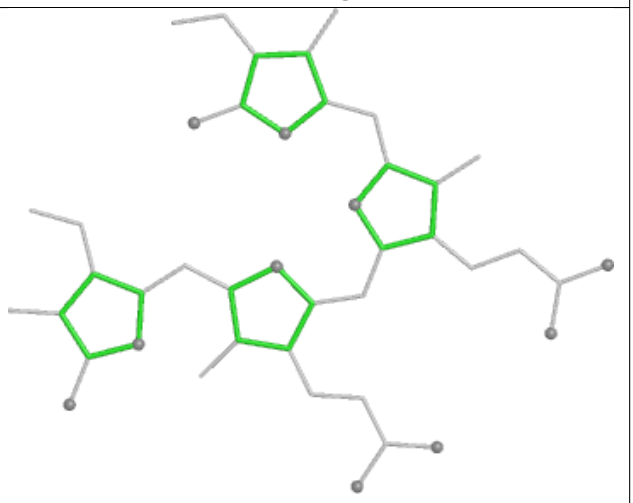
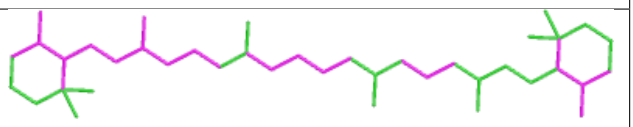


Rings

Ligand BCR BN 839



Bond lengths



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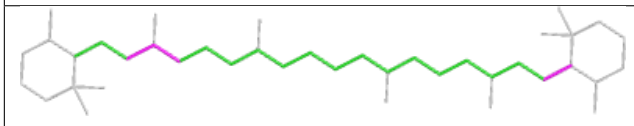

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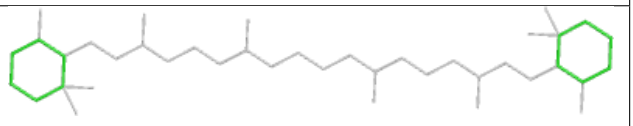
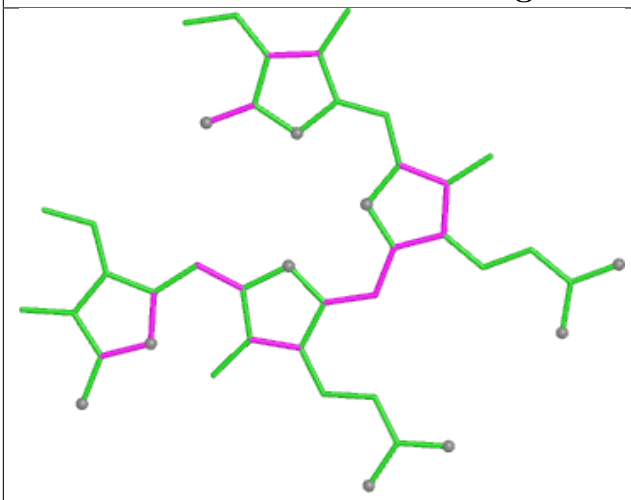


Rings

Ligand PEB O1 203



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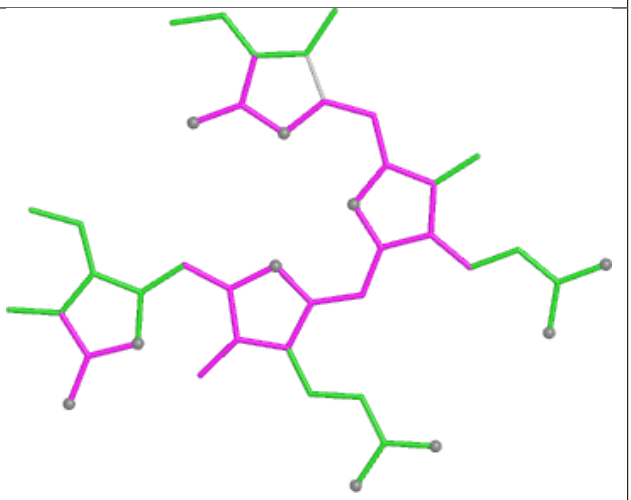
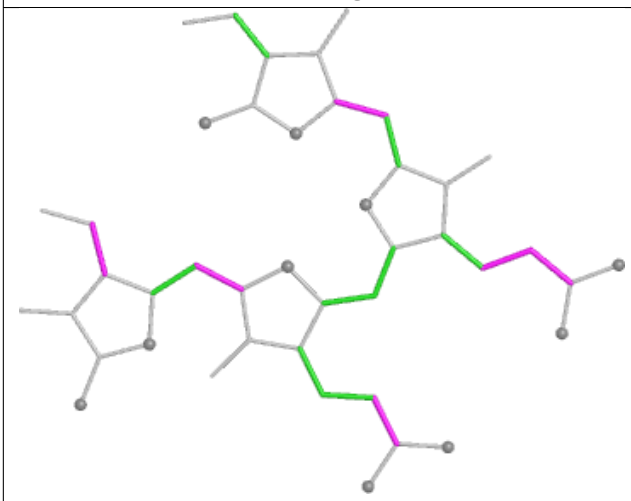


Bond angles



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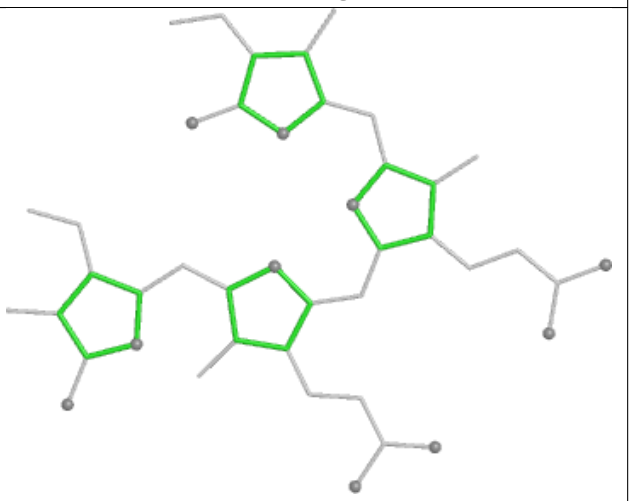
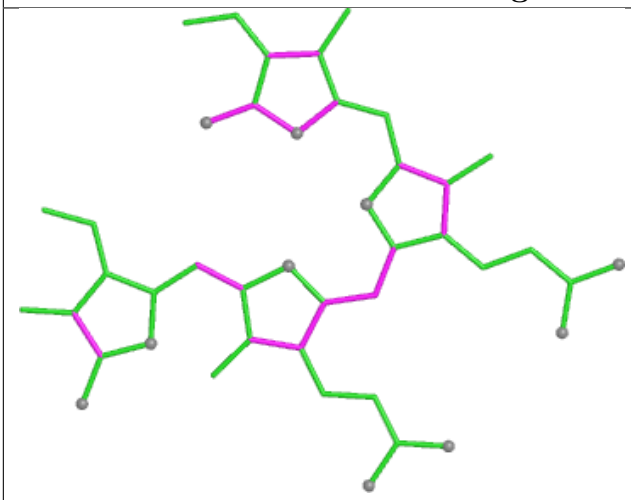


Rings

Ligand PEB BK 201



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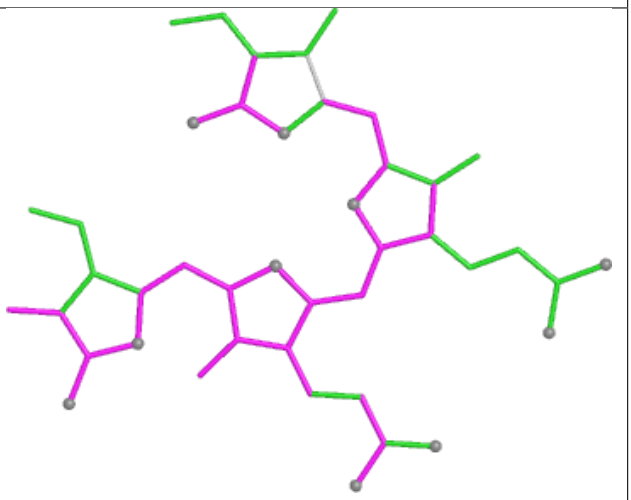

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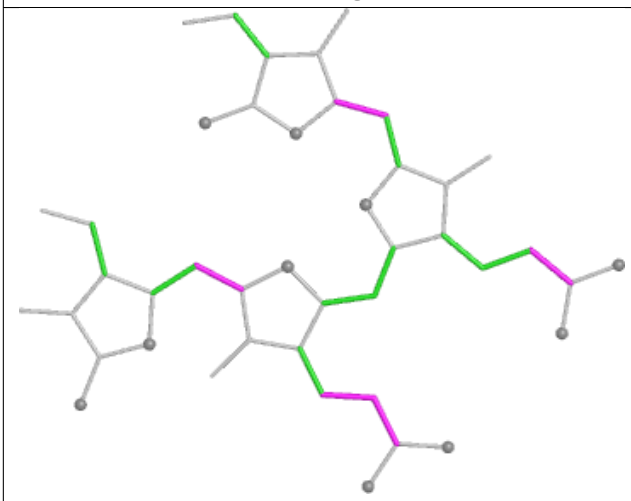

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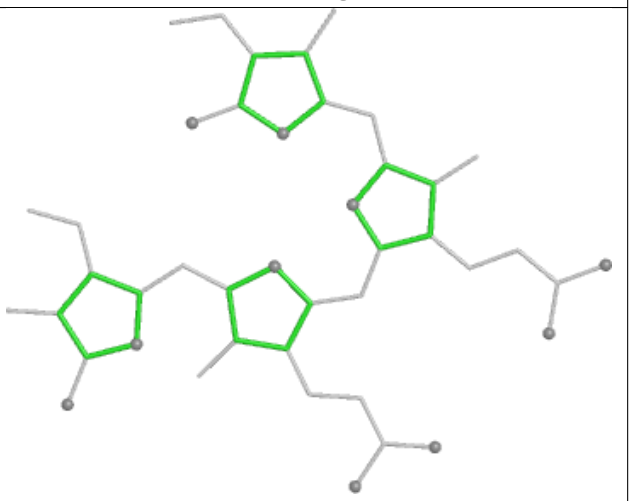
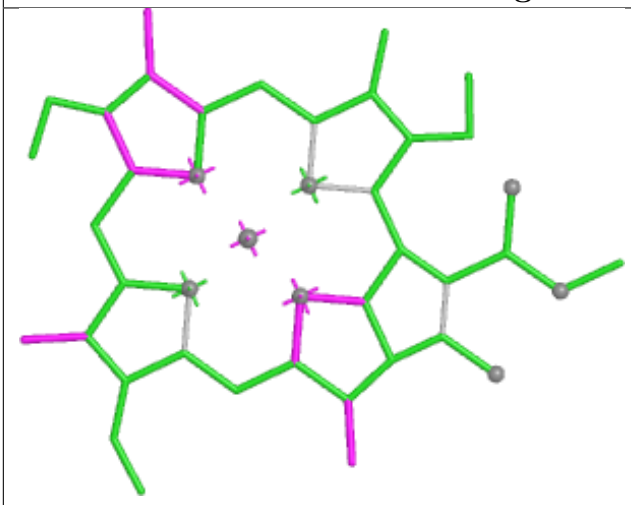


Rings

Ligand CLA 7N 604



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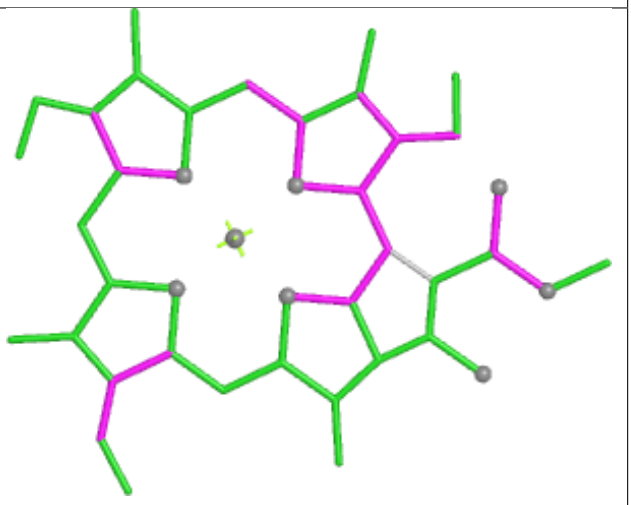

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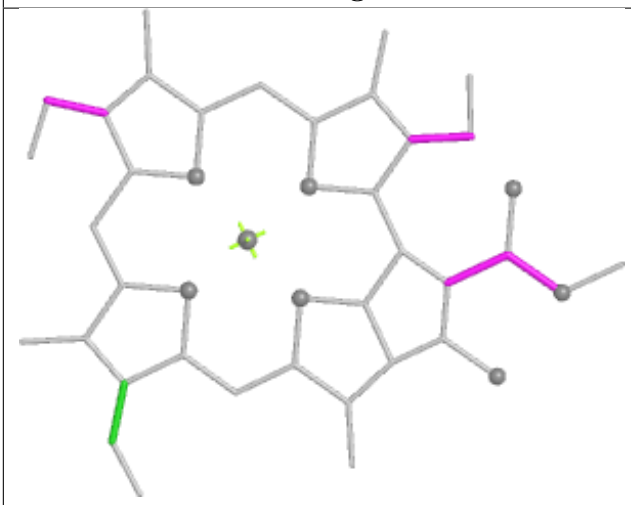
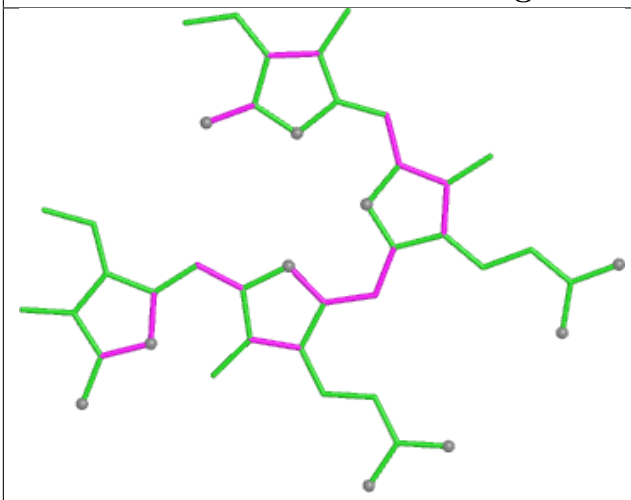


Torsions



Rings

Ligand PEB gK 203



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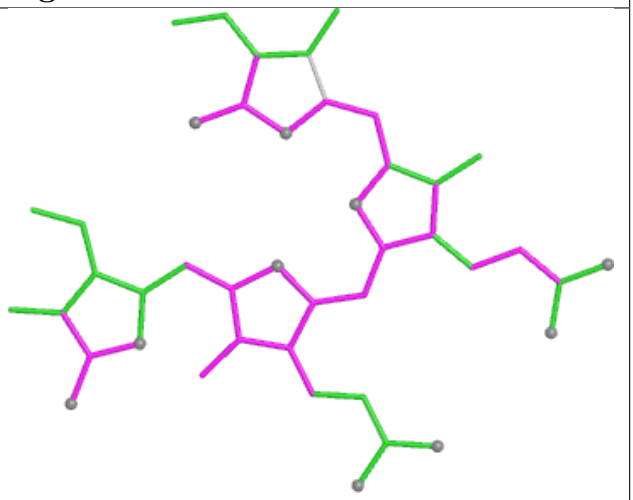

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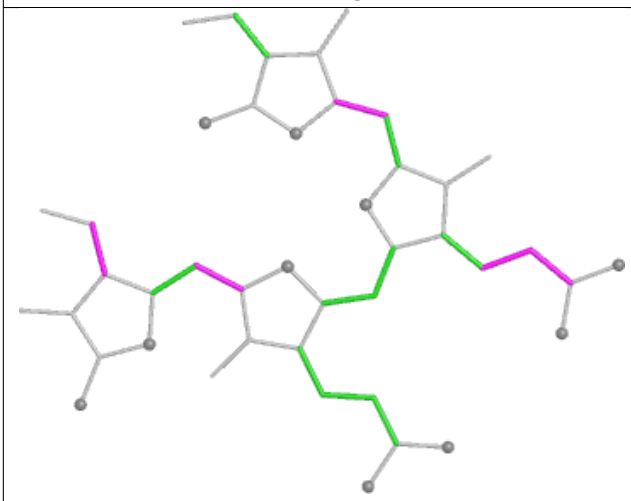

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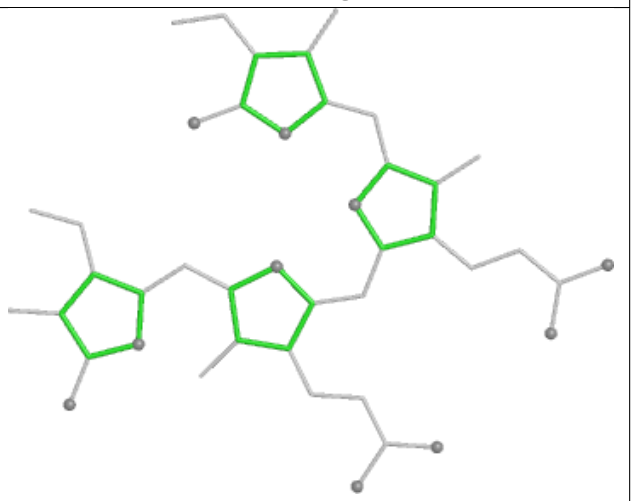

Rings

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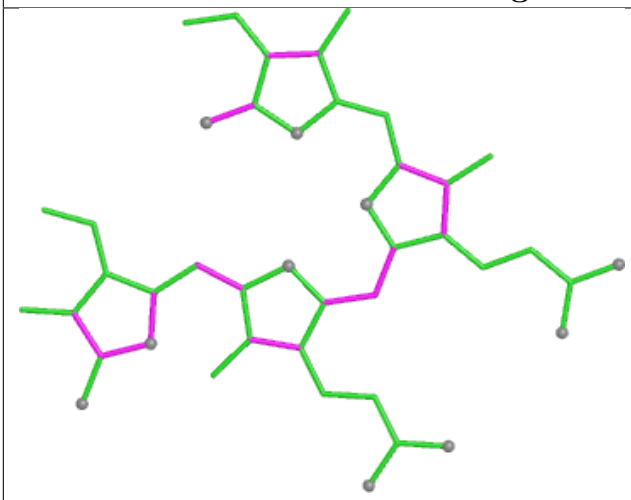

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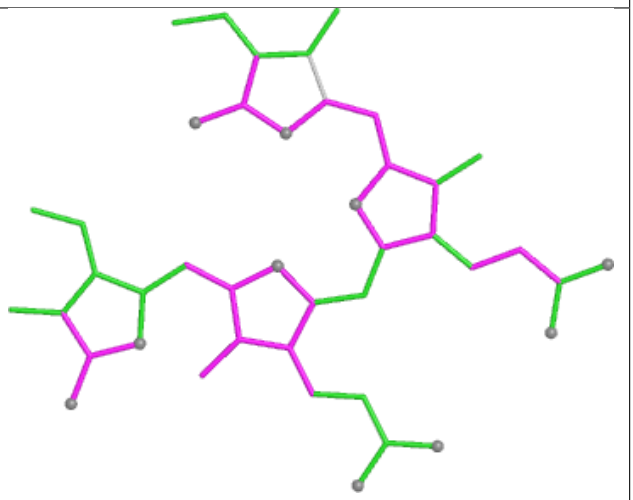

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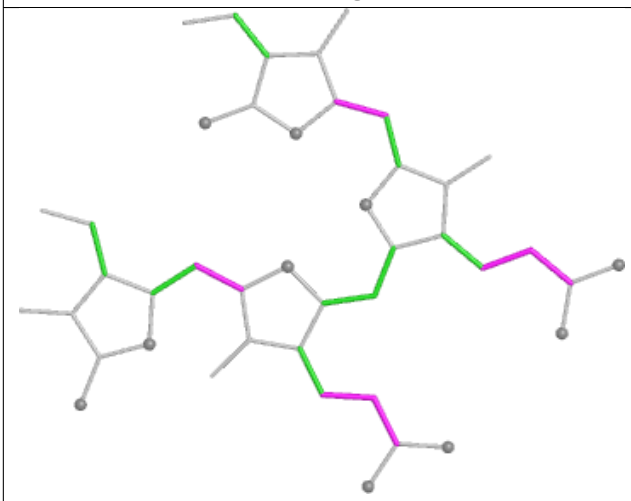

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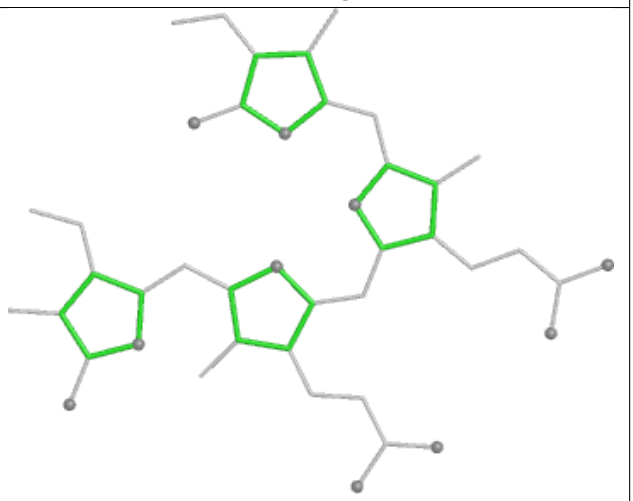
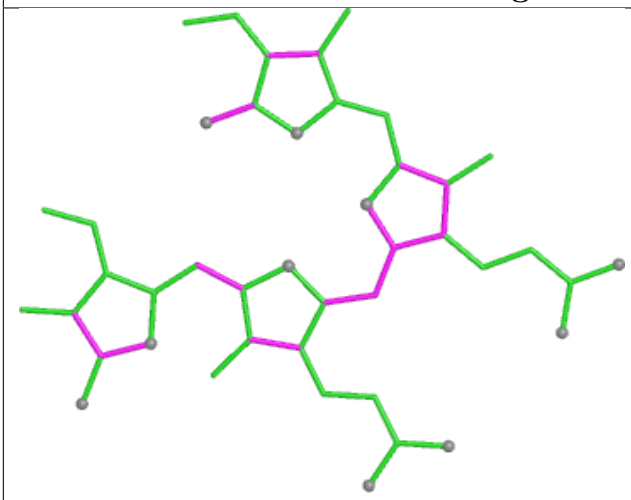


Rings

Ligand PEB M9 301



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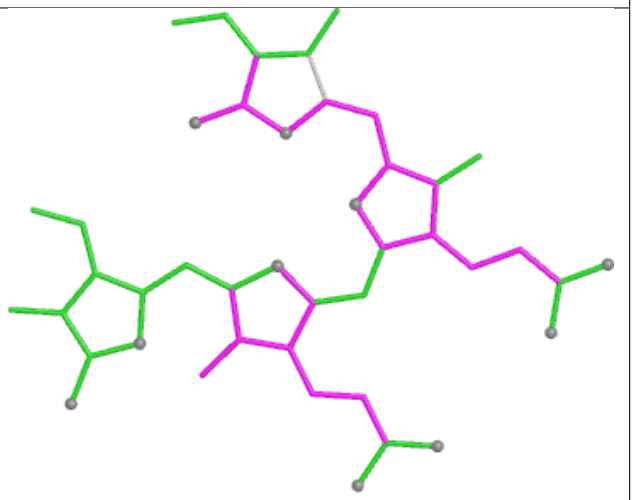

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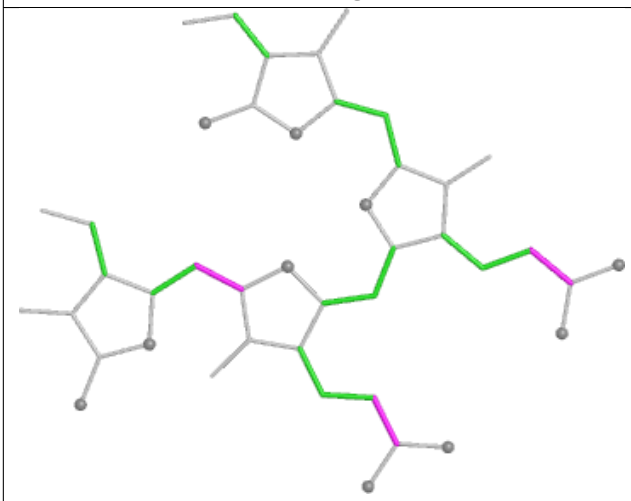

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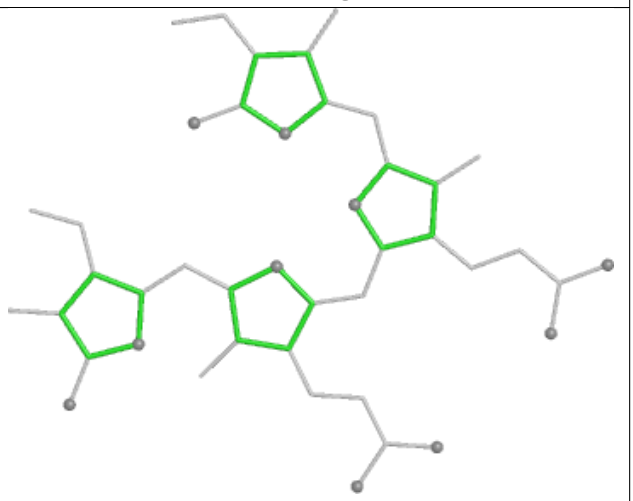
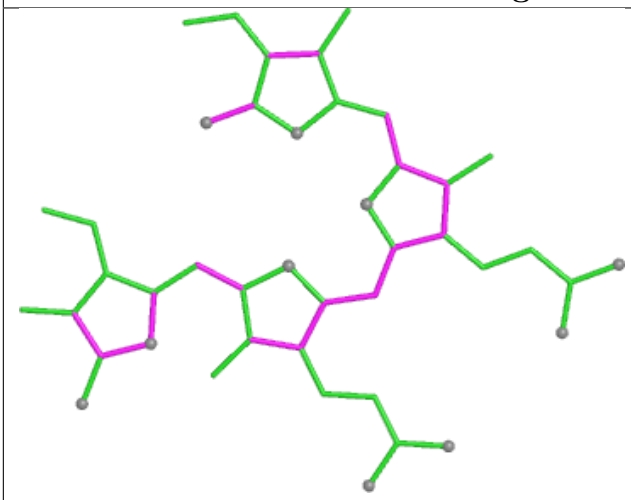


Rings

Ligand PEB EA 201



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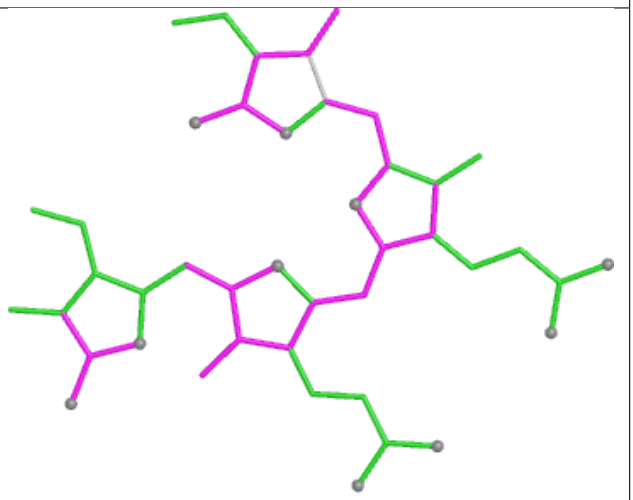

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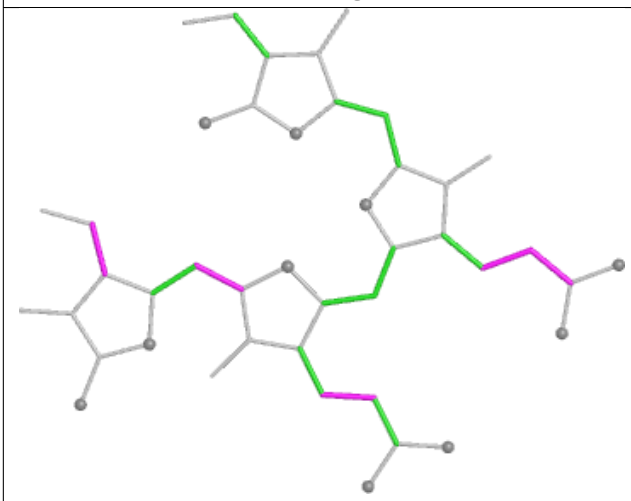

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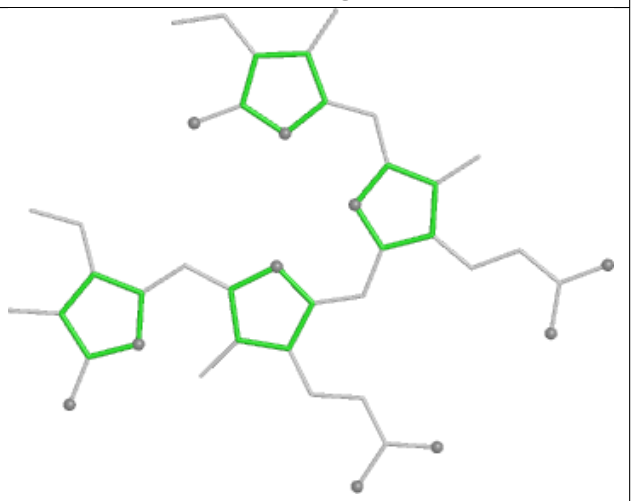
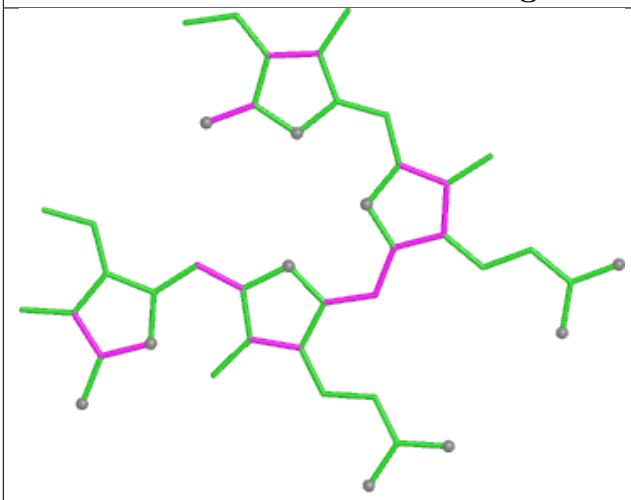


Rings

Ligand PEB 18 203



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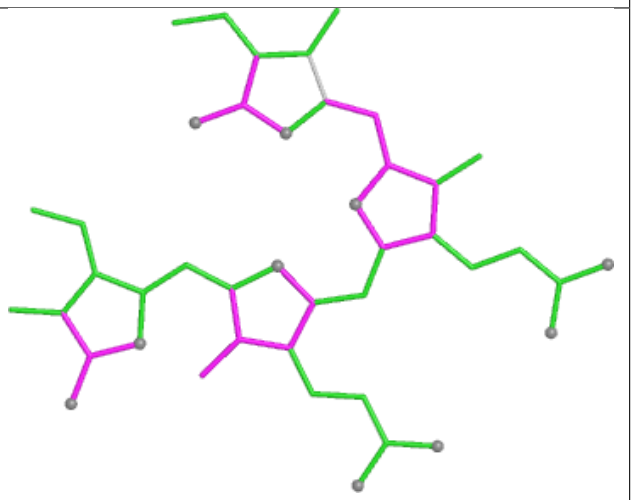

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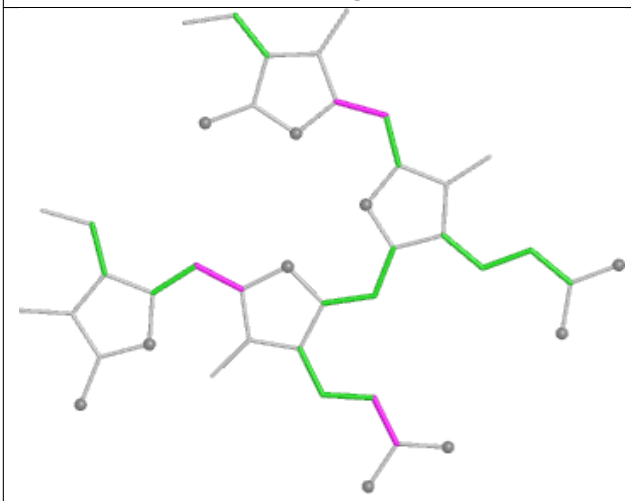

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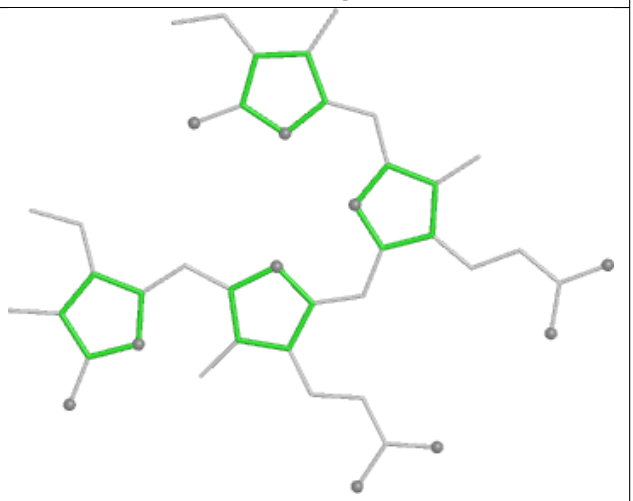

Rings

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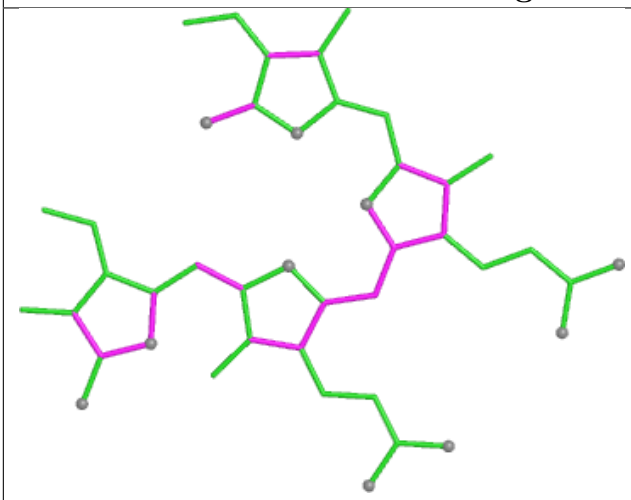

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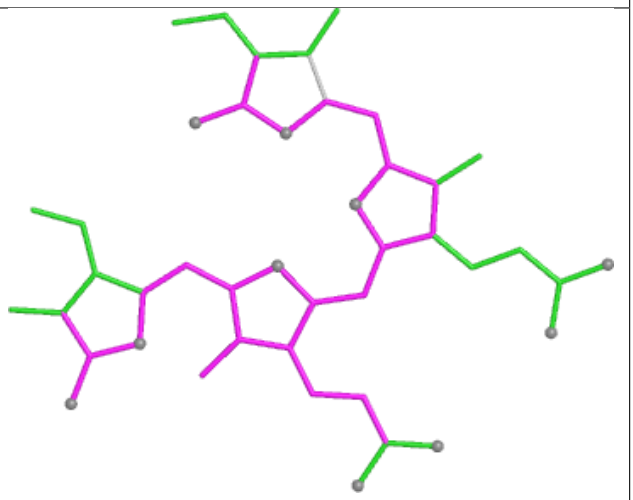
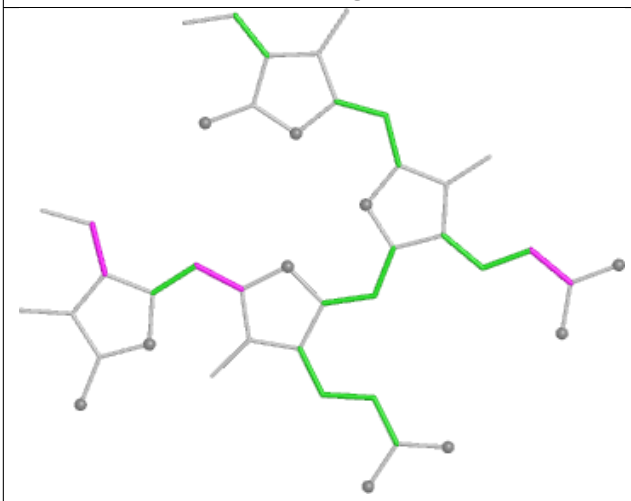


Bond angles



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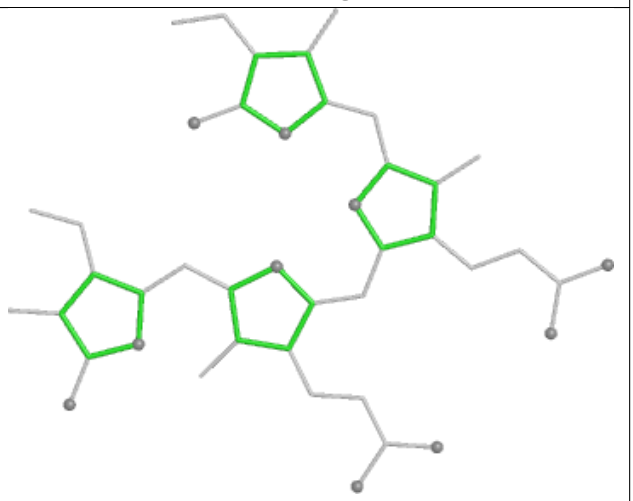
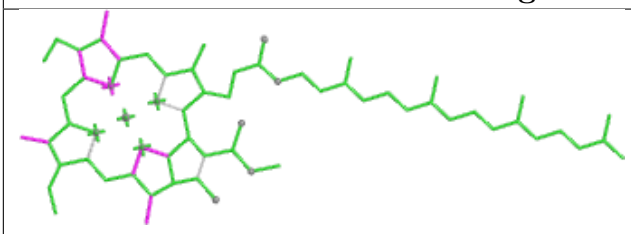


Rings

Ligand CLA cL 505



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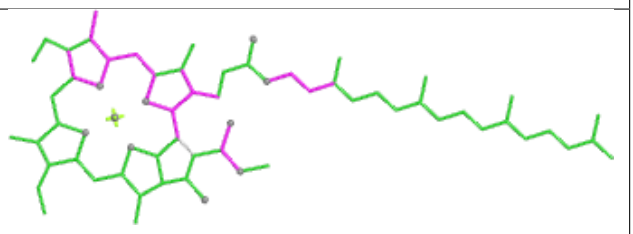
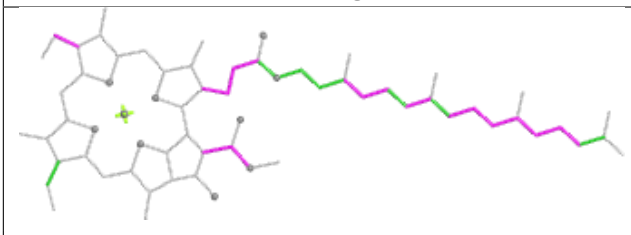


Bond angles



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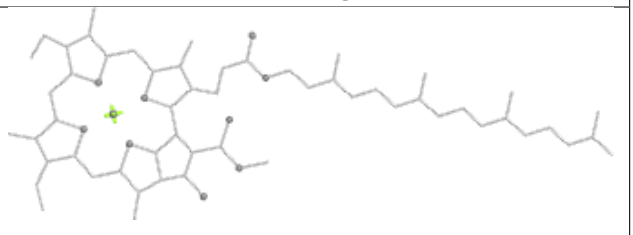
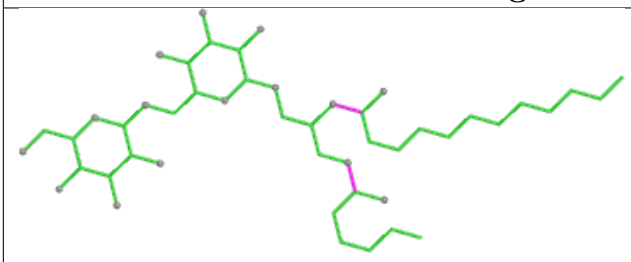


Rings

Ligand DGD CL 523



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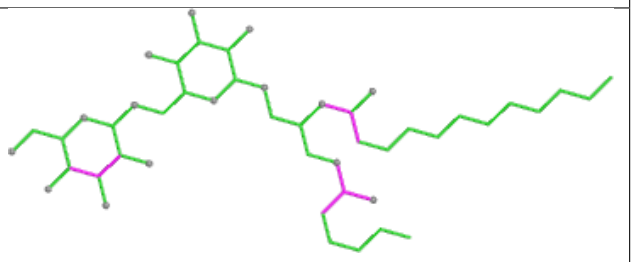
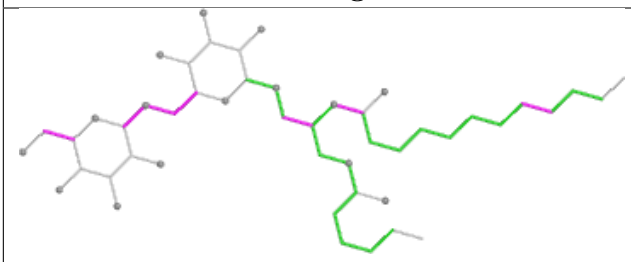


Bond angles



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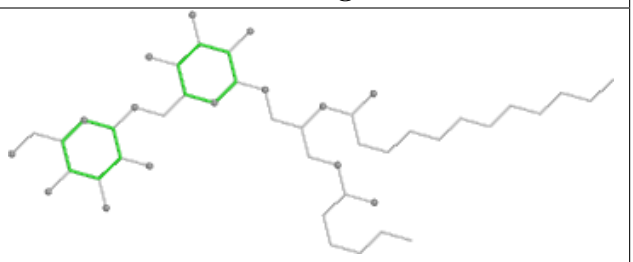
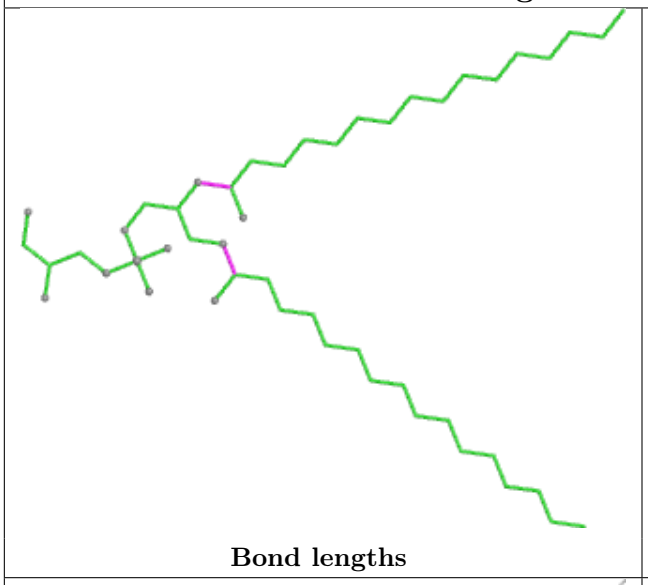


Rings

Ligand LHG dL 405



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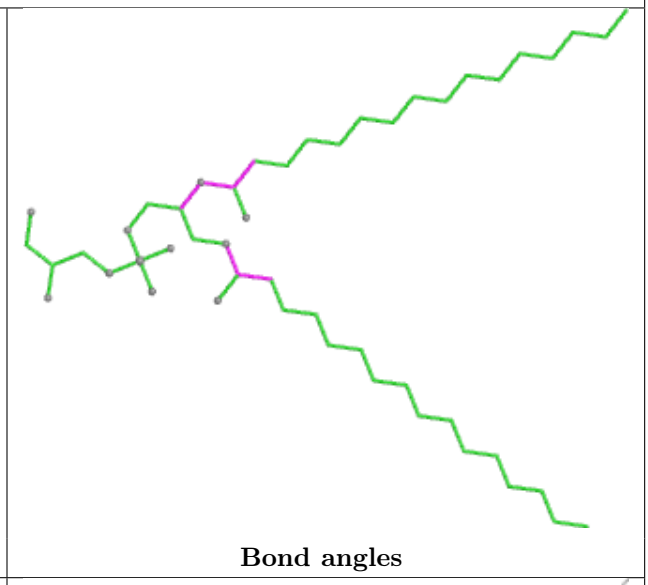
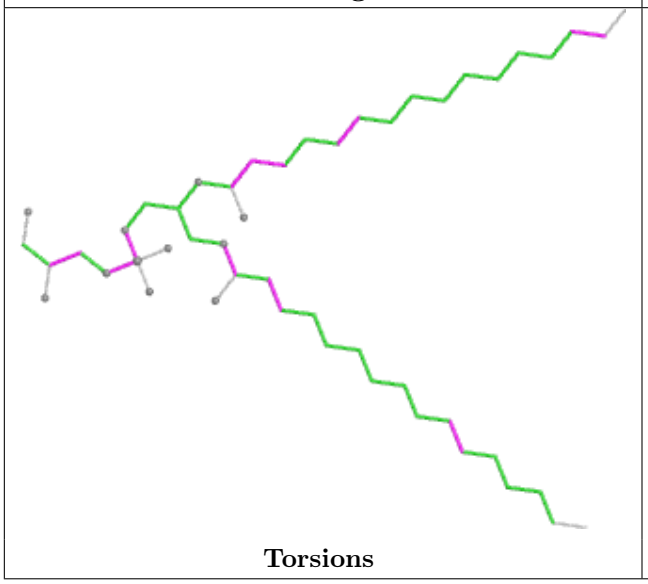
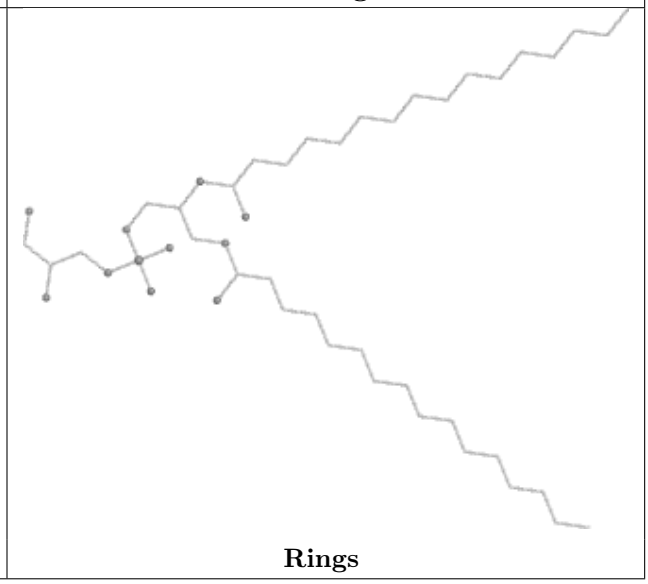


Bond angles

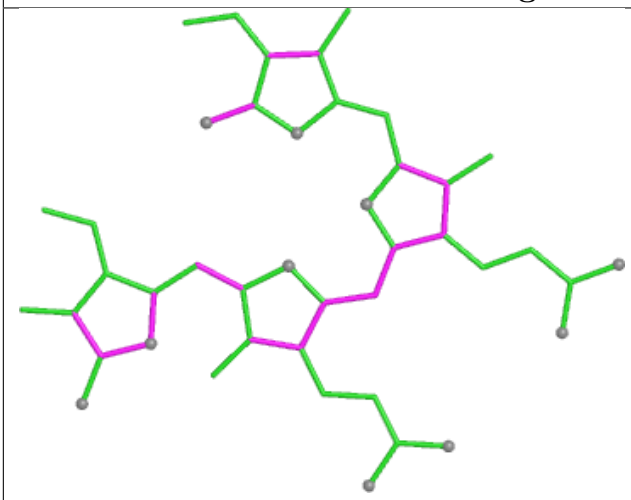


Torsions



Rings

Ligand PEB iK 203



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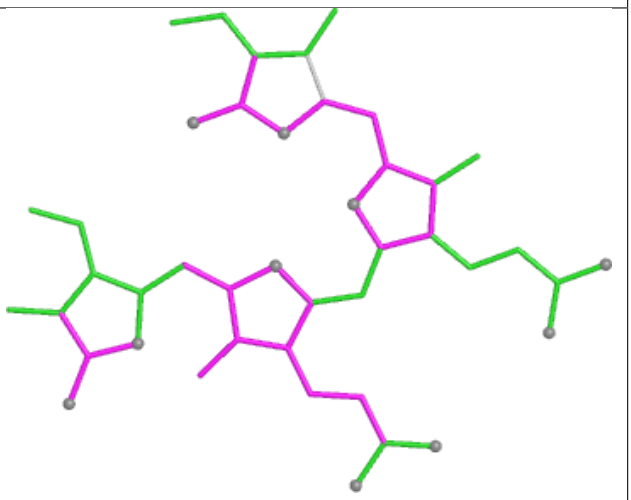

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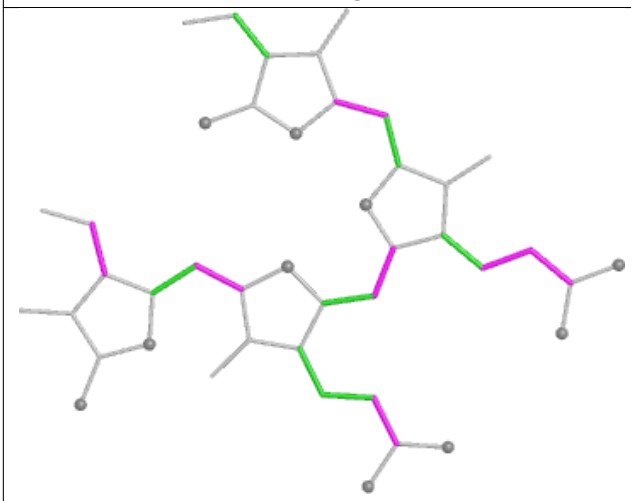

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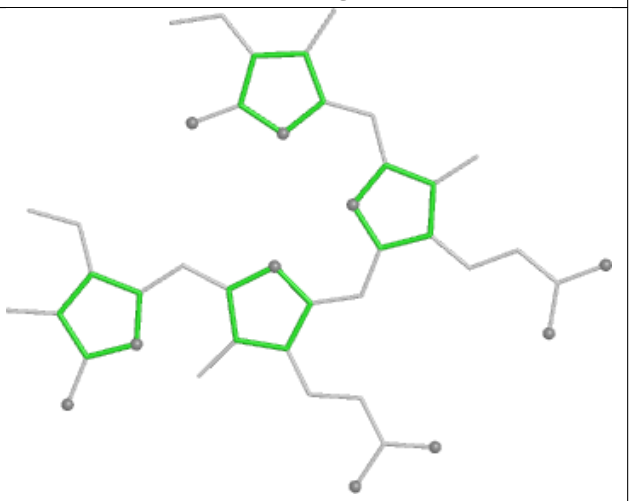

Rings

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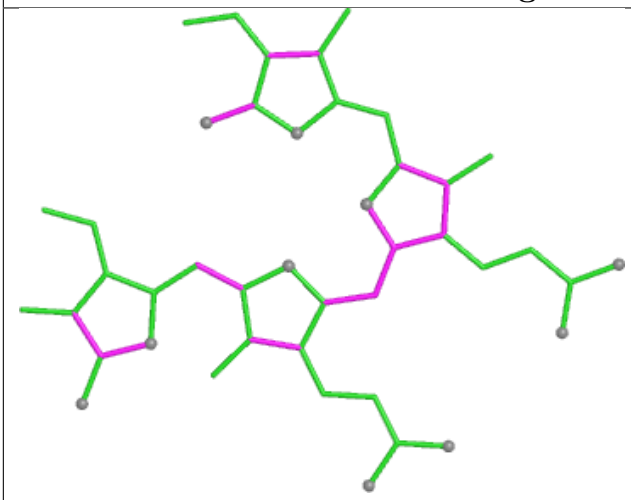

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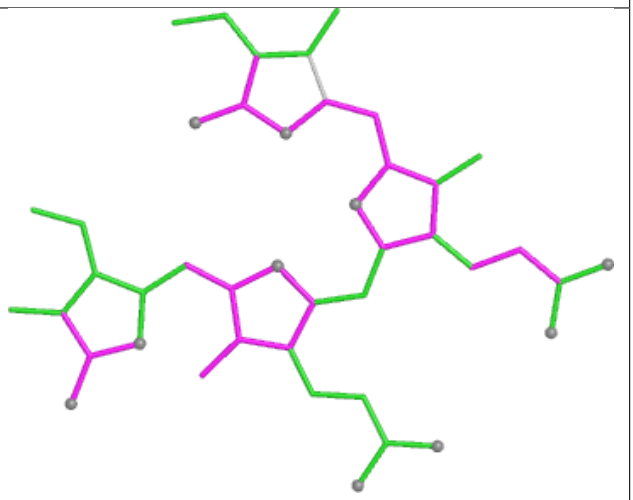

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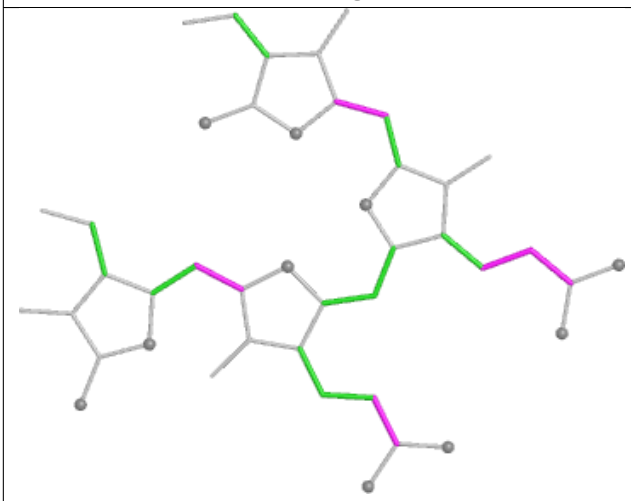

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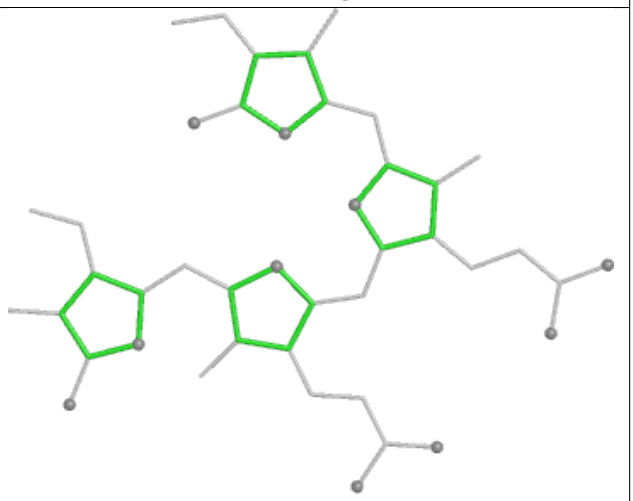
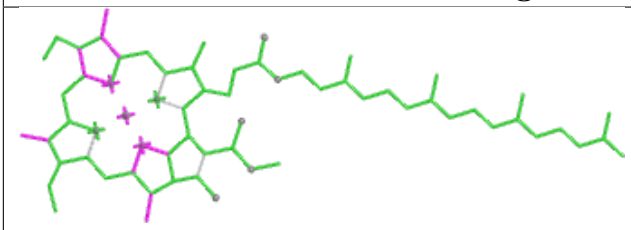


Rings

Ligand CLA B2 806



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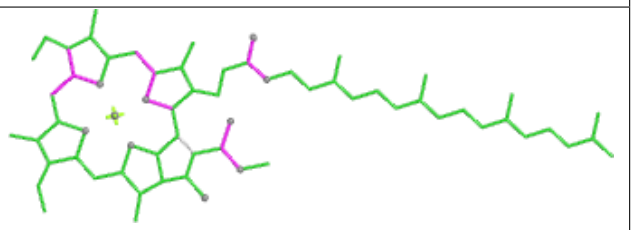

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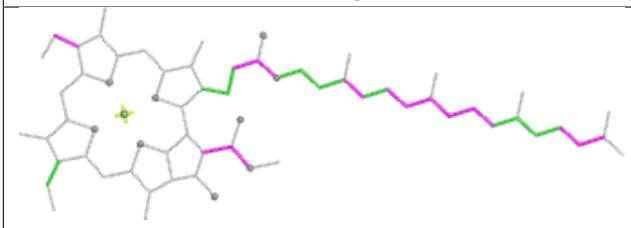

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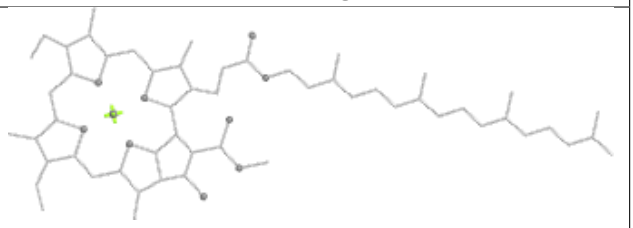
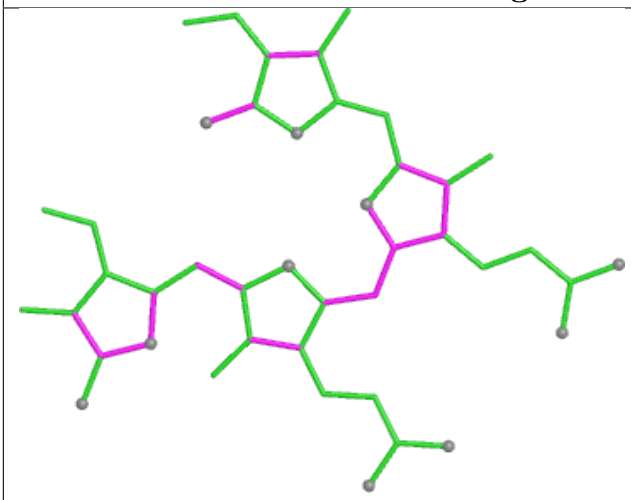


Rings

Ligand PEB J1 1002



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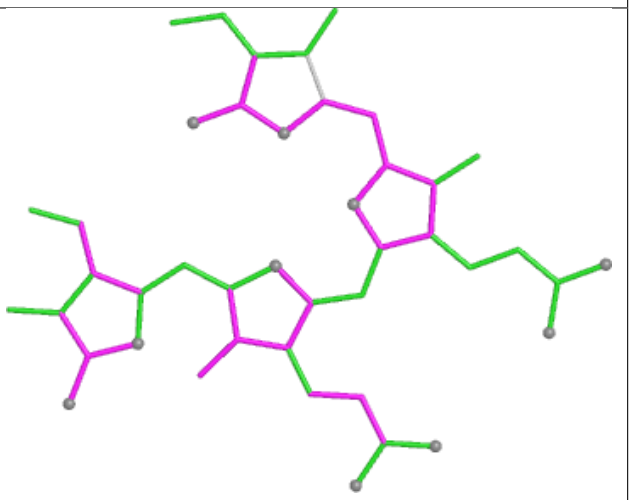

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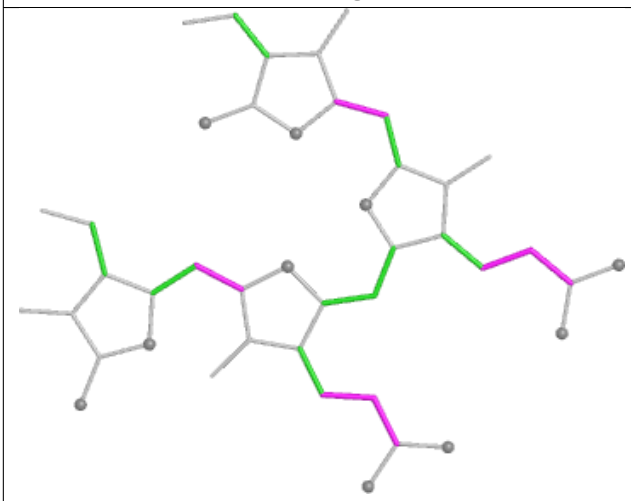

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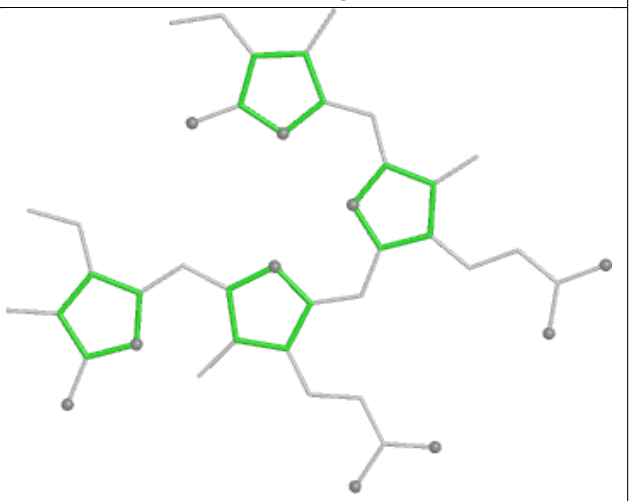
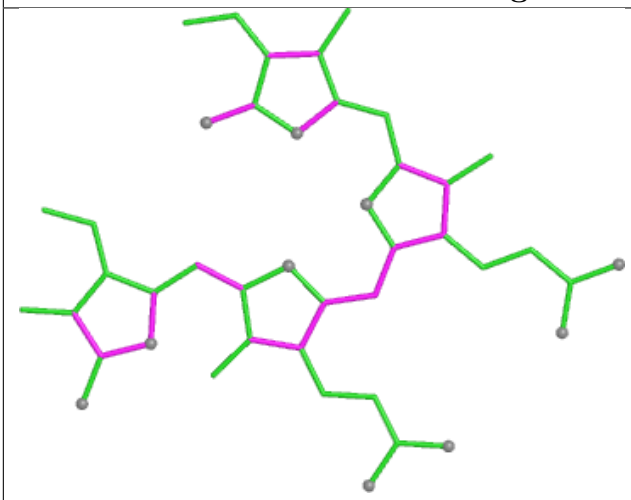


Rings

Ligand PEB OH 201



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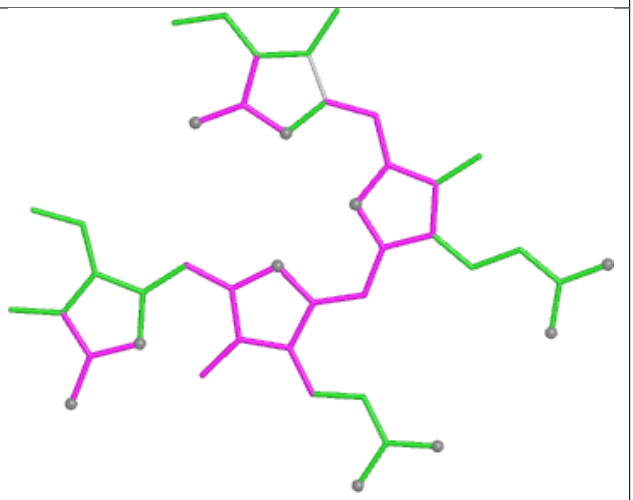

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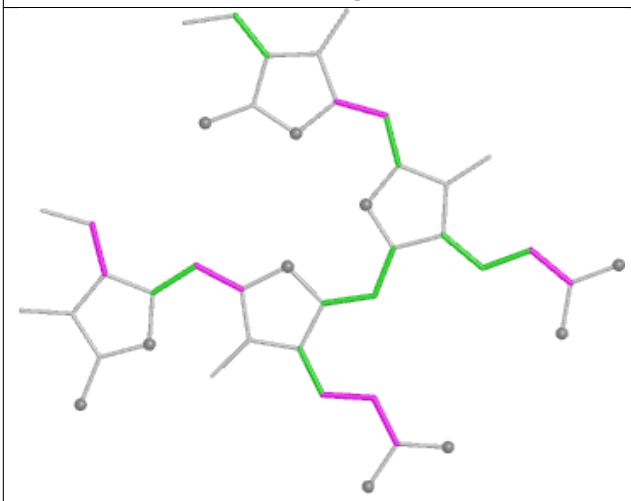

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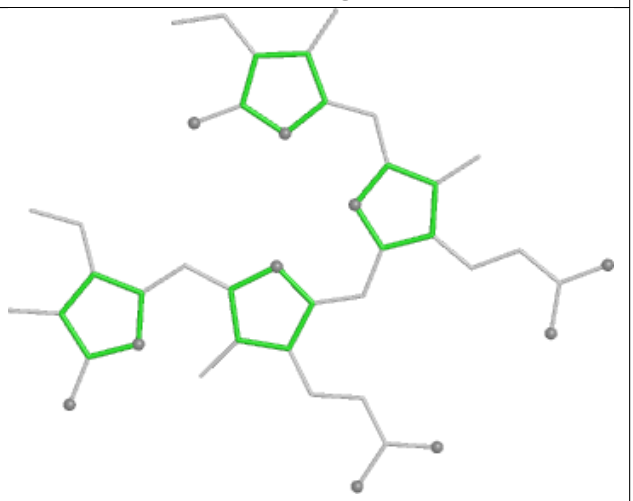
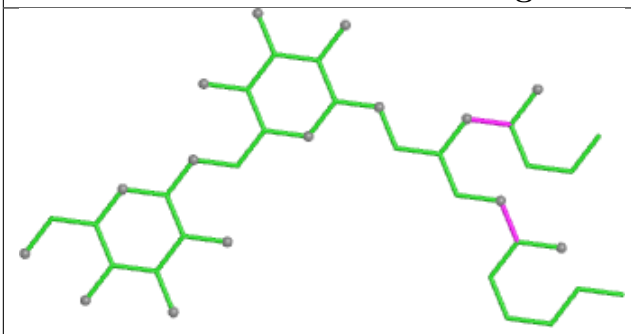


Rings

Ligand DGD a6 602



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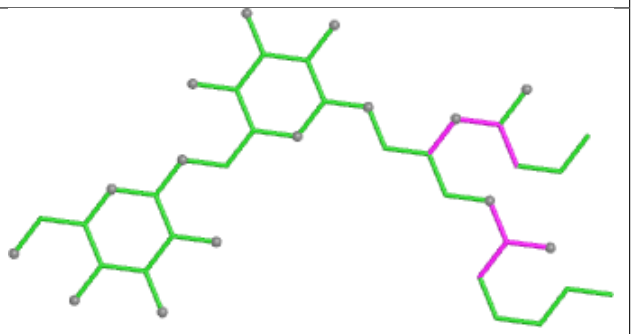

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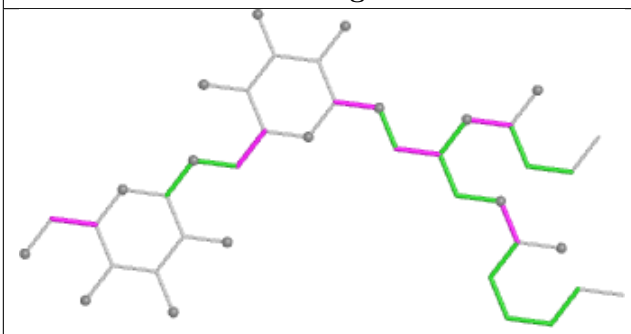

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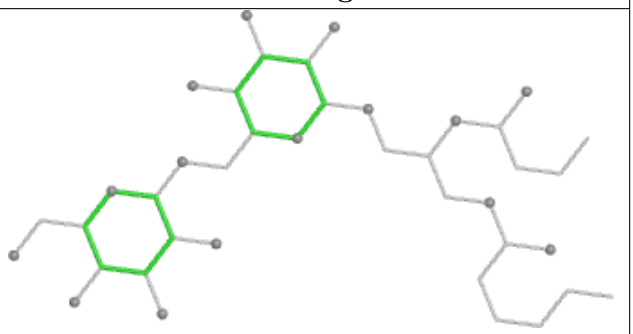
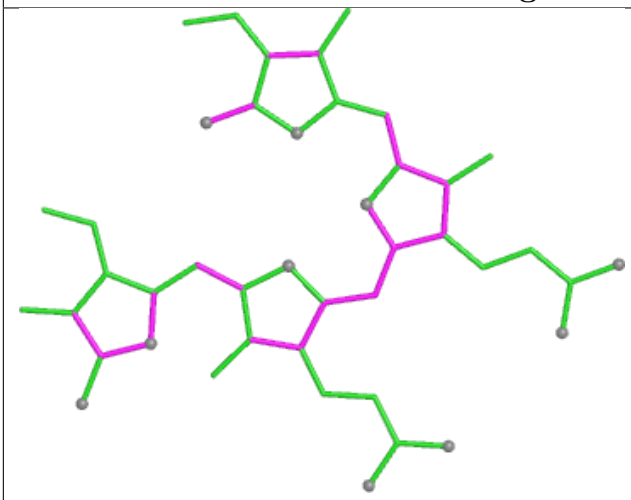


Rings

Ligand PEB J9 201



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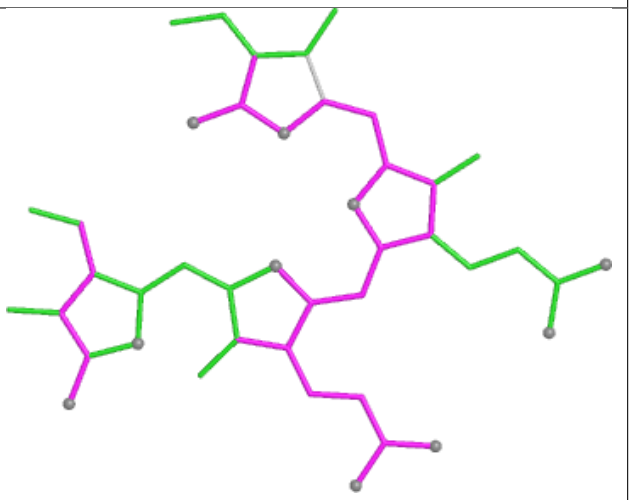

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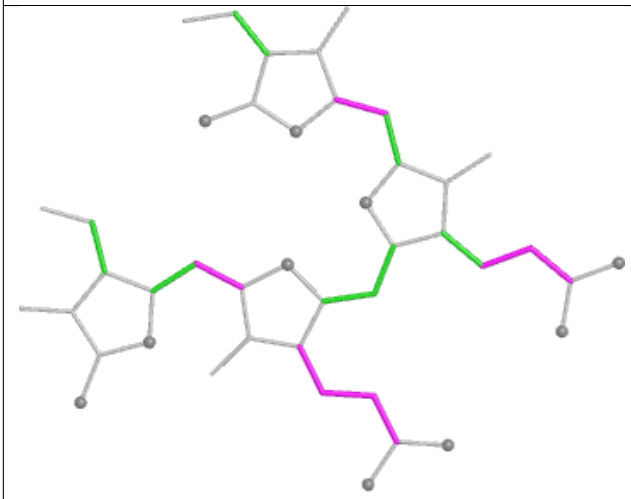

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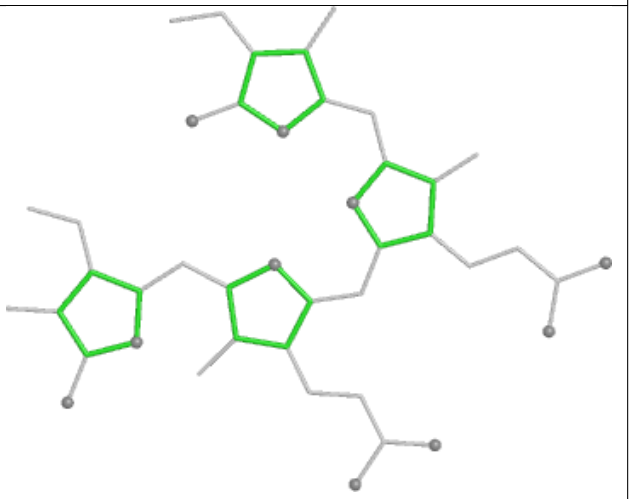
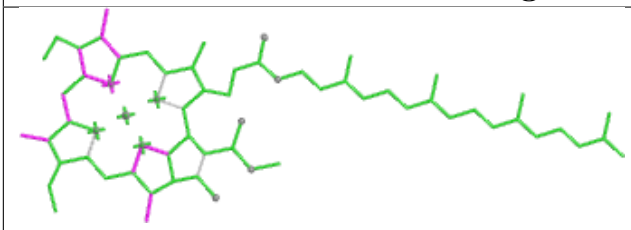


Rings

Ligand CLA c6 613



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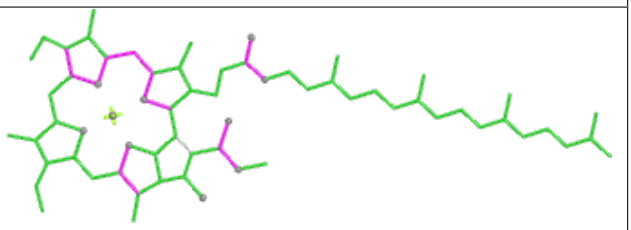

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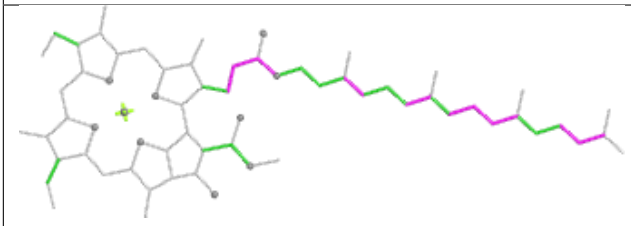

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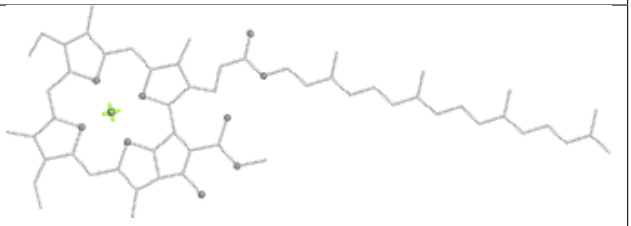
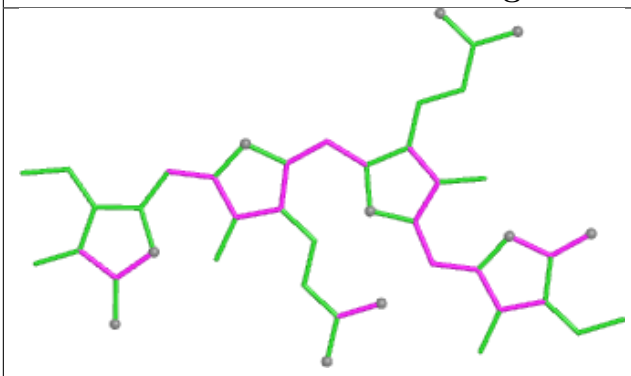


Rings

Ligand CYC U3 1001



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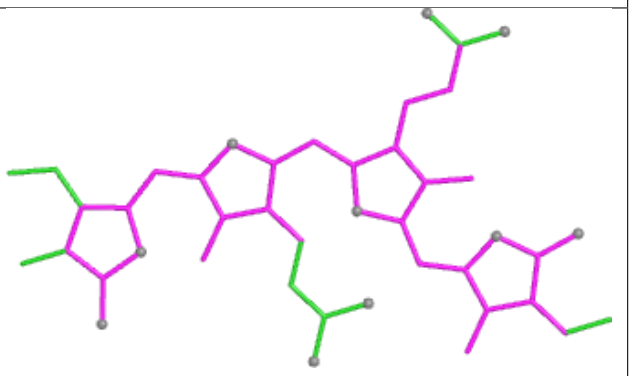

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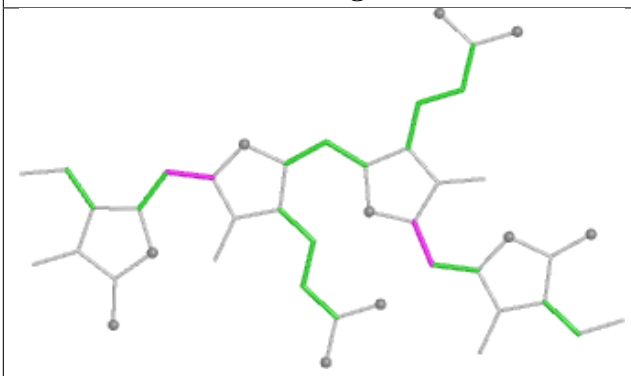

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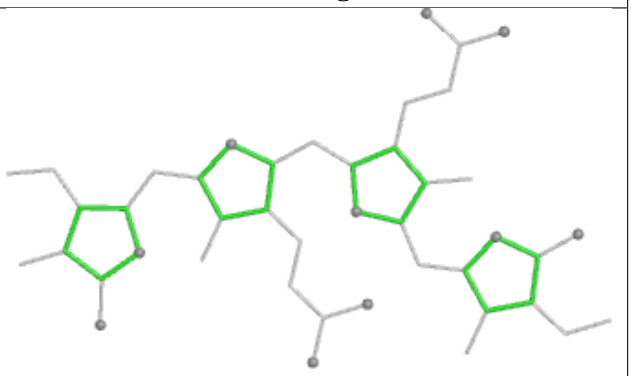
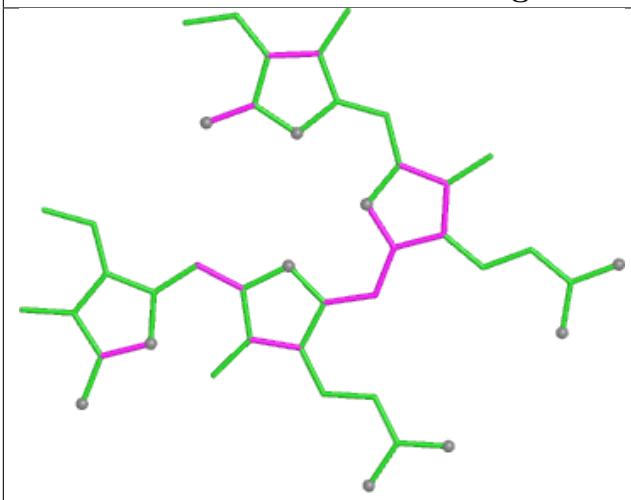


Rings

Ligand PEB TQ 203



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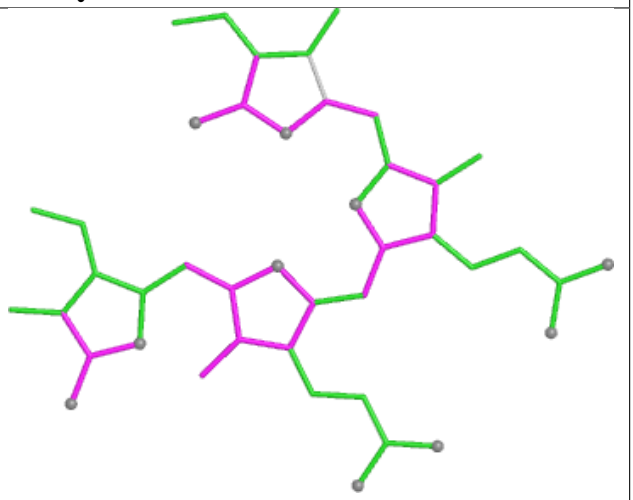

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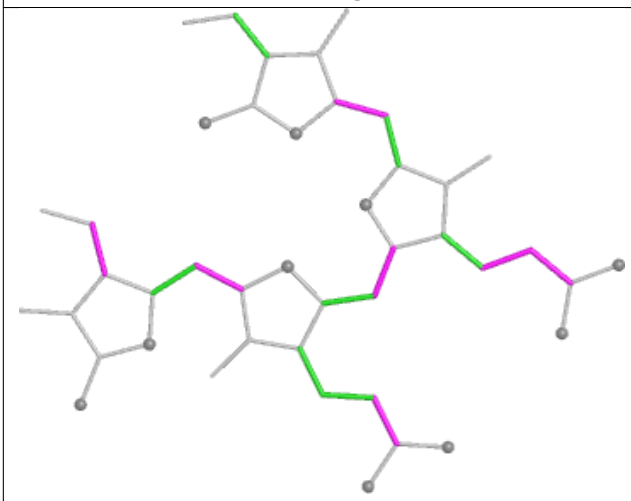

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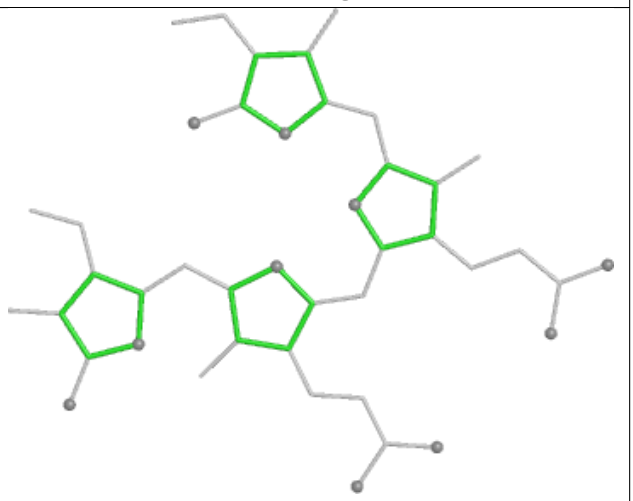
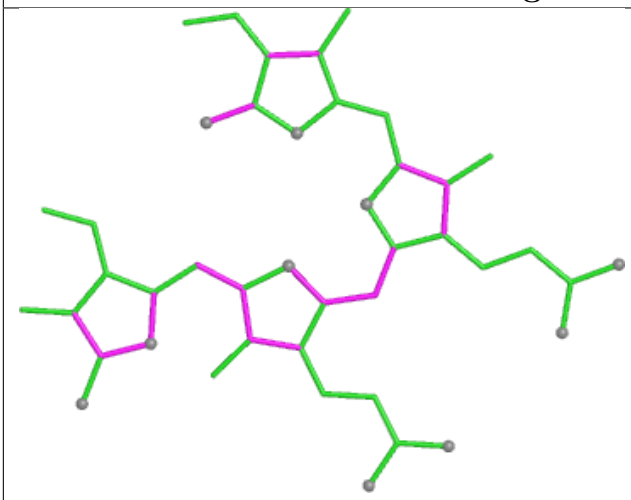


Rings

Ligand PEB lJ 202



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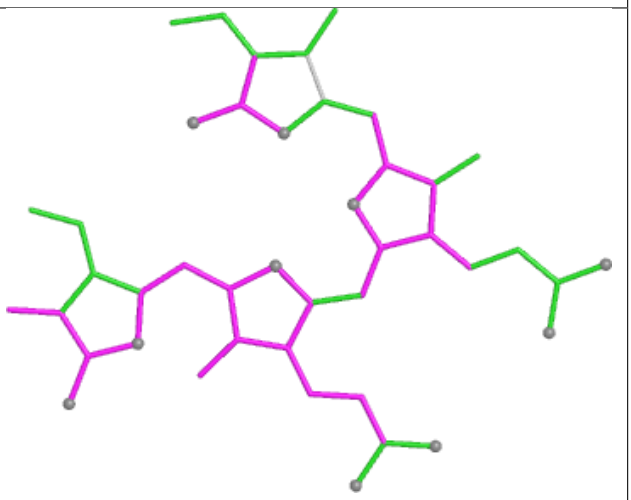

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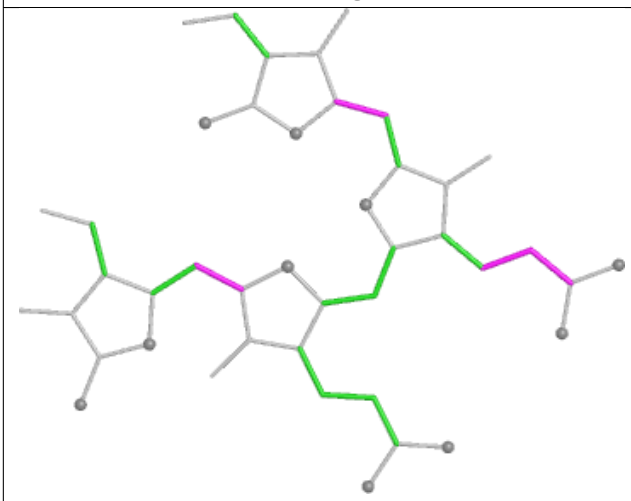

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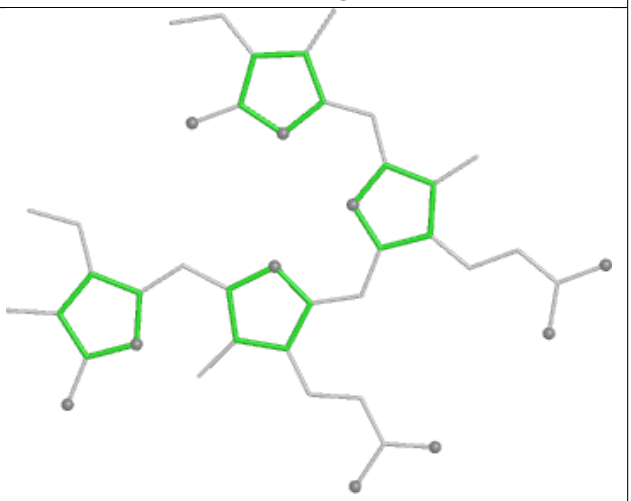
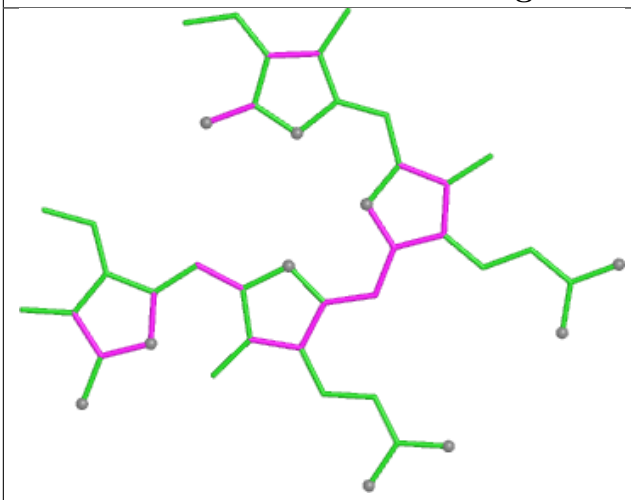


Rings

Ligand PEB eG 201



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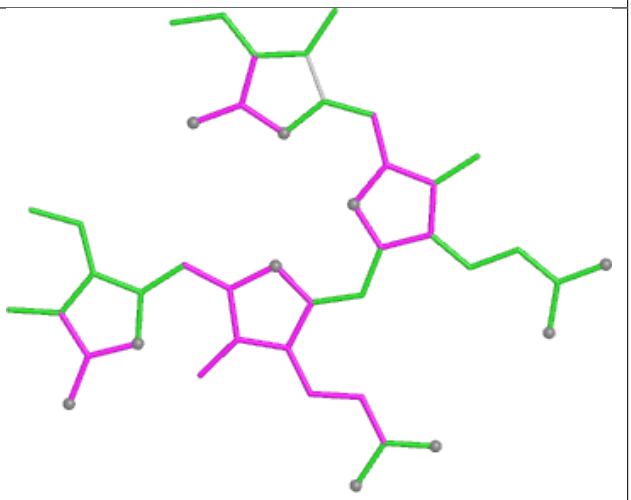
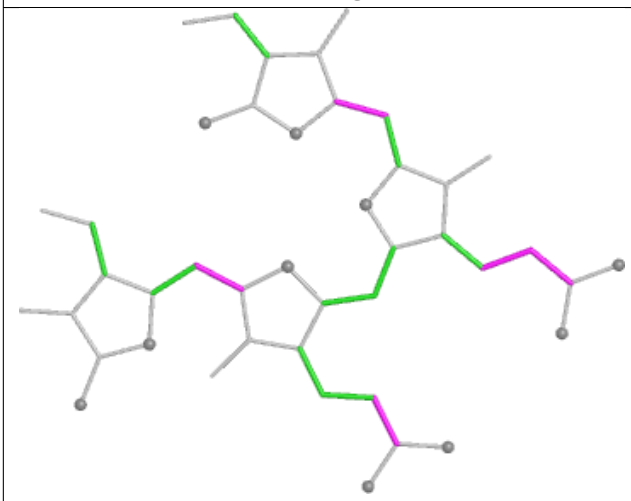


Bond angles



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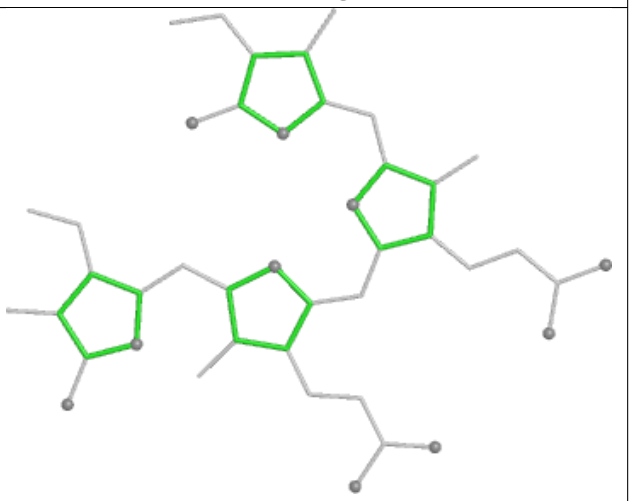
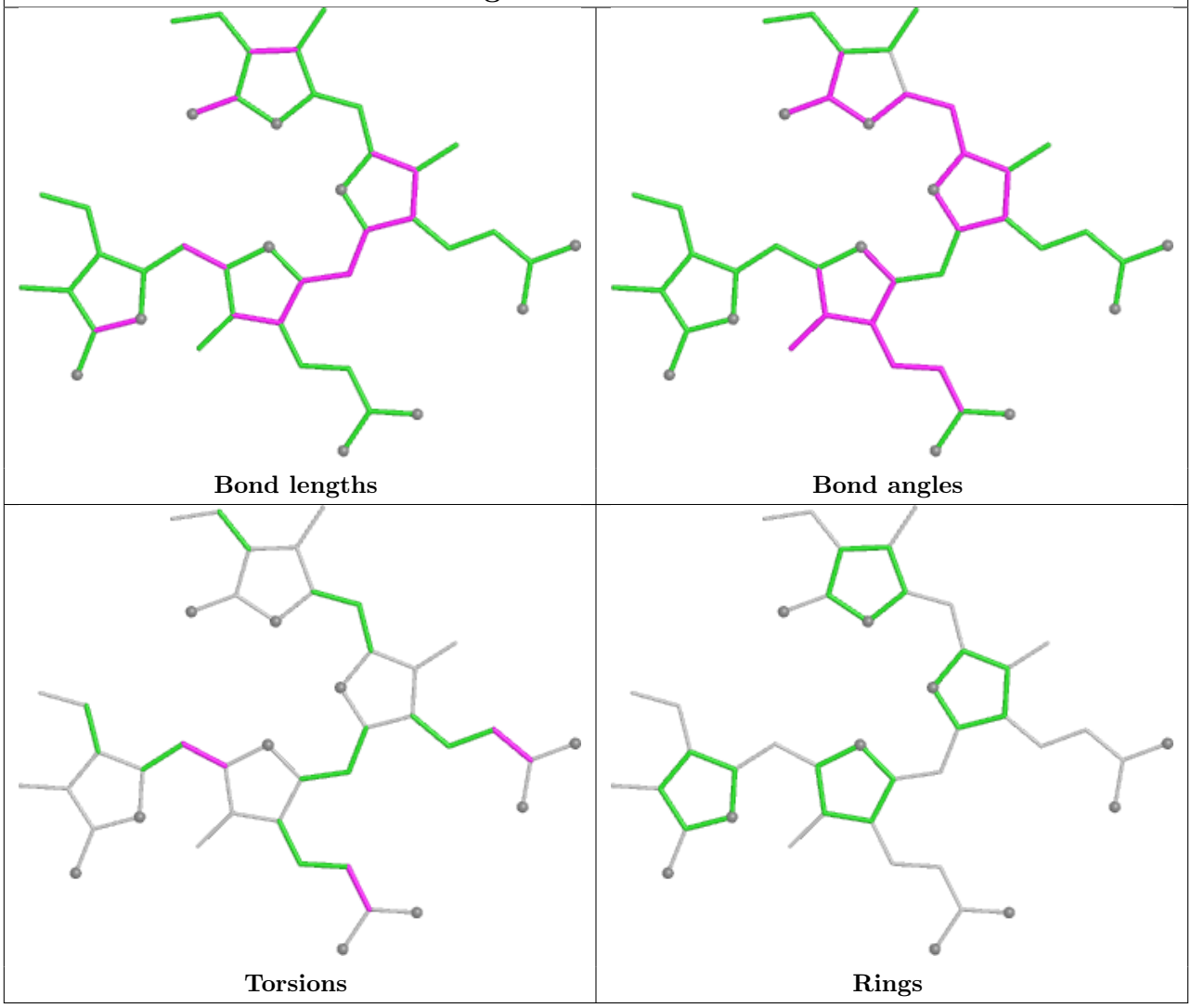
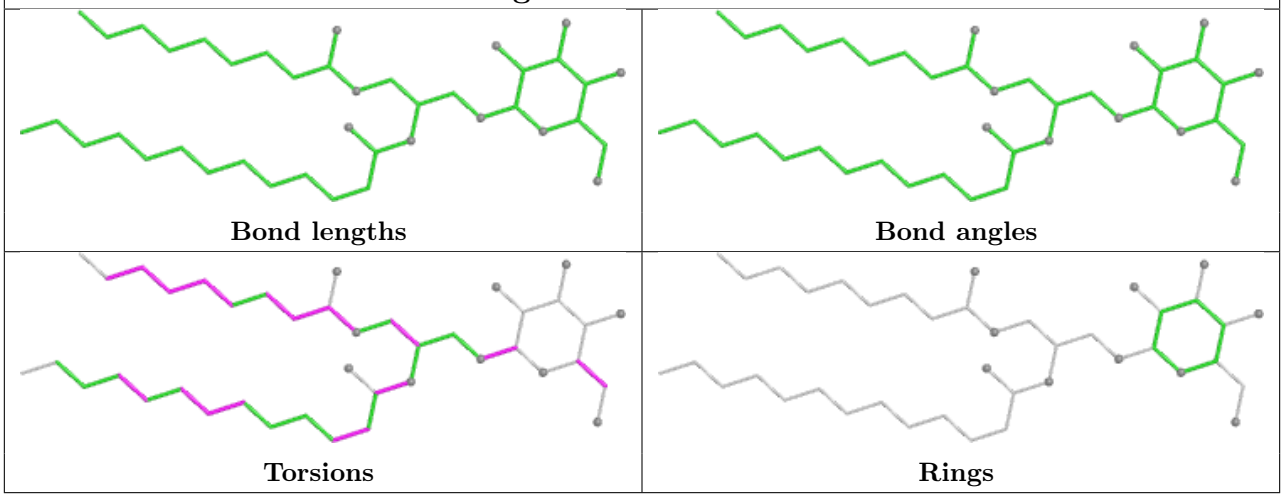


Rings

Ligand PEB e4 203



Ligand LMG bL 609



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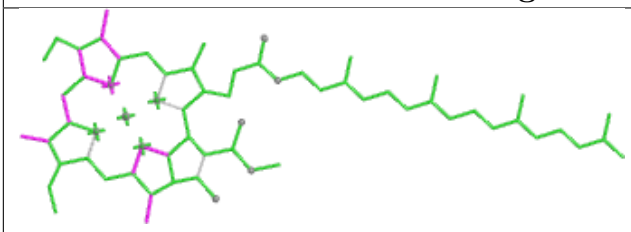

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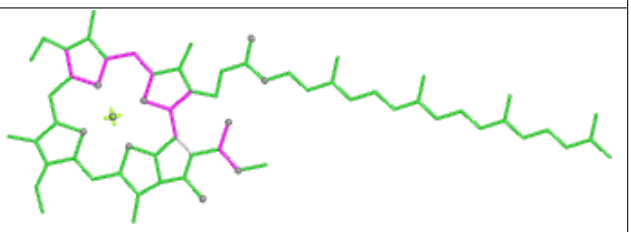
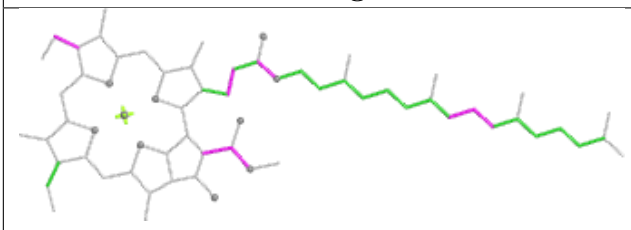


Bond angles



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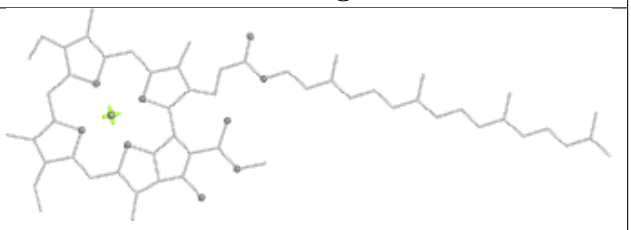
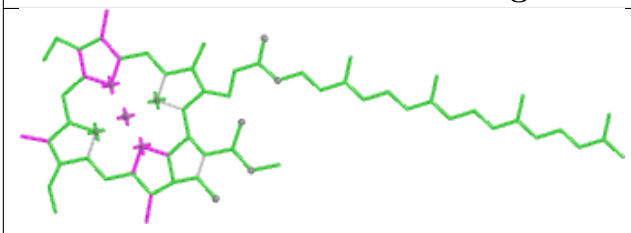


Rings

Ligand CLA BN 823



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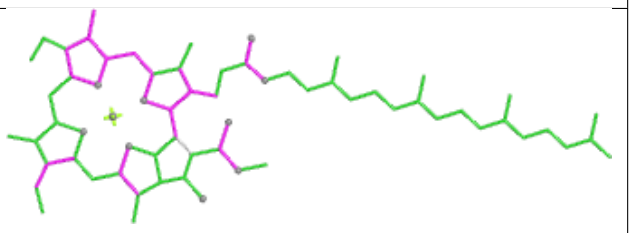
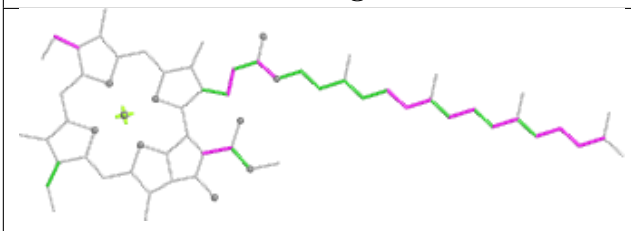
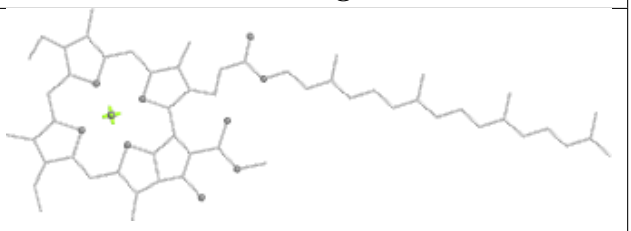


Bond angles

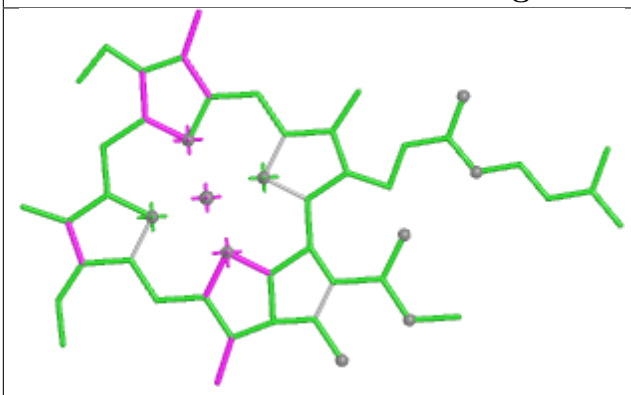


Torsions



Rings

Ligand CLA LN 204



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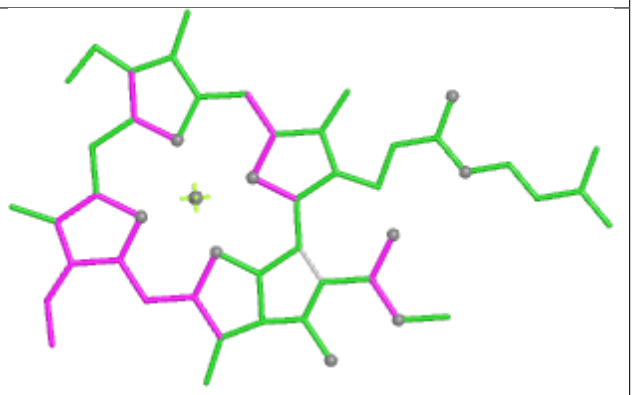
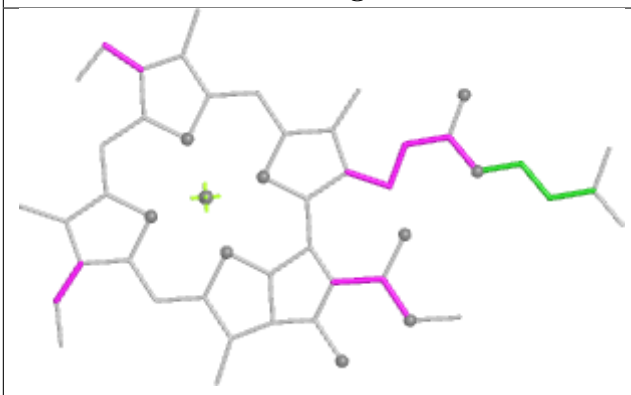


Bond angles



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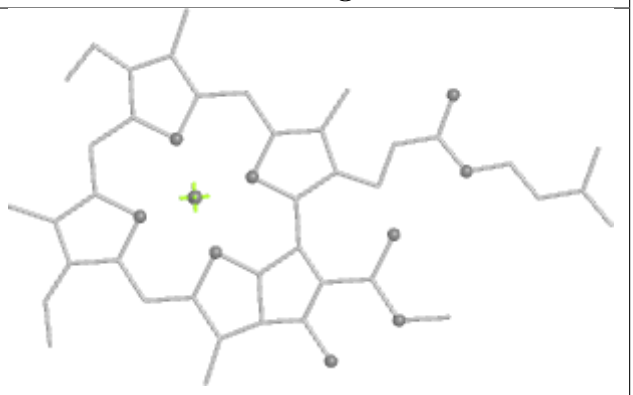
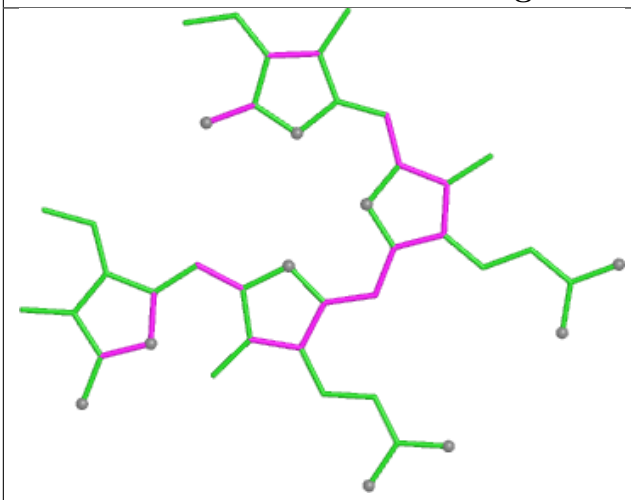


Rings

Ligand PEB gH 203



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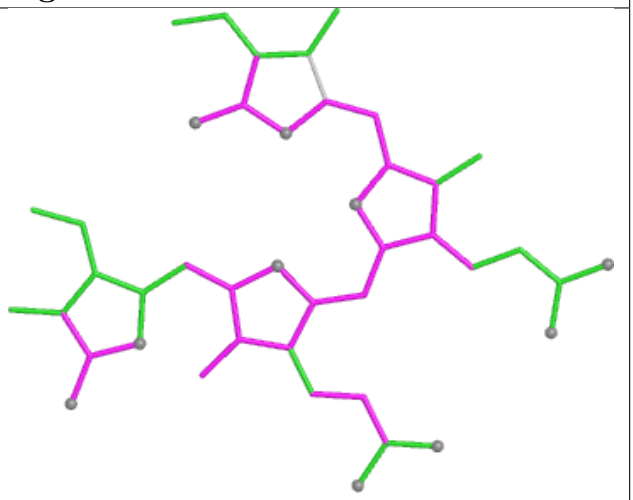
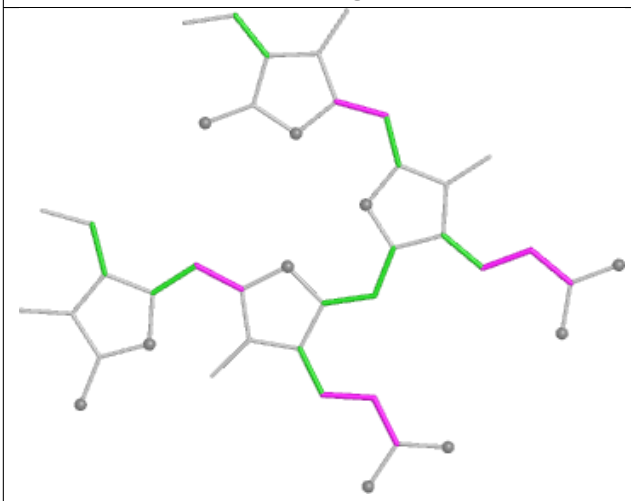


Bond angles



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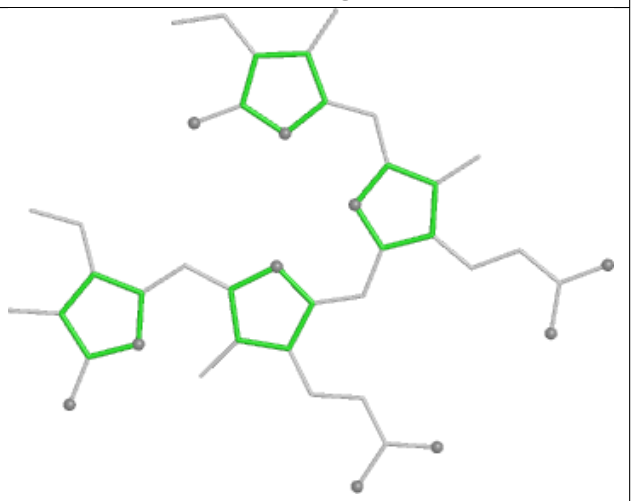
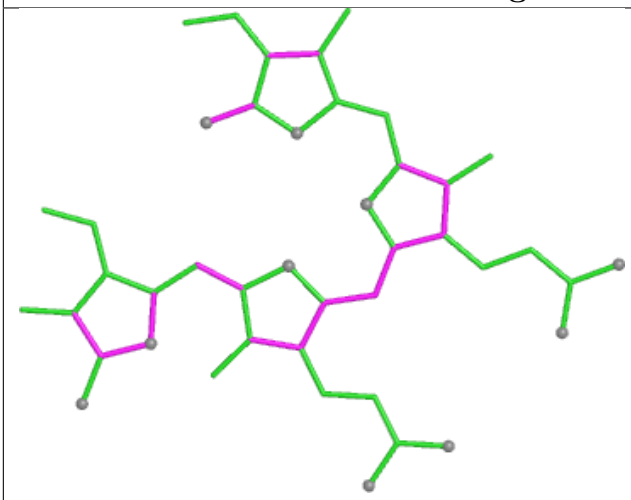


Rings

Ligand PEB EM 201



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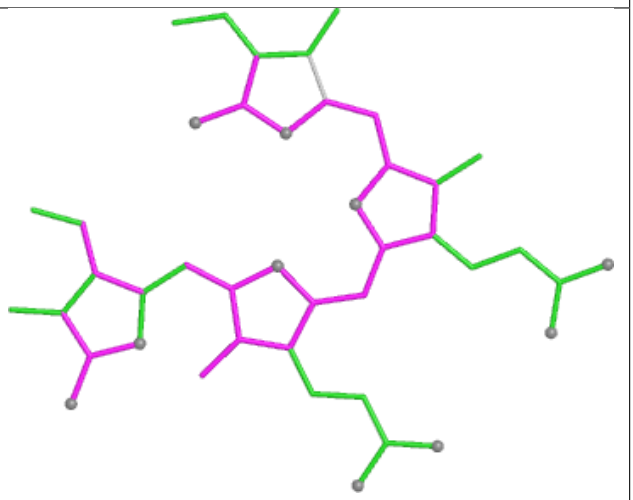

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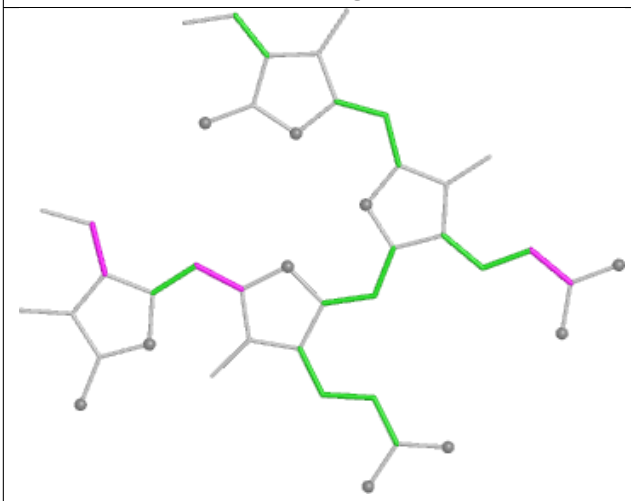

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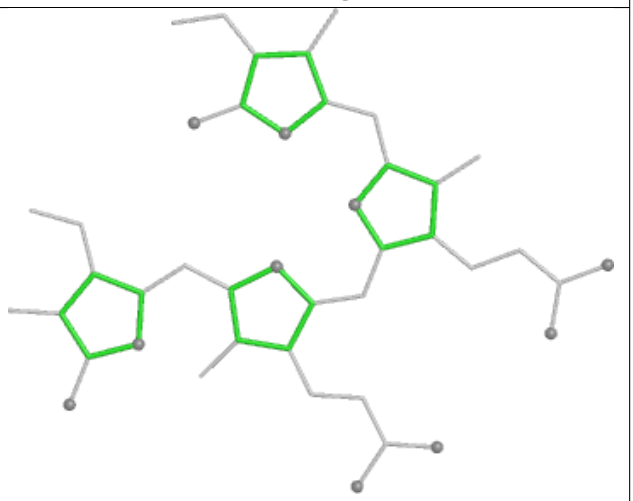
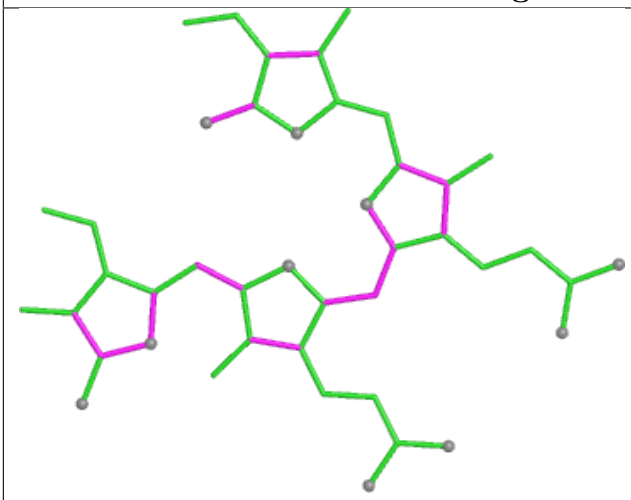


Rings

Ligand PEB CB 201



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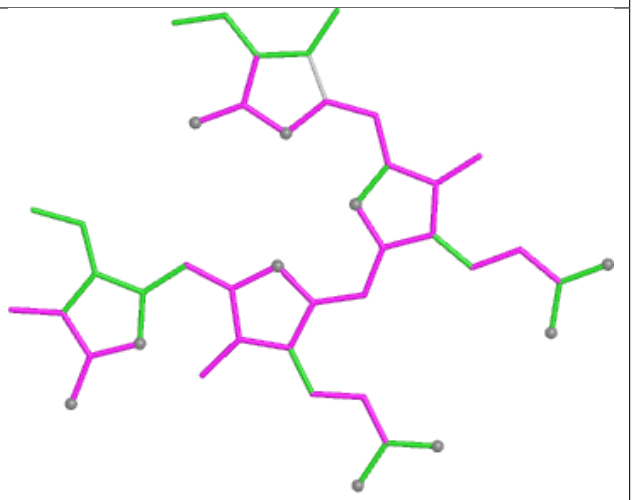

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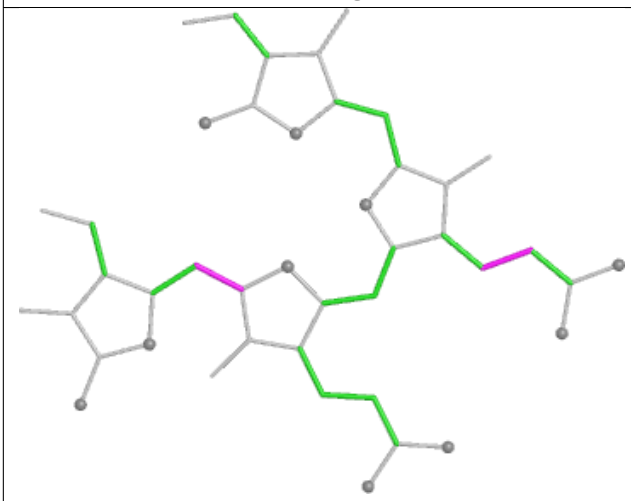

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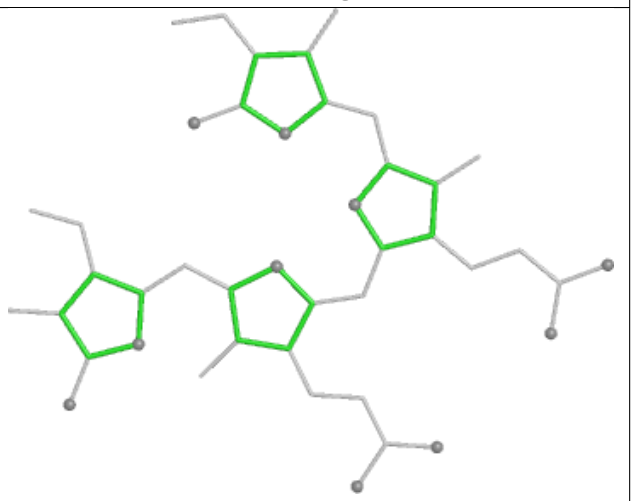
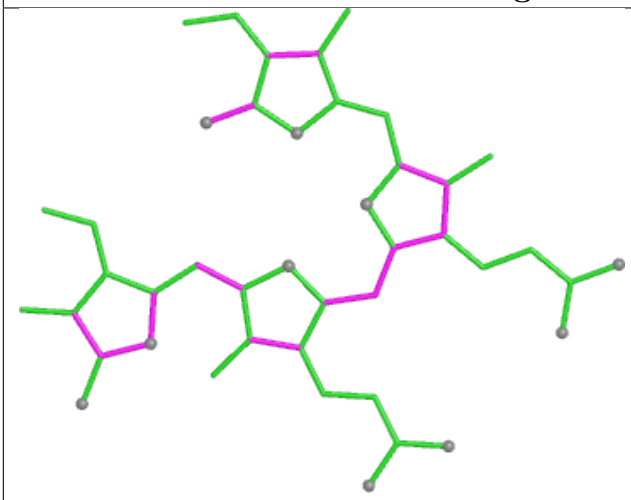


Rings

Ligand PEB EP 202



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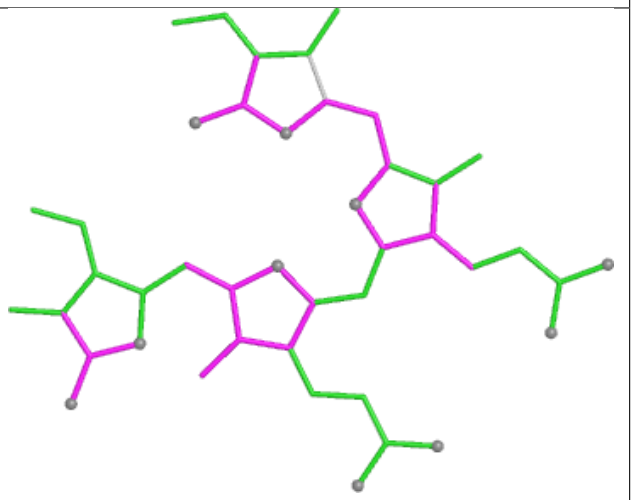

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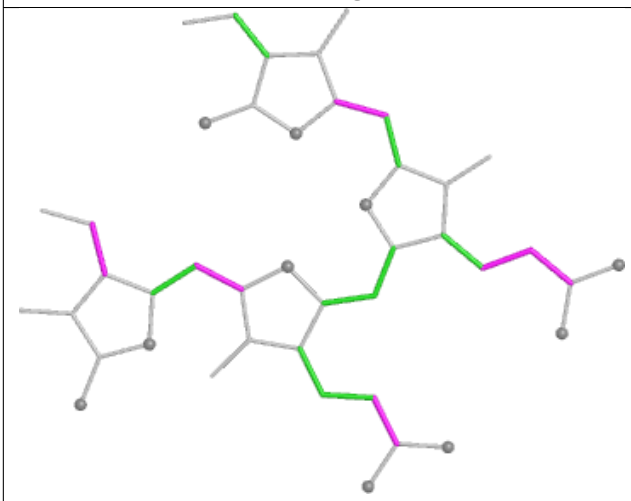

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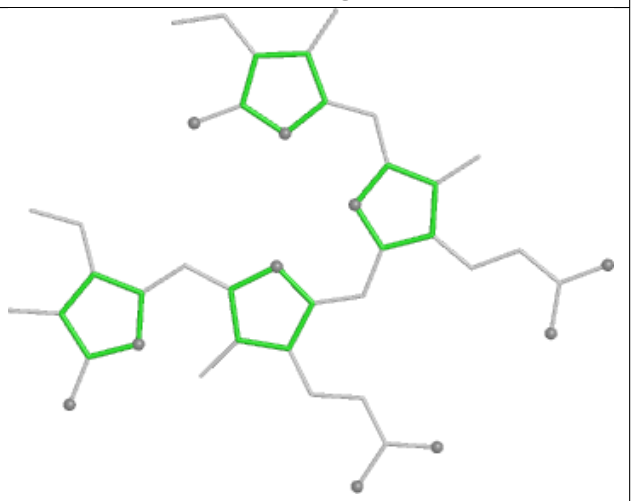
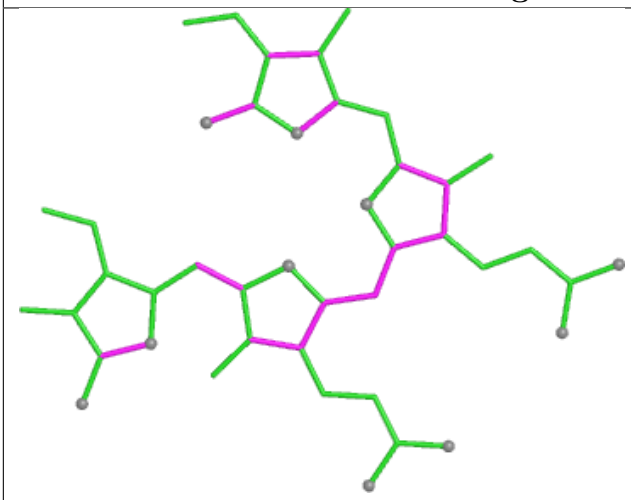


Rings

Ligand PEB VQ 202



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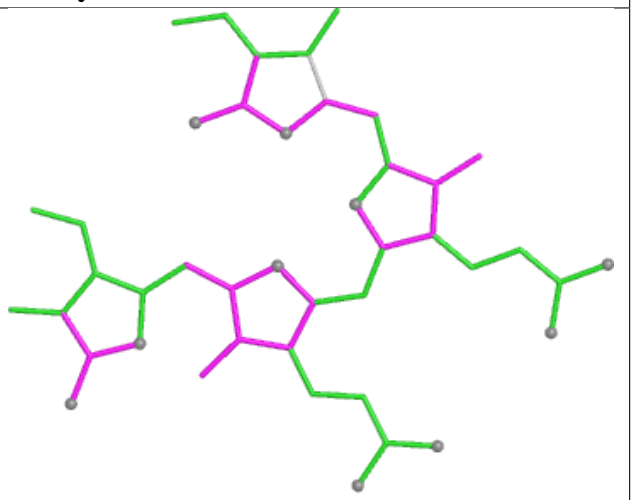
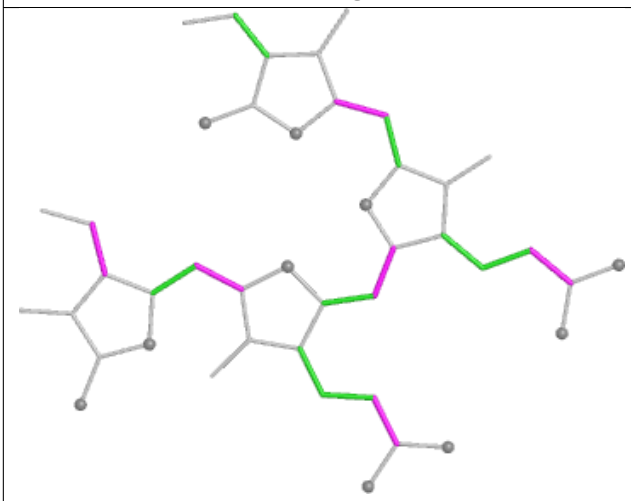


Bond angles



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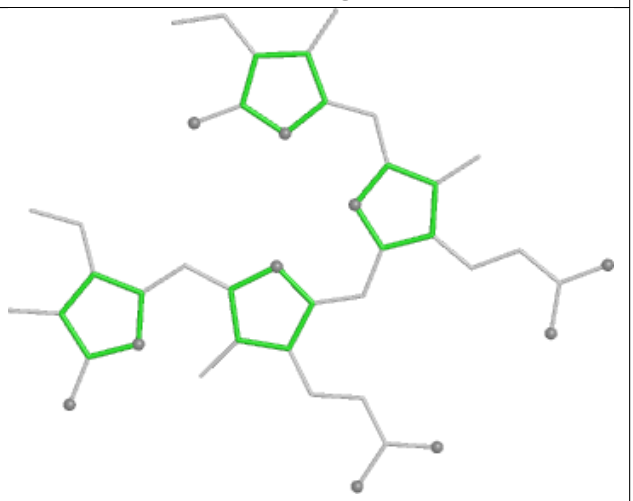
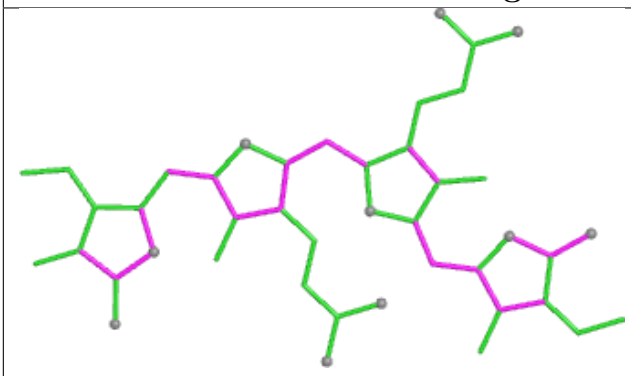


Rings

Ligand CYC R3 1001



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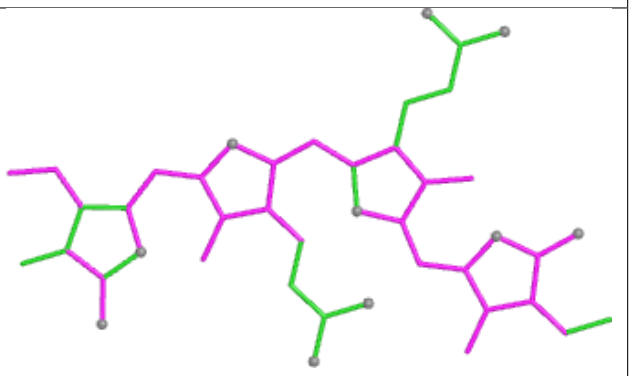

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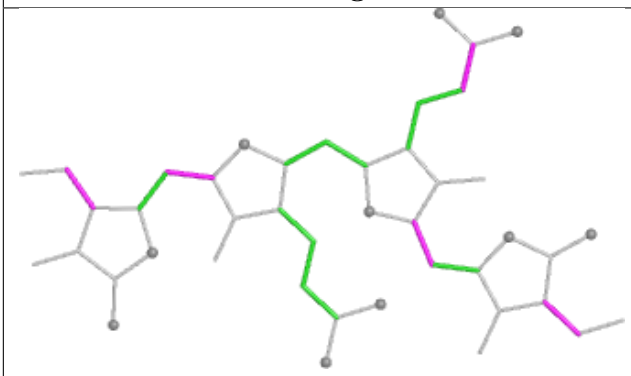

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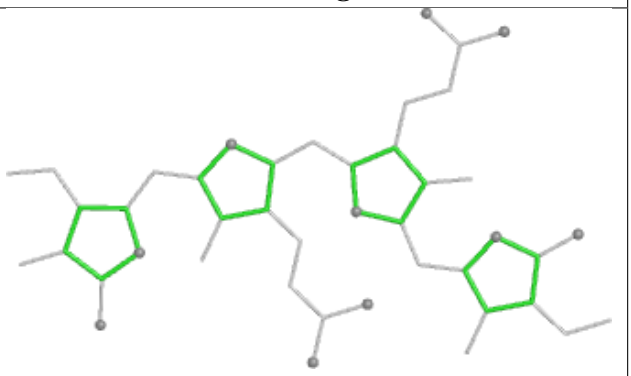
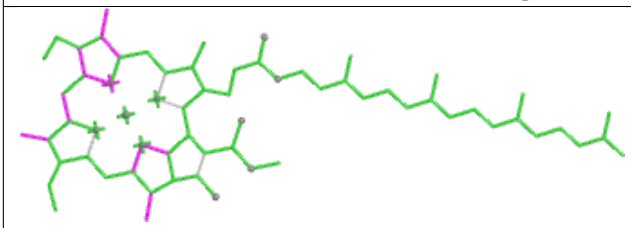


Rings

Ligand CLA bL 615



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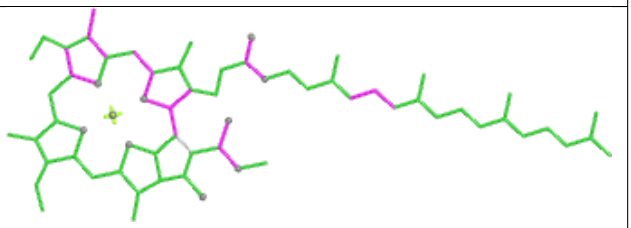

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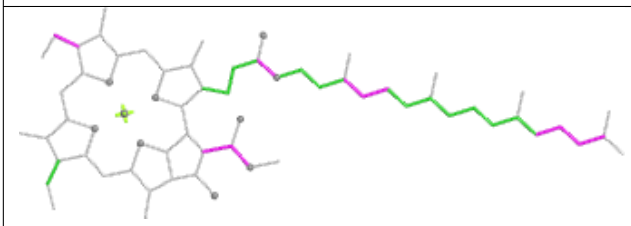

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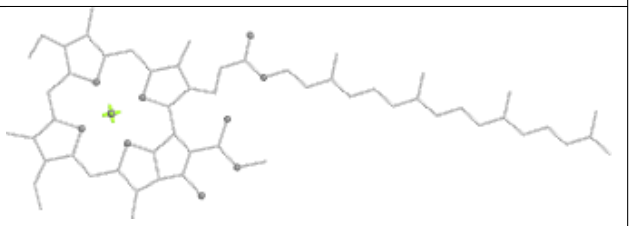
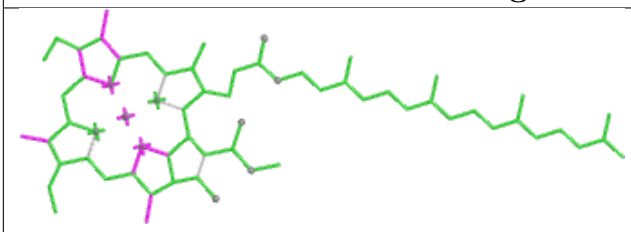


Rings

Ligand CLA AN 851



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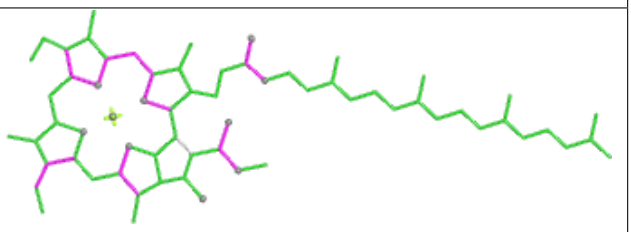

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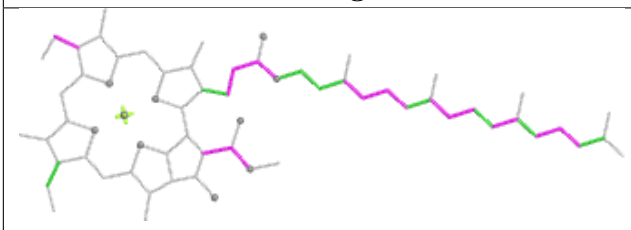

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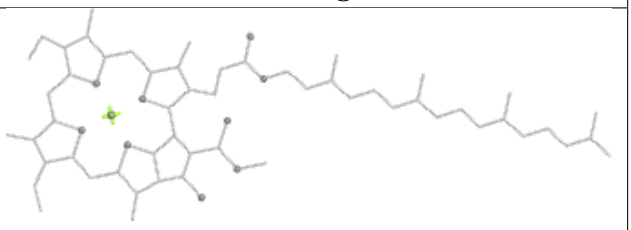
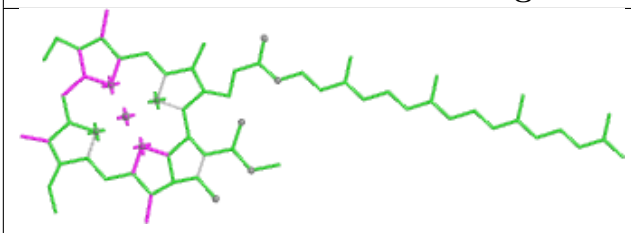


Rings

Ligand CLA A2 831



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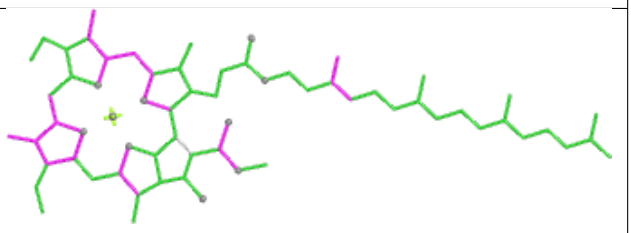

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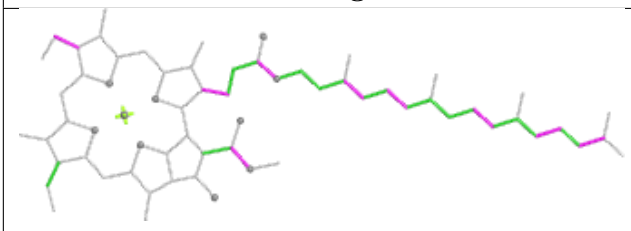

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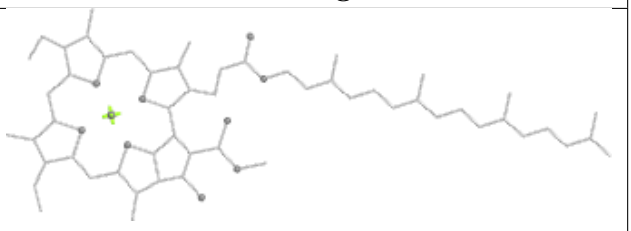
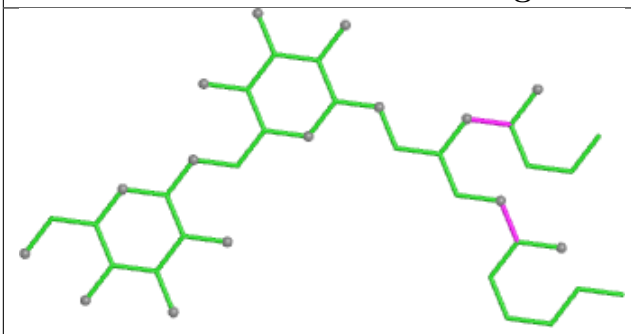


Rings

Ligand DGD b6 621



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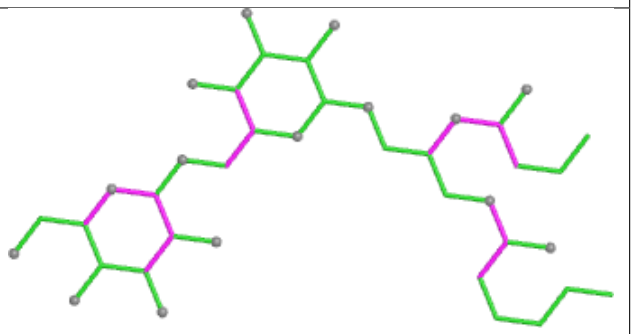

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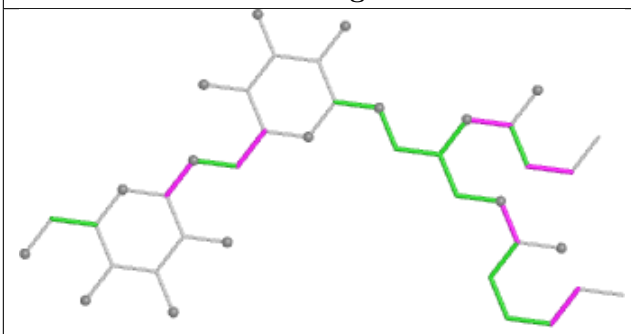

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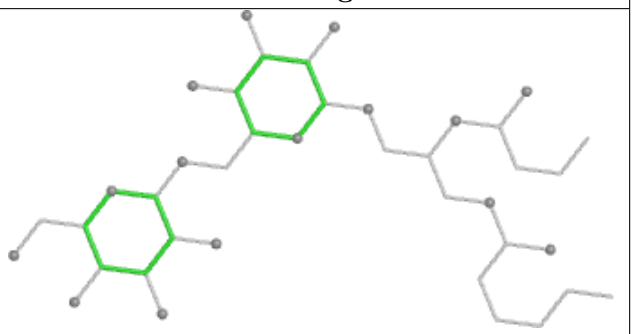
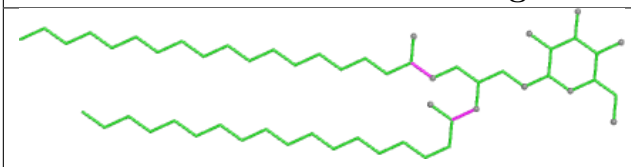


Rings

Ligand LMG CL 519



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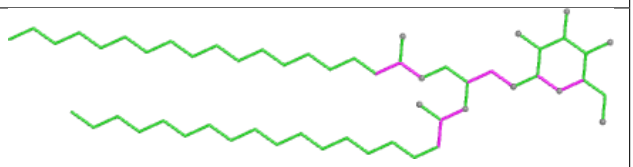
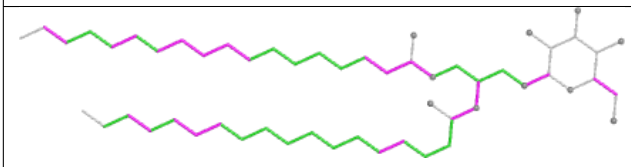


Bond angles



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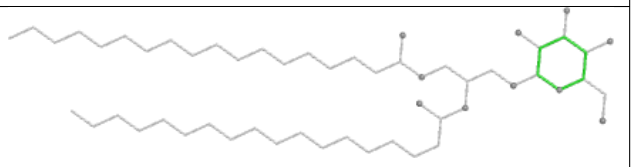
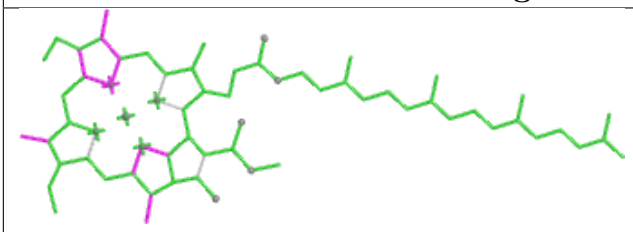


Rings

Ligand CLA CL 508



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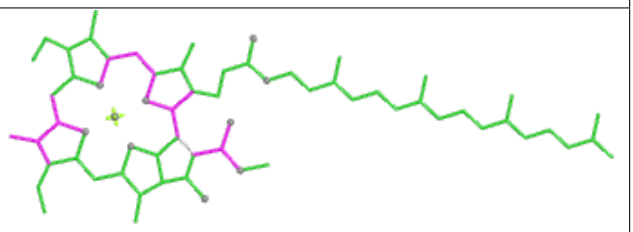
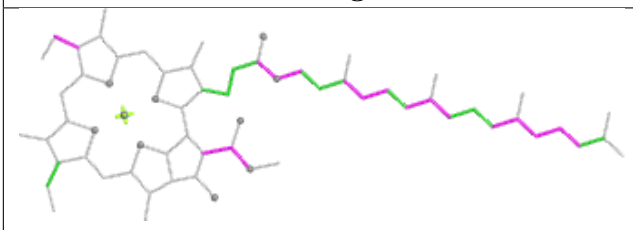


Bond angles



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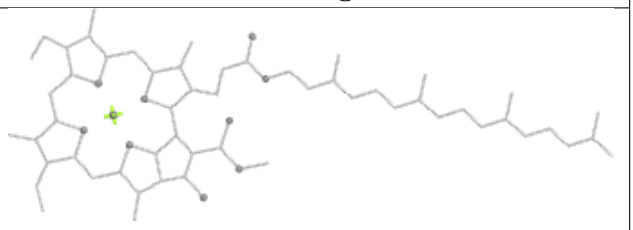
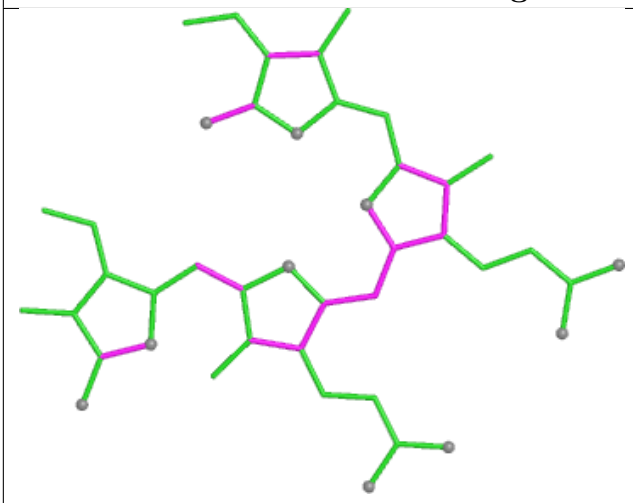


Rings

Ligand PEB VD 202



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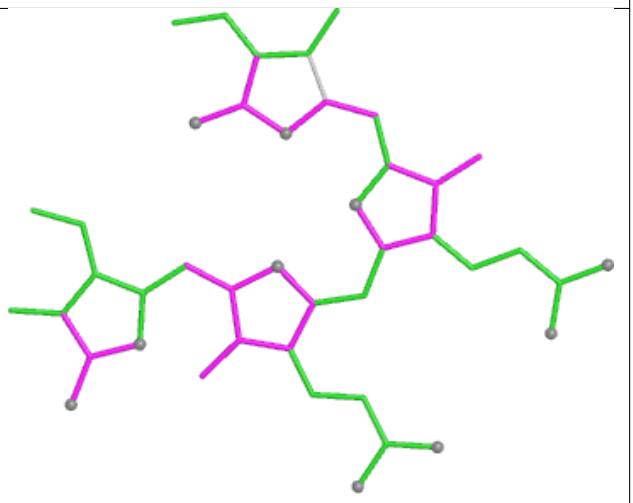
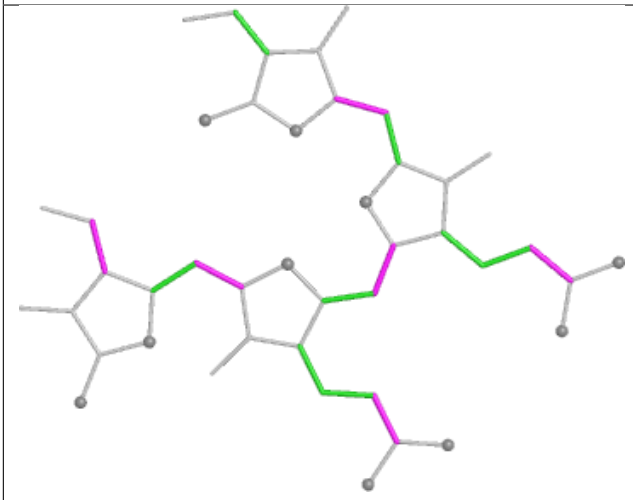


Bond angles



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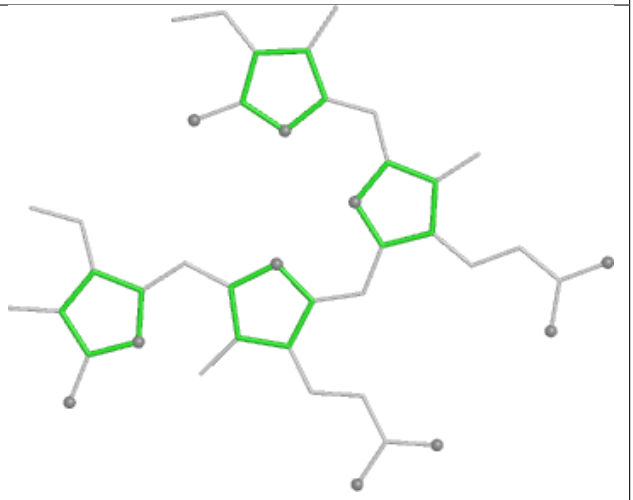
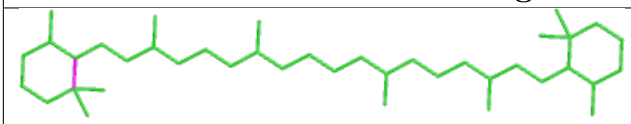
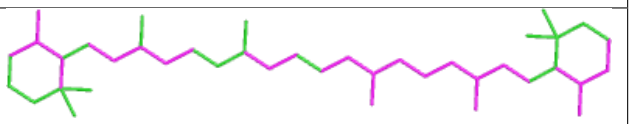


Rings

Ligand BCR F6 101	
	
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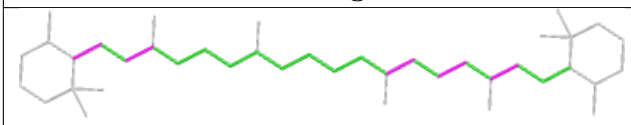	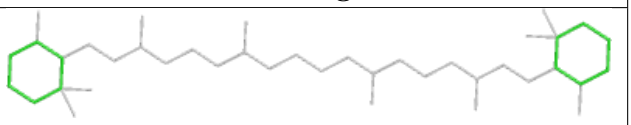
Torsions	Rings

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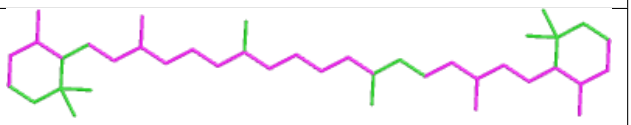
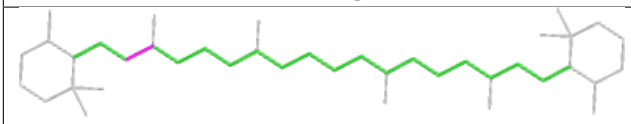
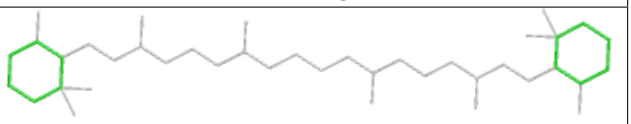
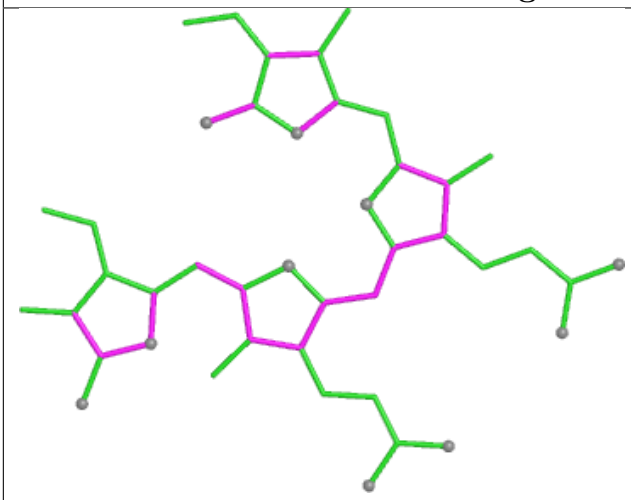
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEB u8 201



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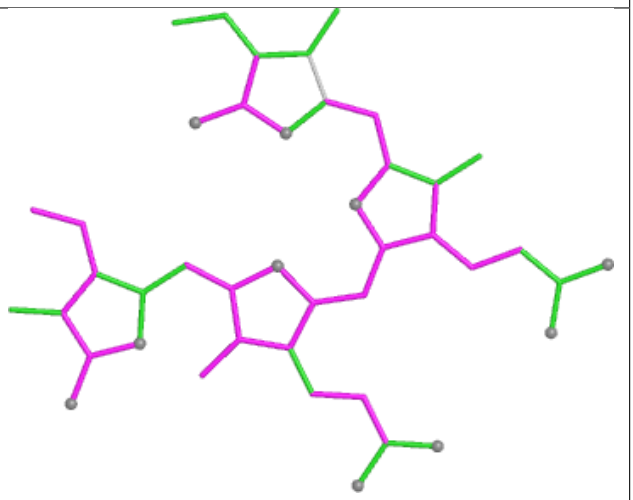

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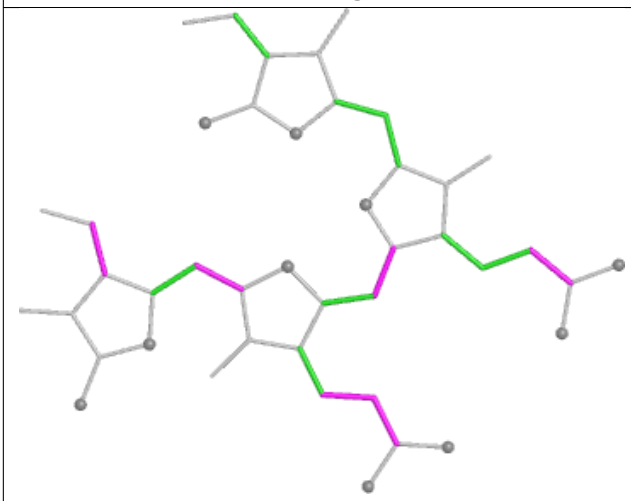

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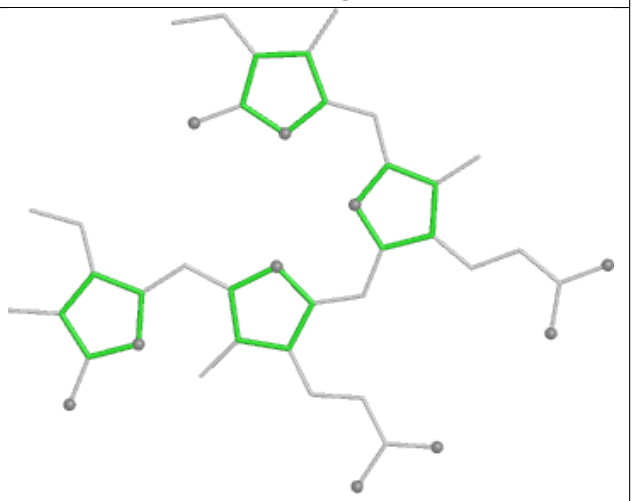
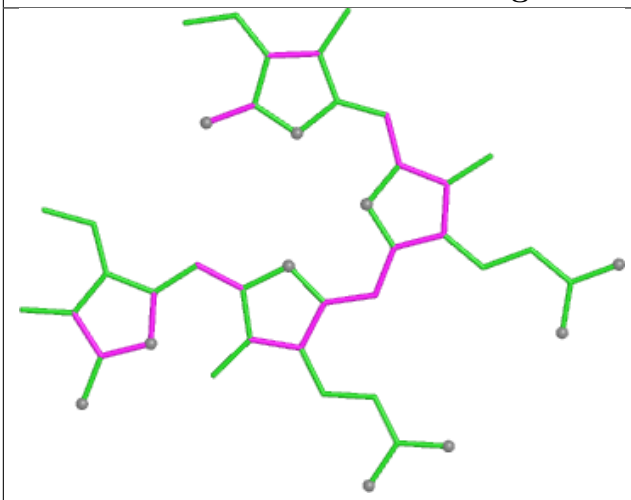


Rings

Ligand PEB XQ 202



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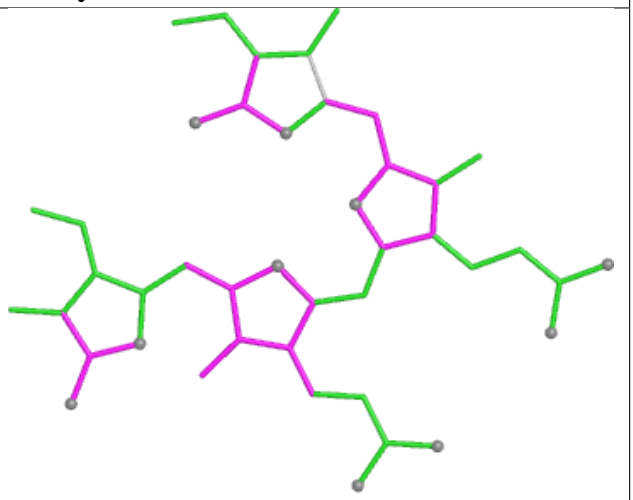

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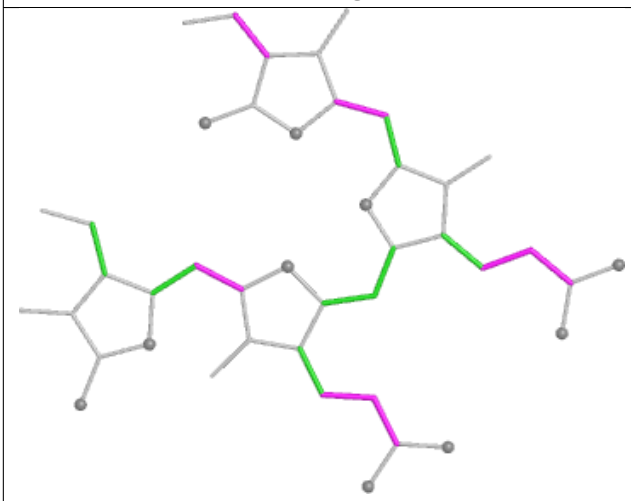

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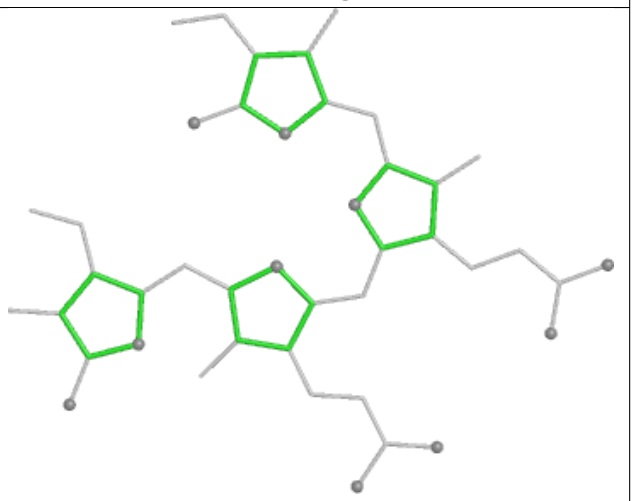
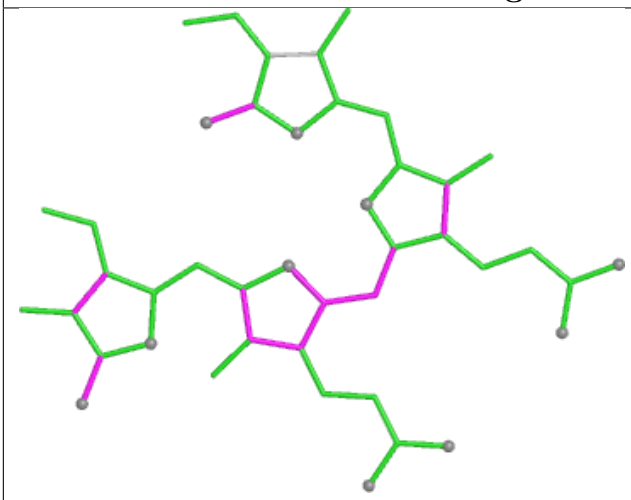


Rings

Ligand PUB QM 201



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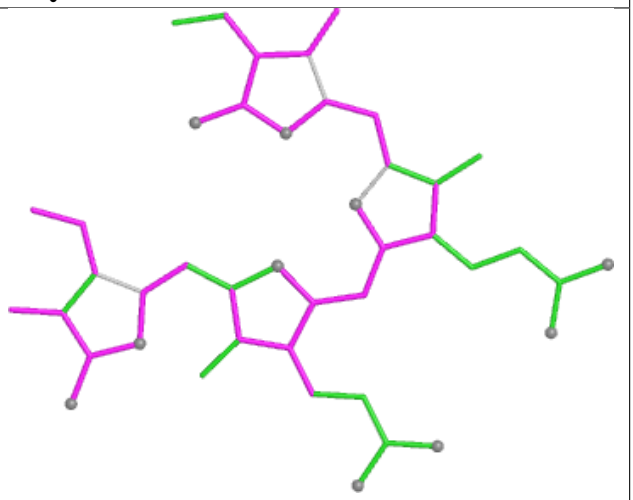

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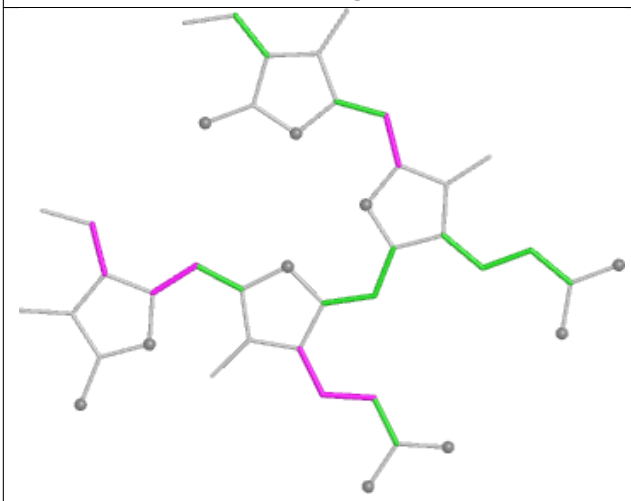

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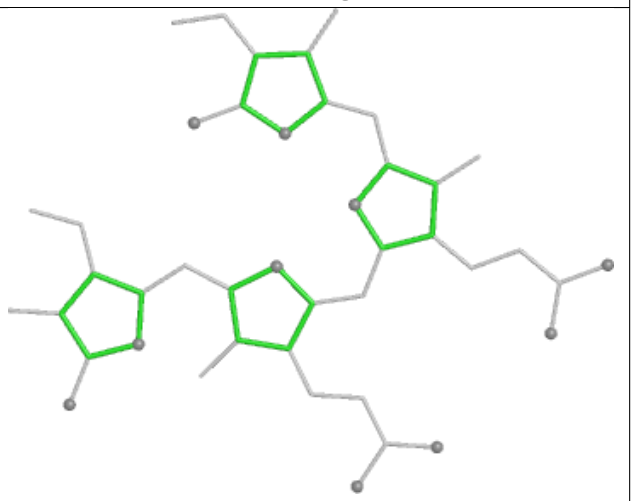
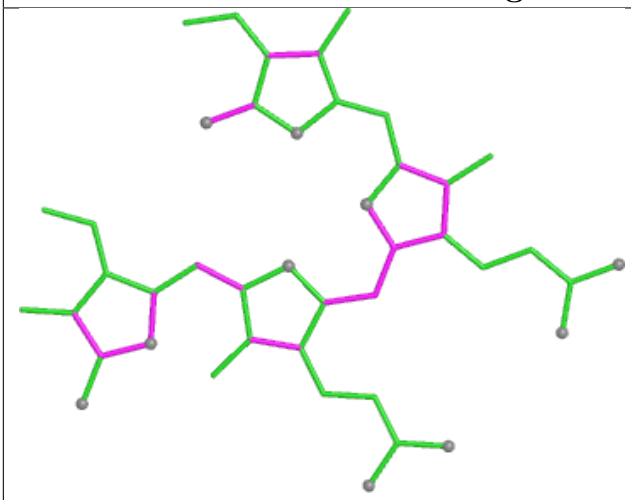


Rings

Ligand PEB N4 1002



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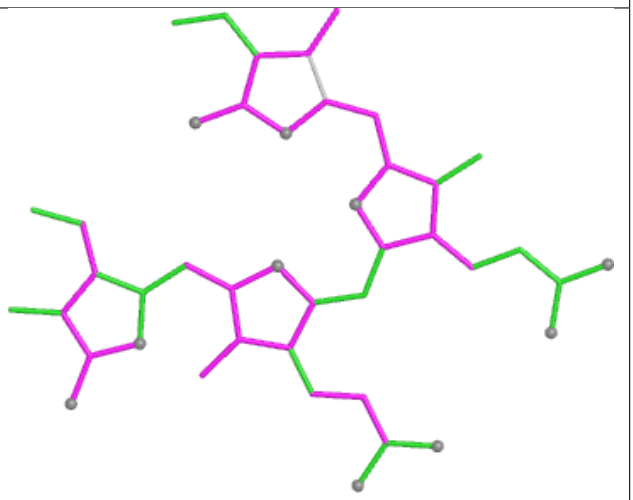

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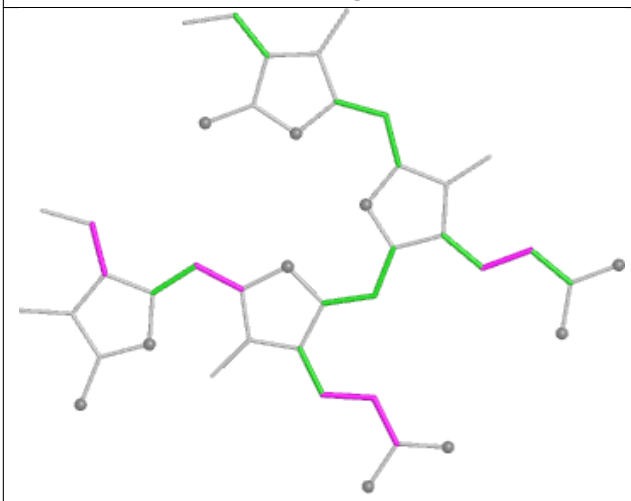

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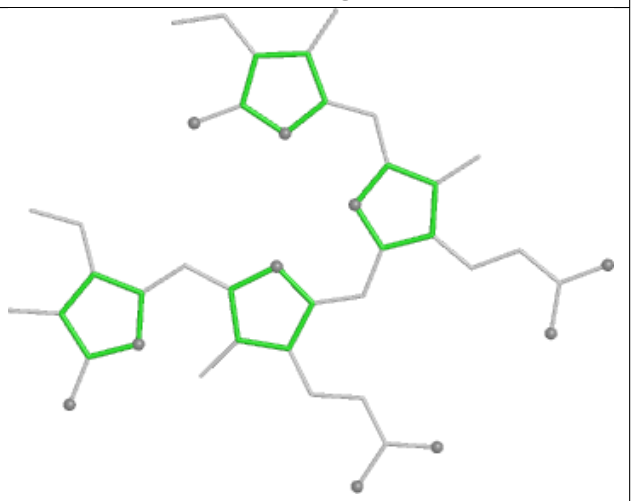

Rings

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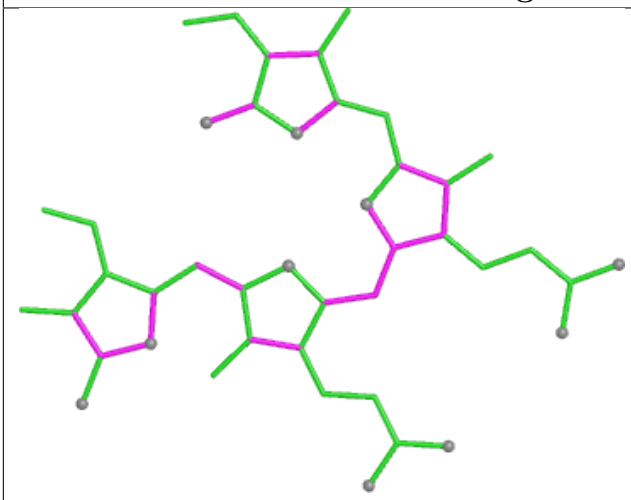

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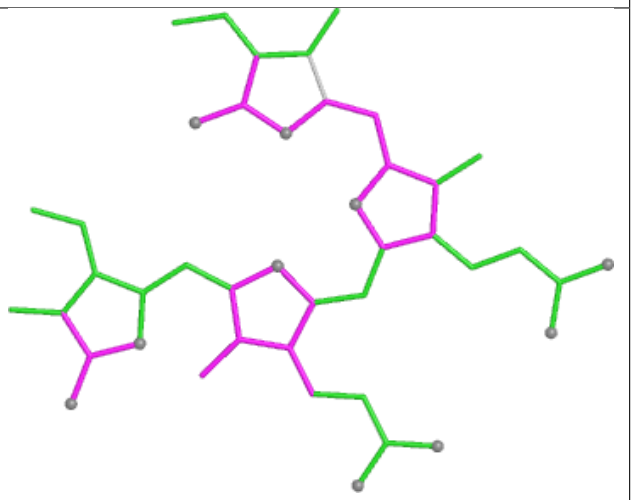

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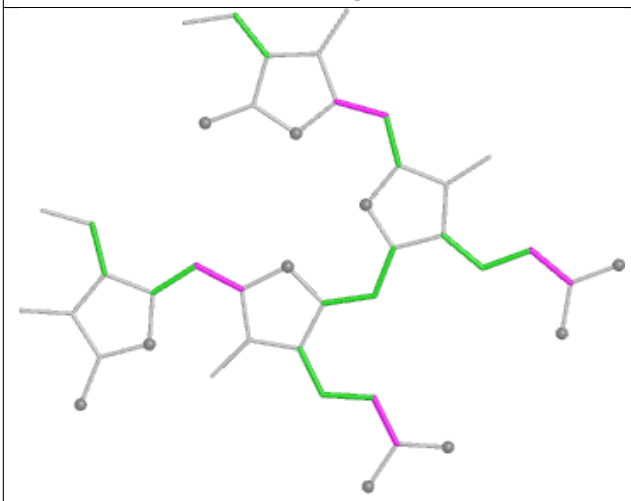

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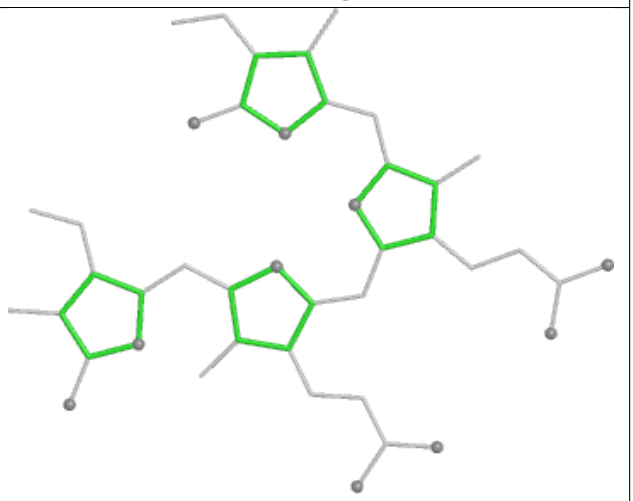

Rings

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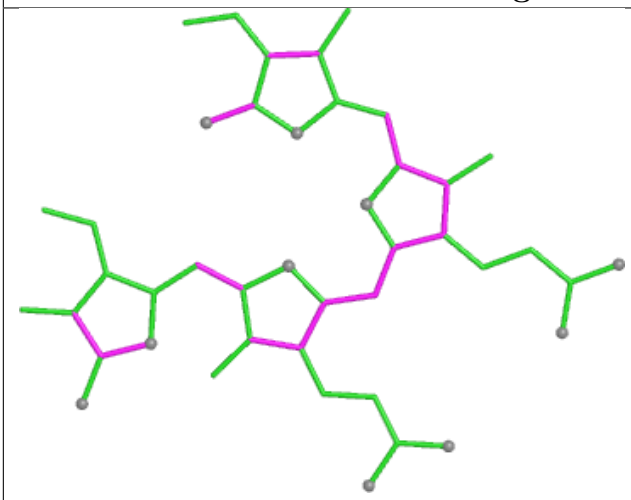

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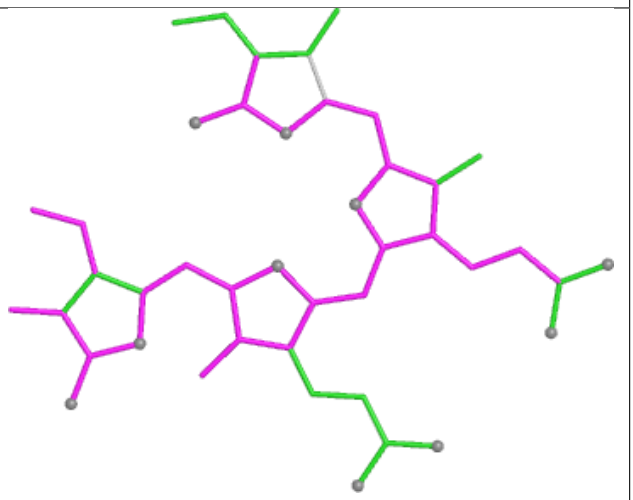

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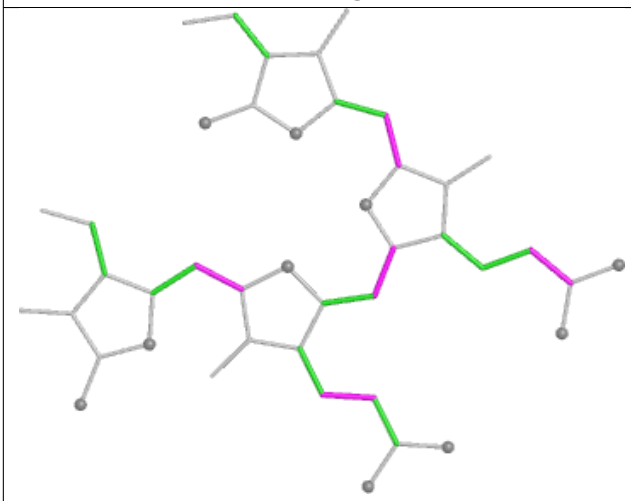

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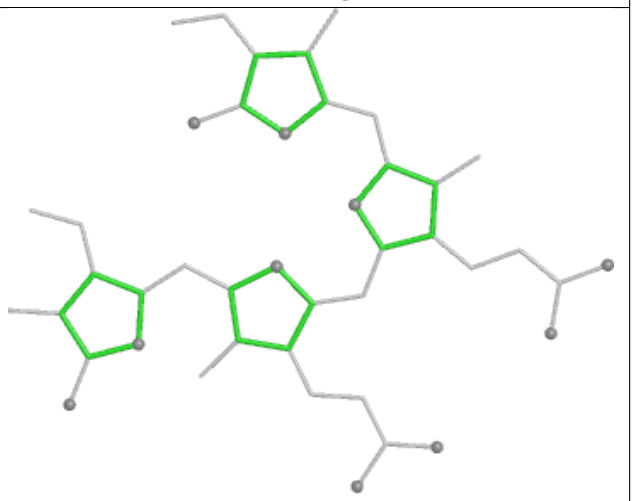
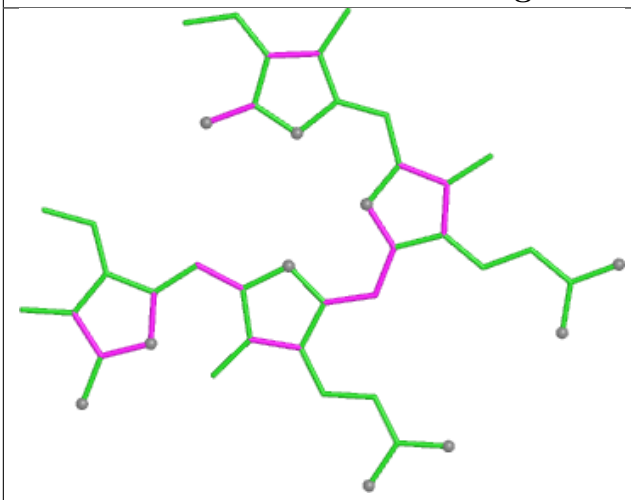


Rings

Ligand PEB LB 201



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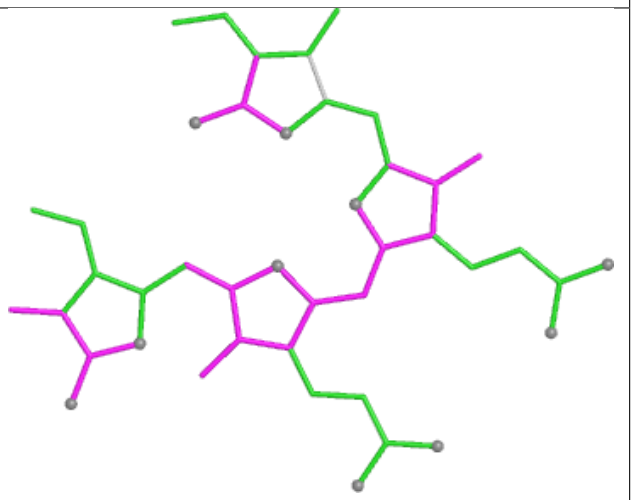

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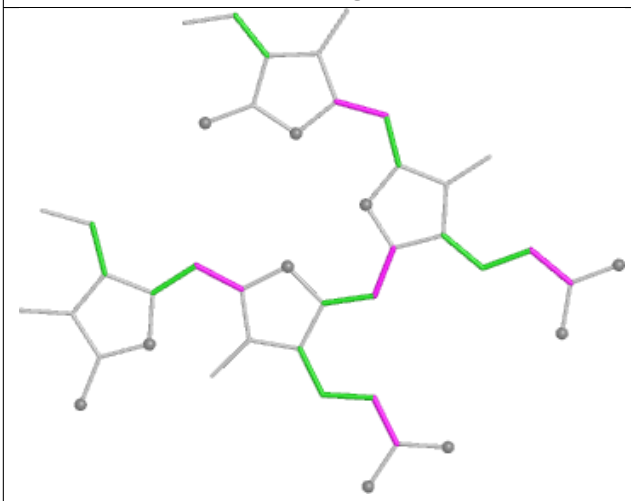

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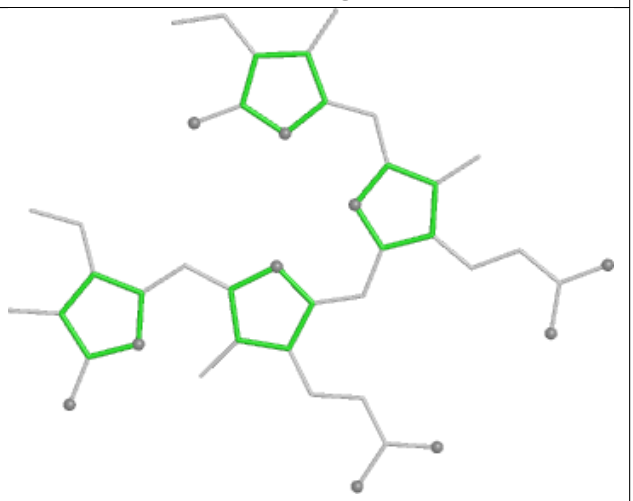
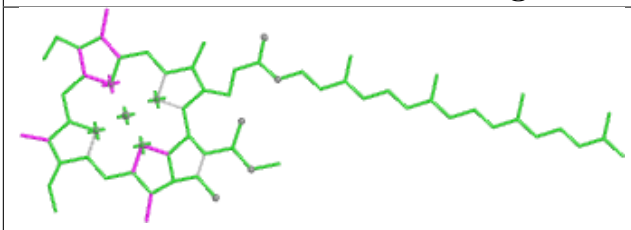


Rings

Ligand CLA AN 813



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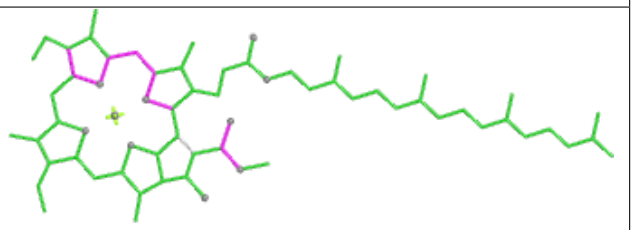

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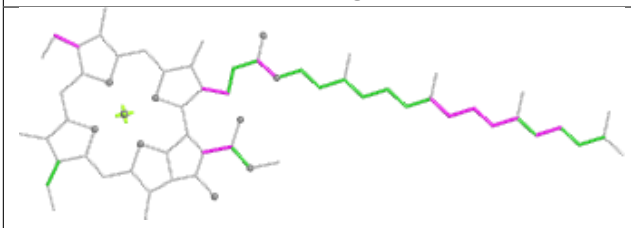

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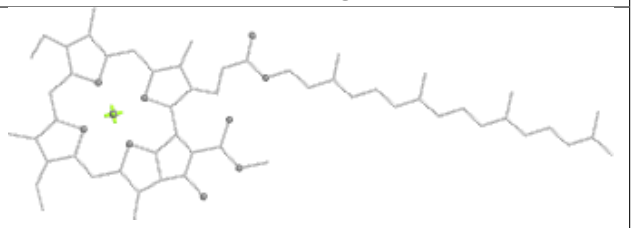
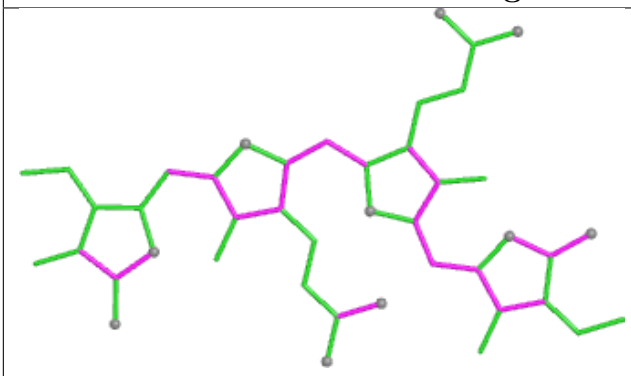


Rings

Ligand CYC Q3 1001



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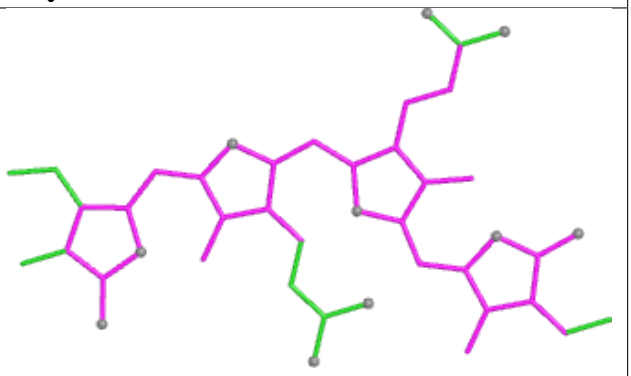

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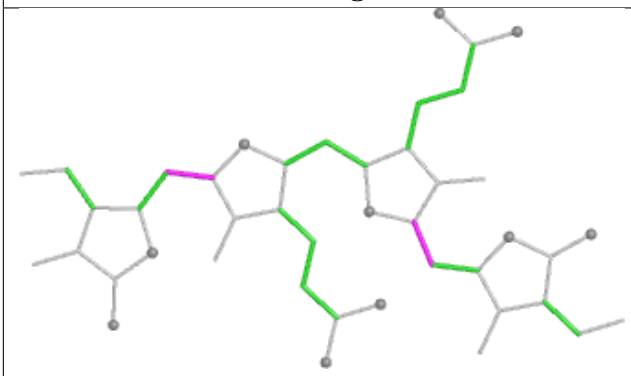

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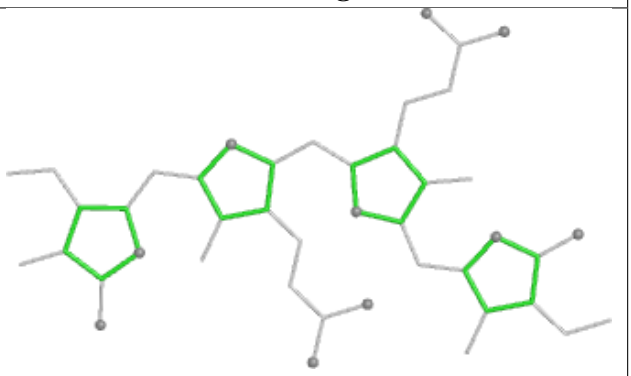
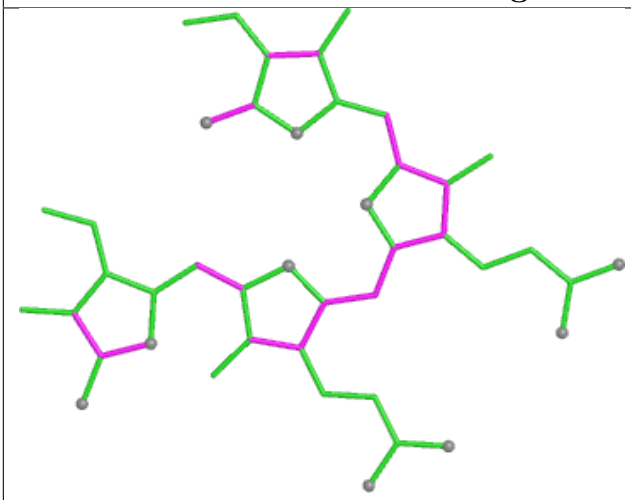


Rings

Ligand PEB RH 202



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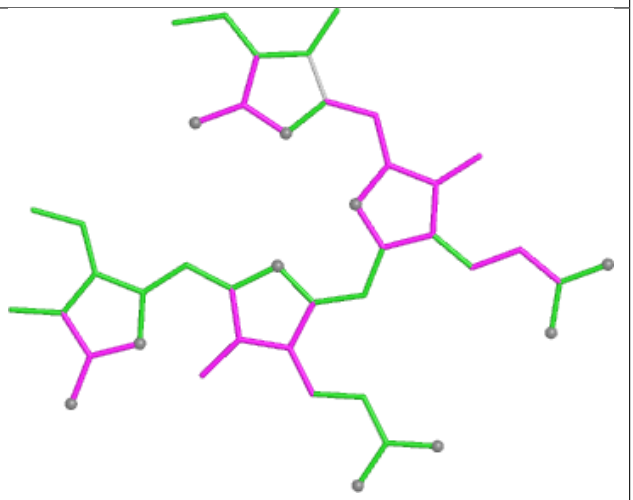

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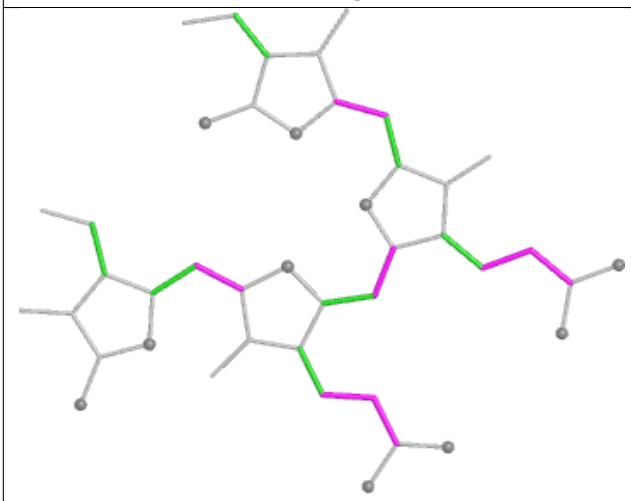

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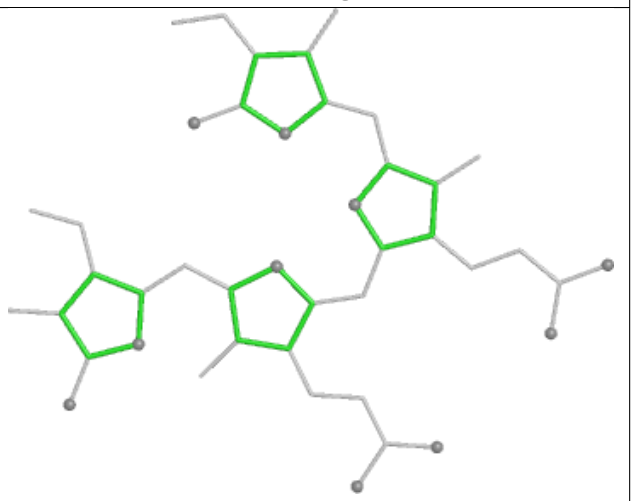
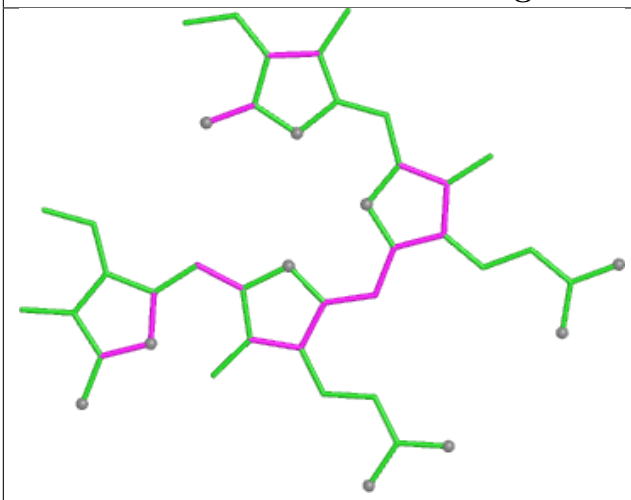


Rings

Ligand PEB xK 303



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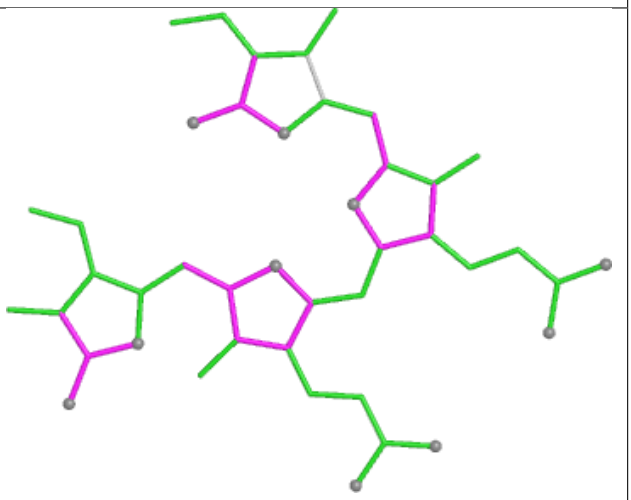
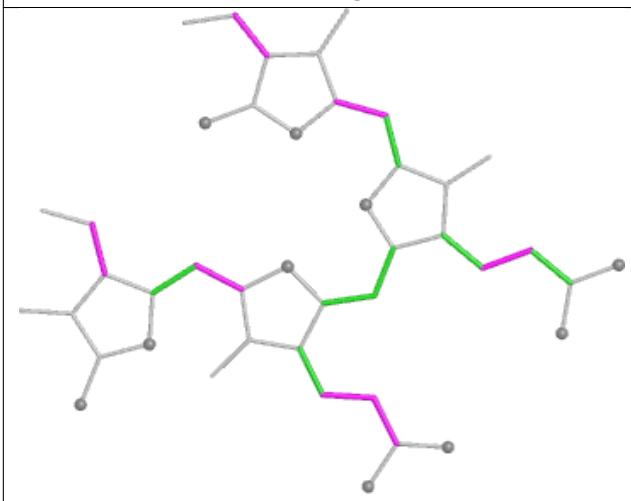


Bond angles



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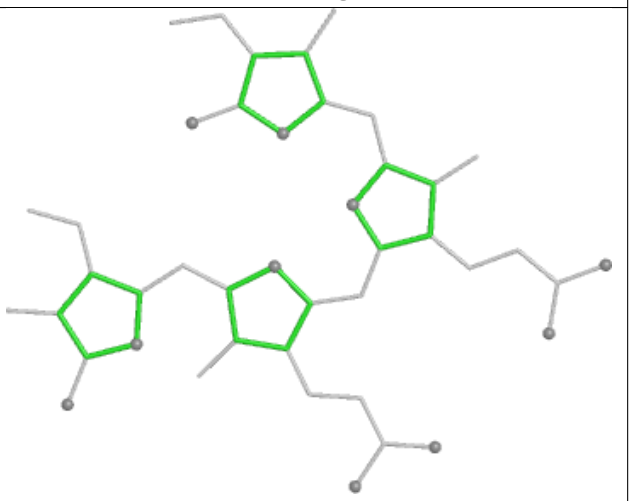
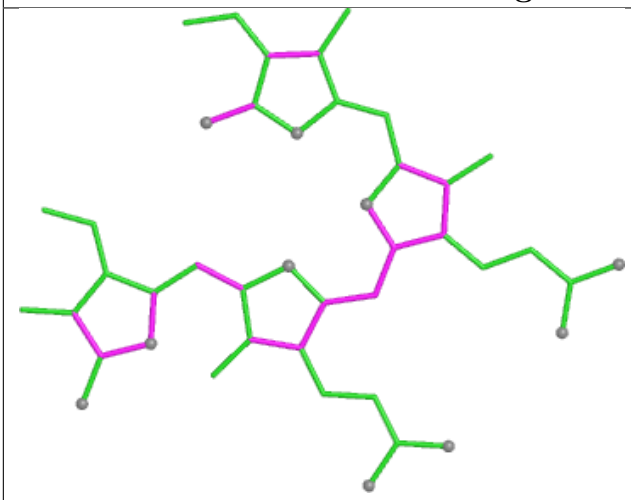


Rings

Ligand PEB FF 202



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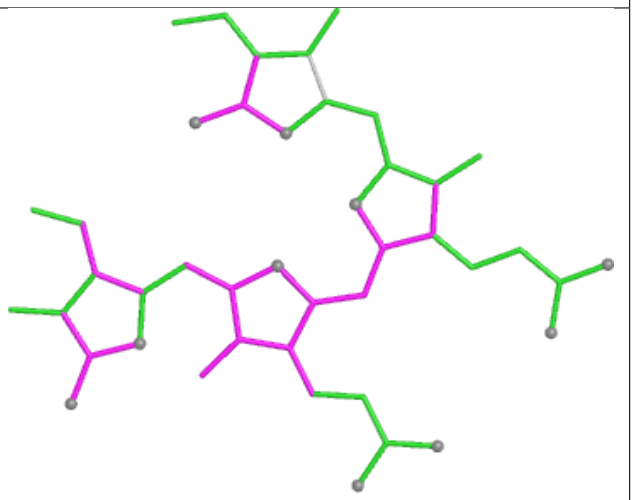
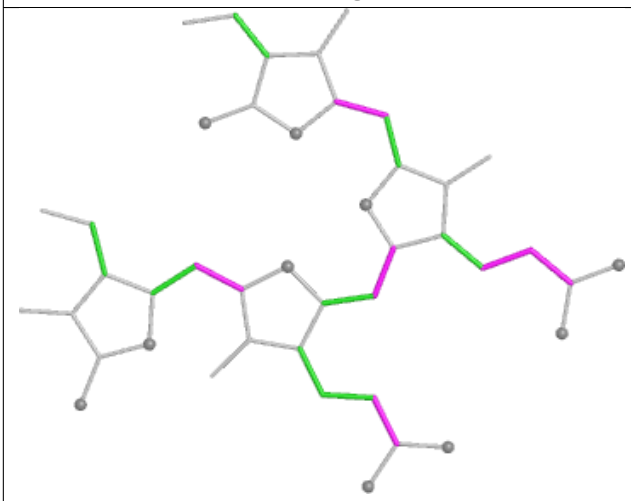


Bond angles



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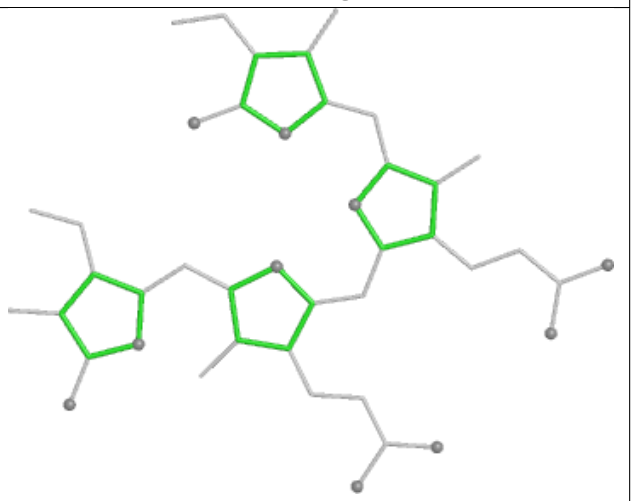
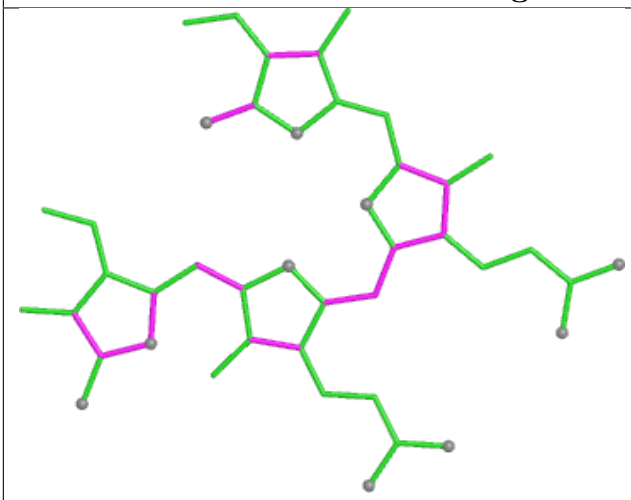


Rings

Ligand PEB NB 202



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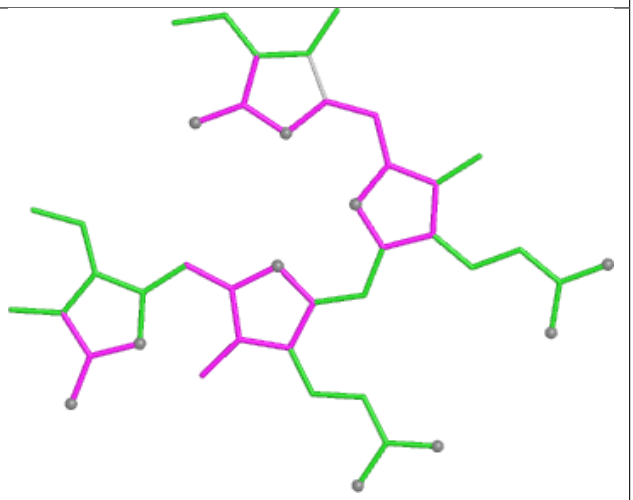
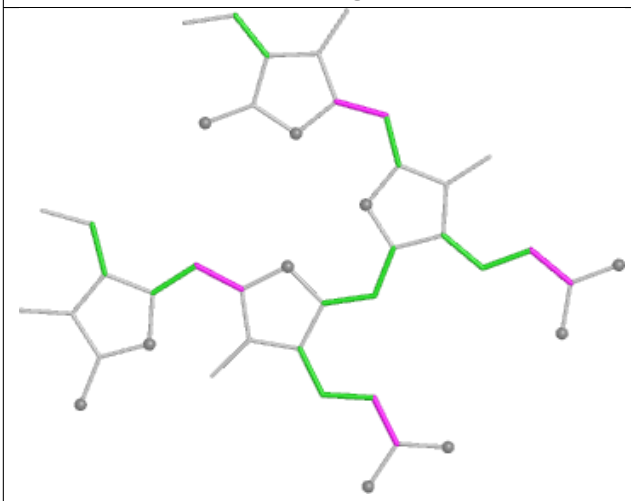


Bond angles



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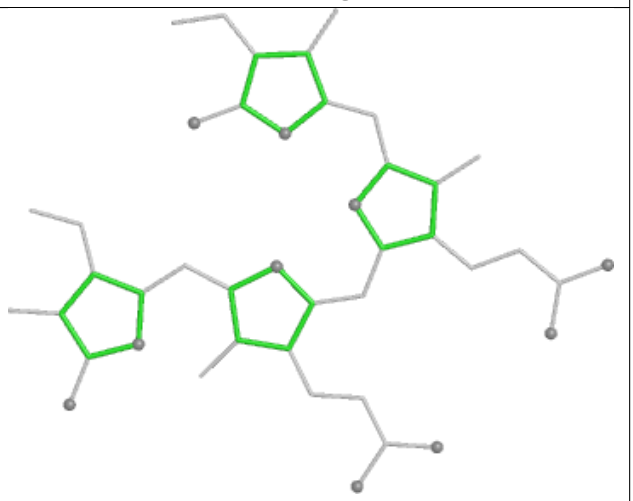
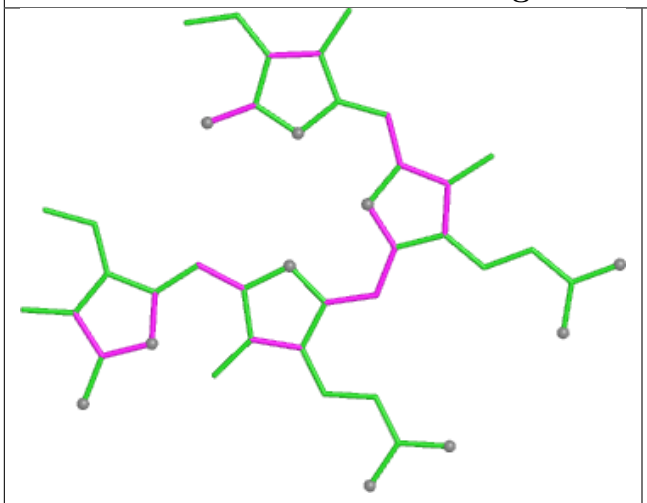


Rings

Ligand PEB JM 201



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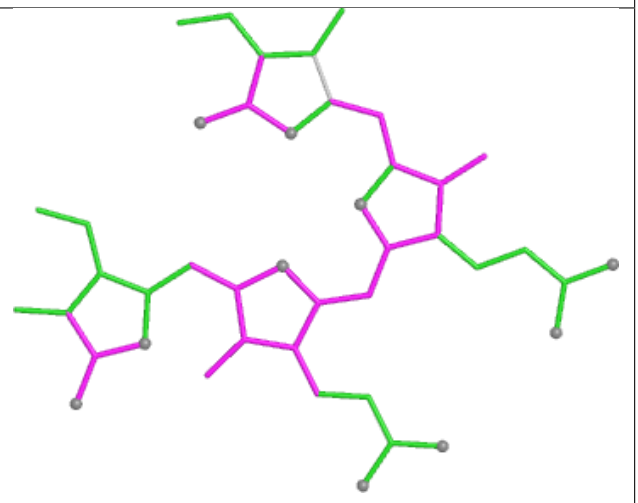

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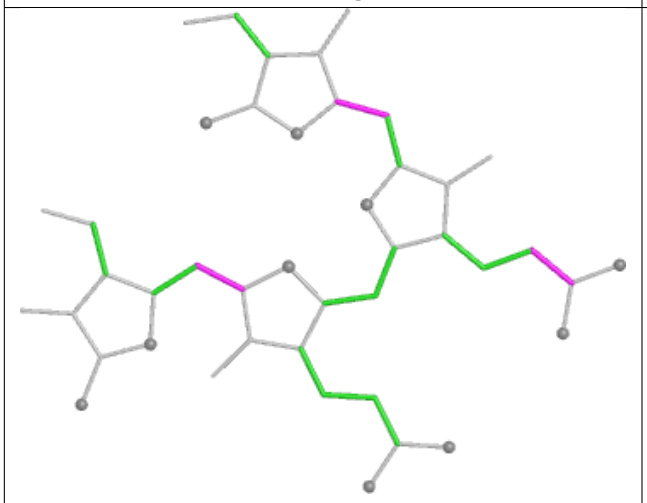
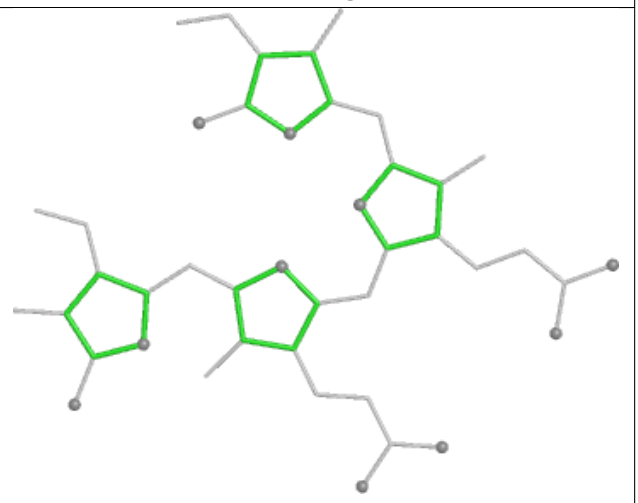
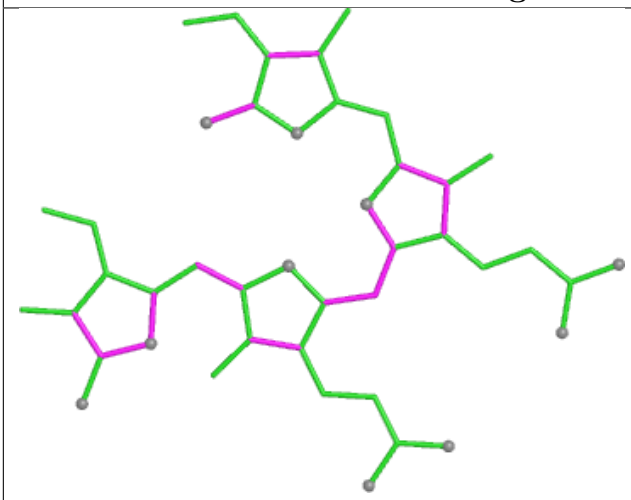


Torsions



Rings

Ligand PEB L1 1002



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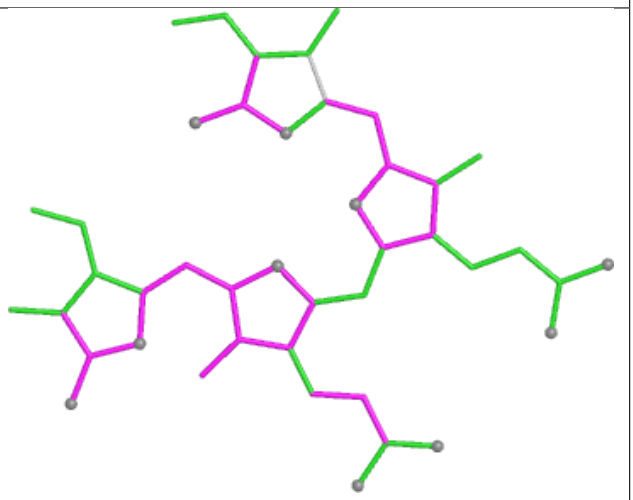

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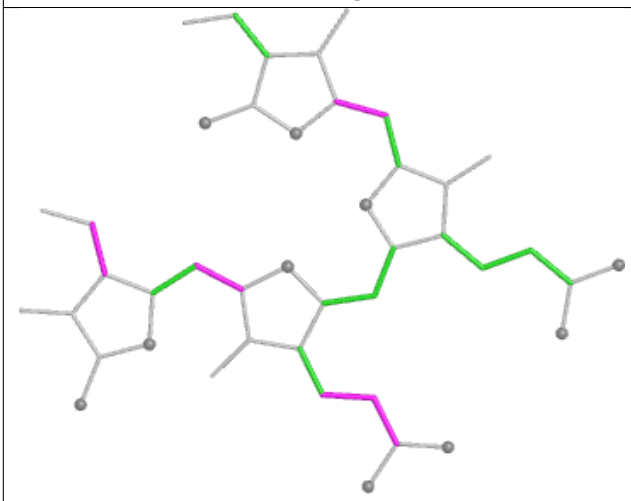

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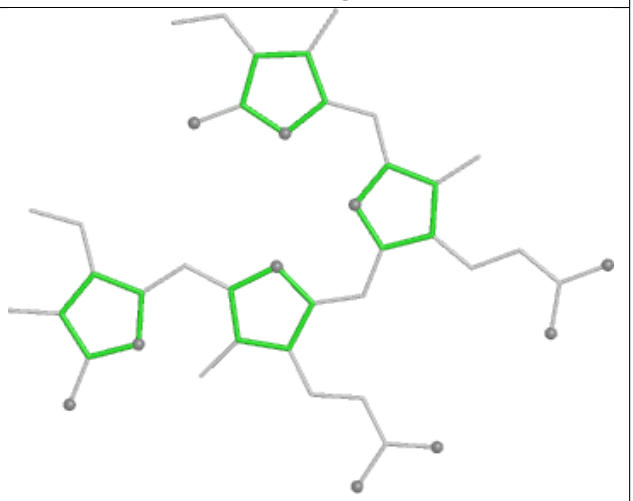
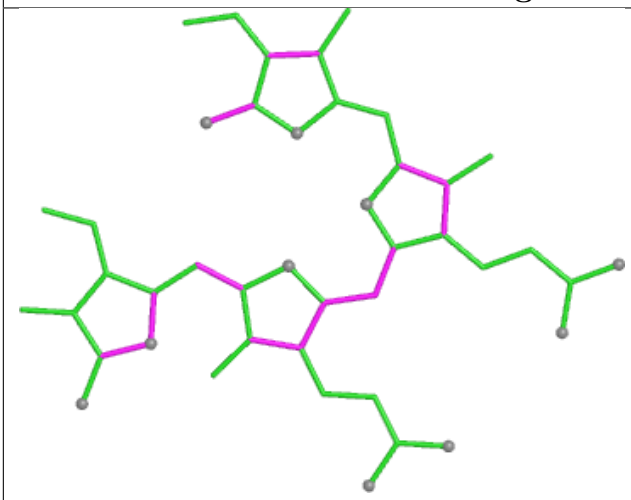


Rings

Ligand PEB U5 202



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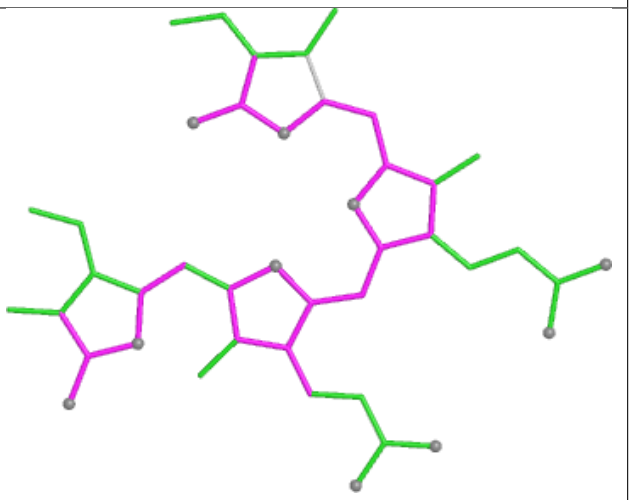

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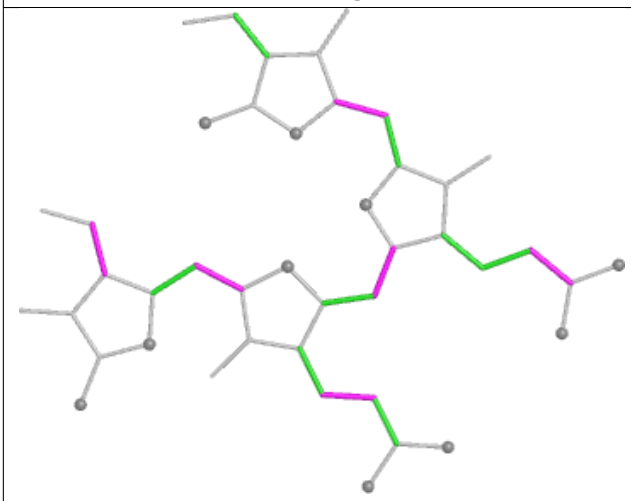

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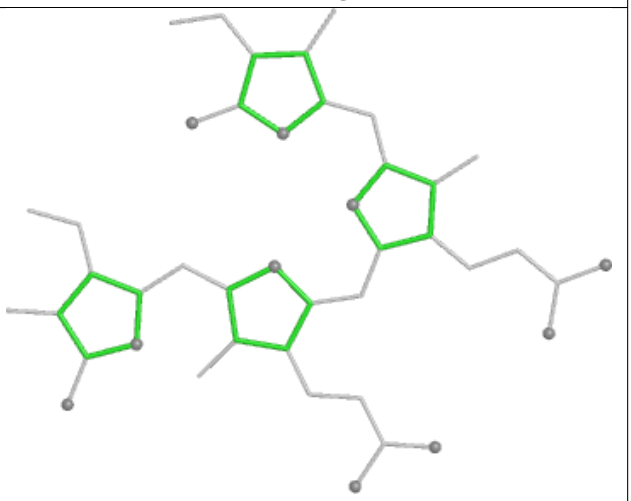
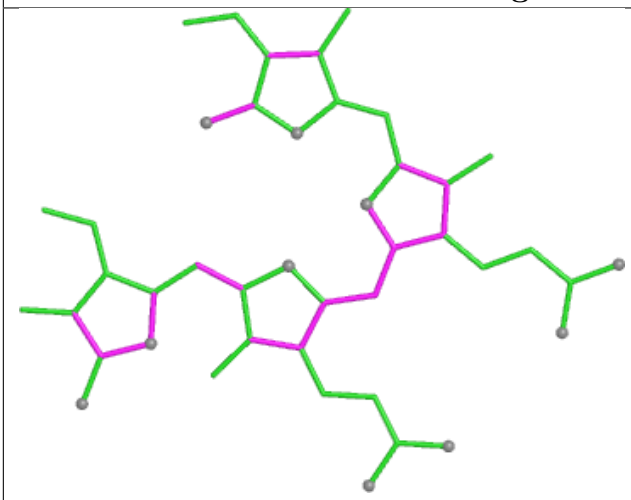


Rings

Ligand PEB GP 203



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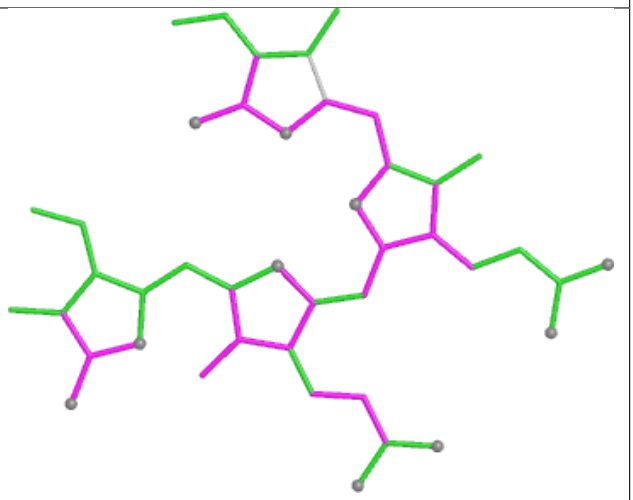

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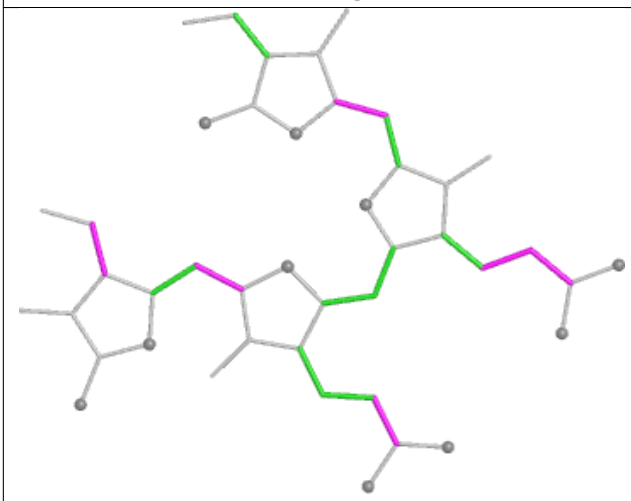

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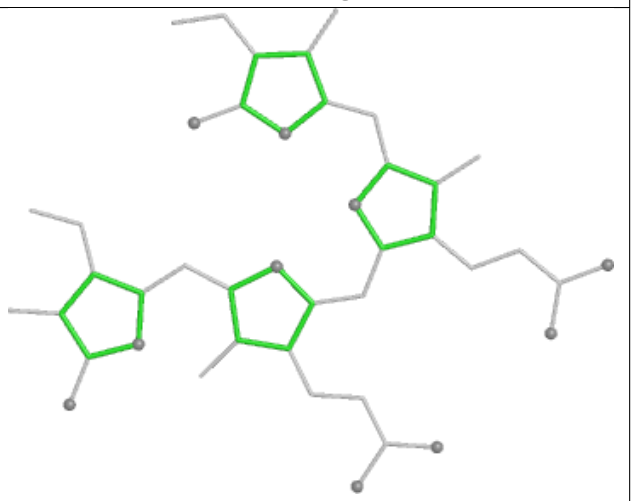

Rings

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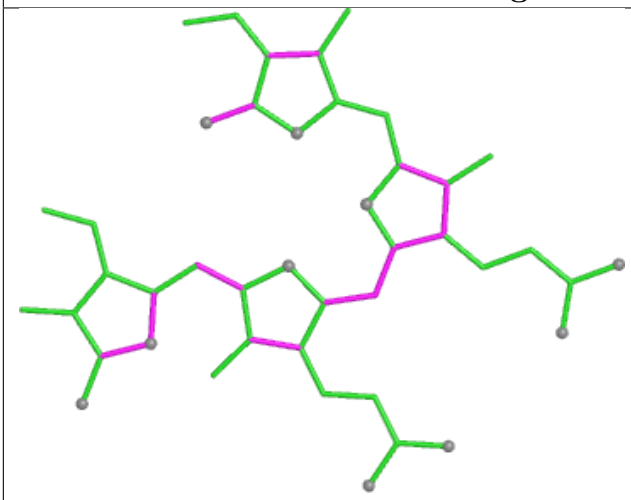

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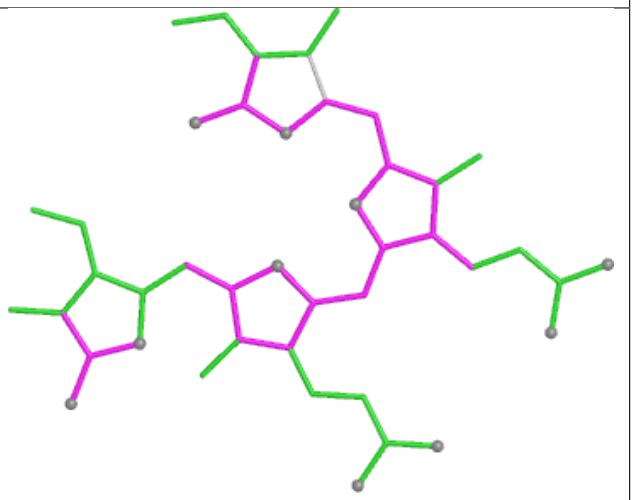

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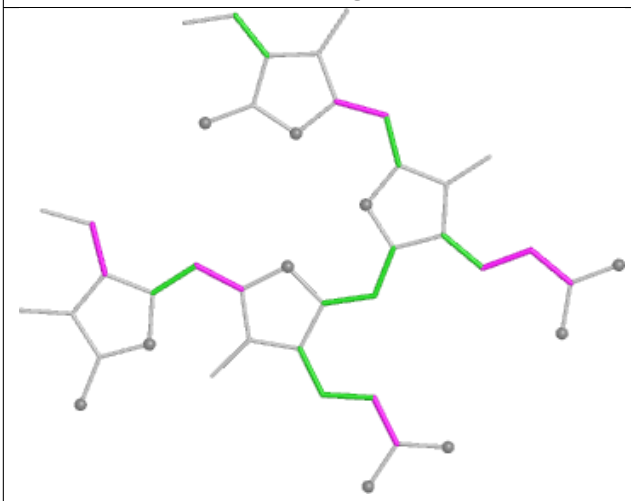

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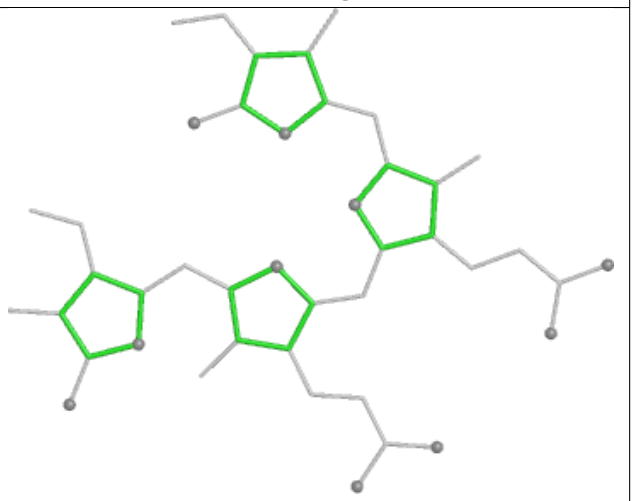

Rings

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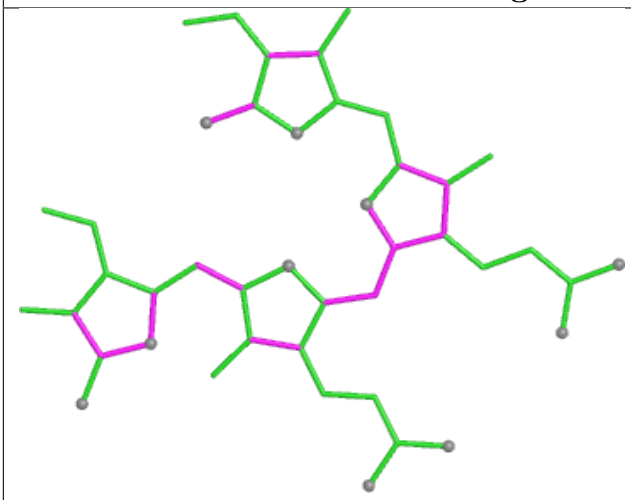

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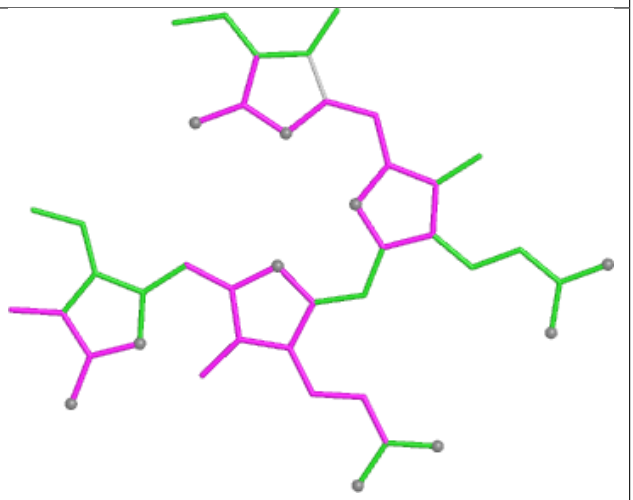

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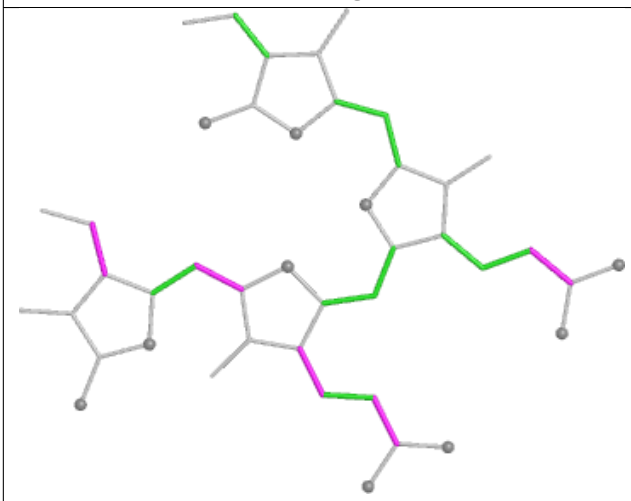

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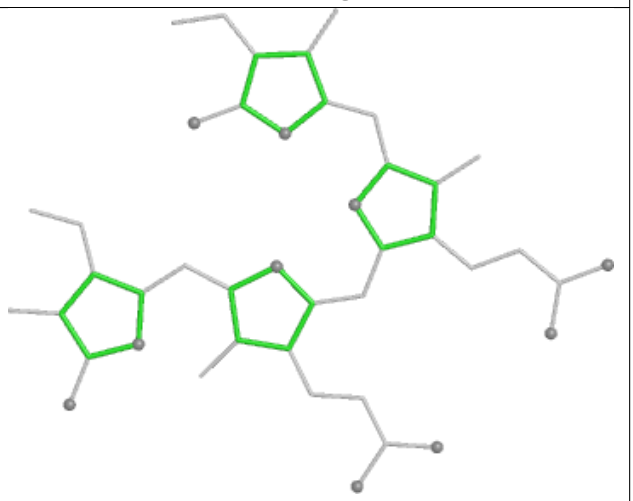

Rings

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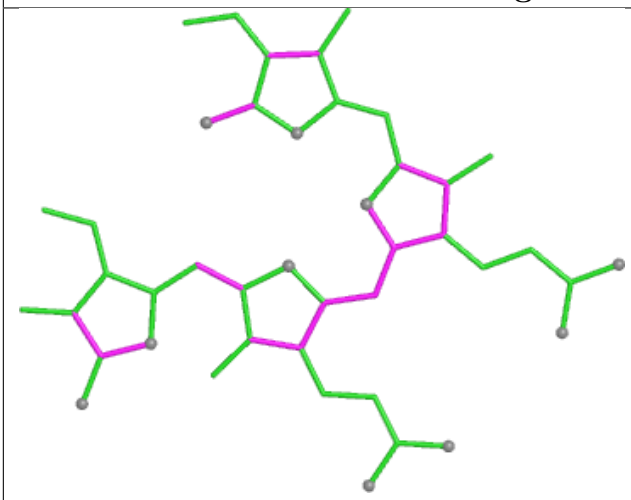

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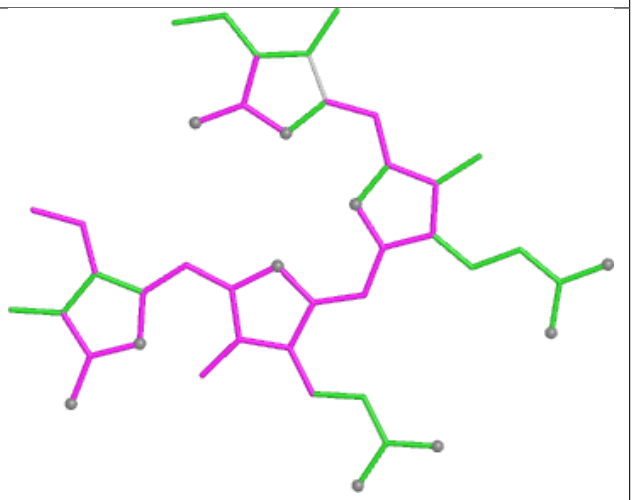

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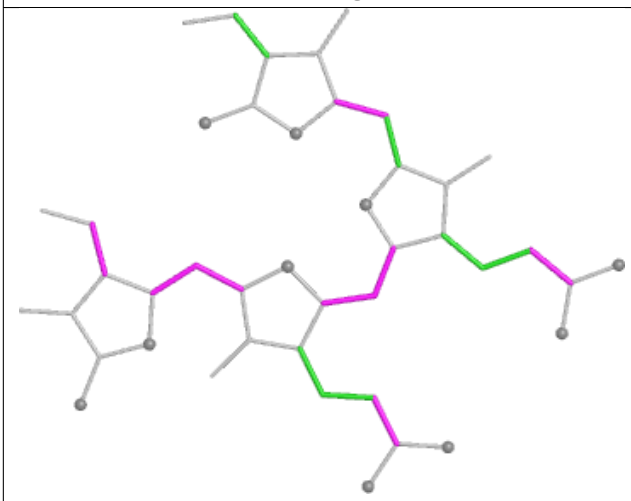

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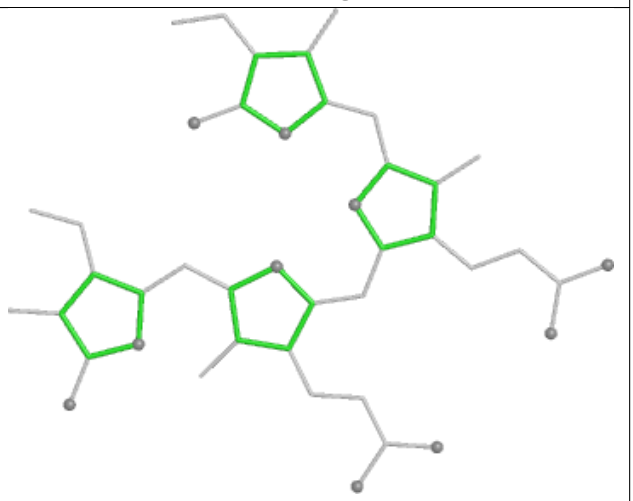

Rings

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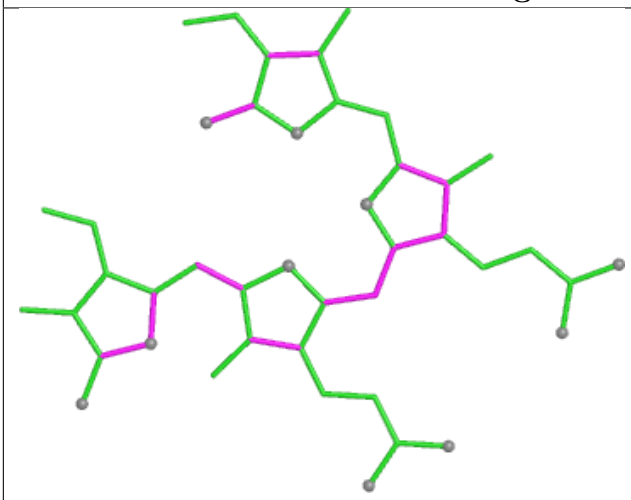

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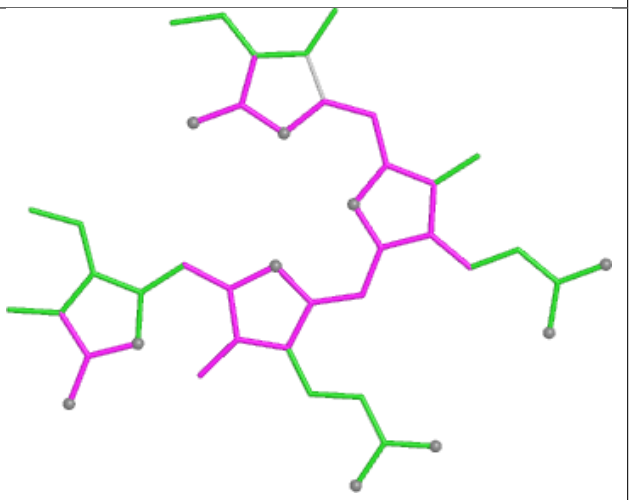

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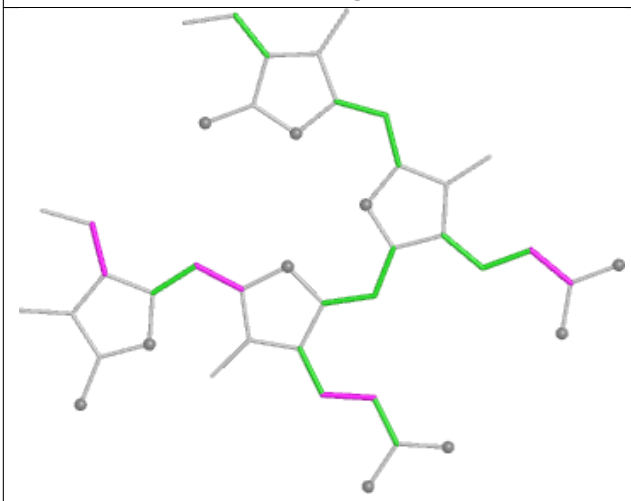

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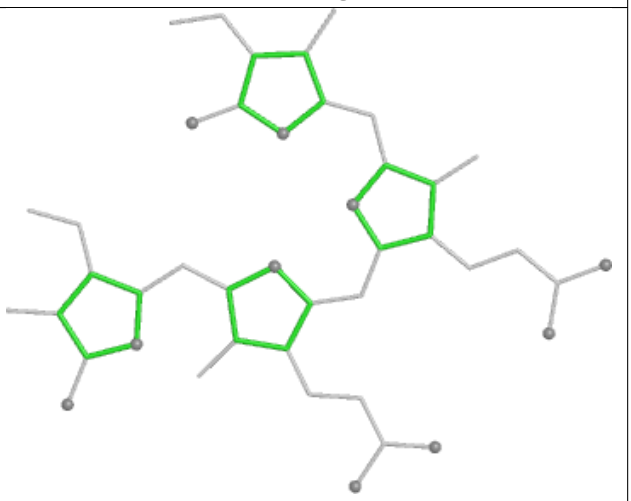
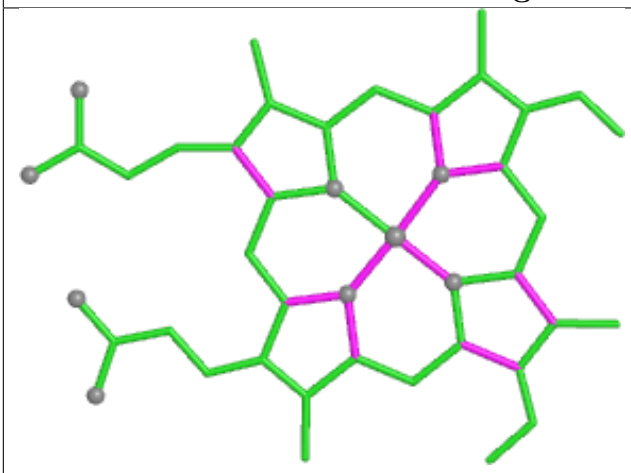


Rings

Ligand HEM v6 201



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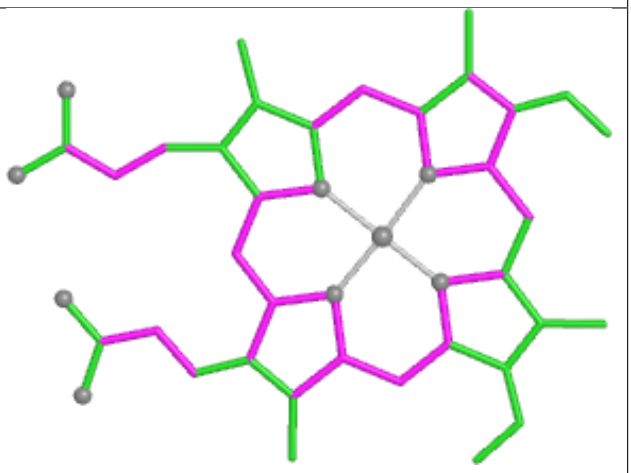

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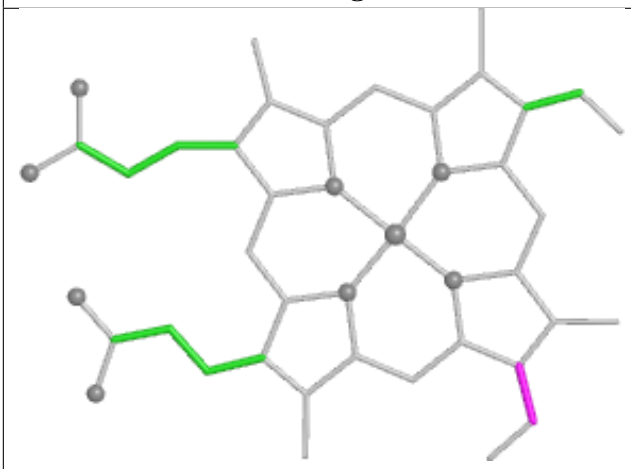

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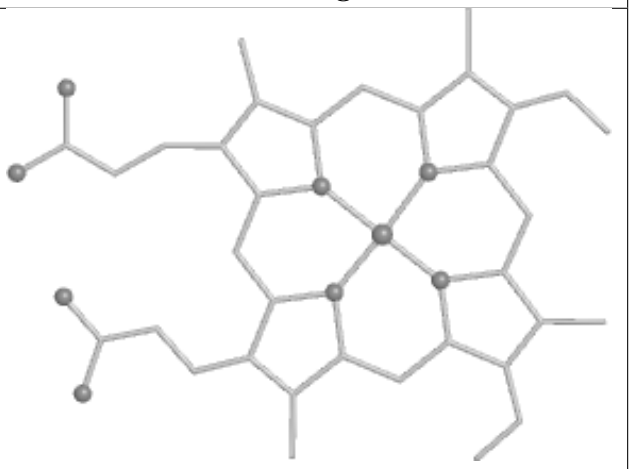
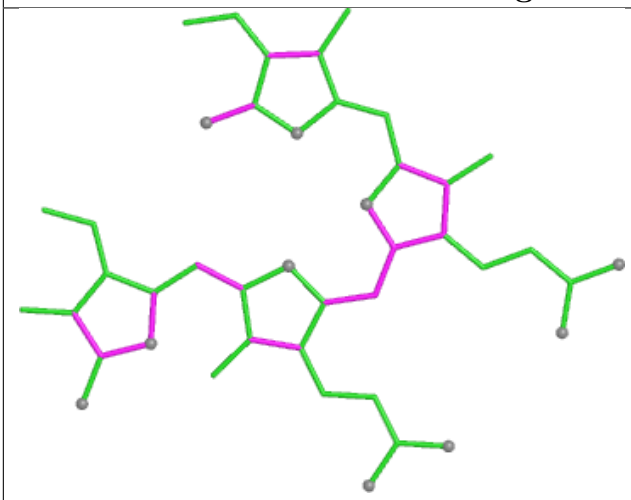


Rings

Ligand PEB V5 202



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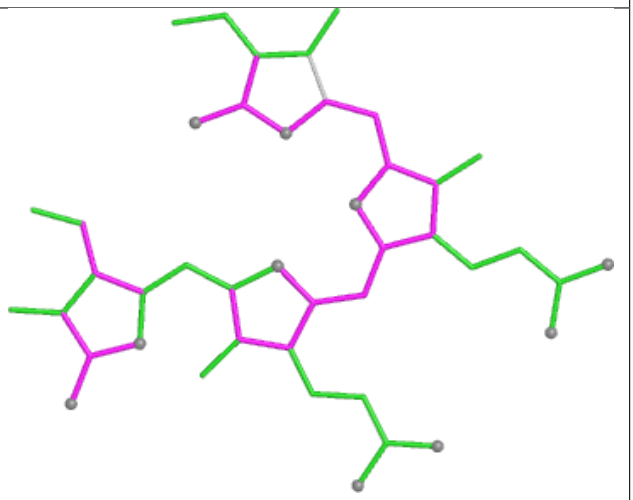

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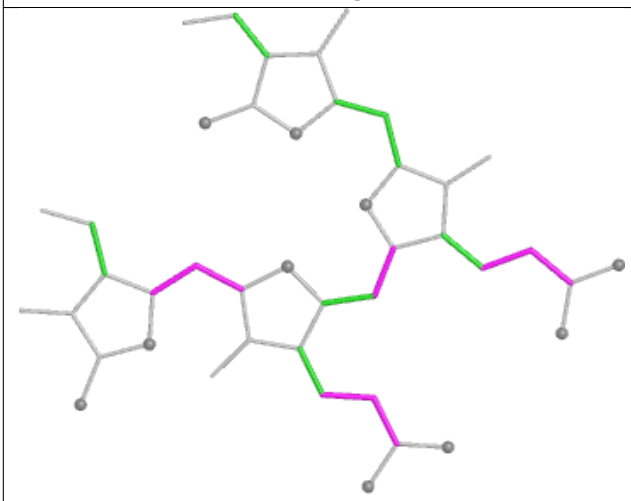

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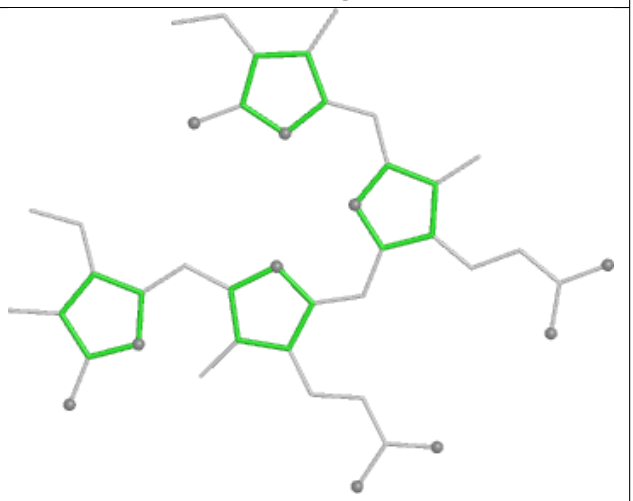
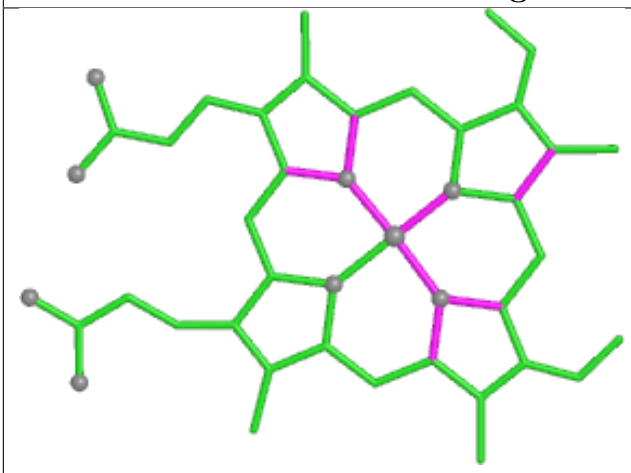


Rings

Ligand HEM FL 102



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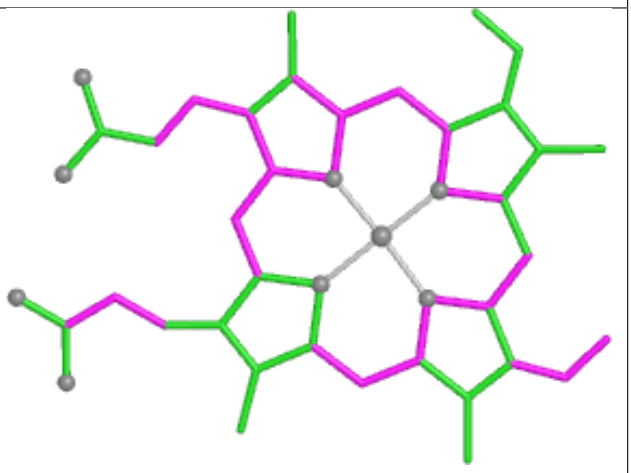

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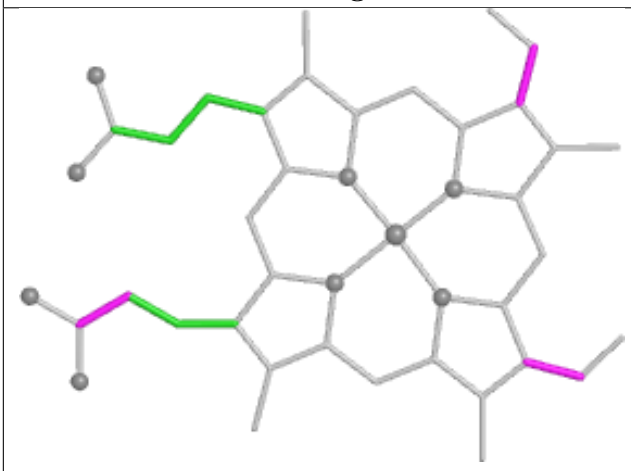

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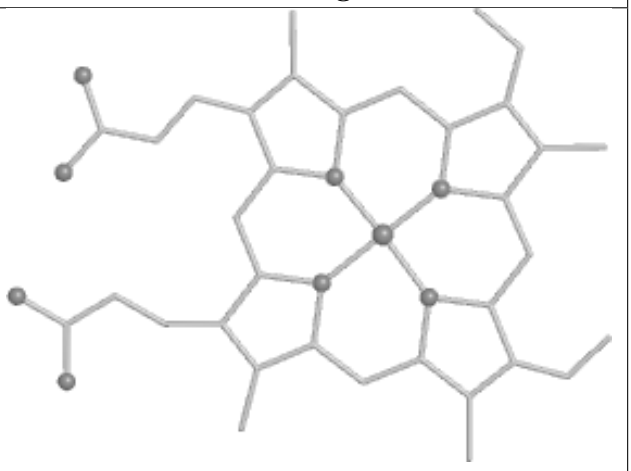
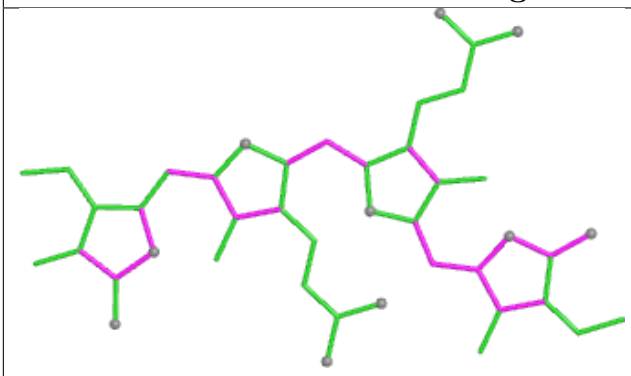


Rings

Ligand CYC NE 201



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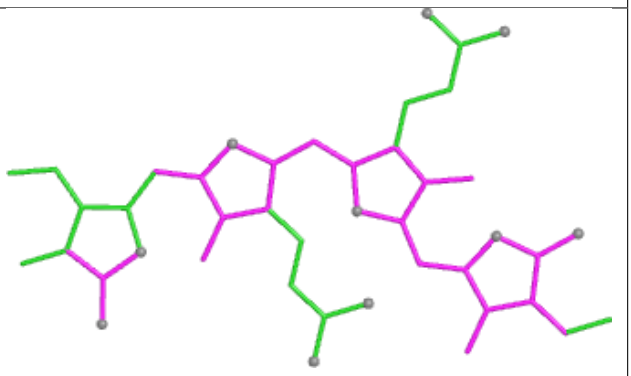

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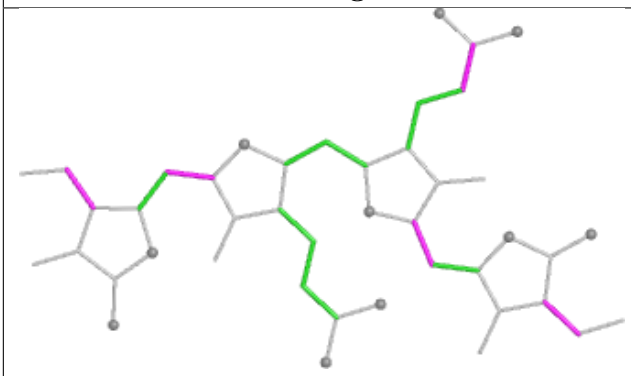

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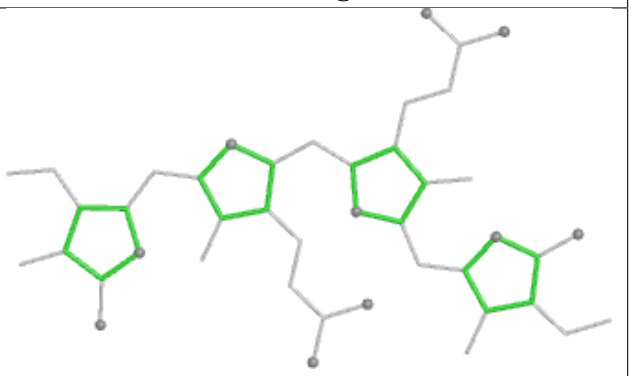
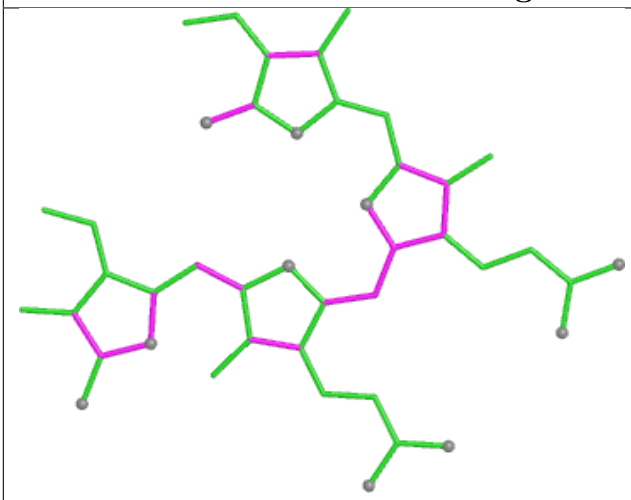


Rings

Ligand PEB JA 201



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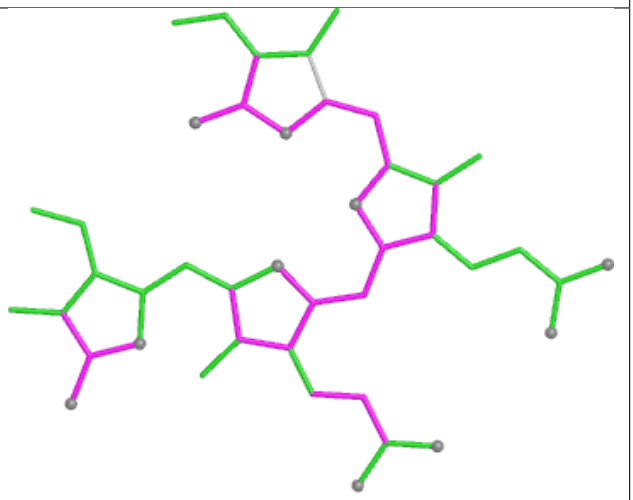

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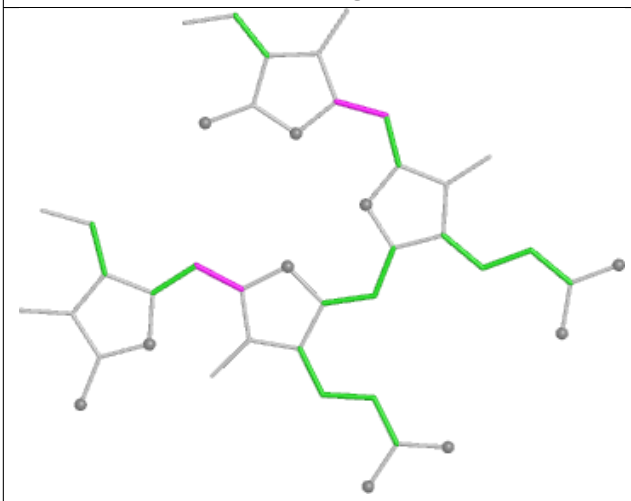

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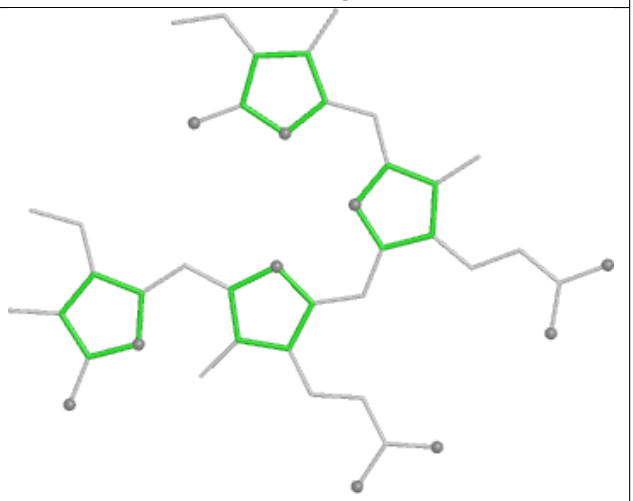
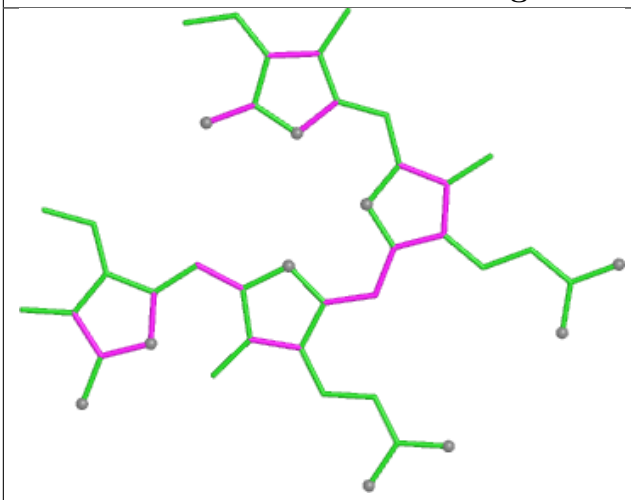


Rings

Ligand PEB W7 202



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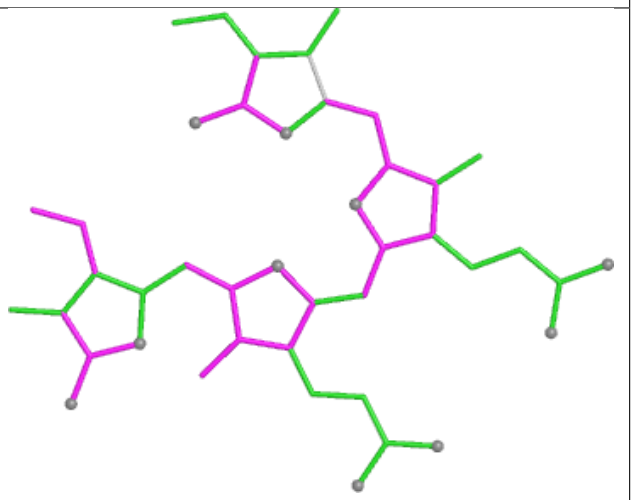
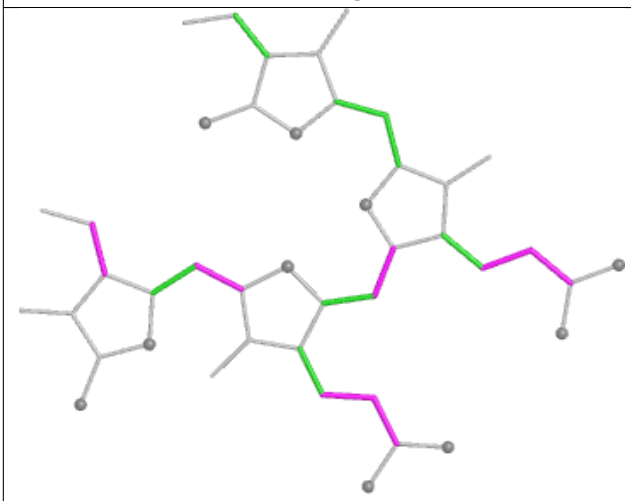


Bond angles



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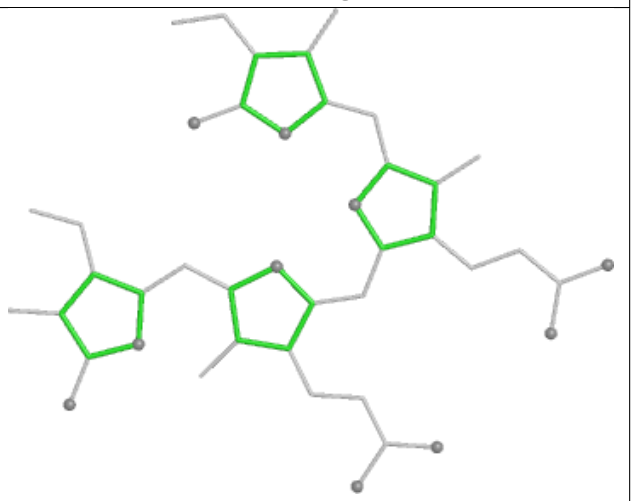
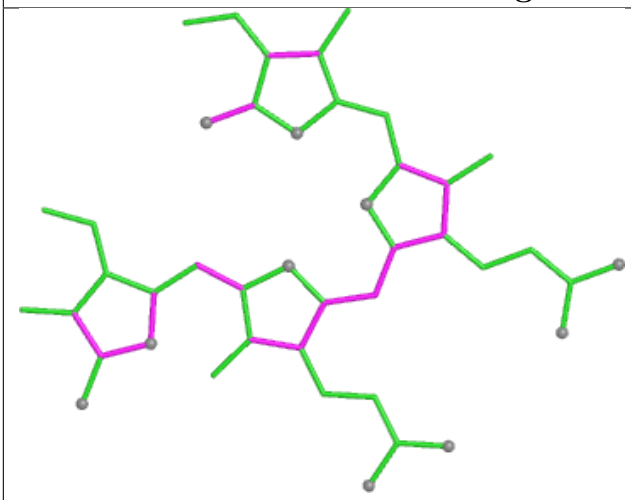


Rings

Ligand PEB FA 203



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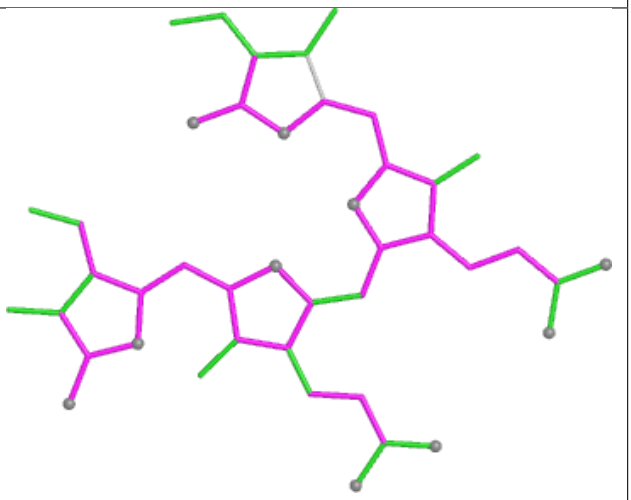
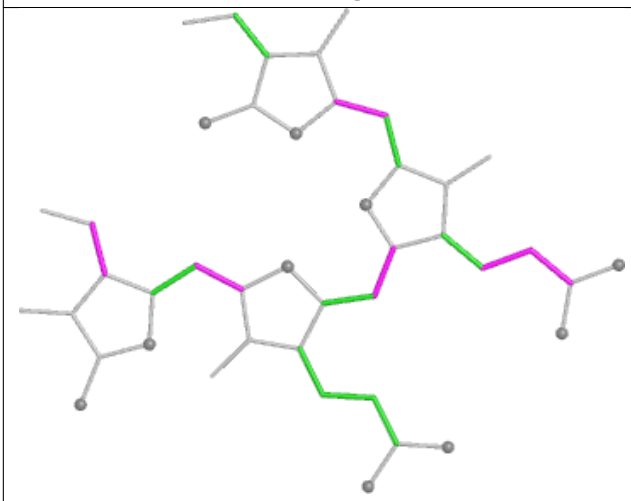
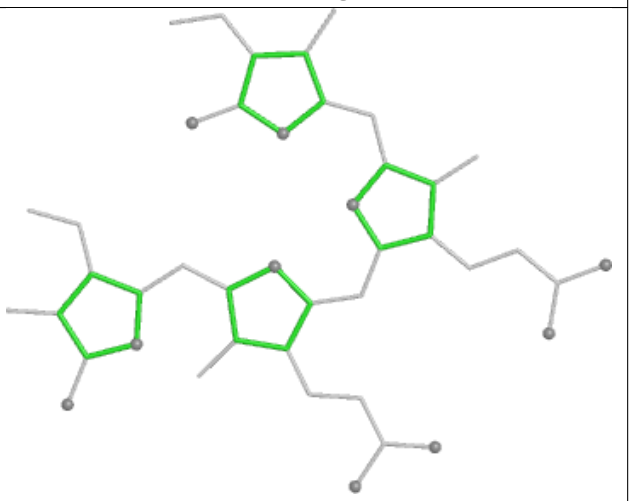


Bond angles

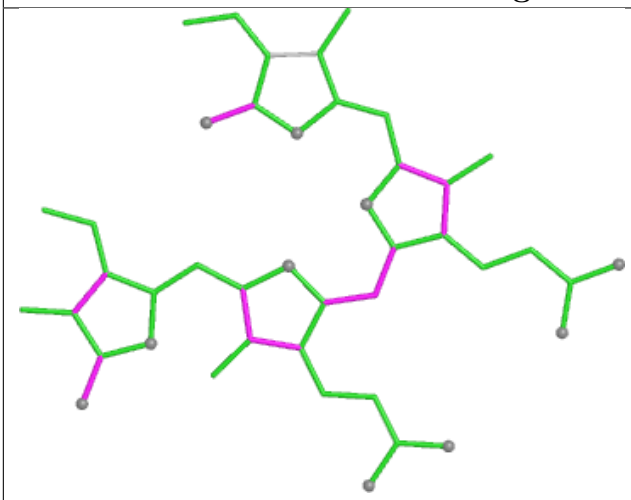


Torsions



Rings

Ligand PUB AJ 303



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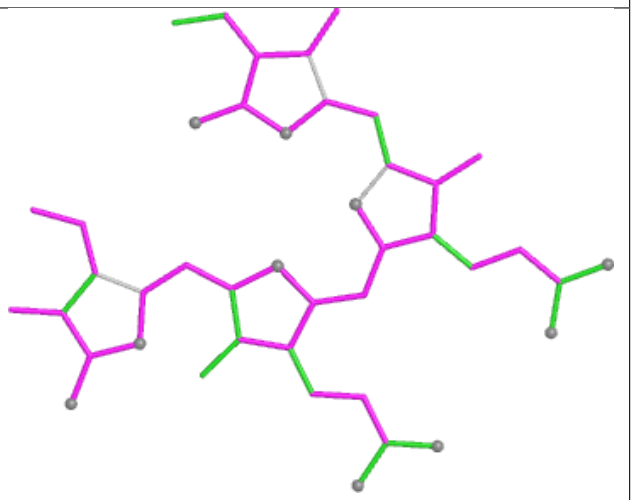
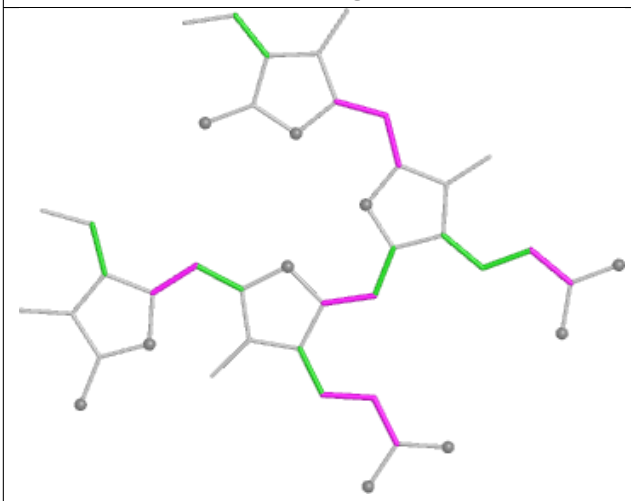


Bond angles



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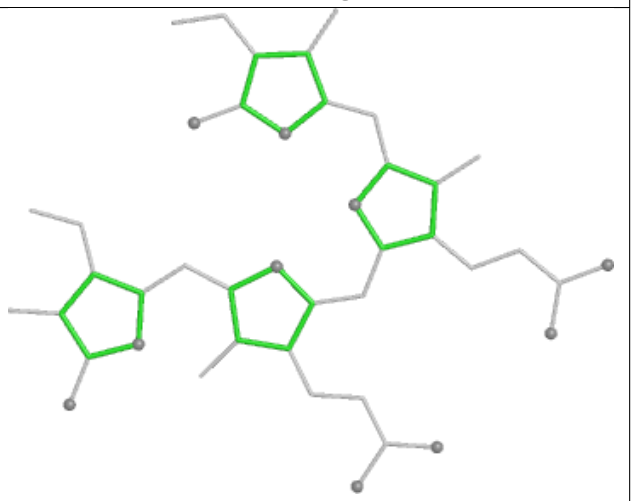
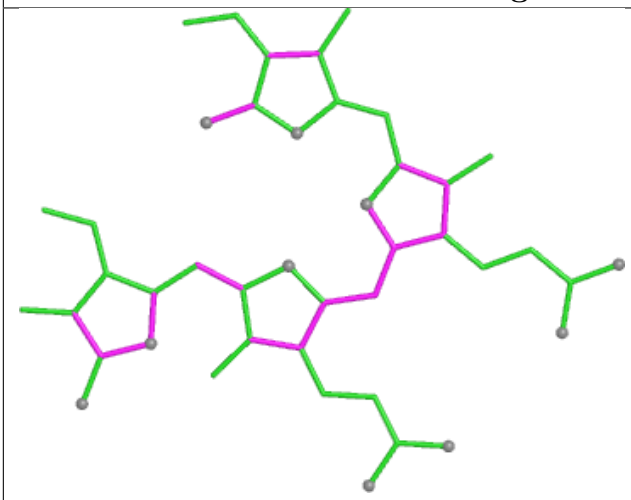


Rings

Ligand PEB VG 201



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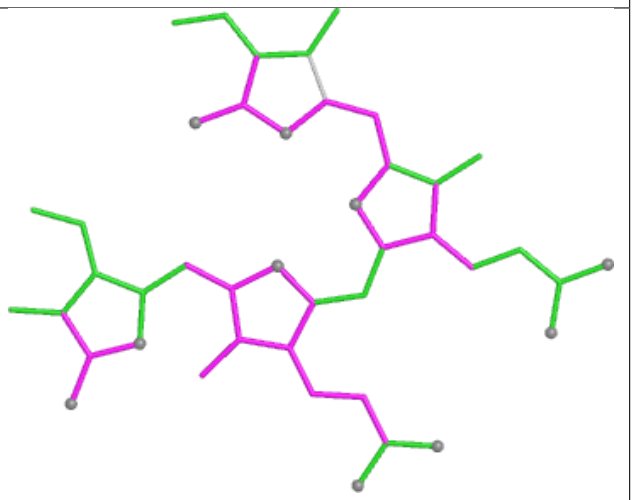

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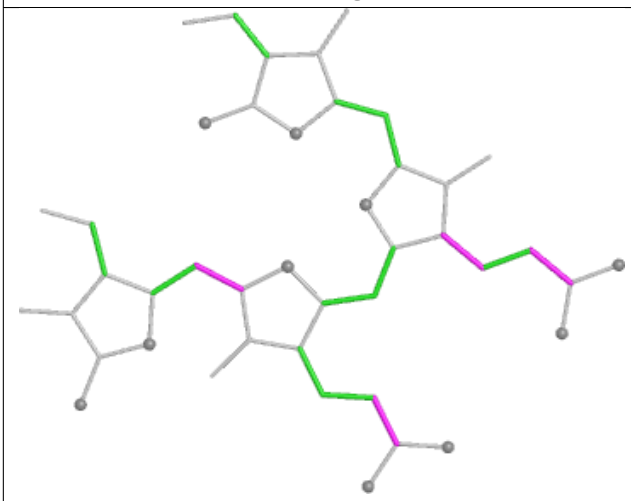

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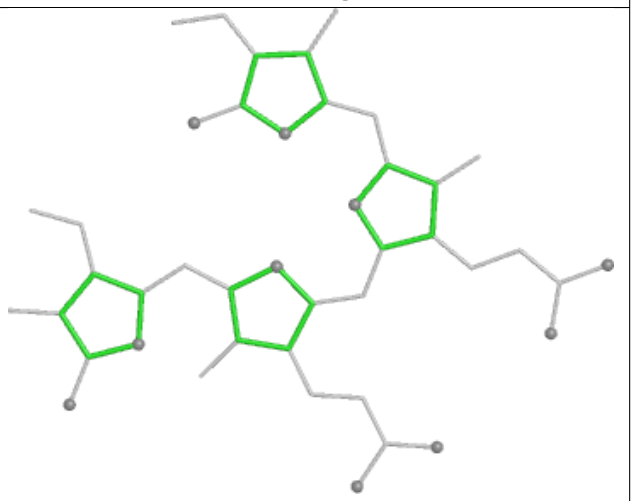
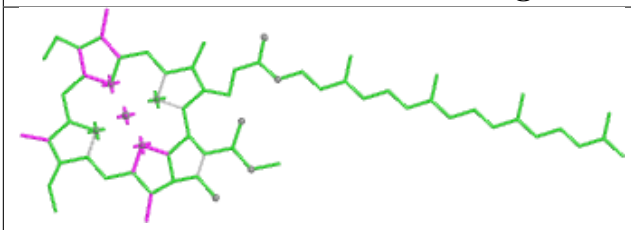


Rings

Ligand CLA A2 805



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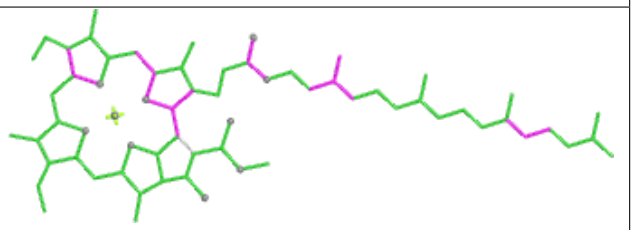

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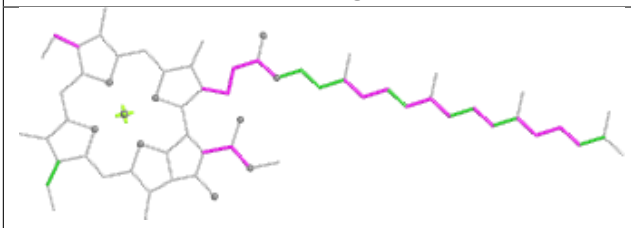

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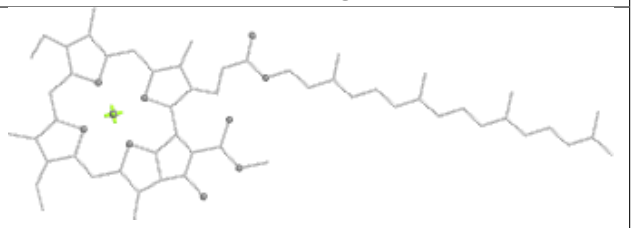
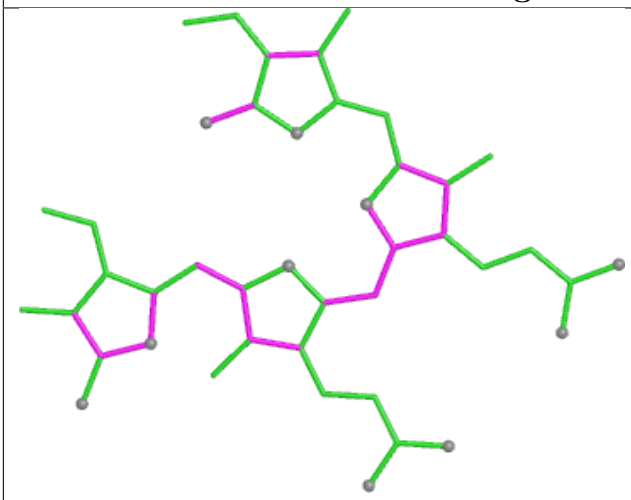


Rings

Ligand PEB EP 201



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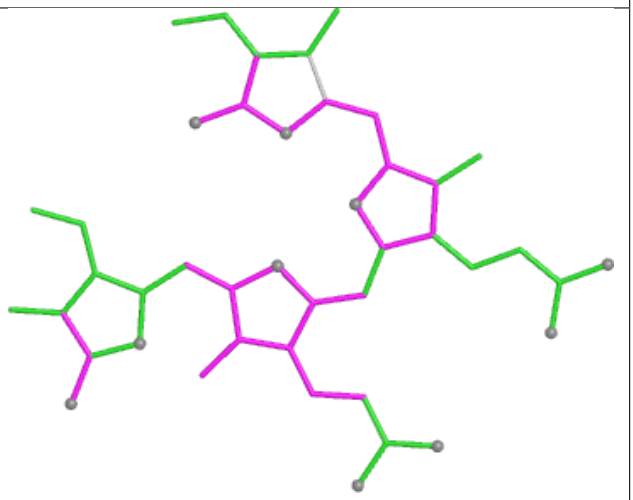

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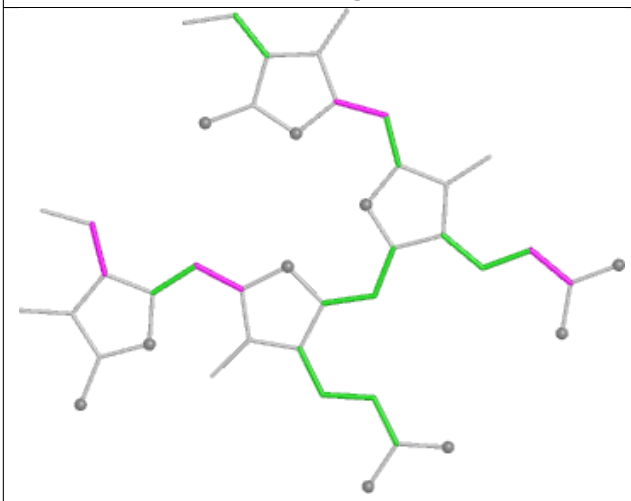

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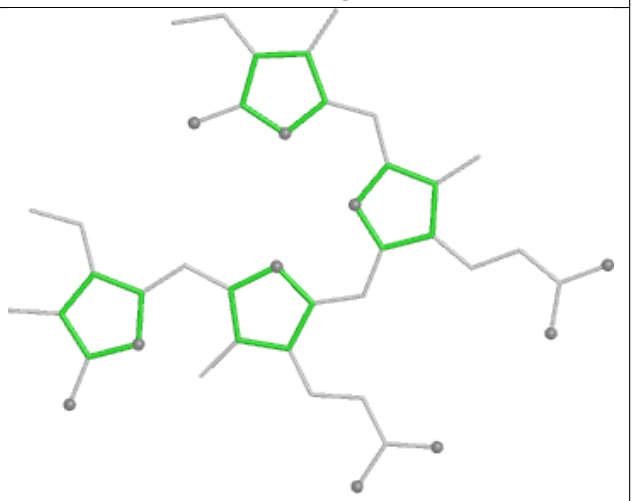
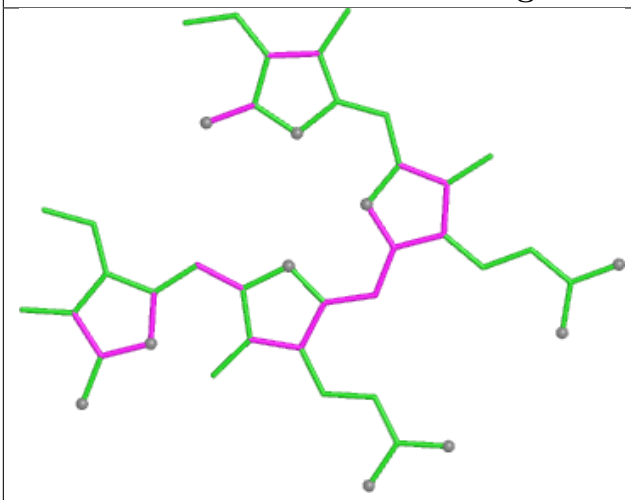


Rings

Ligand PEB HI 201



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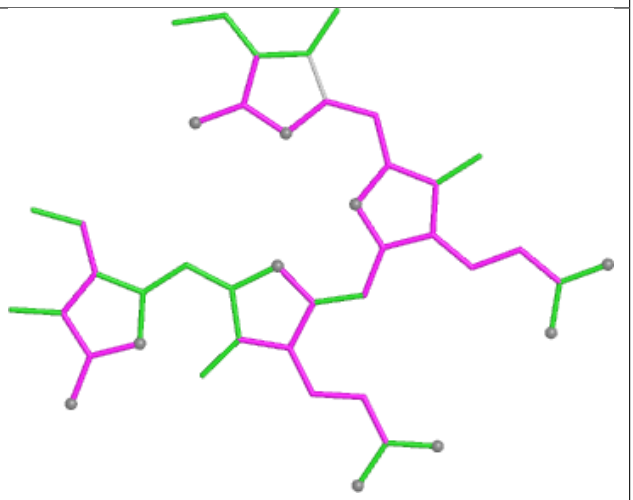

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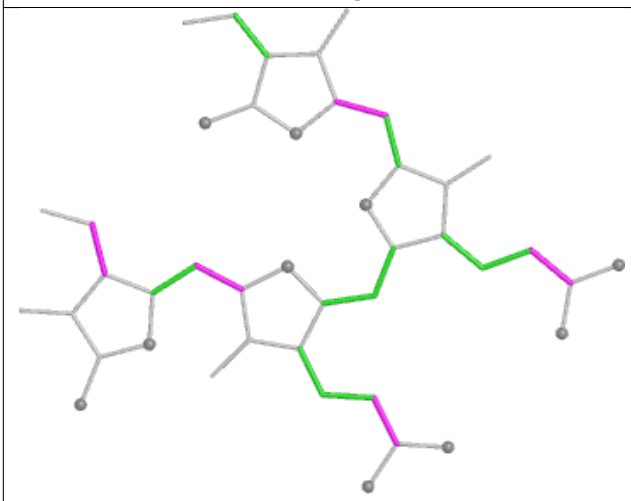

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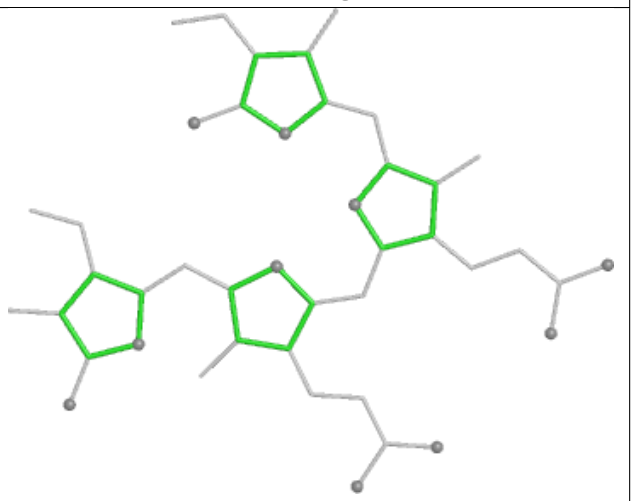
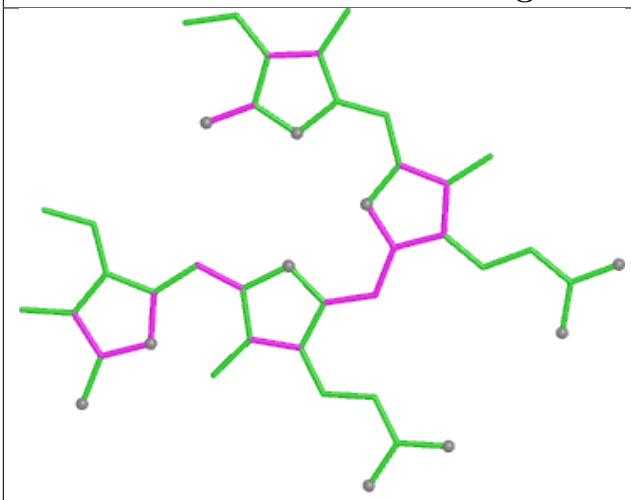


Rings

Ligand PEB bE 201



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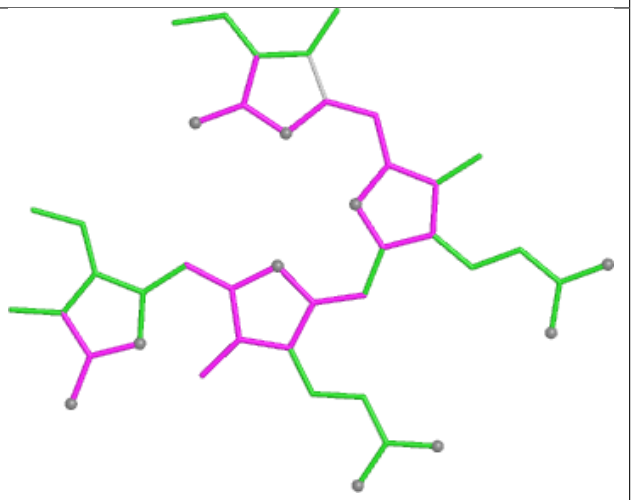

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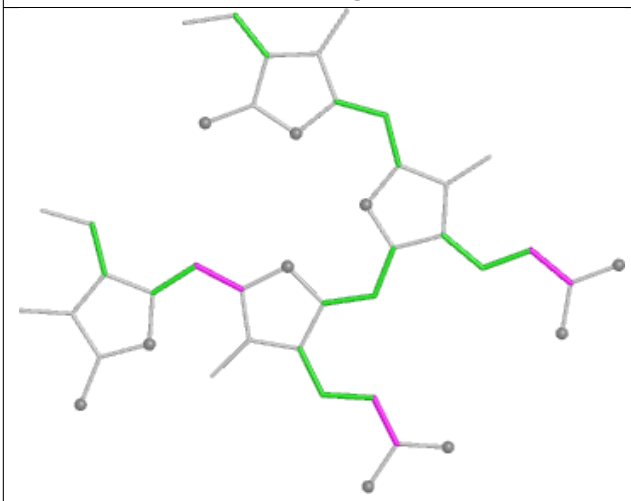

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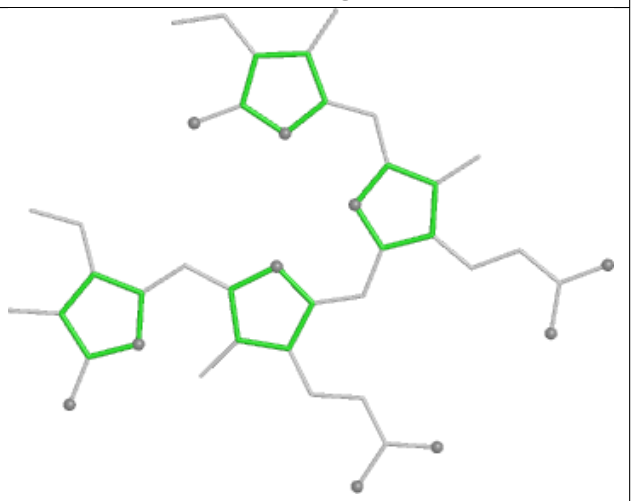
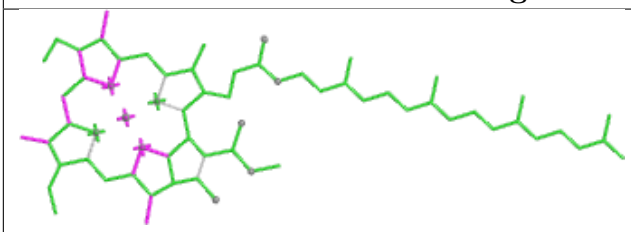


Rings

Ligand CLA AN 821



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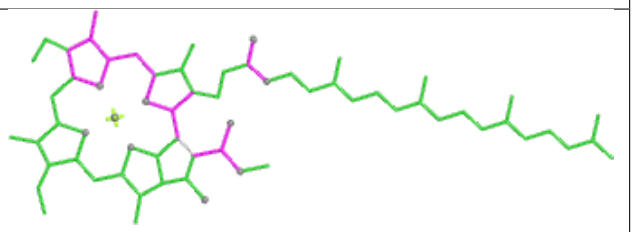

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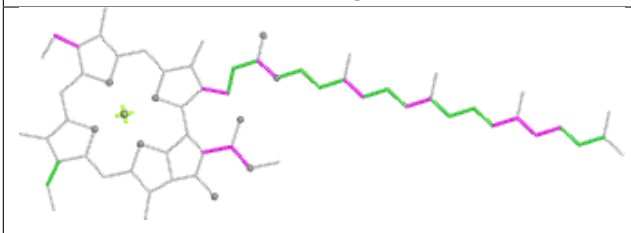

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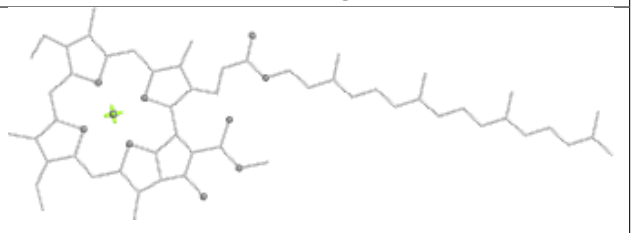
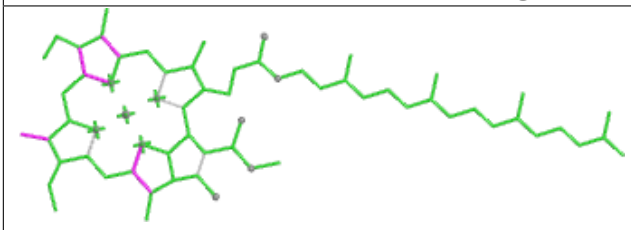


Rings

Ligand CLA 2N 303



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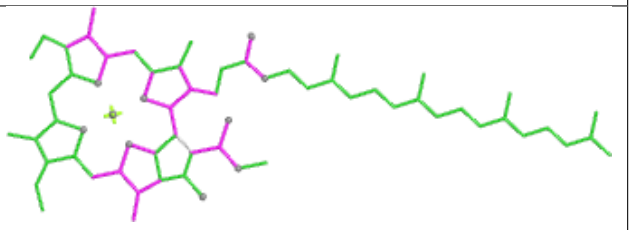
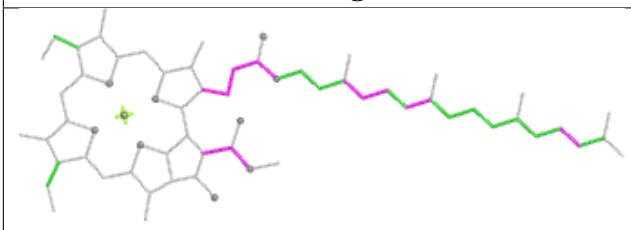


Bond angles



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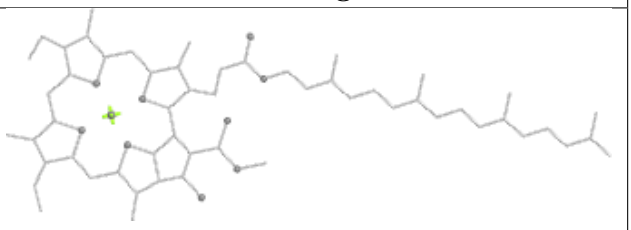
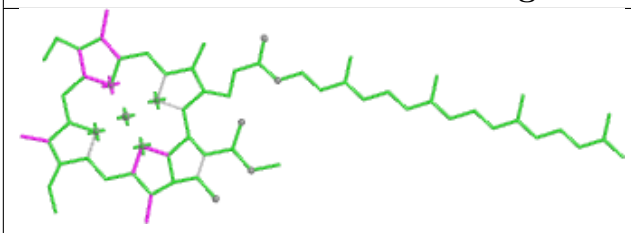


Rings

Ligand CLA b6 613



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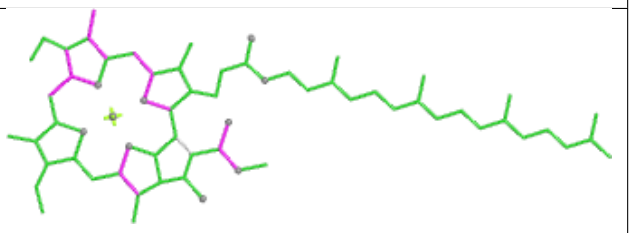

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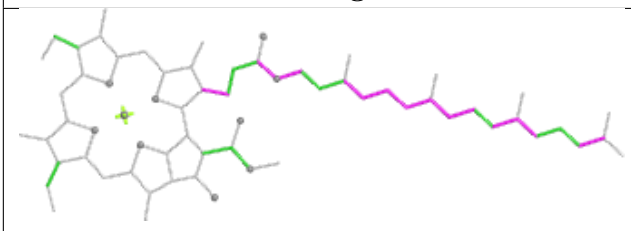

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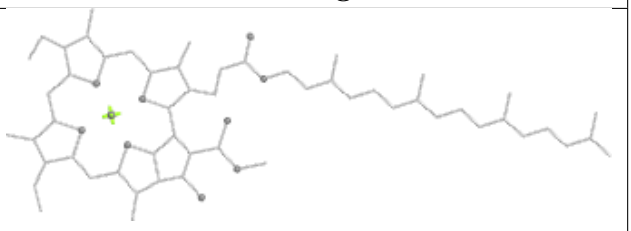
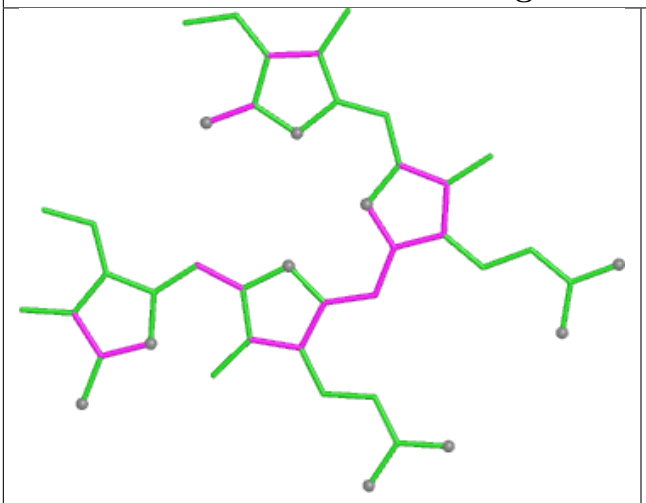


Rings

Ligand PEB A9 202



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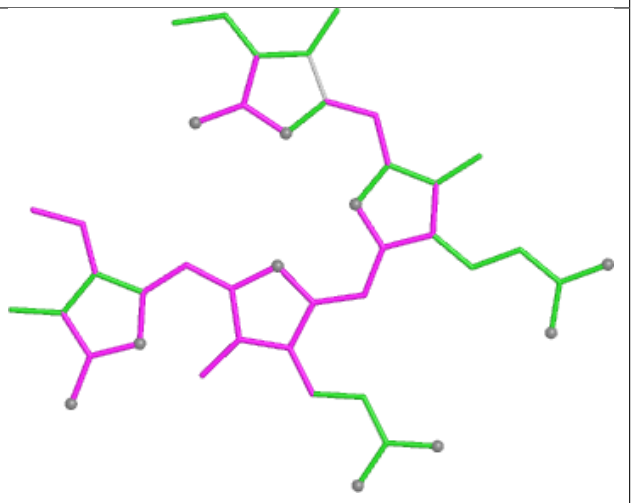

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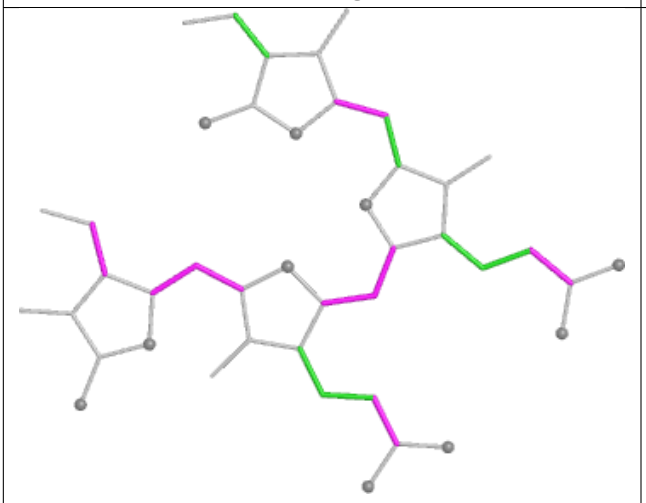

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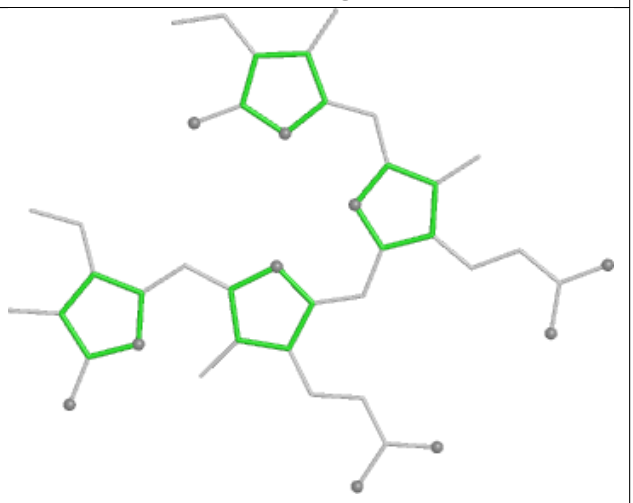
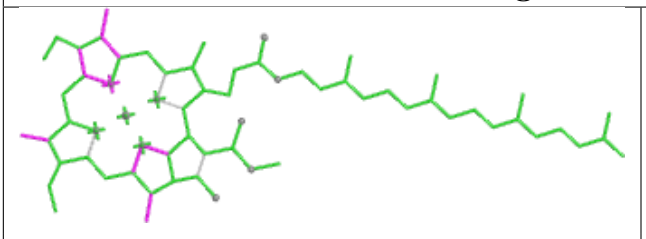


Rings

Ligand CLA A2 833



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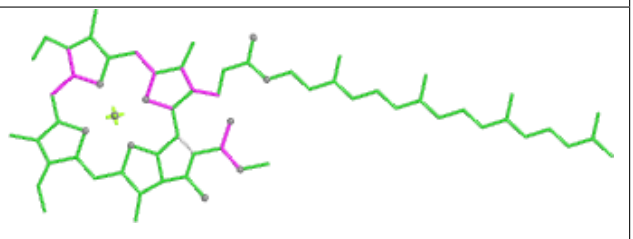
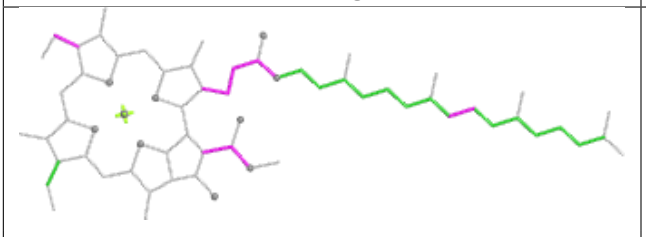


Bond angles



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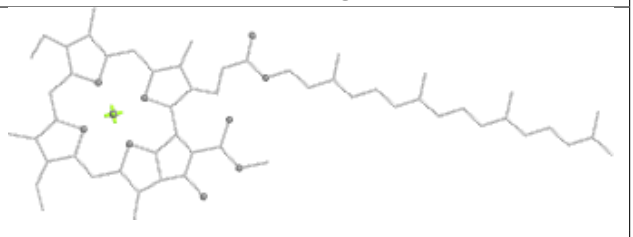
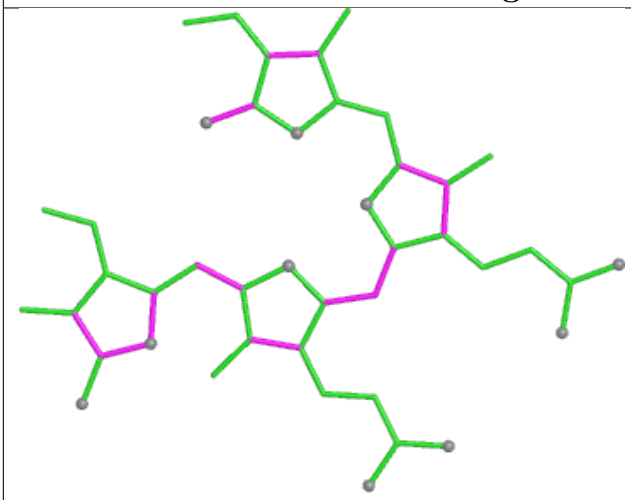


Rings

Ligand PEB WM 203



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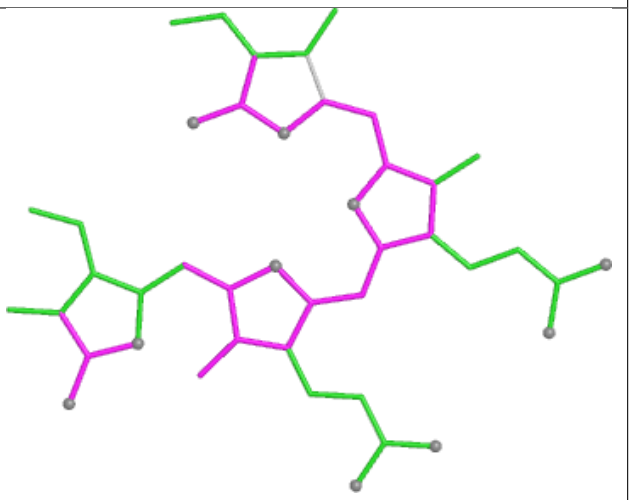
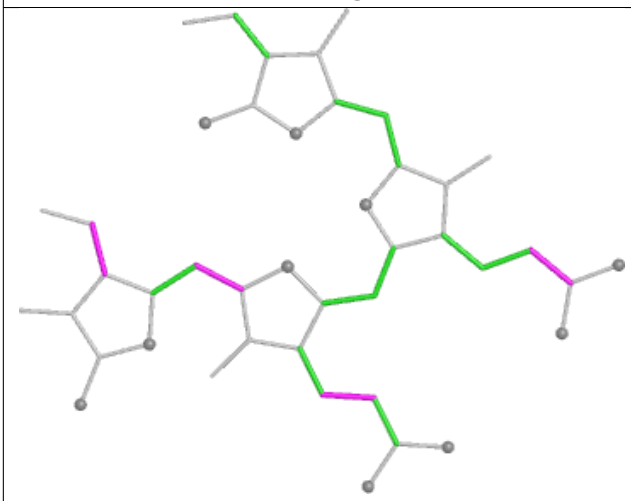


Bond angles



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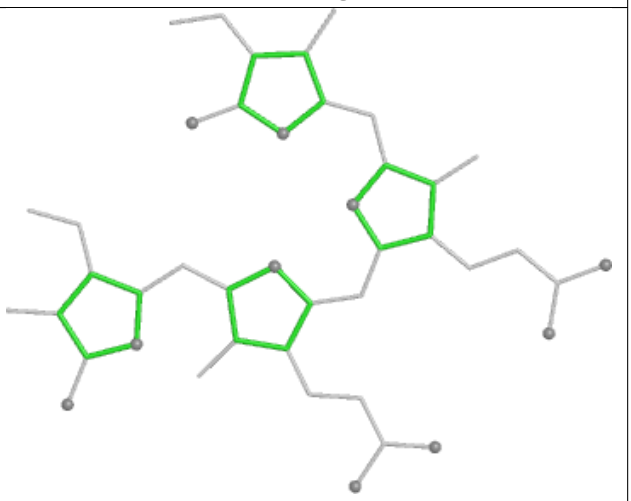
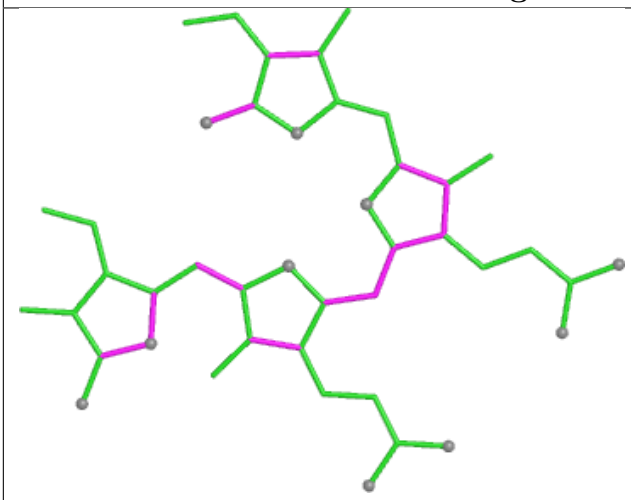


Rings

Ligand PEB GA 201



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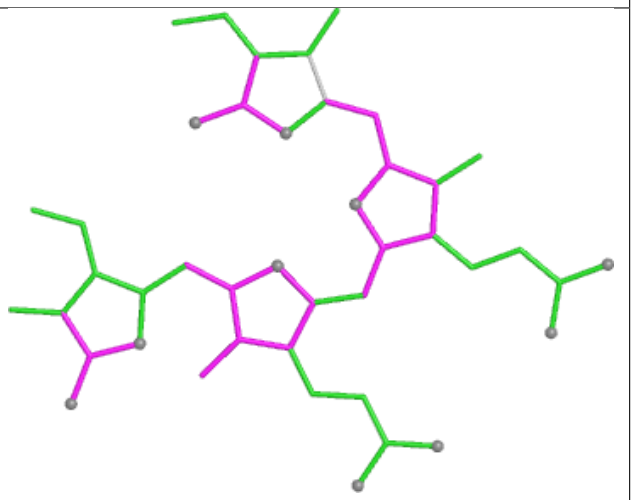
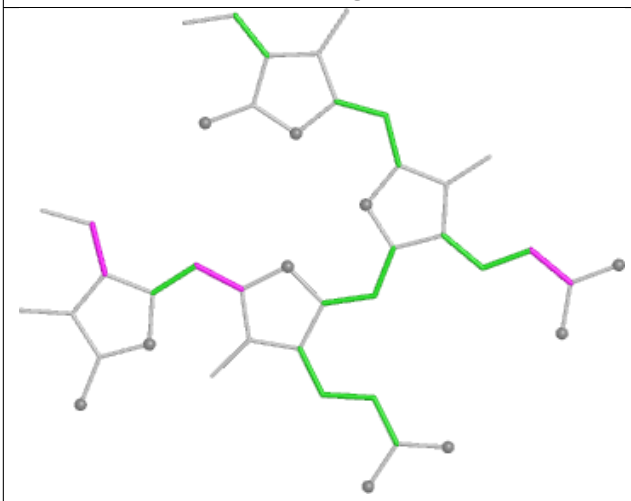


Bond angles



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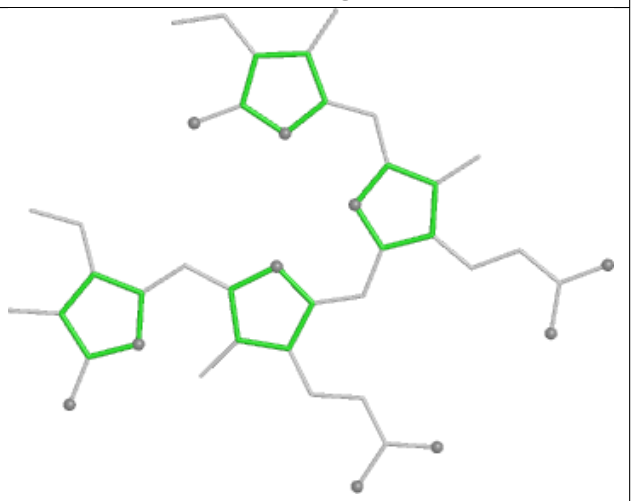
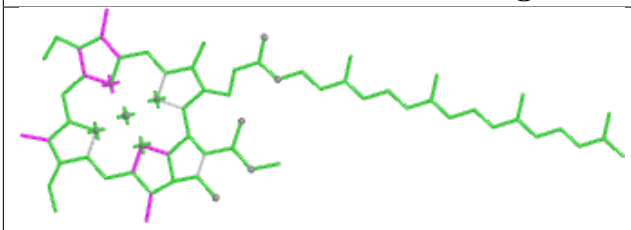


Rings

Ligand CLA C6 512



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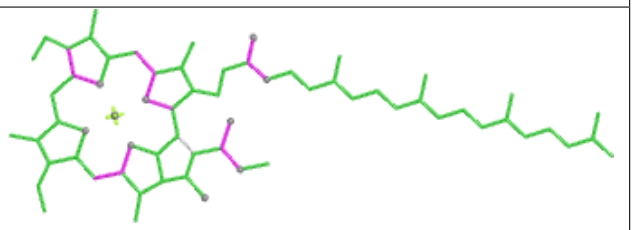
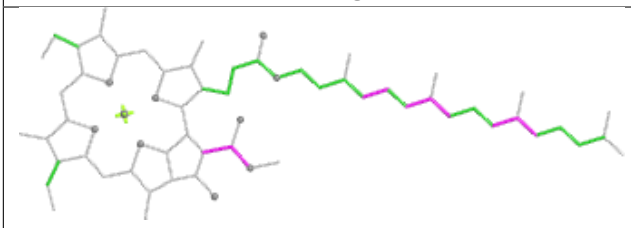


Bond angles



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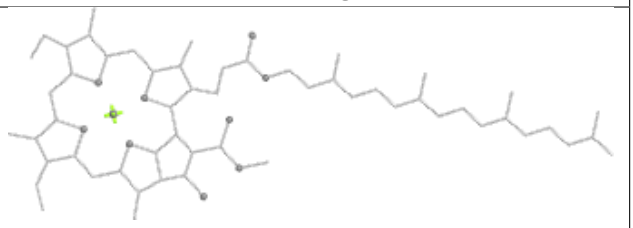
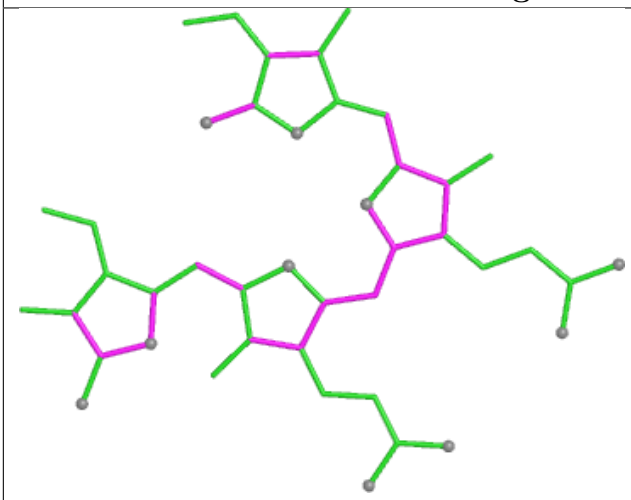


Rings

Ligand PEB ZK 202



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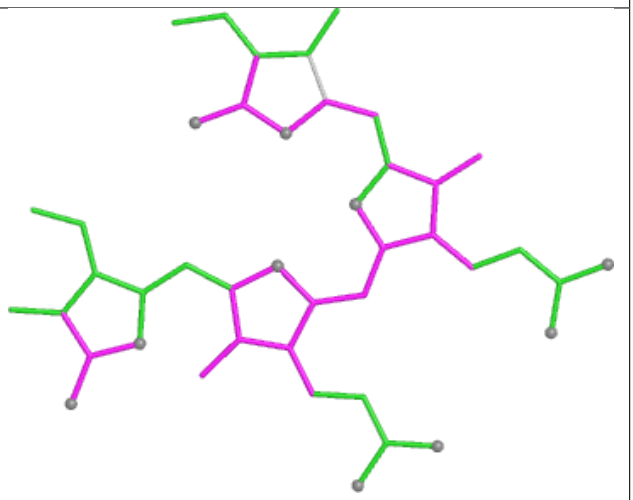

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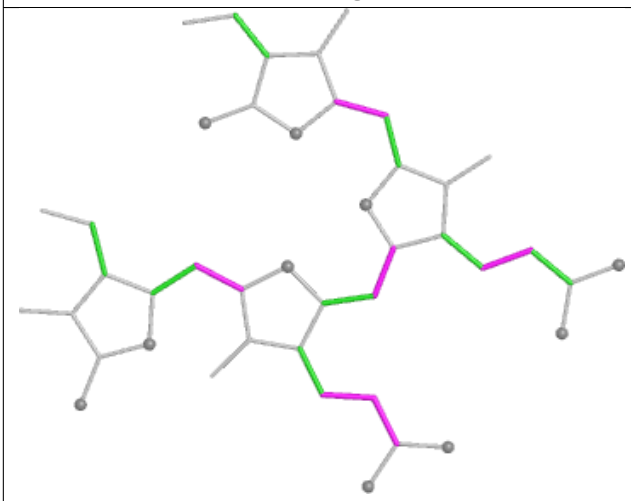

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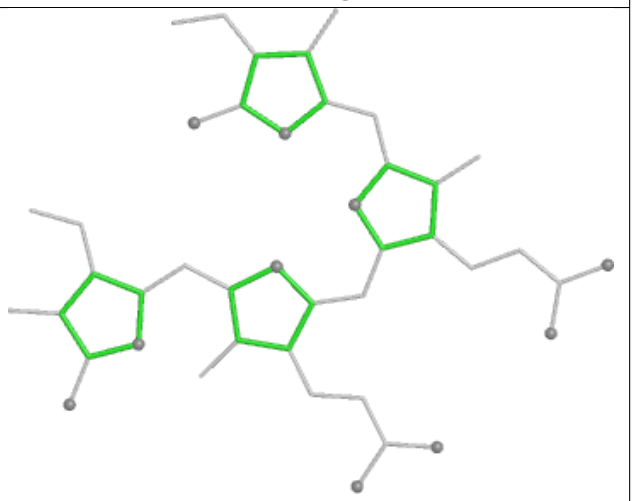
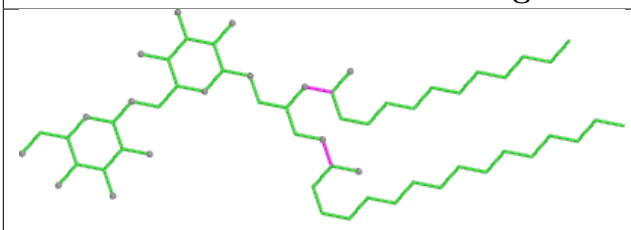


Rings

Ligand DGD L6 102



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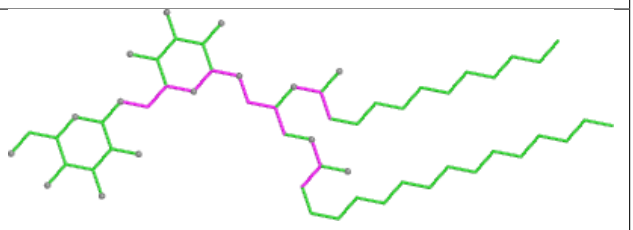

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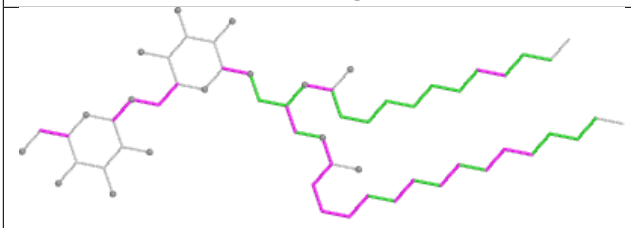

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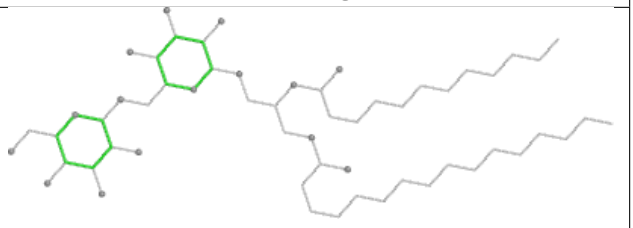
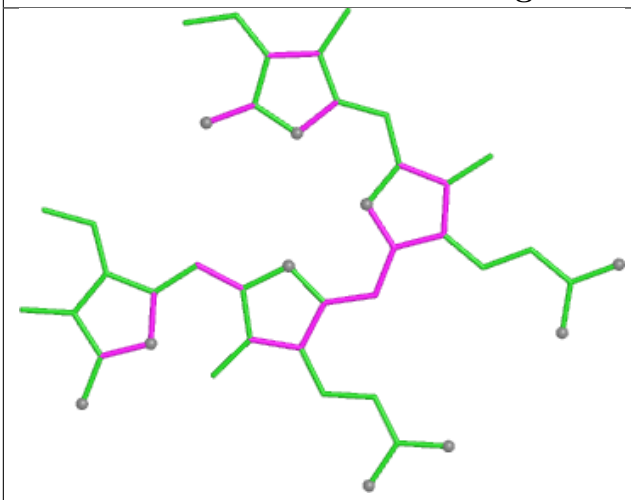


Rings

Ligand PEB A1 305



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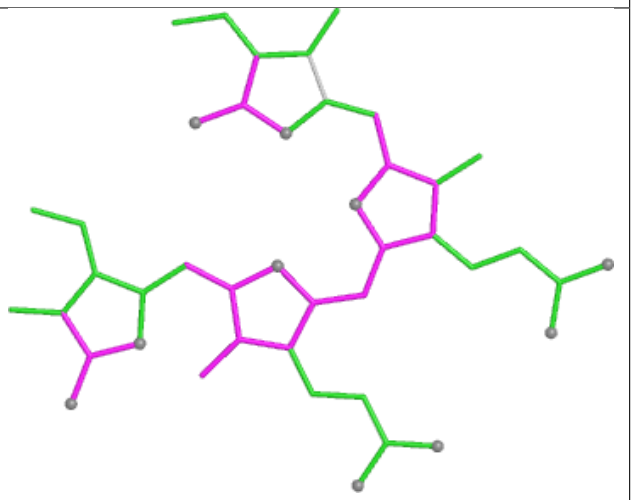

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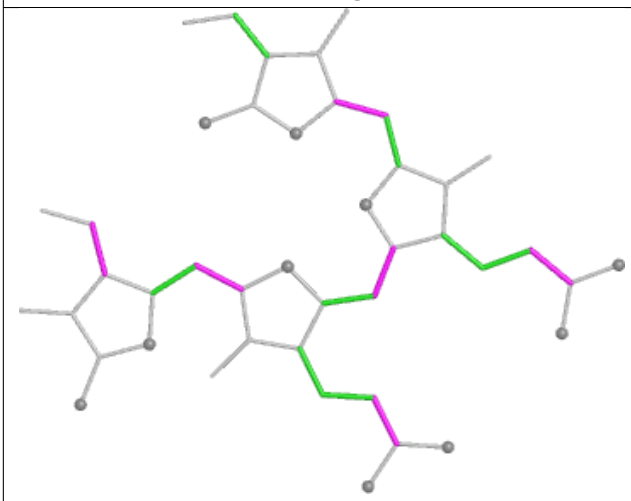

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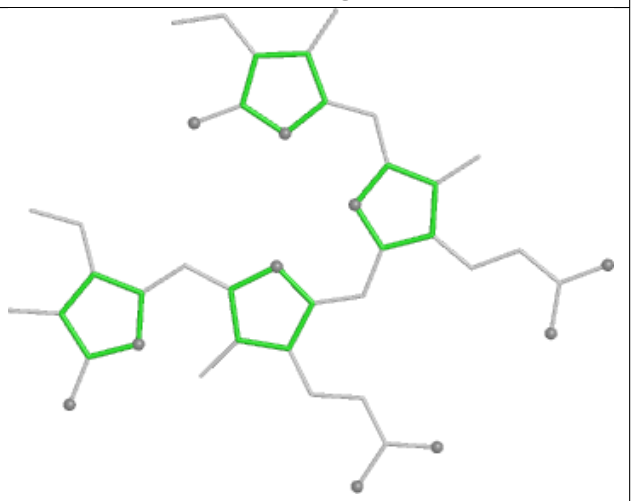
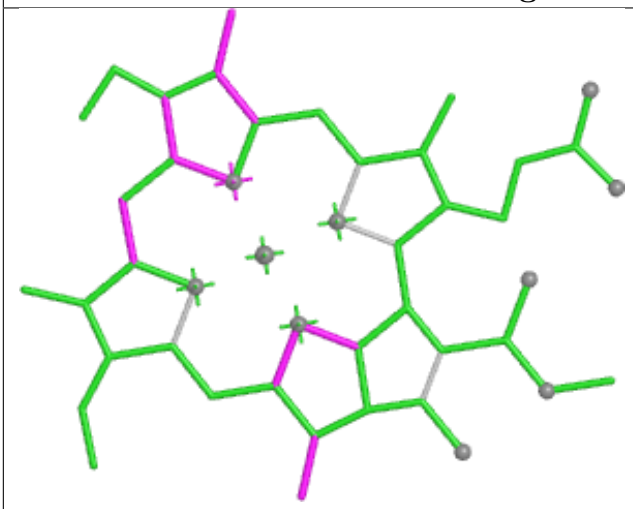


Rings

Ligand CLA 52 605



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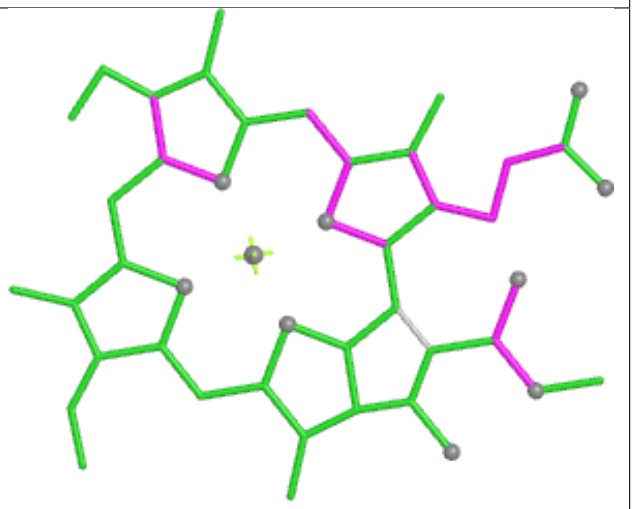

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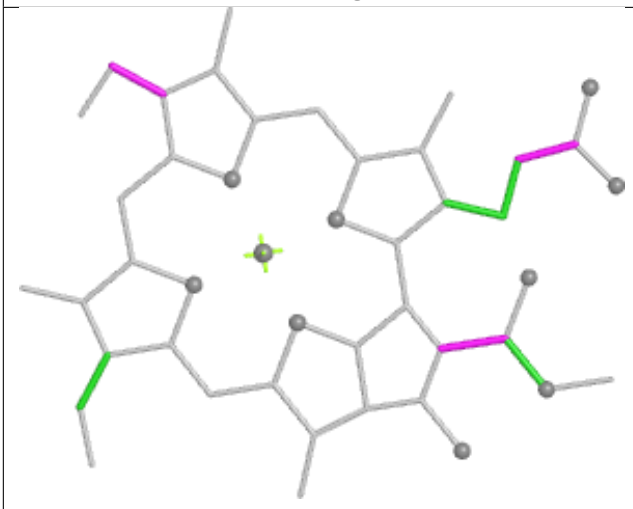
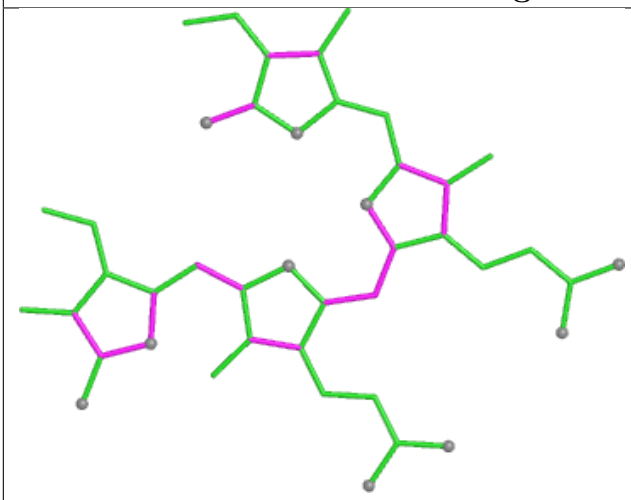


Torsions



Rings

Ligand PEB ZO 202



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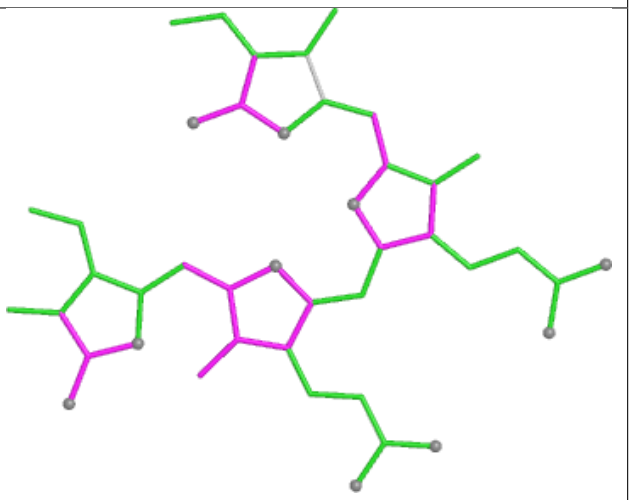

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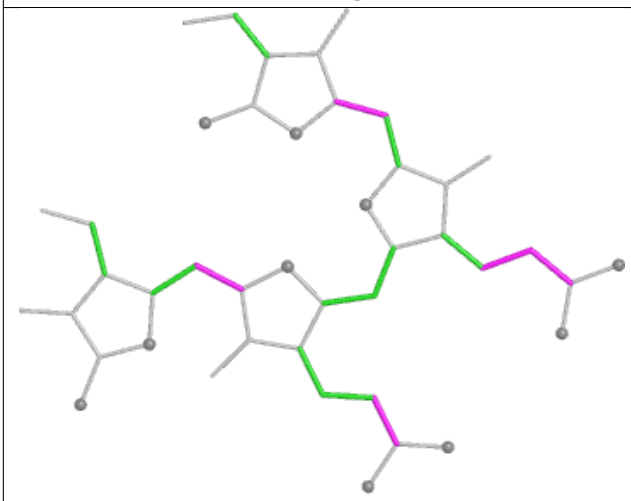

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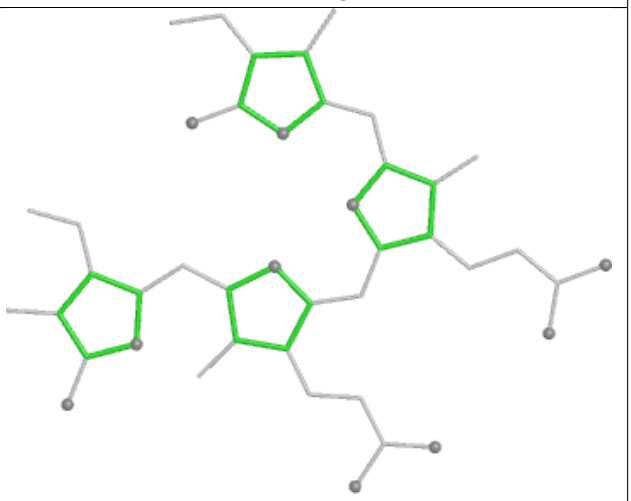
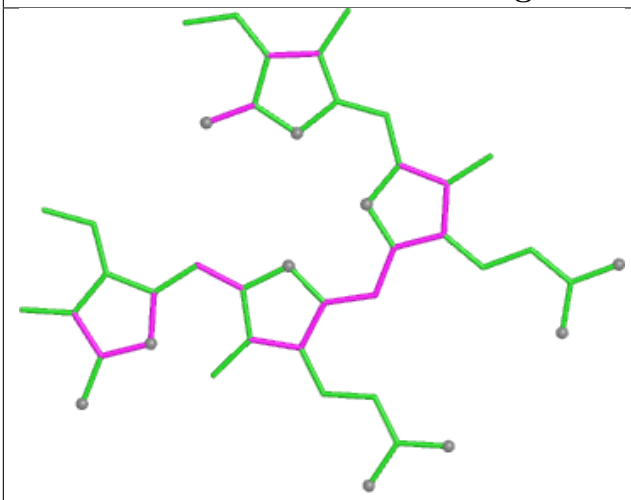


Rings

Ligand PEB kO 202



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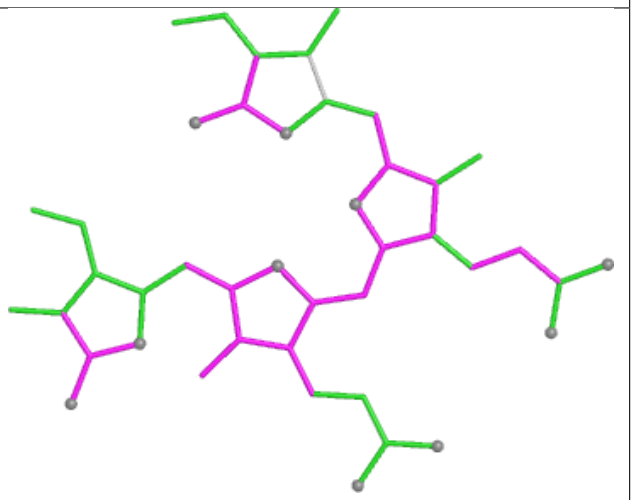

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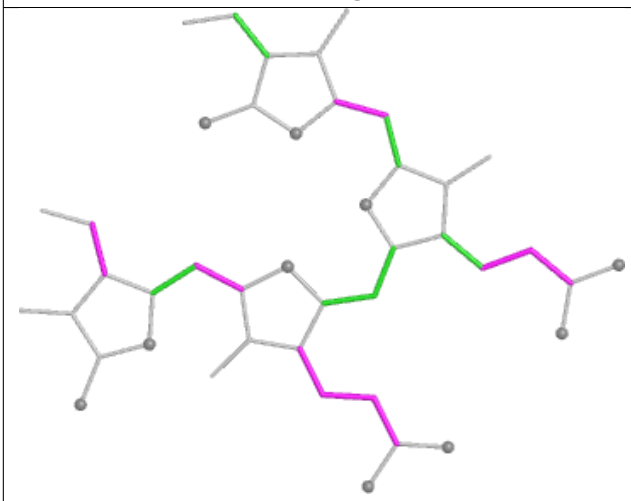

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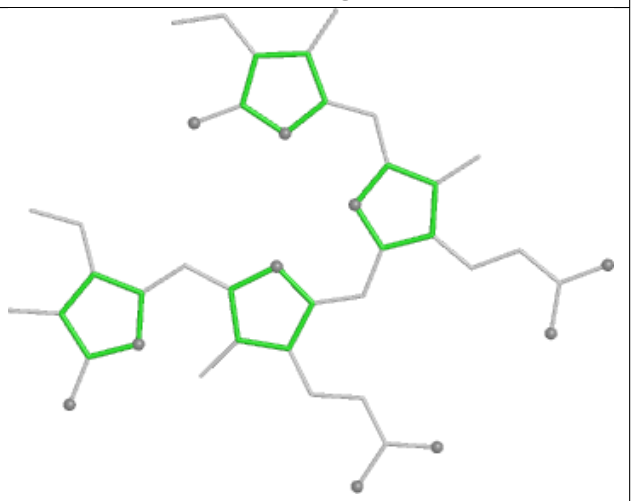

Rings

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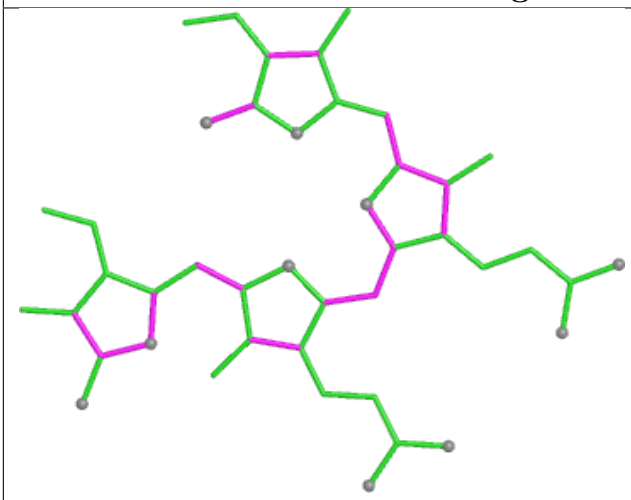

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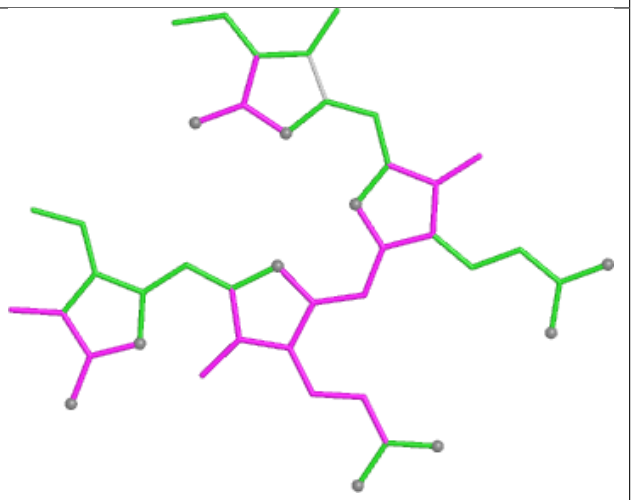

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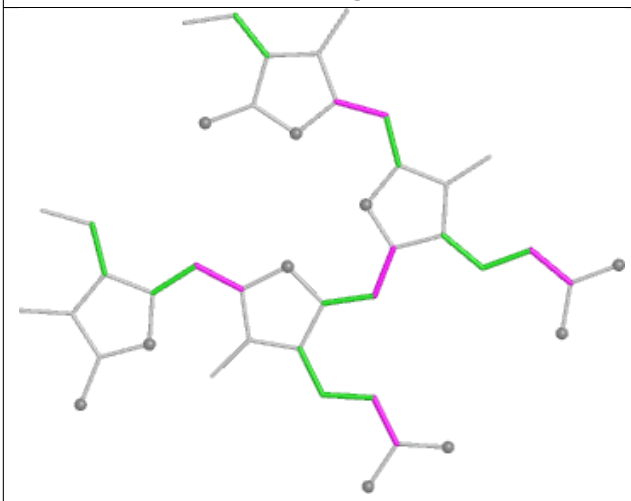

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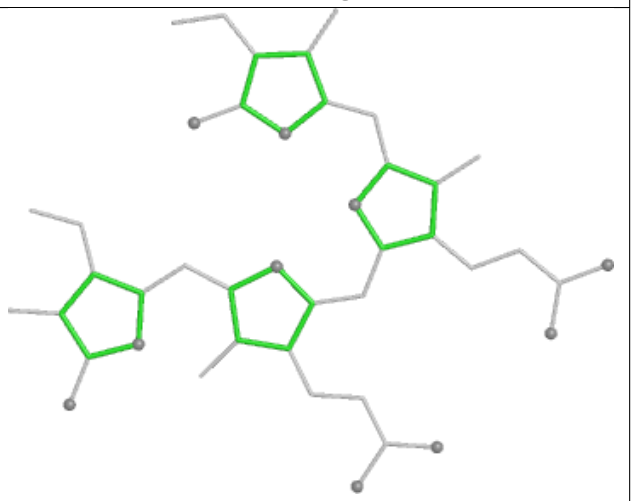
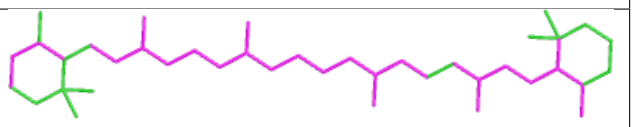


Rings

Ligand BCR A2 848



Bond lengths



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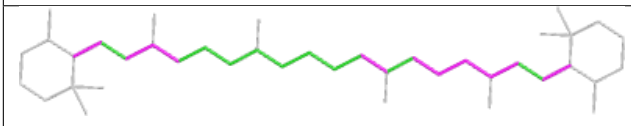

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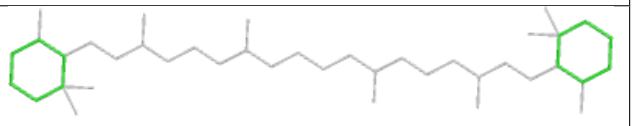
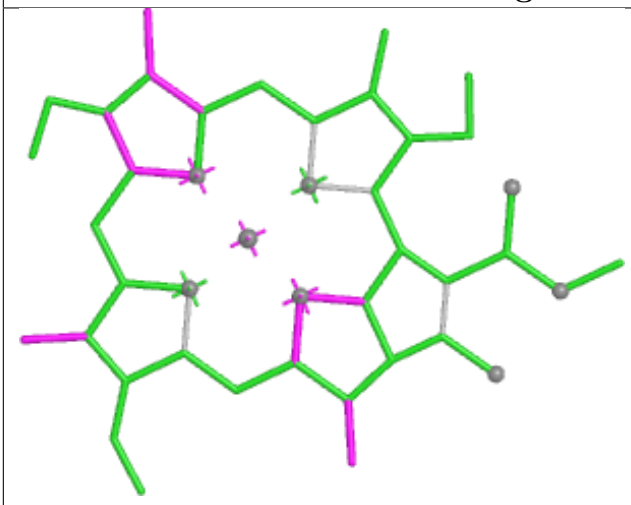


Rings

Ligand CLA B2 814



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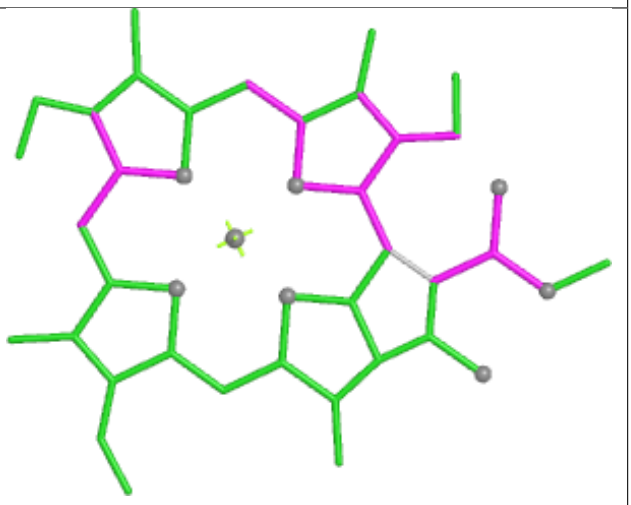

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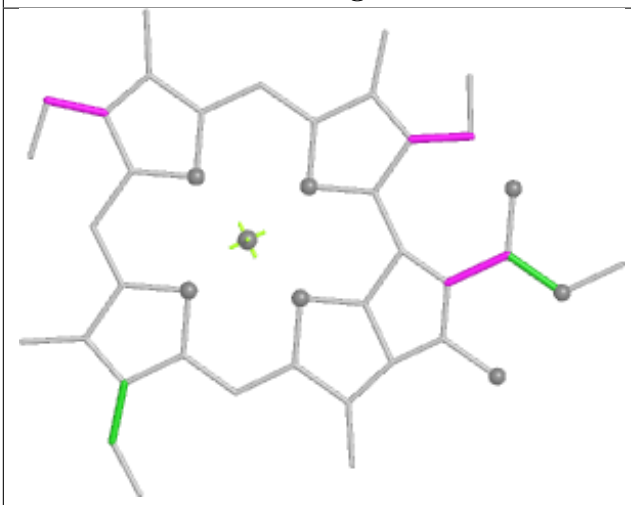
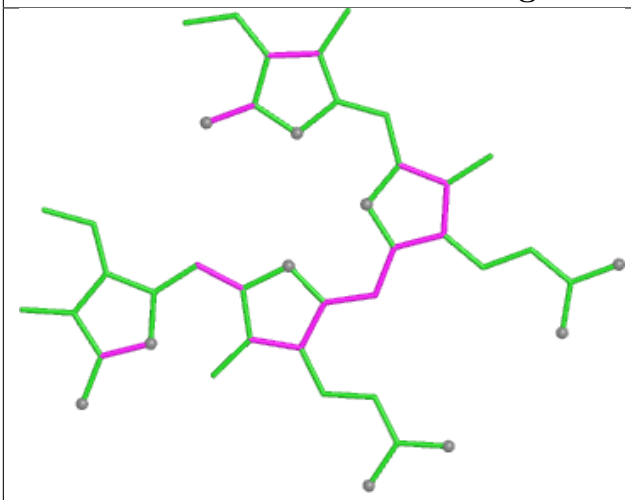


Torsions



Rings

Ligand PEB b1 202



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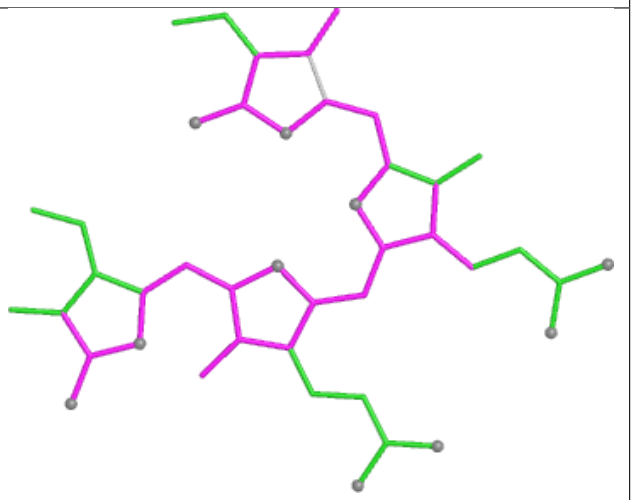

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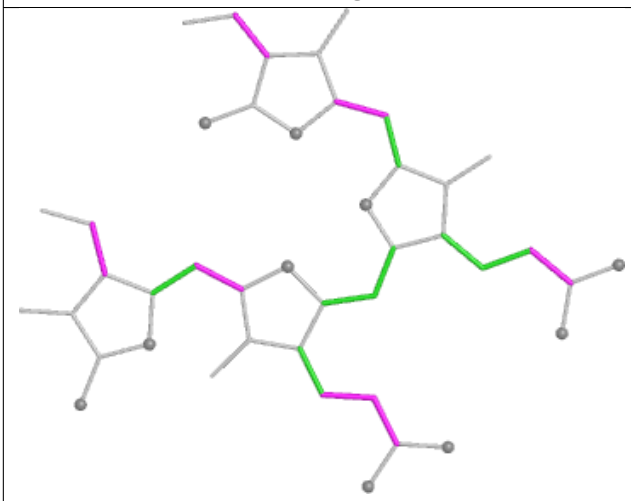

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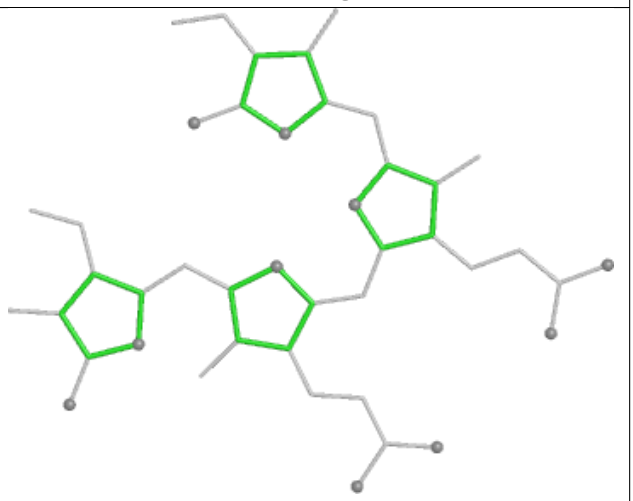
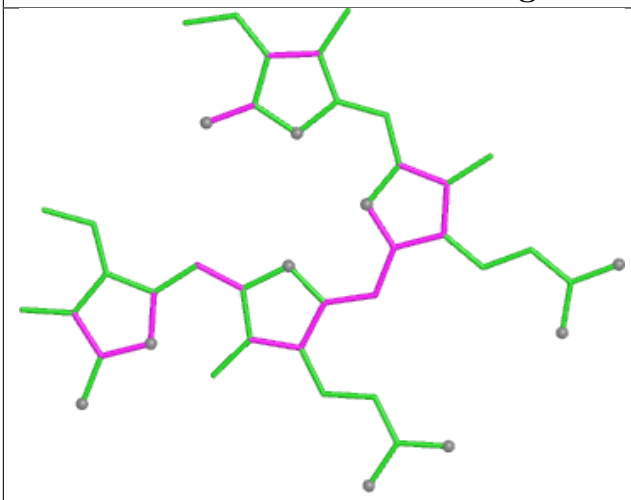


Rings

Ligand PEB S5 201



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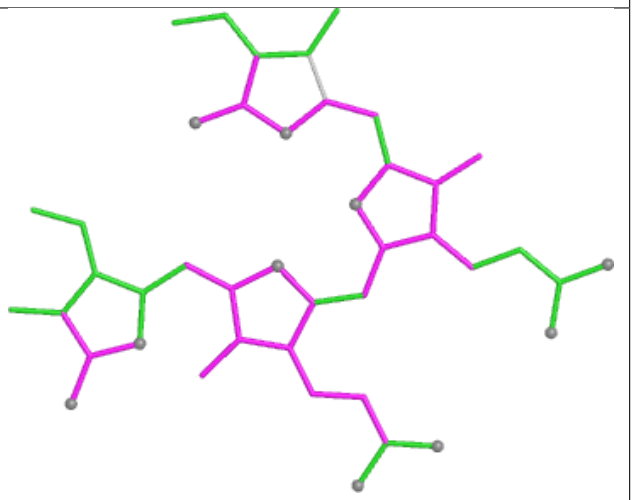

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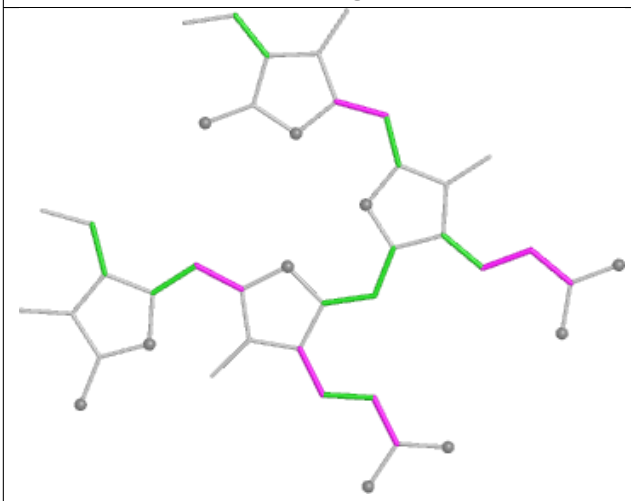

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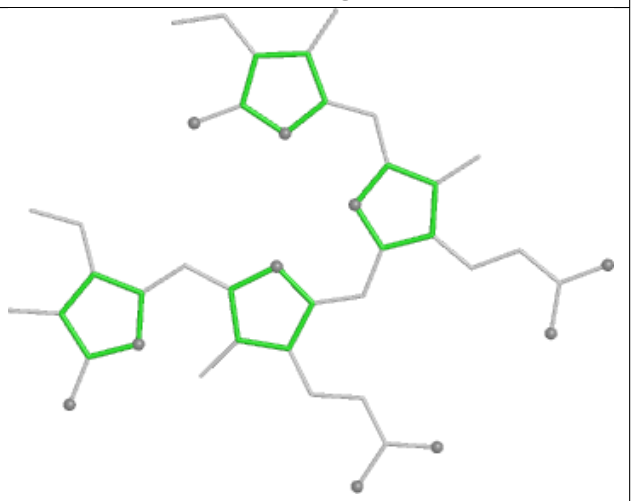
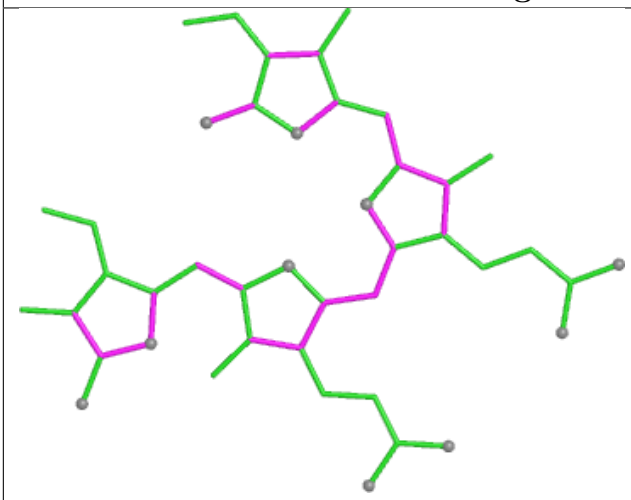


Rings

Ligand PEB TF 202



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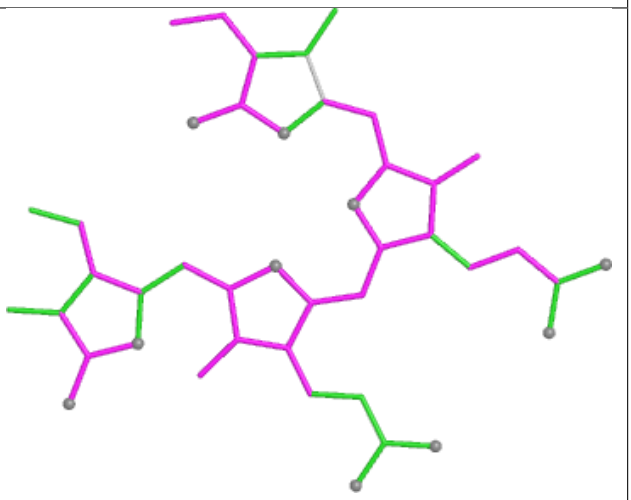
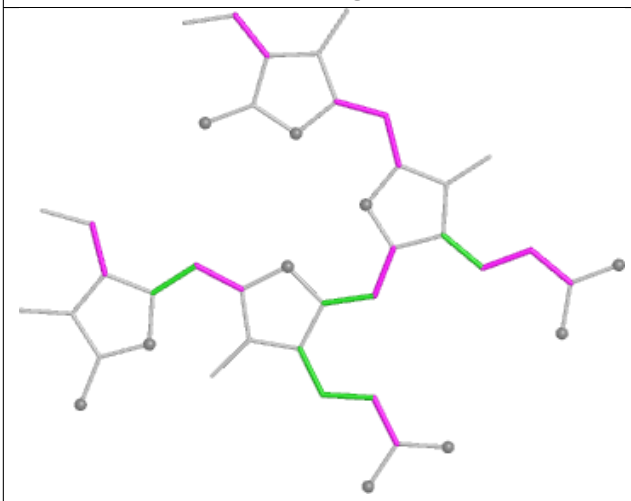


Bond angles



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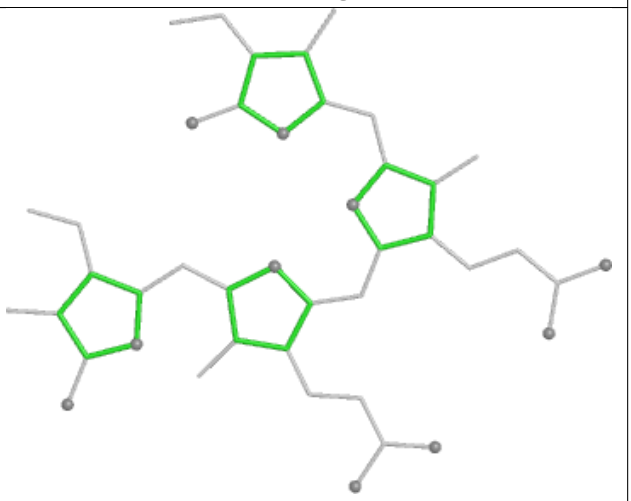
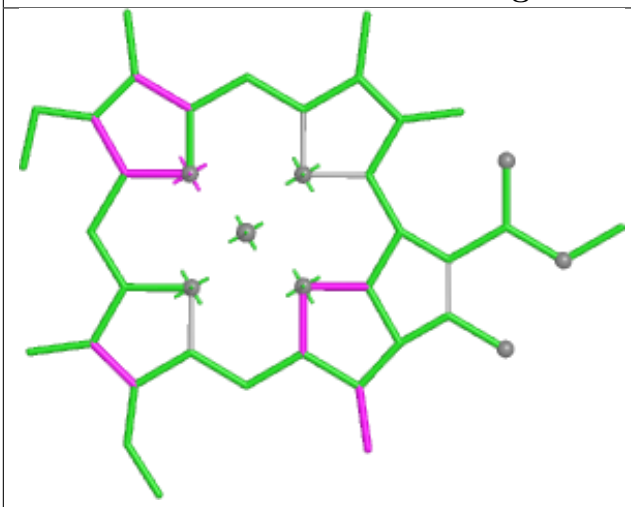


Rings

Ligand CLA FN 201



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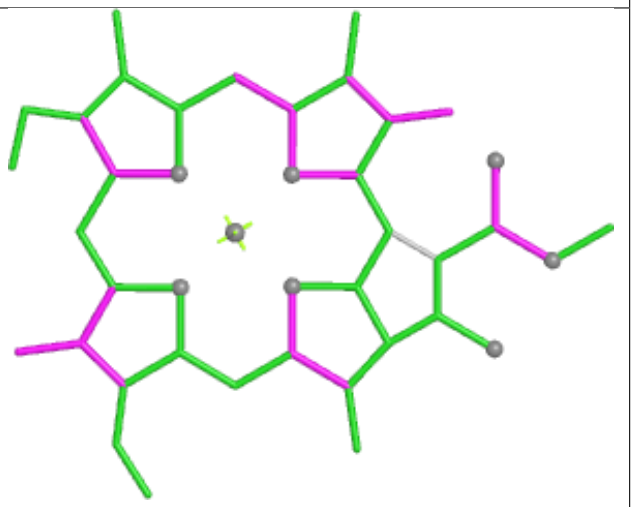
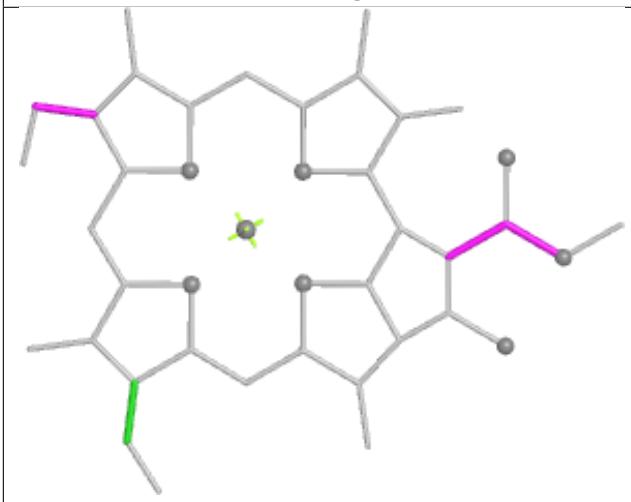


Bond angles



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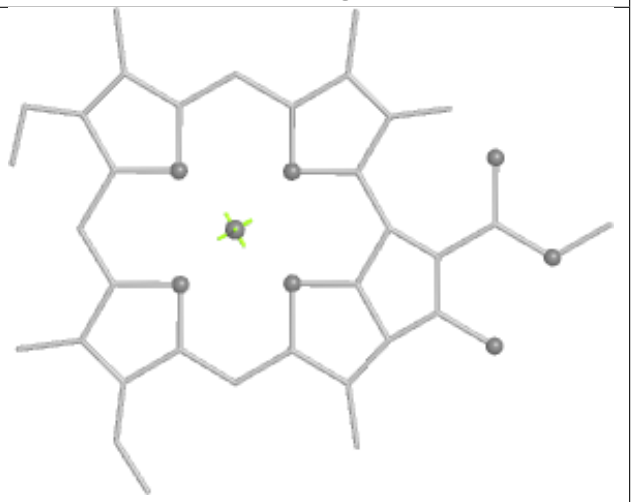
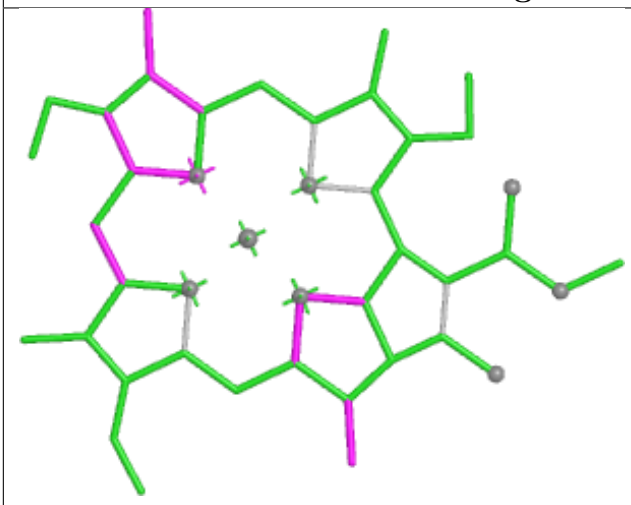


Rings

Ligand CLA 2N 311



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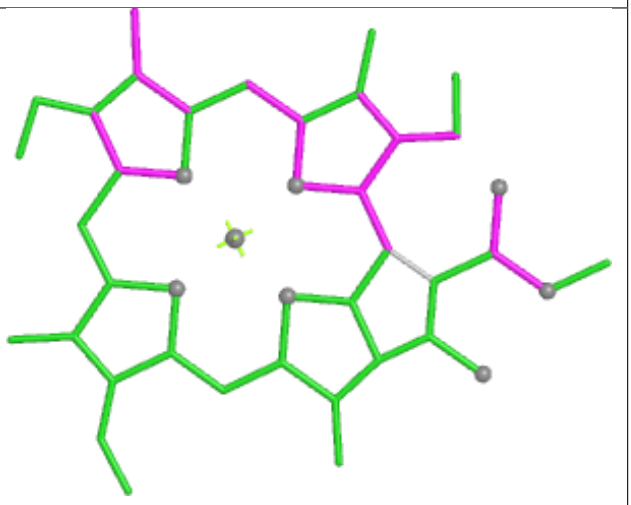
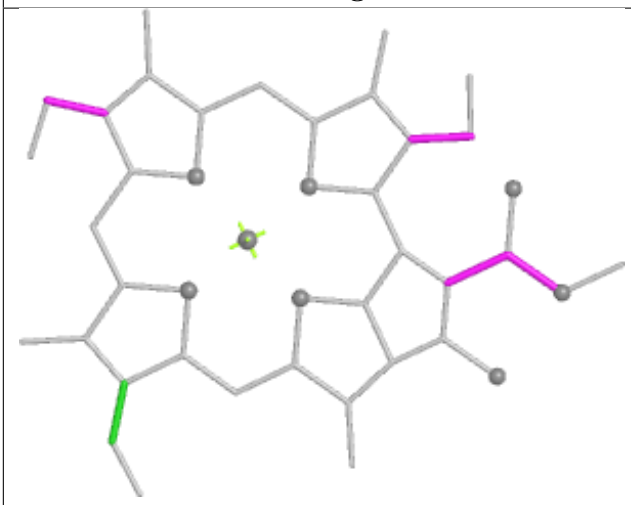


Bond angles

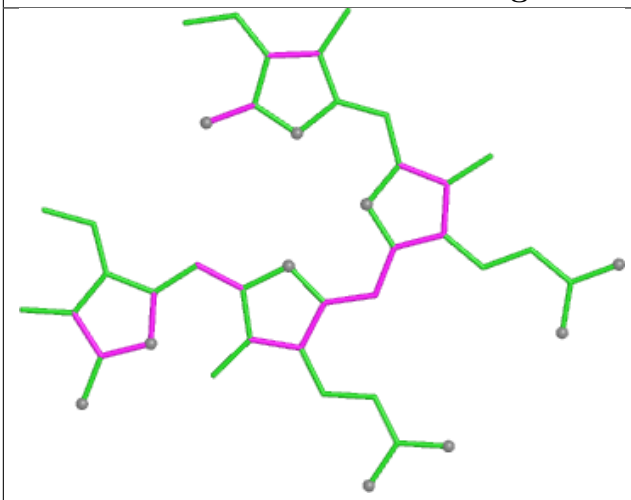


Torsions



Rings

Ligand PEB hM 201



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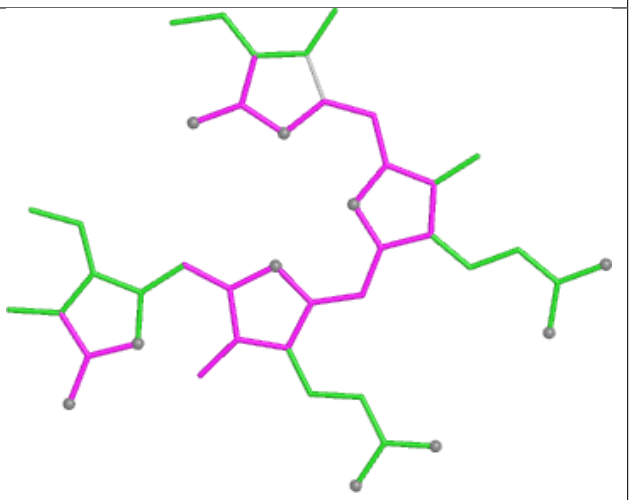
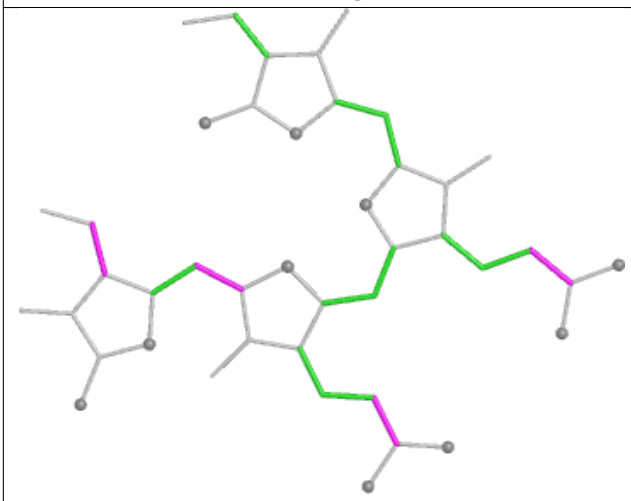


Bond angles



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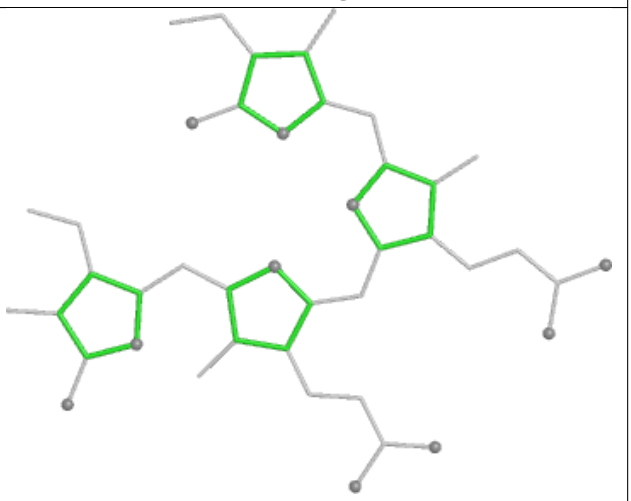
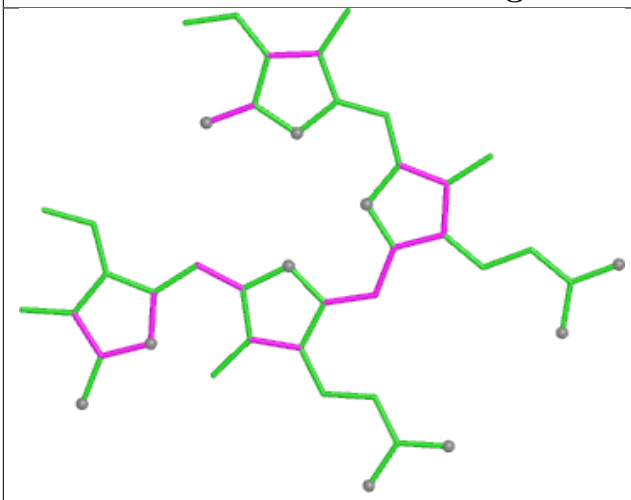


Rings

Ligand PEB D4 1002



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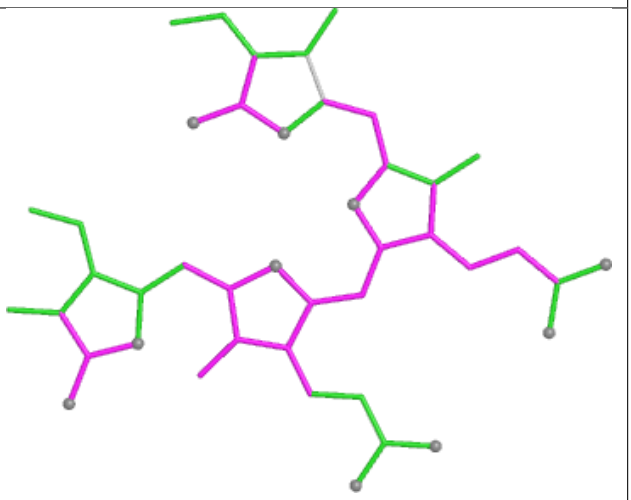
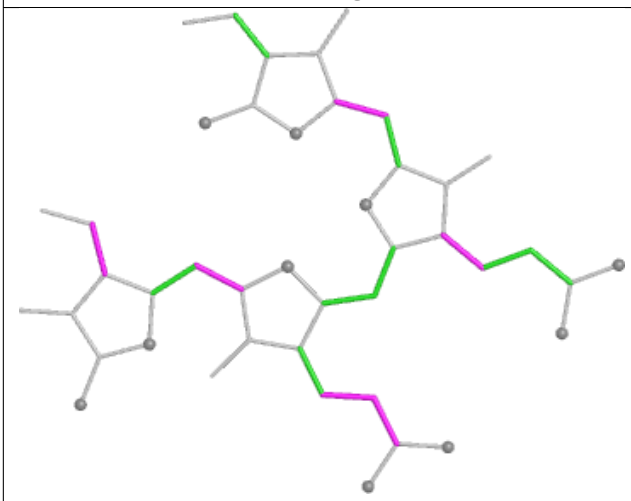


Bond angles



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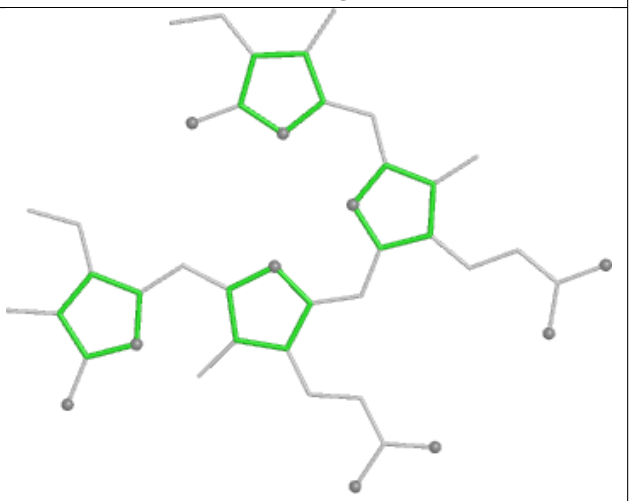
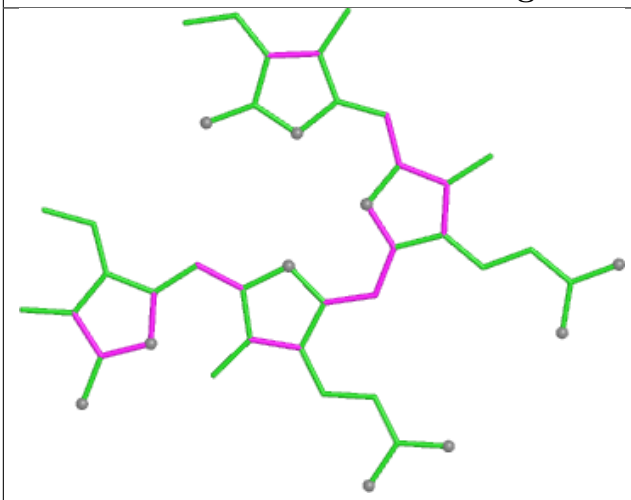


Rings

Ligand PEB FJ 201



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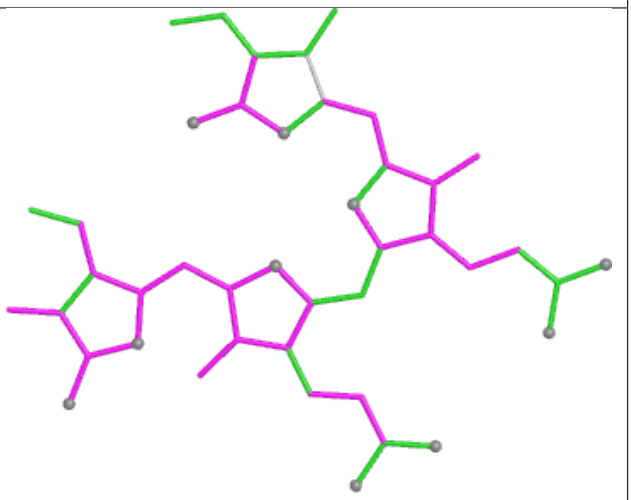

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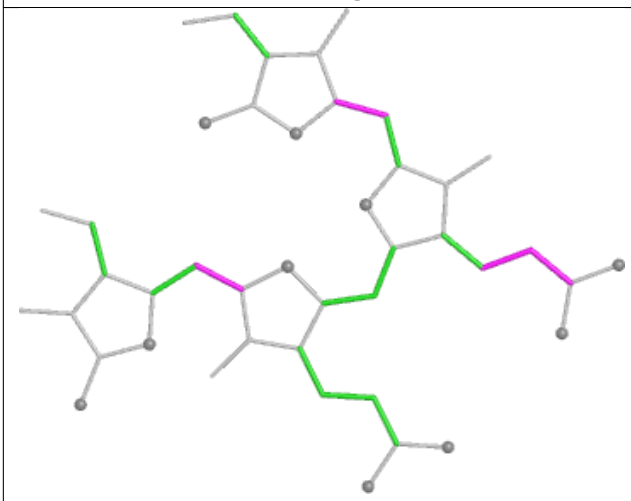

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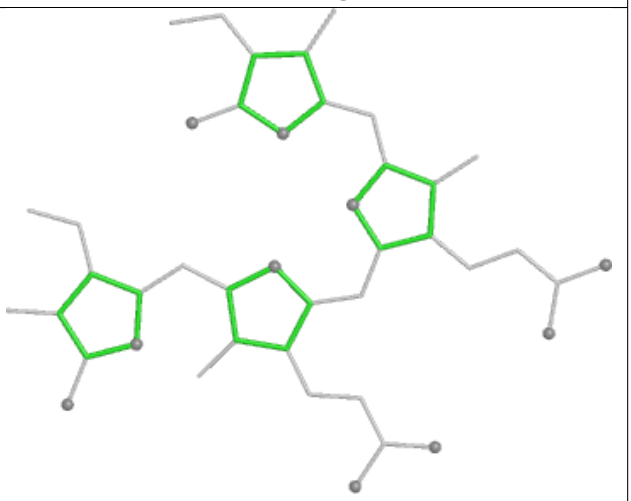
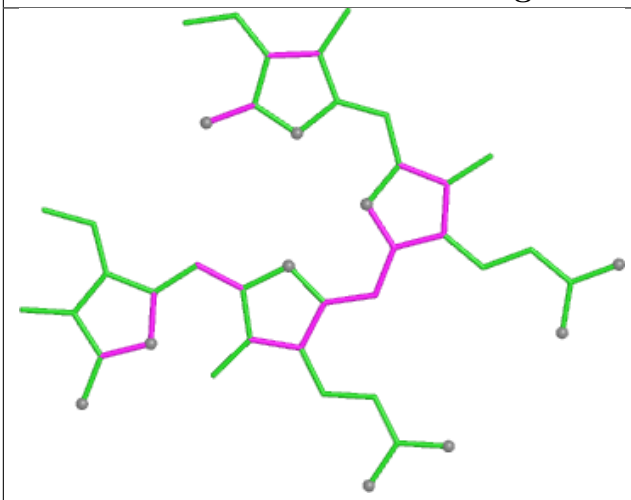


Rings

Ligand PEB kH 201



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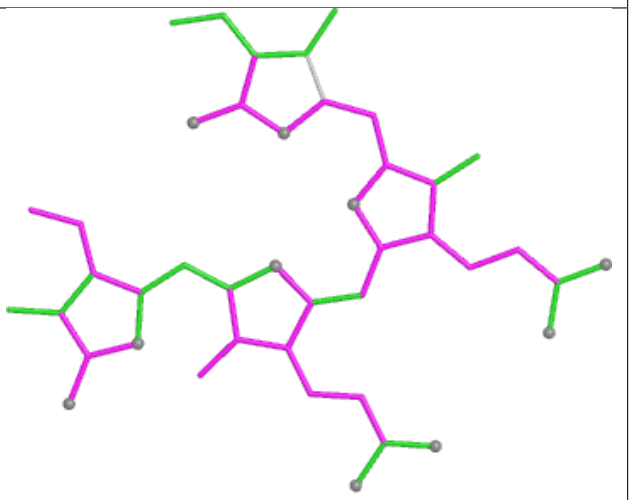

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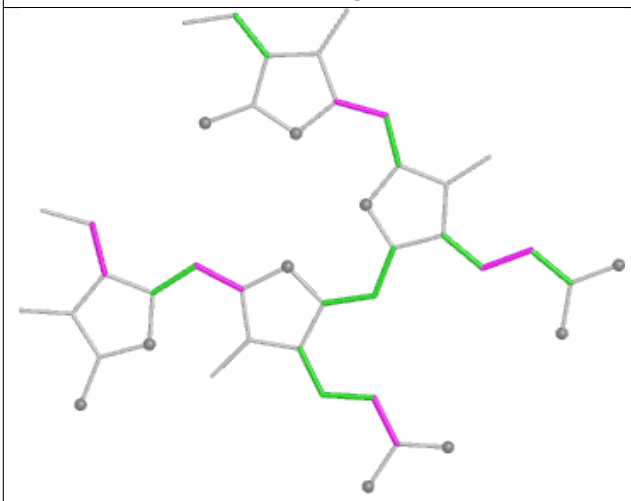

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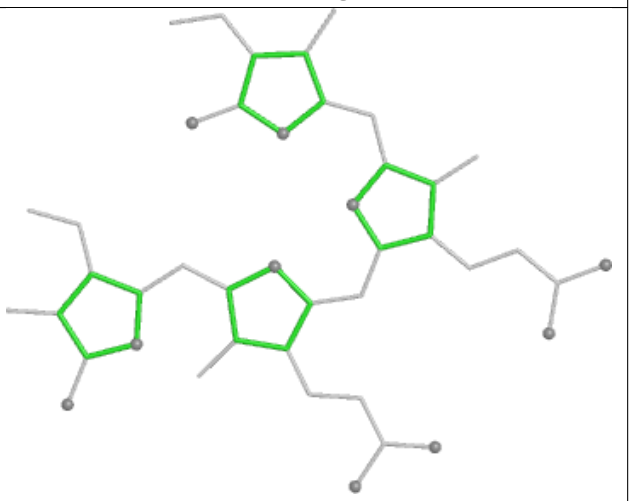
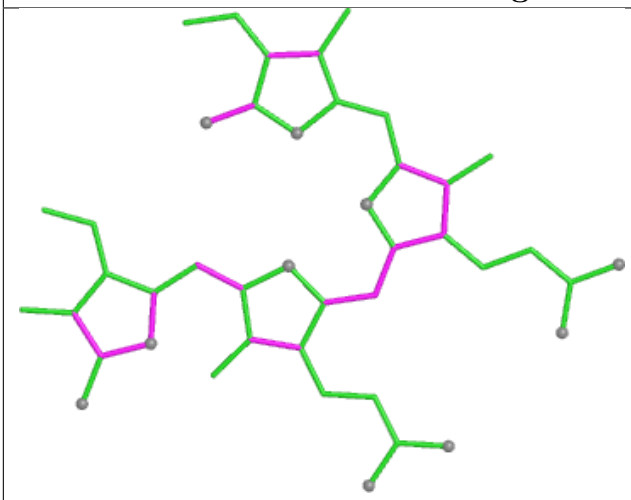


Rings

Ligand PEB AO 305



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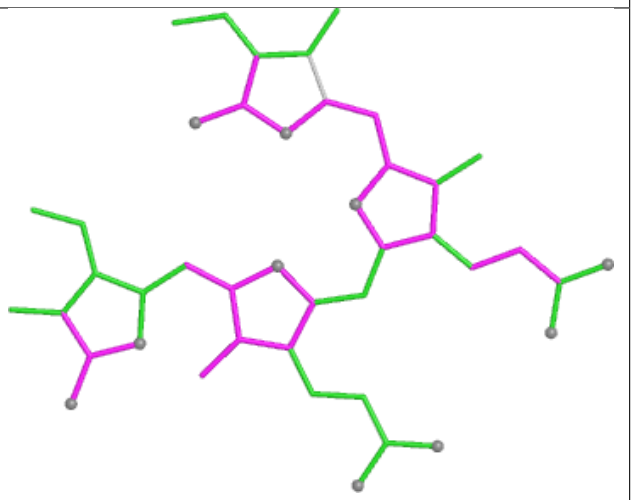

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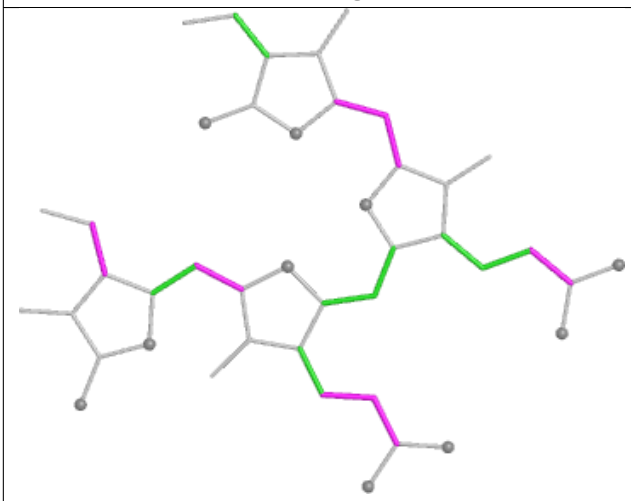

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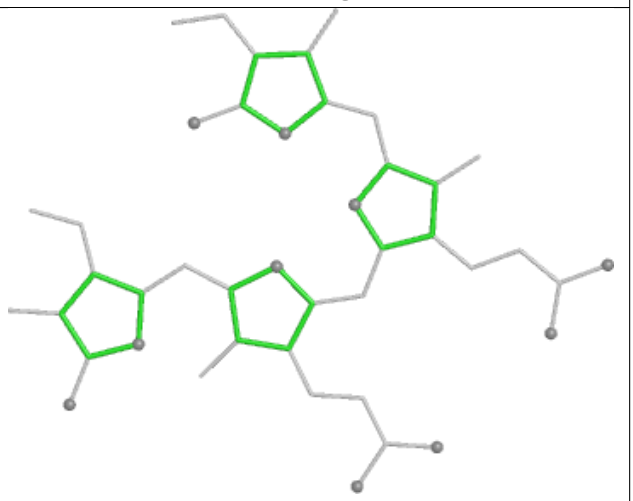
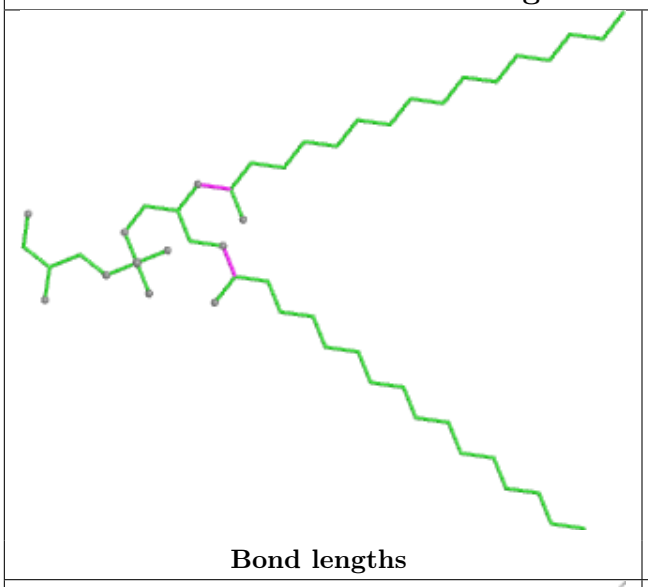


Rings

Ligand LHG i6 101



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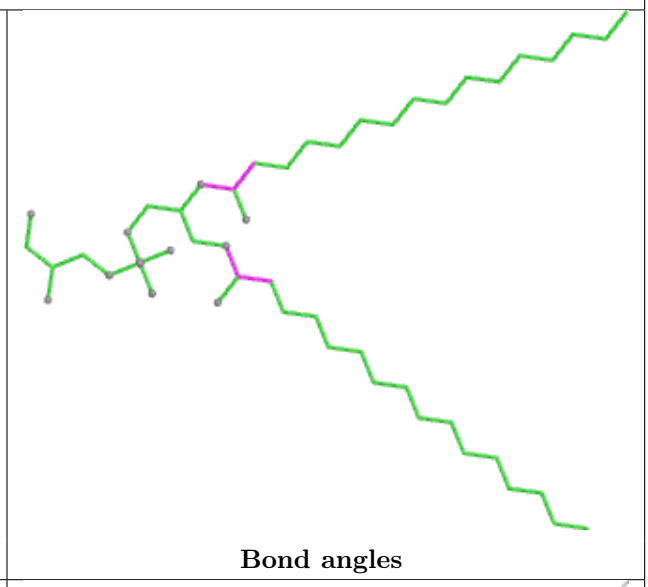

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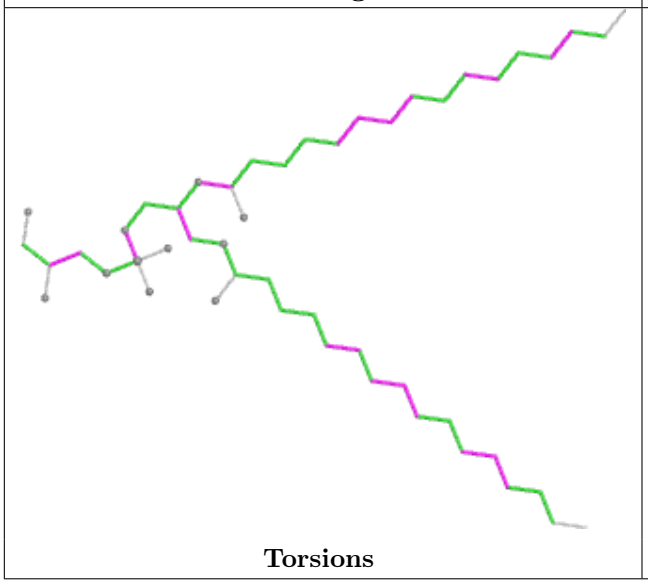

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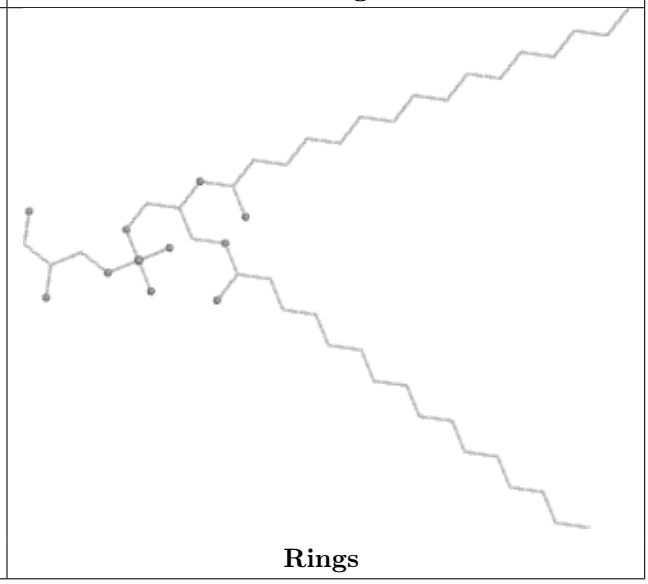
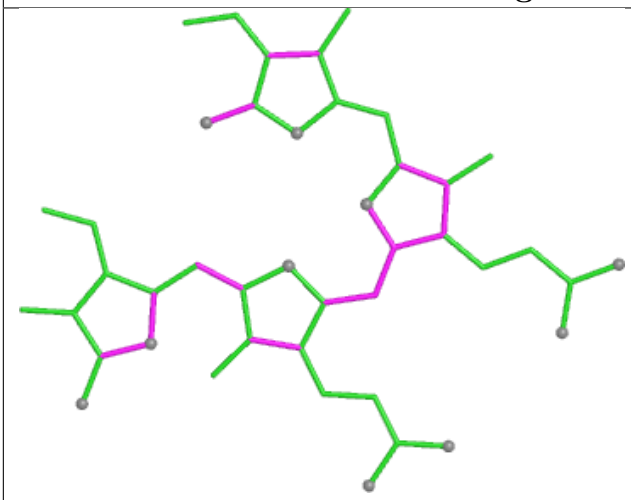


Rings

Ligand PEB Y5 203



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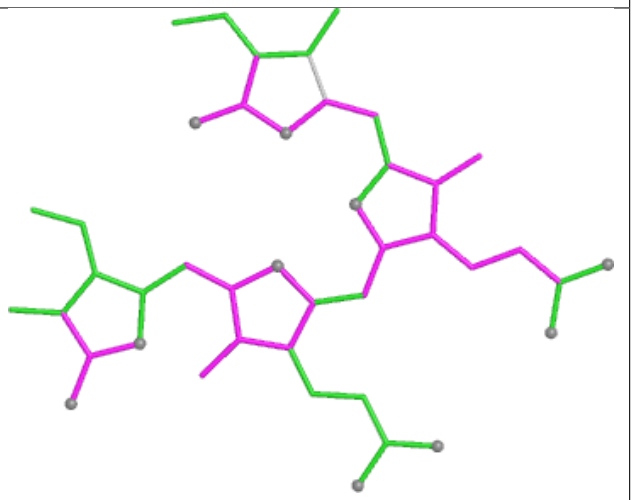

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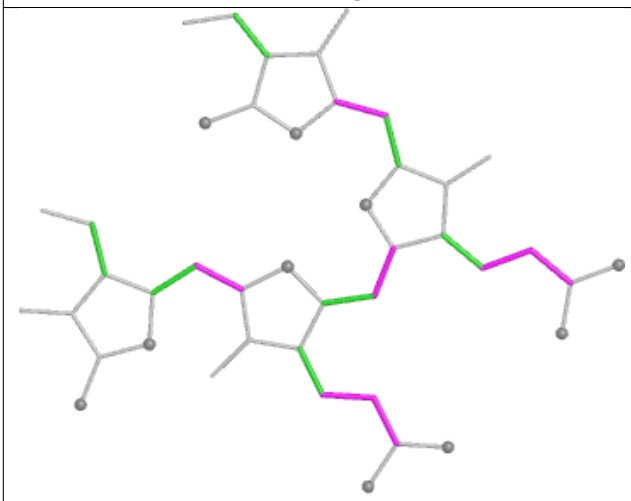

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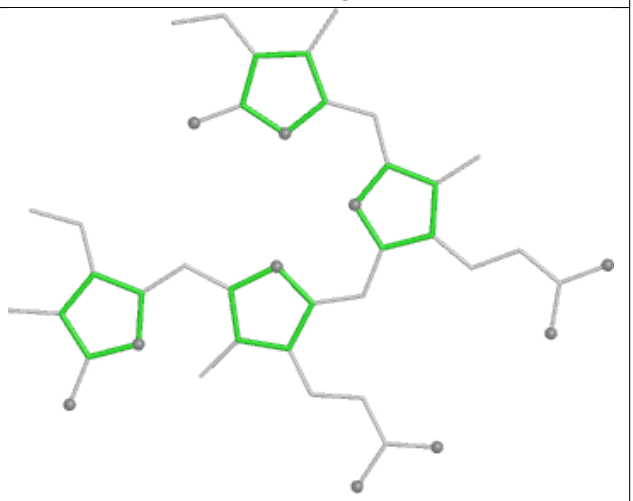
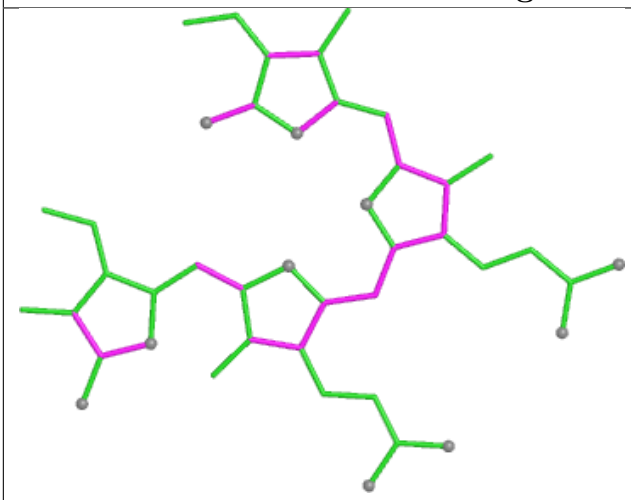


Rings

Ligand PEB uF 201



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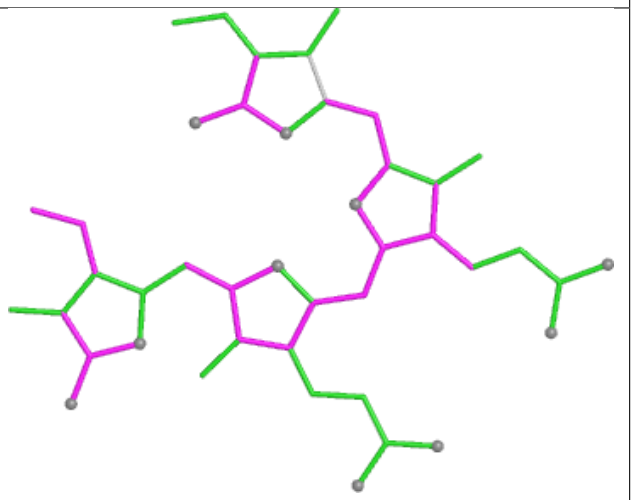

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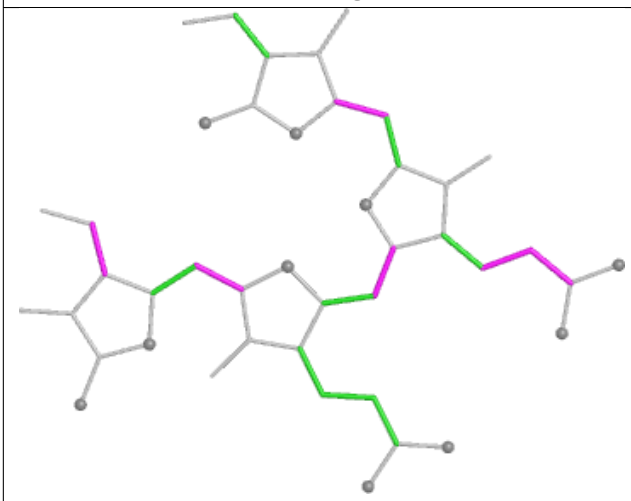

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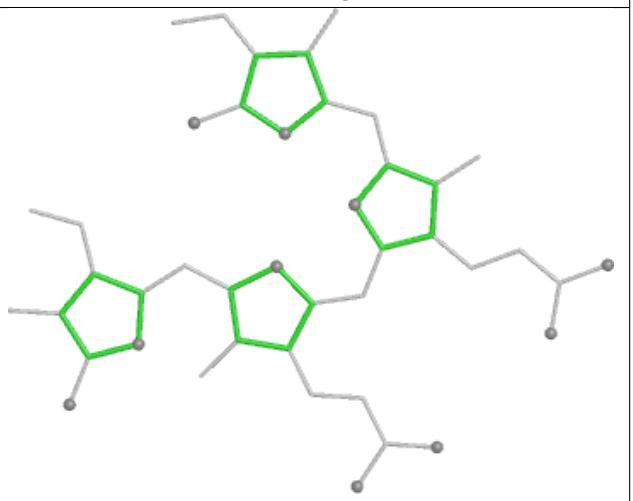
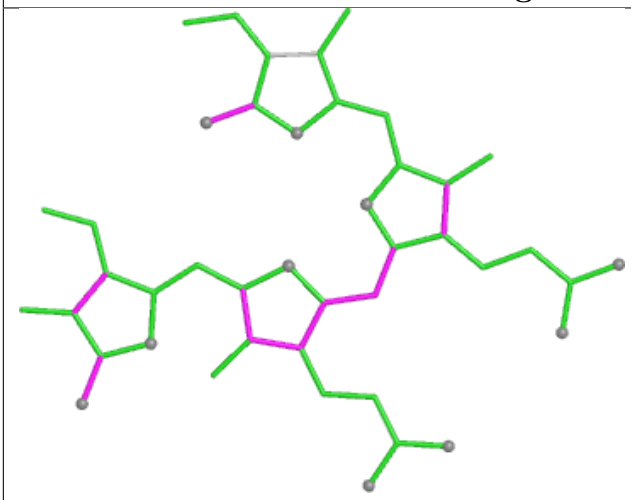


Rings

Ligand PUB xF 305



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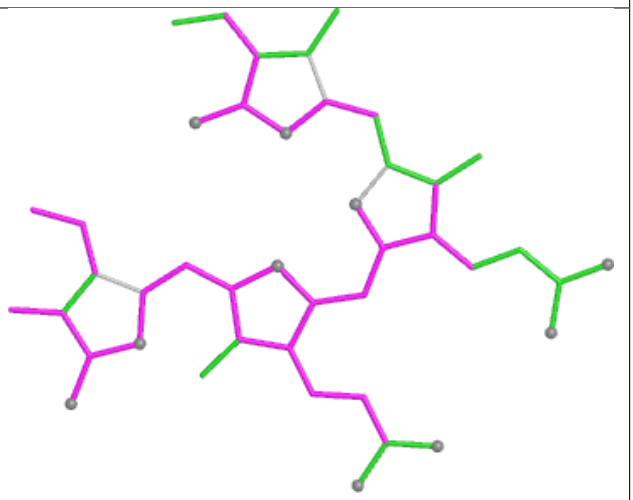

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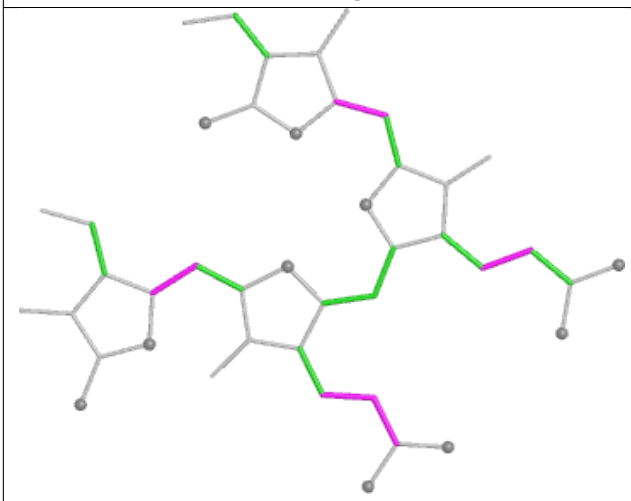

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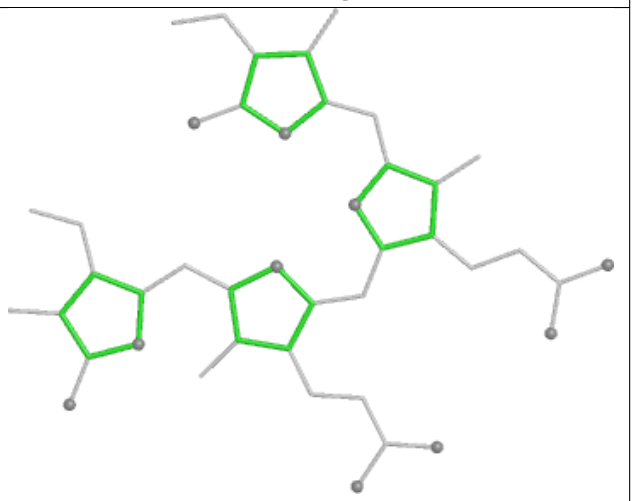
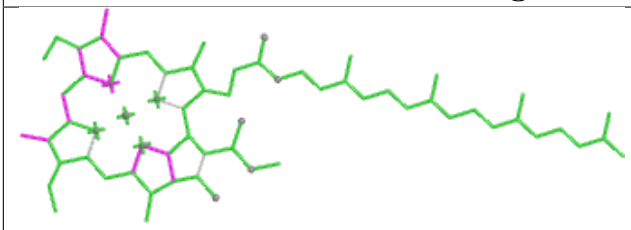


Rings

Ligand CLA AN 810



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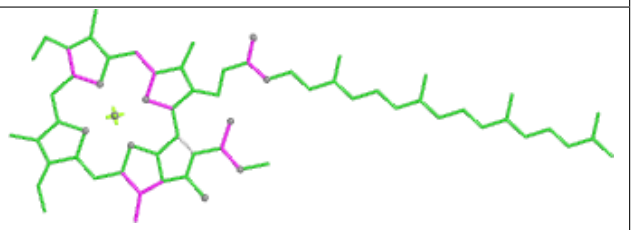

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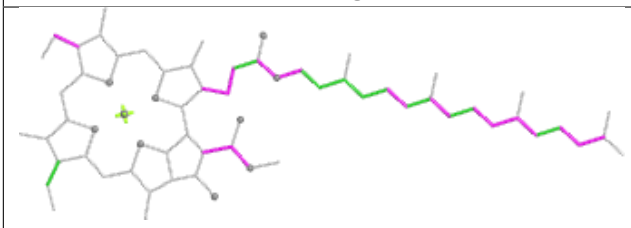

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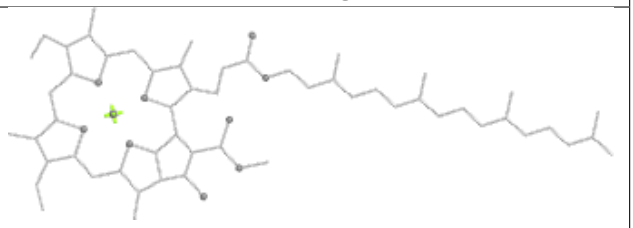
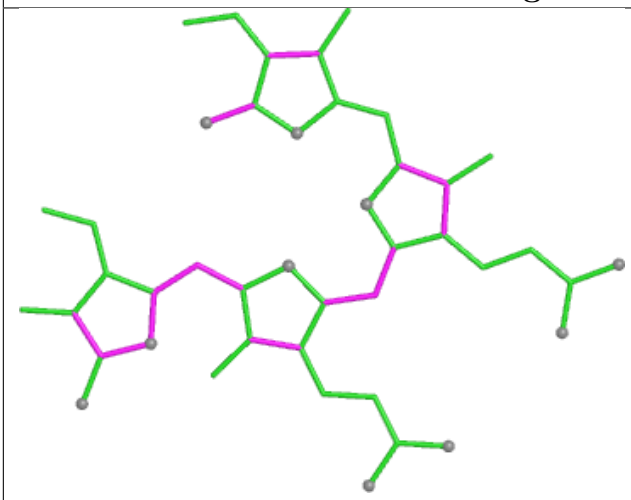


Rings

Ligand PEB f4 201



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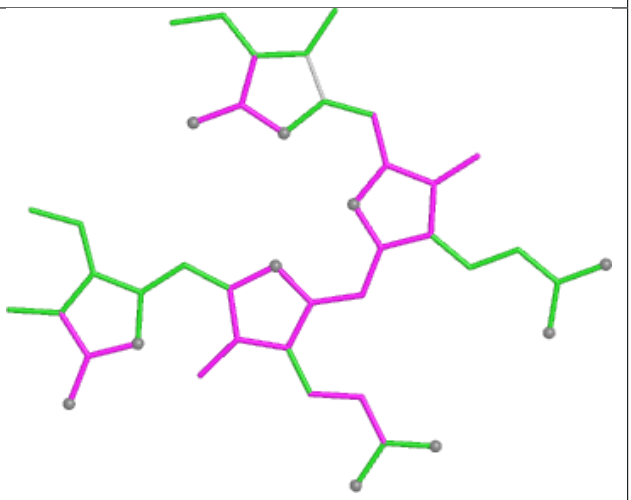

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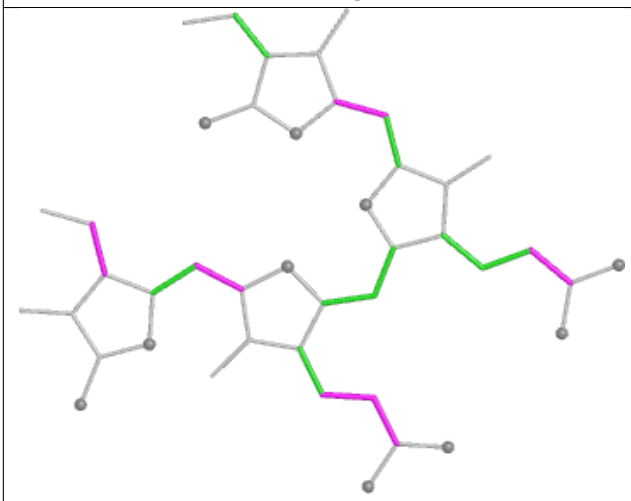

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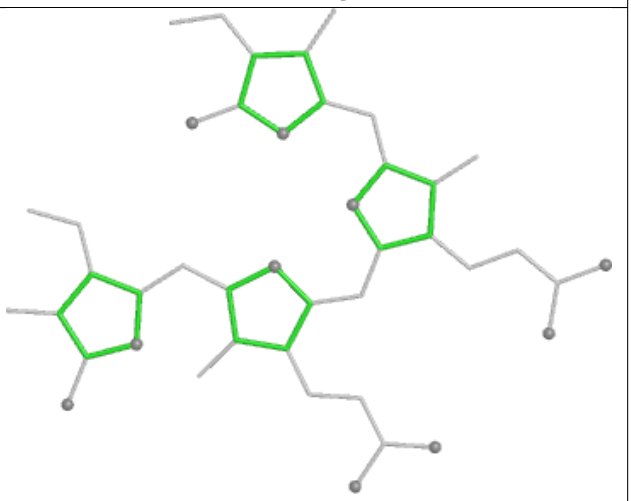
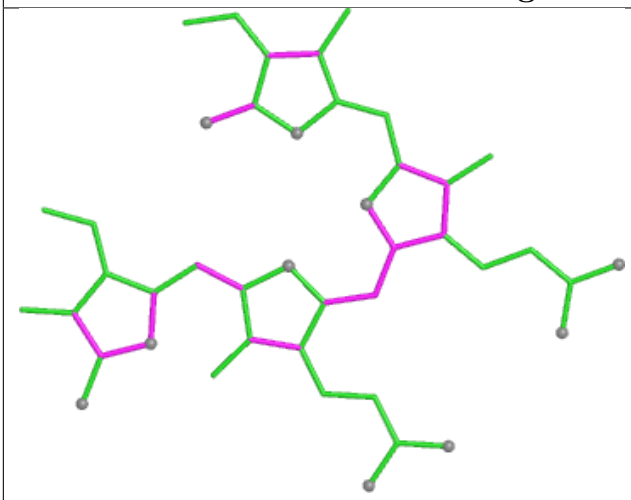


Rings

Ligand PEB RI 202



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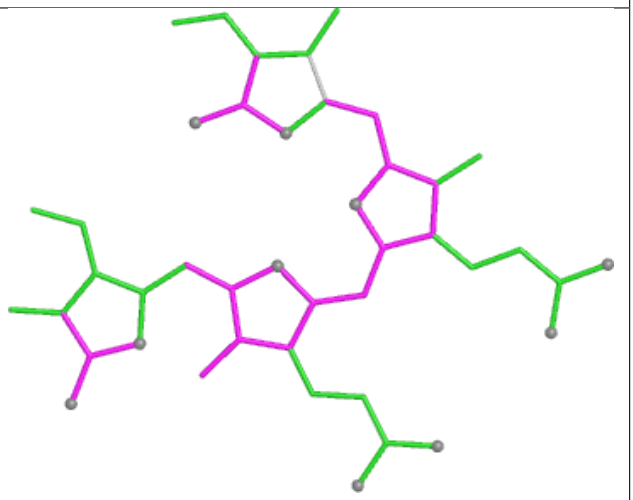

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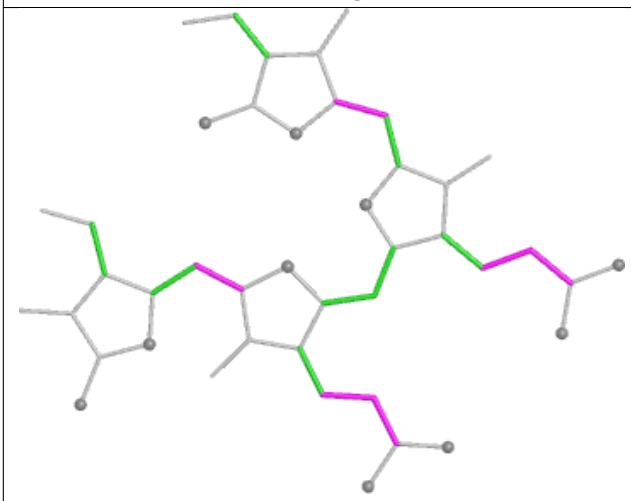

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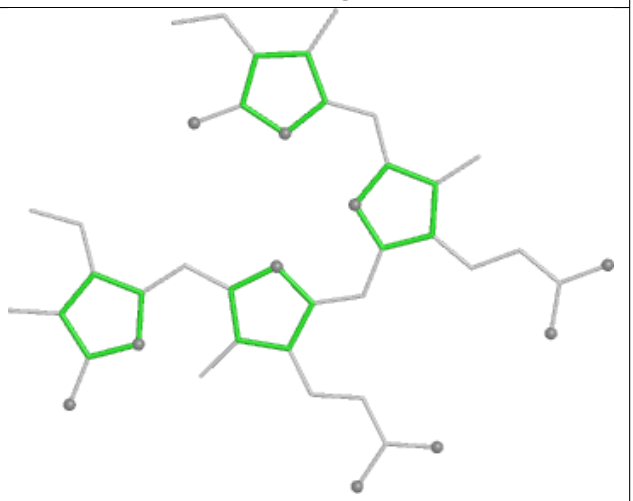

Rings

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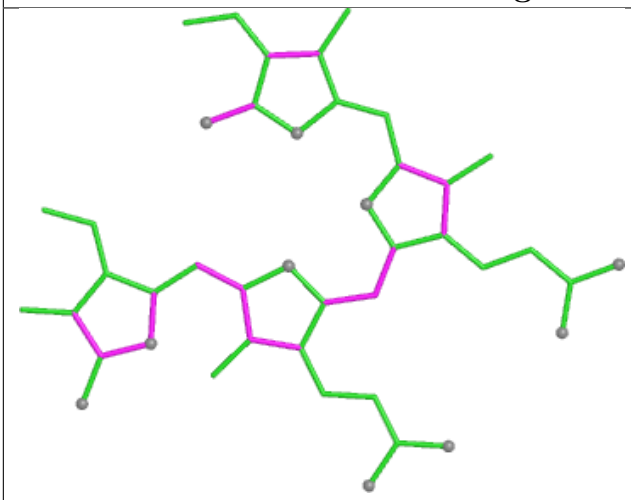

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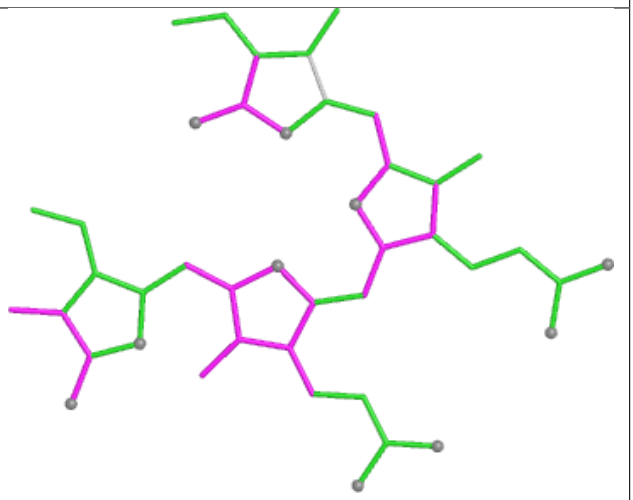

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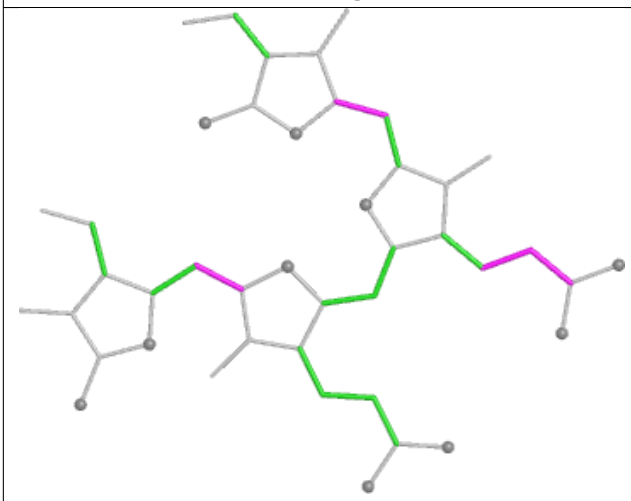

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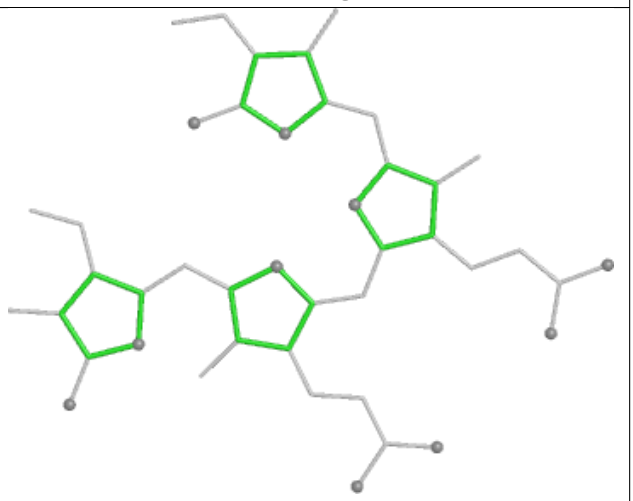
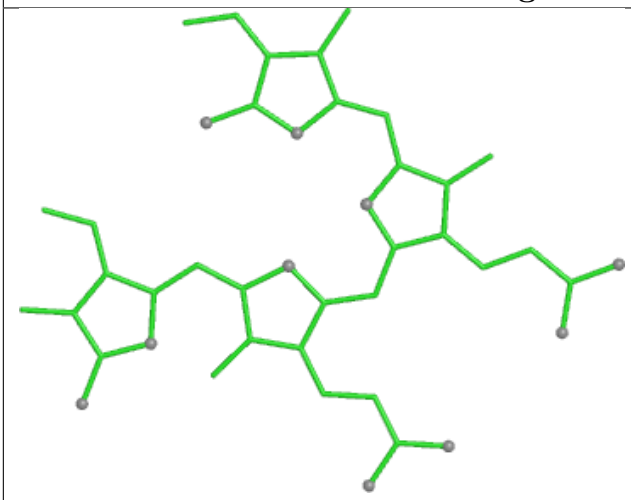


Rings

Ligand PEB cF 202



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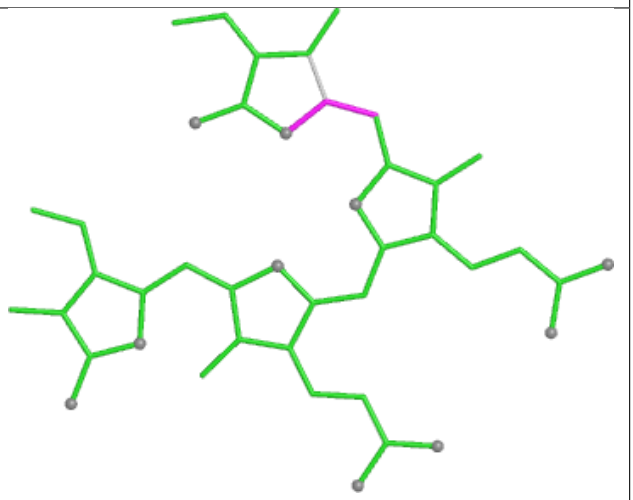

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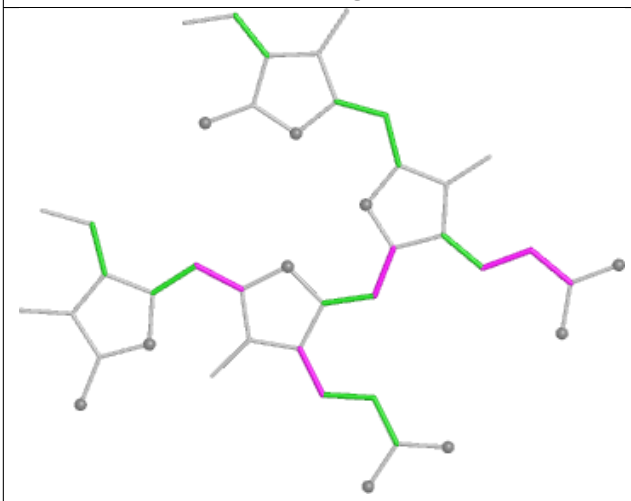

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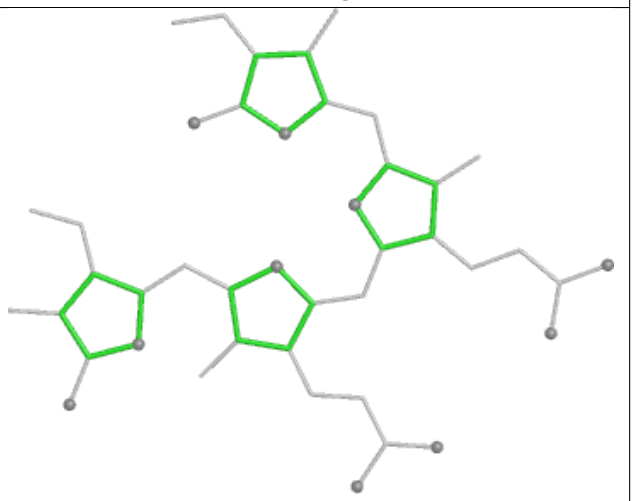
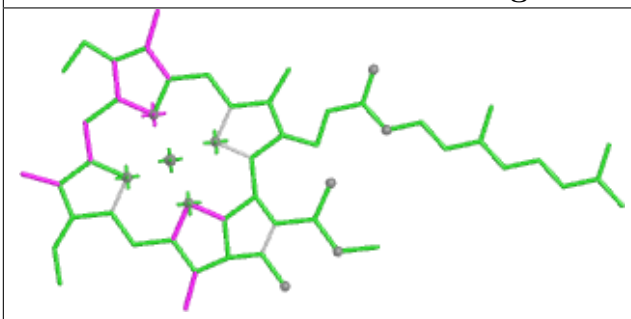
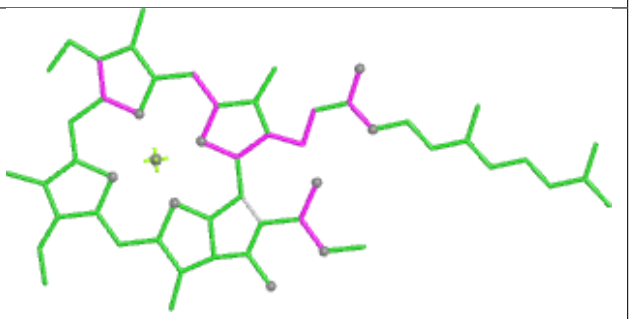


Rings

Ligand CLA BN 822	
	
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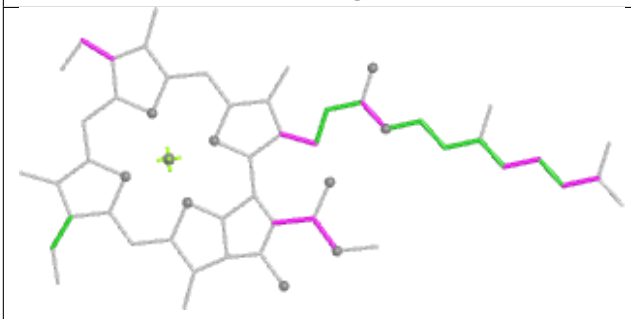
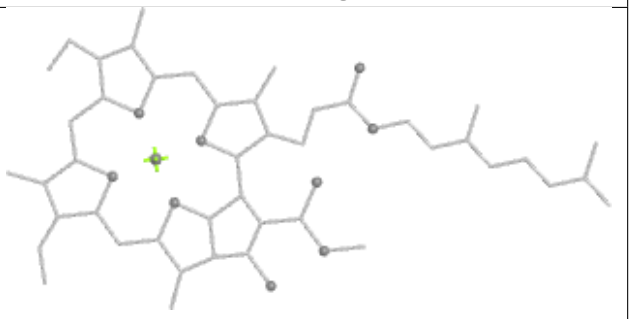
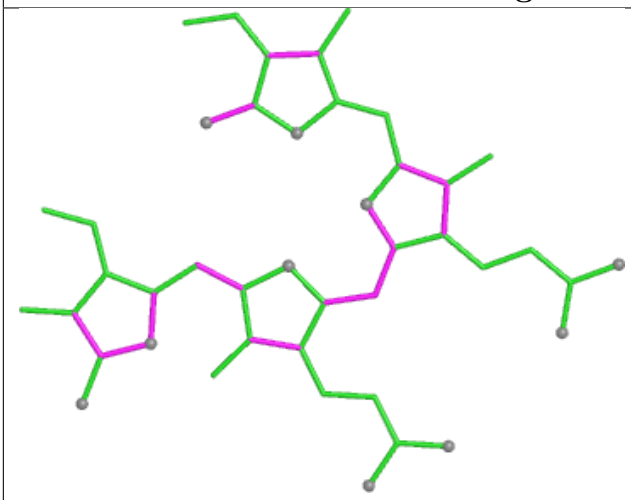
	
Torsions	**Rings**

Ligand PEB eK 202



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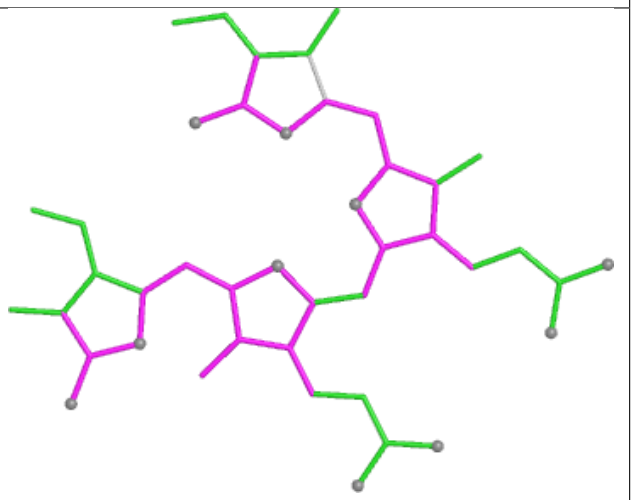
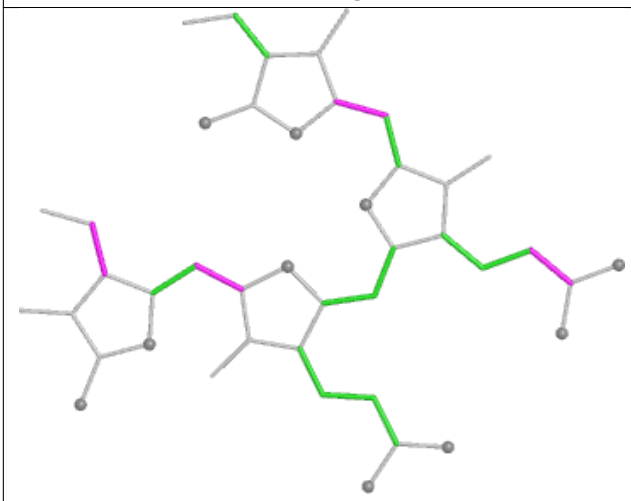


Bond angles



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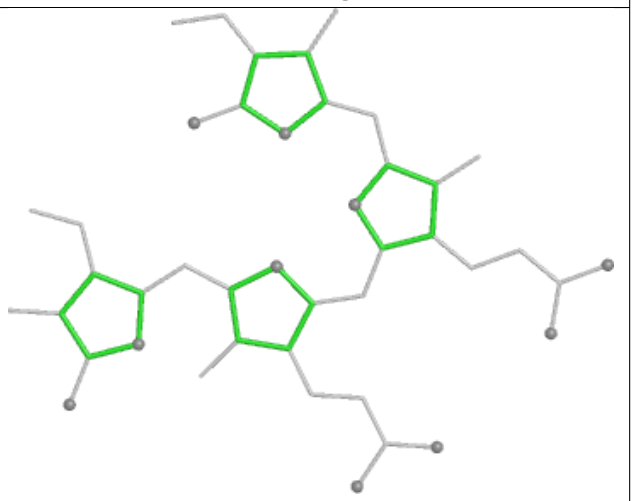
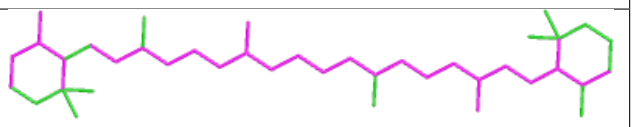


Rings

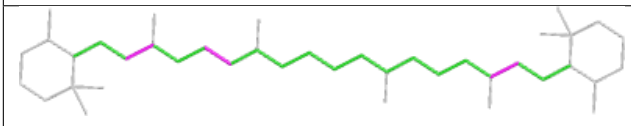
Ligand BCR BN 838



Bond lengths



Bond angles



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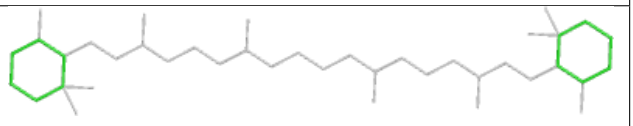
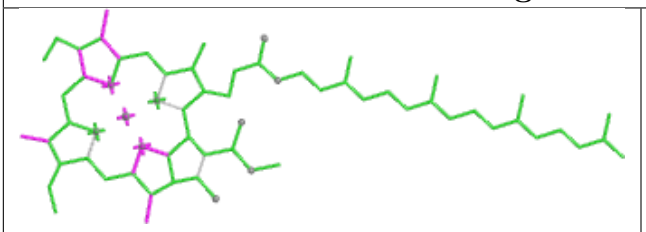


Rings

Ligand CLA A2 851



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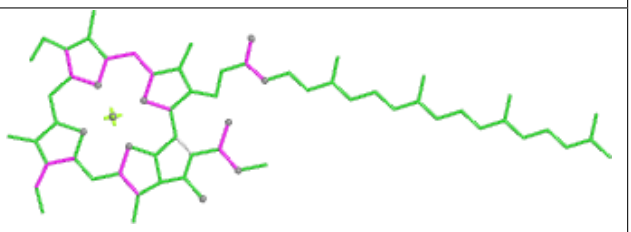

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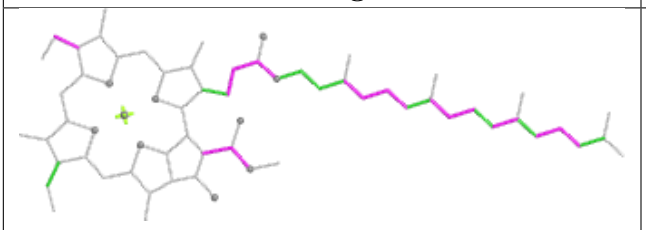

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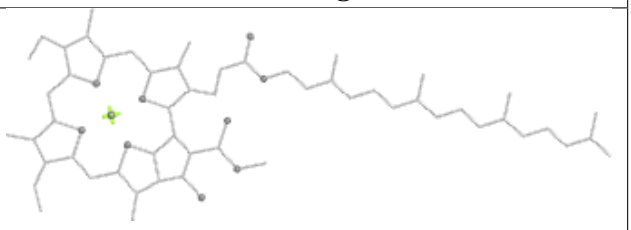
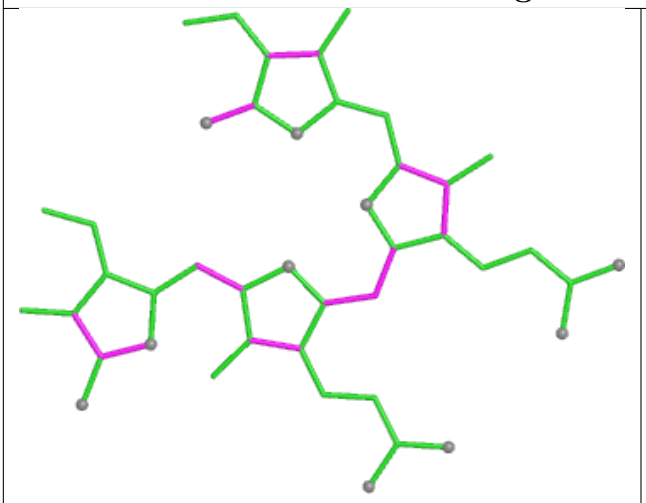


Rings

Ligand PEB N7 202



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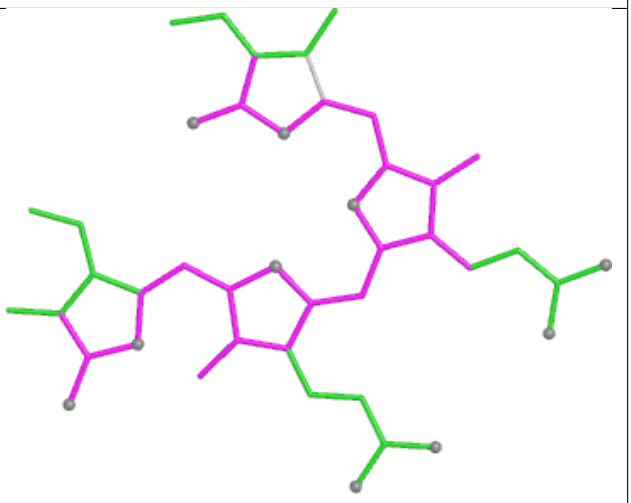

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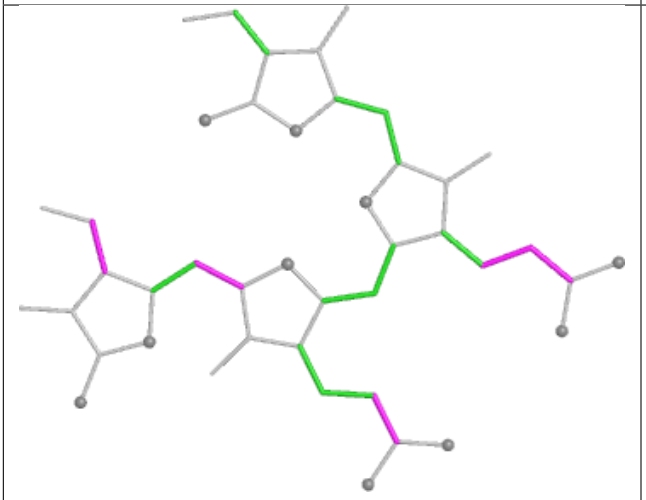

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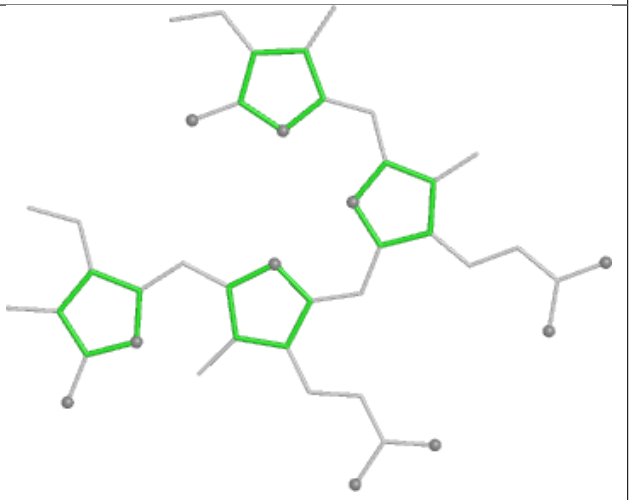
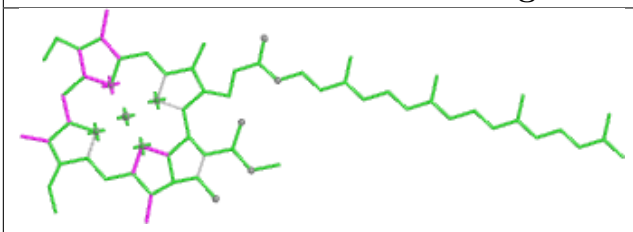


Rings

Ligand CLA b6 615



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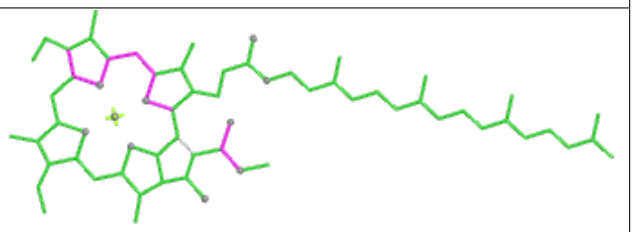

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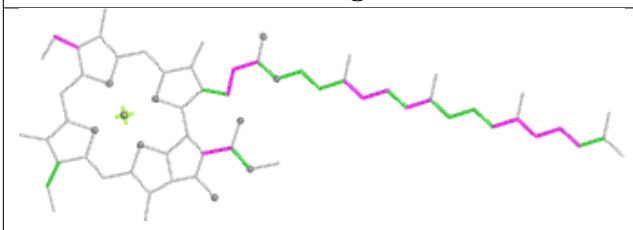

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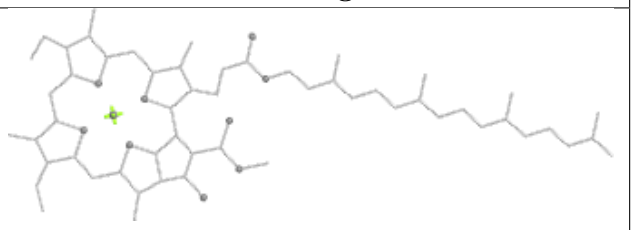
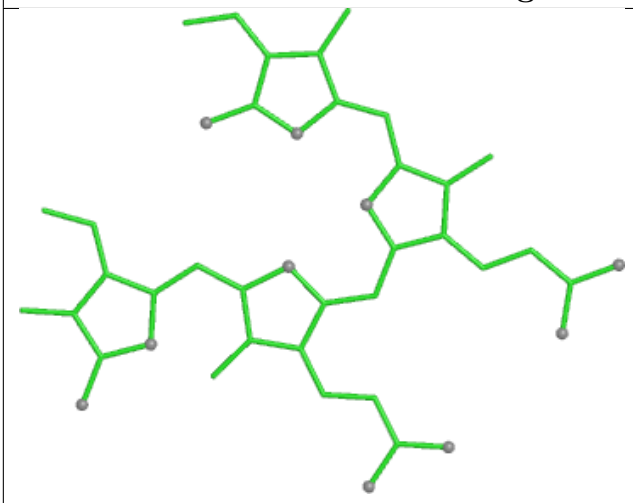


Rings

Ligand PEB IK 202



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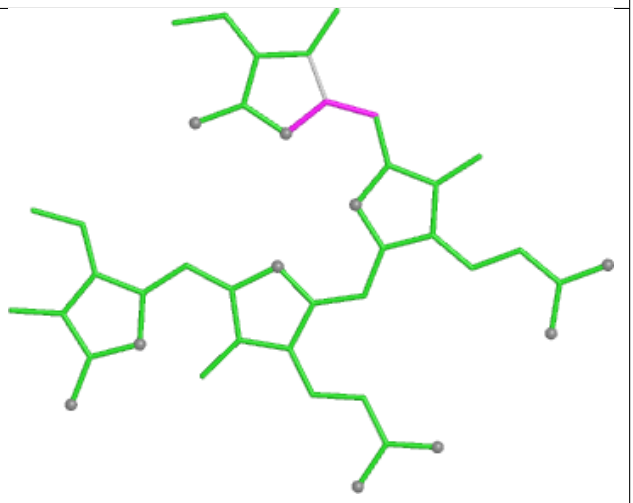

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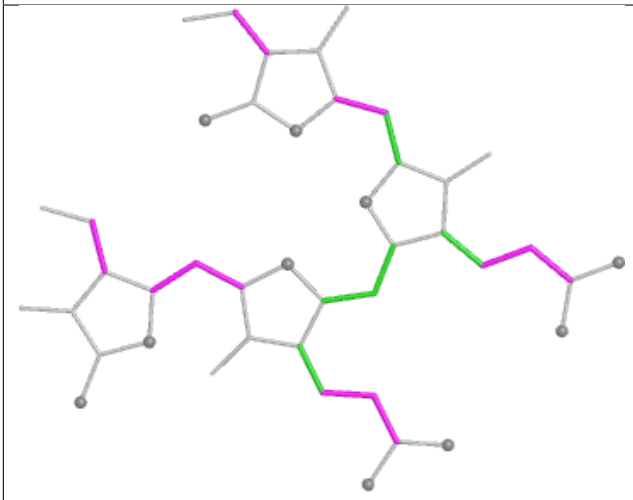

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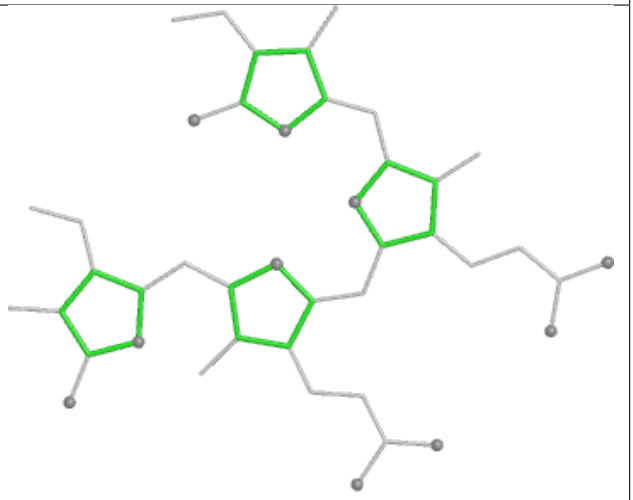
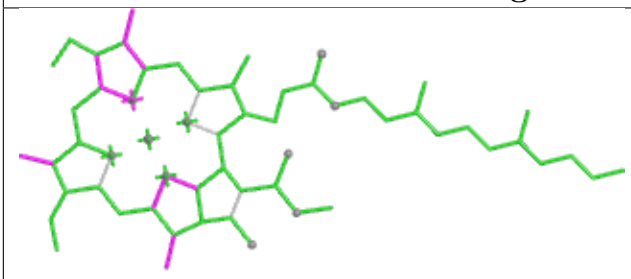


Rings

Ligand CLA BN 802



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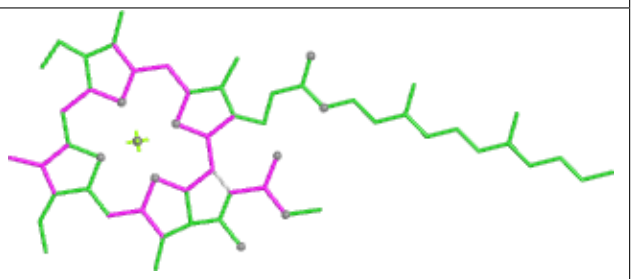

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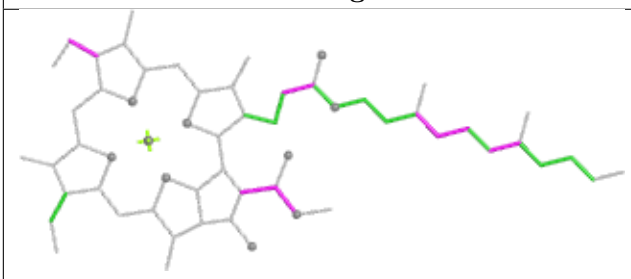

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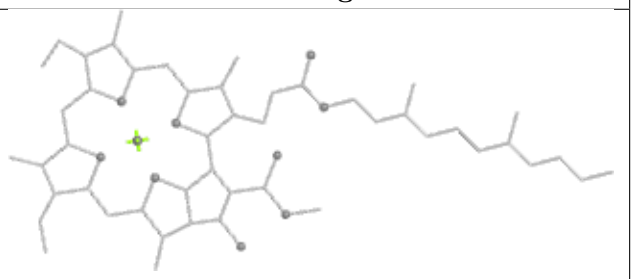
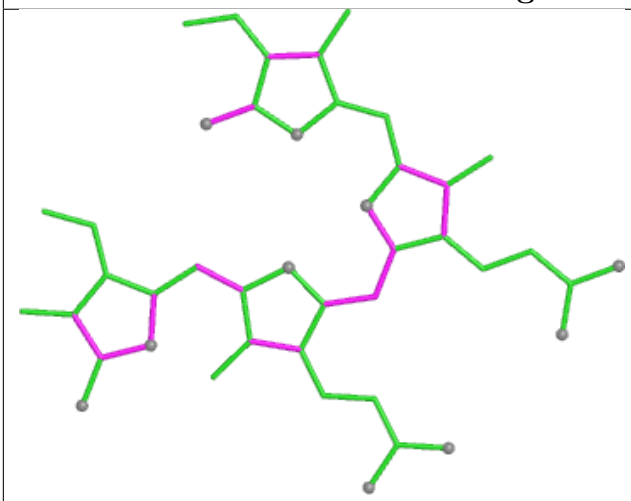


Rings

Ligand PEB HI 203



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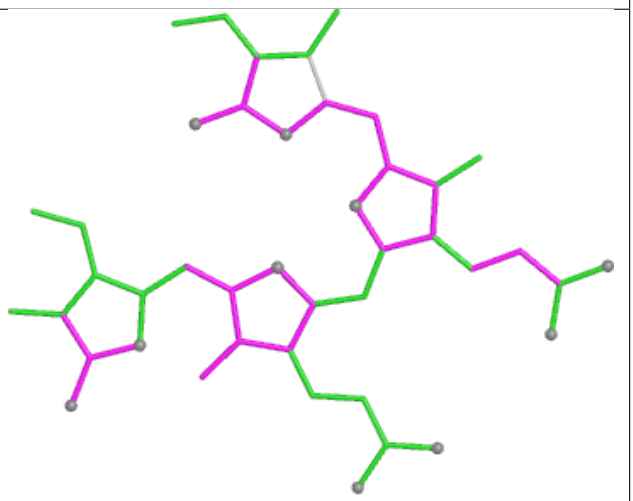

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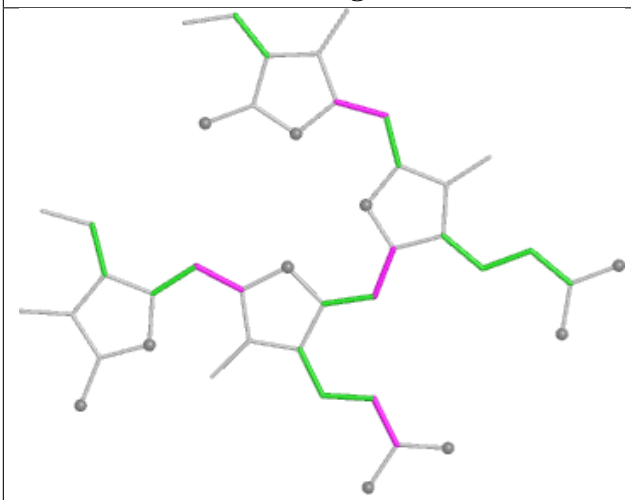

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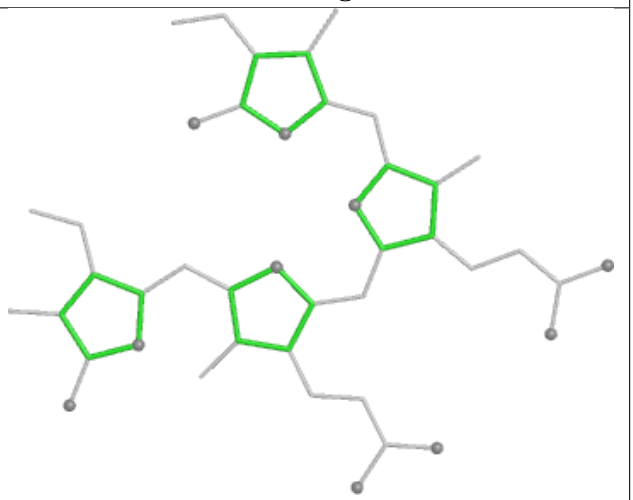

Rings

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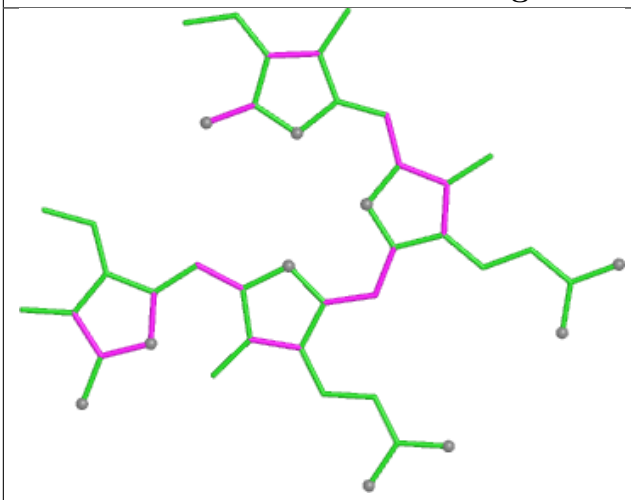

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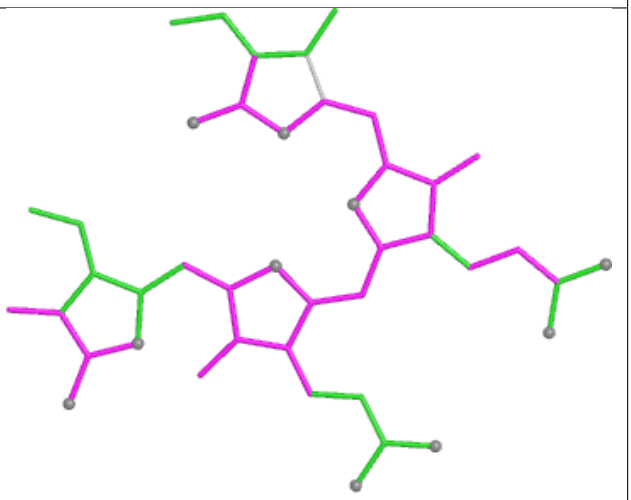

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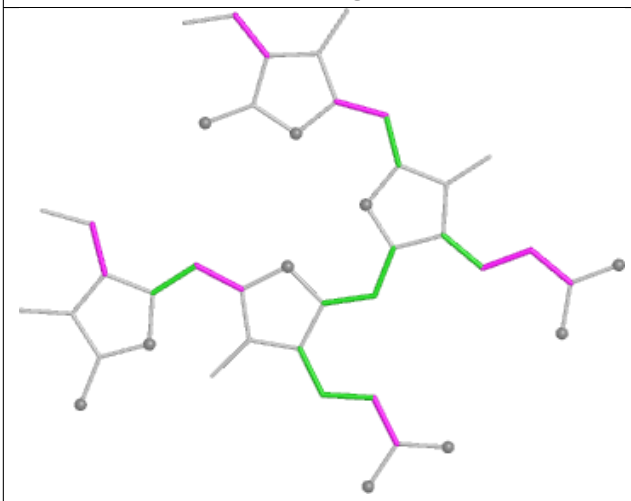

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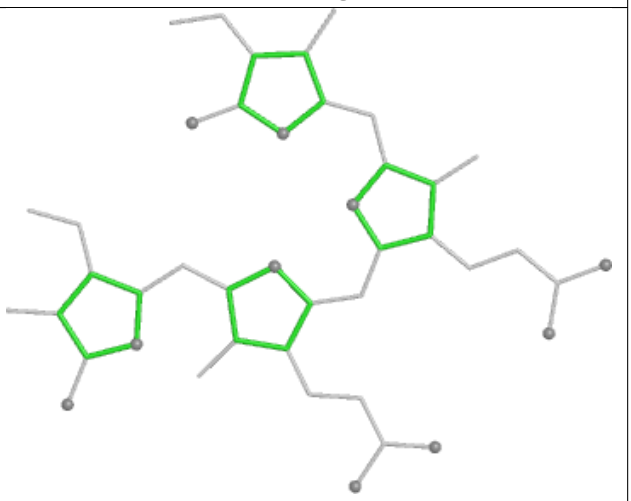
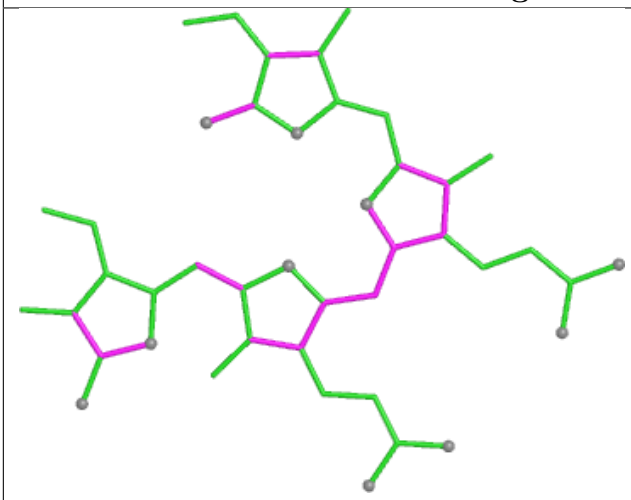


Rings

Ligand PEB AQ 304



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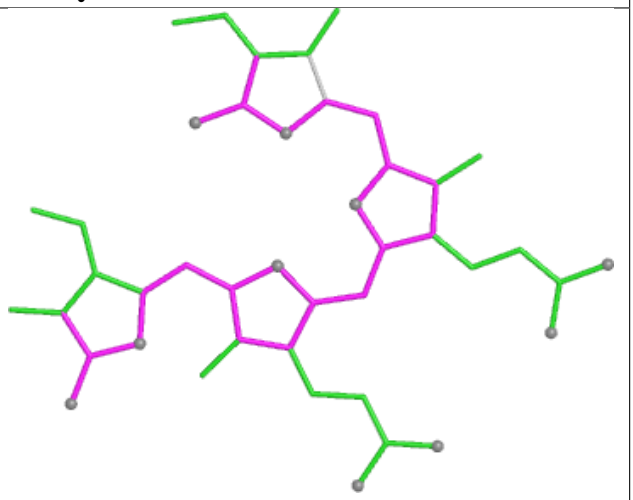

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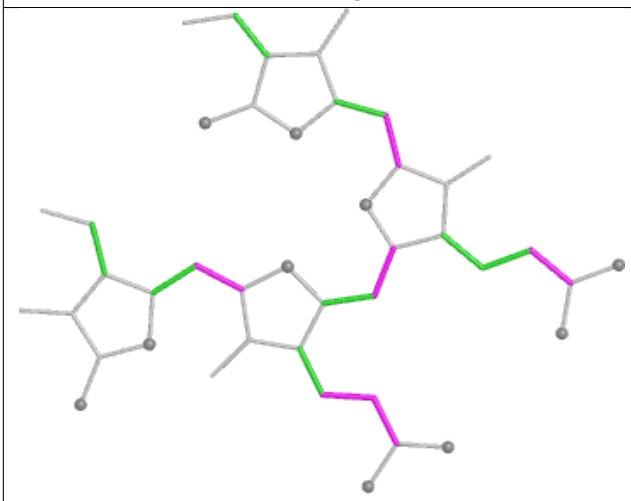

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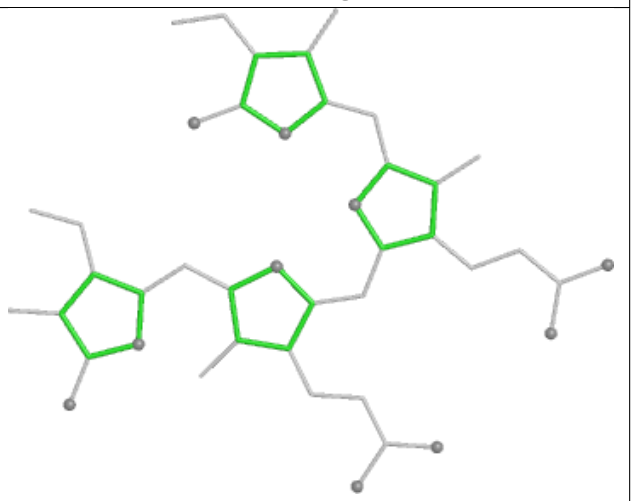
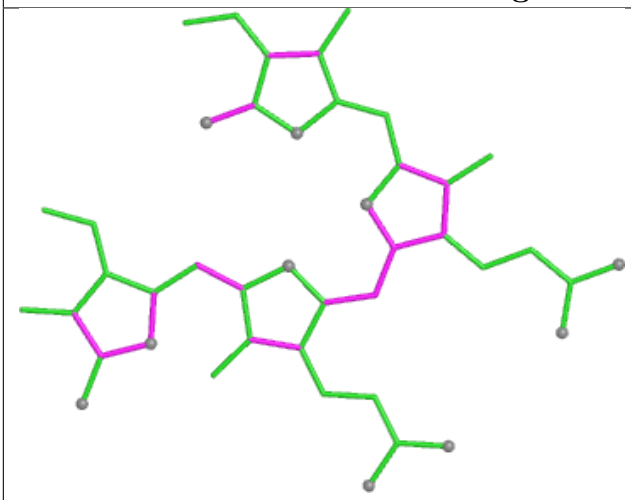


Rings

Ligand PEB VP 202



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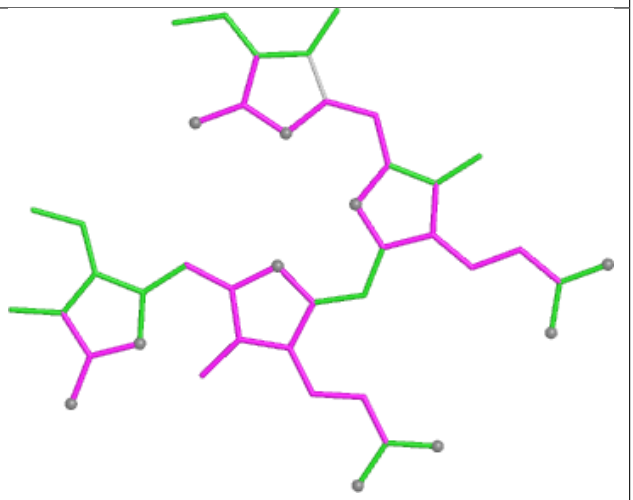

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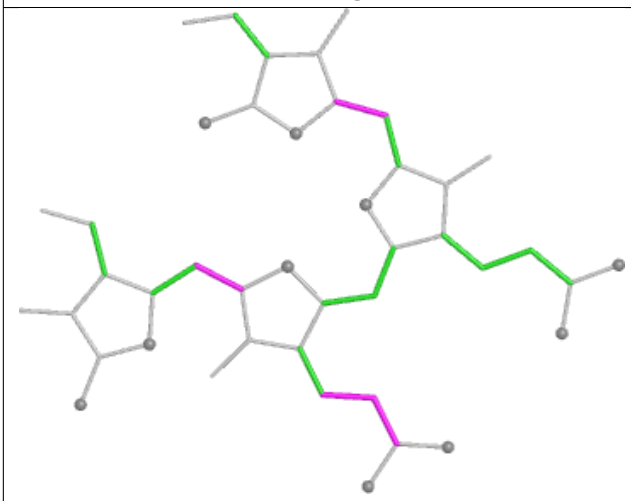

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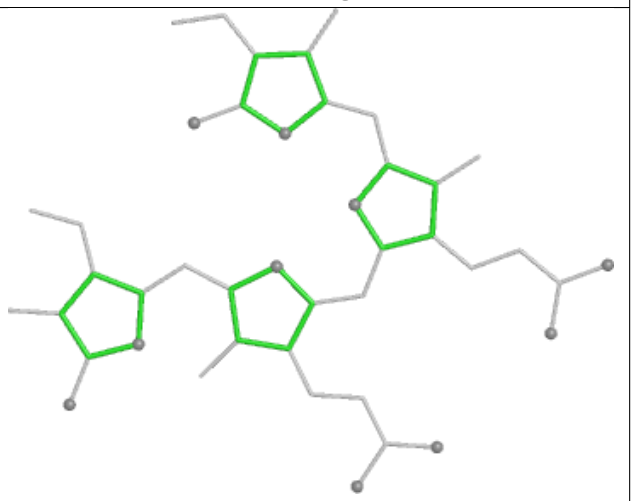
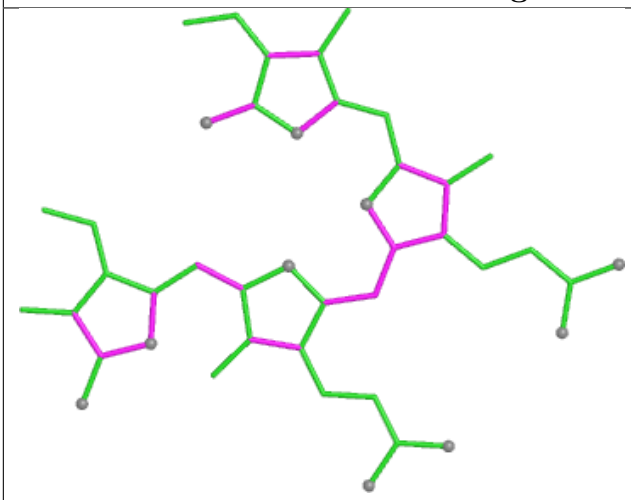


Rings

Ligand PEB AD 303



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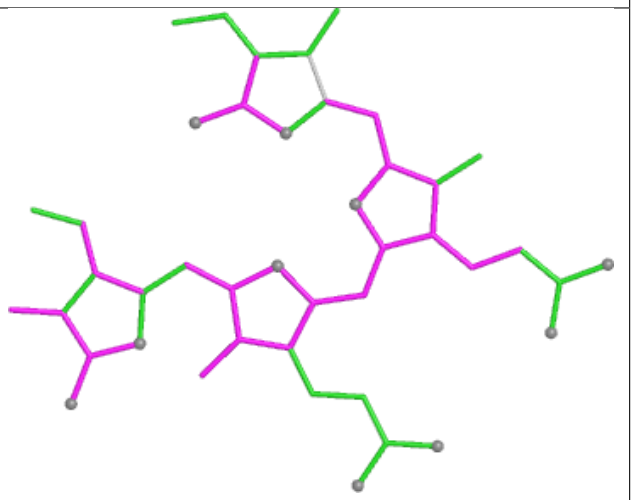

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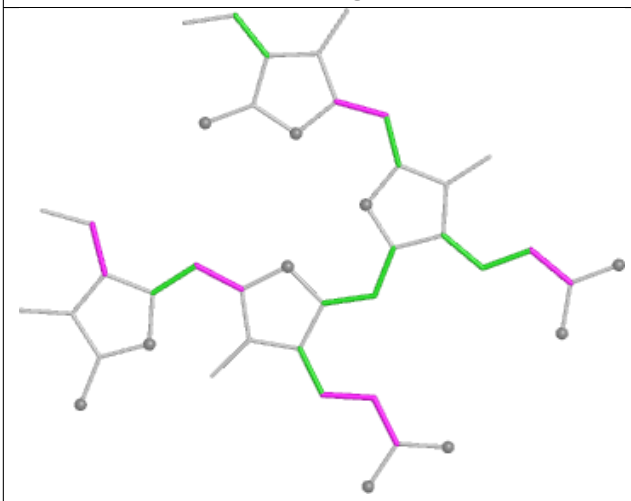

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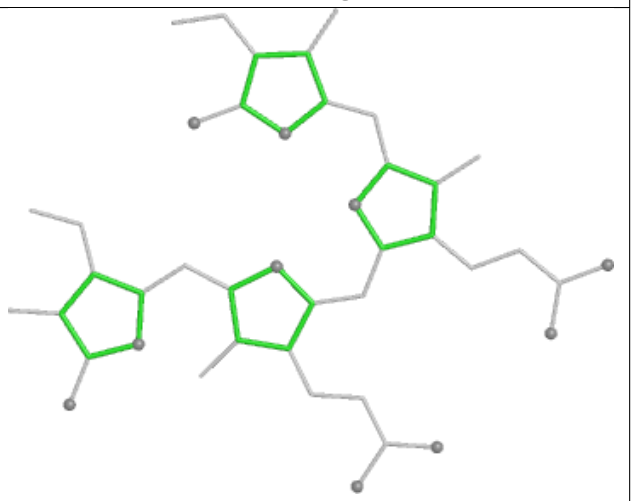
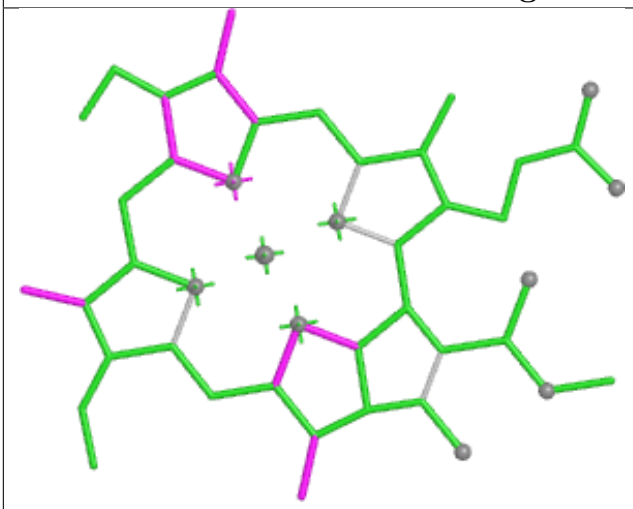


Rings

Ligand CLA 72 610



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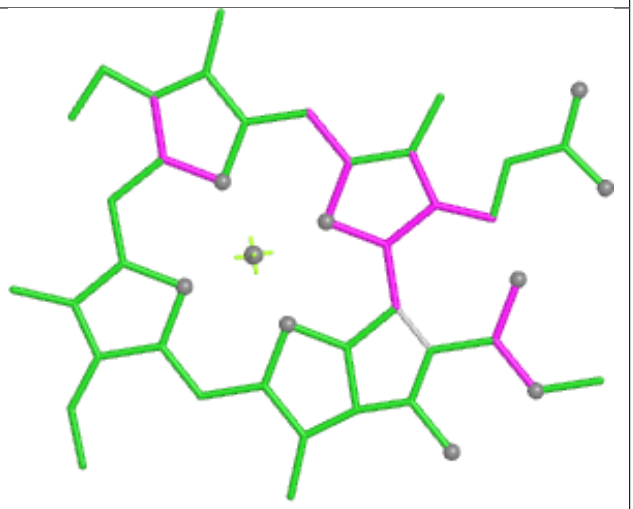

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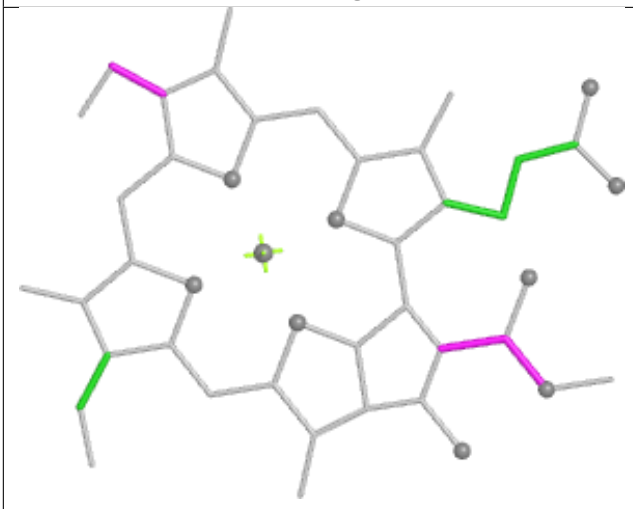
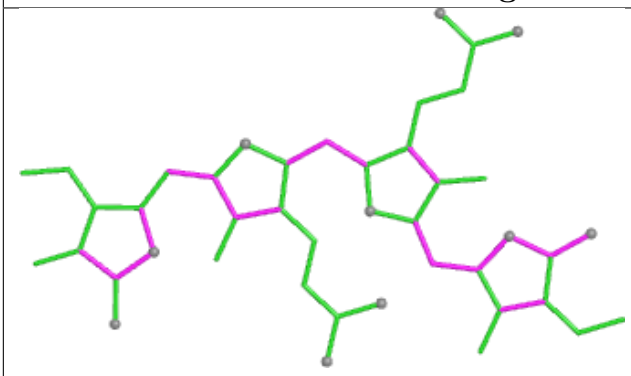


Torsions



Rings

Ligand CYC DO 1001



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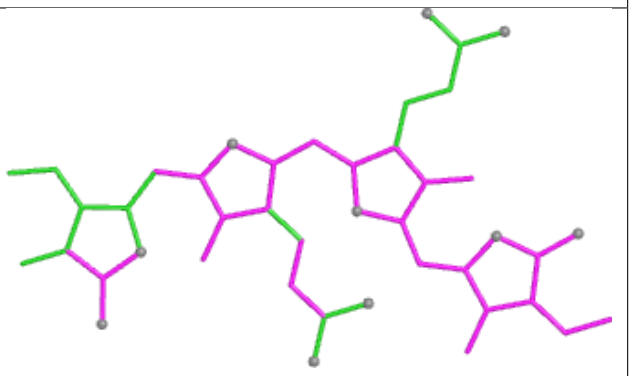

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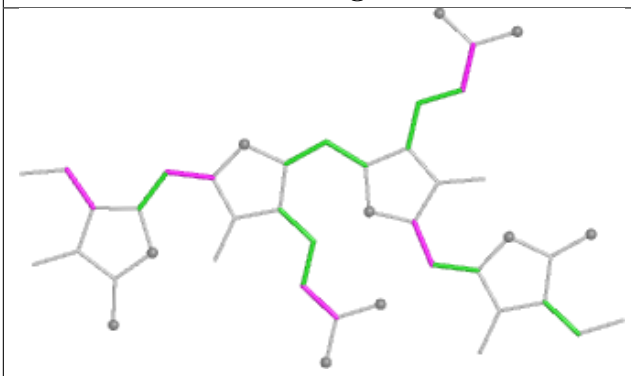

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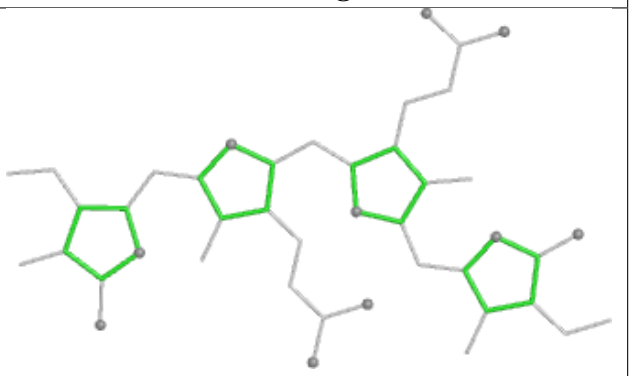
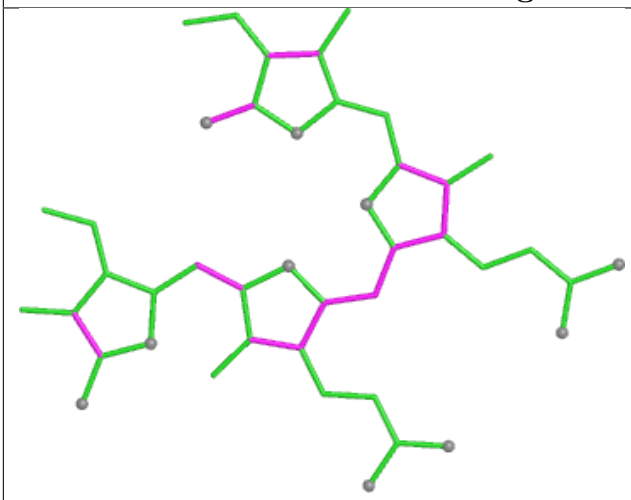


Rings

Ligand PEB tK 201



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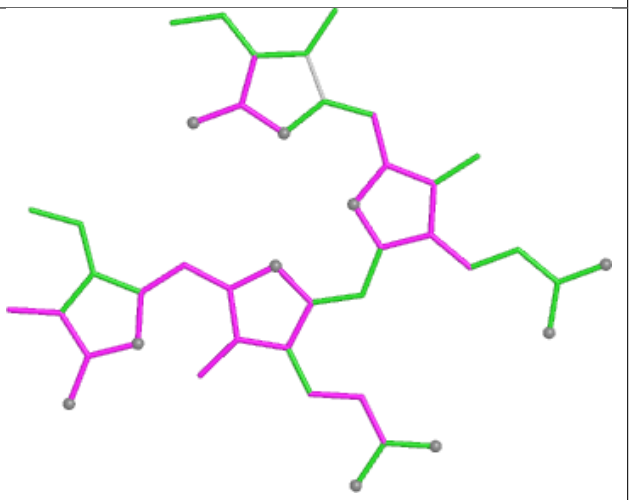
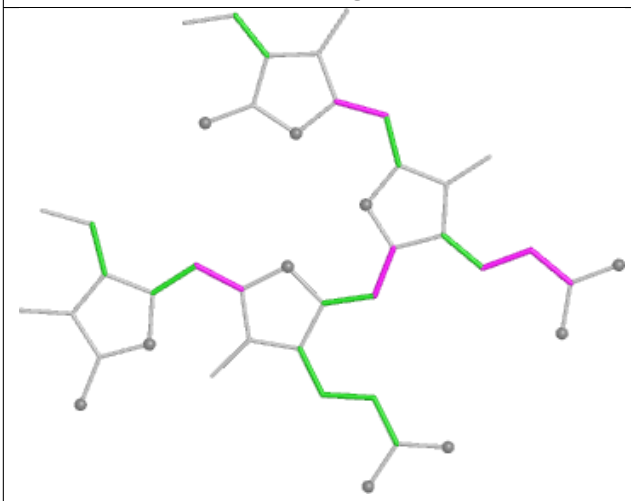


Bond angles



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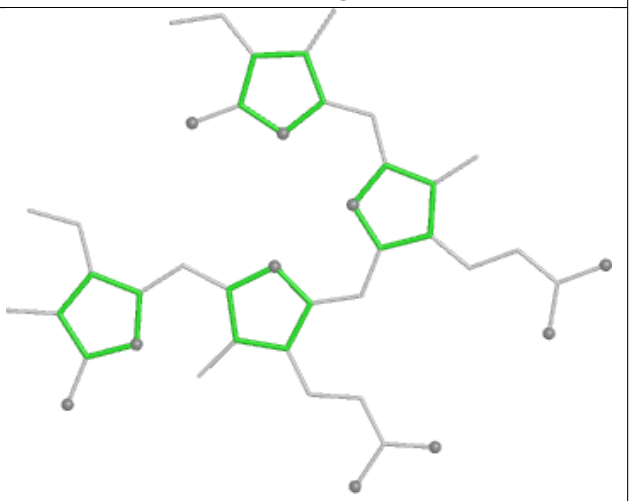
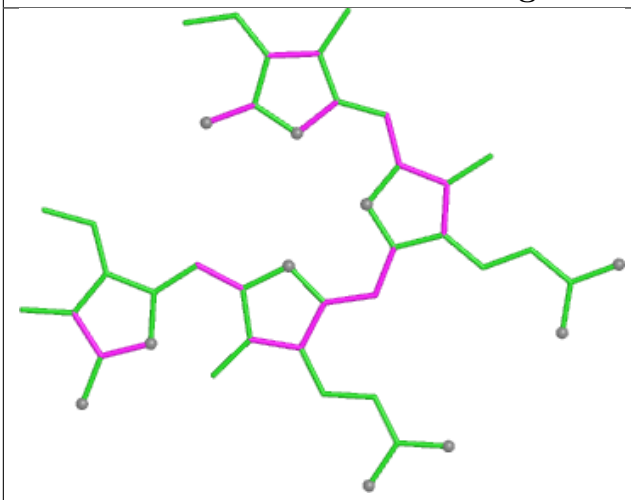


Rings

Ligand PEB lK 202



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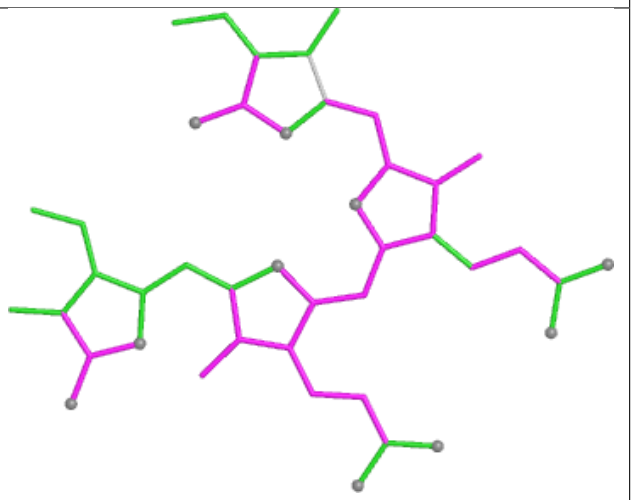
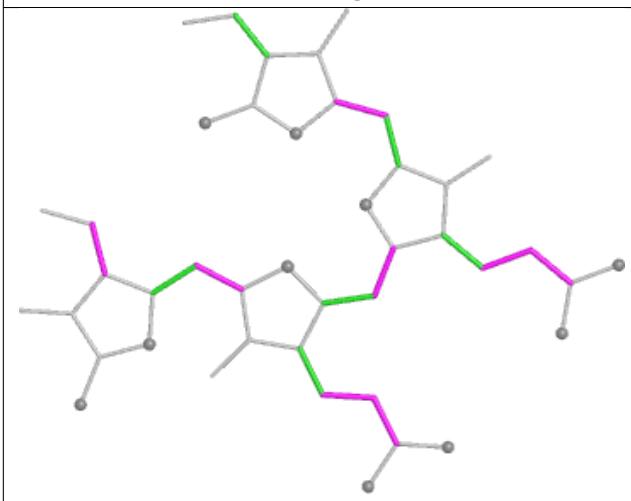


Bond angles



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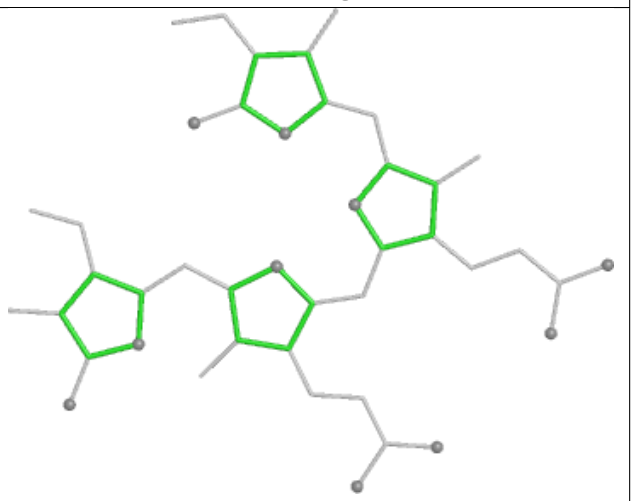
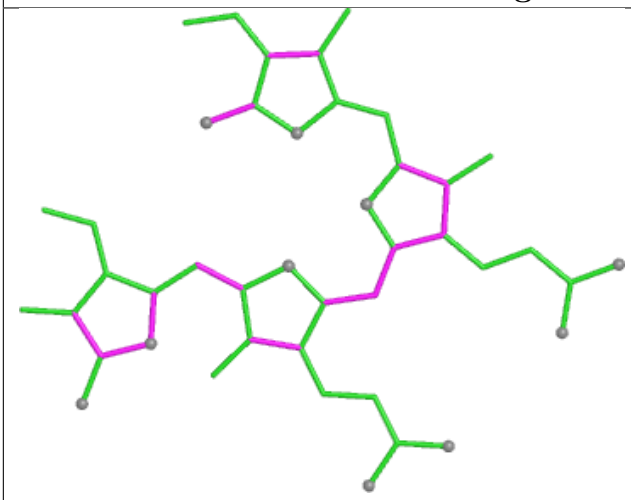


Rings

Ligand PEB FP 202



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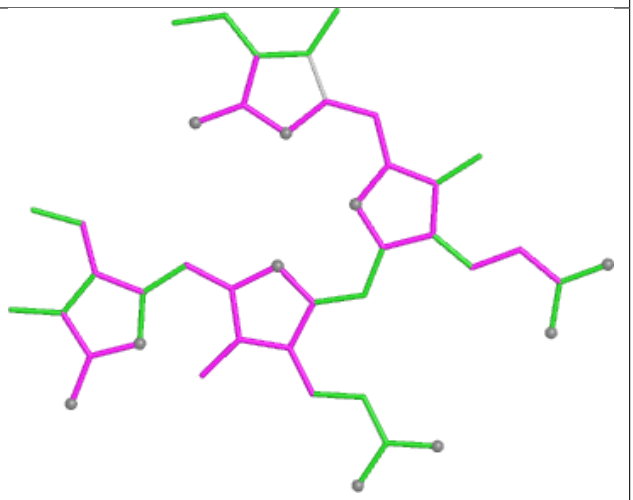
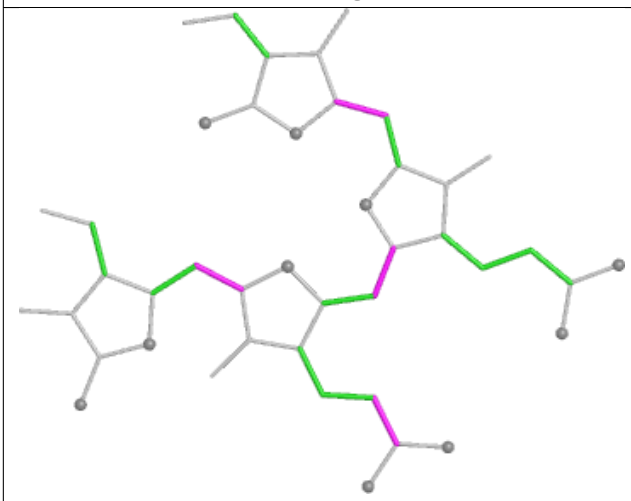


Bond angles



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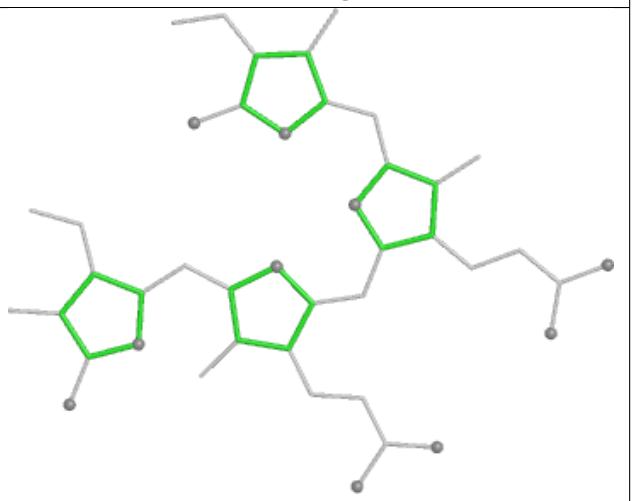
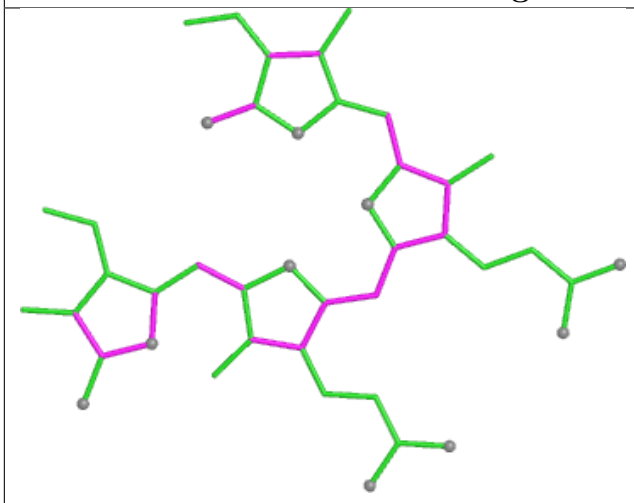


Rings

Ligand PEB AA 201



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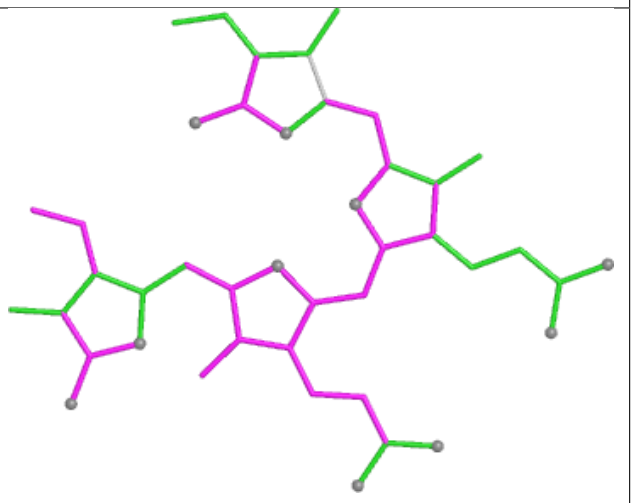

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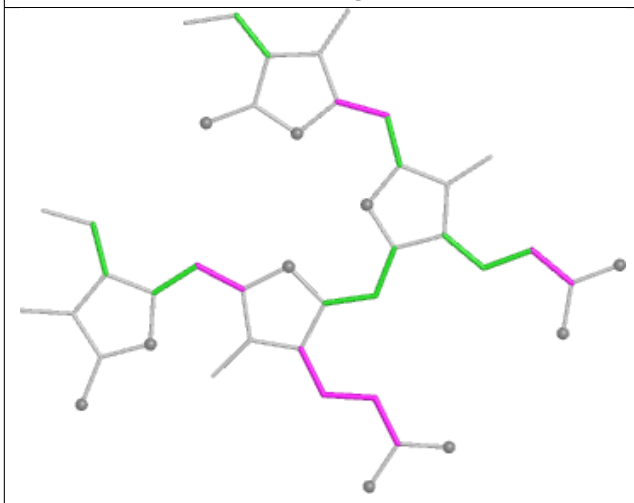

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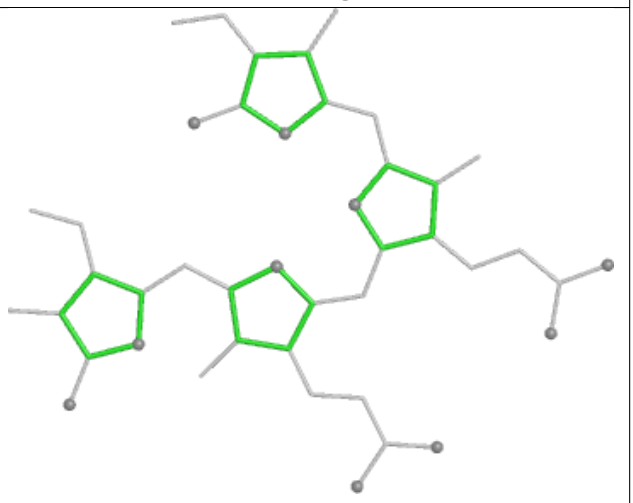
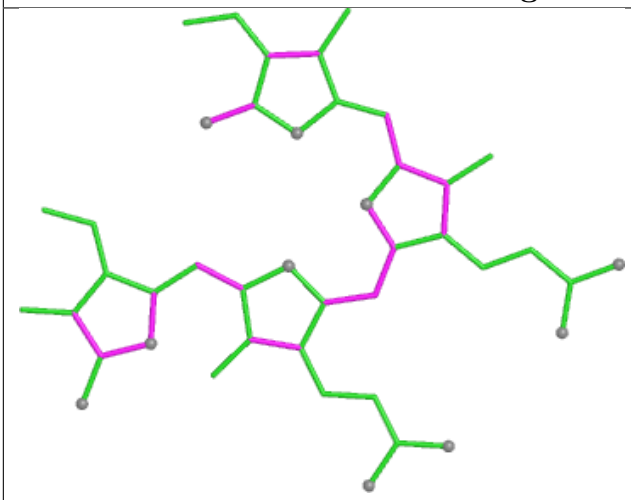


Rings

Ligand PEB eJ 201



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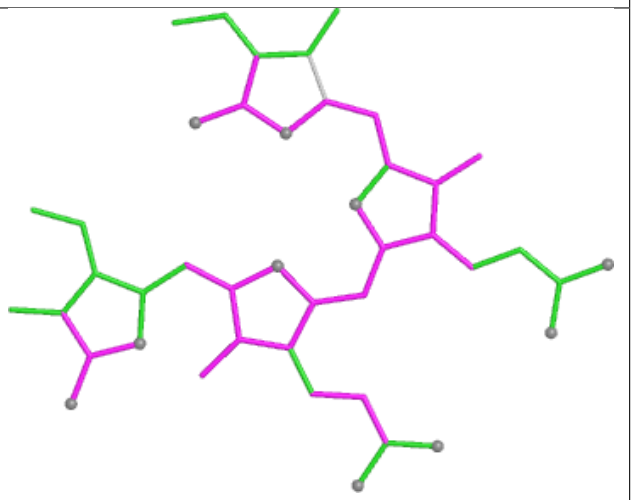

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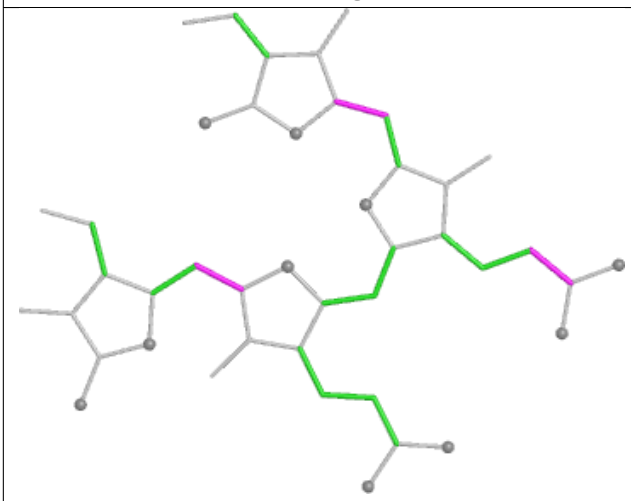

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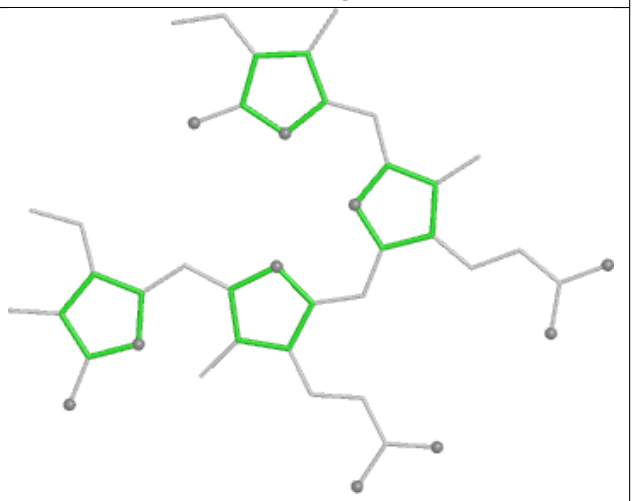
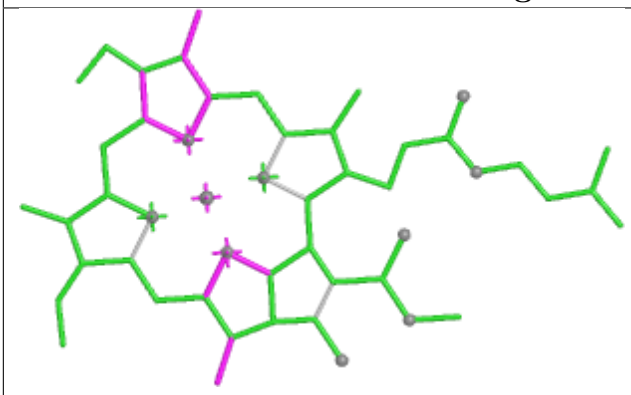


Rings

Ligand CLA 4N 608



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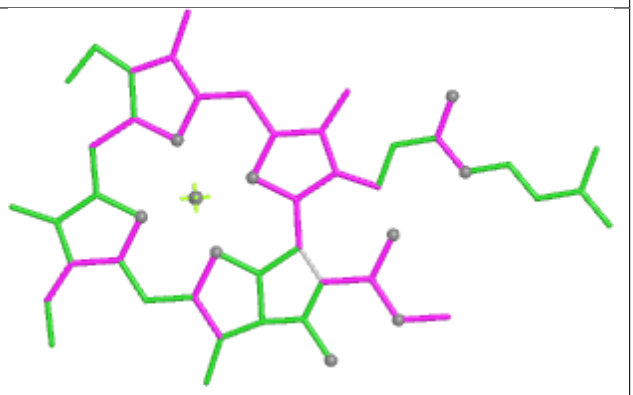

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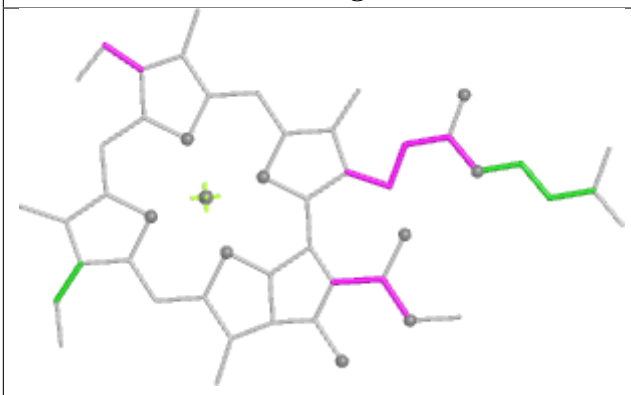

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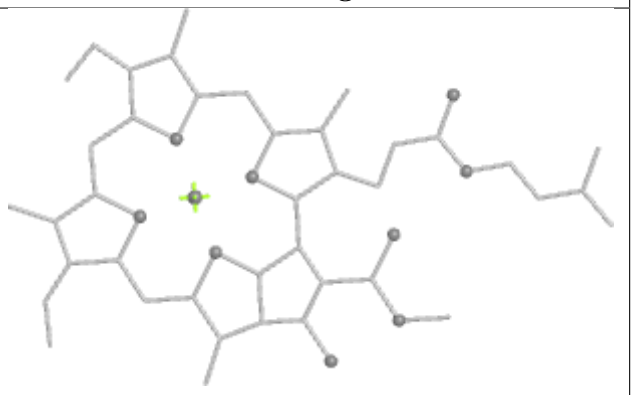
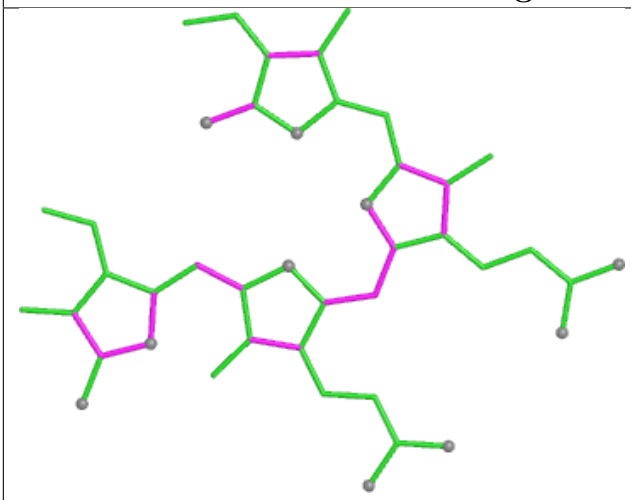


Rings

Ligand PEB bB 201



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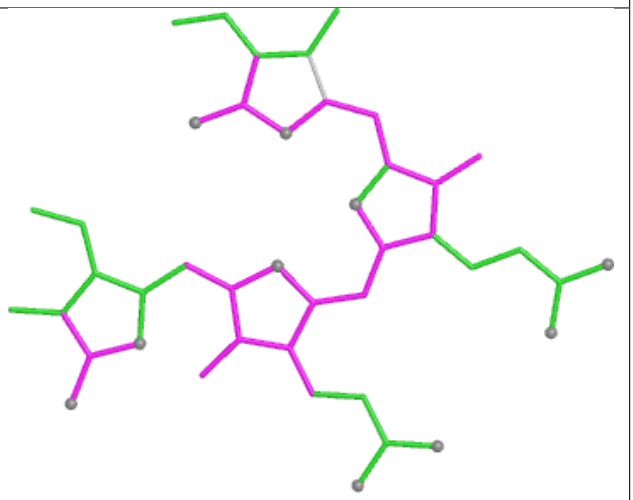

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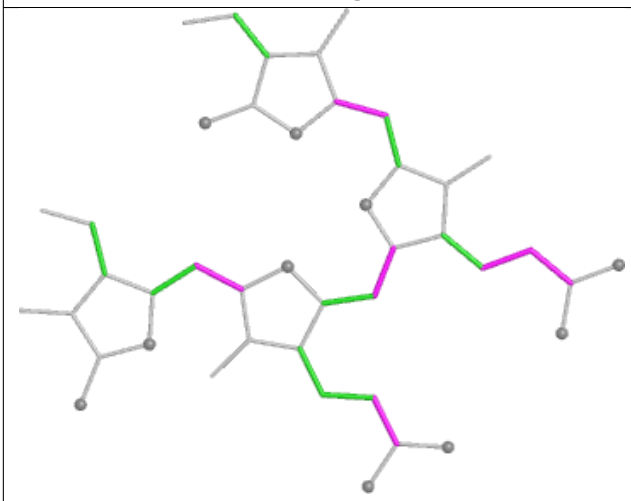

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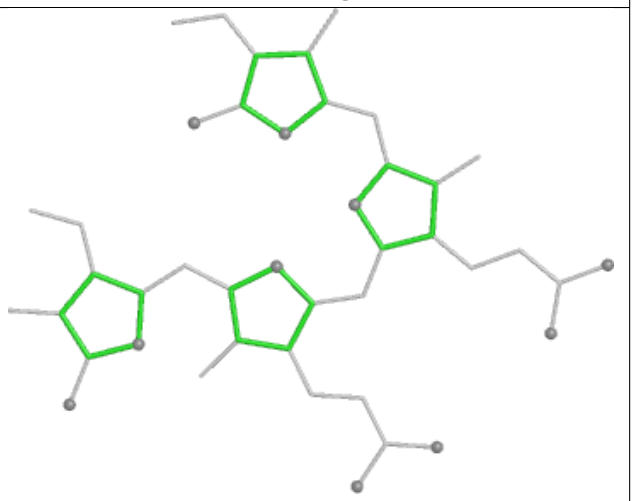
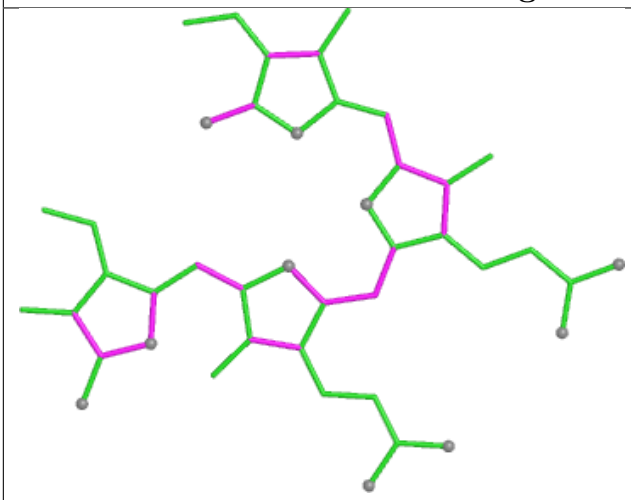


Rings

Ligand PEB S1 201



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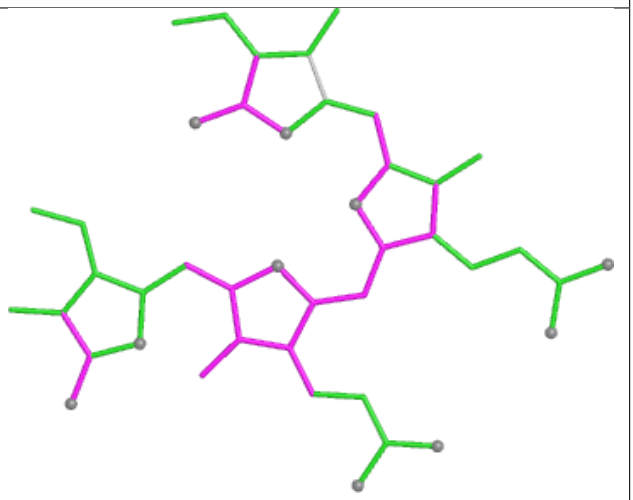

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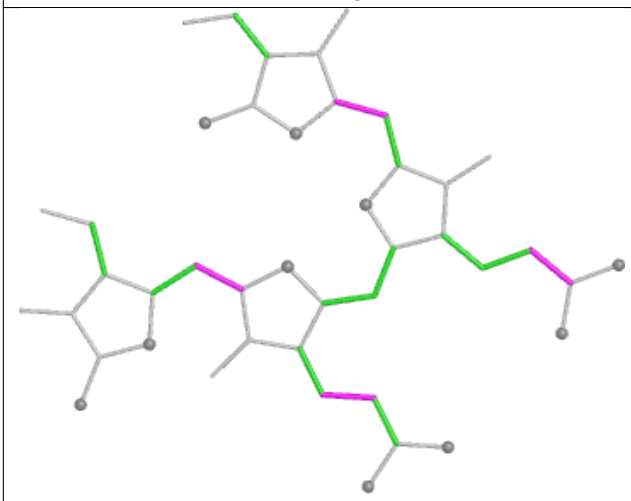

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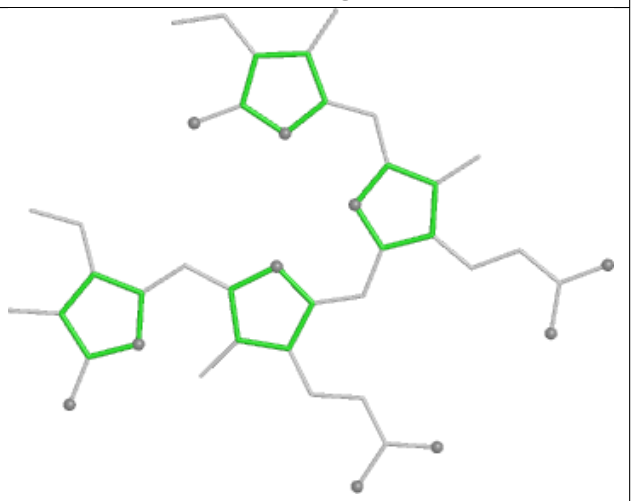
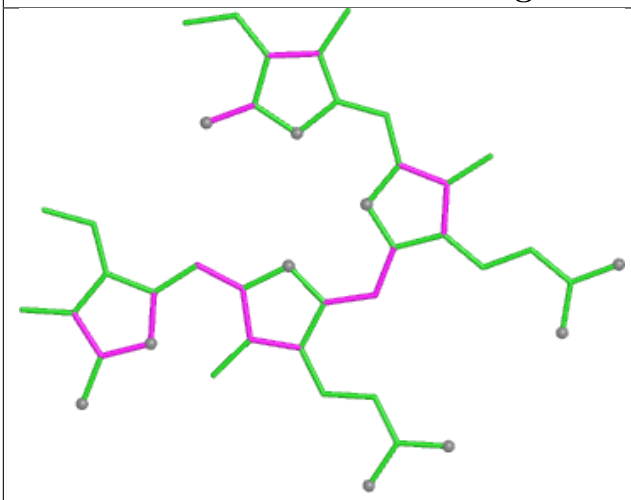


Rings

Ligand PEB aK 202



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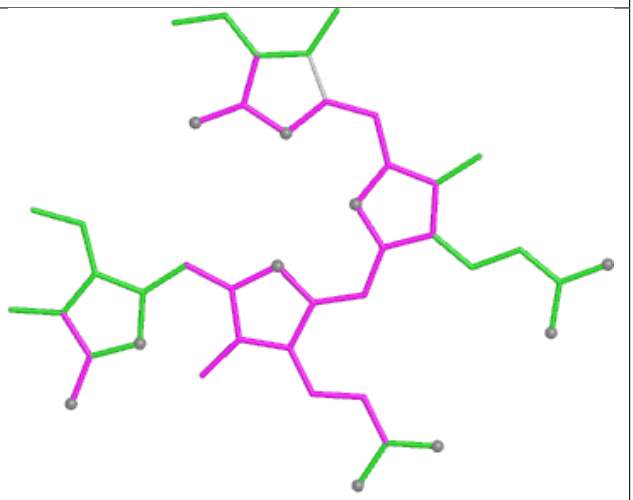

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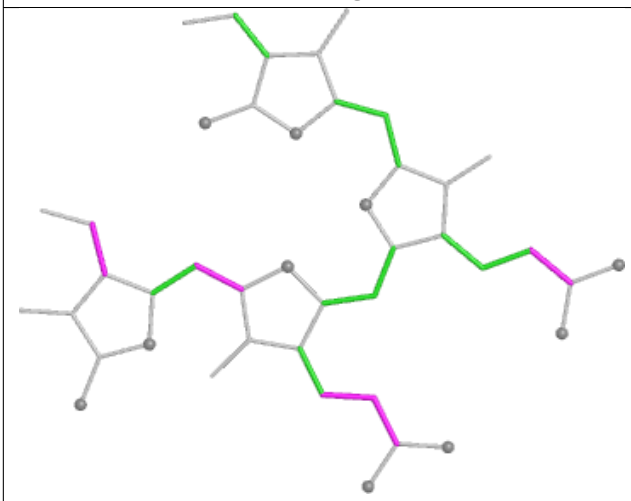

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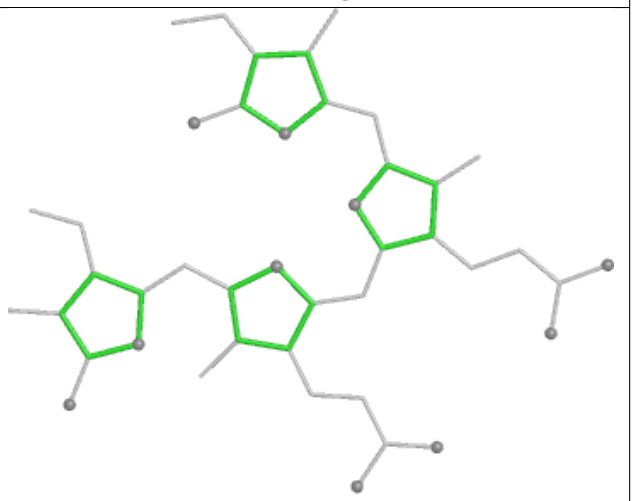
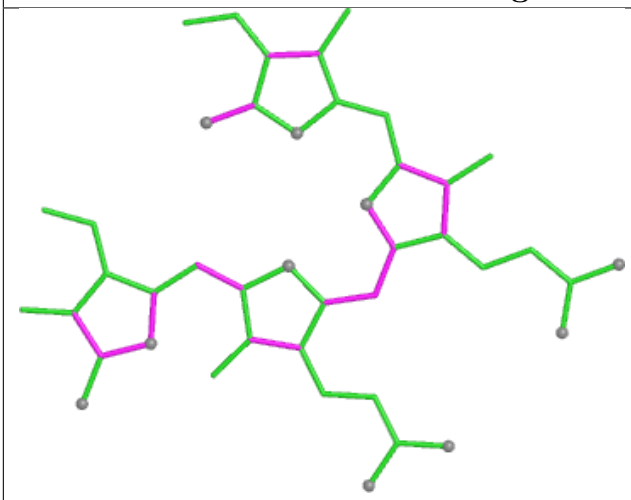


Rings

Ligand PEB KP 202



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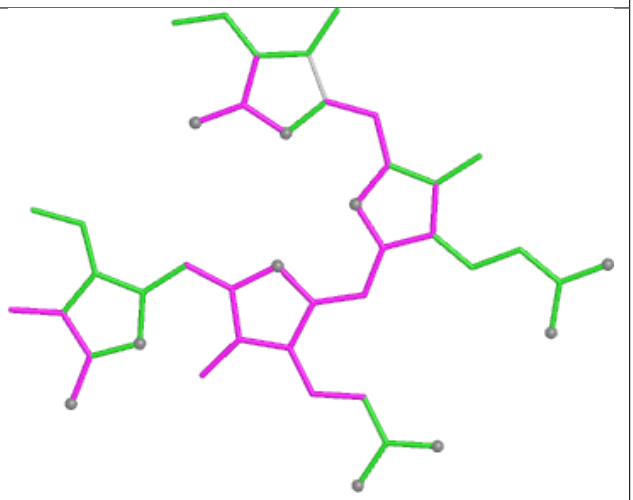

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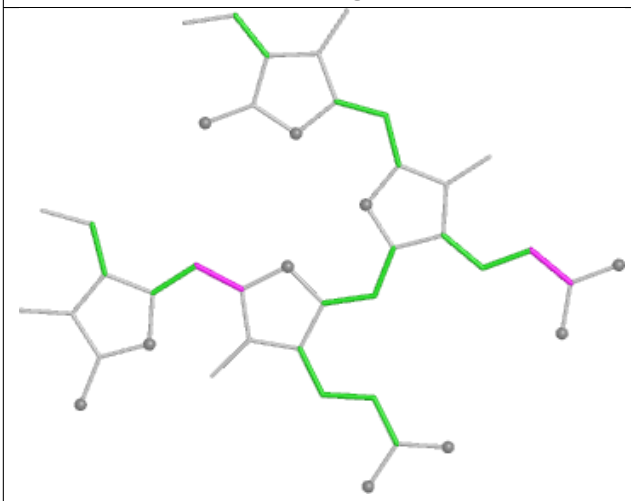

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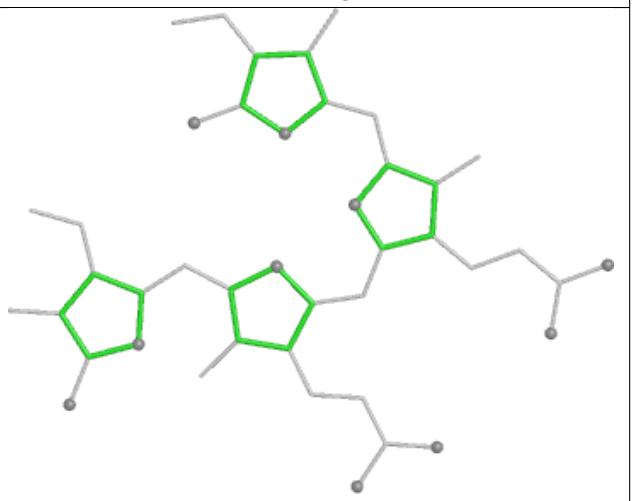
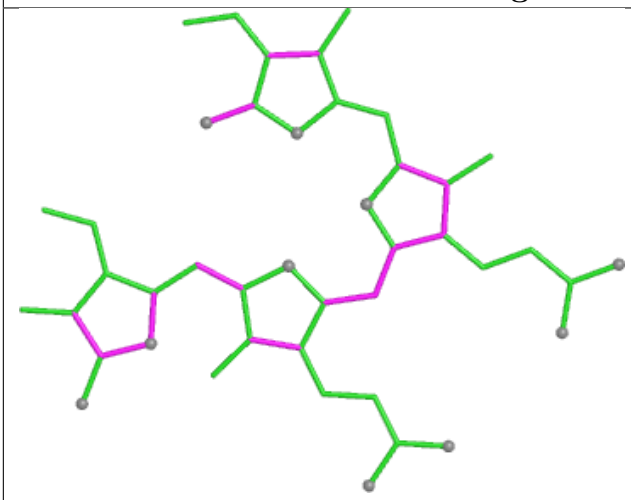


Rings

Ligand PEB KB 304



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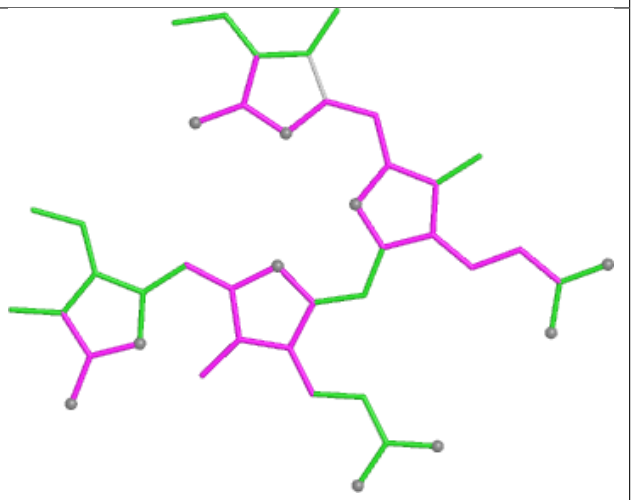

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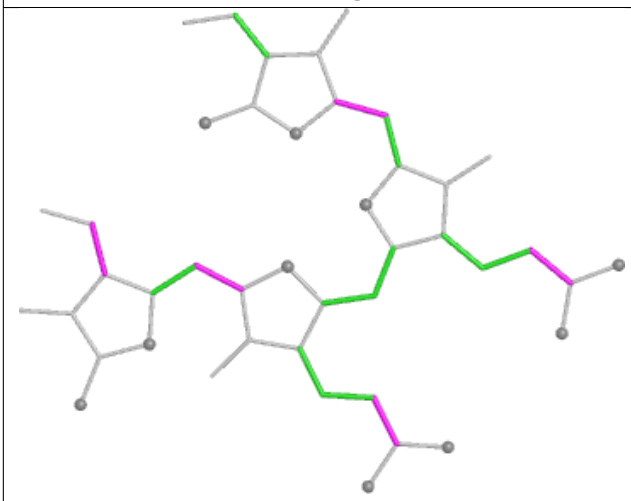

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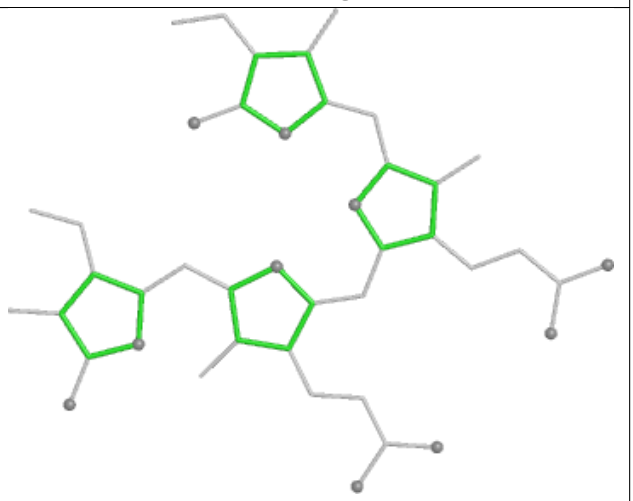
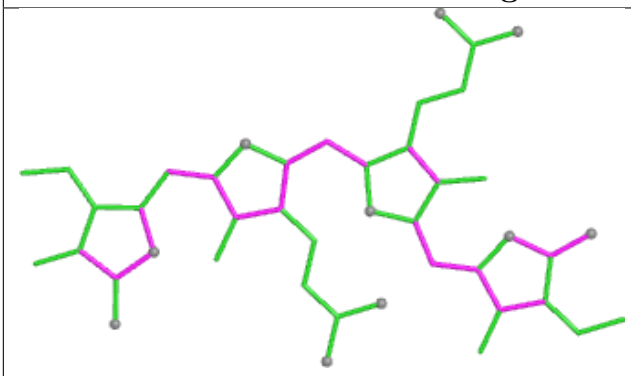


Rings

Ligand CYC FH 1001



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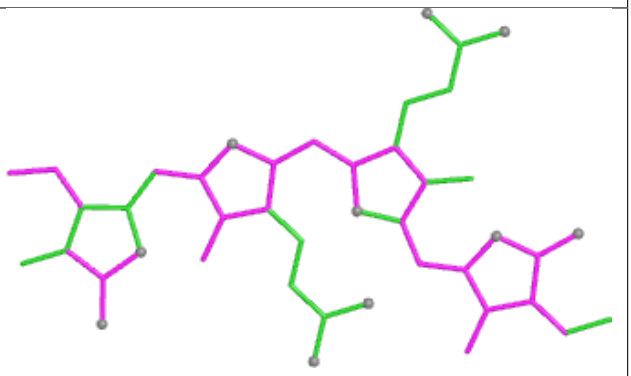

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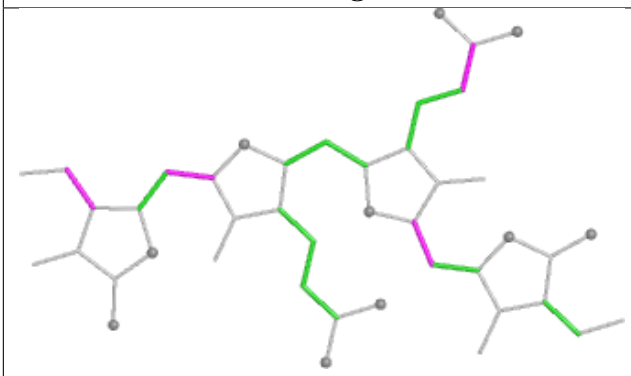

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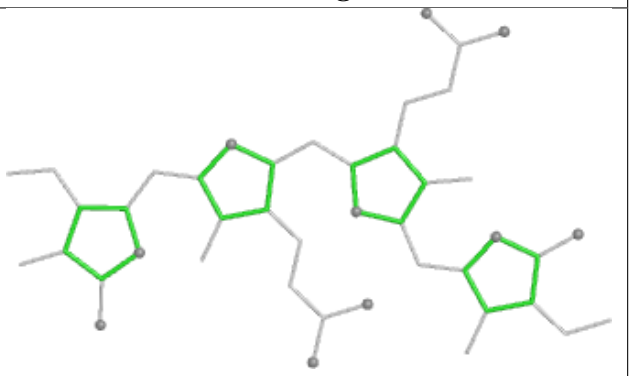
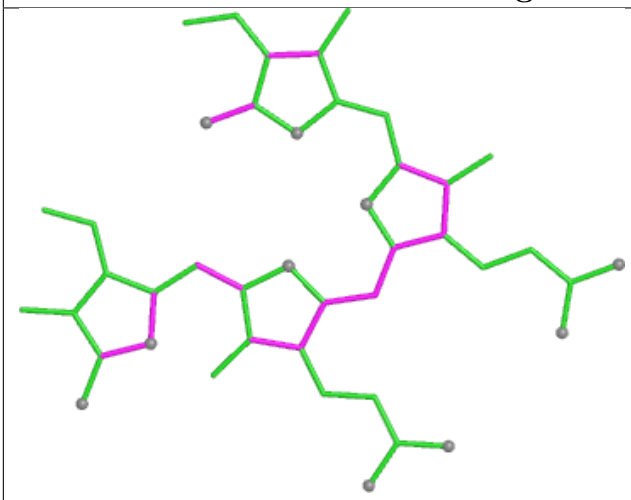


Rings

Ligand PEB cG 202



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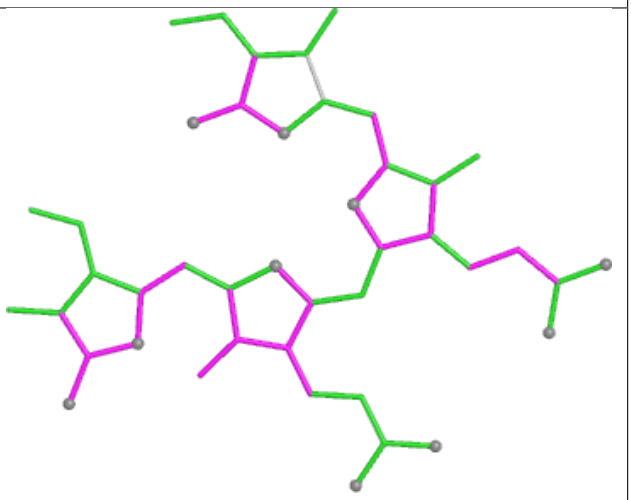

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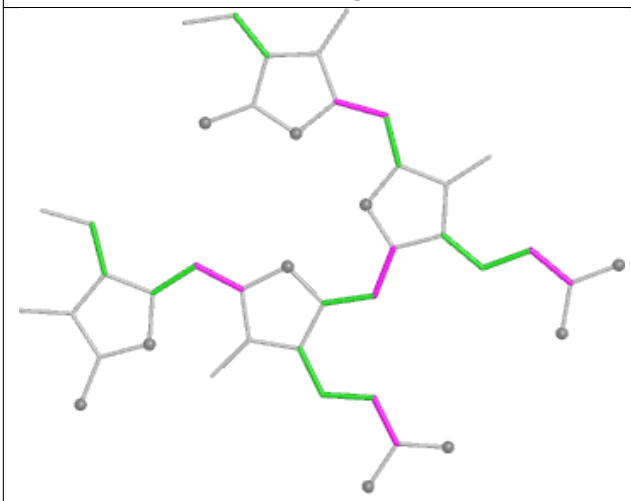

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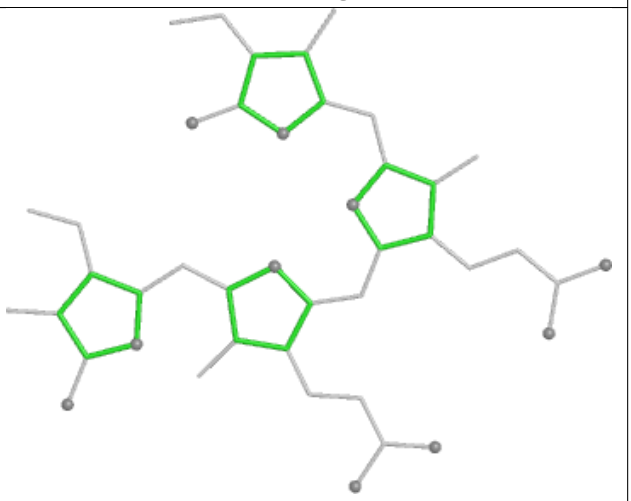
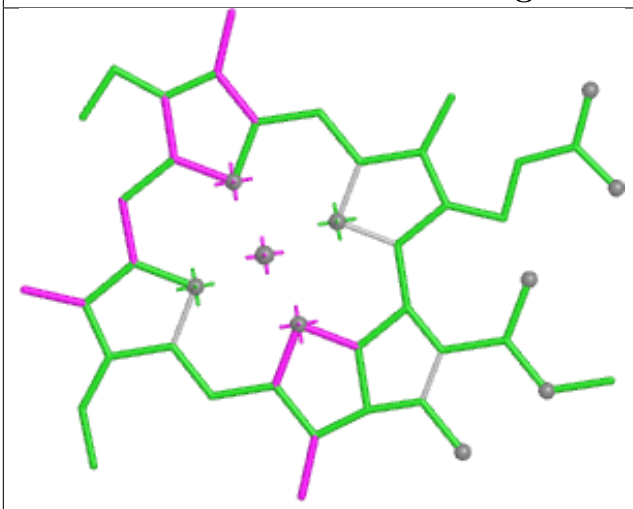


Rings

Ligand CLA B2 828



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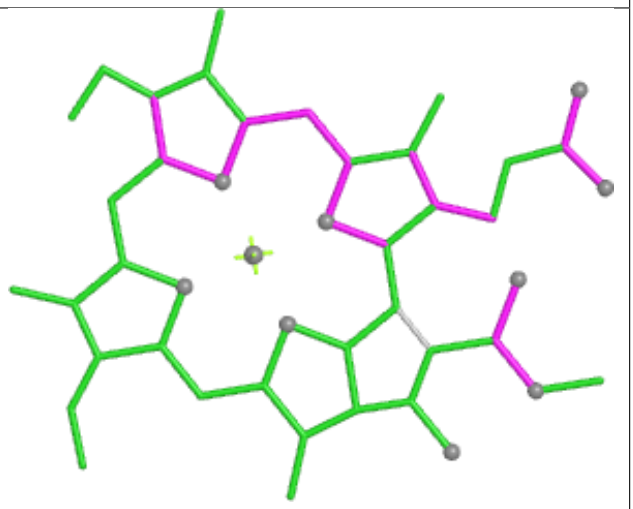

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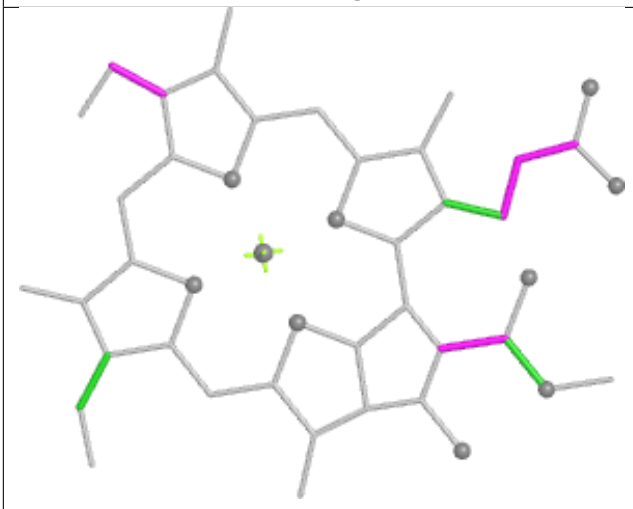
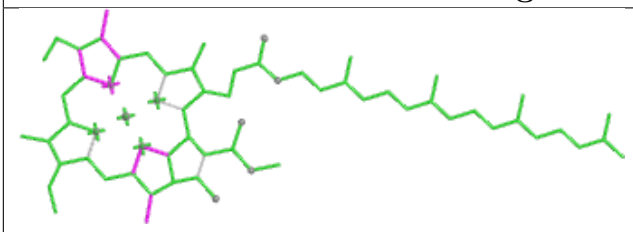


Torsions



Rings

Ligand CLA dL 404



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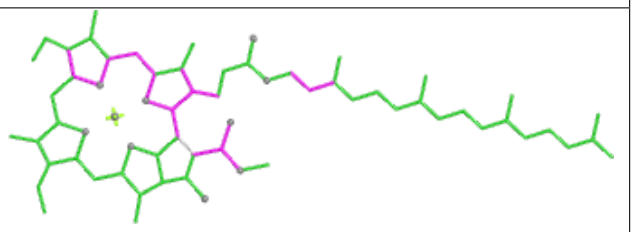

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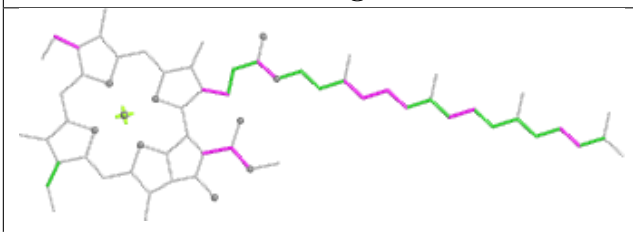

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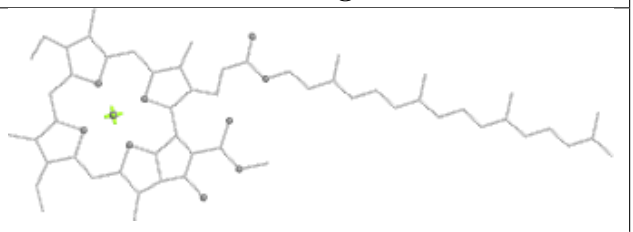
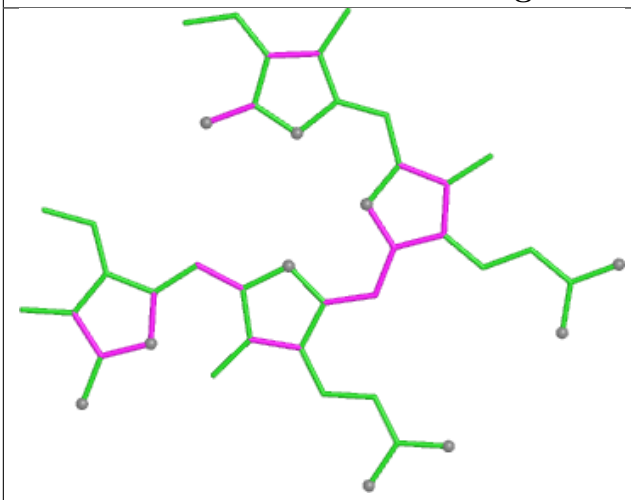


Rings

Ligand PEB LP 202



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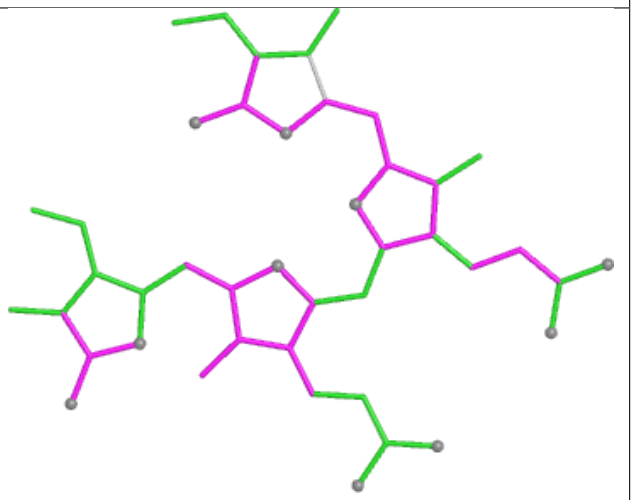

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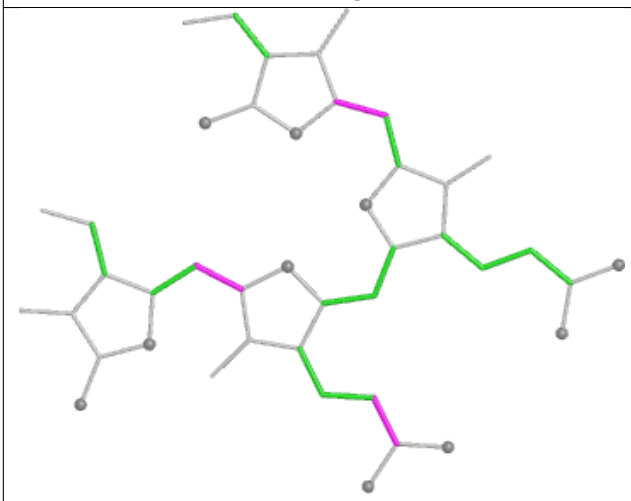

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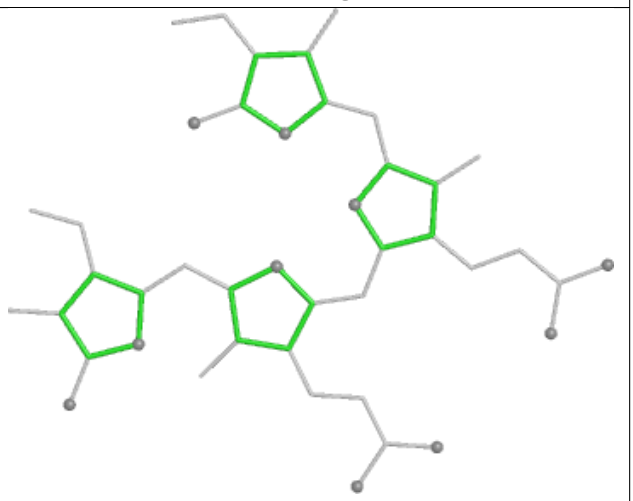
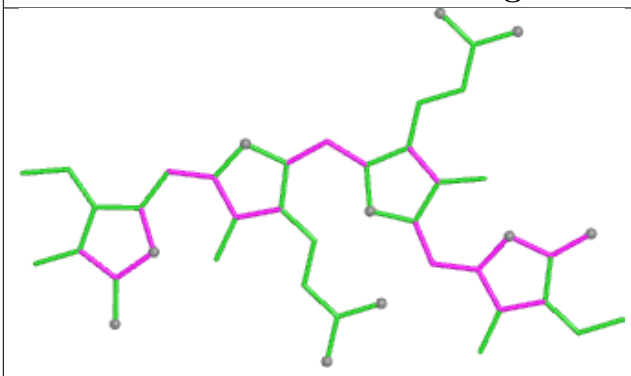


Rings

Ligand CYC C4 1001



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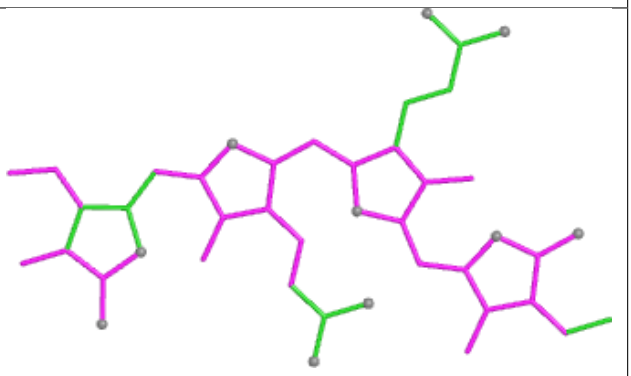
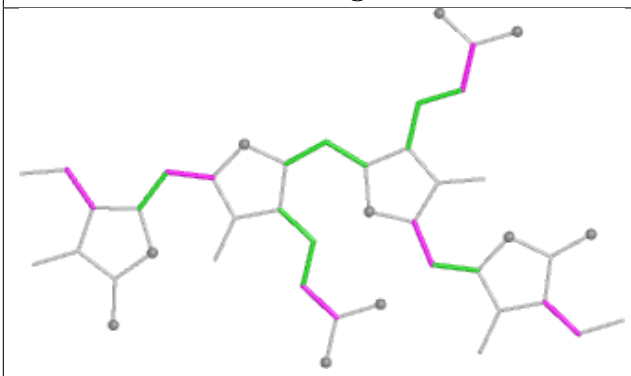


Bond angles



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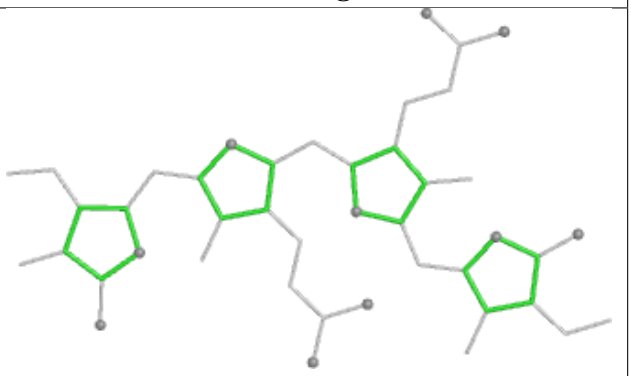
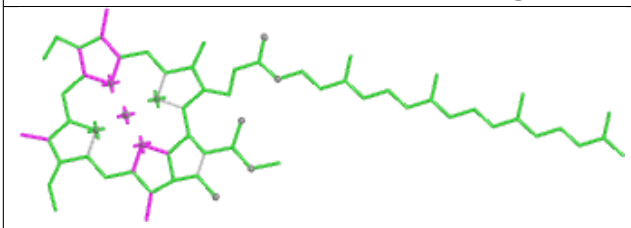


Rings

Ligand CLA AN 823



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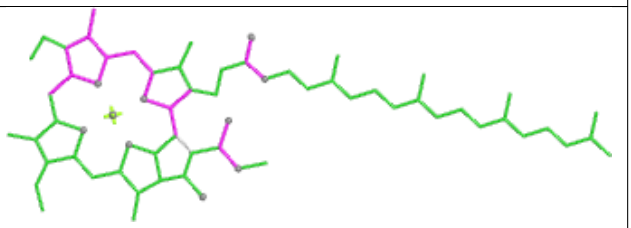
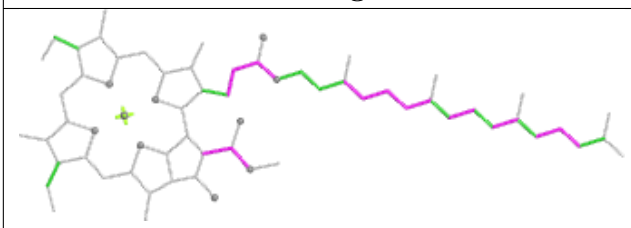


Bond angles



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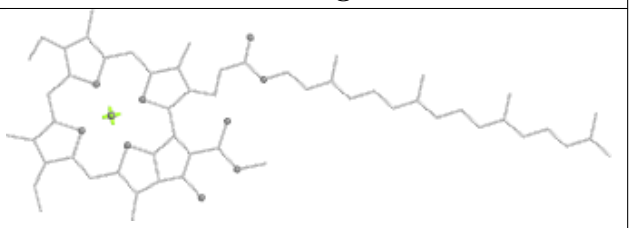
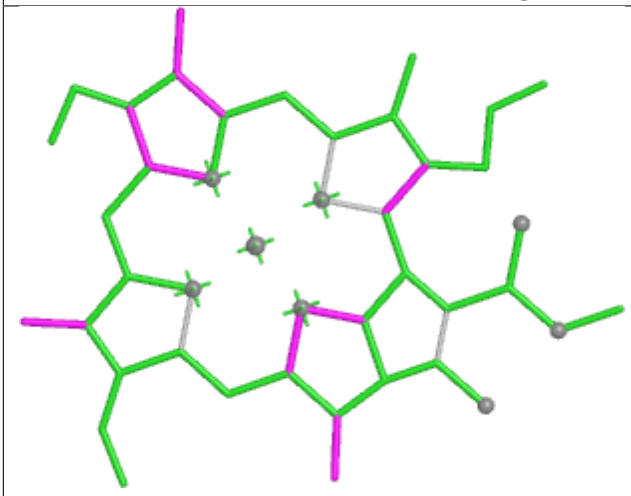


Rings

Ligand CLA B2 820



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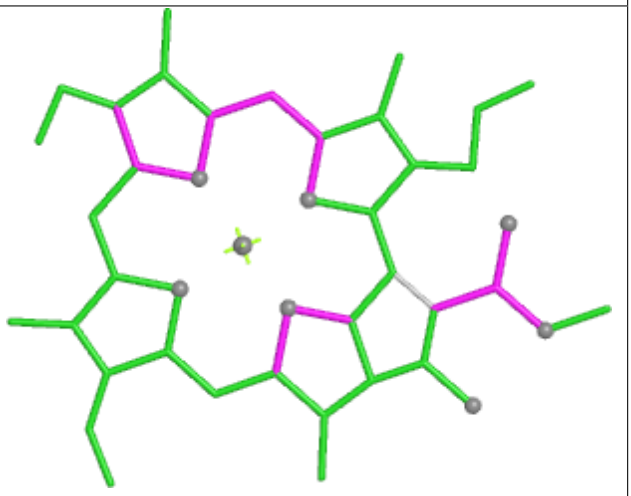

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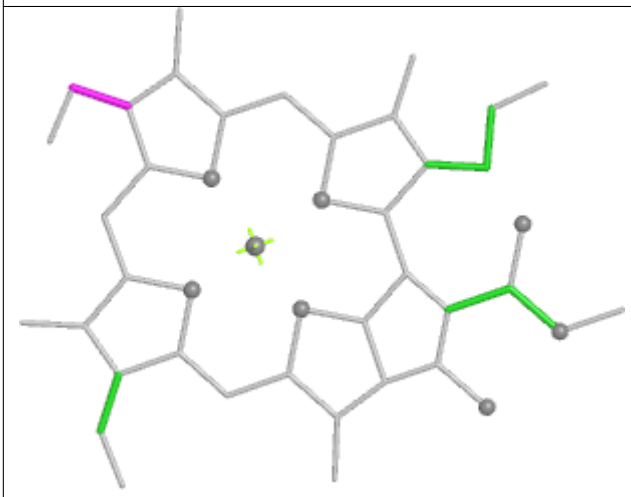

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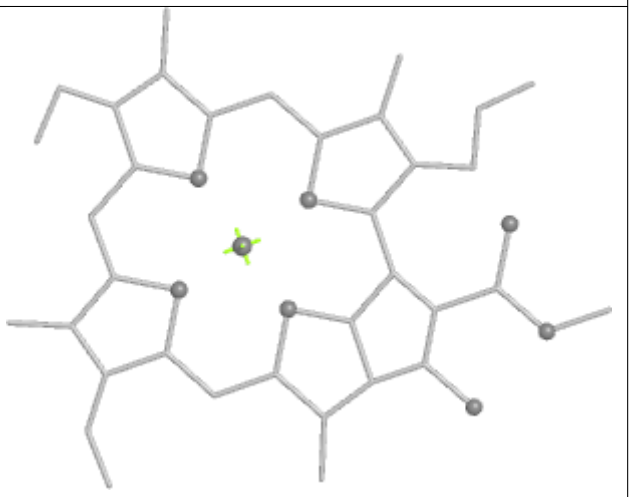
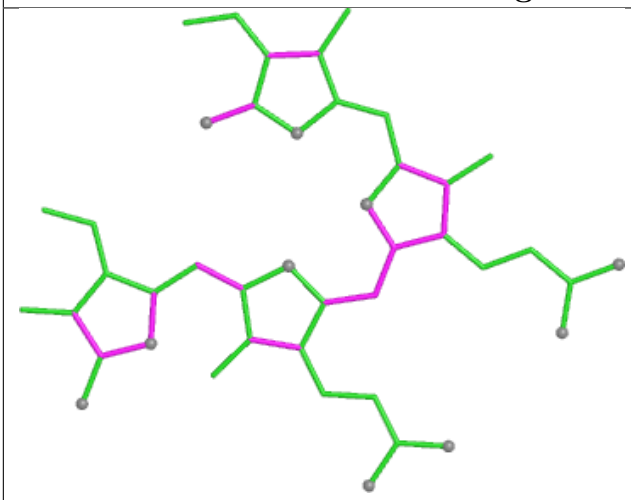


Rings

Ligand PEB U5 203



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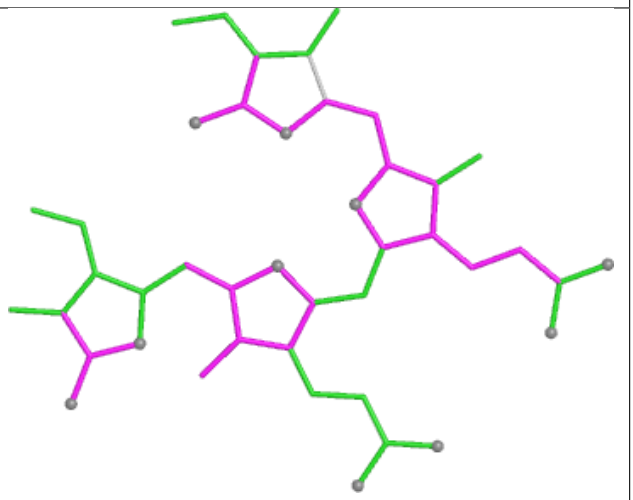

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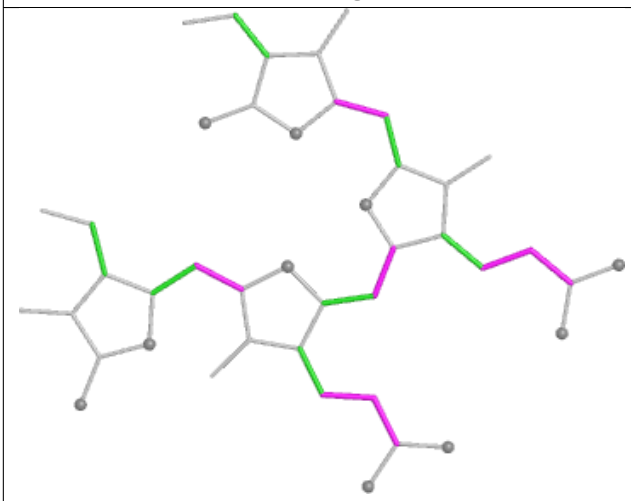

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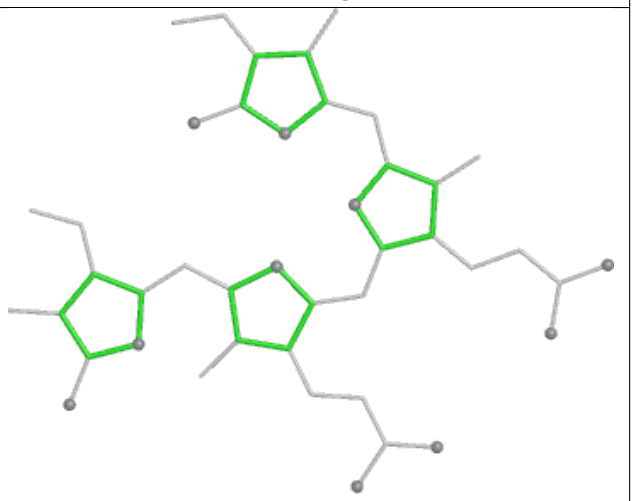
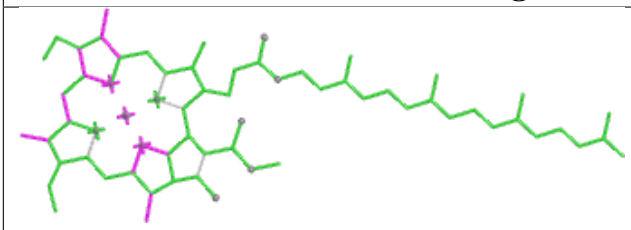


Rings

Ligand CLA BN 807



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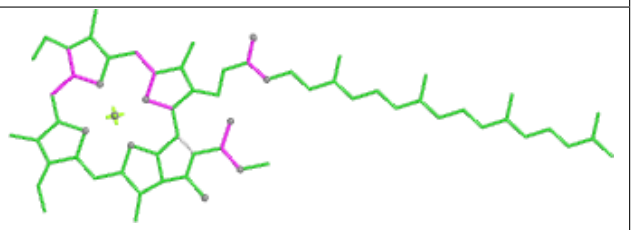

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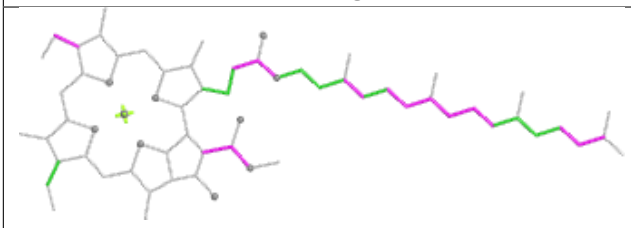

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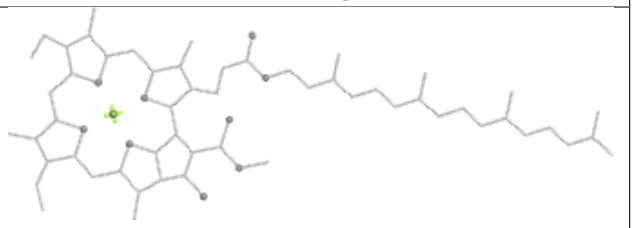
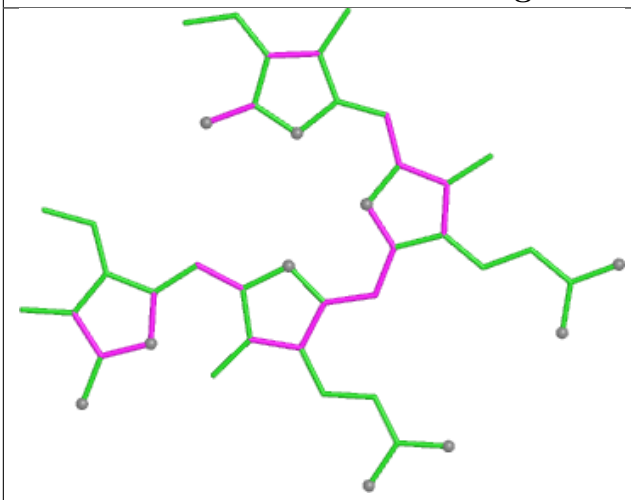


Rings

Ligand PEB JK 202



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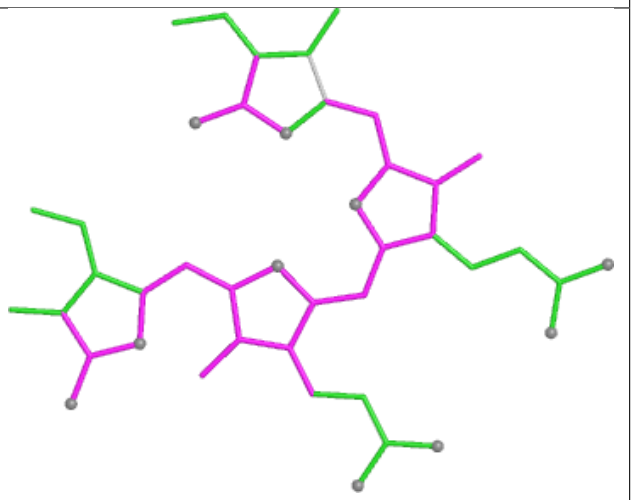

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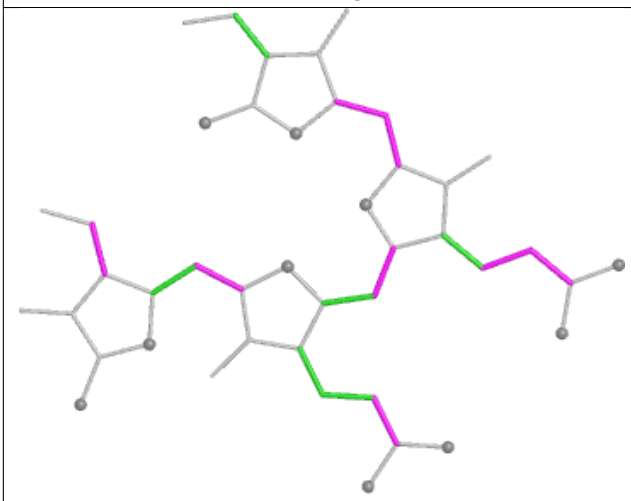

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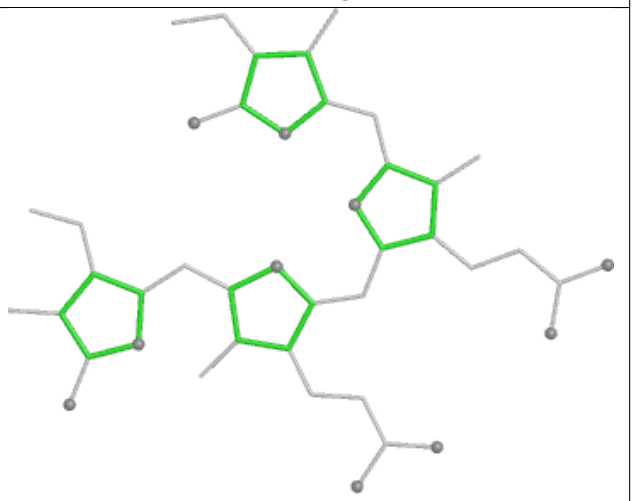
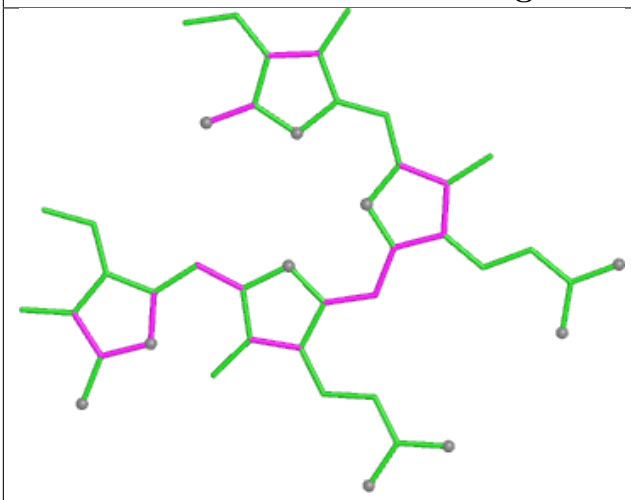


Rings

Ligand PEB Y5 202



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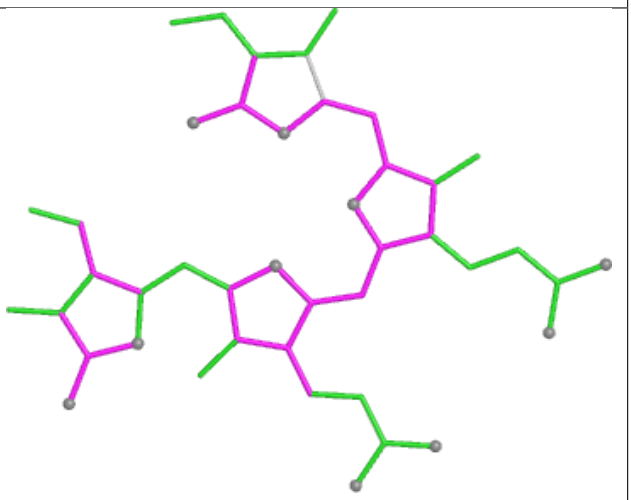

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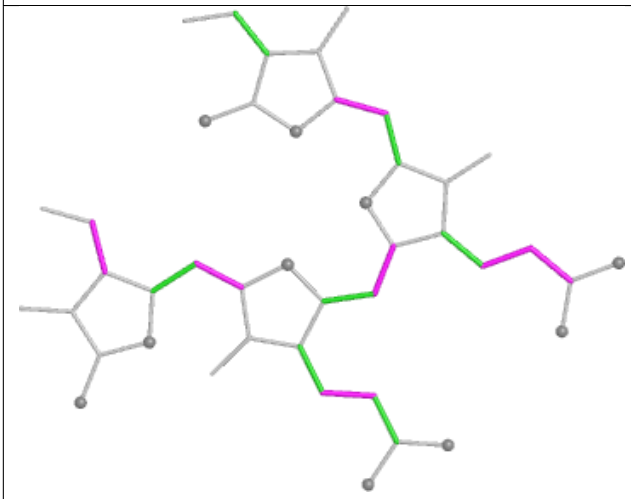

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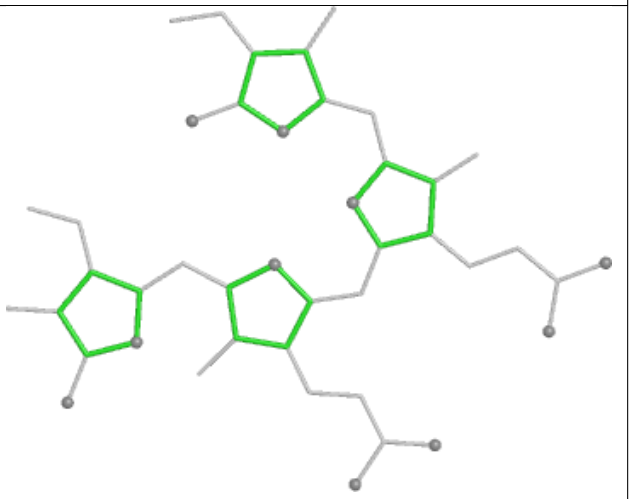
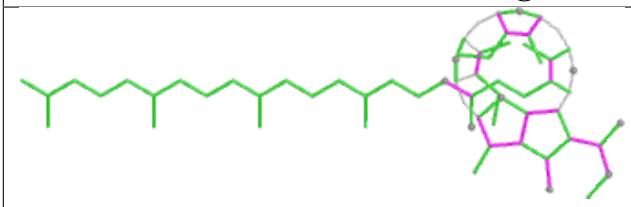


Rings

Ligand PHO d6 404



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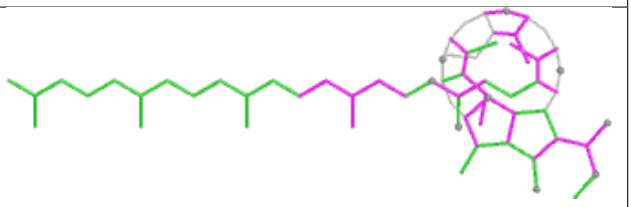

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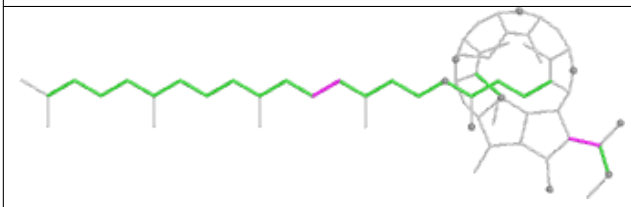

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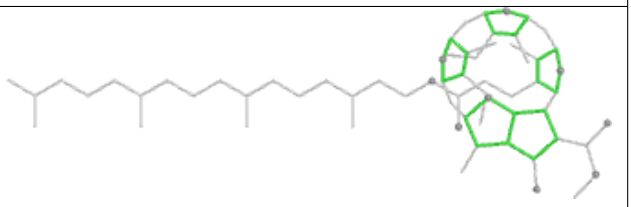
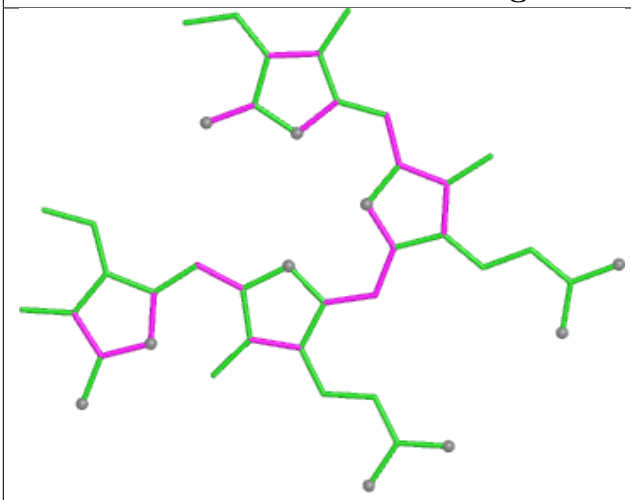


Rings

Ligand PEB ZM 201



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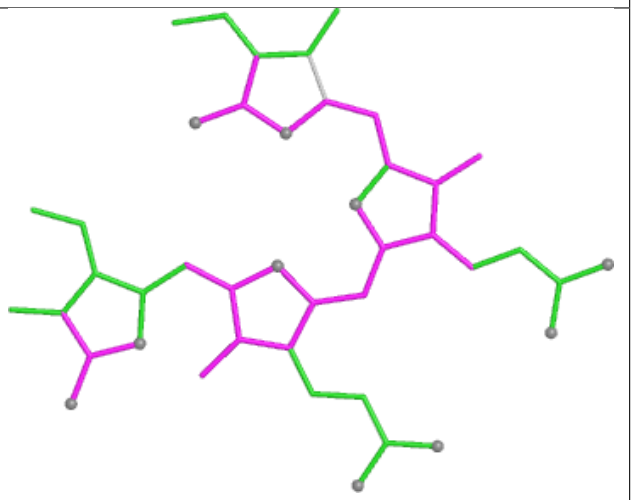

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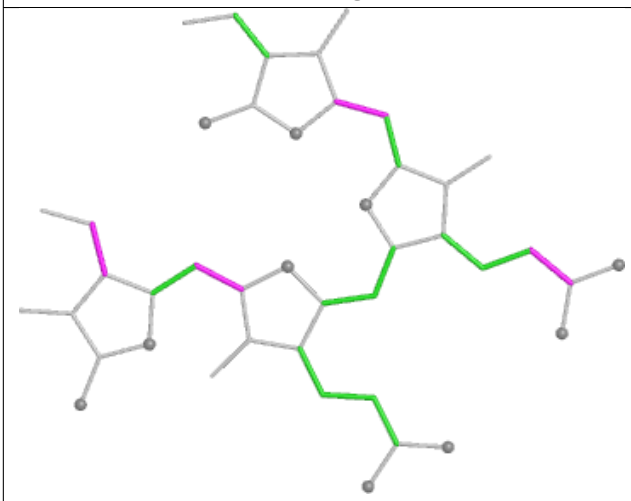

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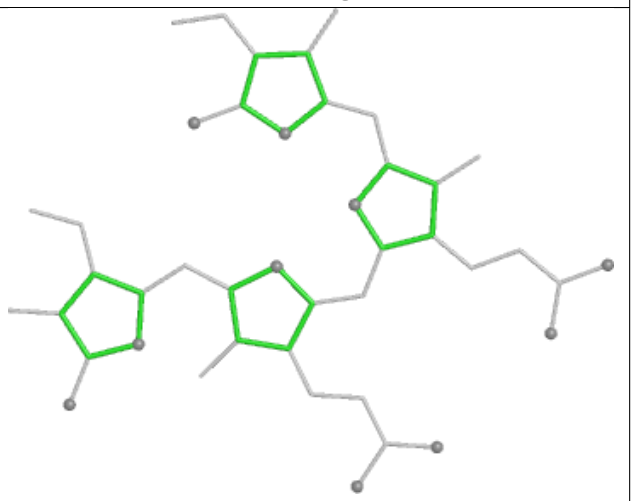
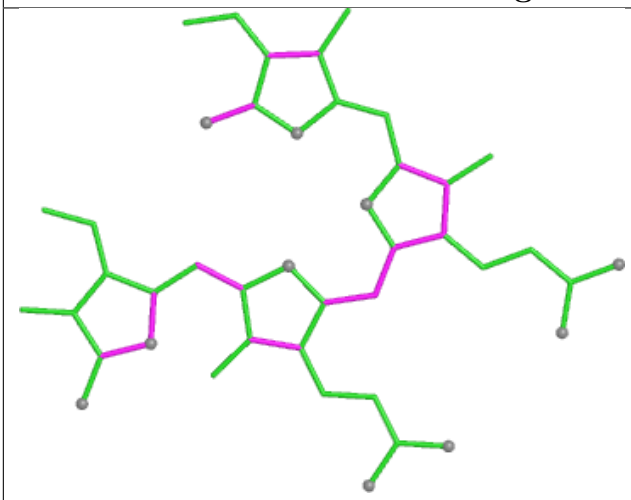


Rings

Ligand PEB H5 203



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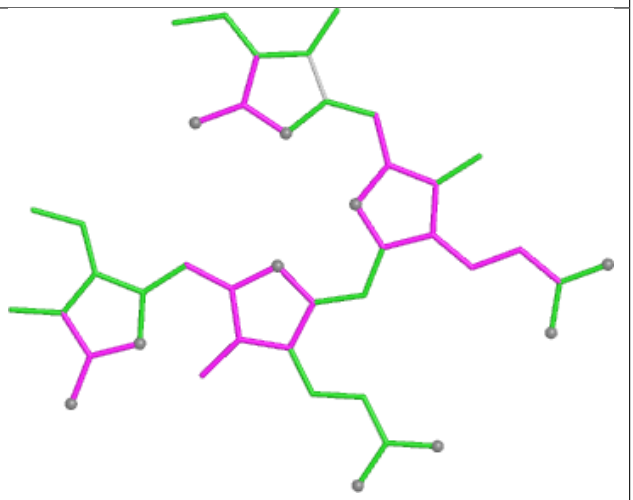

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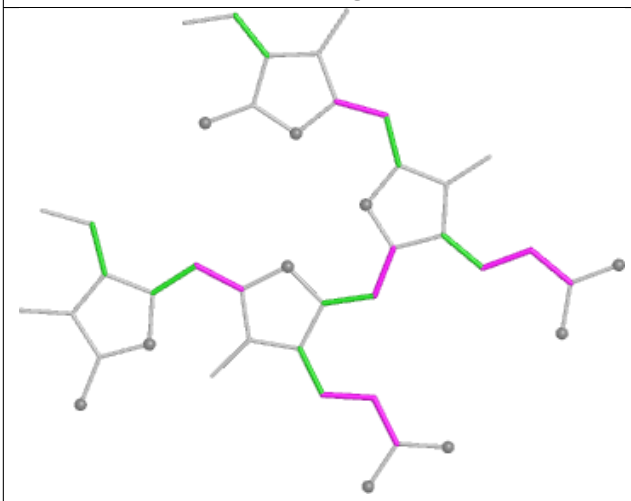

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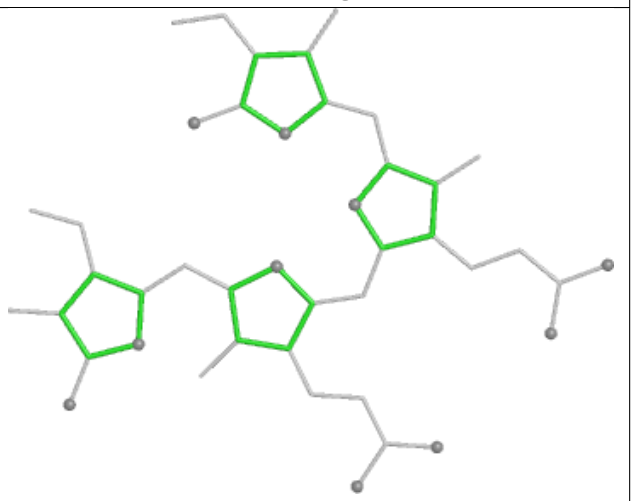

Rings

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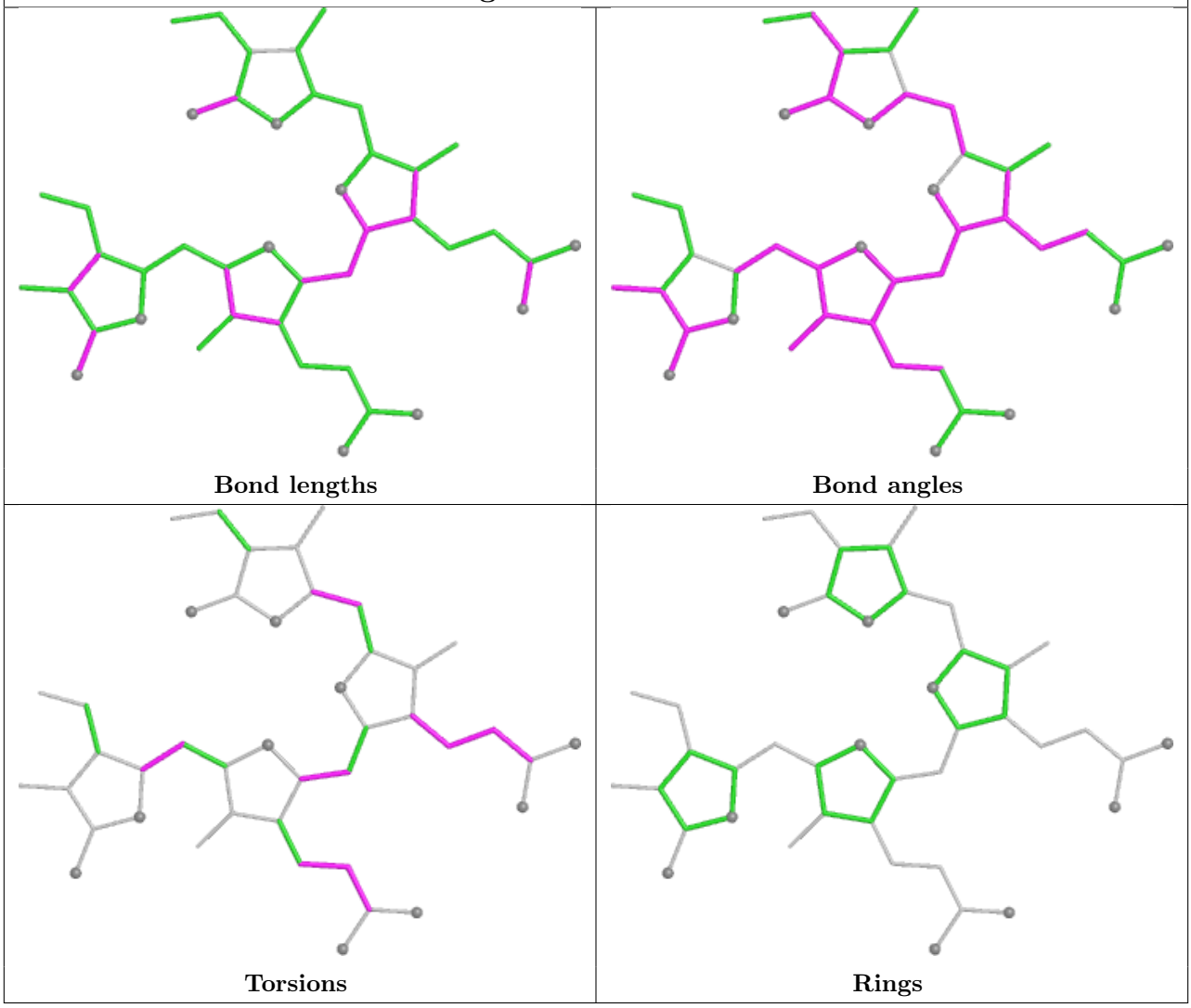

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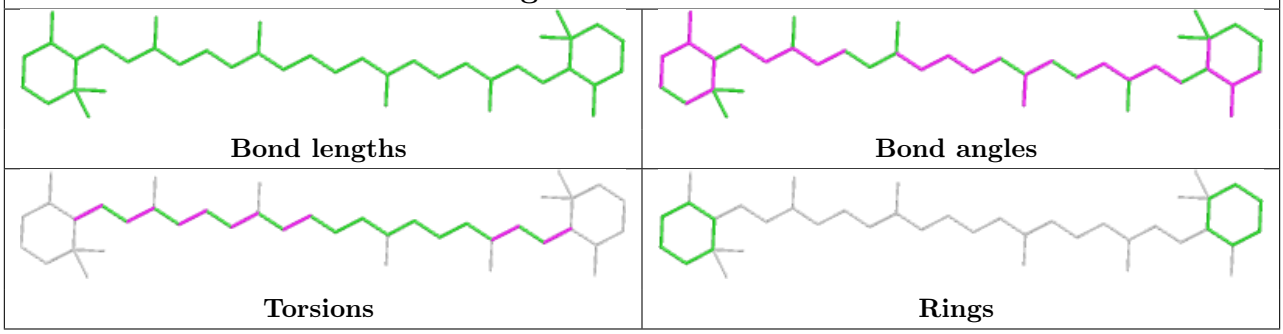

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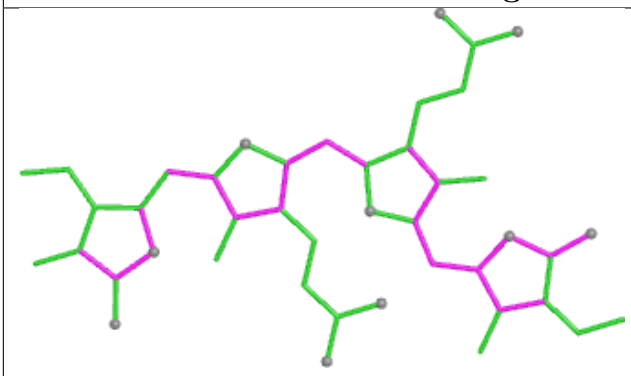

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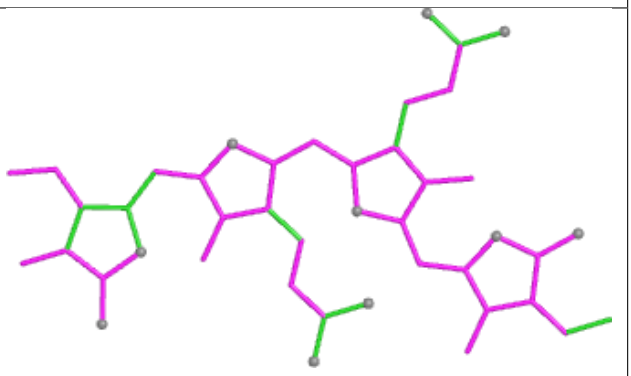

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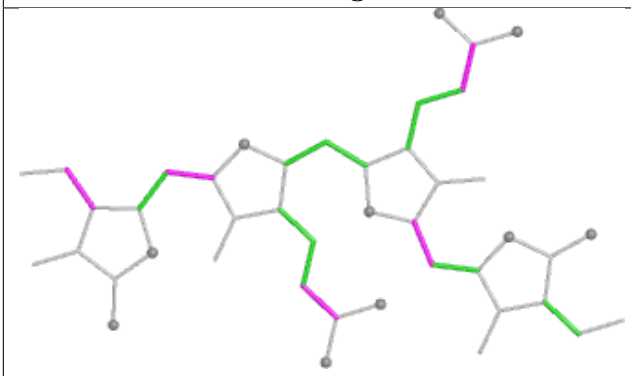

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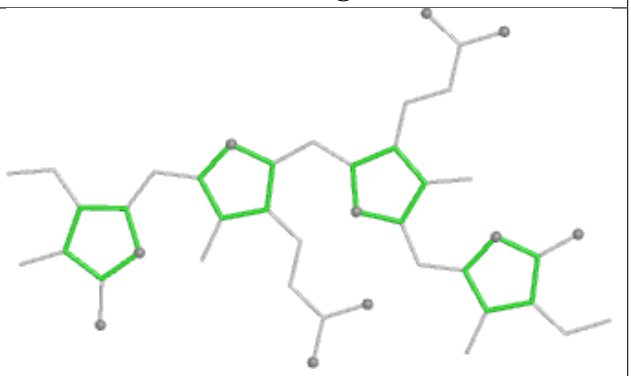
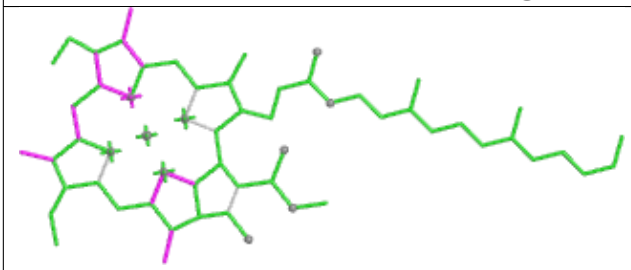


Rings

Ligand CLA b6 614



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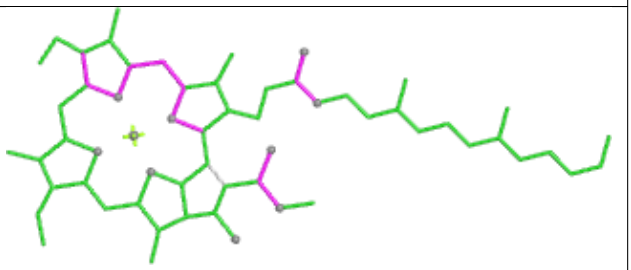

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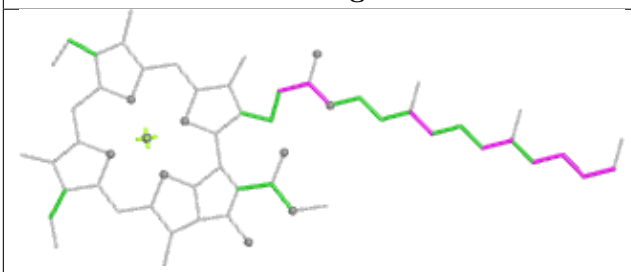

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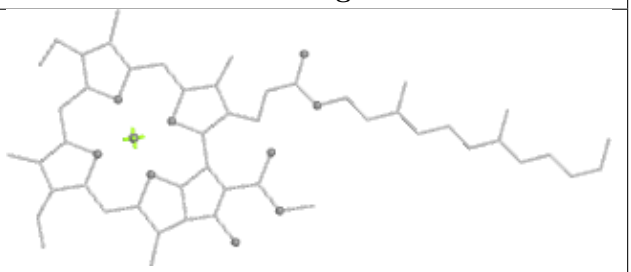
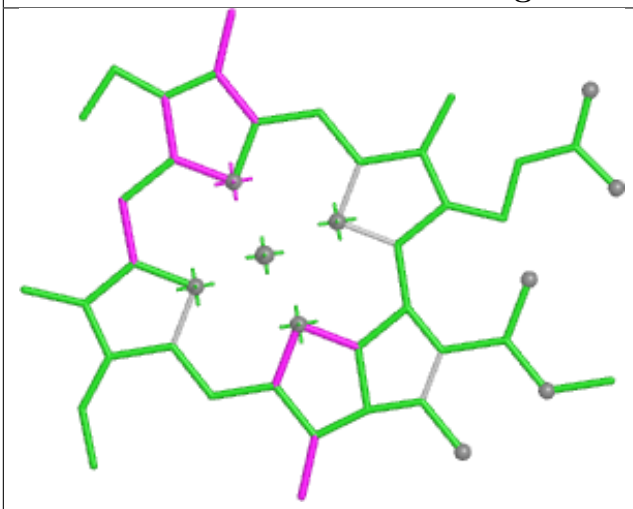


Rings

Ligand CLA 7N 606



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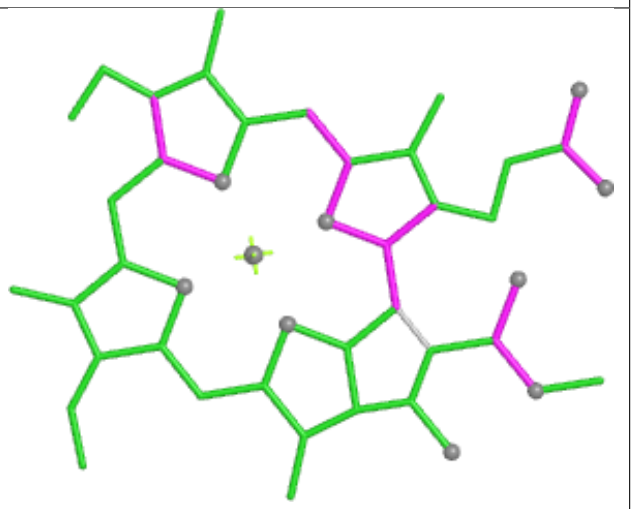

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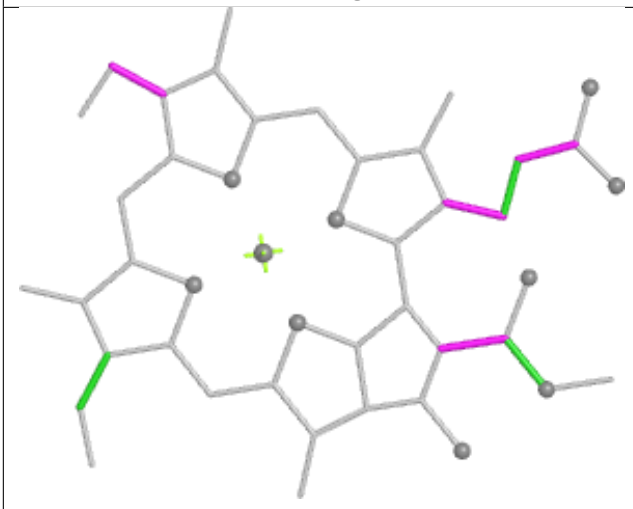
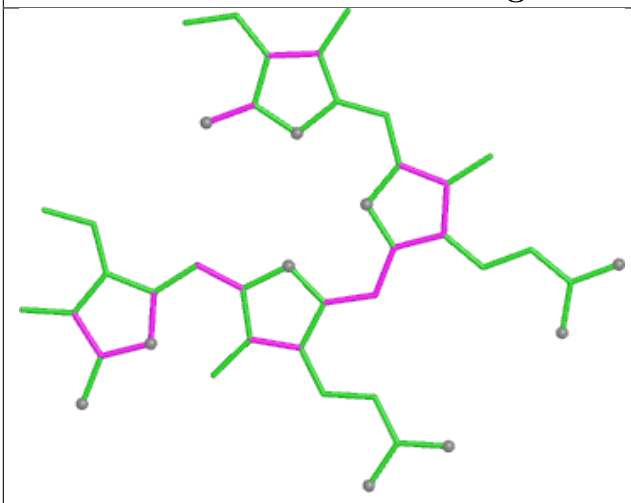


Torsions



Rings

Ligand PEB OM 203



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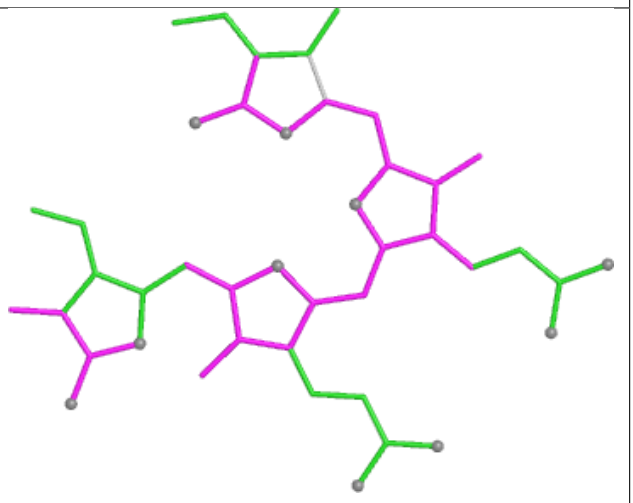

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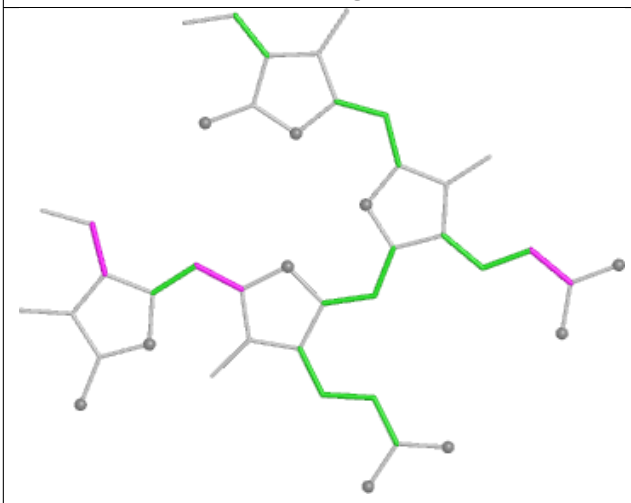

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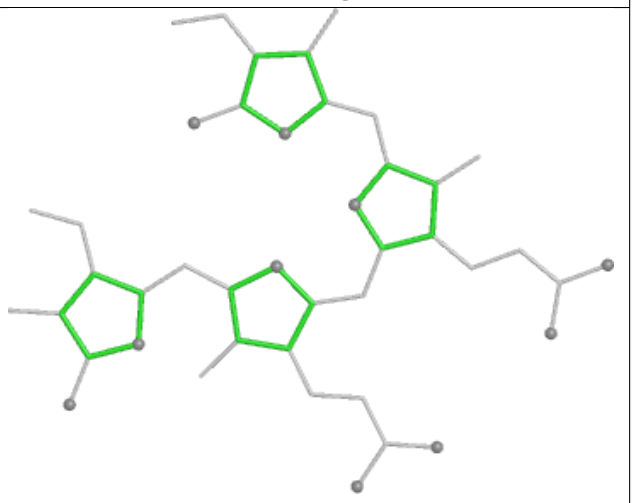
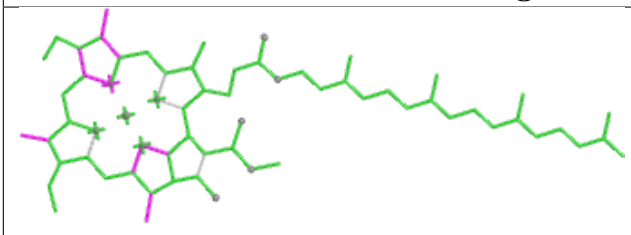


Rings

Ligand CLA C6 509



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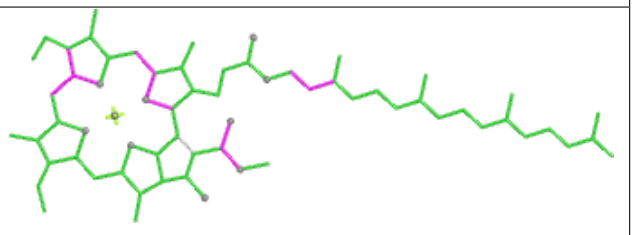
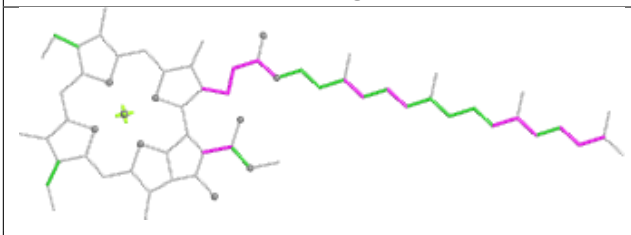


Bond angles



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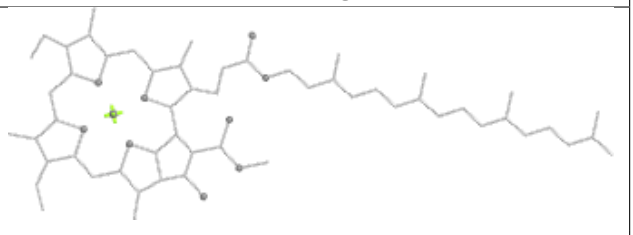
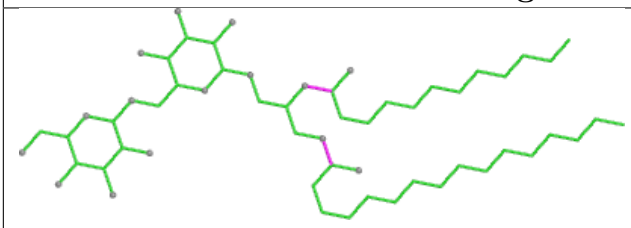


Rings

Ligand DGD lL 101



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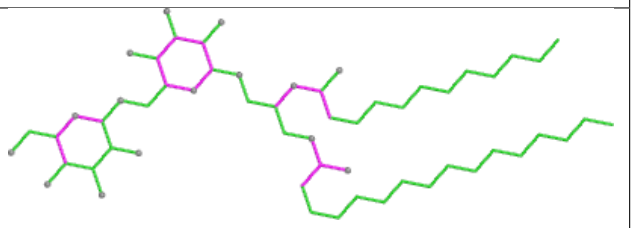
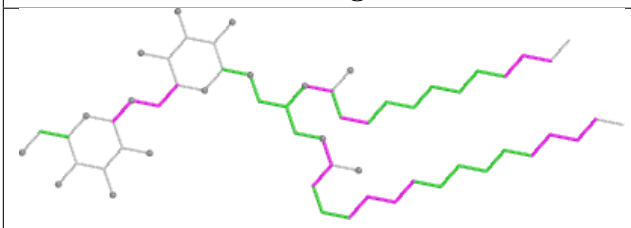


Bond angles



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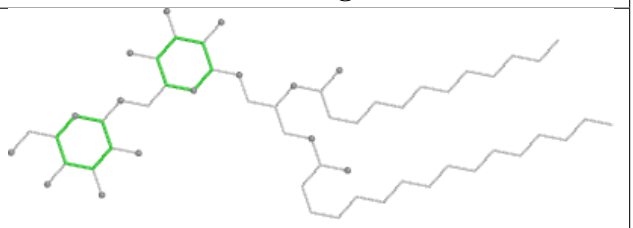
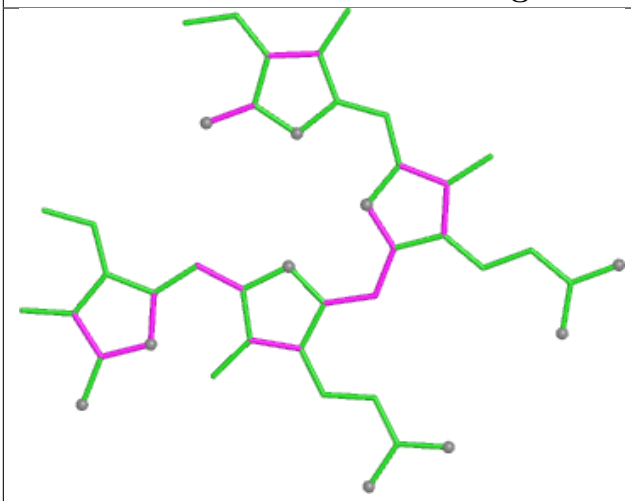


Rings

Ligand PEB YB 202



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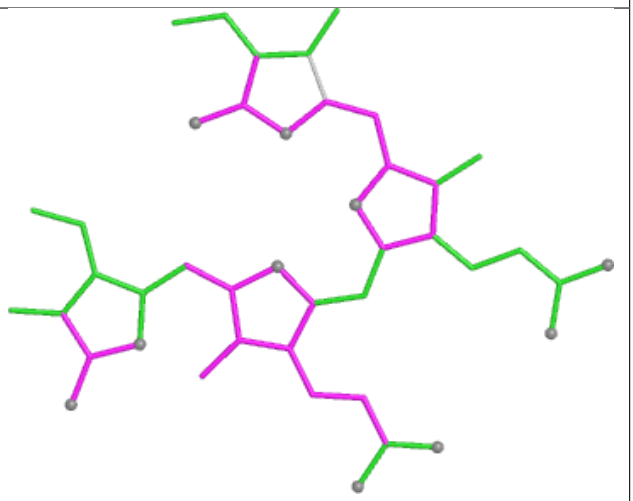
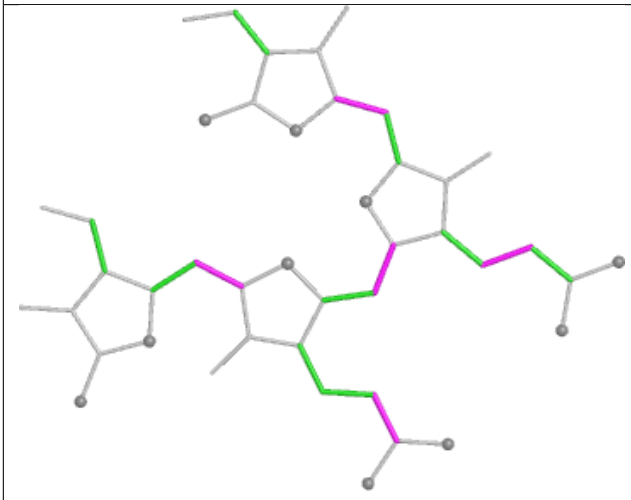
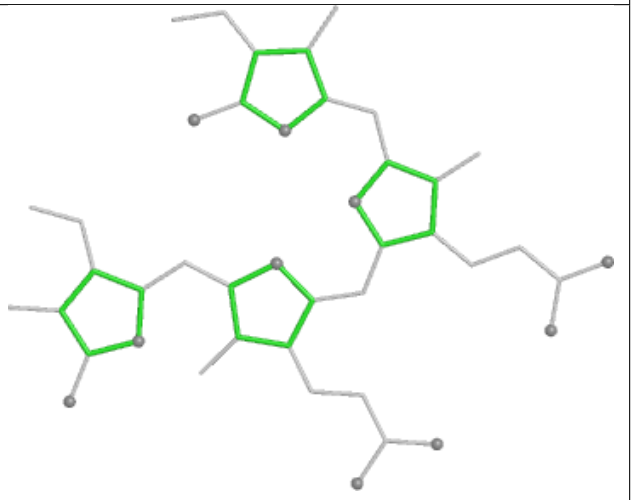


Bond angles

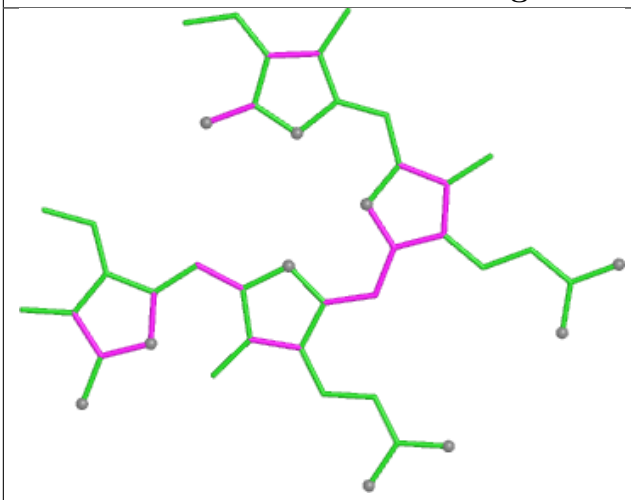


Torsions



Rings

Ligand PEB YO 201



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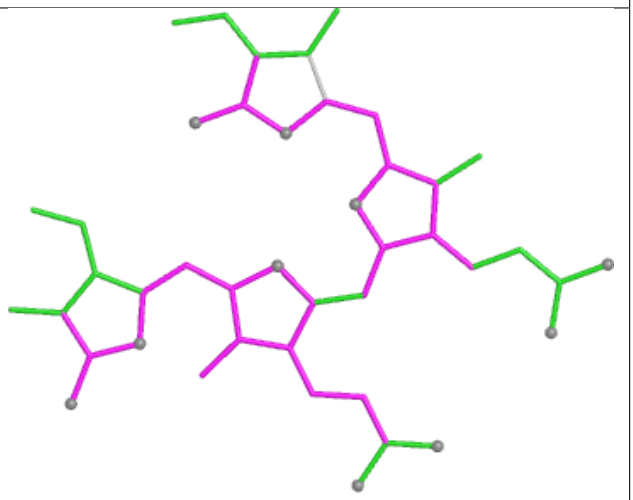

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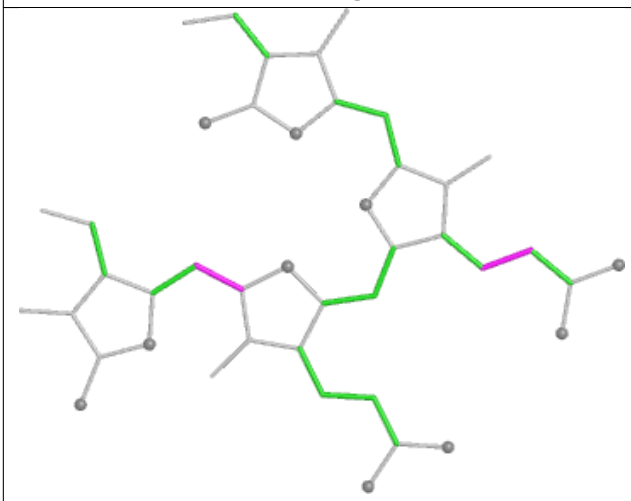

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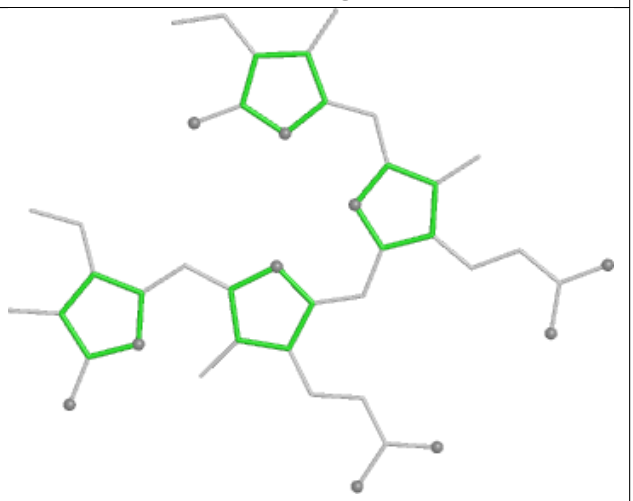
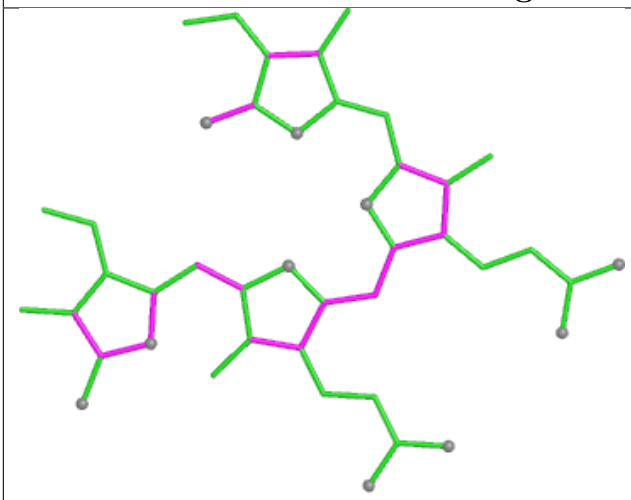


Rings

Ligand PEB V7 203



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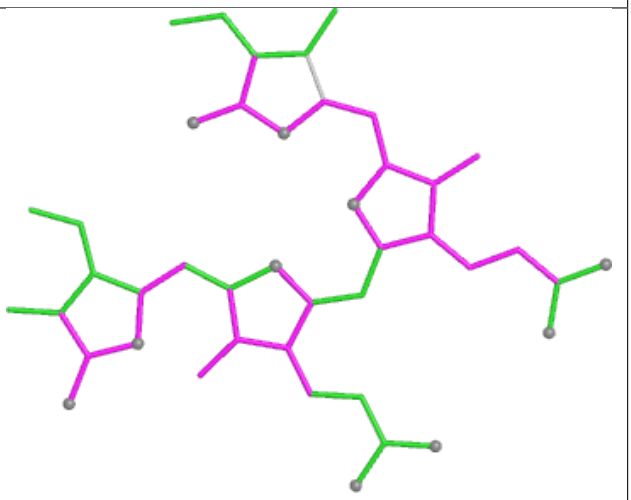

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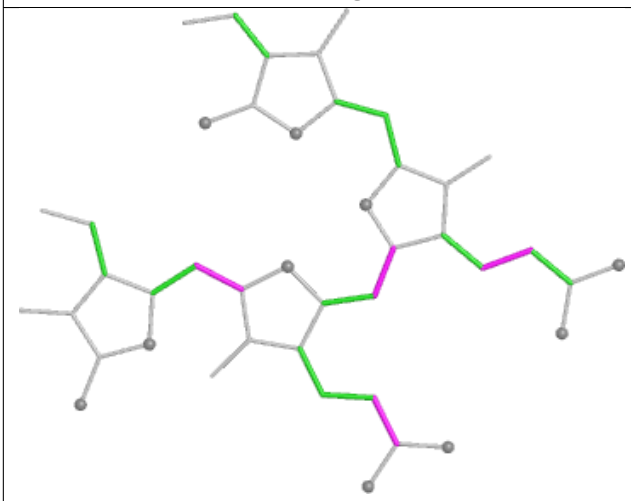

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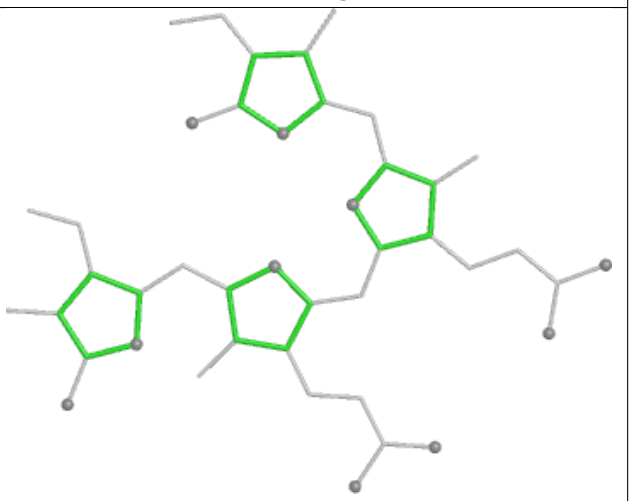
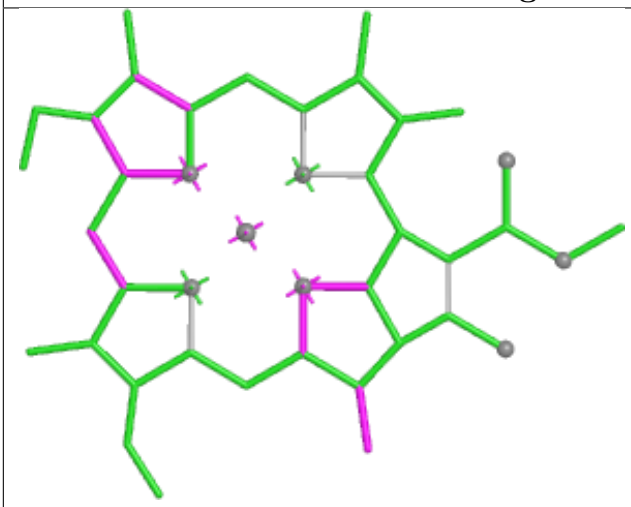


Rings

Ligand CLA 32 310



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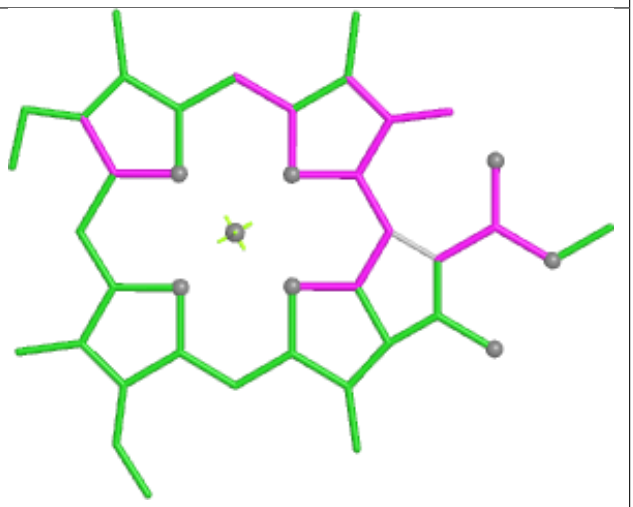
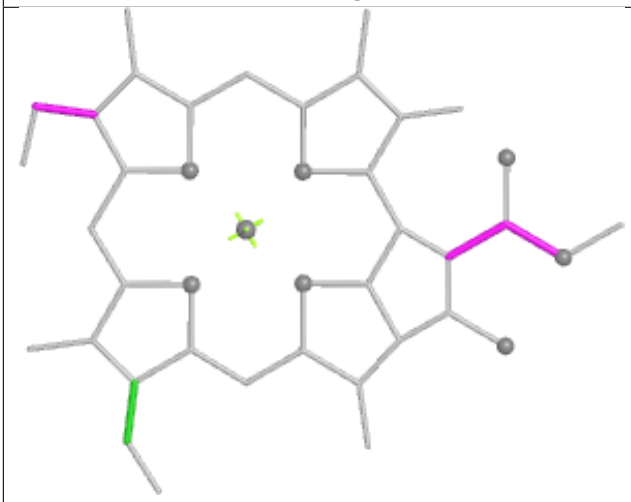


Bond angles



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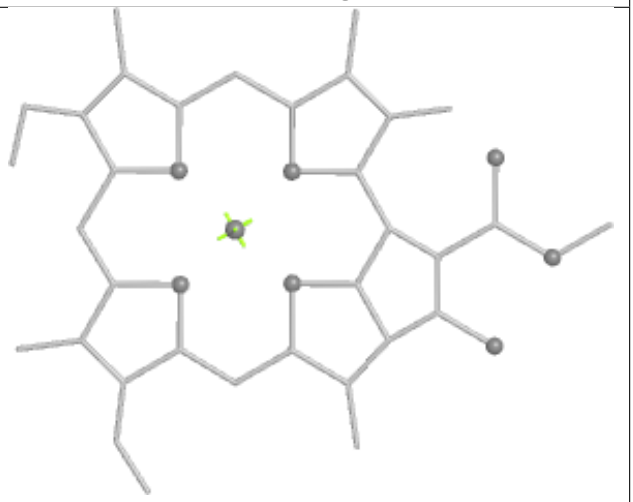
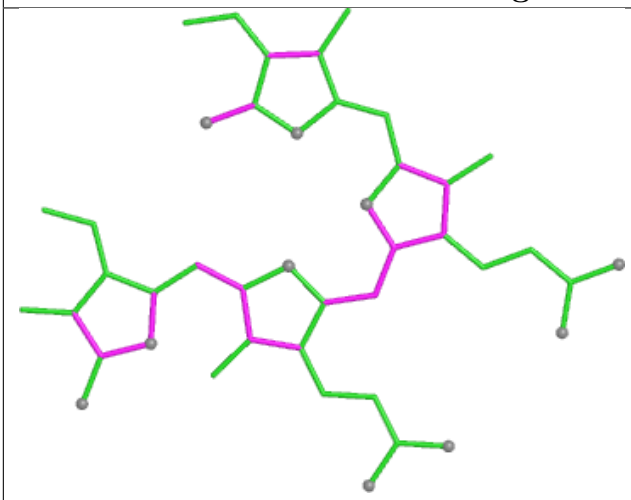


Rings

Ligand PEB QP 201



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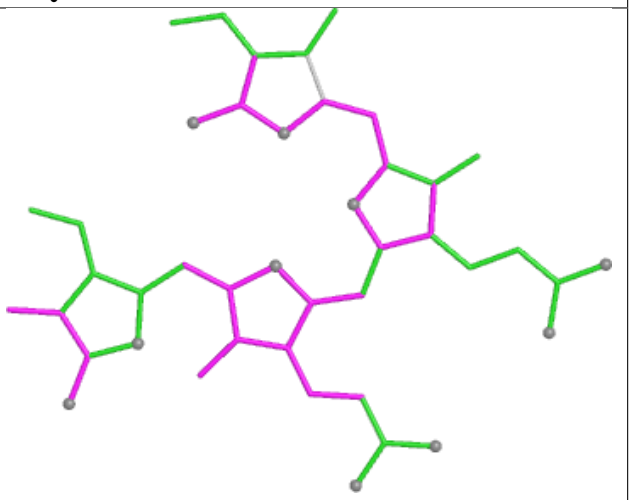
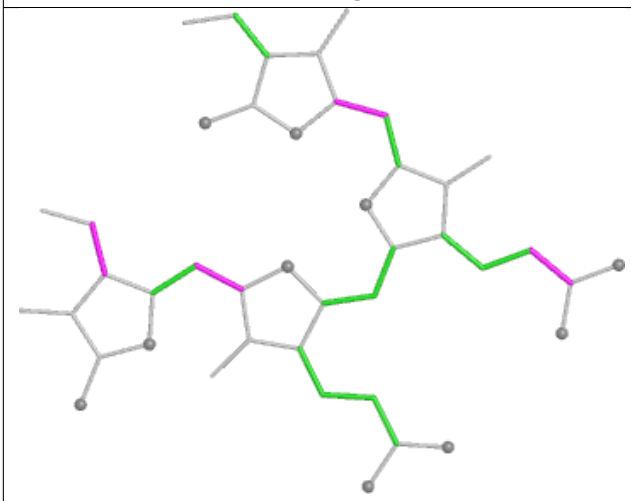


Bond angles



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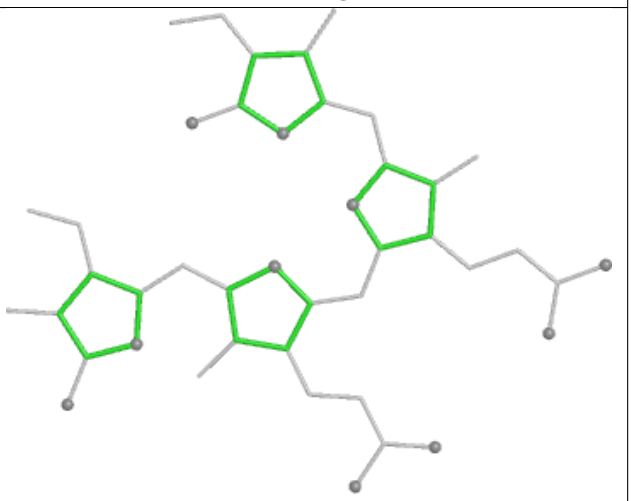
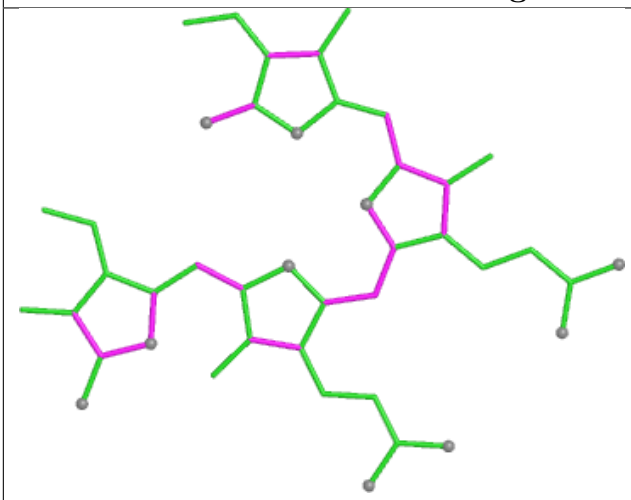


Rings

Ligand PEB FM 201



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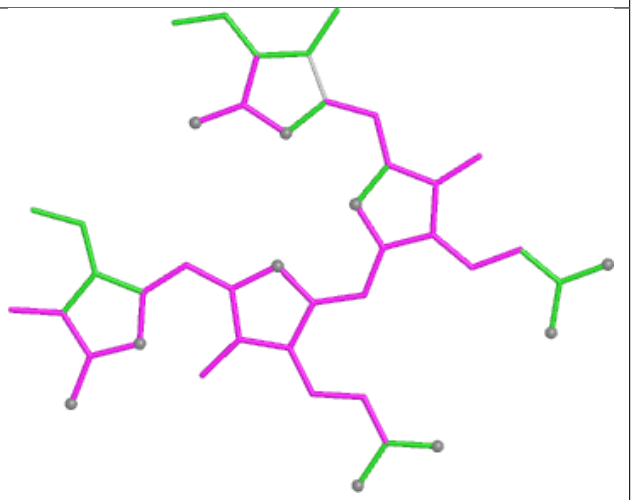
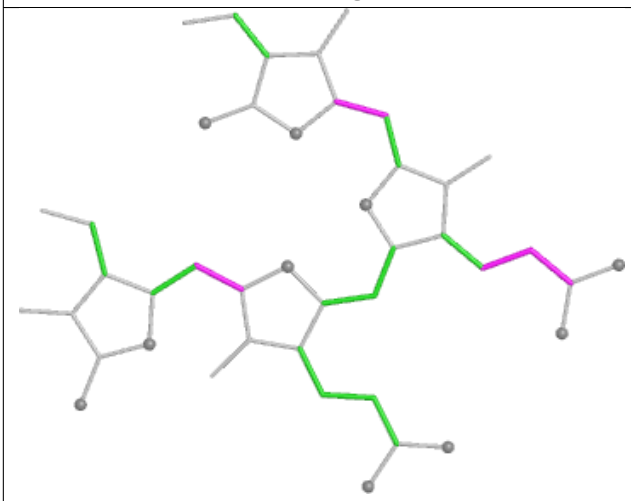


Bond angles



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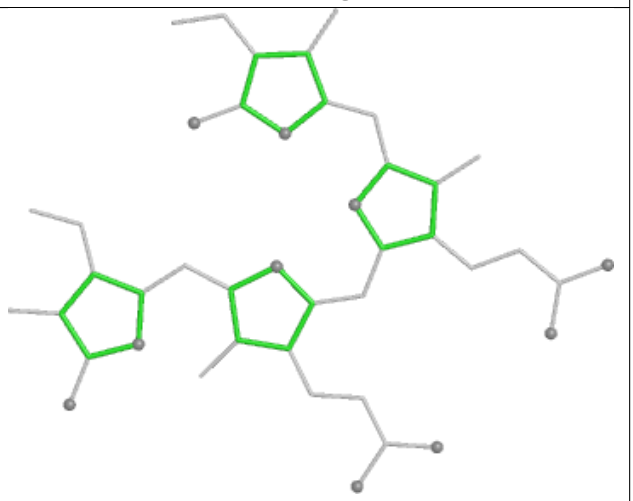

Rings

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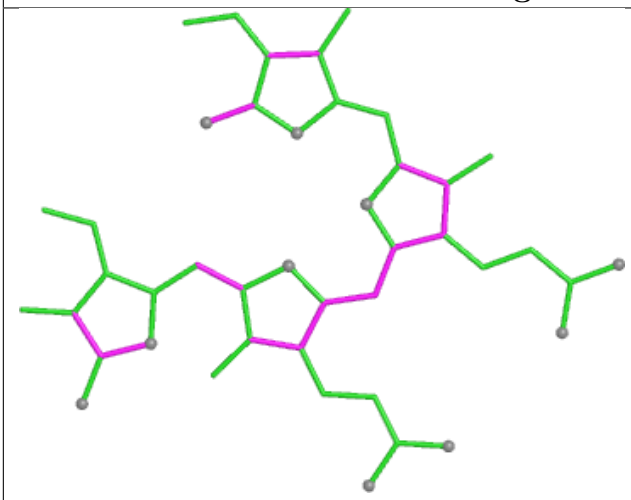

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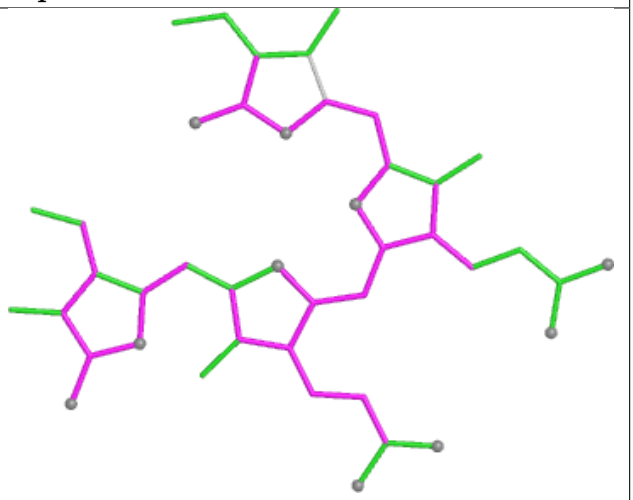
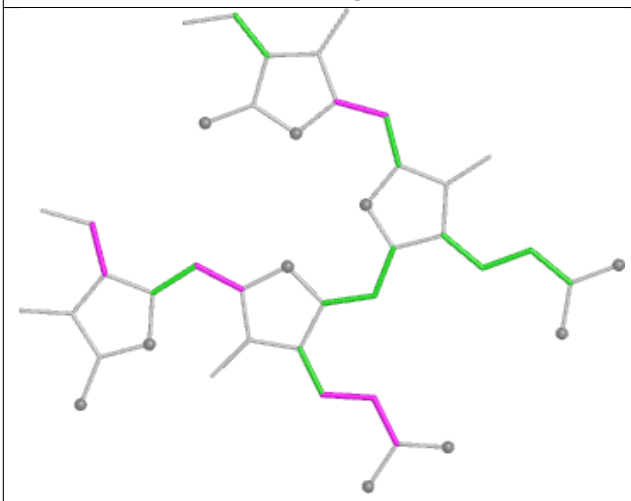


Bond angles



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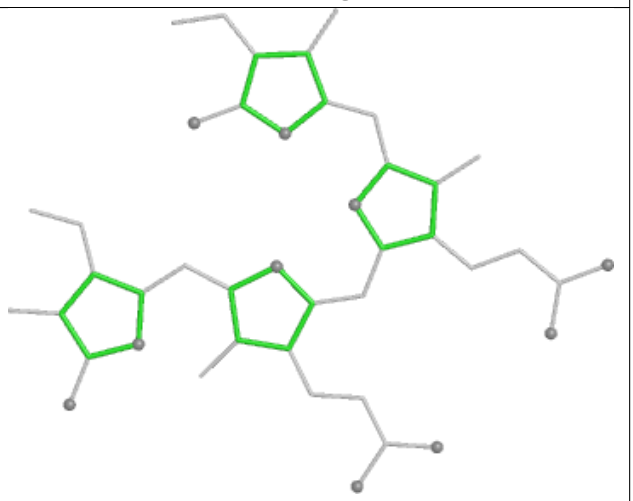
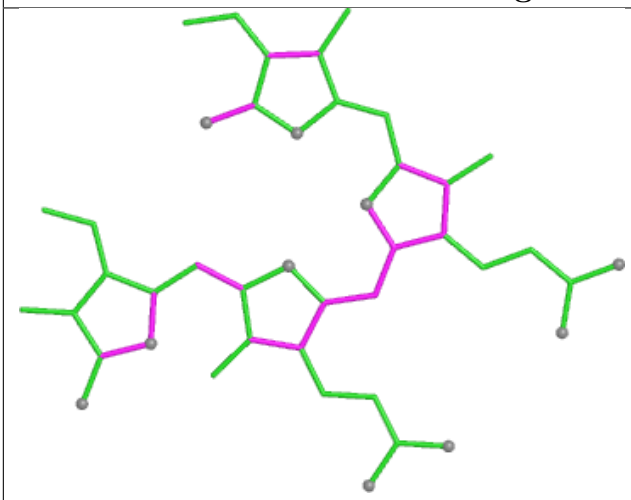


Rings

Ligand PEB H9 201



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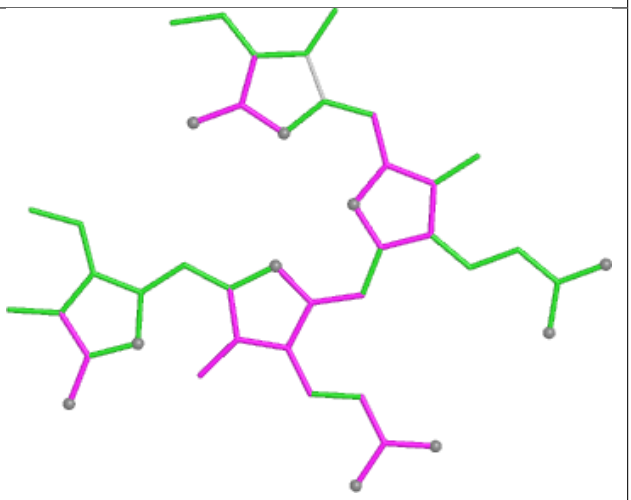

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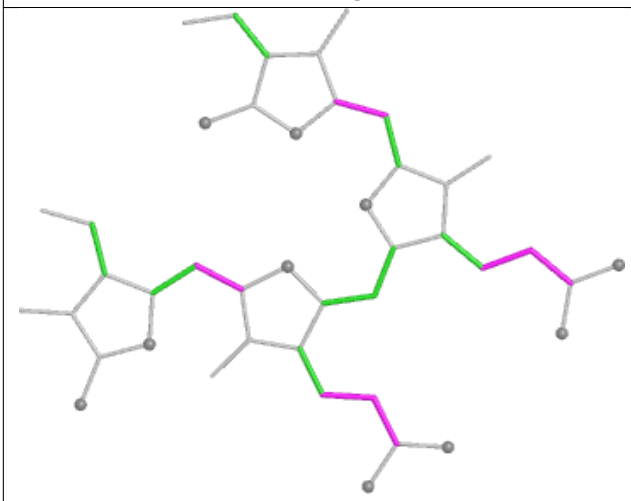

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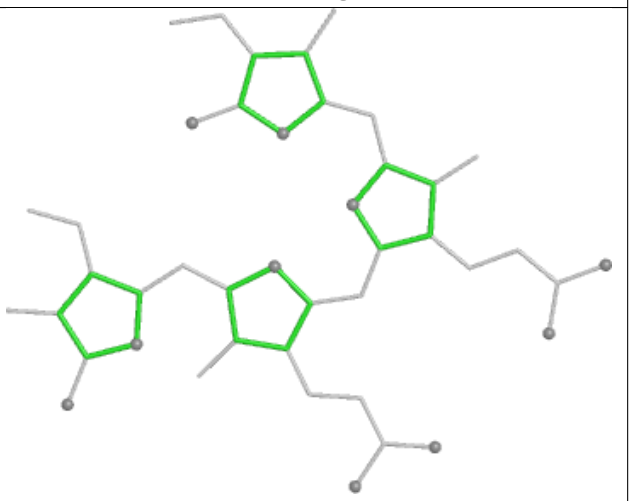
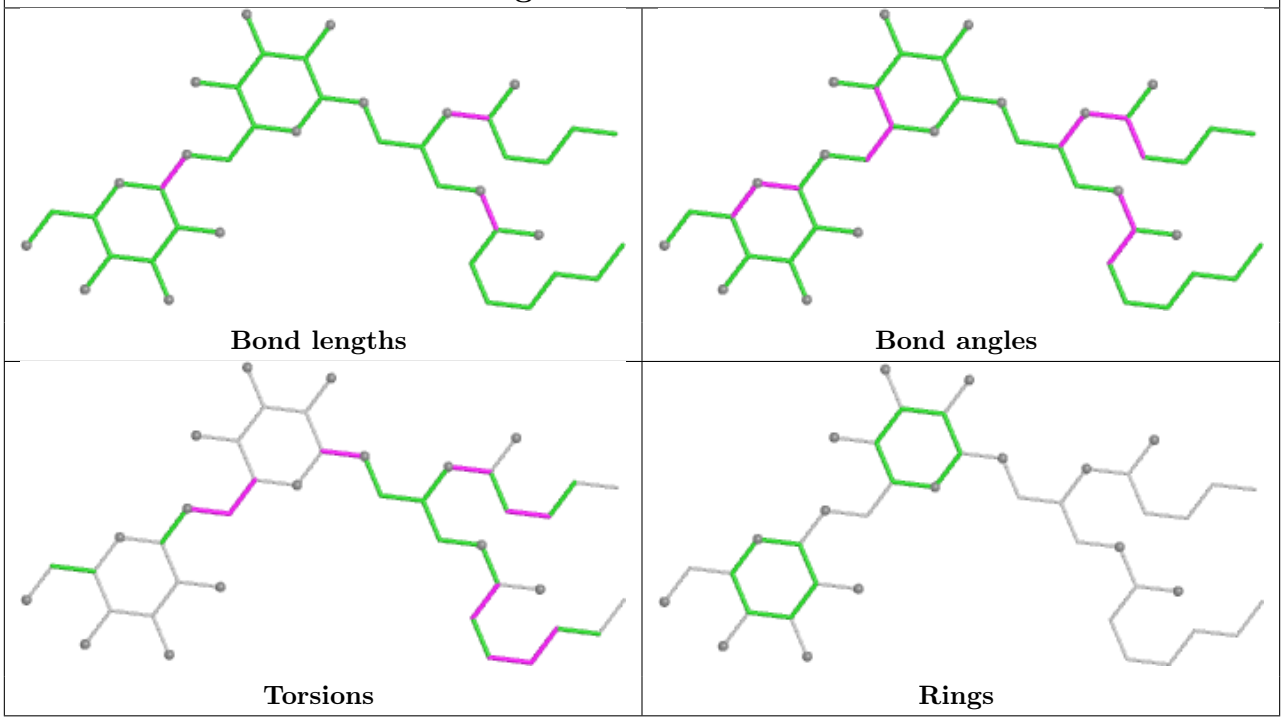
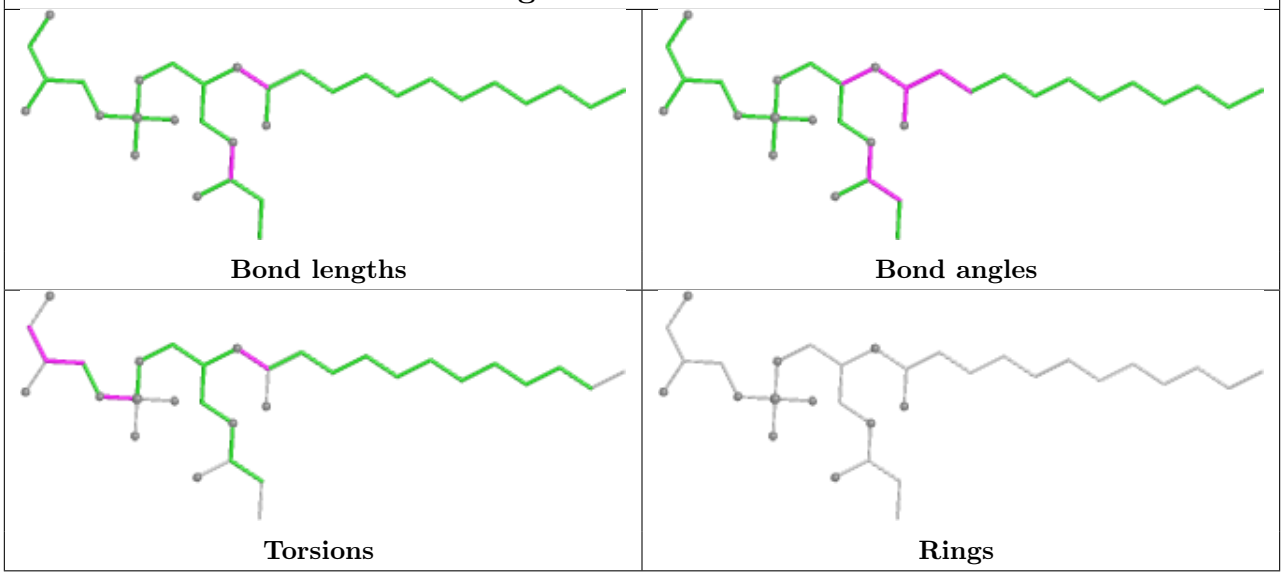


Rings

Ligand DGD b6 622



Ligand LHG cL 501



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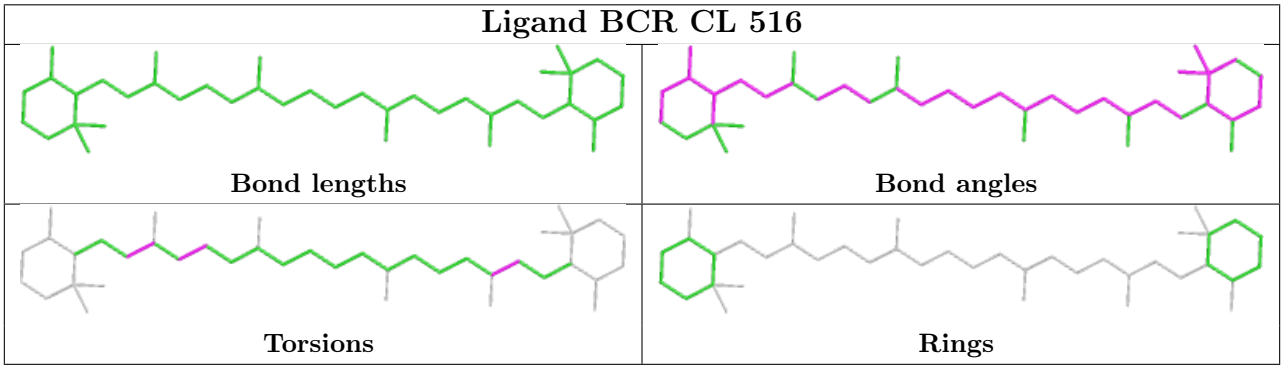
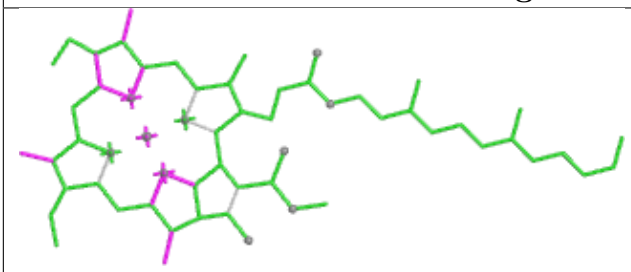


Ligand CLA B2 816



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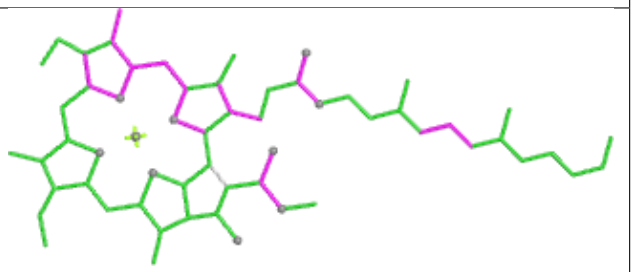
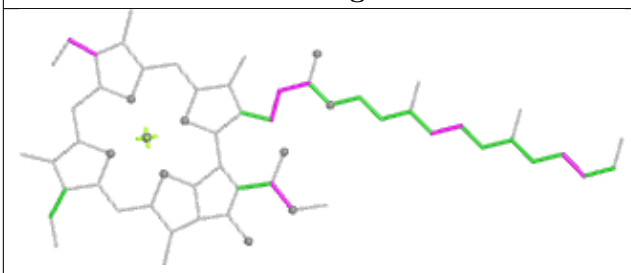


Bond angles



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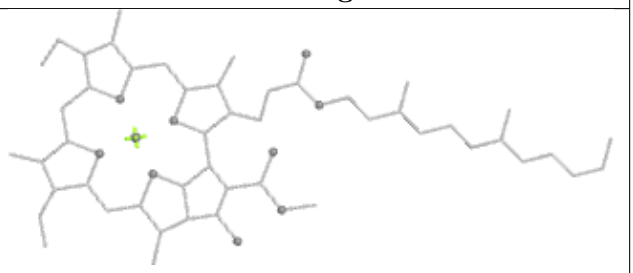
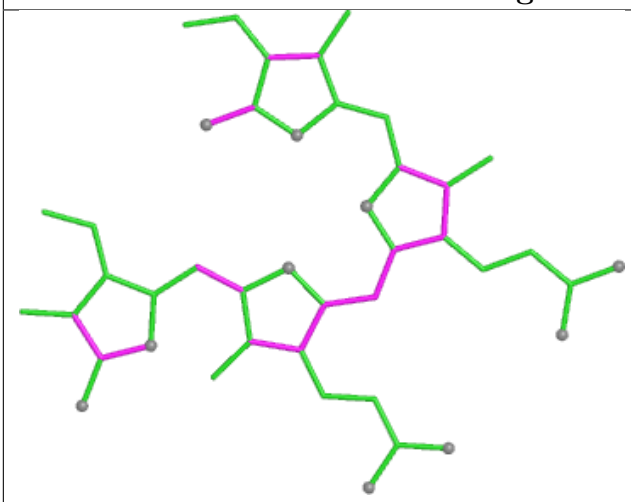


Rings

Ligand PEB P7 202



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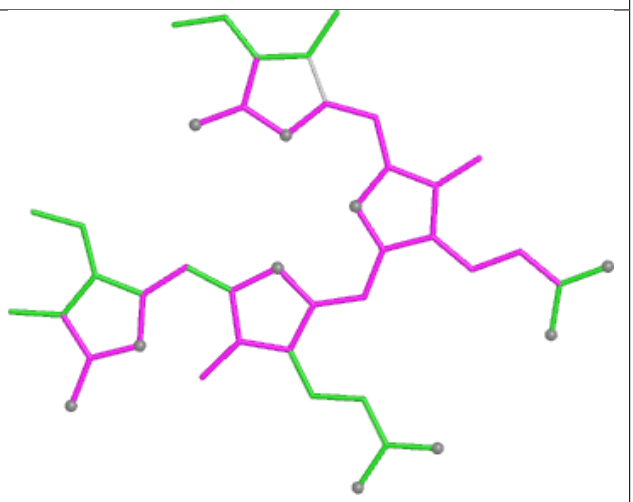
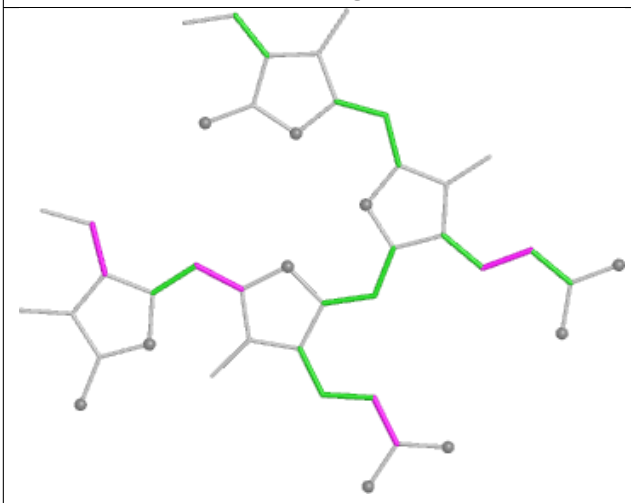


Bond angles



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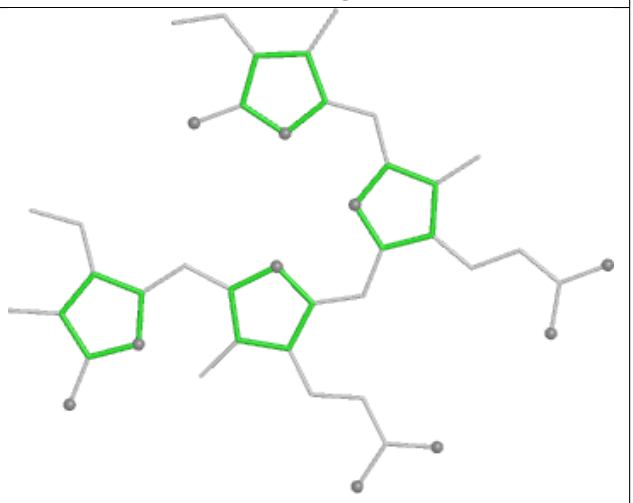
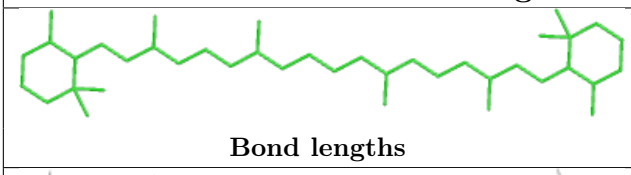


Rings

Ligand BCR IN 101



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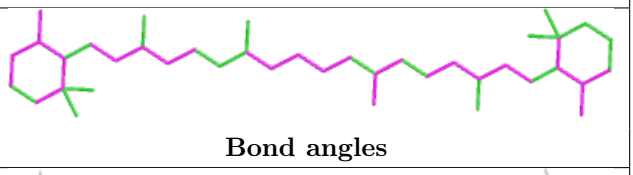
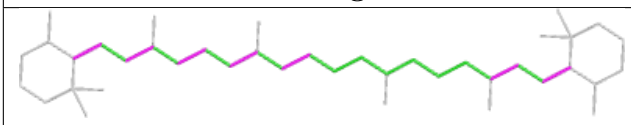


Bond angles



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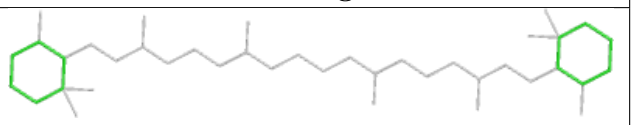
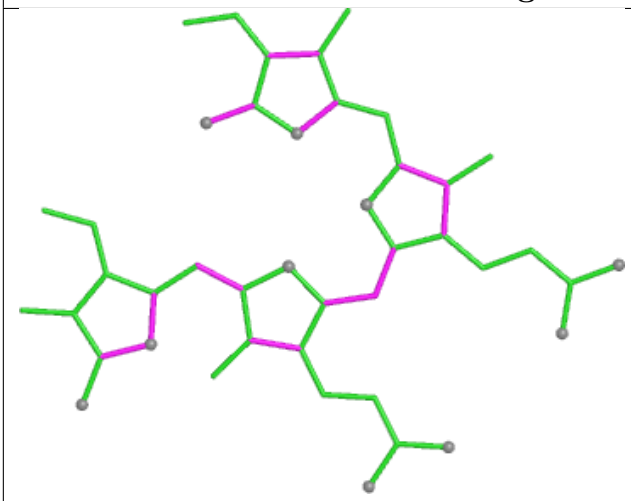


Rings

Ligand PEB Z9 301



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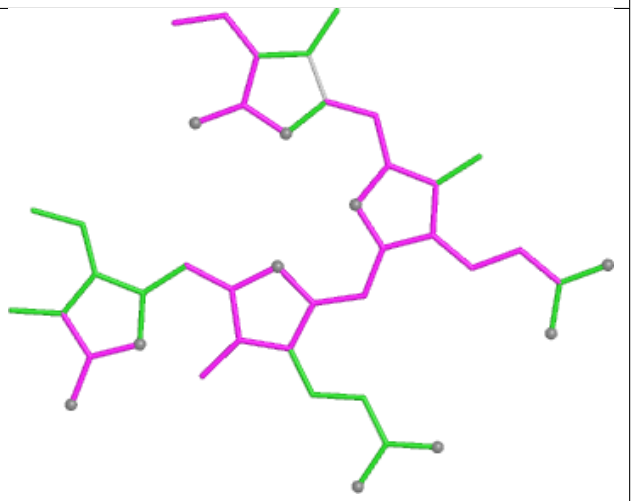
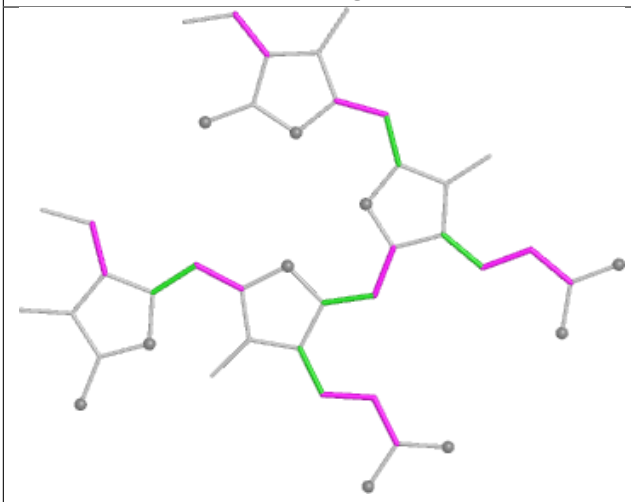


Bond angles



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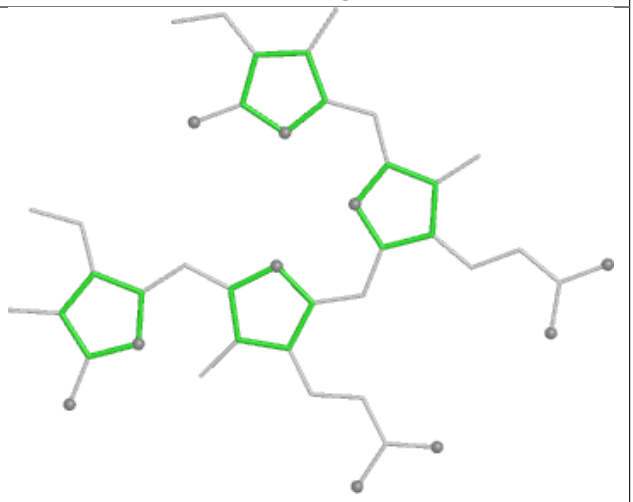
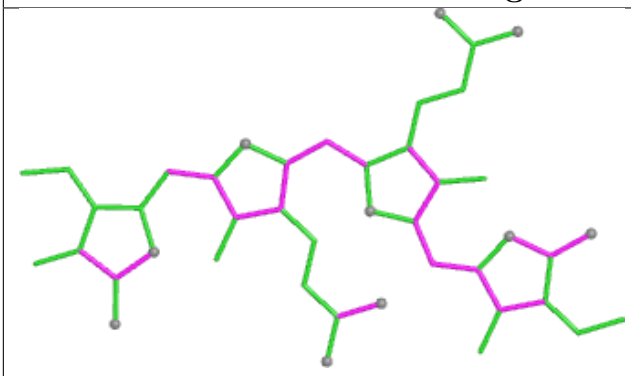


Rings

Ligand CYC F3 1001



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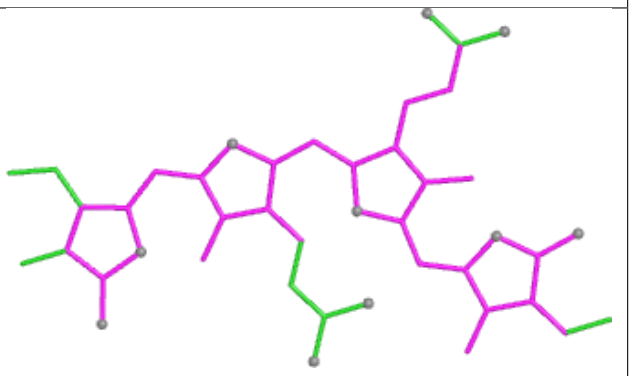
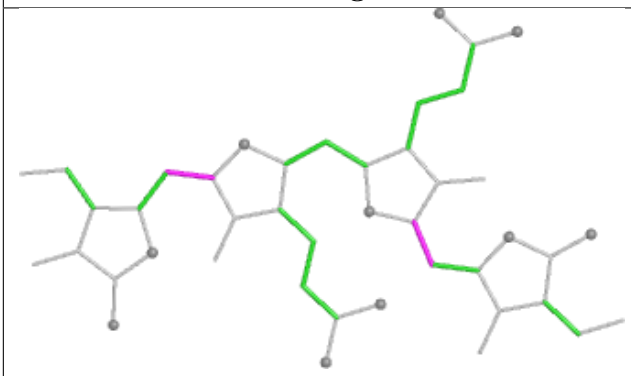


Bond angles



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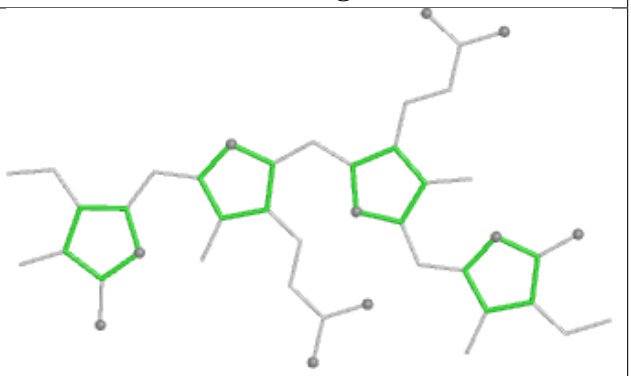
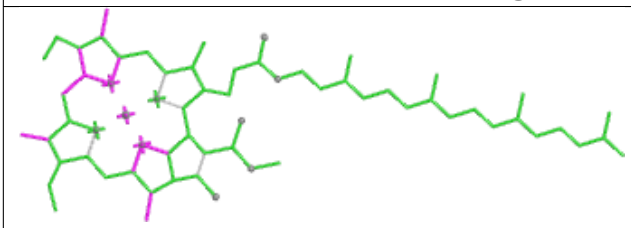


Rings

Ligand CLA AN 831



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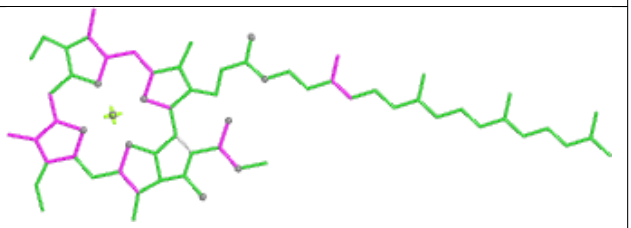
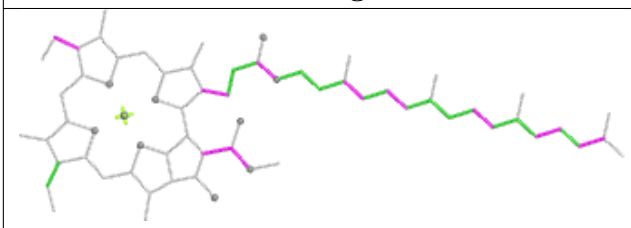


Bond angles



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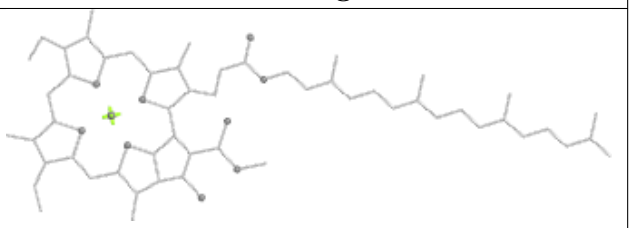
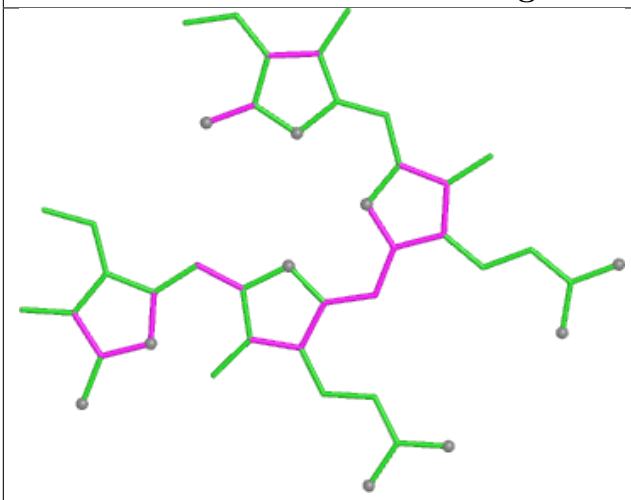
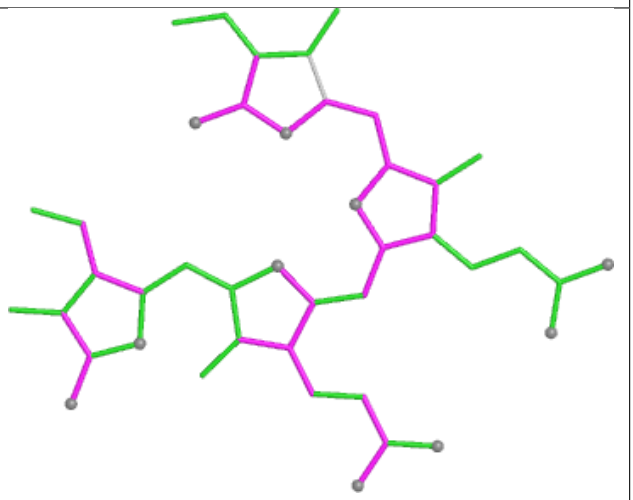


Rings

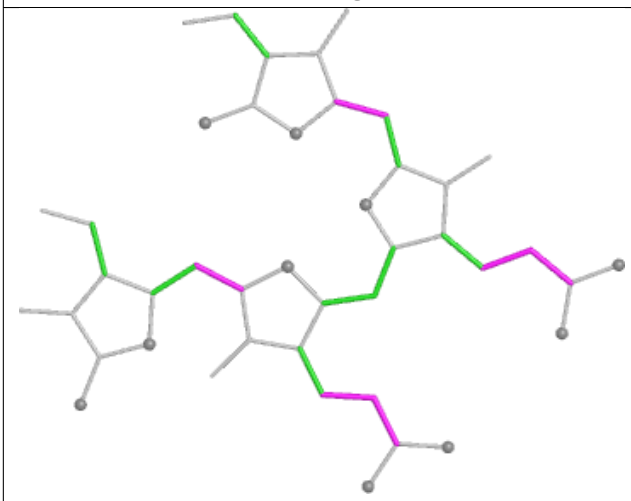
Ligand PEB L9 201



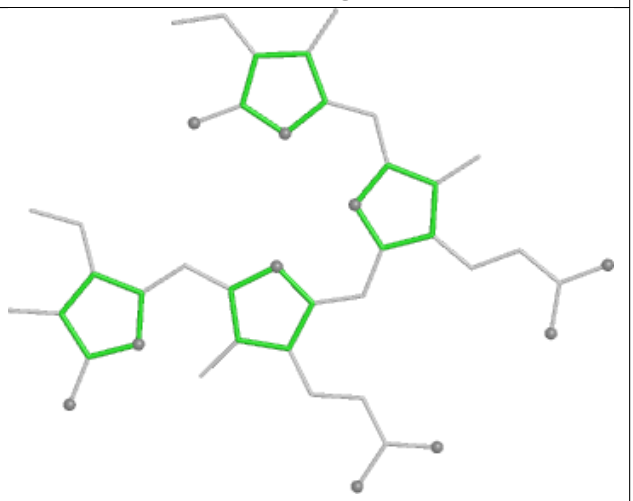
Bond lengths



Bond angles

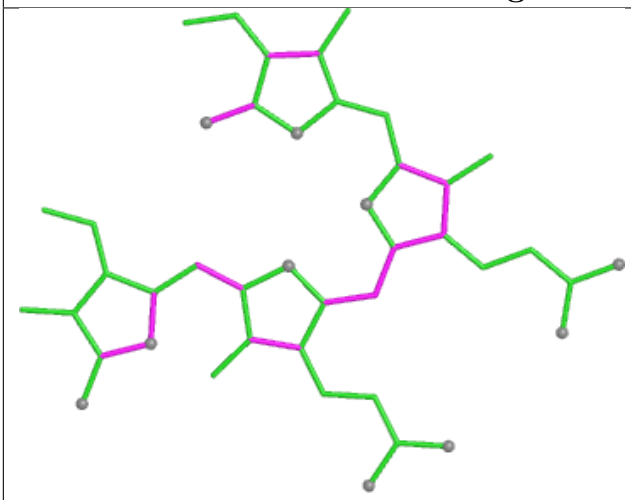


Torsions



Rings

Ligand PEB MQ 202



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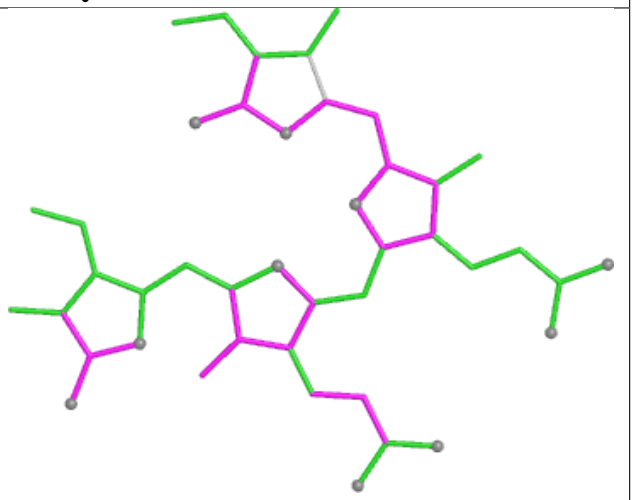

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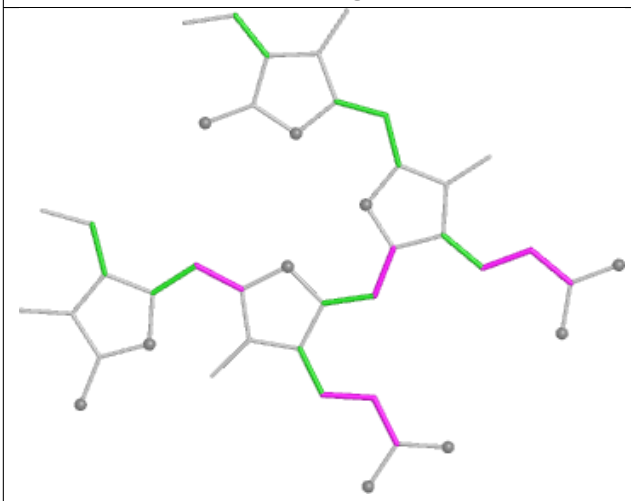

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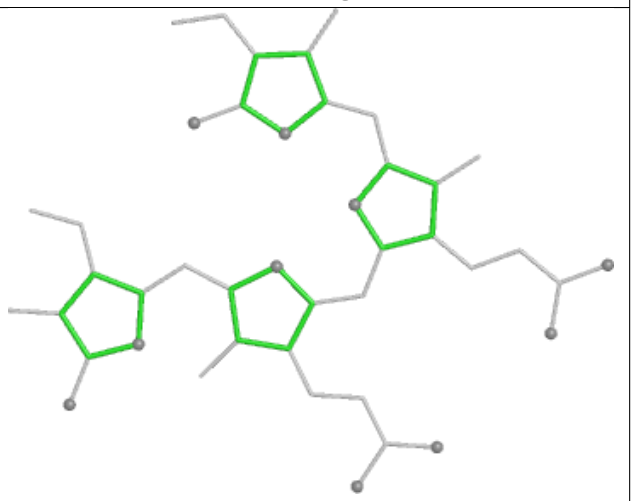
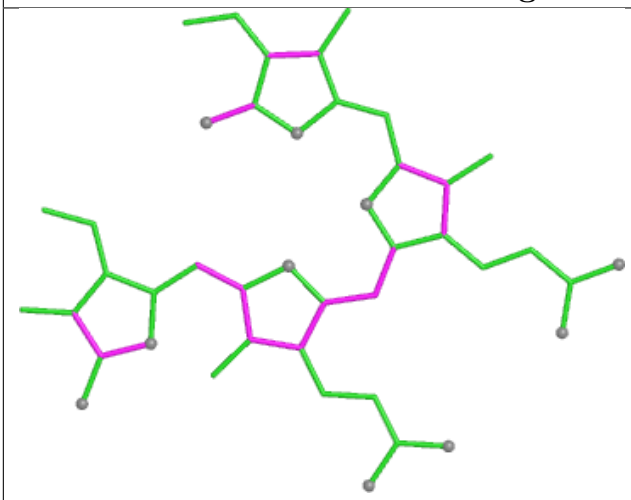


Rings

Ligand PEB iH 202



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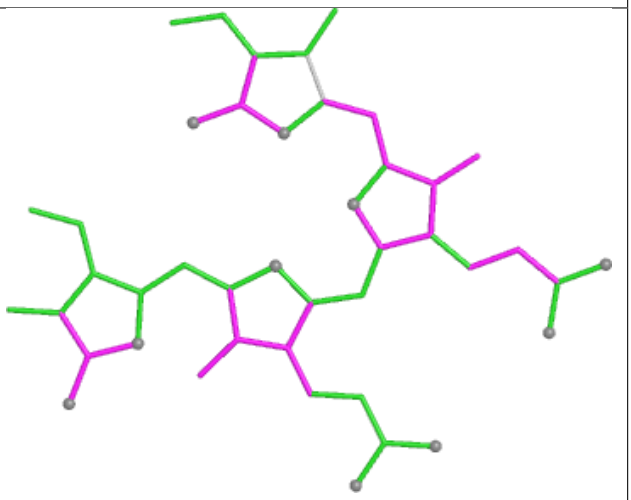

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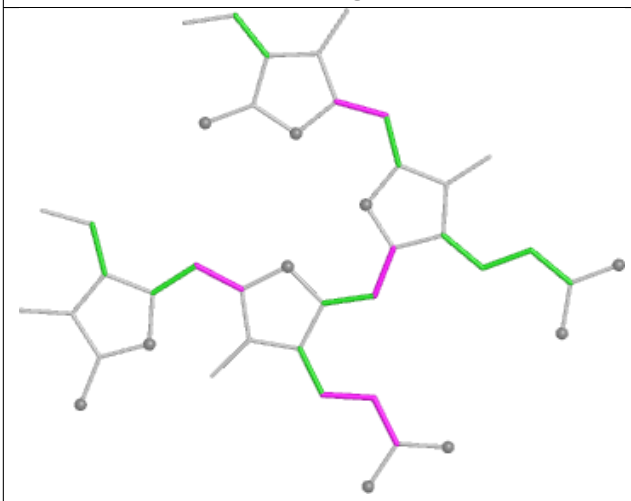

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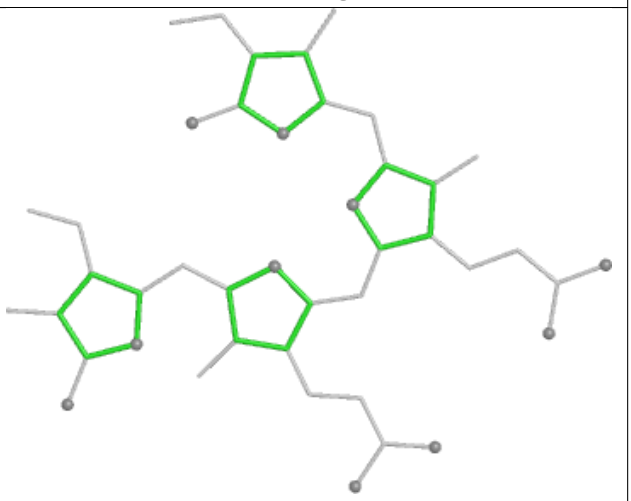
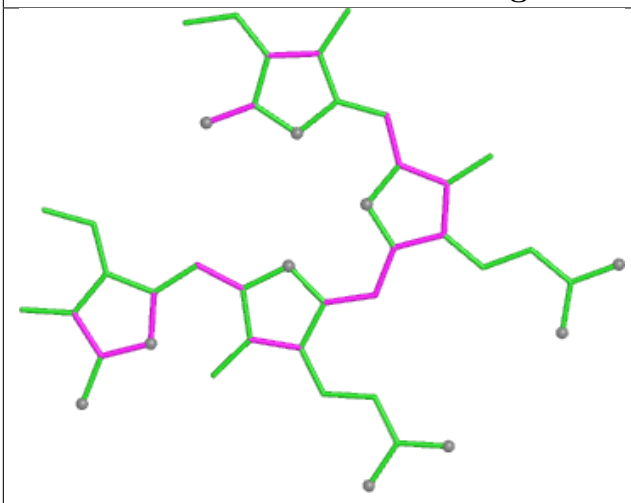


Rings

Ligand PEB HA 201



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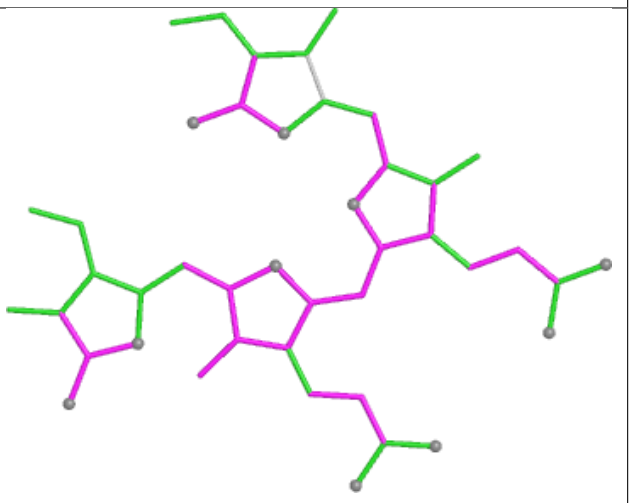

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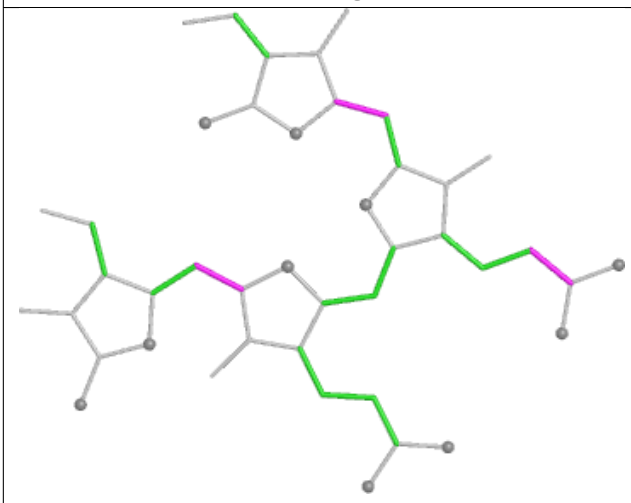

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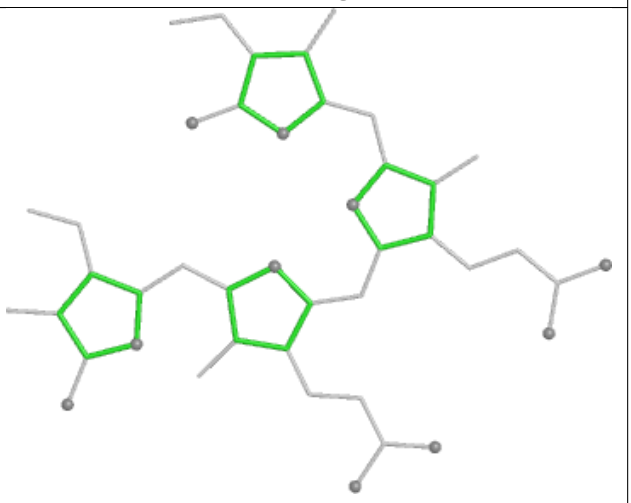
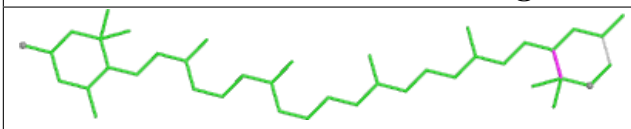


Rings

Ligand ZEX 8N 309



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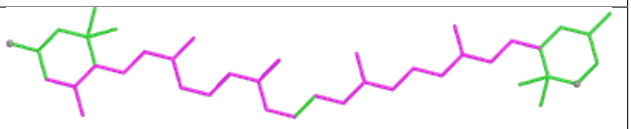

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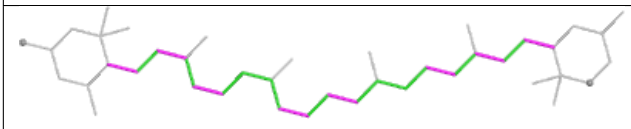

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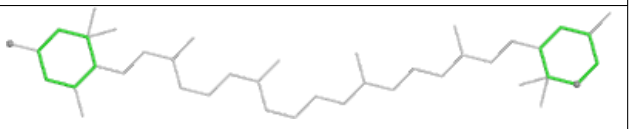
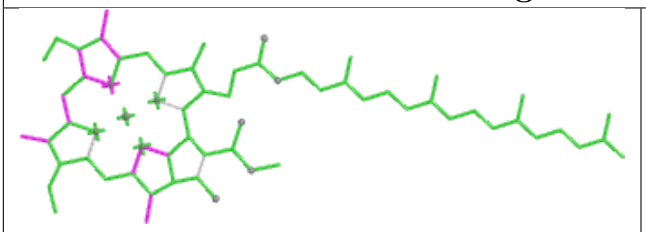


Rings

Ligand CLA C6 510



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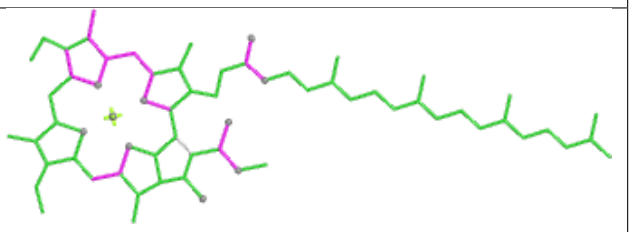

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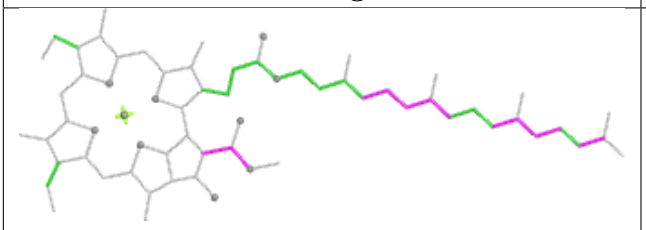

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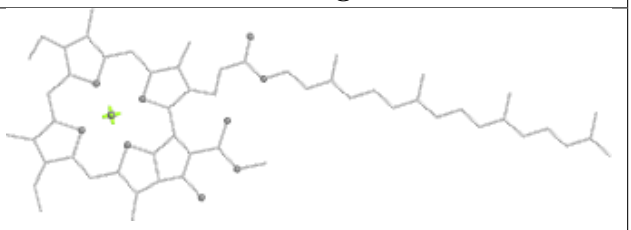
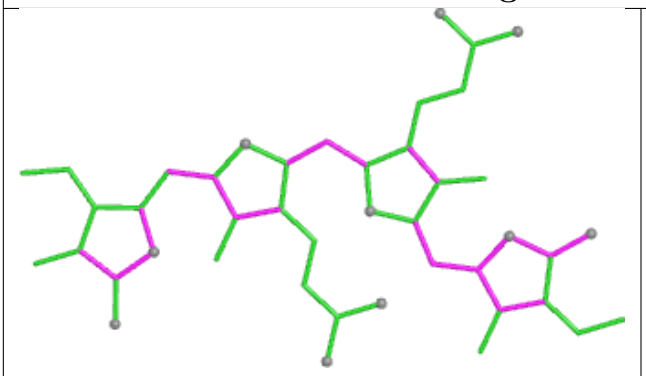


Rings

Ligand CYC CO 1001



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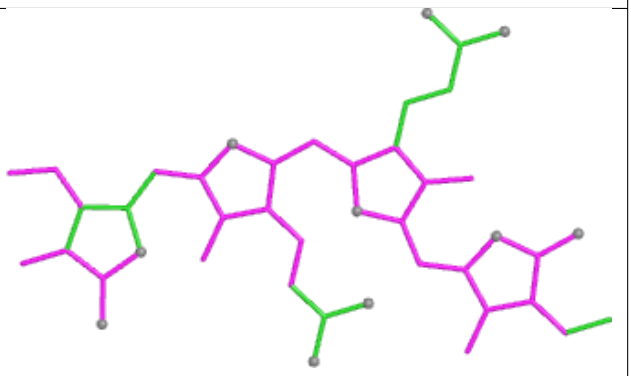

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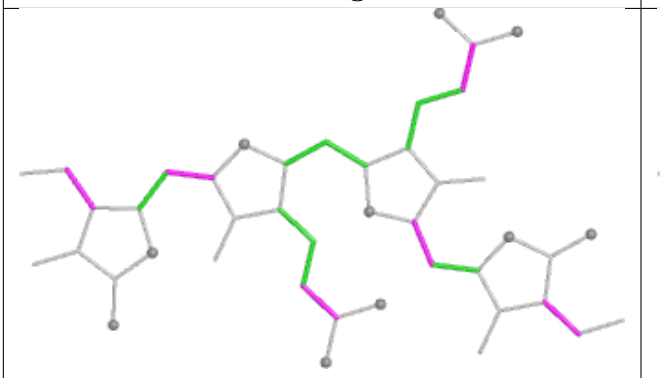

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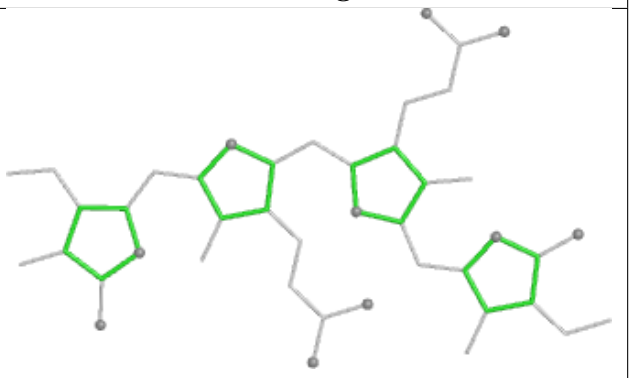
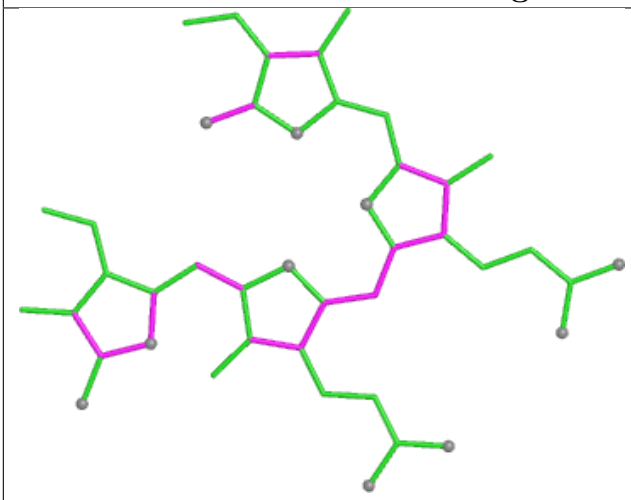


Rings

Ligand PEB kM 202



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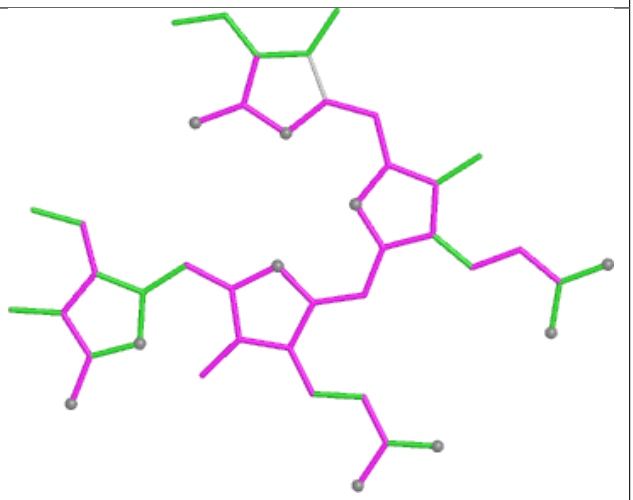

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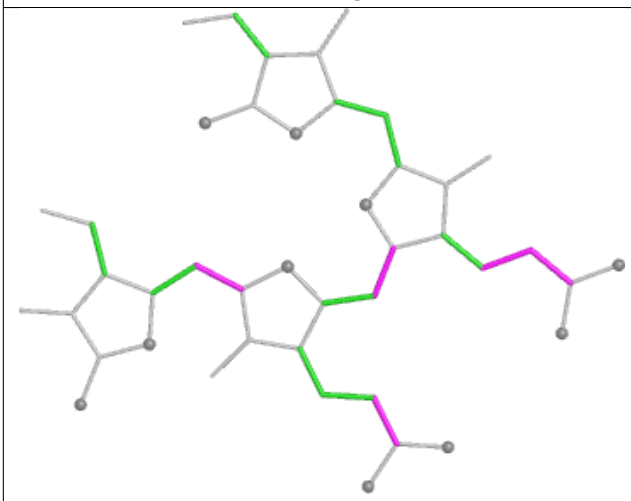

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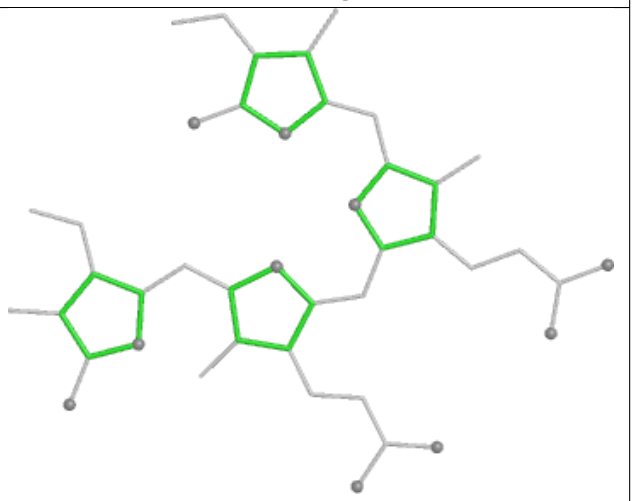
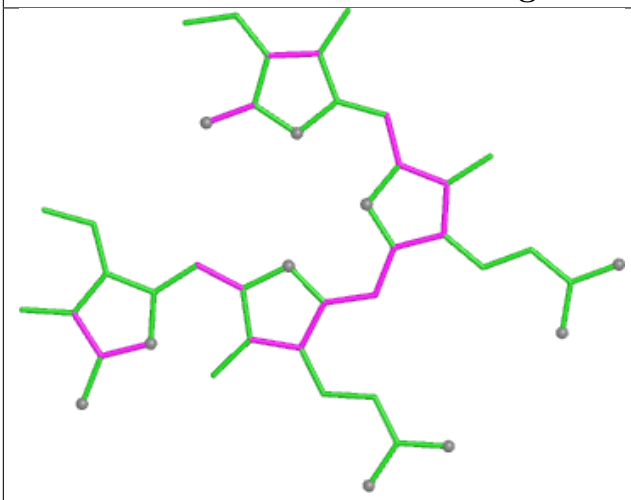


Rings

Ligand PEB lH 202



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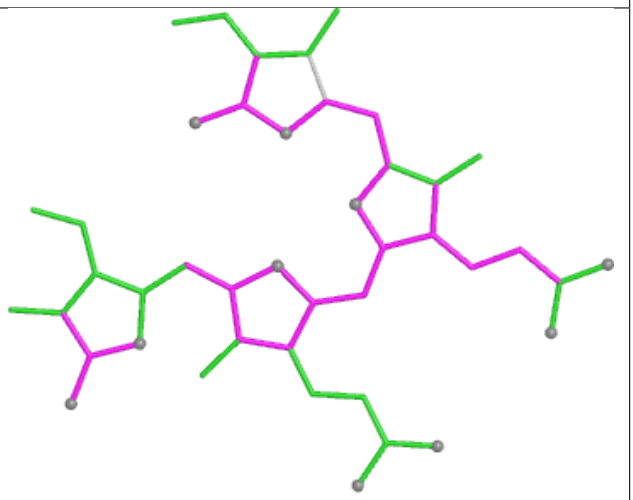

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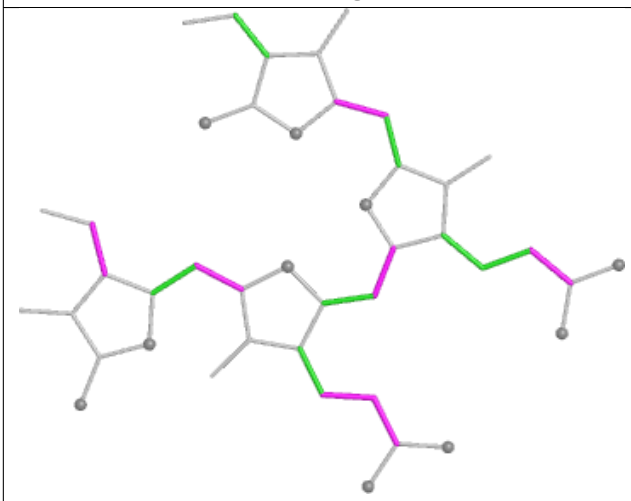

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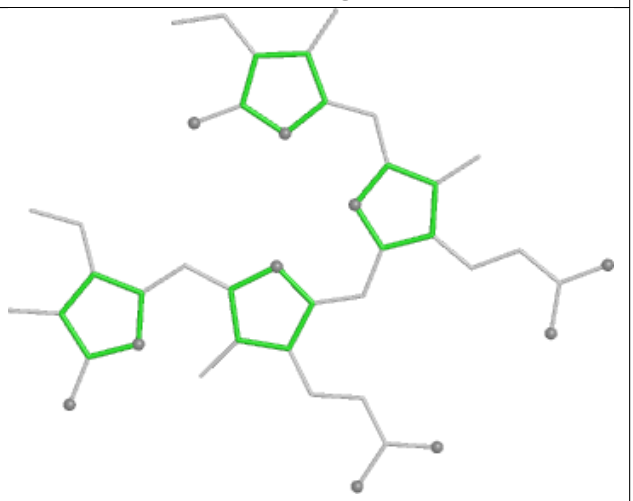
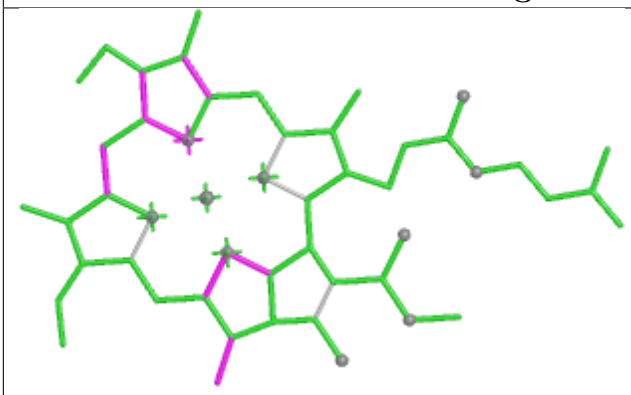


Rings

Ligand CLA 1N 607



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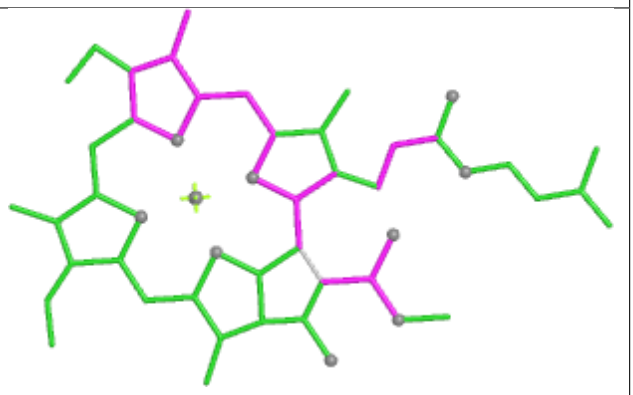

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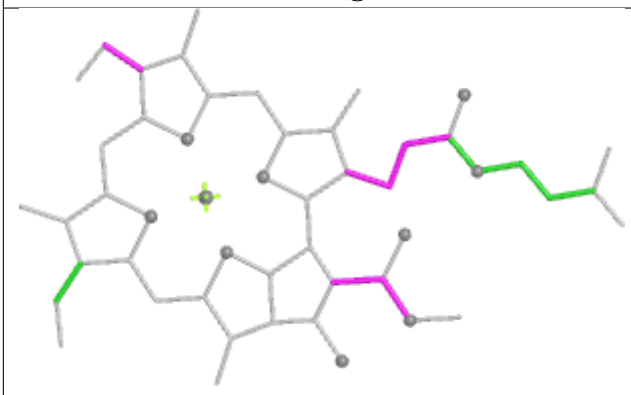

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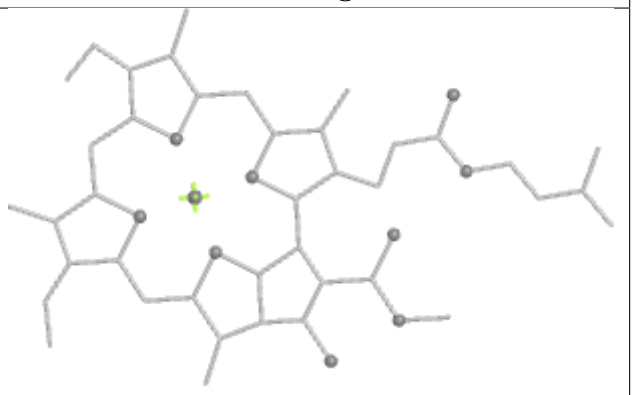
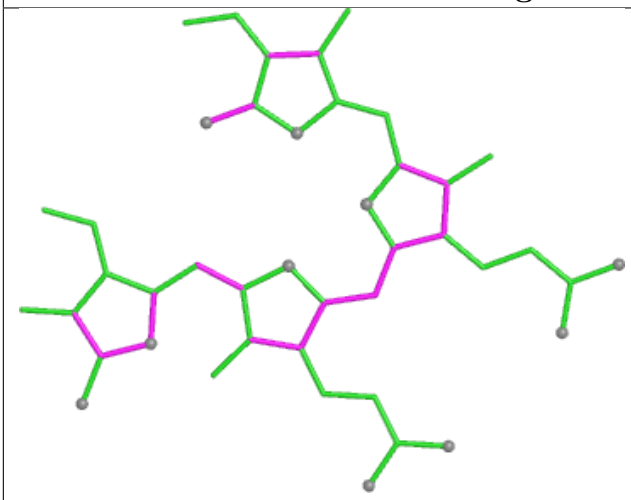


Rings

Ligand PEB yC 203



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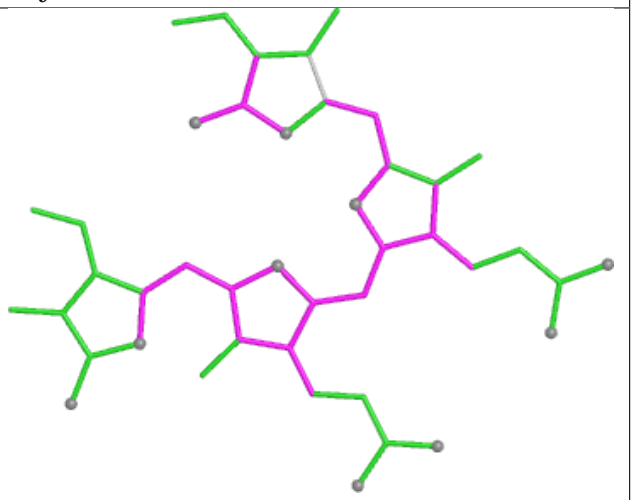

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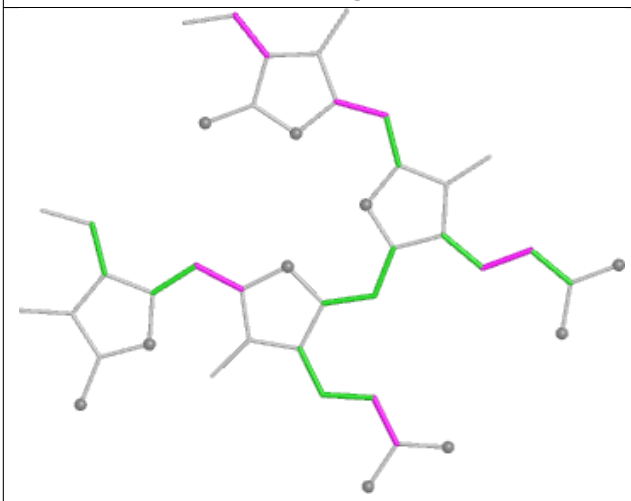

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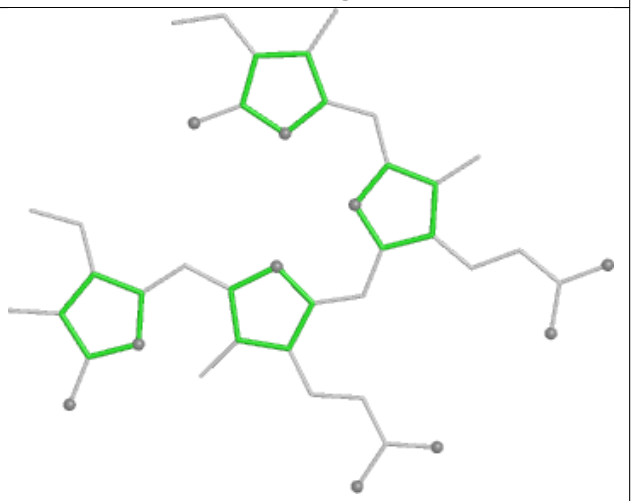
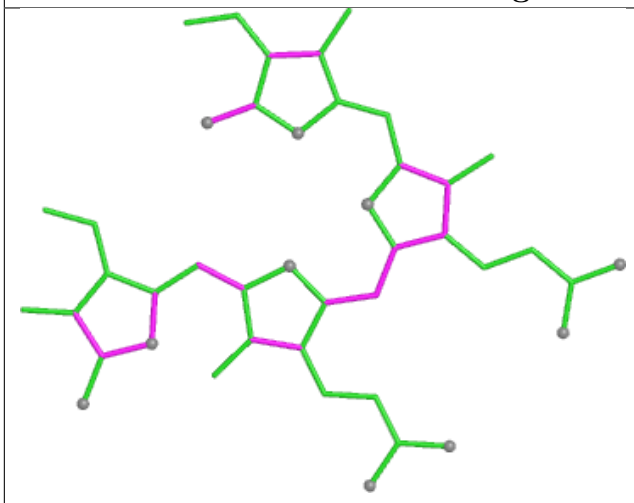


Rings

Ligand PEB GP 202



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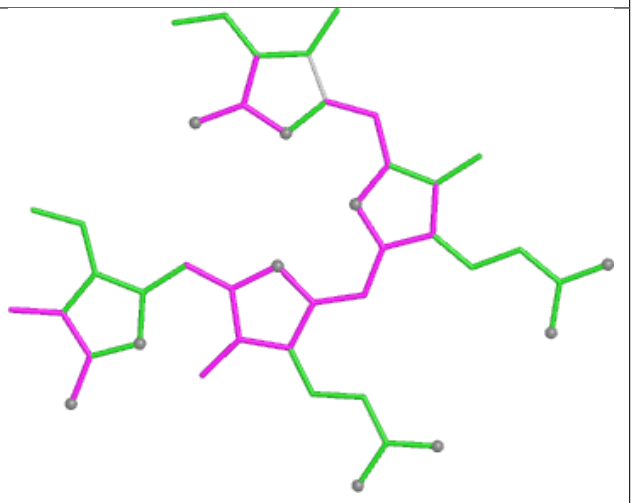

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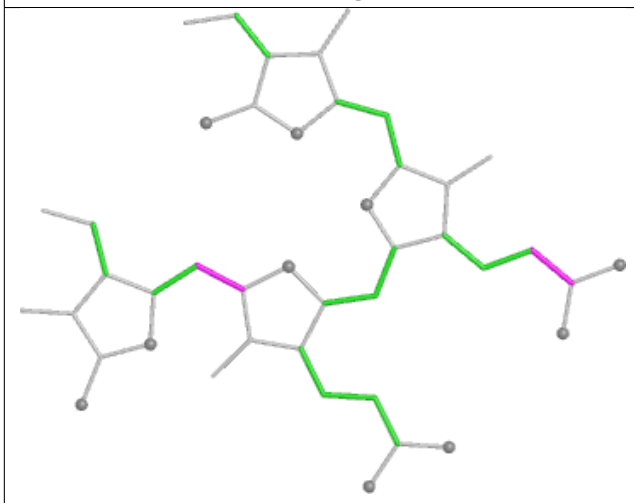

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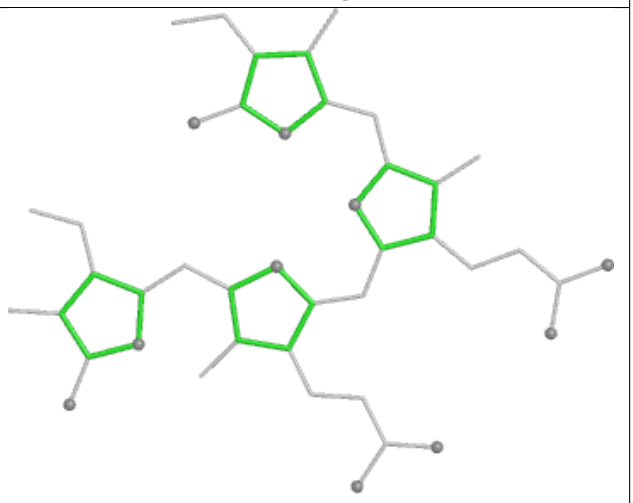
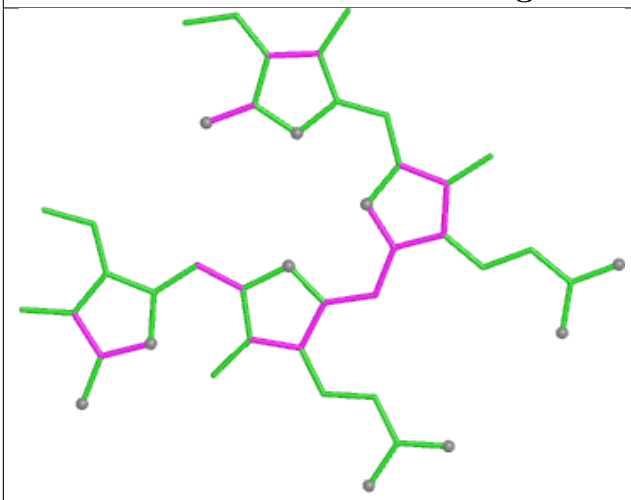


Rings

Ligand PEB C9 202



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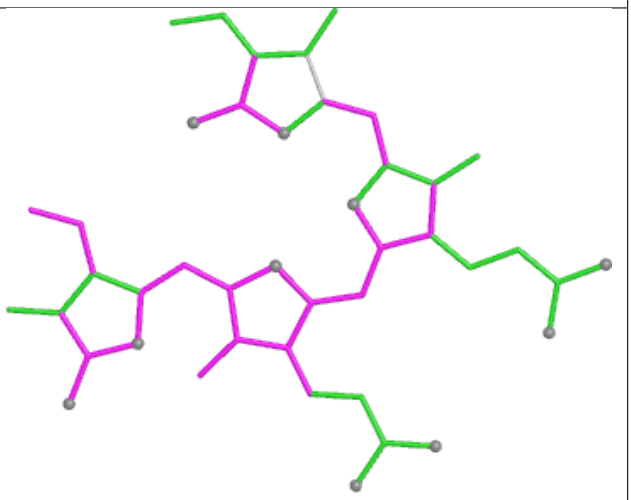

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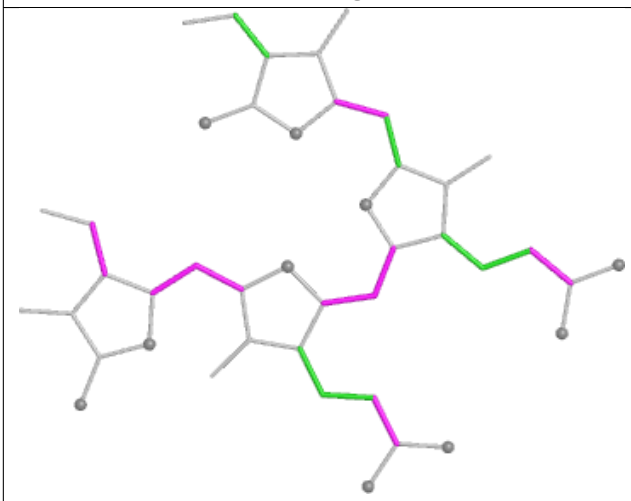

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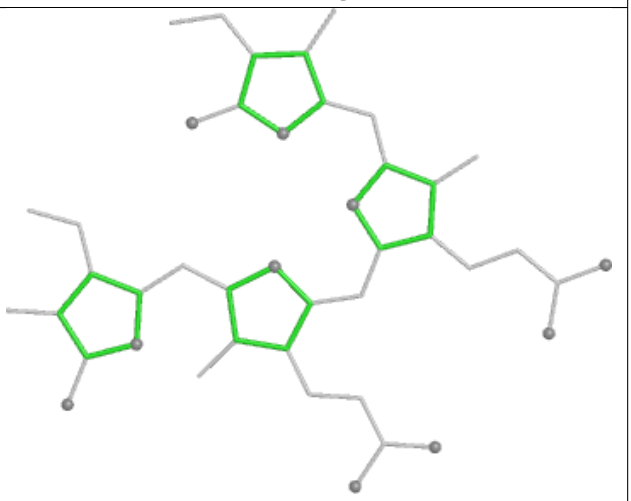
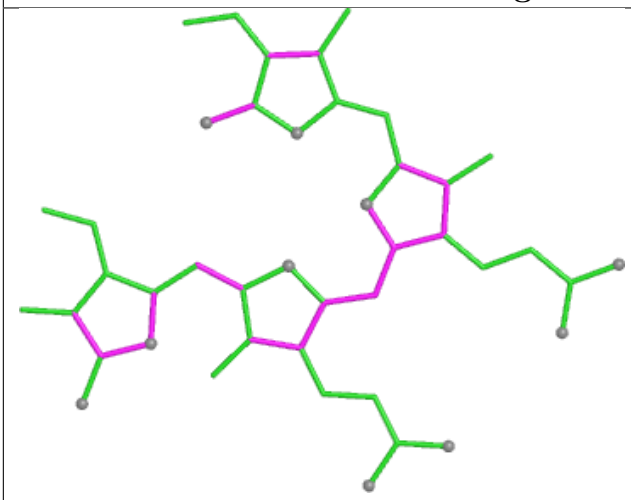


Rings

Ligand PEB kG 202



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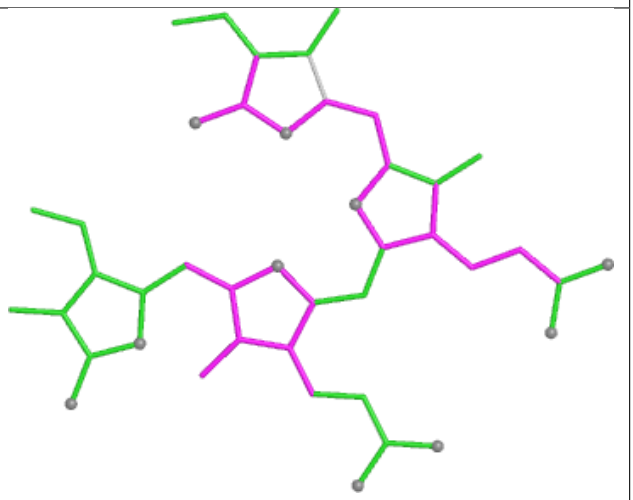
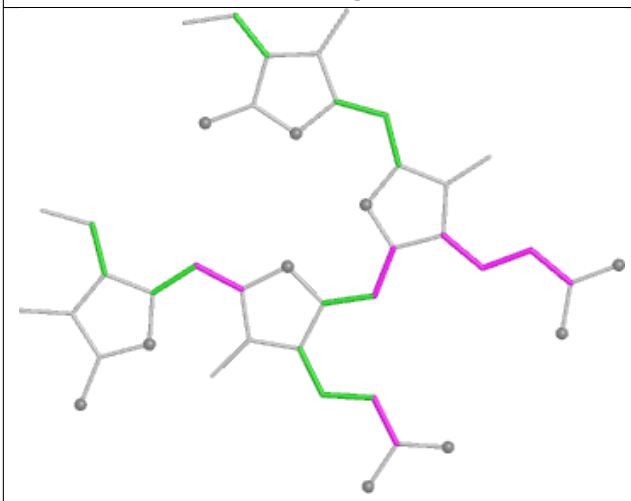


Bond angles



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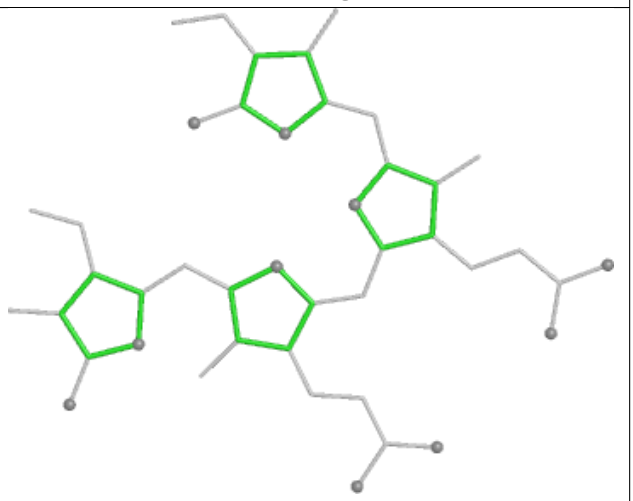
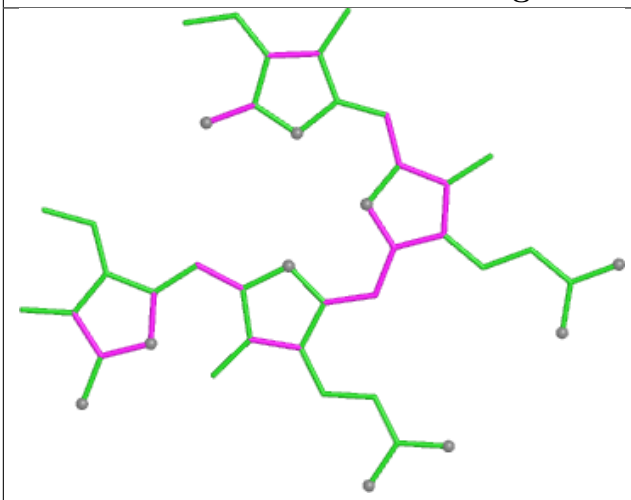


Rings

Ligand PEB DF 203



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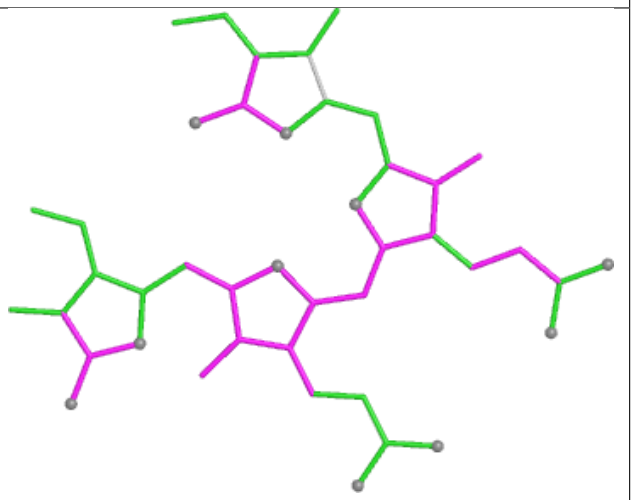
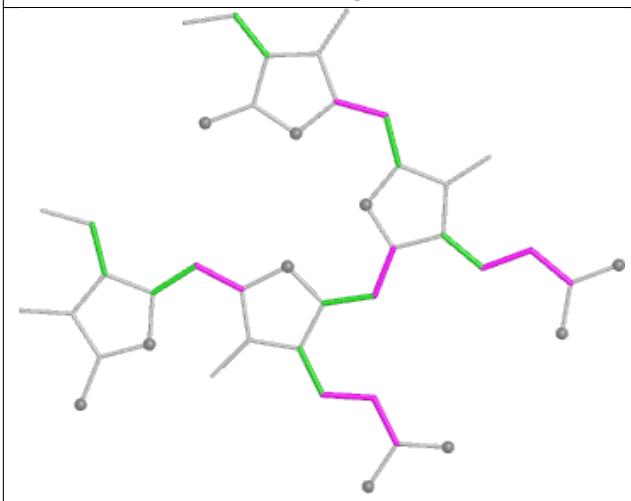
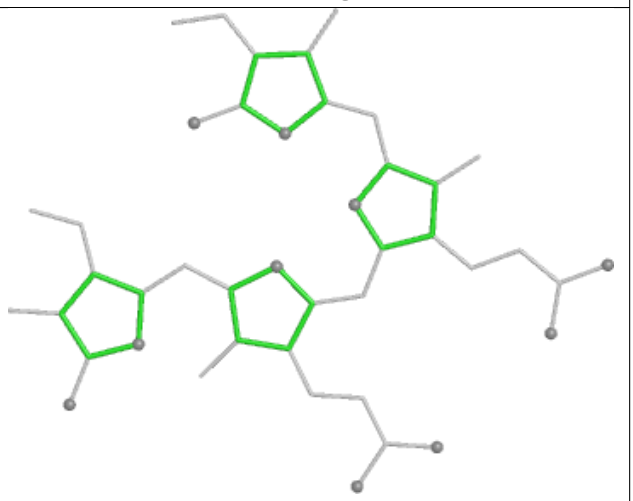


Bond angles

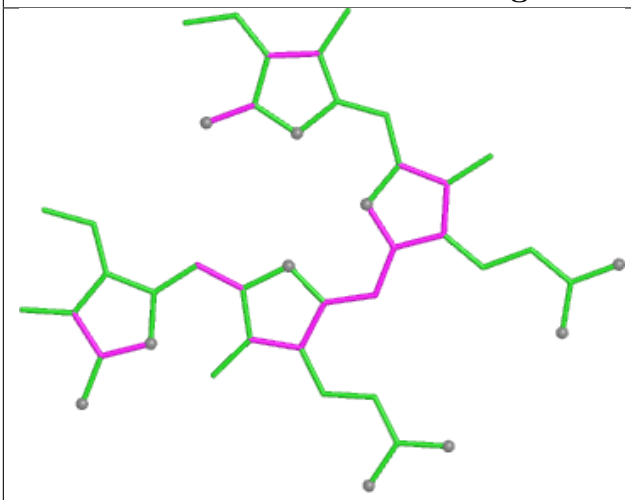


Torsions



Rings

Ligand PEB CK 201



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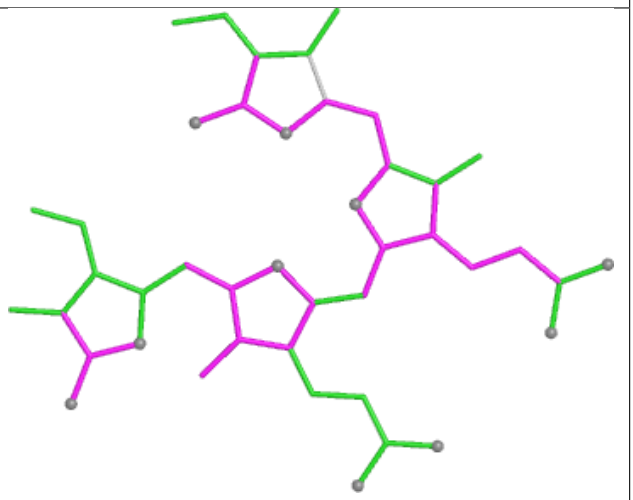

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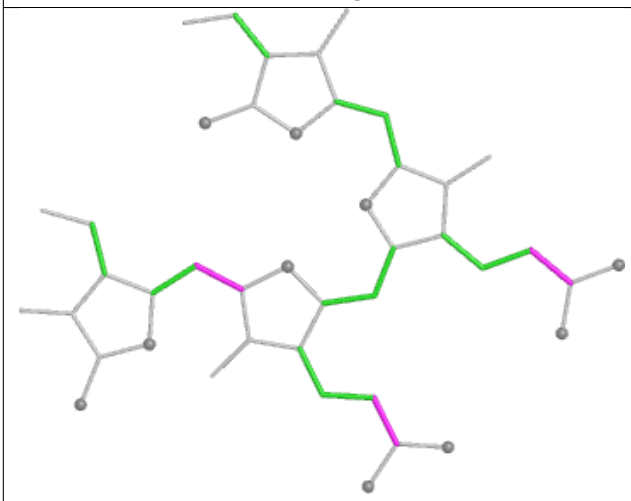

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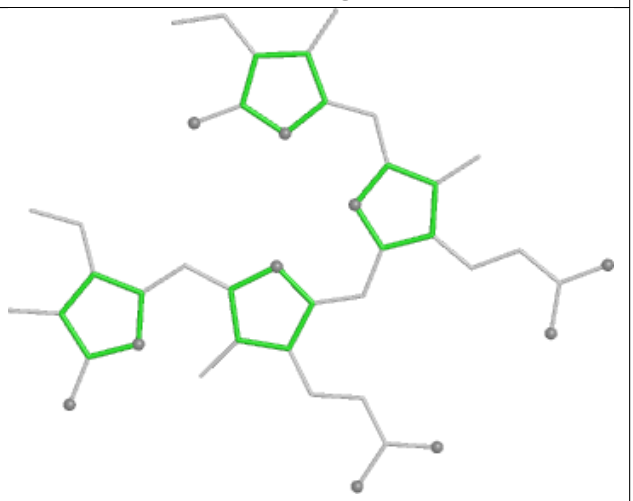
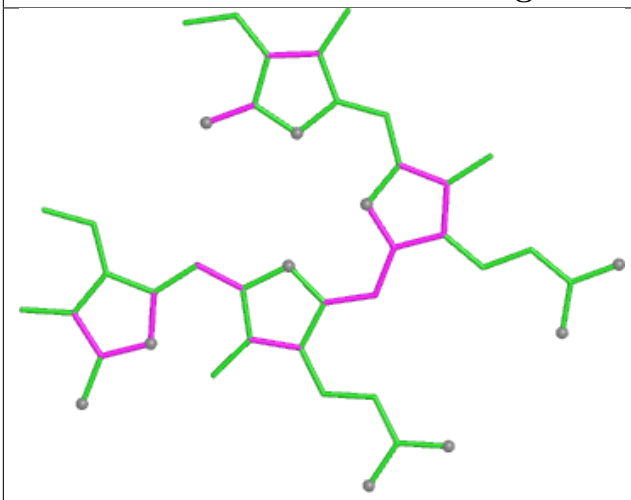


Rings

Ligand PEB A5 202



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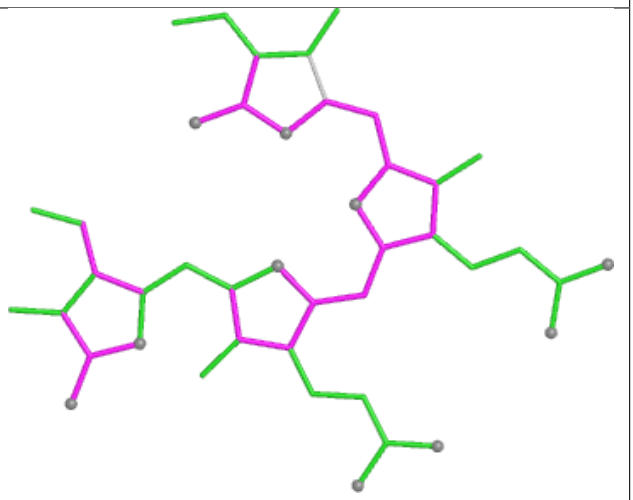

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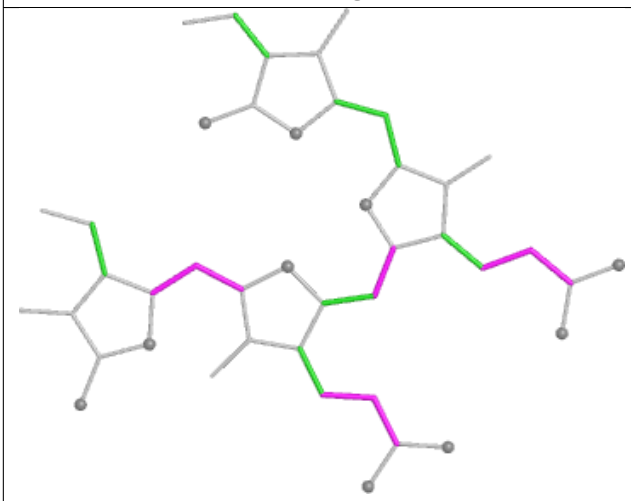

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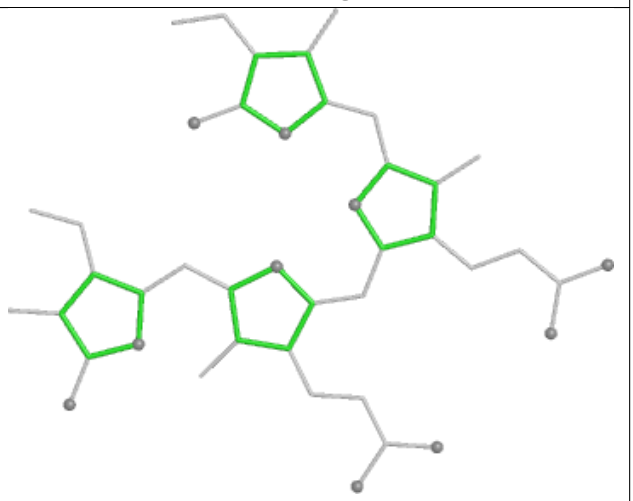
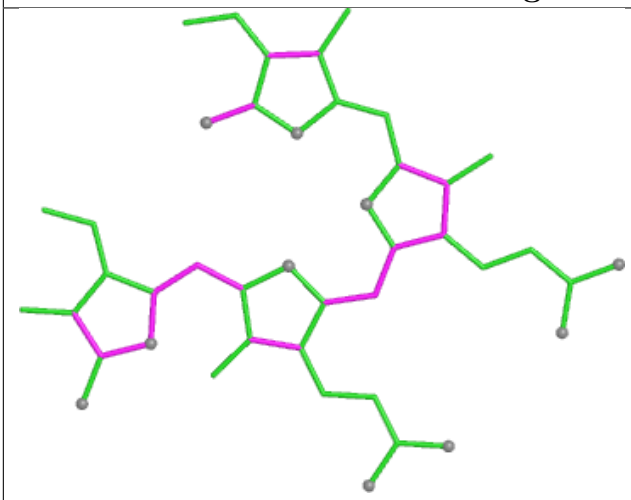


Rings

Ligand PEB j4 201



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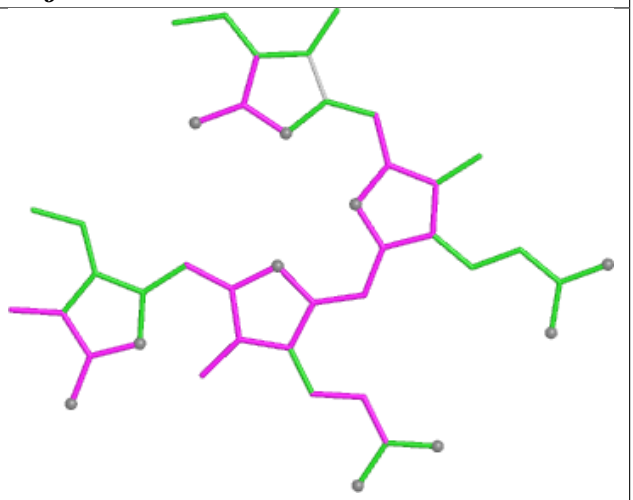

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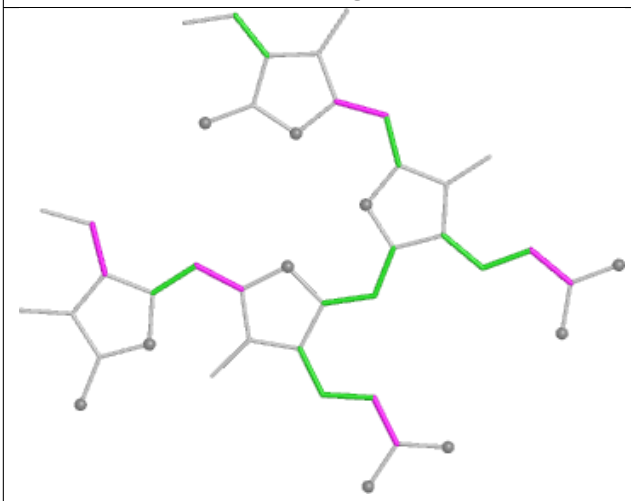

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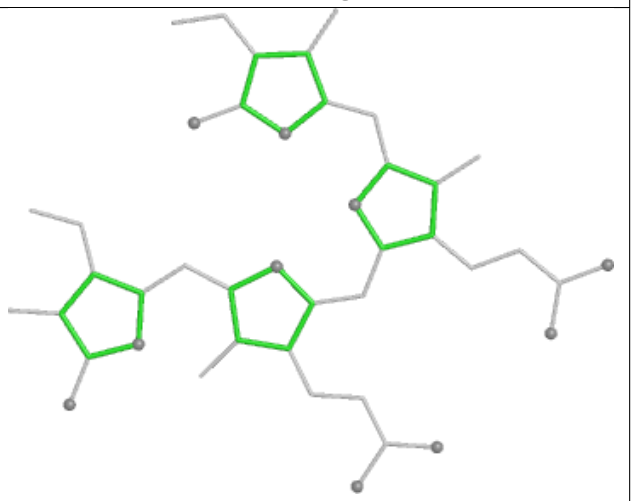
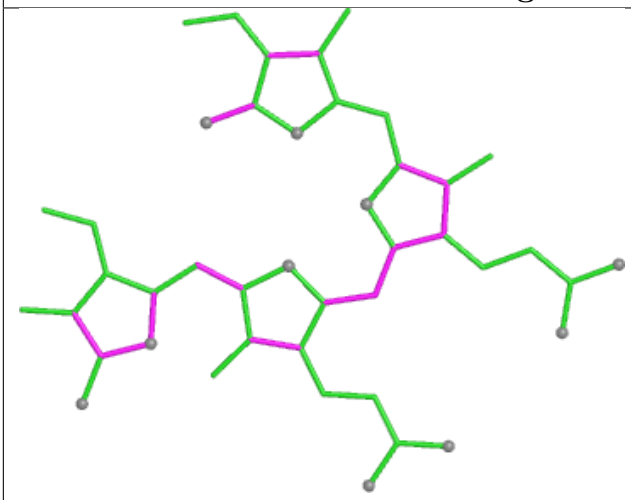


Rings

Ligand PEB gE 201



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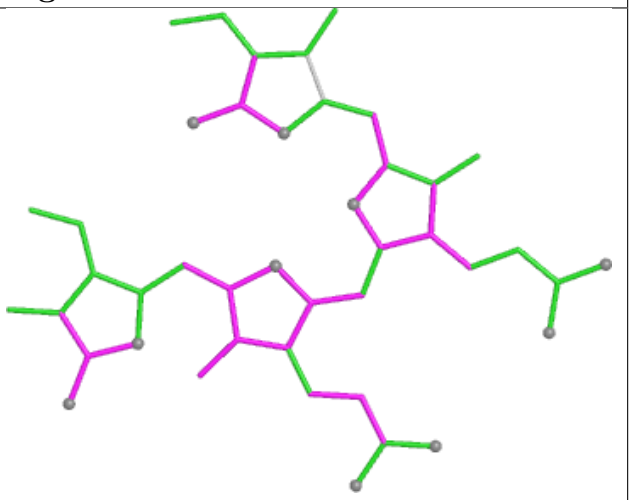

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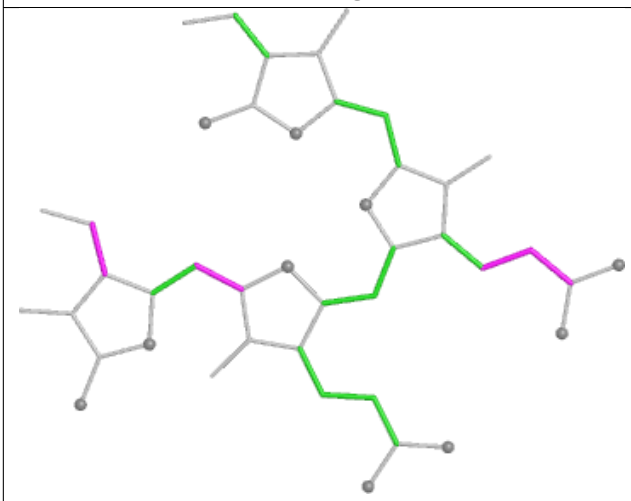

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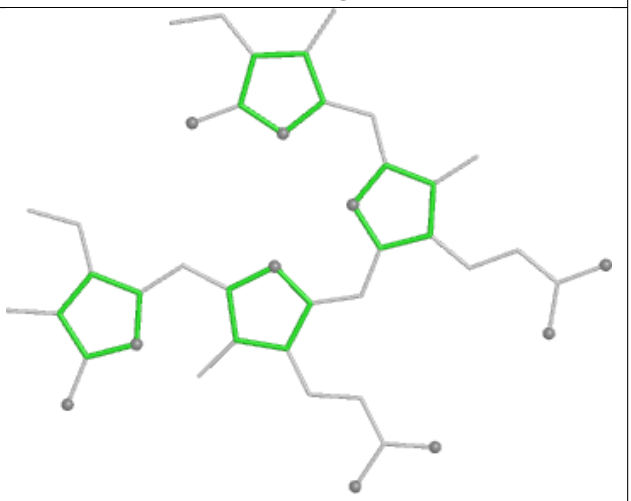
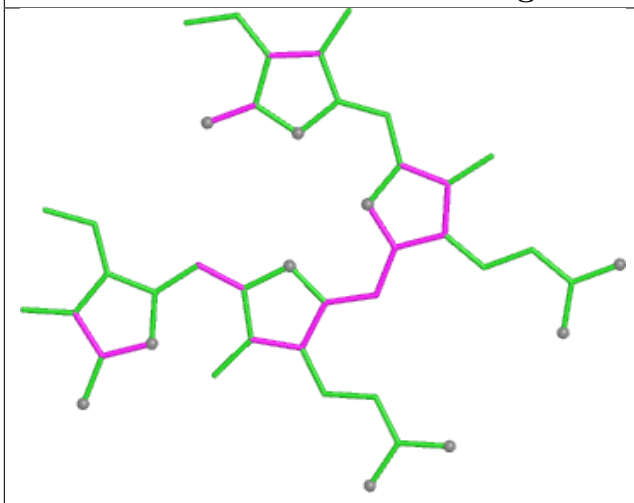


Rings

Ligand PEB P9 202



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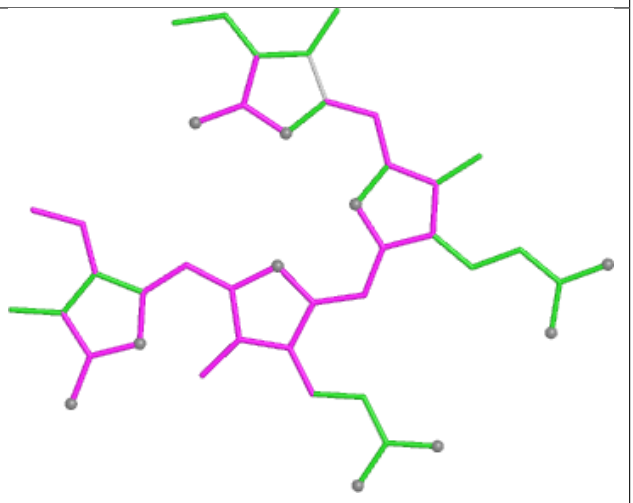

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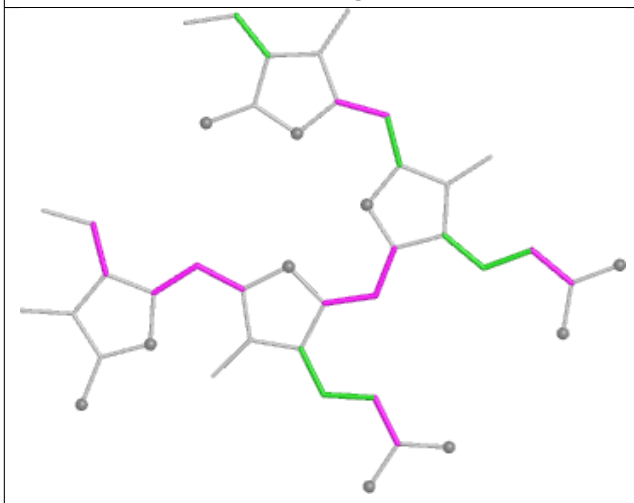

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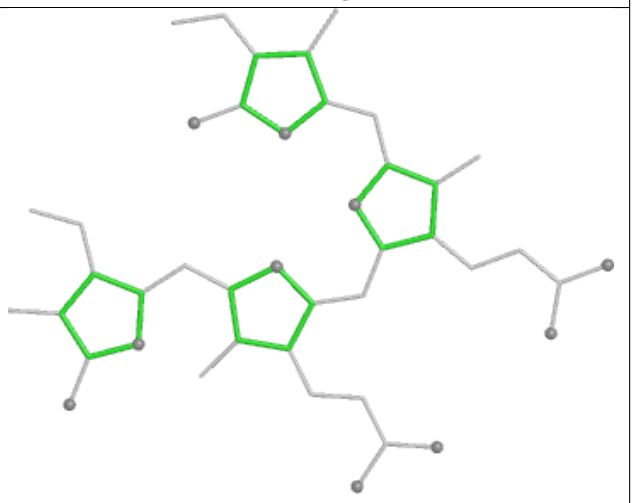
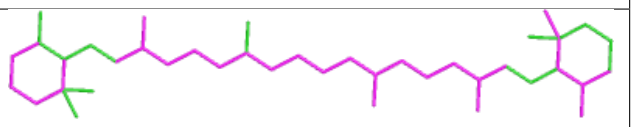


Rings

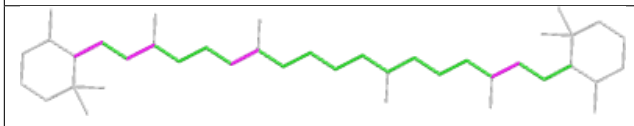
Ligand BCR A2 847



Bond lengths



Bond angles



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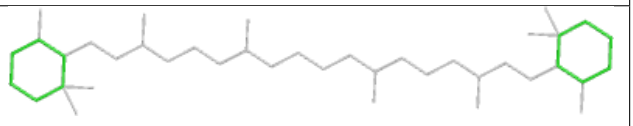
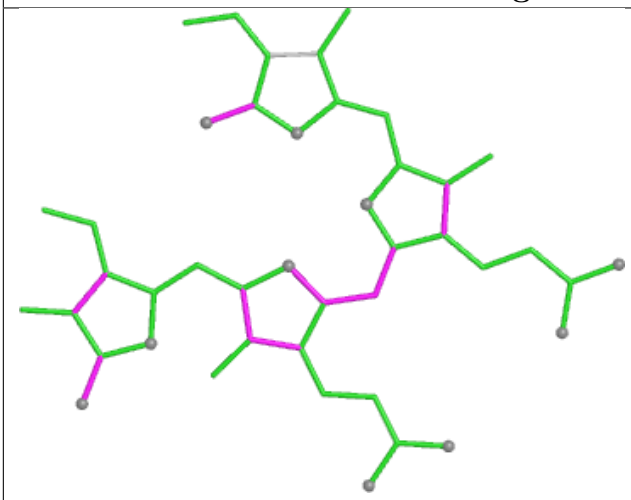


Rings

Ligand PUB K7 203



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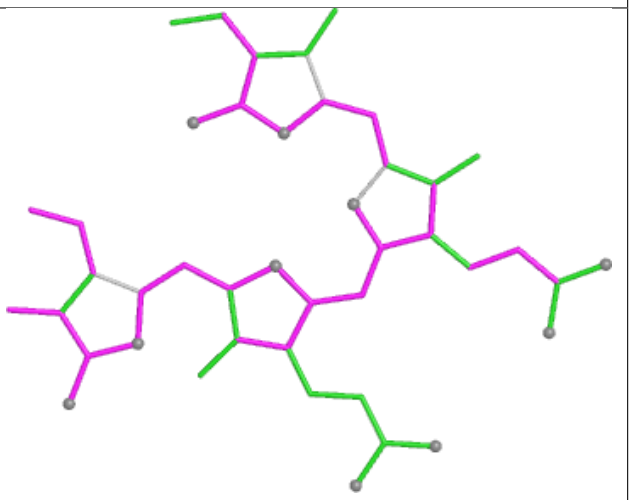

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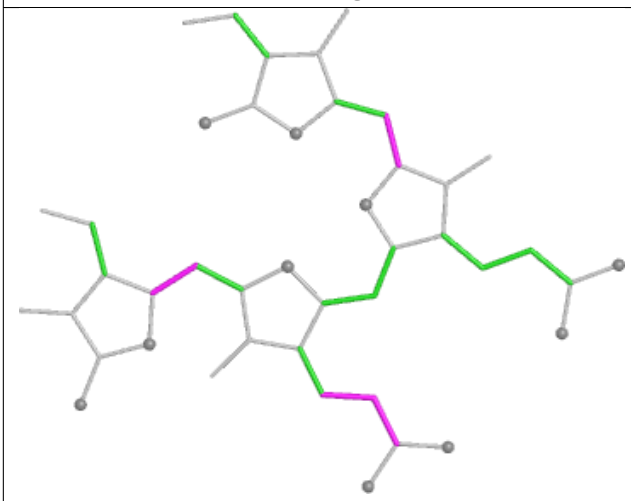

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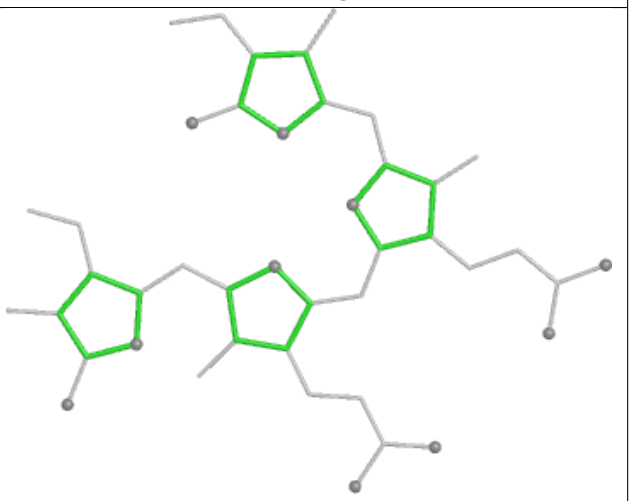
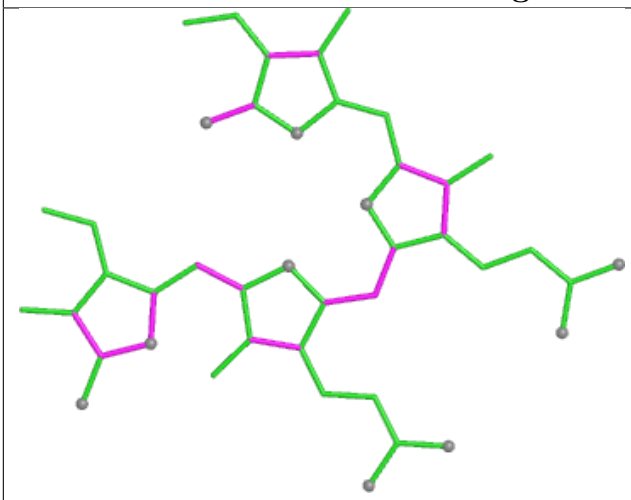


Rings

Ligand PEB AP 201



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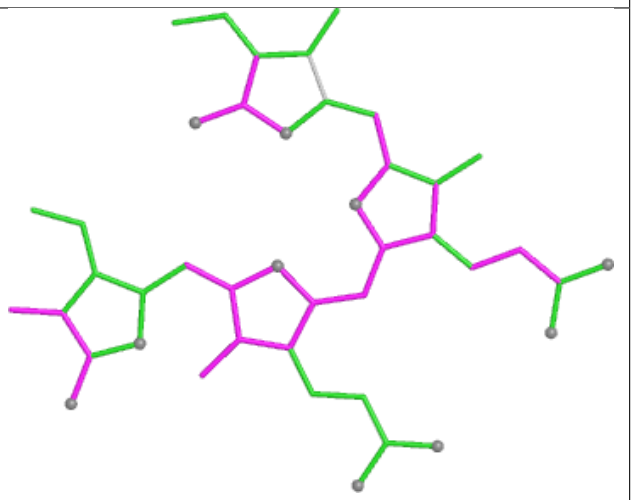

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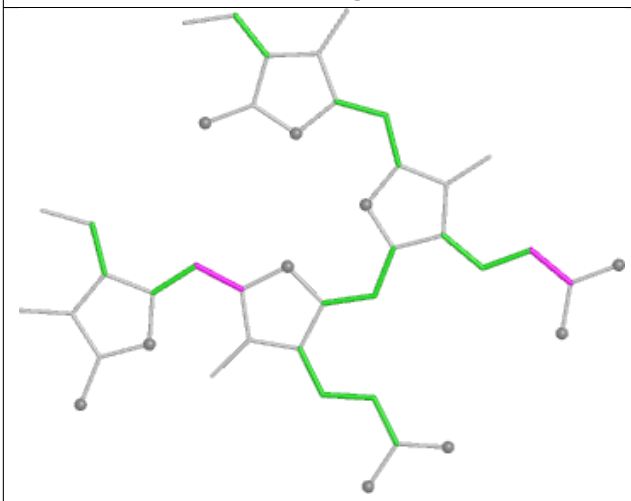

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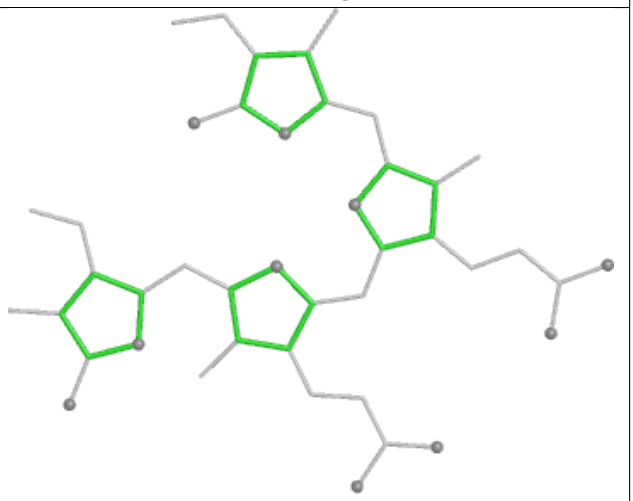
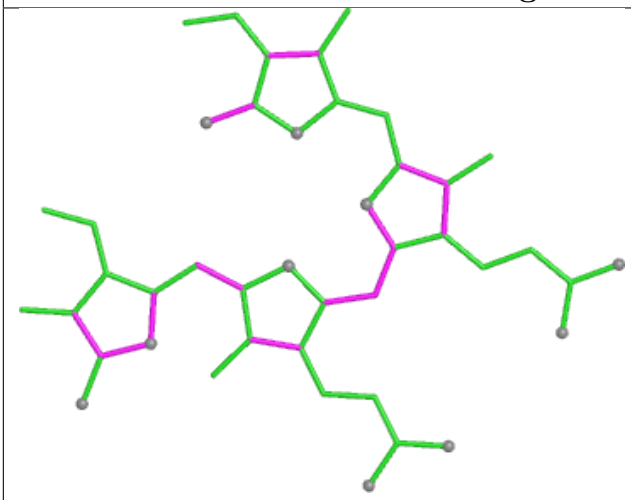


Rings

Ligand PEB iO 201



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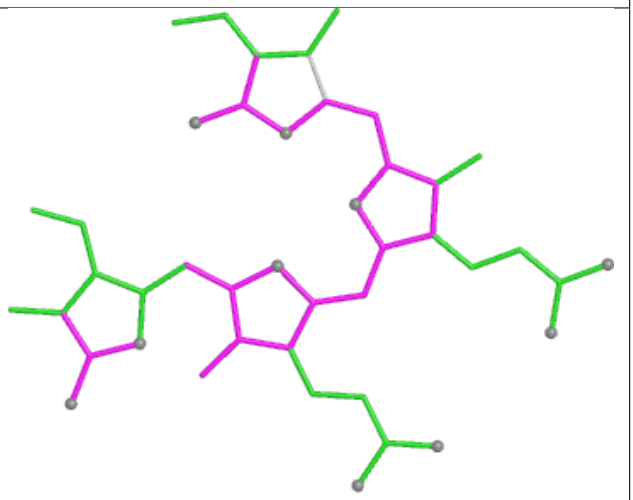

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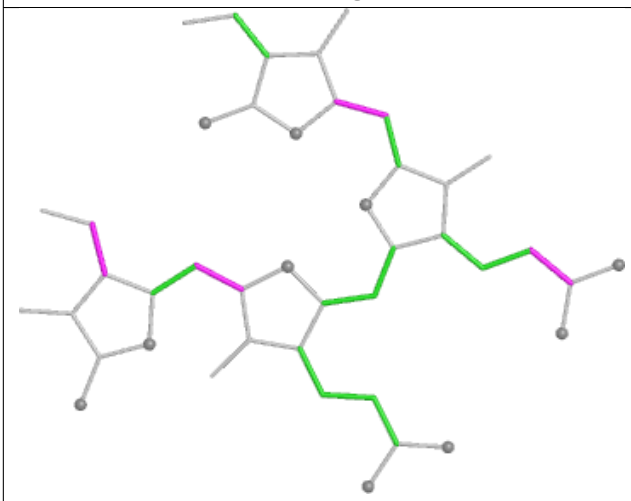

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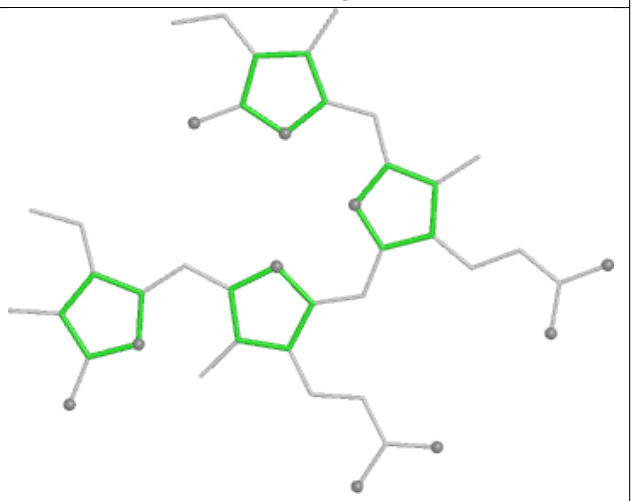
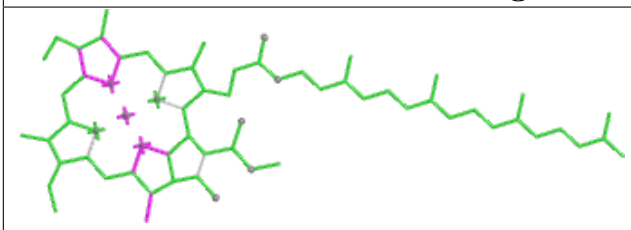


Rings

Ligand CLA AN 850



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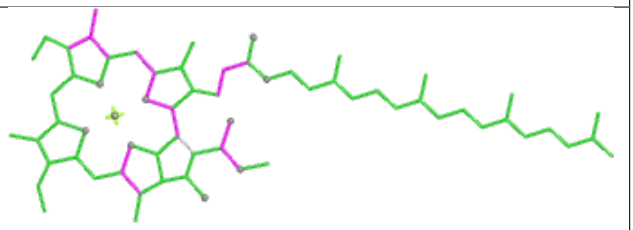

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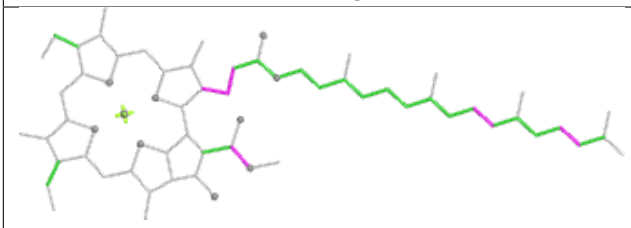

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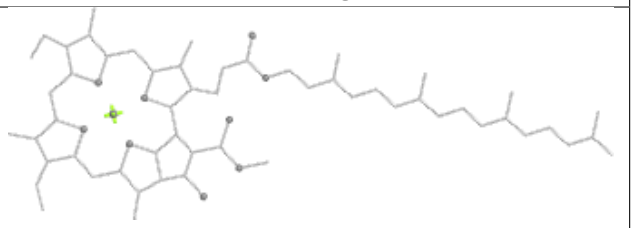
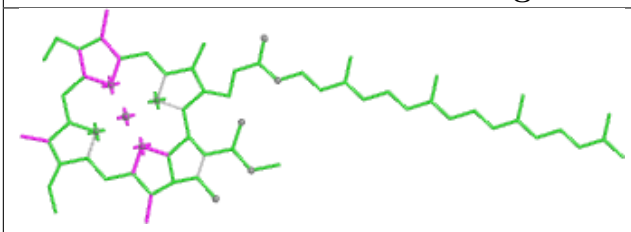


Rings

Ligand CLA BL 601



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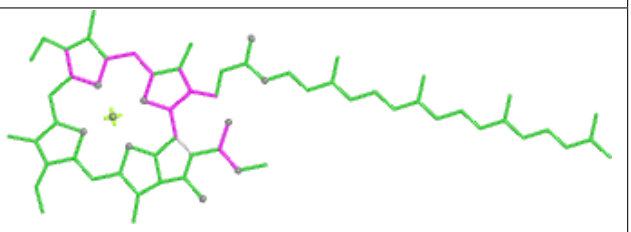

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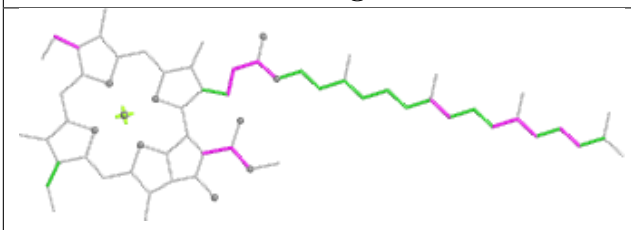

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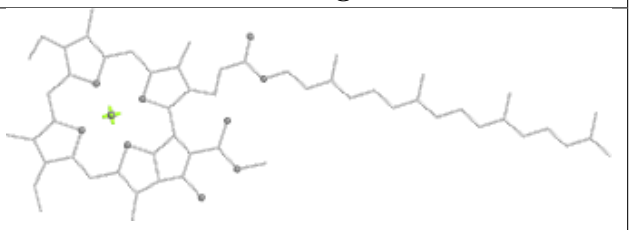
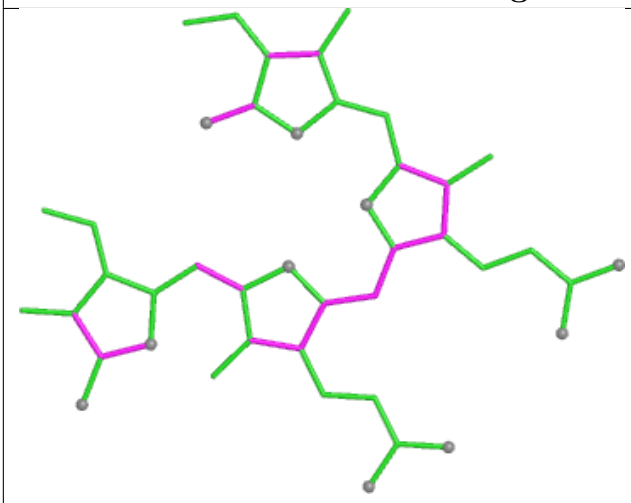


Rings

Ligand PEB XD 203



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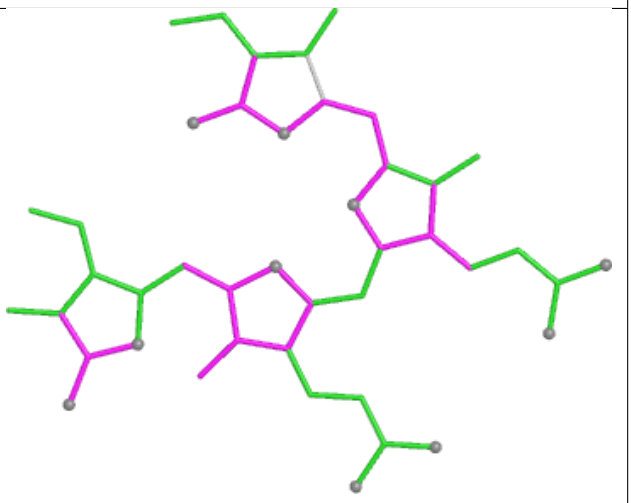

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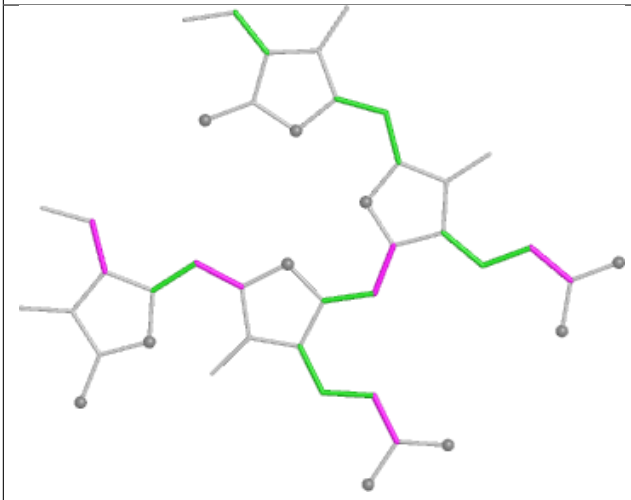

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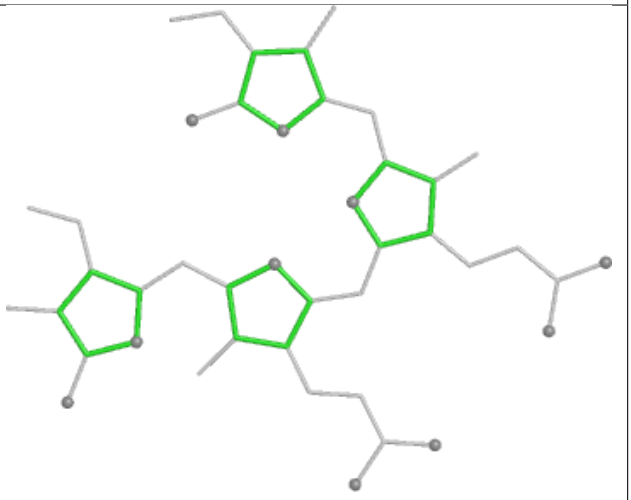
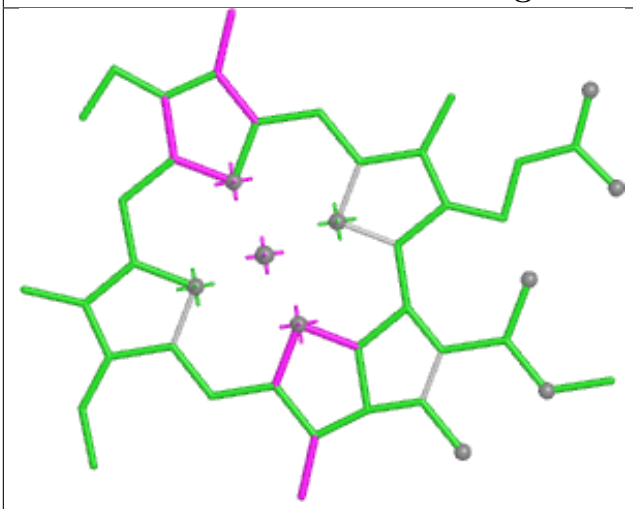


Rings

Ligand CLA 3N 312



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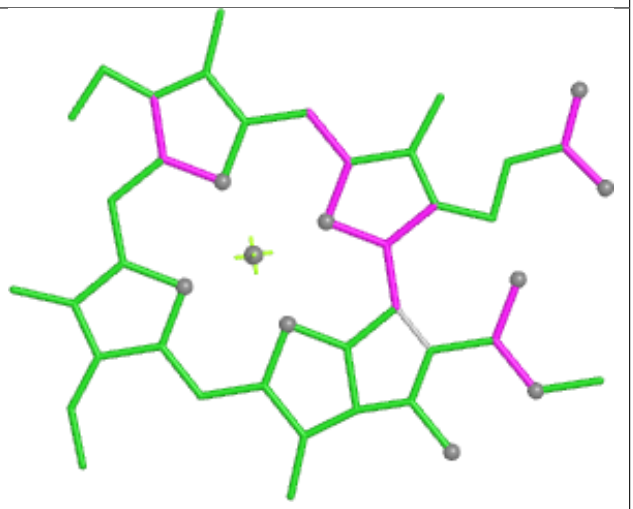
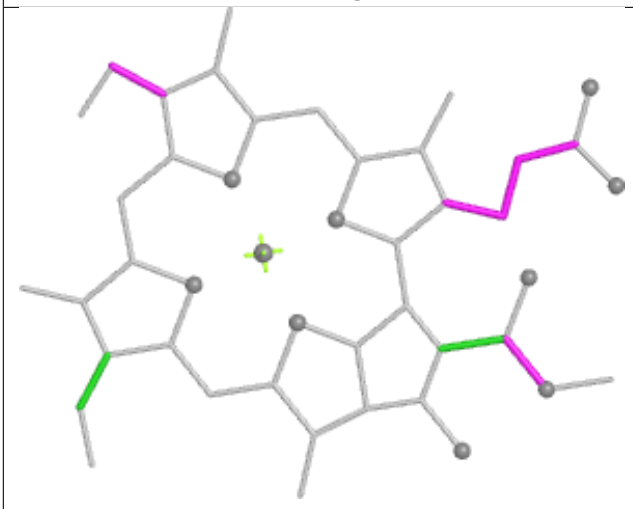


Bond angles

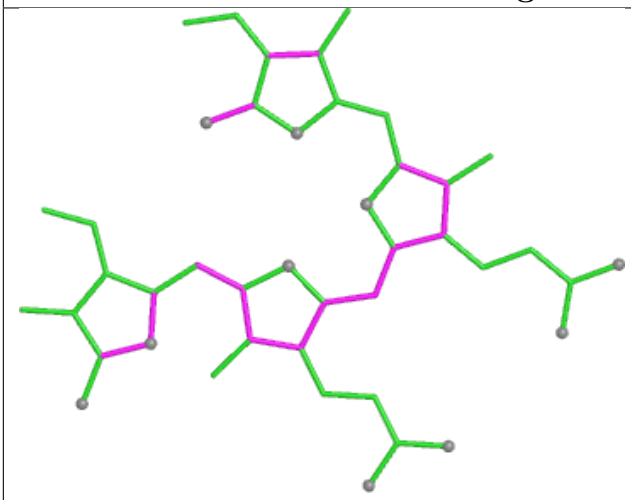


Torsions



Rings

Ligand PEB qF 202



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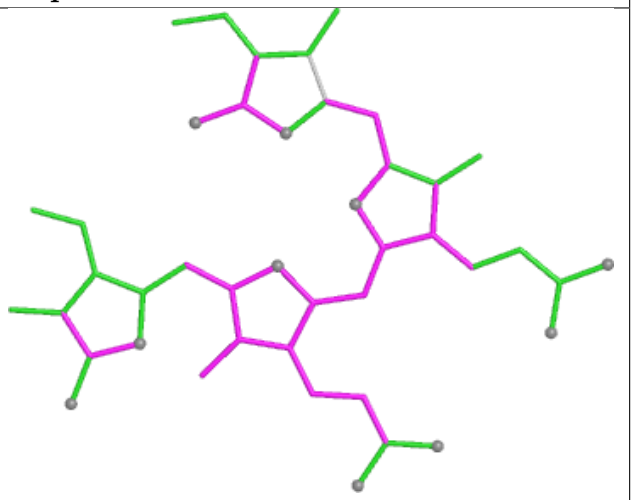
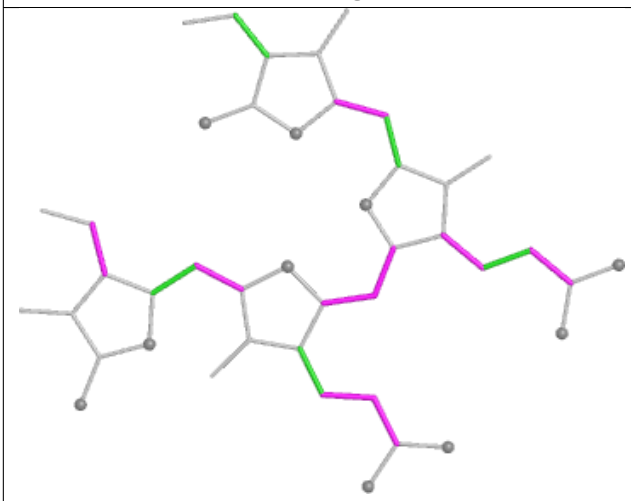


Bond angles



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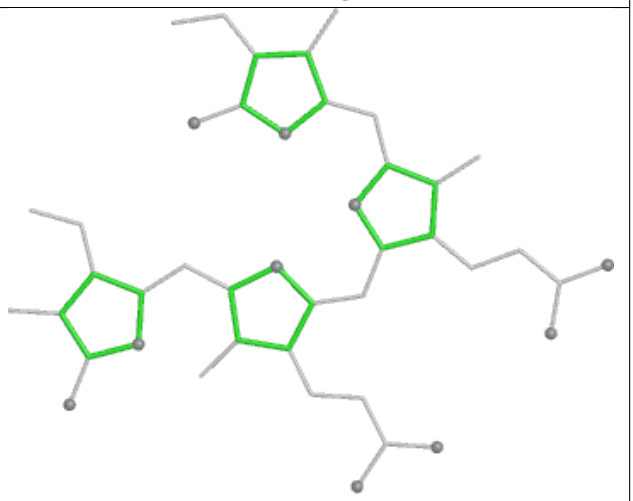
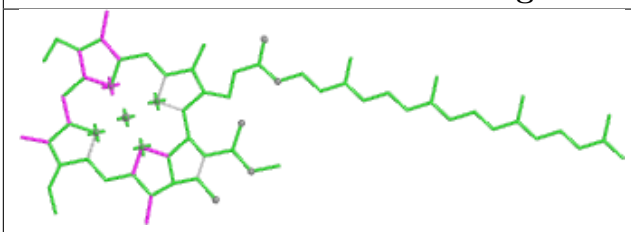


Rings

Ligand CLA dL 402



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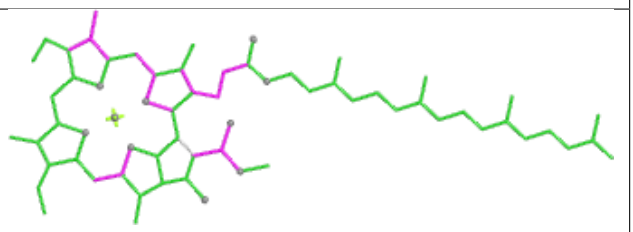
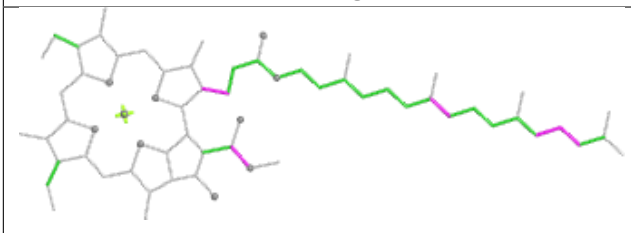
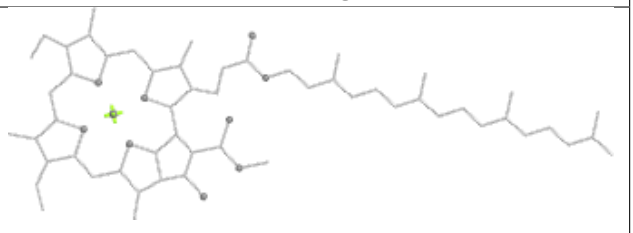


Bond angles



Torsions



Rings

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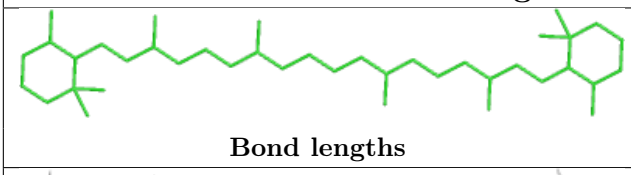

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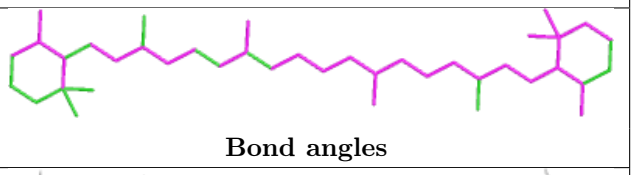

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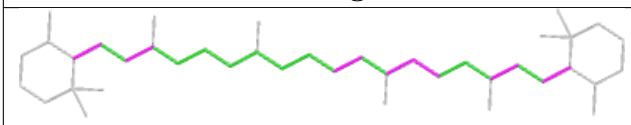

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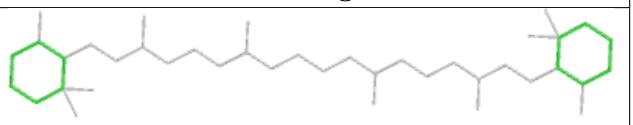

Rings

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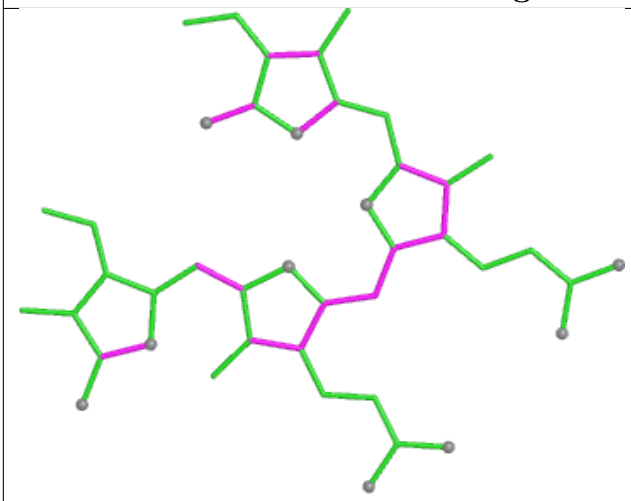

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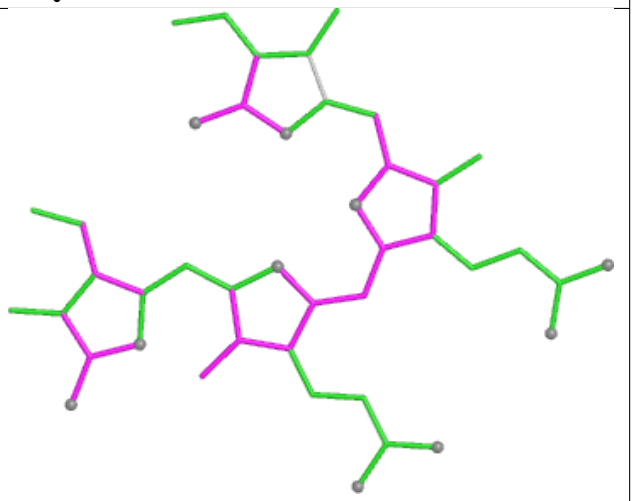

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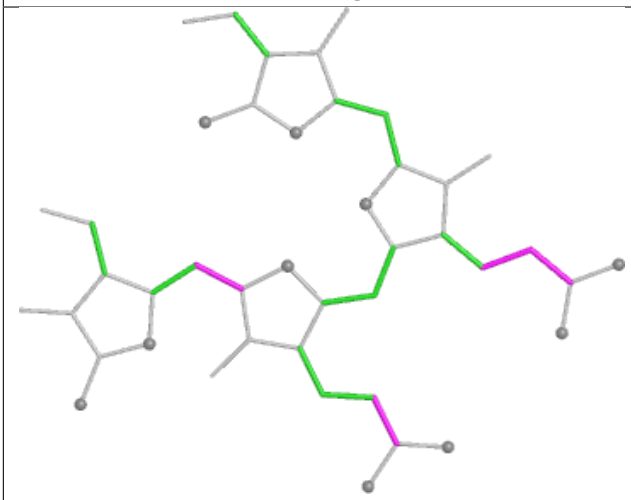

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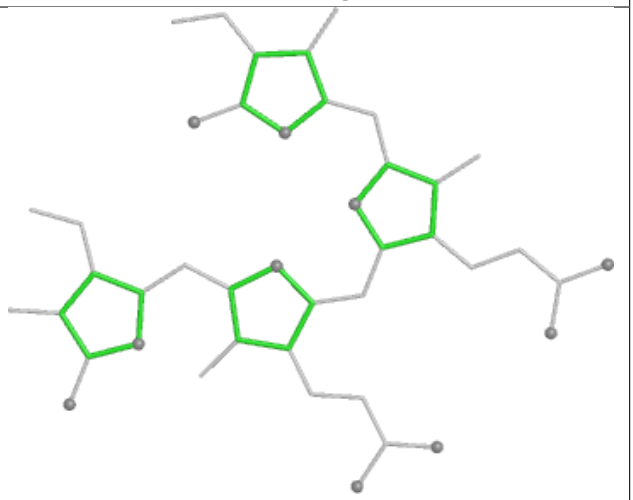

Rings

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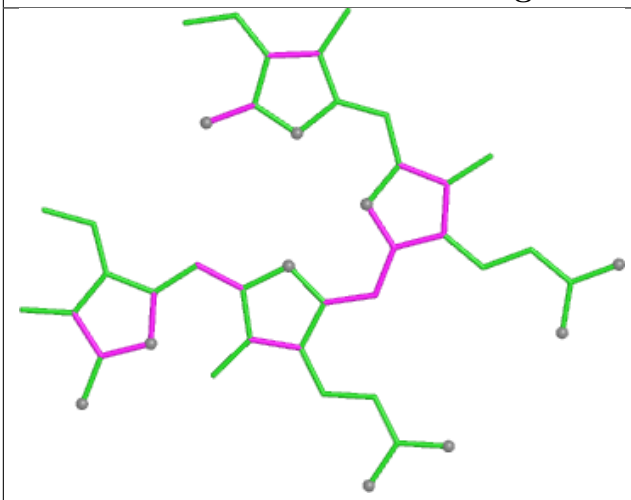

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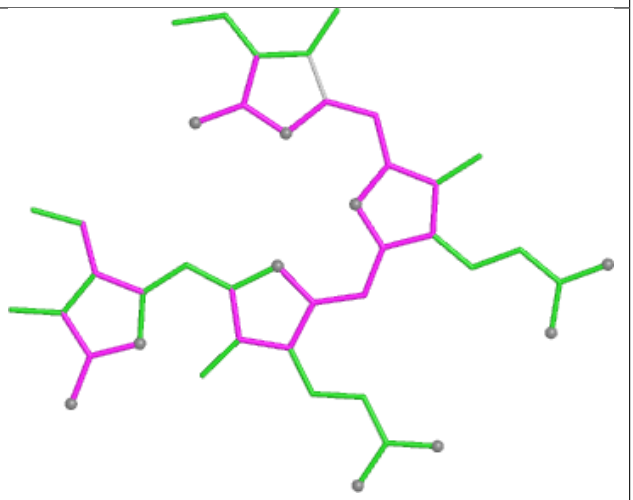

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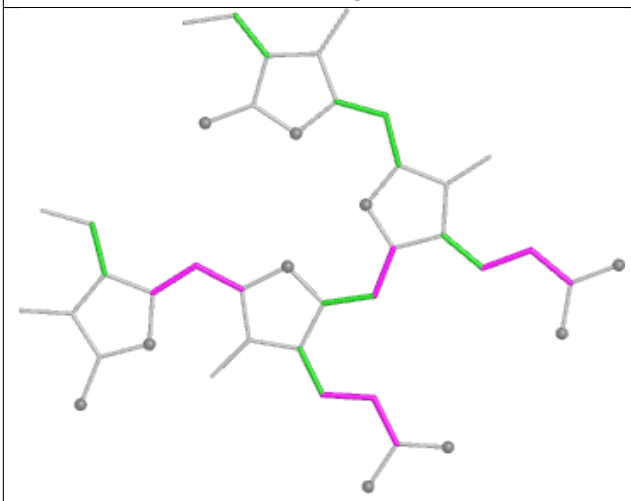

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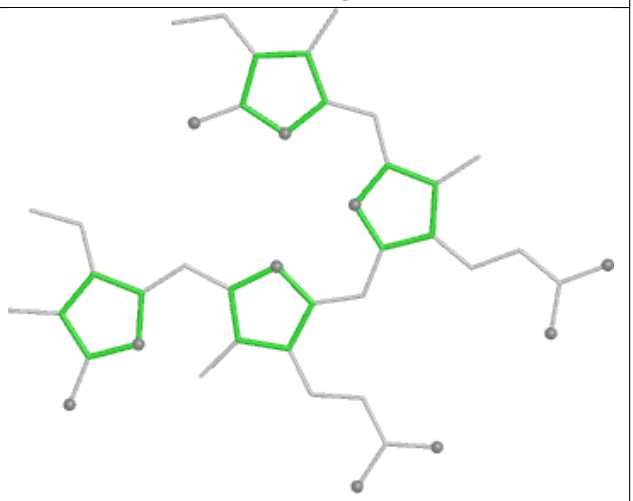

Rings

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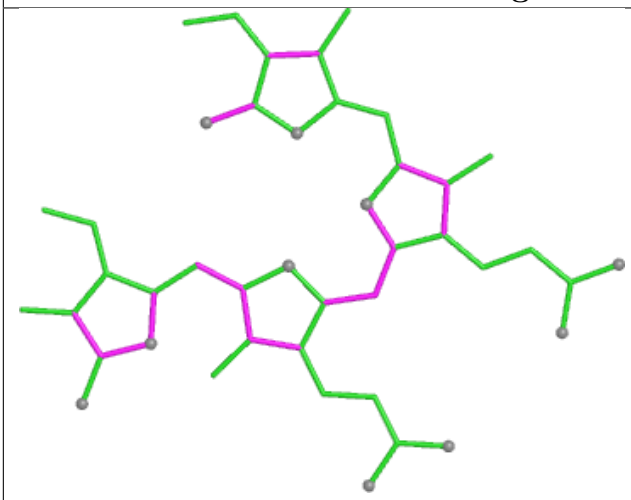

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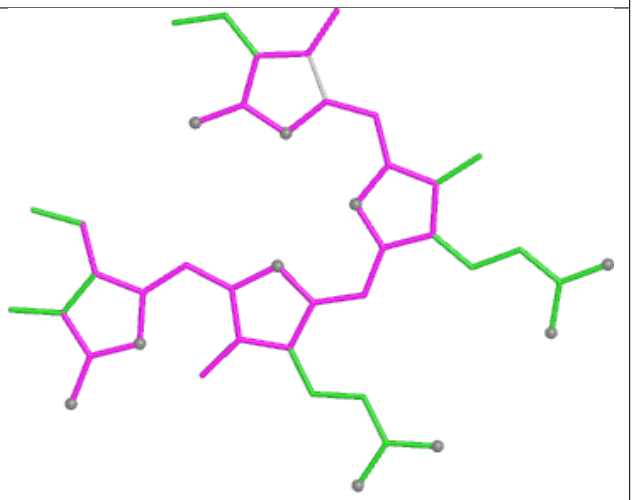

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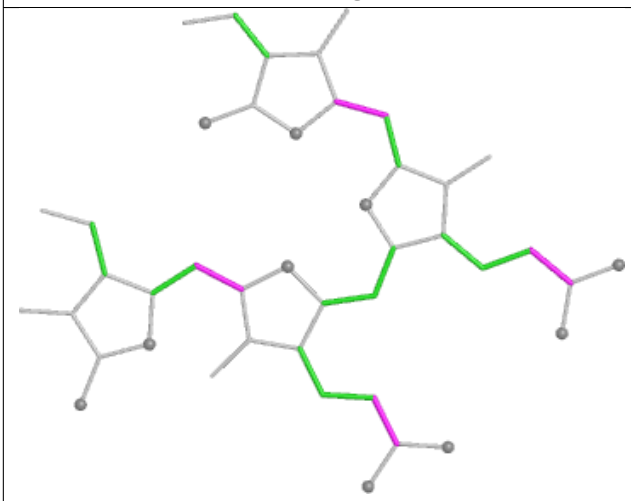

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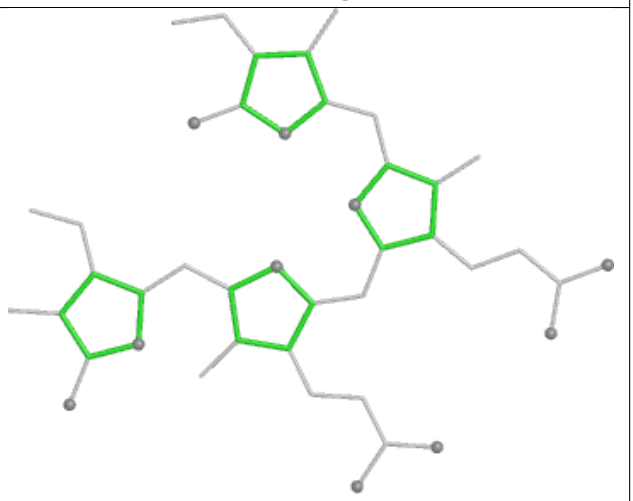

Rings

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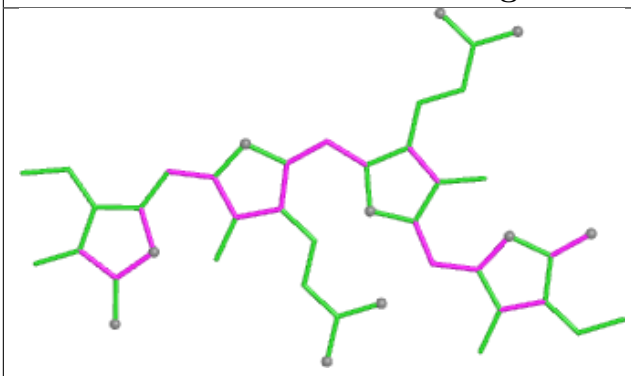

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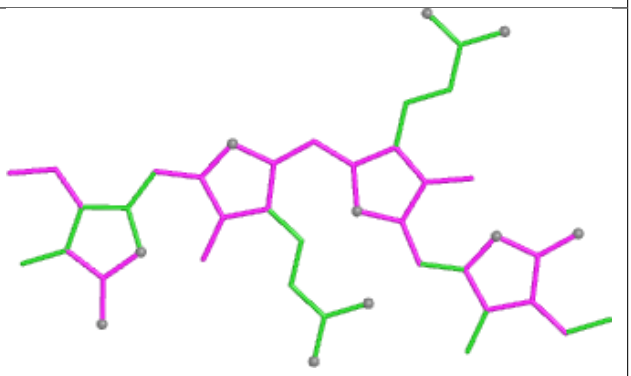

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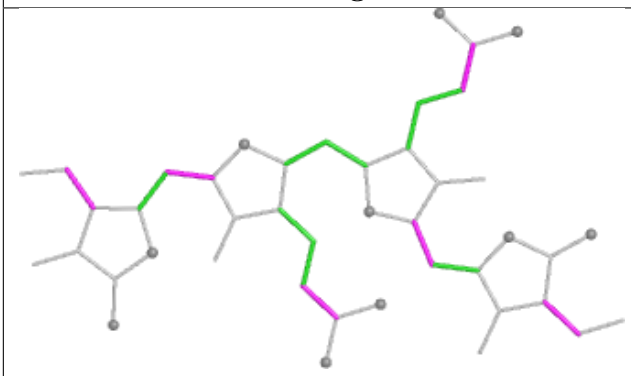

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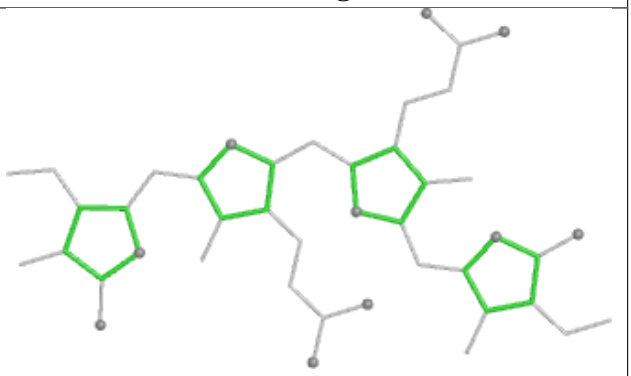

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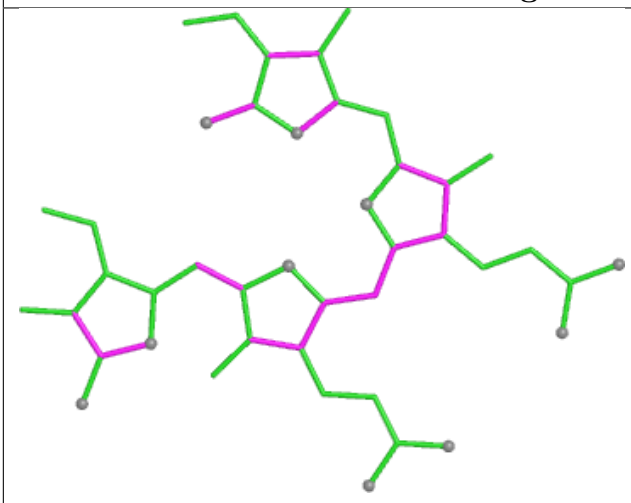

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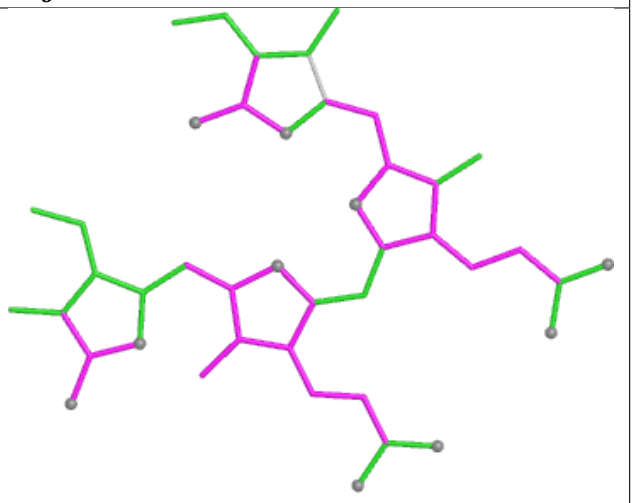

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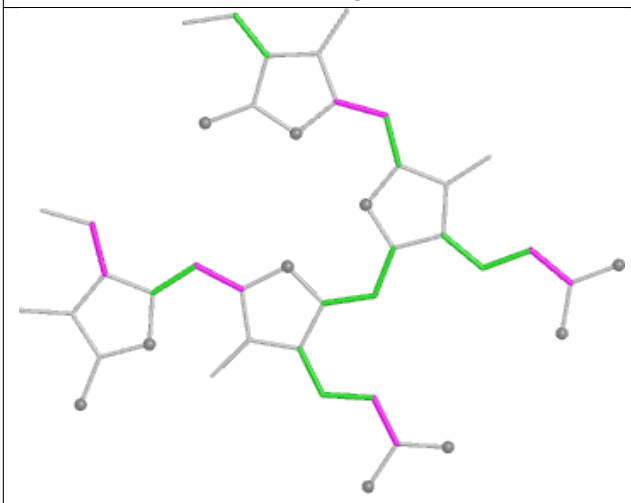

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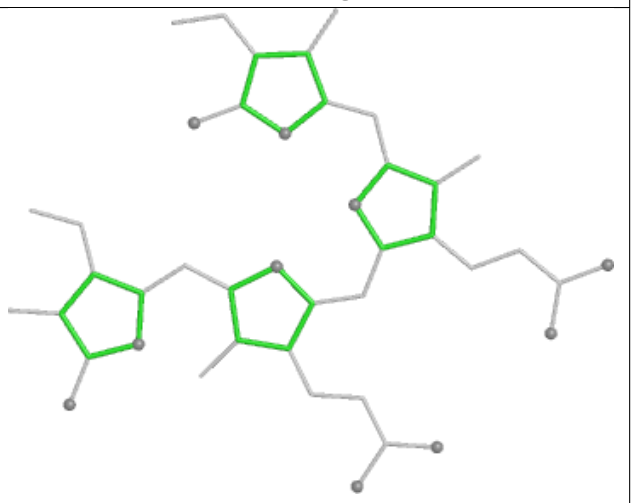

Rings

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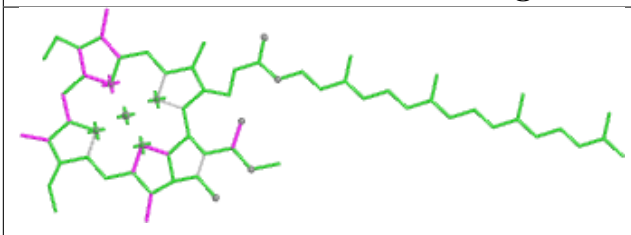

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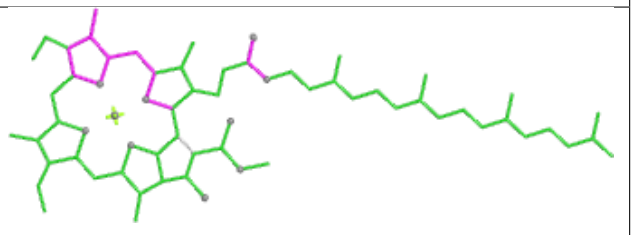

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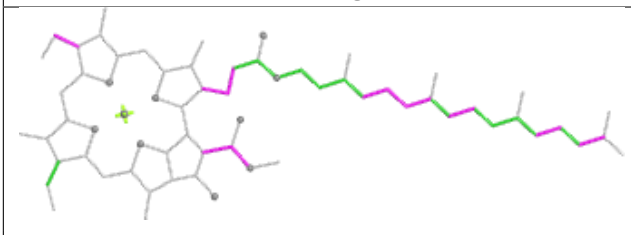

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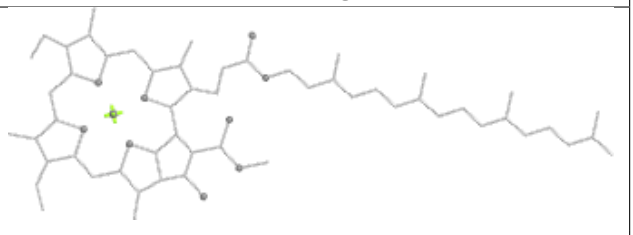

Rings

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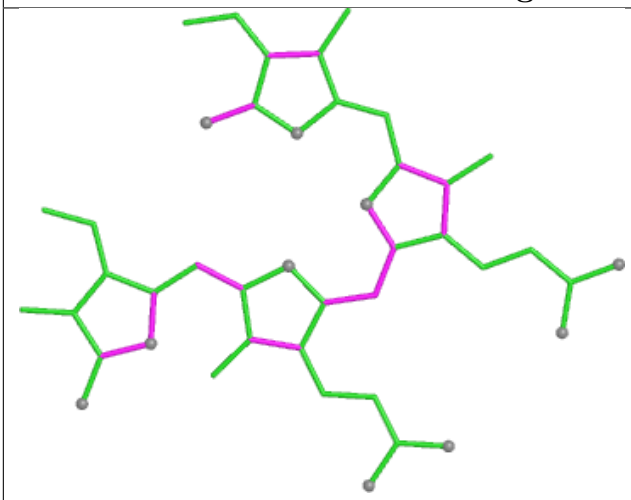

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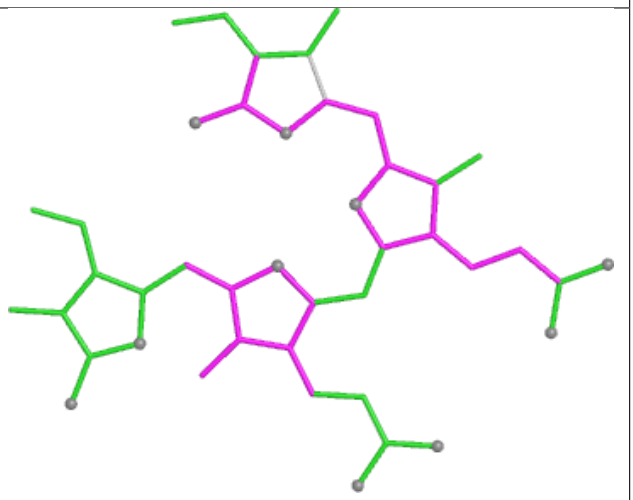

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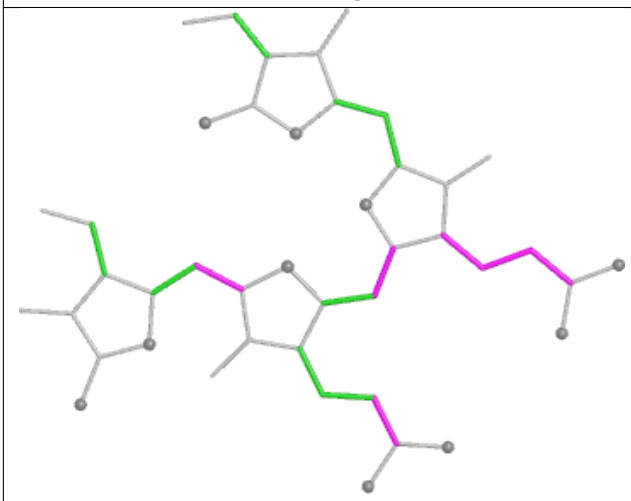

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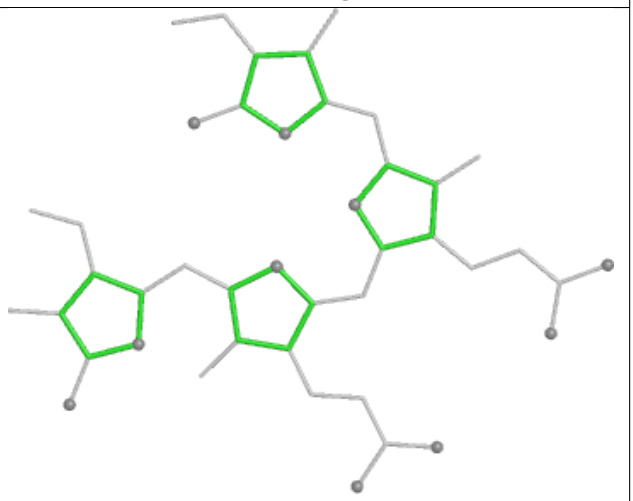

Rings

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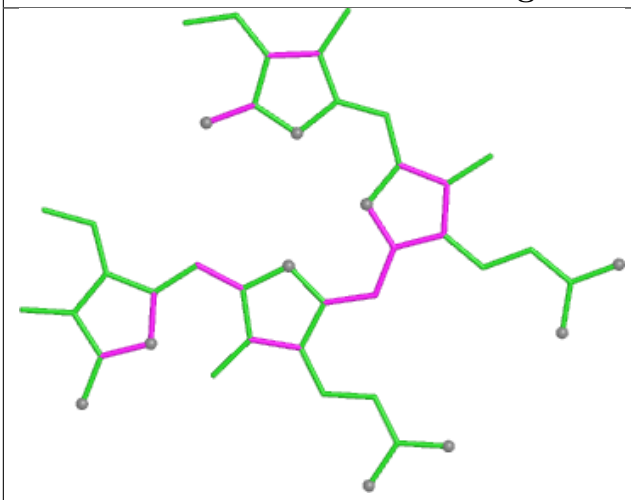

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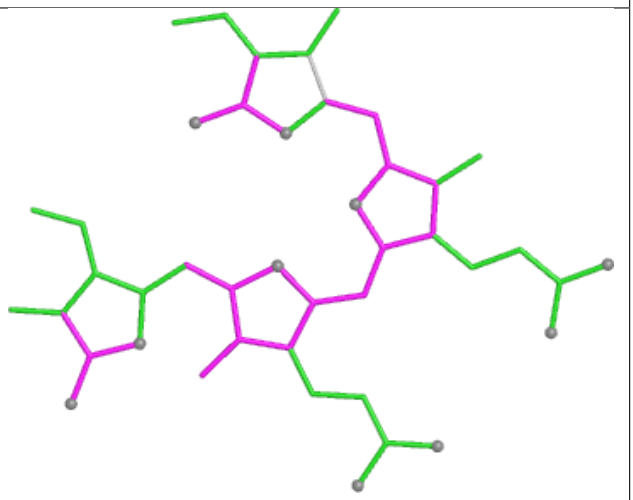

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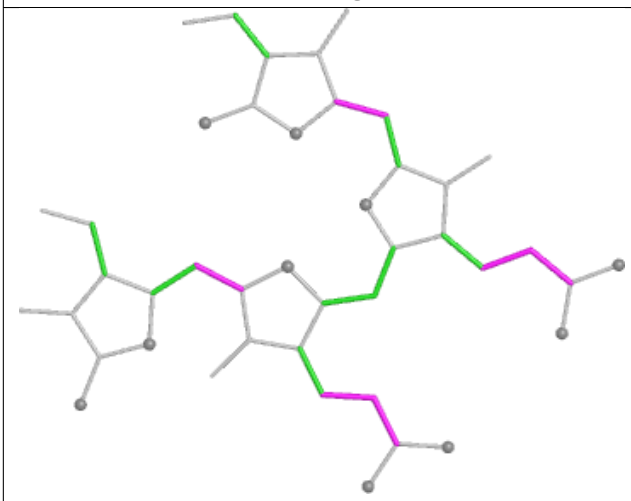

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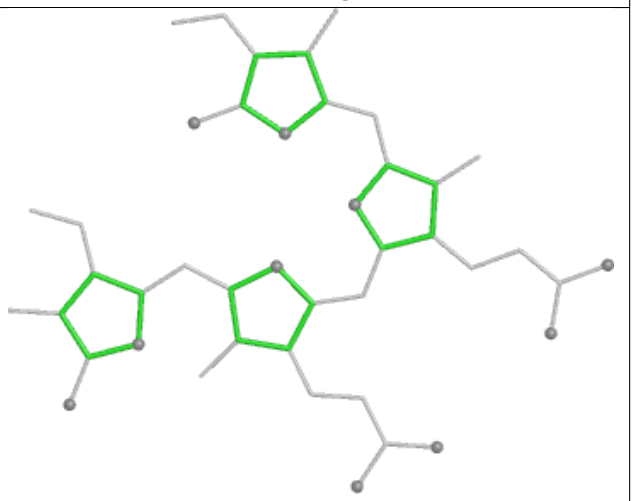

Rings

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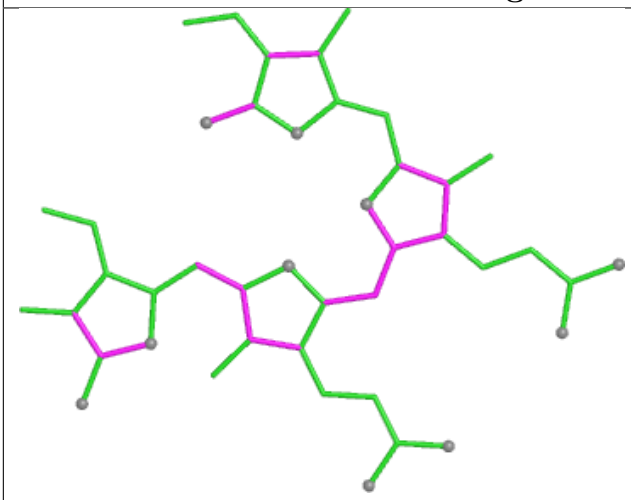

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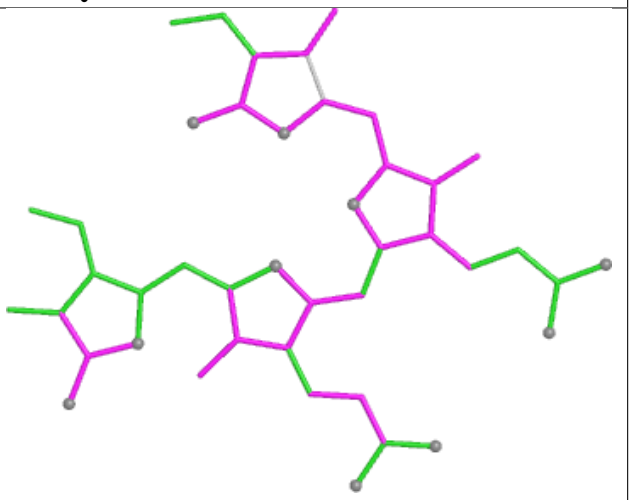

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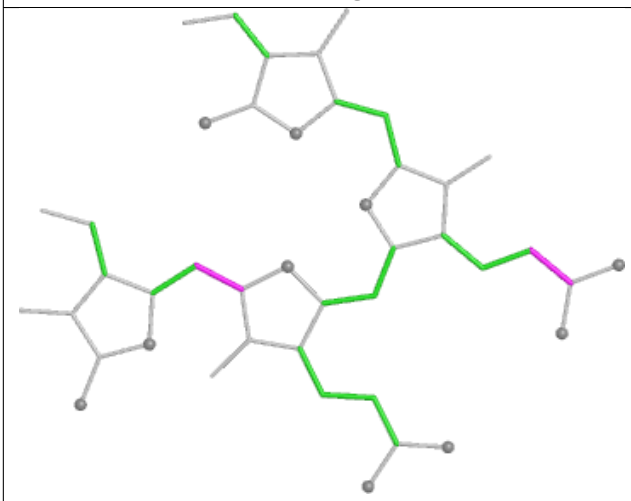

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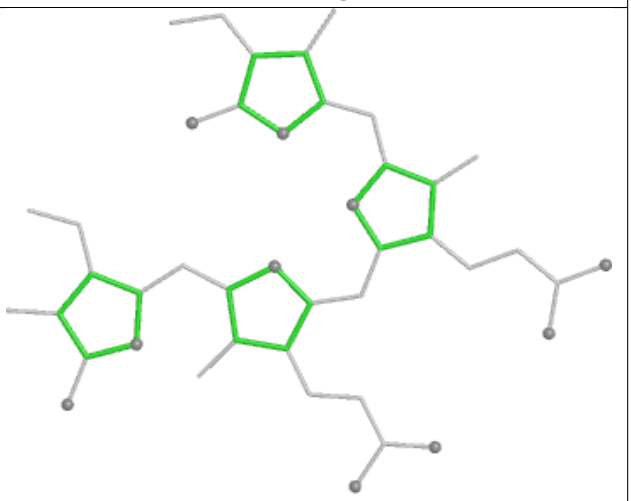

Rings

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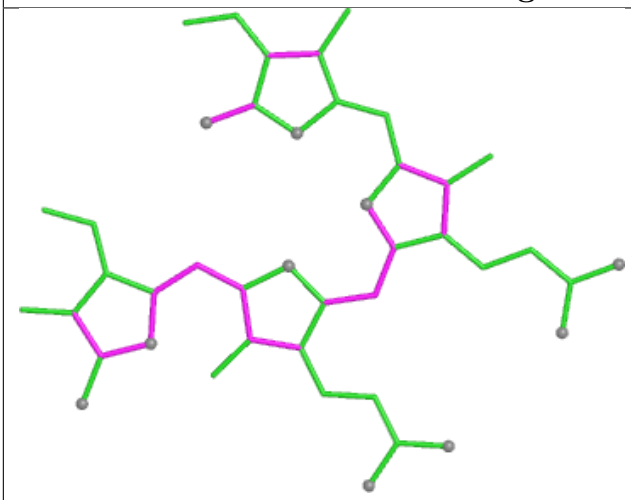

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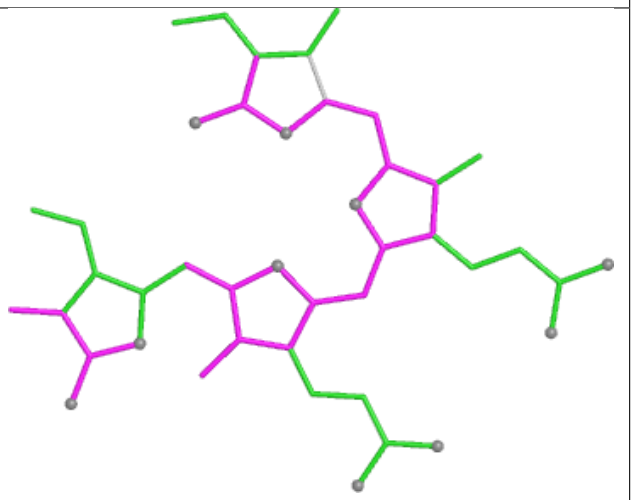

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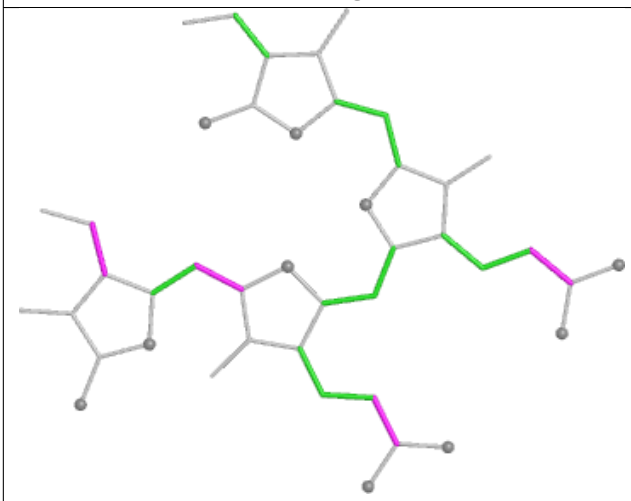

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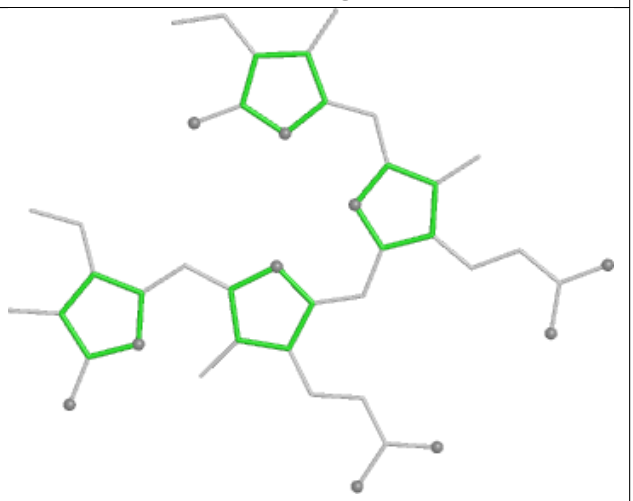

Rings

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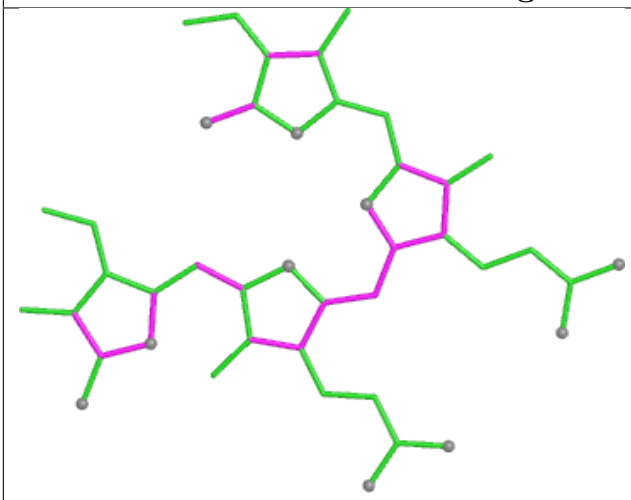

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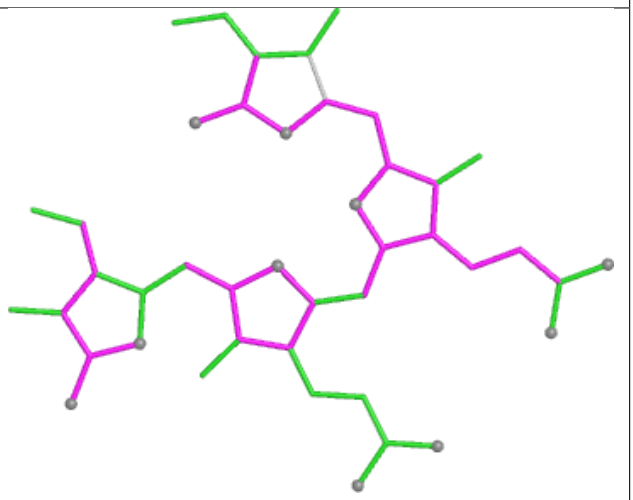

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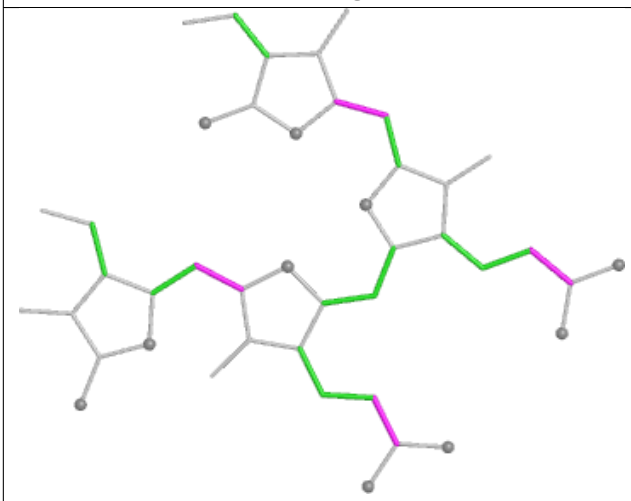

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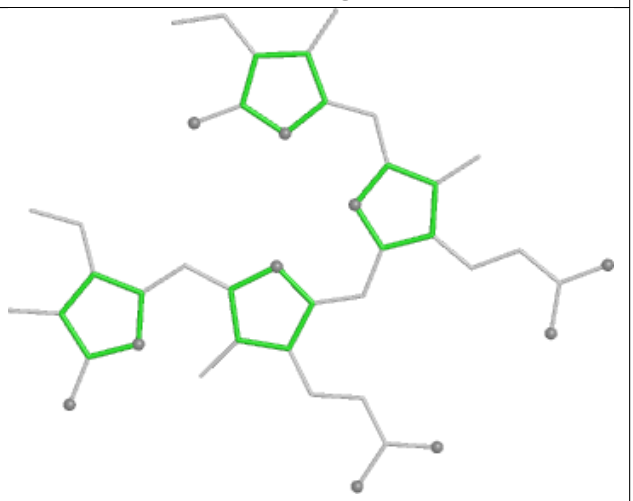

Rings

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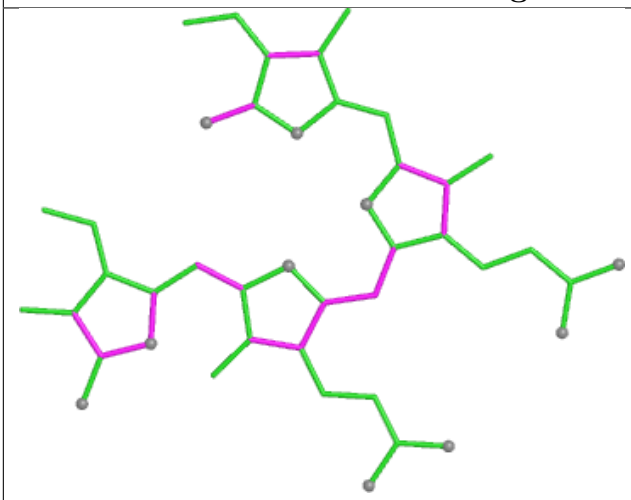

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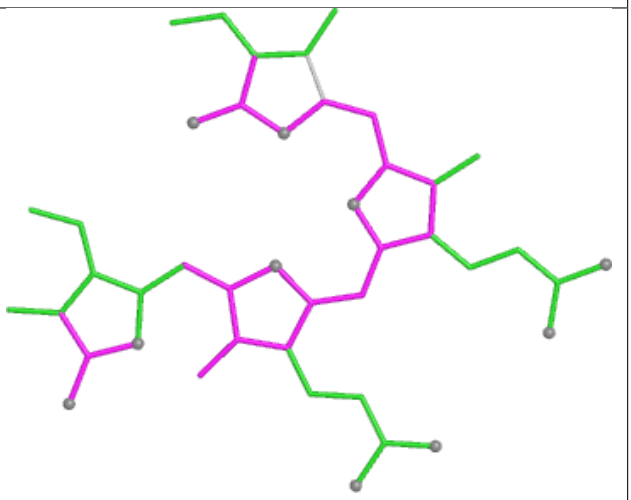

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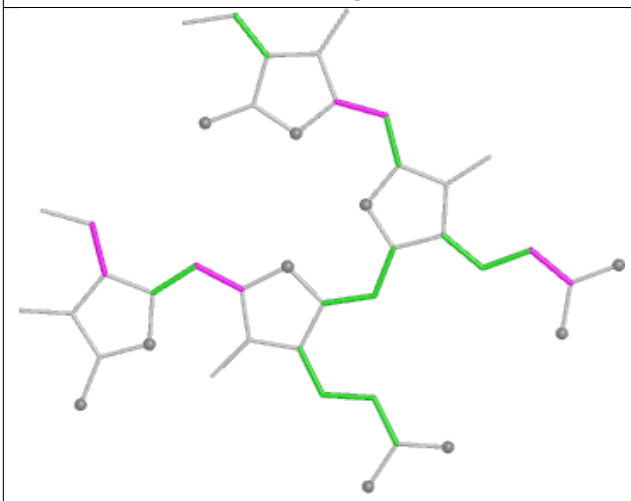

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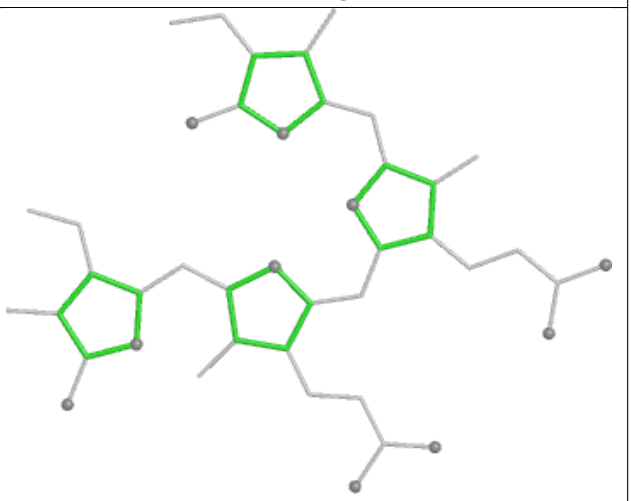

Rings

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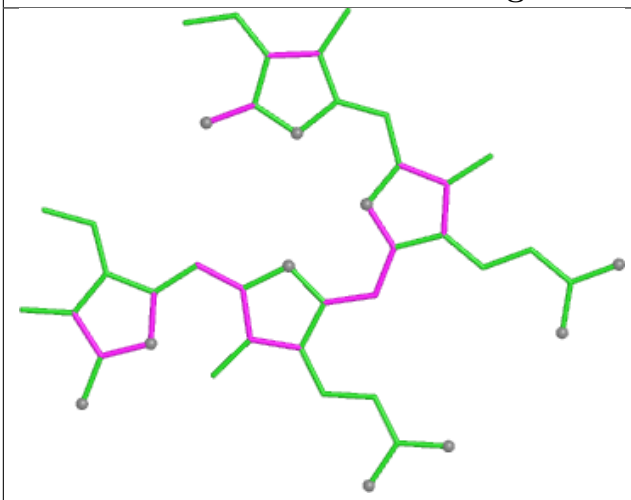

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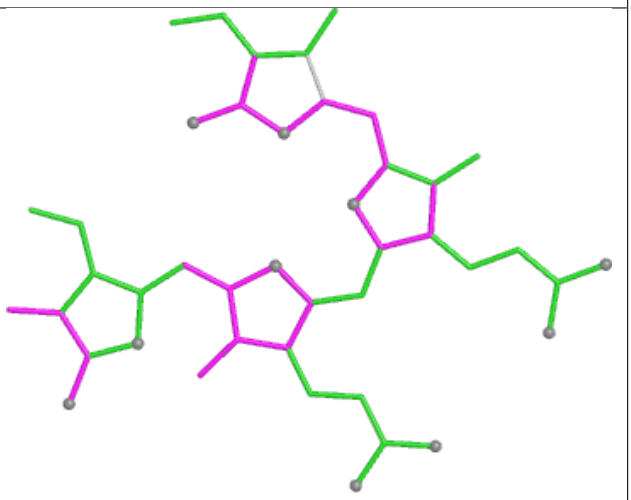

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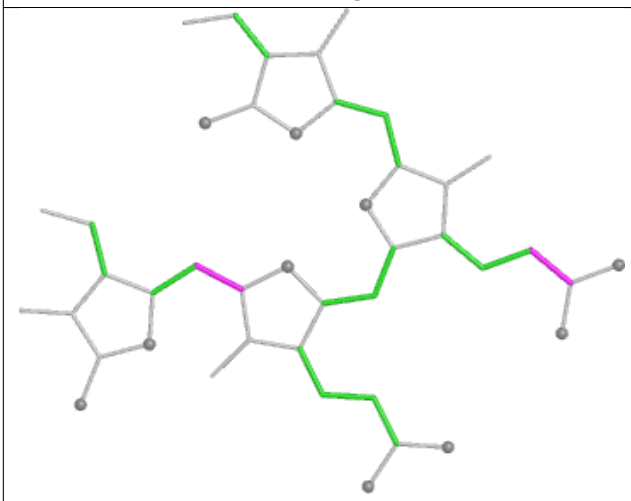

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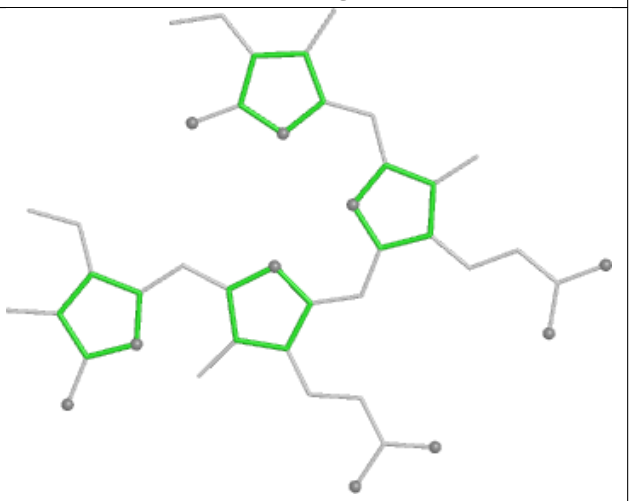

Rings

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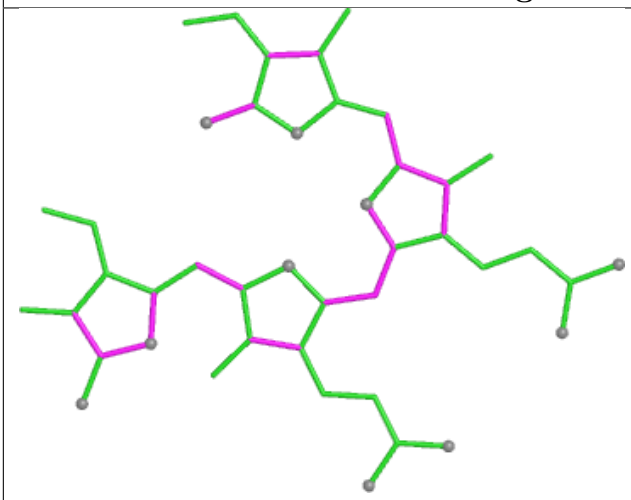
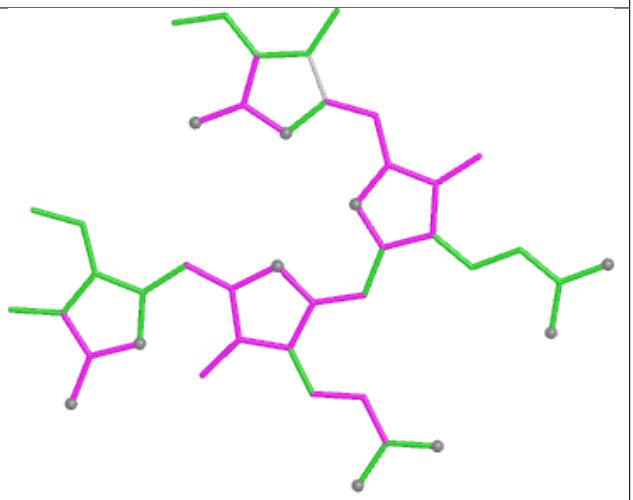
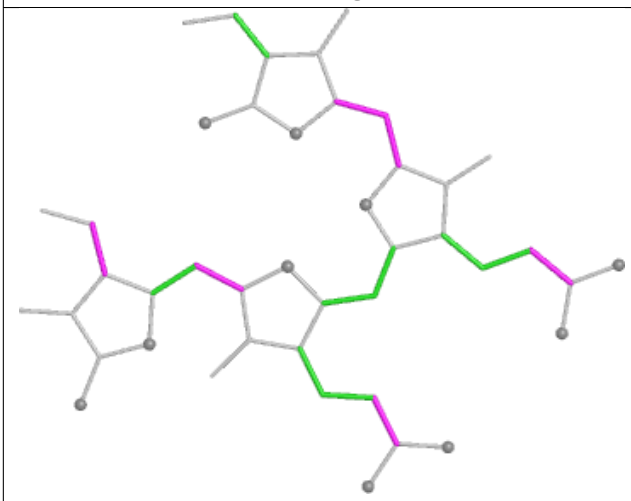


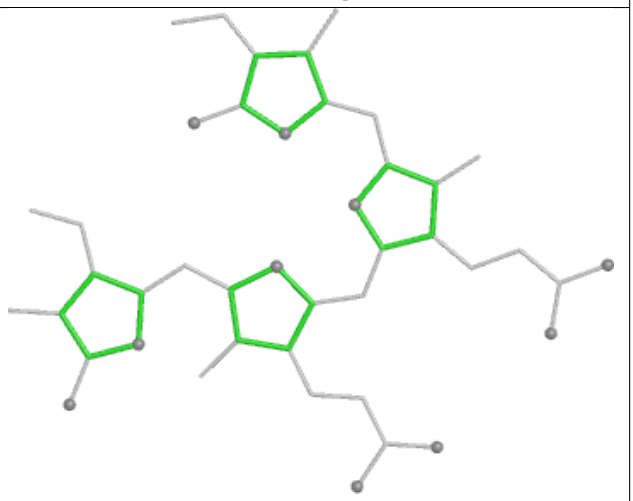
Bond lengths



Bond angles

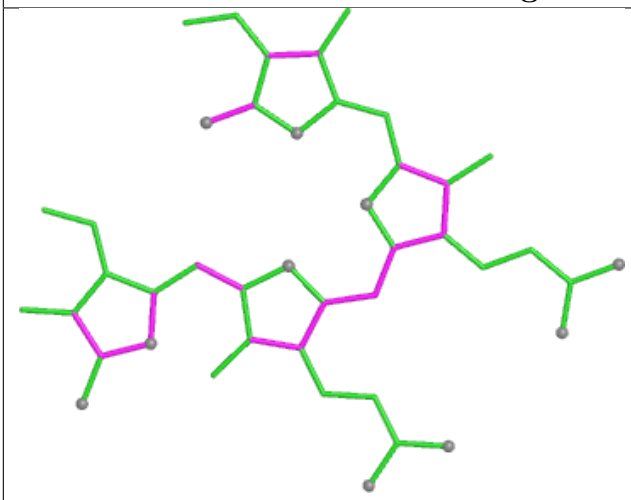


Torsions



Rings

Ligand PEB c4 203



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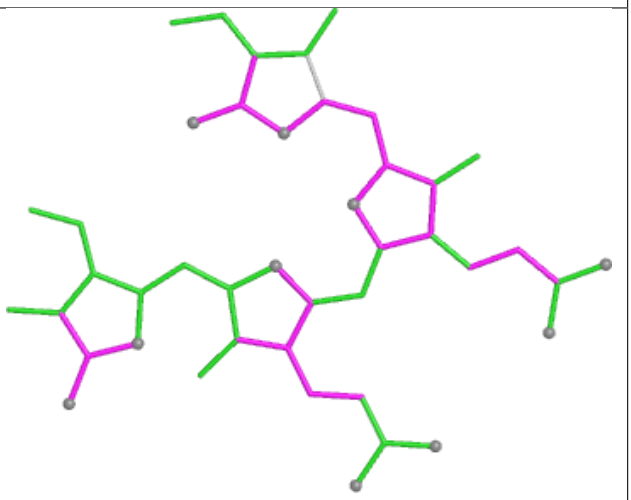

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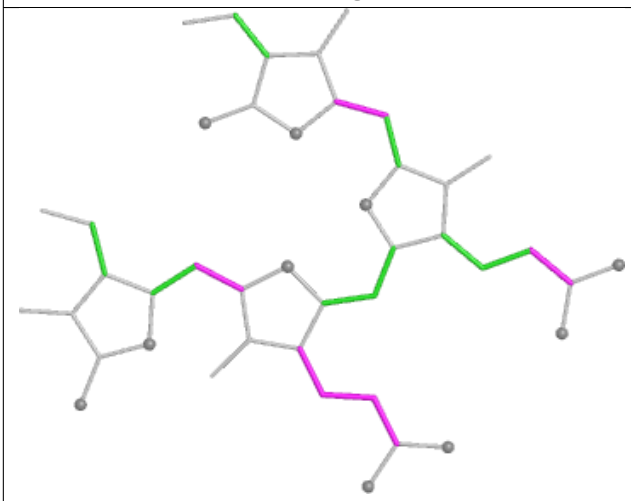

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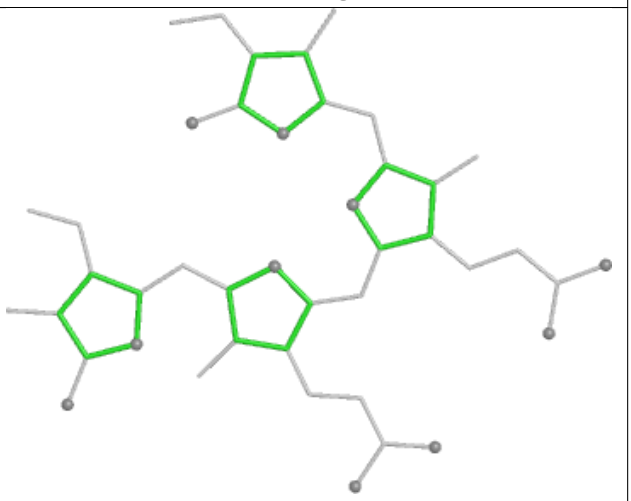
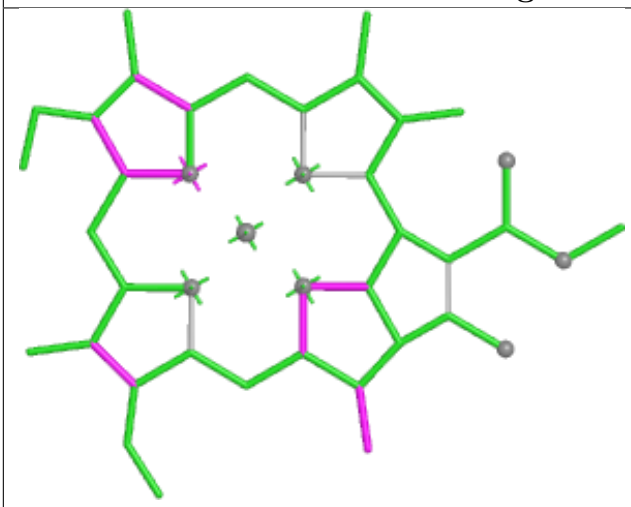


Rings

Ligand CLA F2 202



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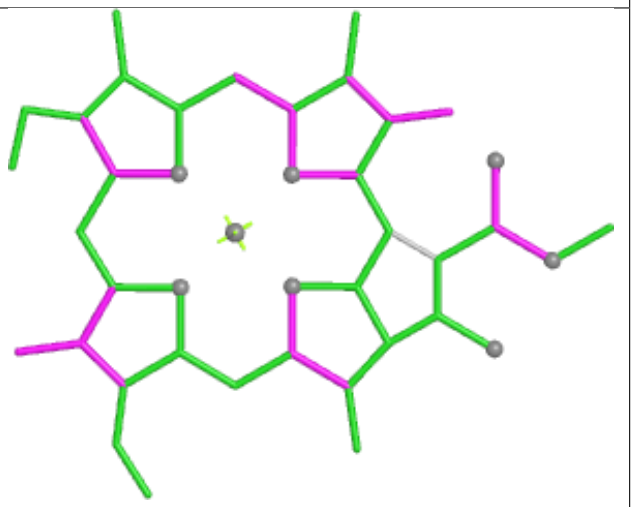

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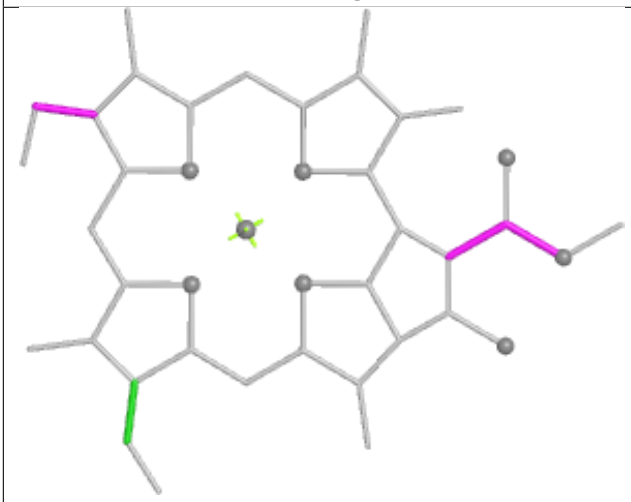

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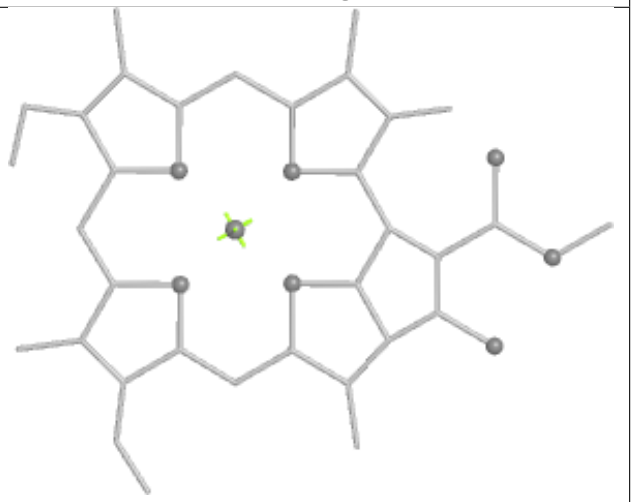
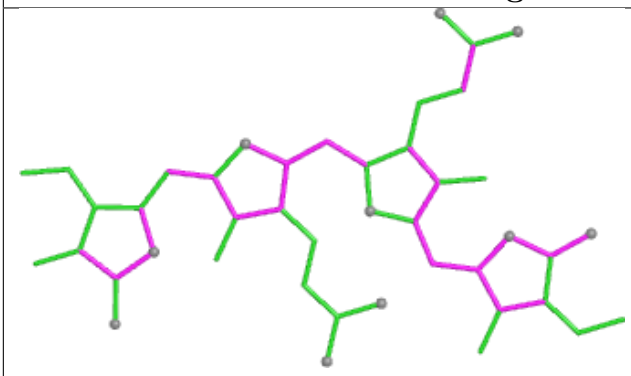


Rings

Ligand CYC L1 1001



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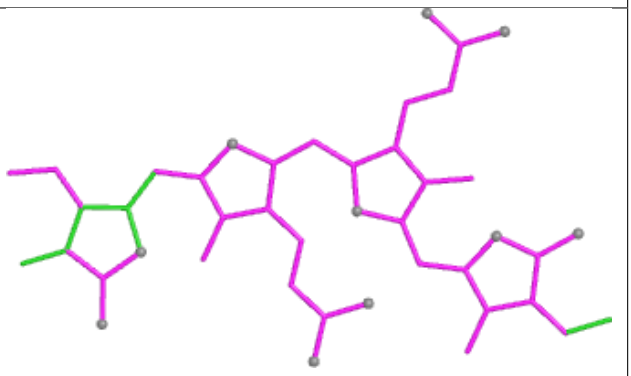

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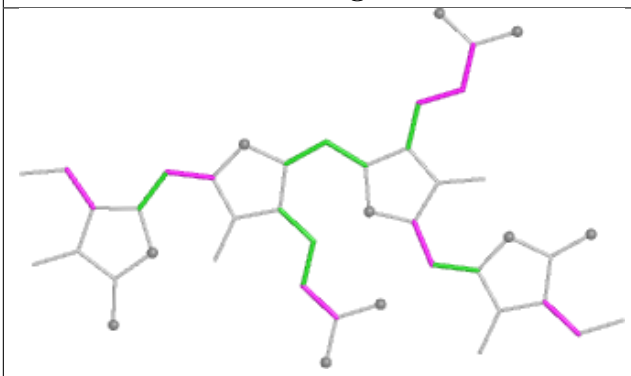

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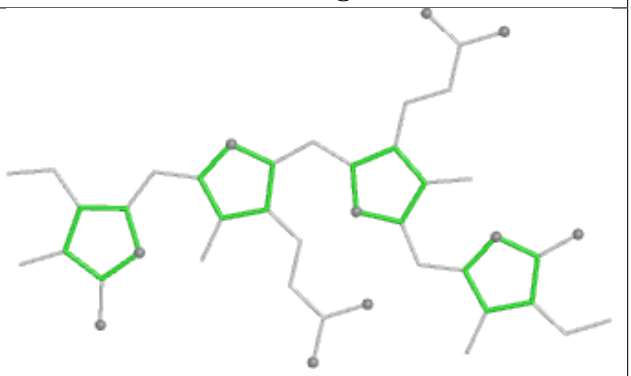
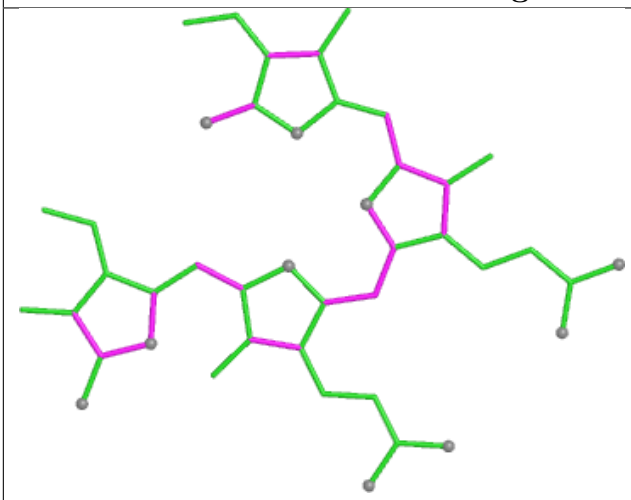


Rings

Ligand PEB QB 204



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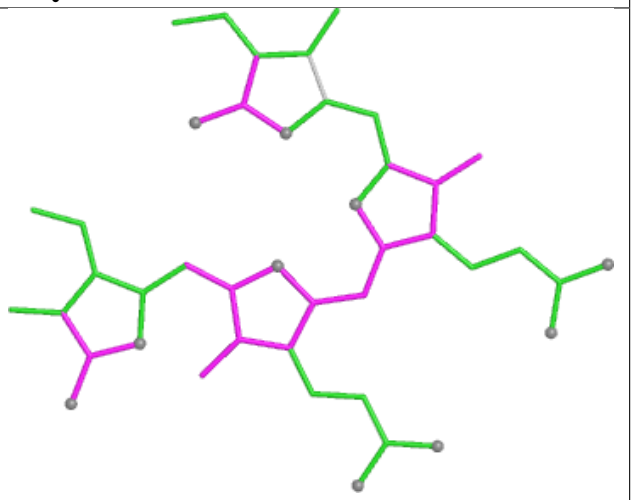
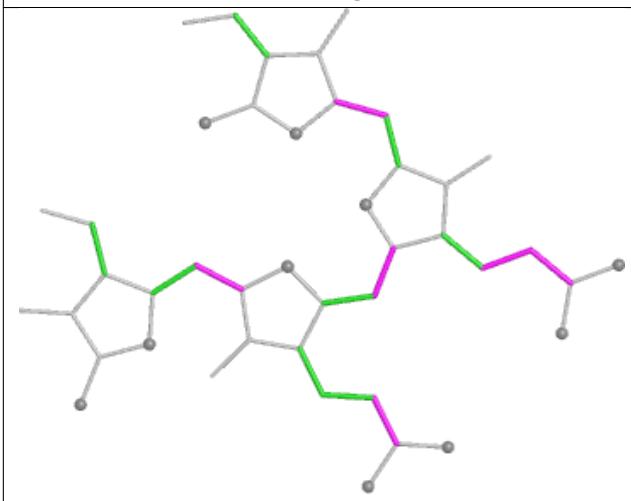


Bond angles



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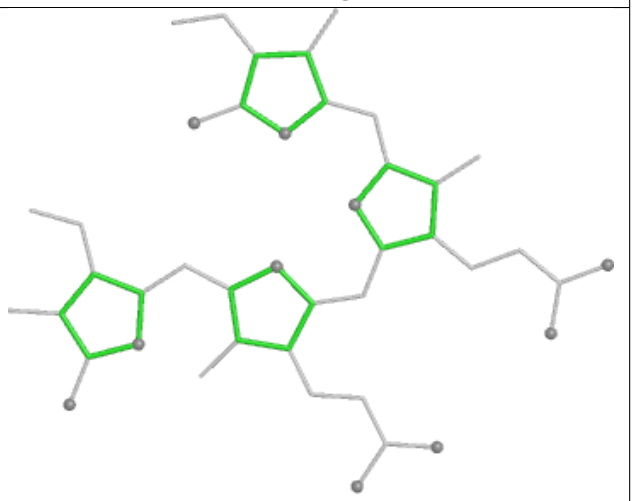
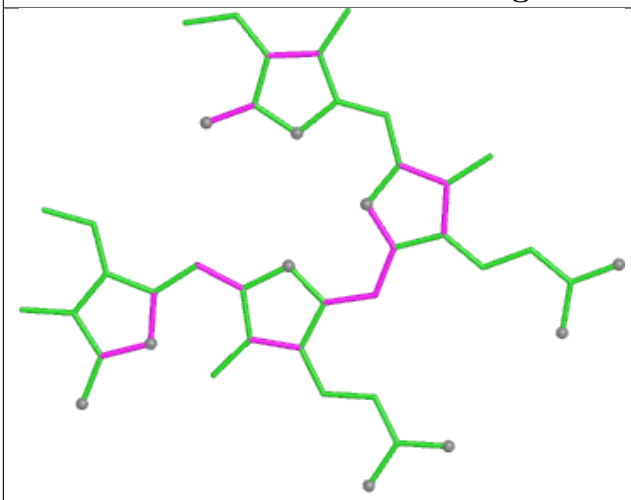


Rings

Ligand PEB EK 201



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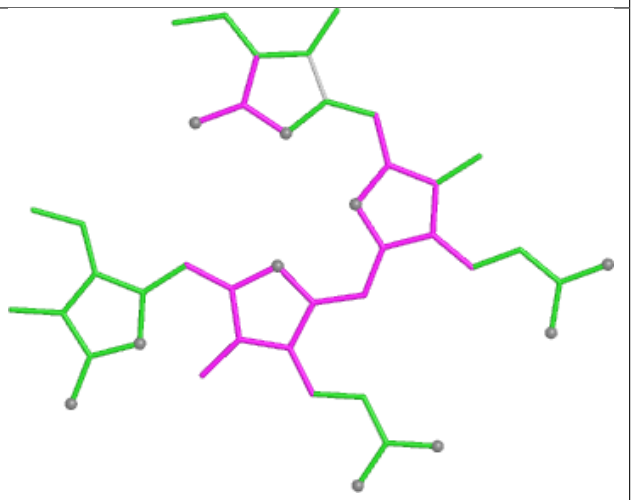

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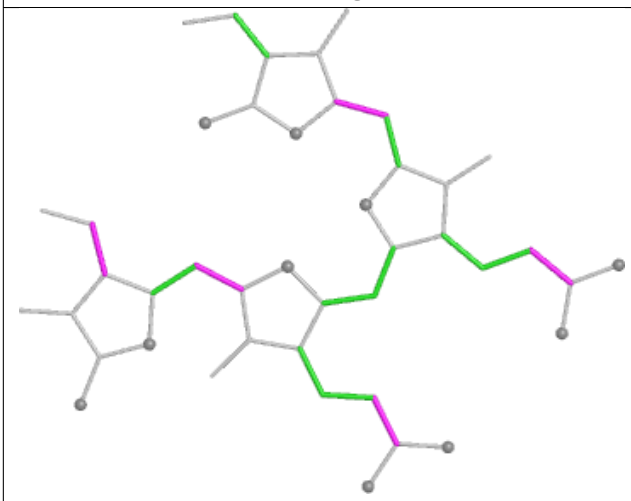

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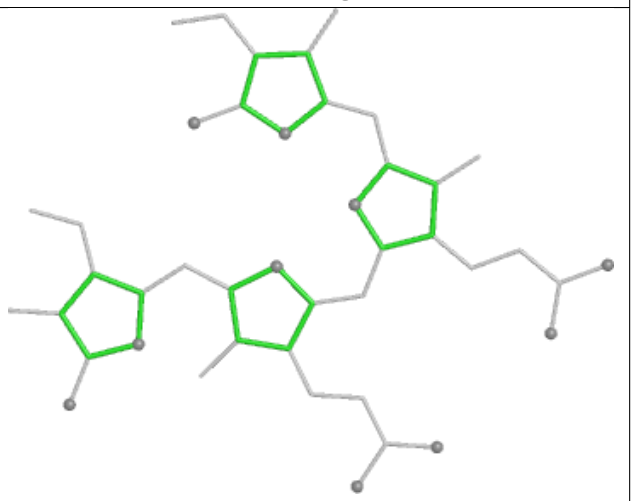
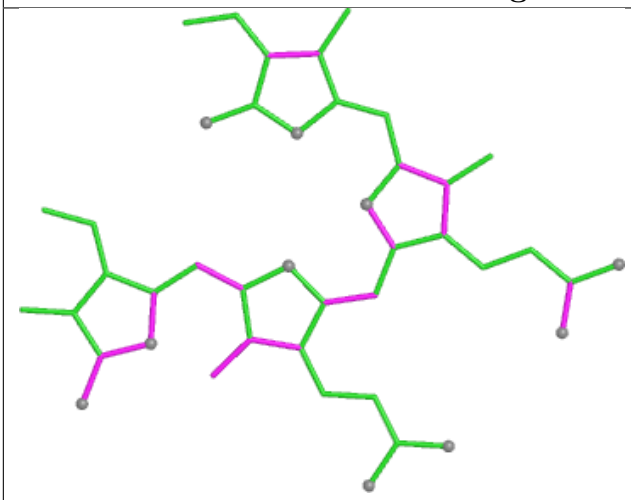


Rings

Ligand PEB GK 202



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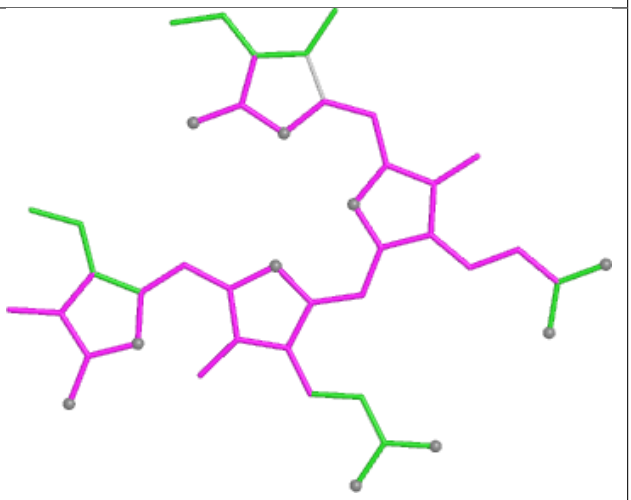
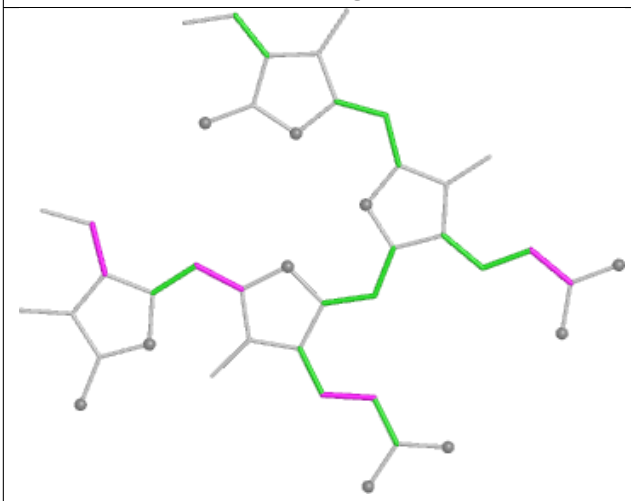


Bond angles



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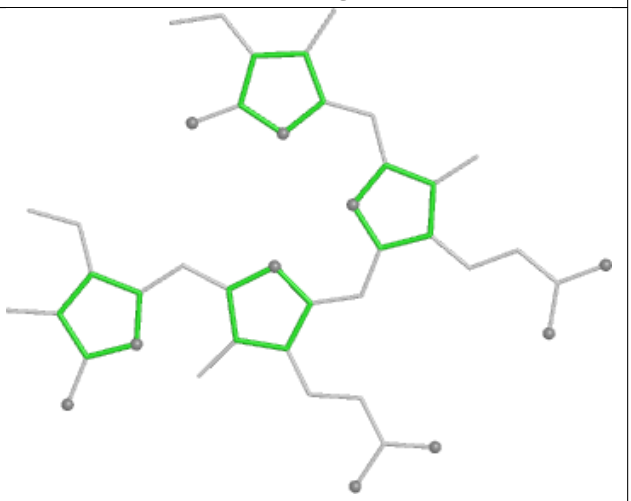
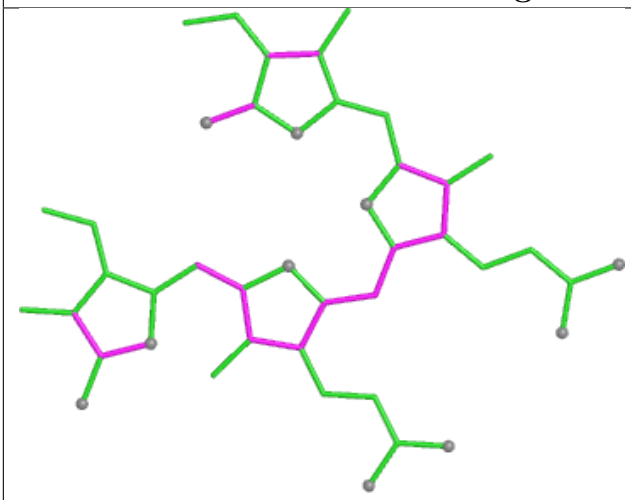


Rings

Ligand PEB qK 201



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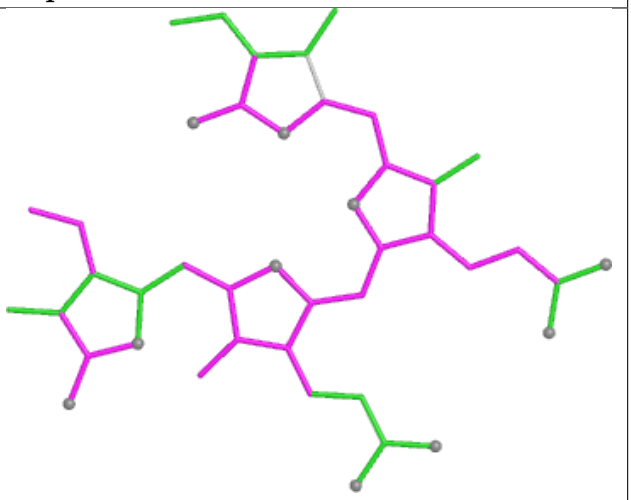
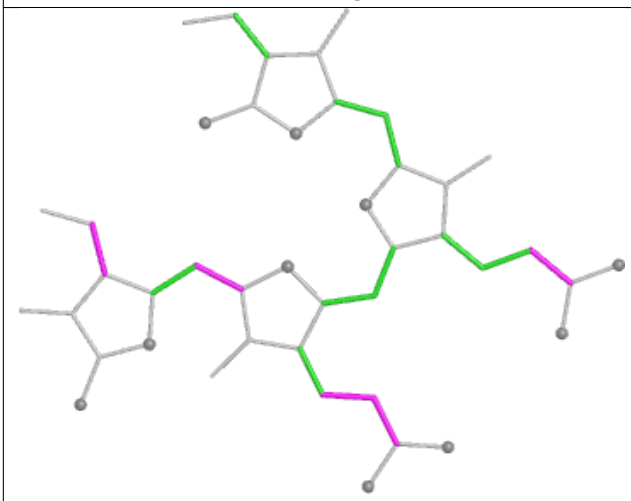


Bond angles



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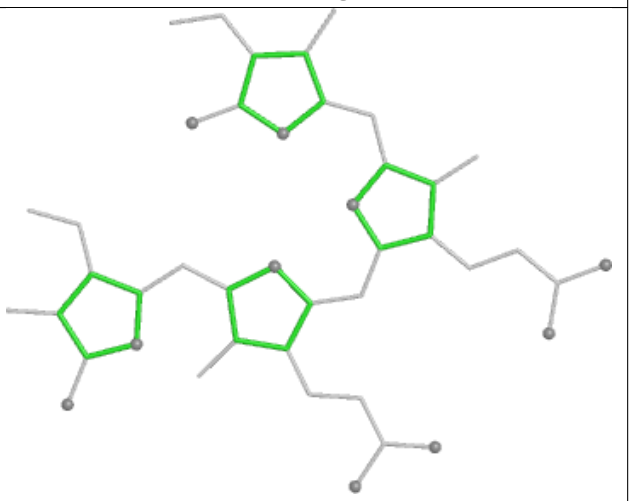
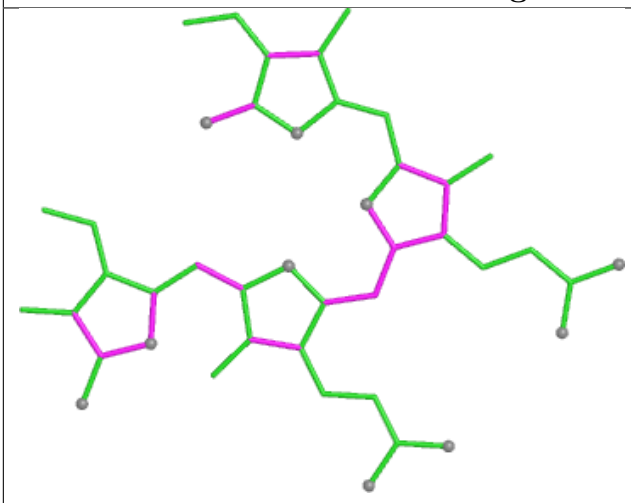


Rings

Ligand PEB UG 203



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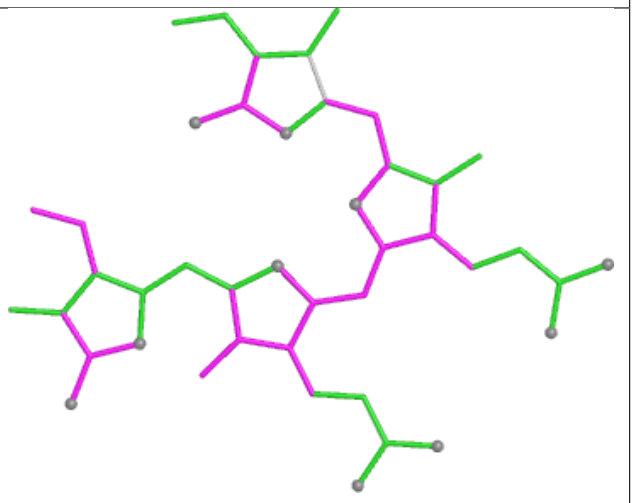

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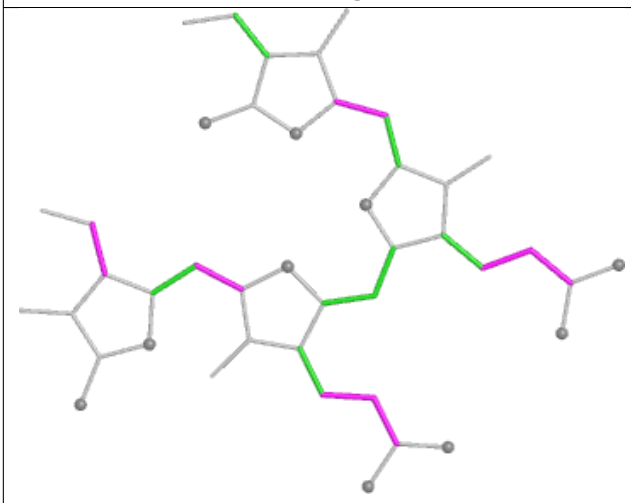

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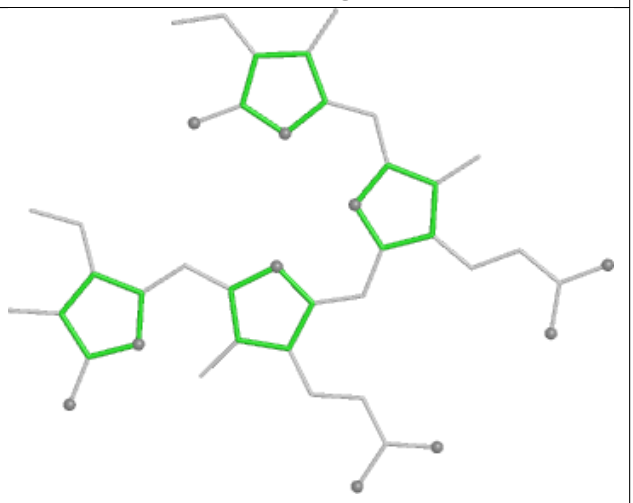
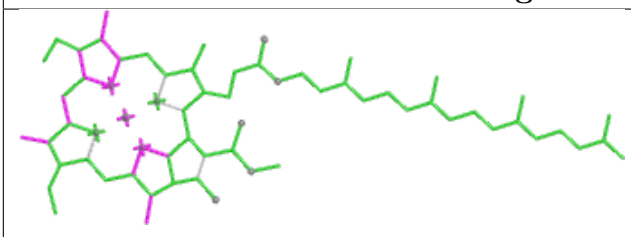


Rings

Ligand CLA B2 825



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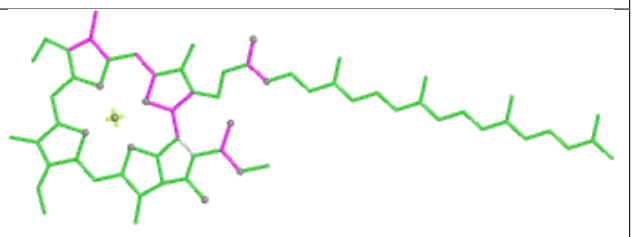
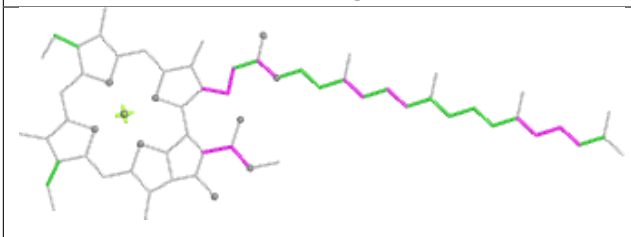


Bond angles



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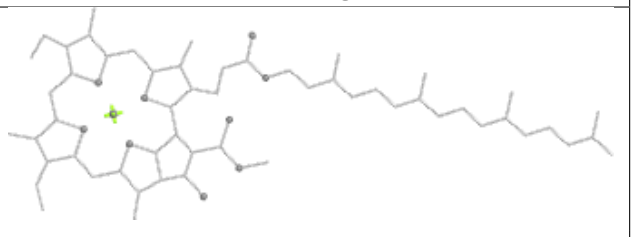
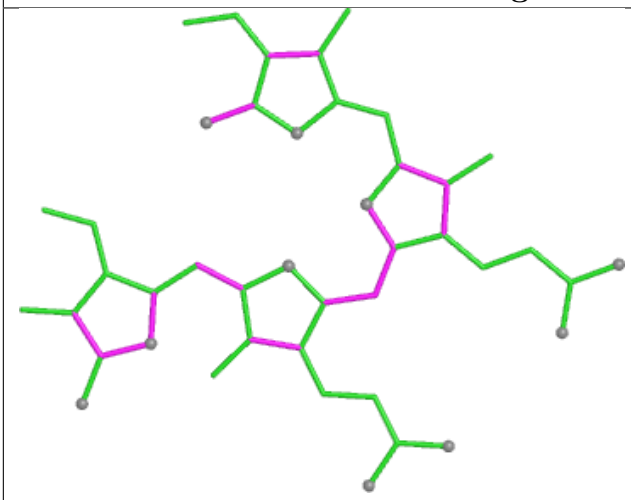


Rings

Ligand PEB HB 202



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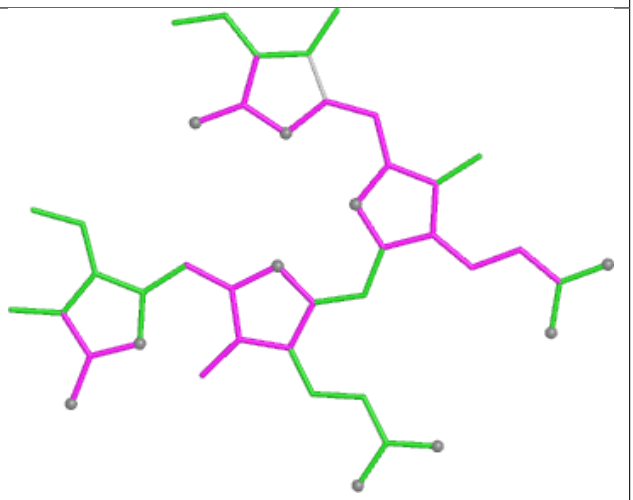

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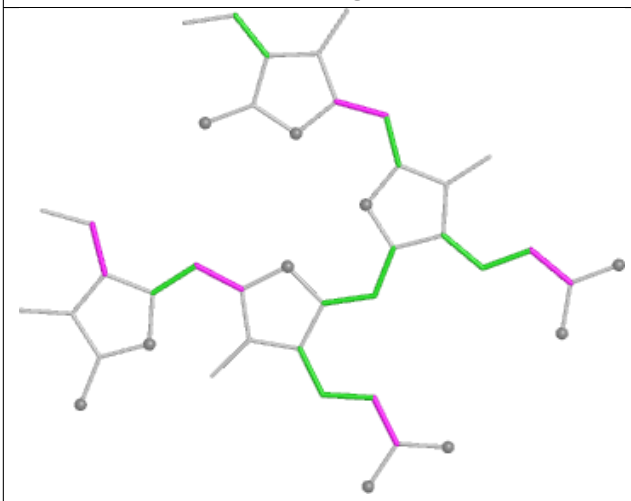

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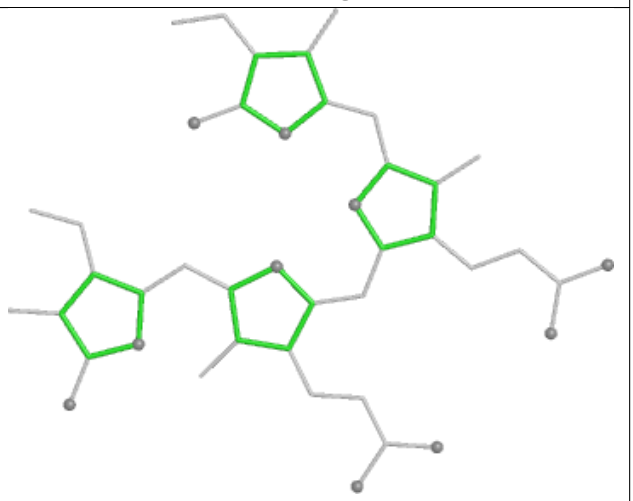
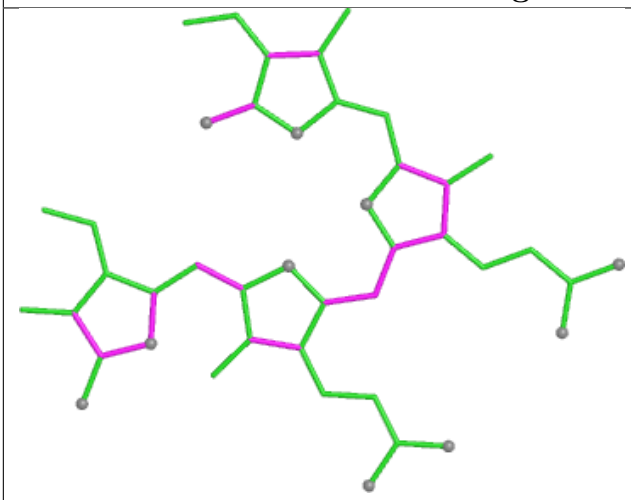


Rings

Ligand PEB XP 202



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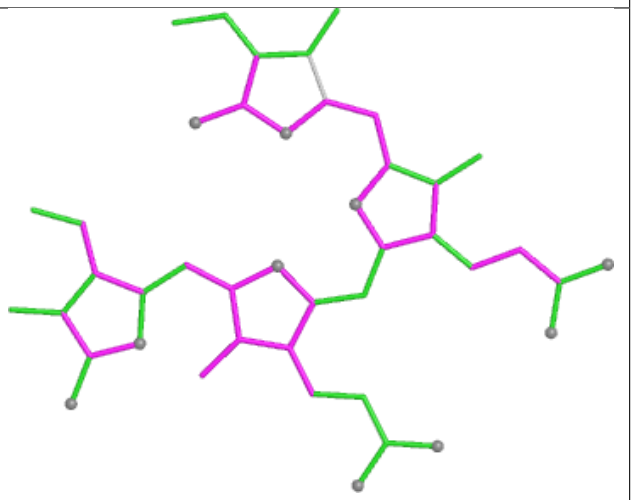
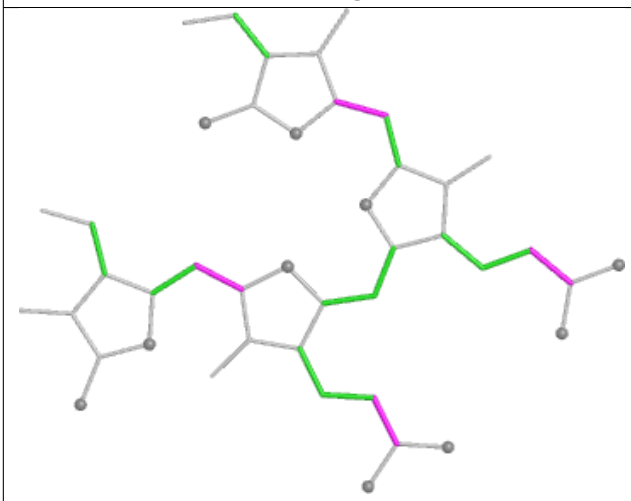


Bond angles



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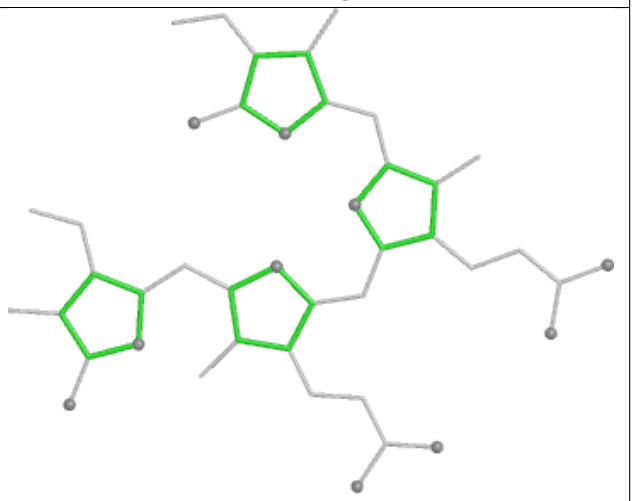
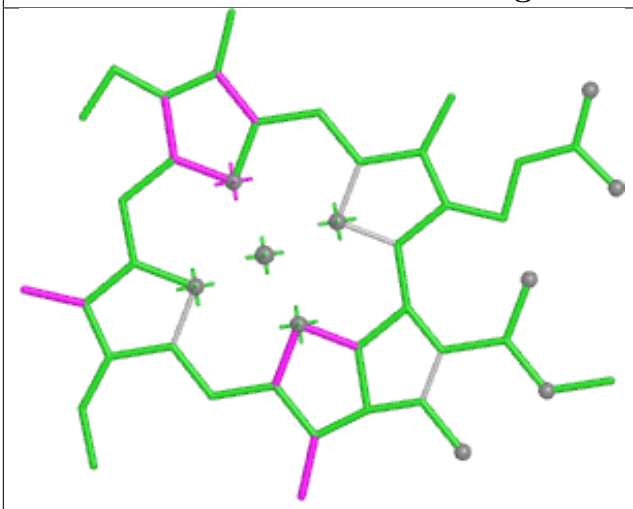


Rings

Ligand CLA 2N 308



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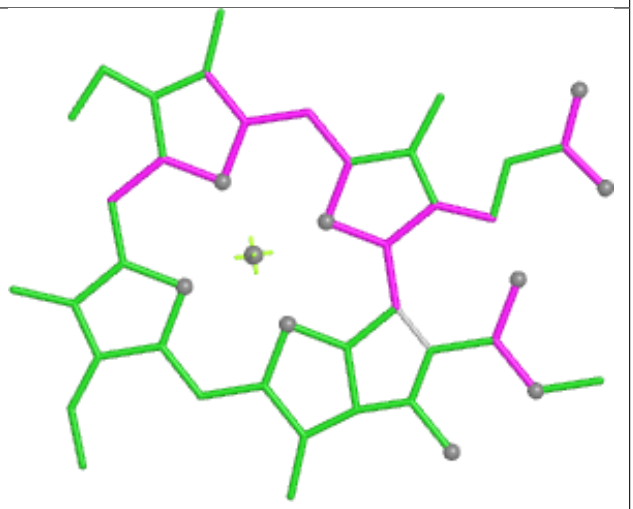
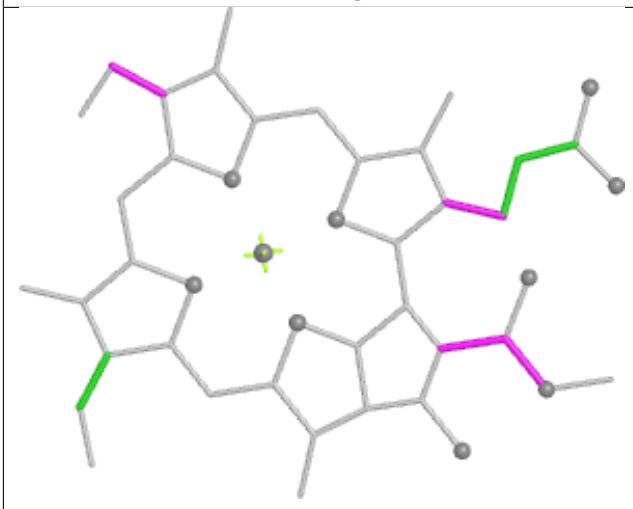


Bond angles

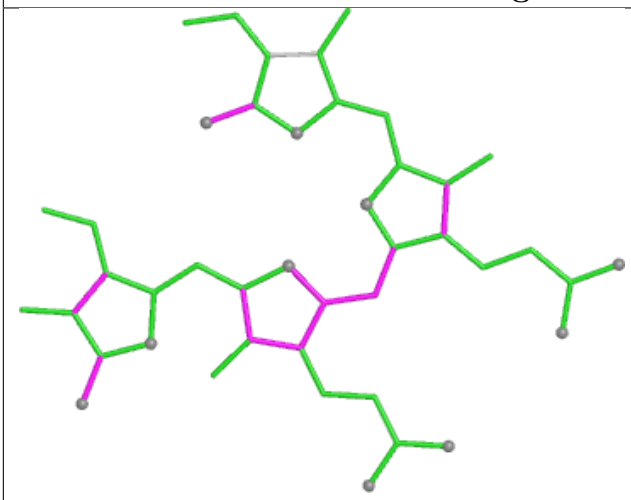


Torsions



Rings

Ligand PUB xK 306



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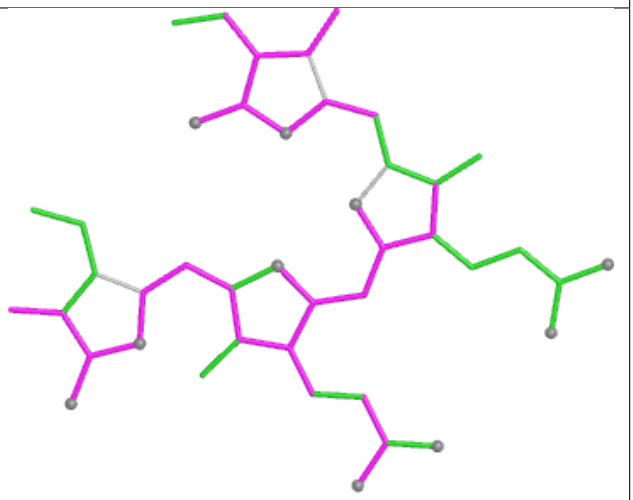
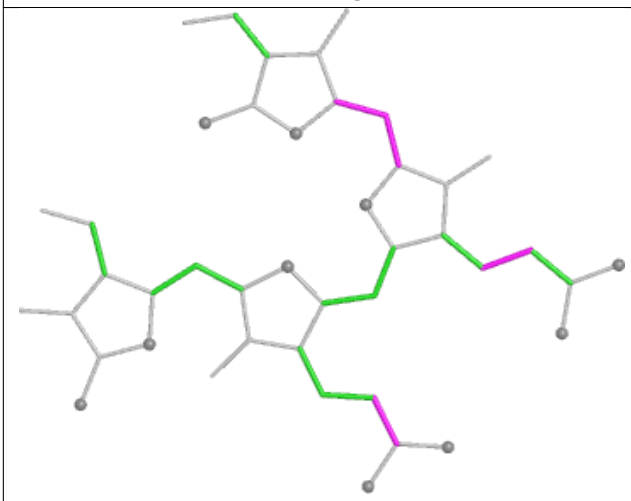


Bond angles



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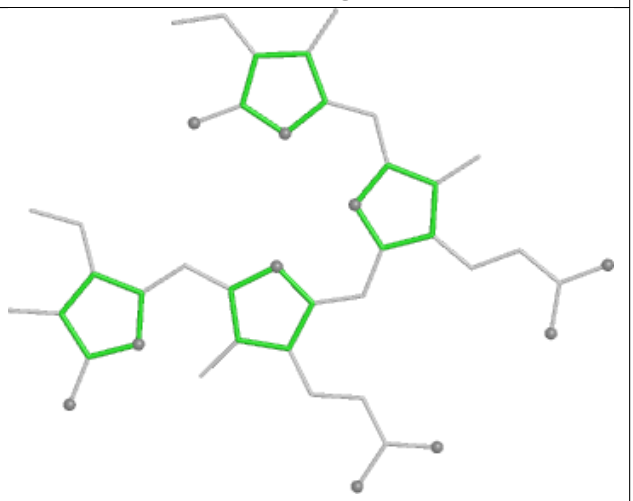
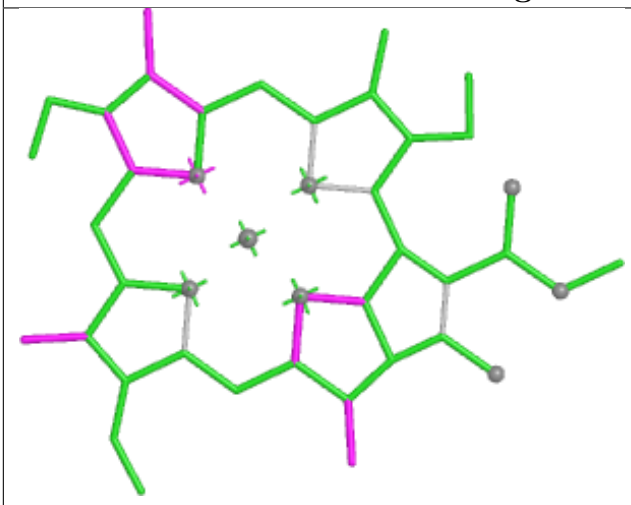


Rings

Ligand CLA 5N 609



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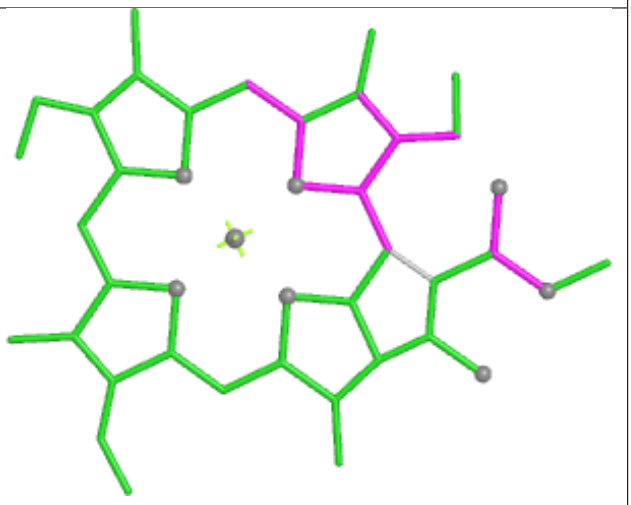
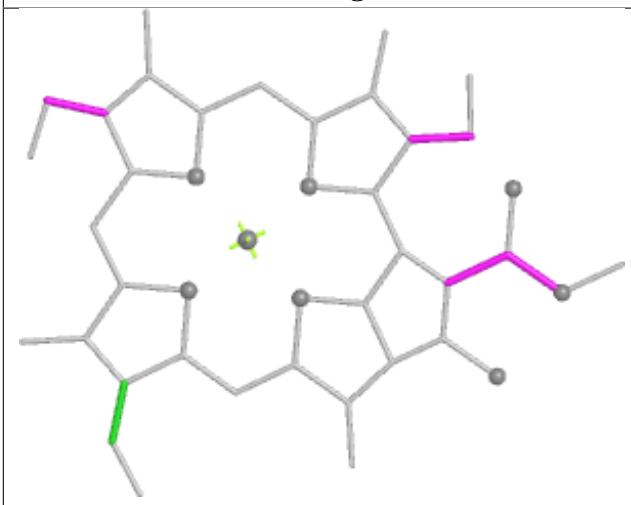


Bond angles

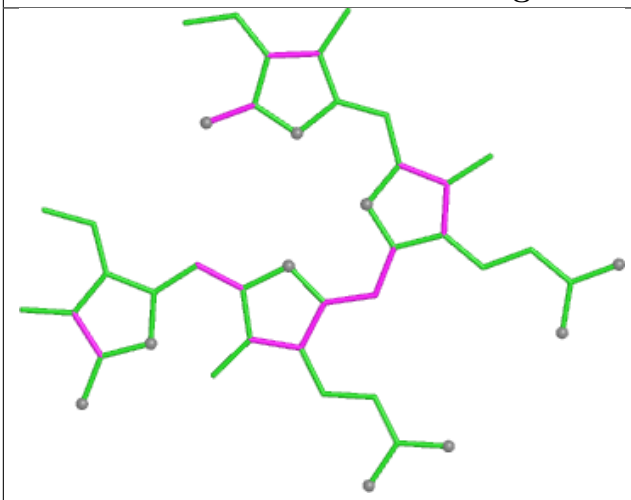


Torsions

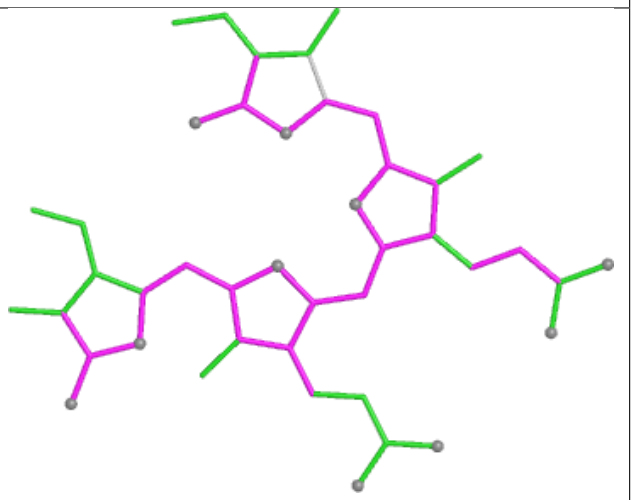


Rings

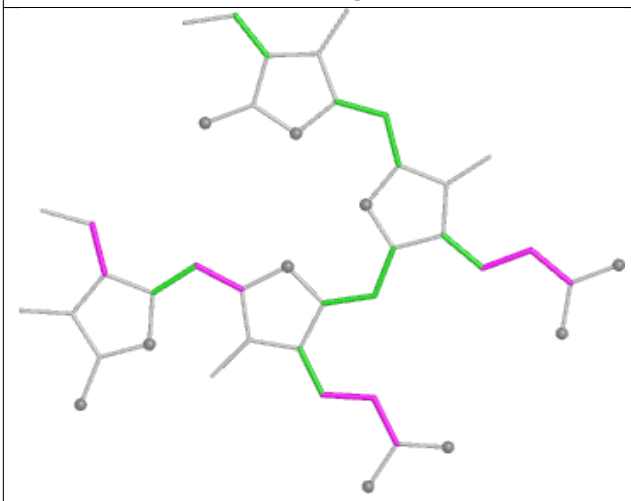
Ligand PEB XF 201



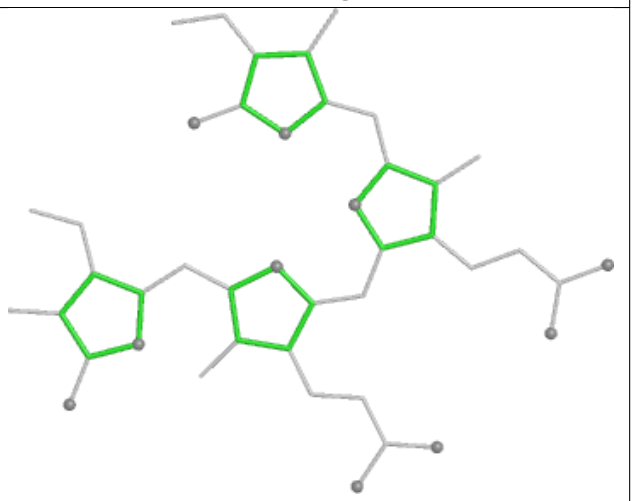
Bond lengths



Bond angles

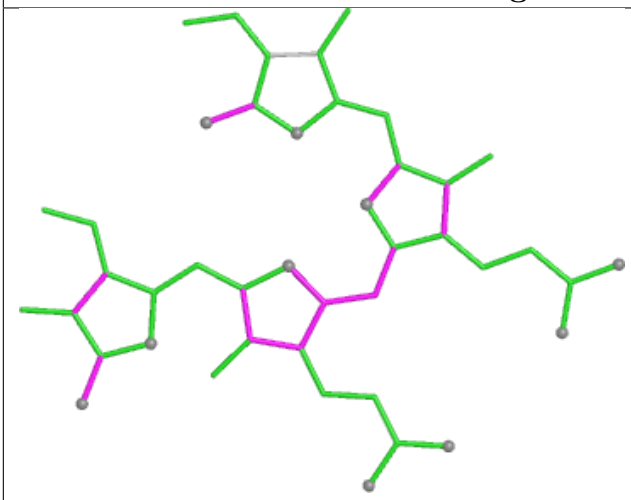


Torsions



Rings

Ligand PUB M5 303



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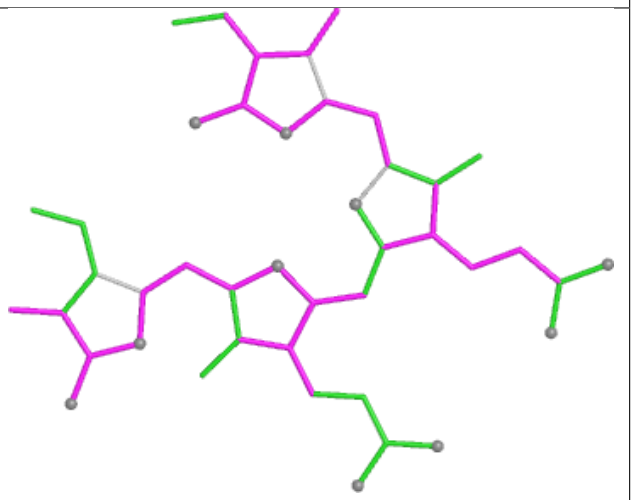

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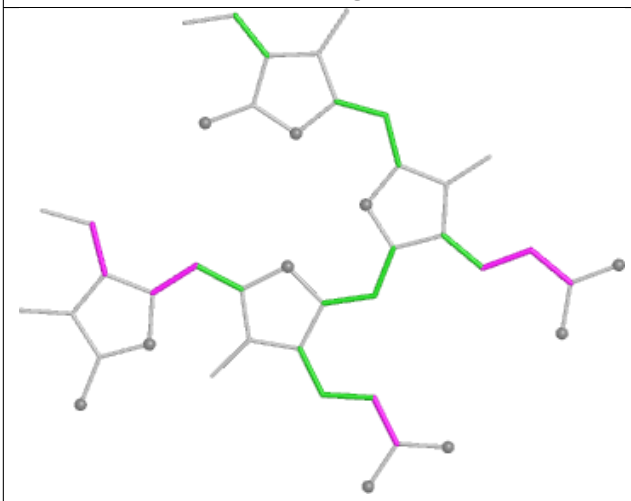

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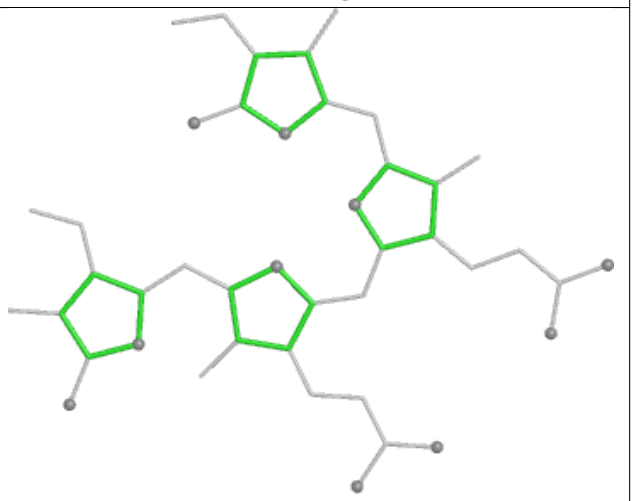
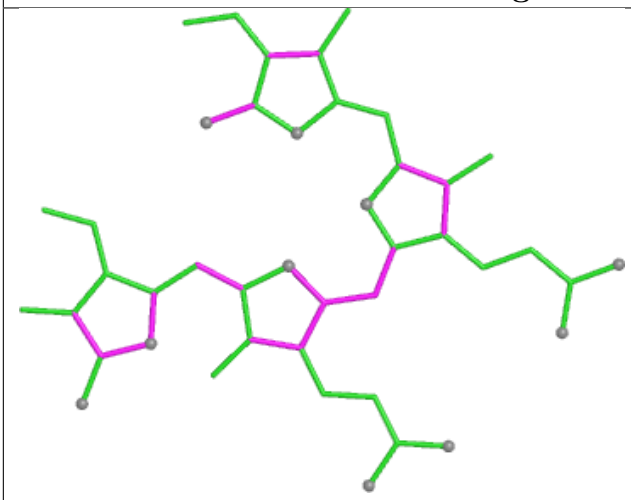


Rings

Ligand PEB HF 201



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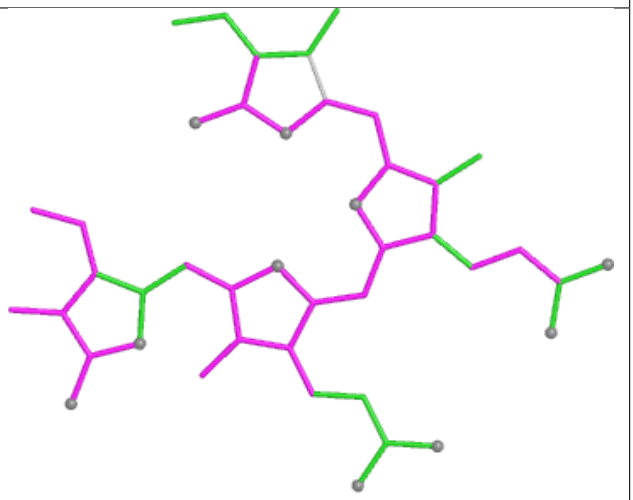

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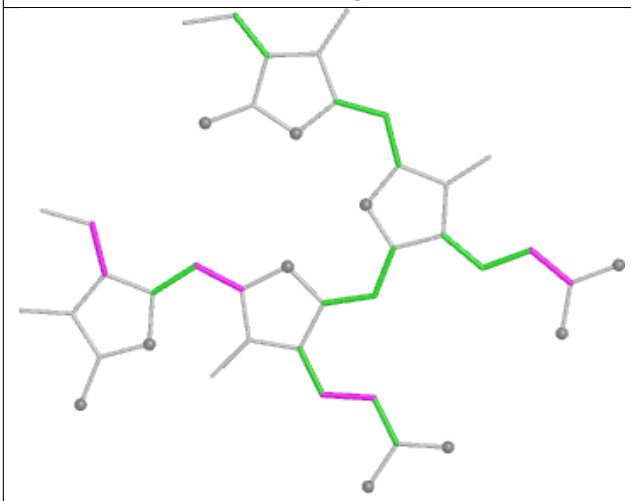

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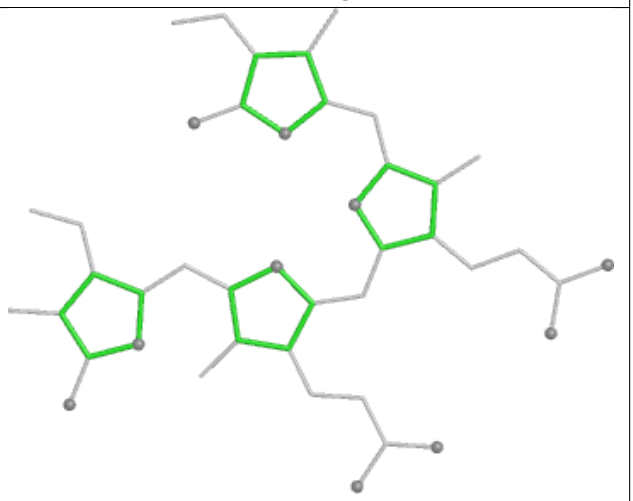
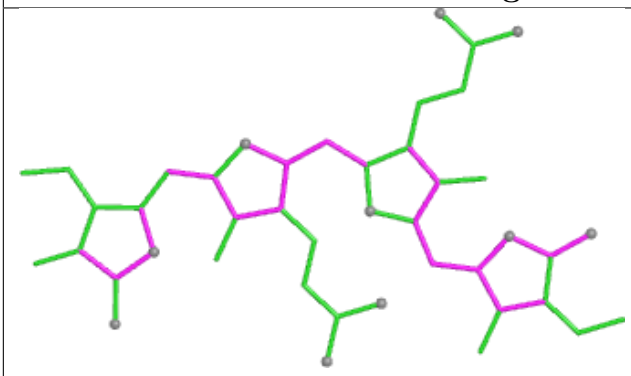


Rings

Ligand CYC EE 1001



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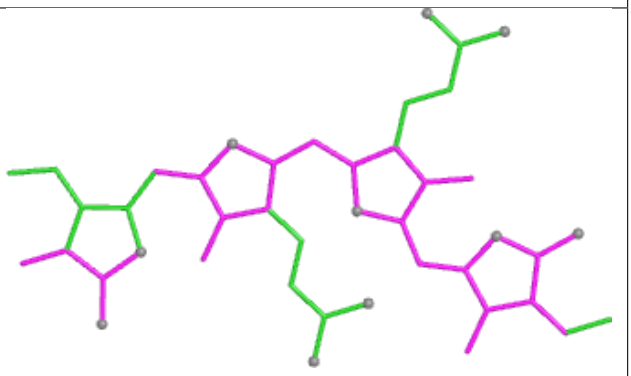

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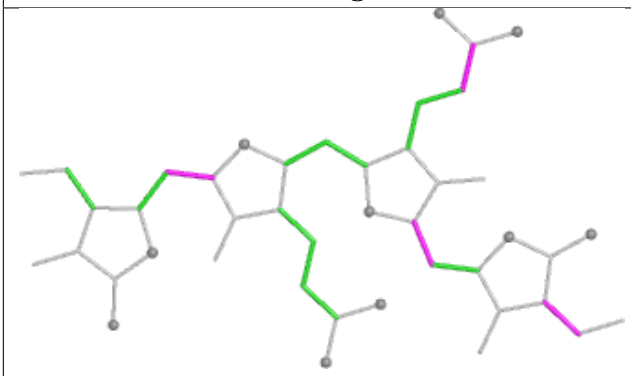

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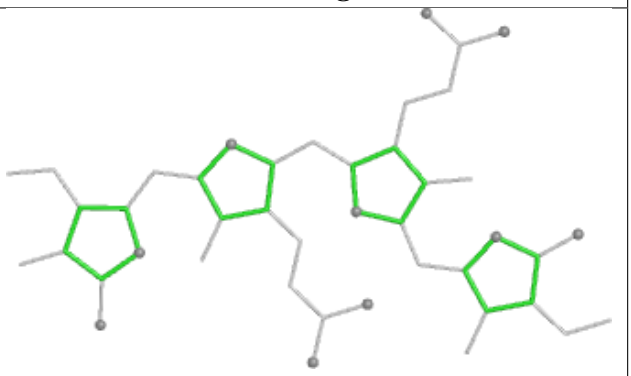
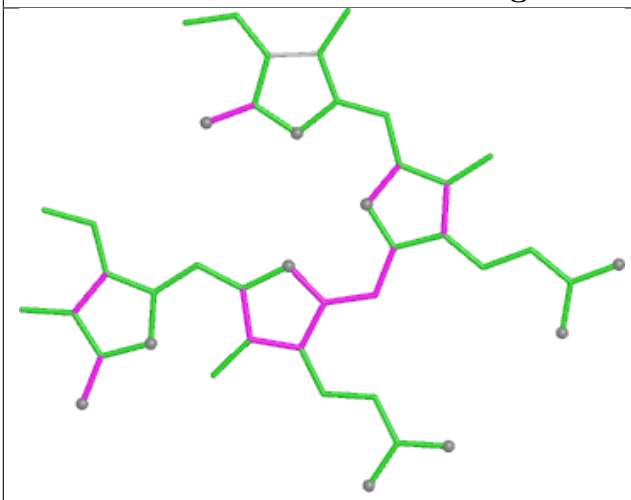


Rings

Ligand PUB YA 302



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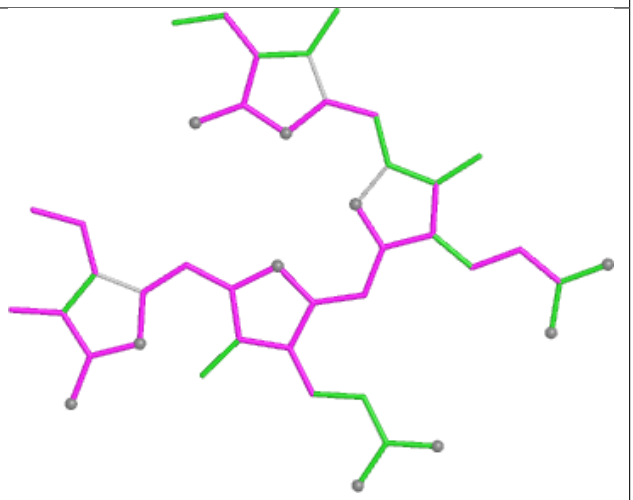

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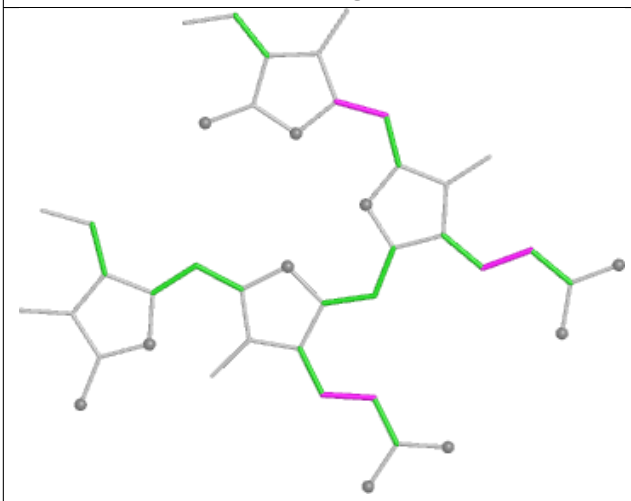

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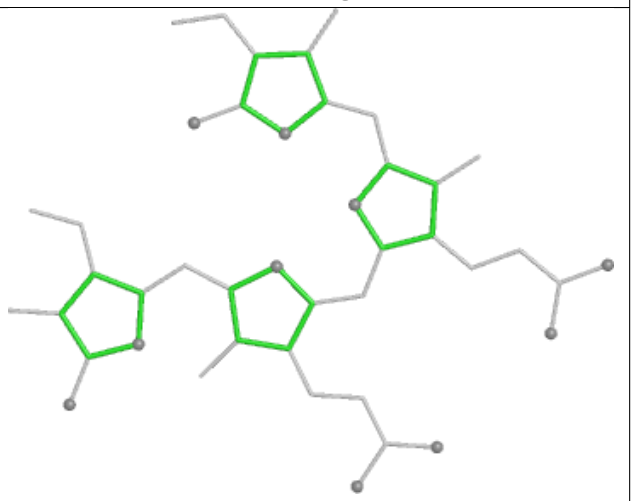
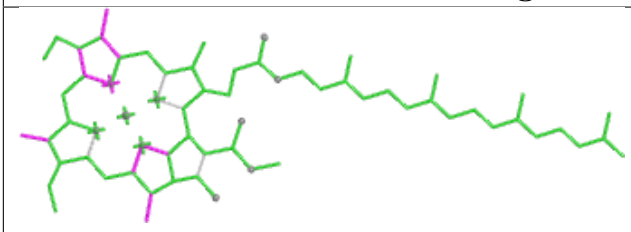


Rings

Ligand CLA IN 102



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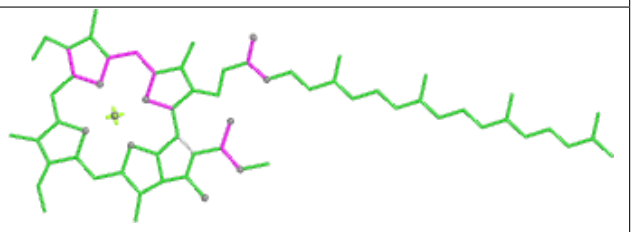

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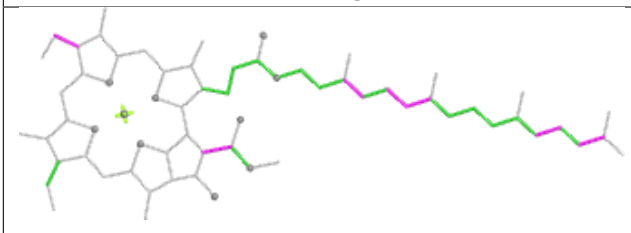

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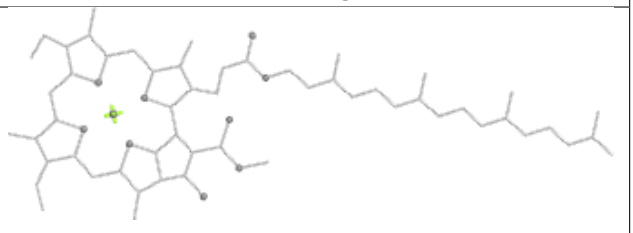
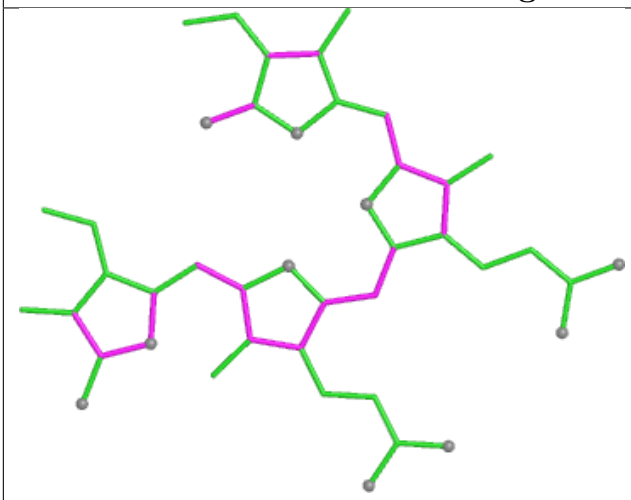


Rings

Ligand PEB iH 201



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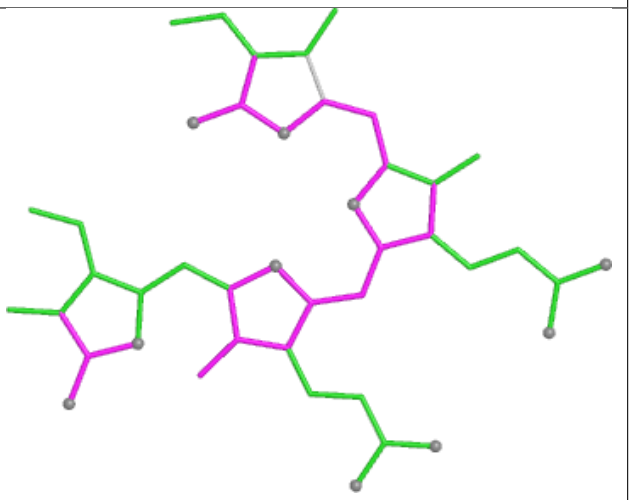

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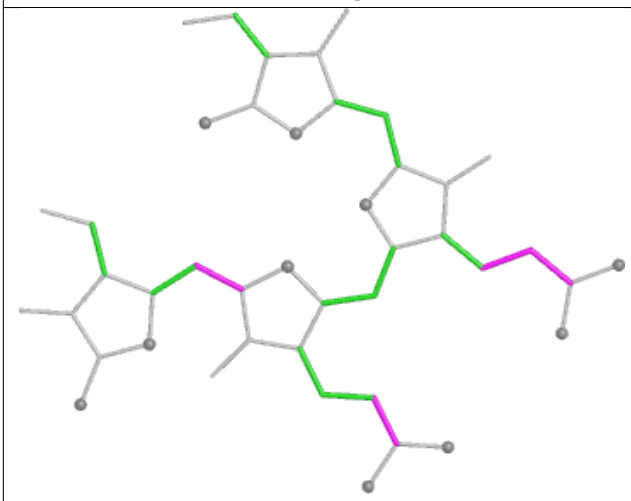

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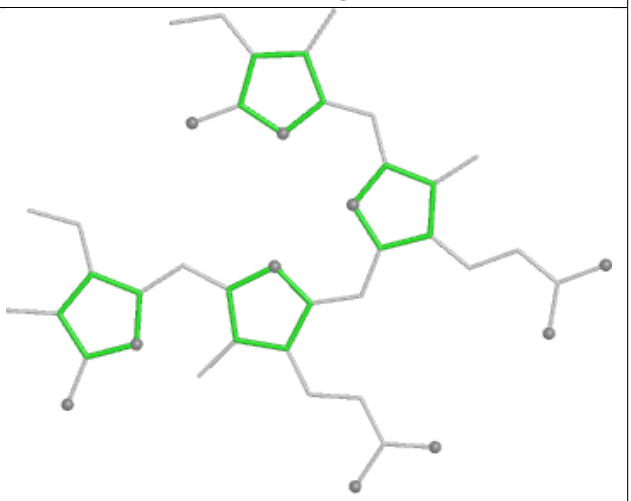
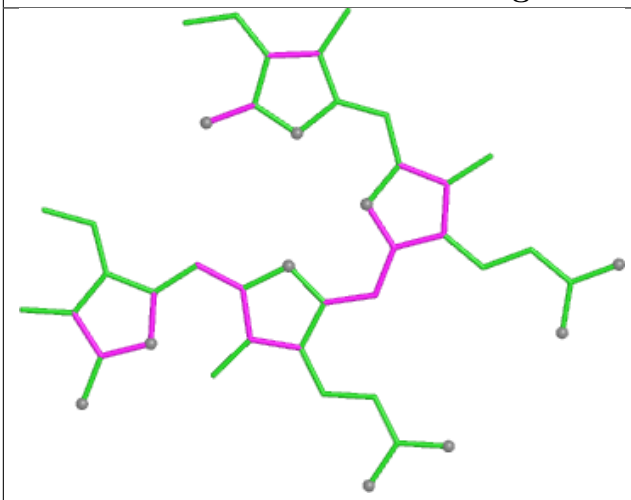


Rings

Ligand PEB EQ 201



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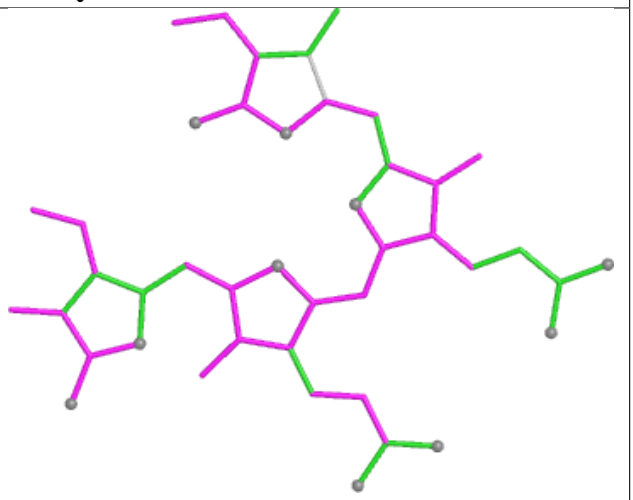

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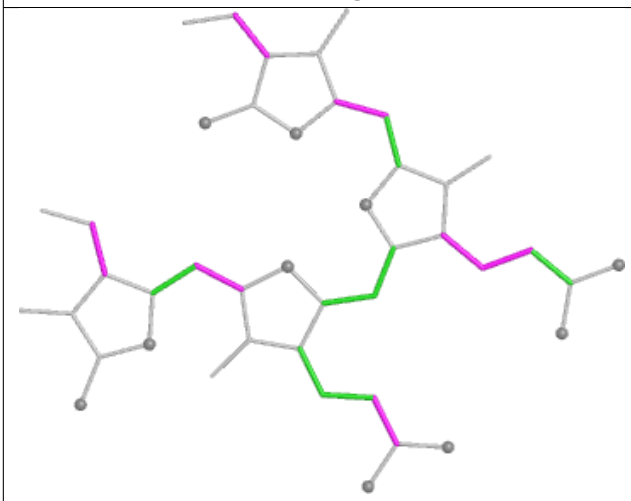

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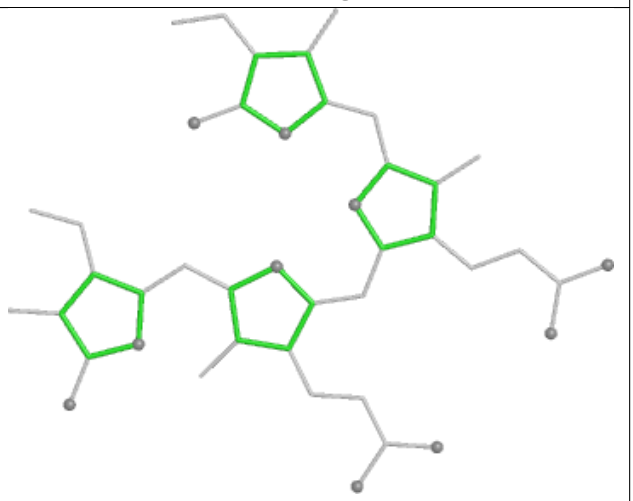
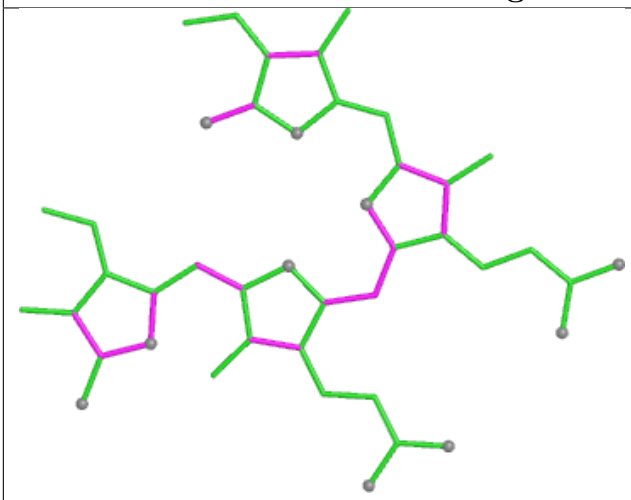


Rings

Ligand PEB WP 202



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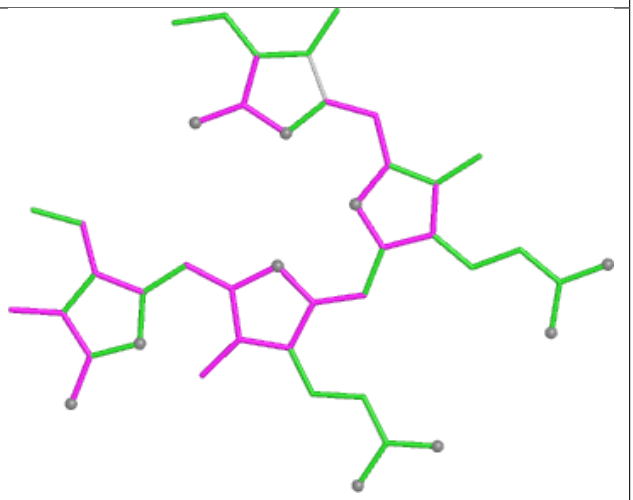

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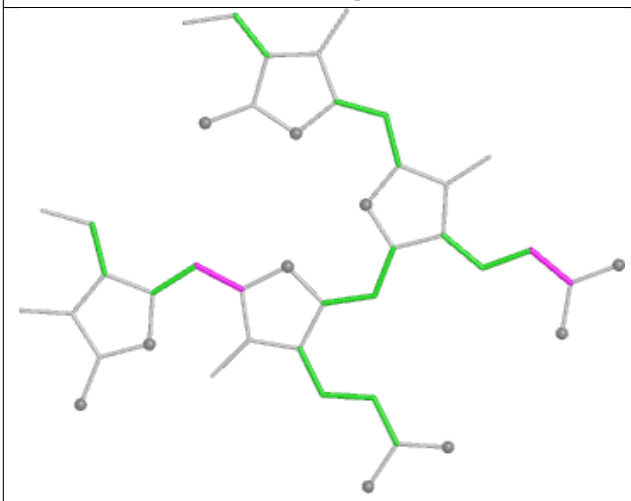

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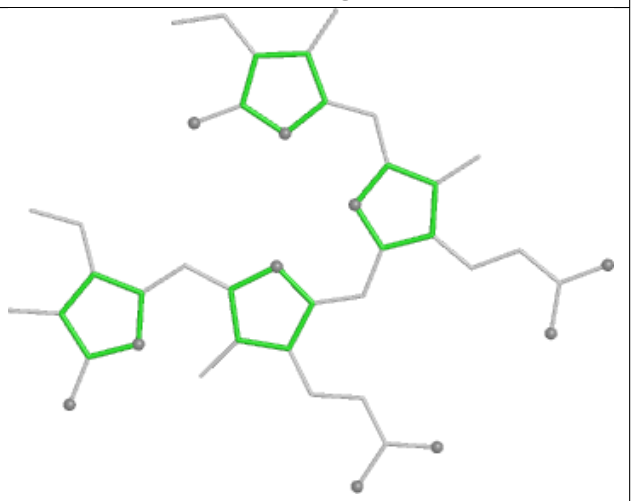
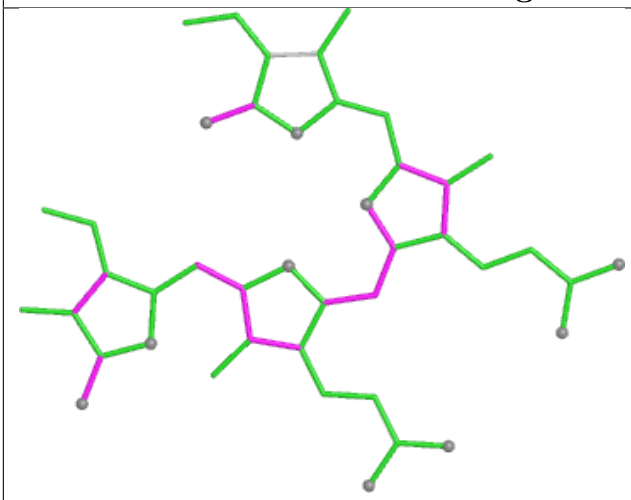


Rings

Ligand PUB Z9 302



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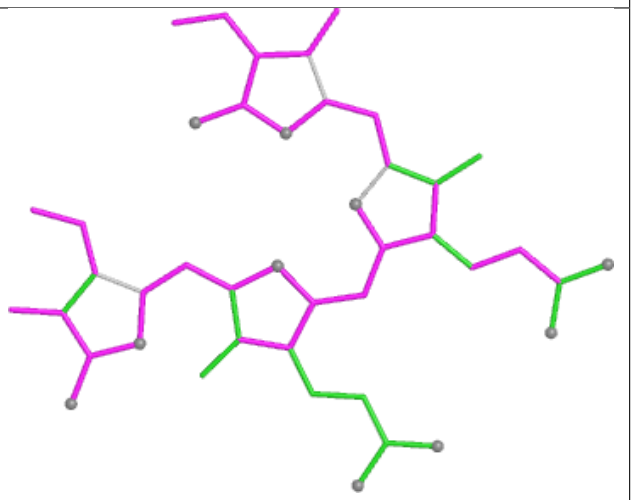

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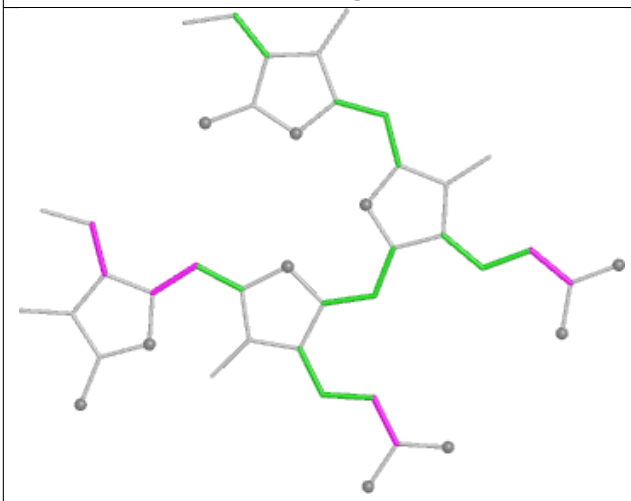

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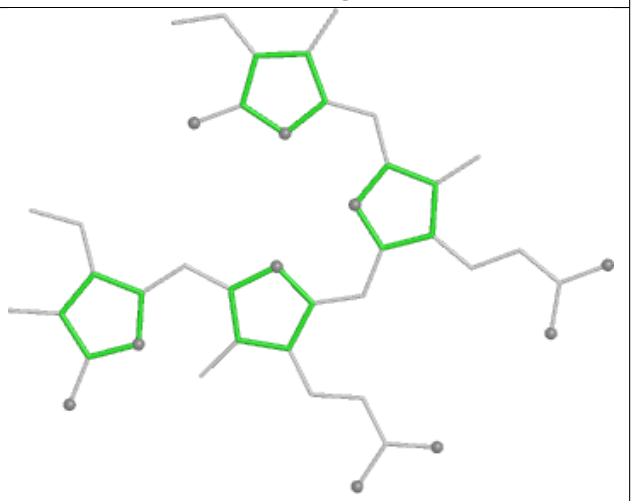
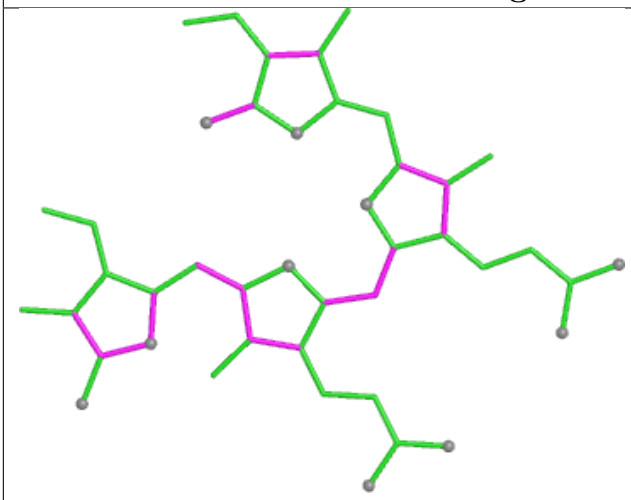


Rings

Ligand PEB KK 202



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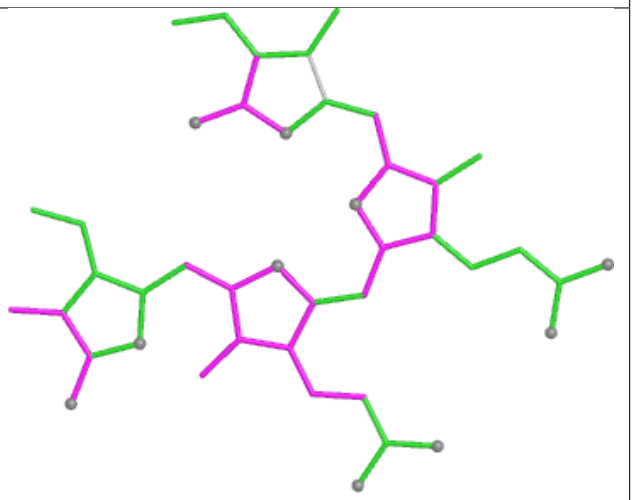

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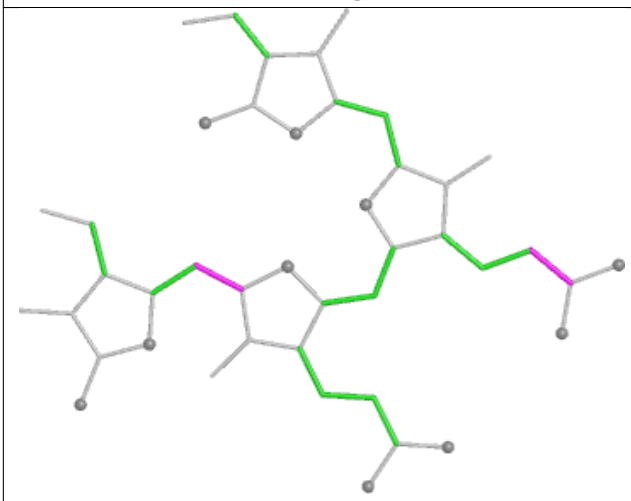

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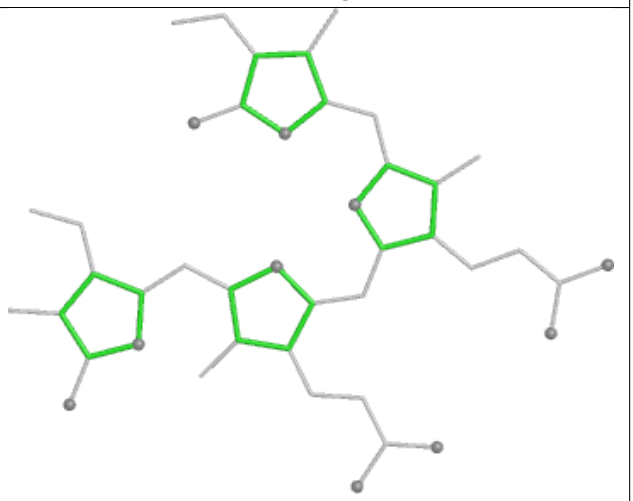
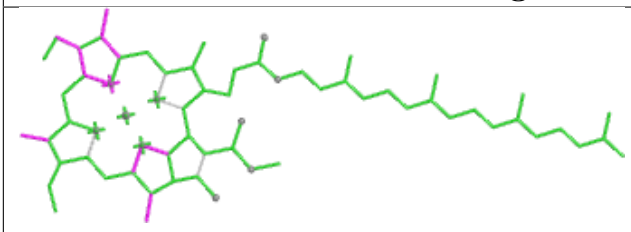


Rings

Ligand CLA AN 834



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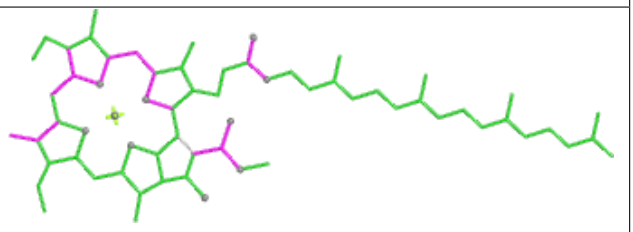
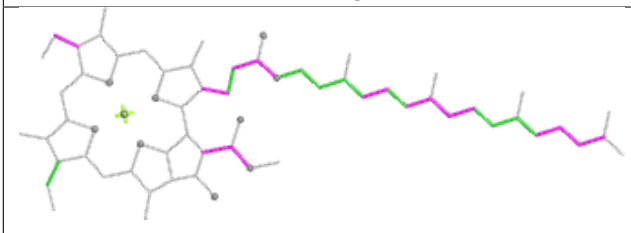


Bond angles



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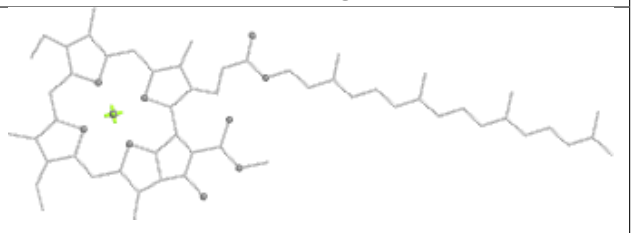
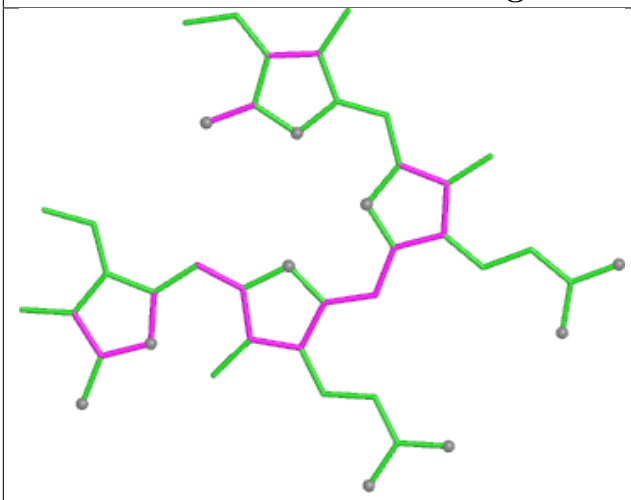


Rings

Ligand PEB MK 203



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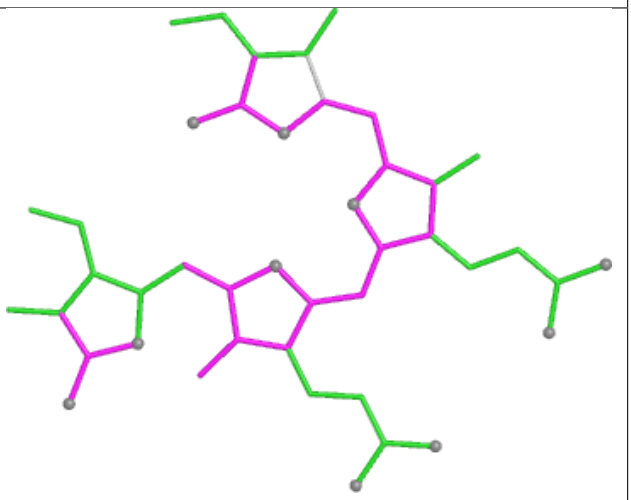
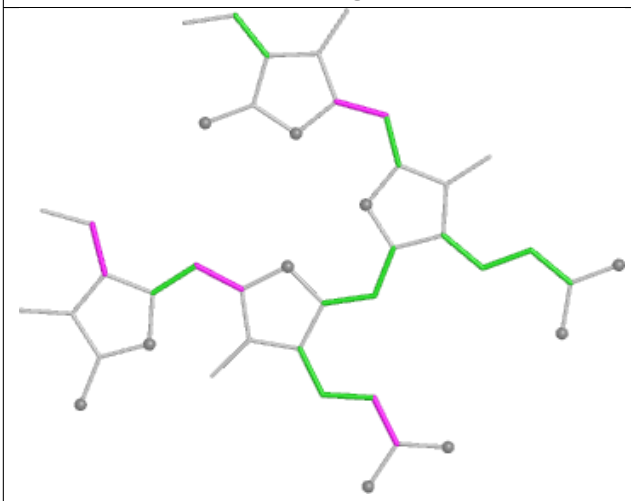


Bond angles



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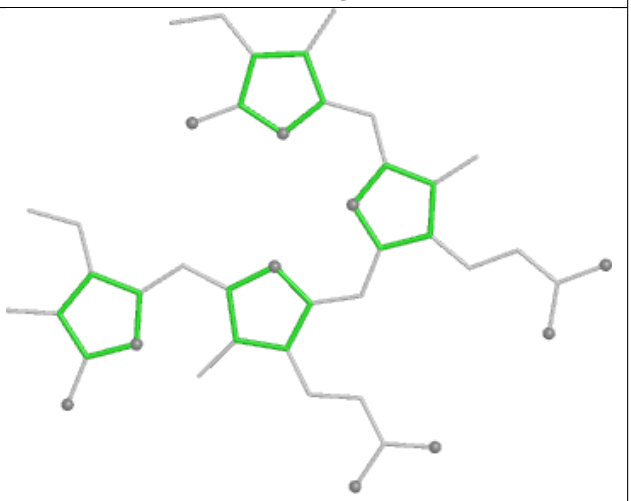
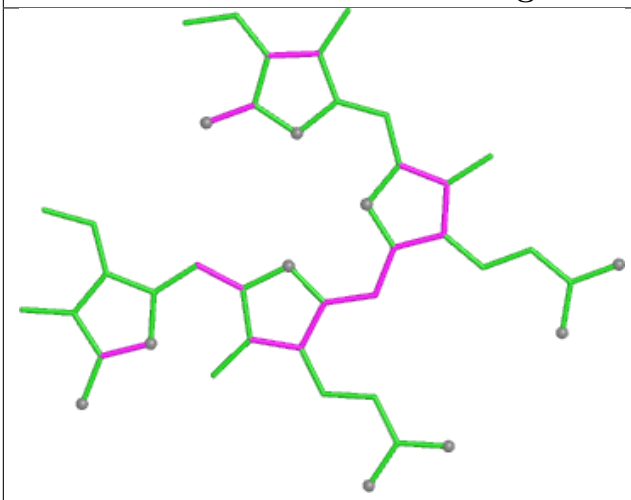


Rings

Ligand PEB xF 303



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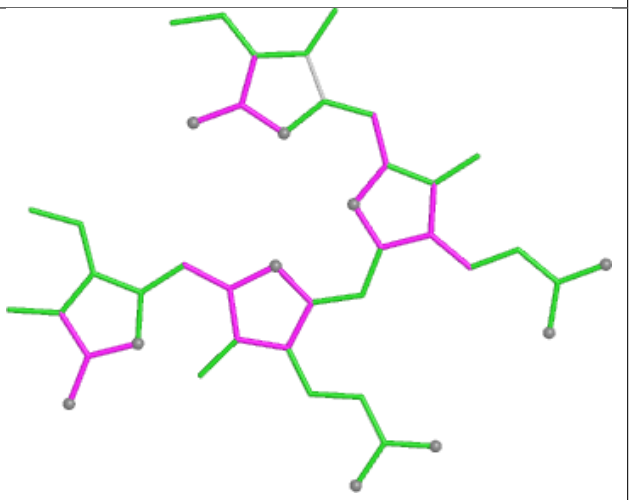
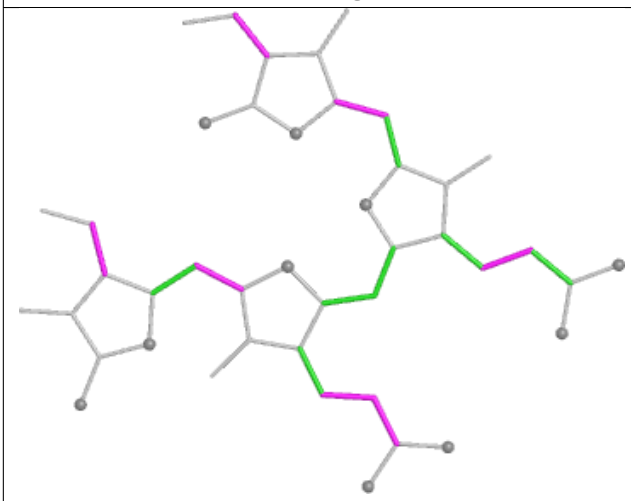


Bond angles



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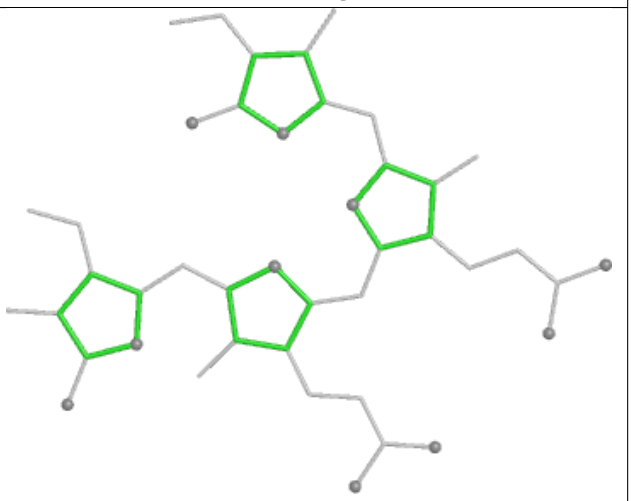
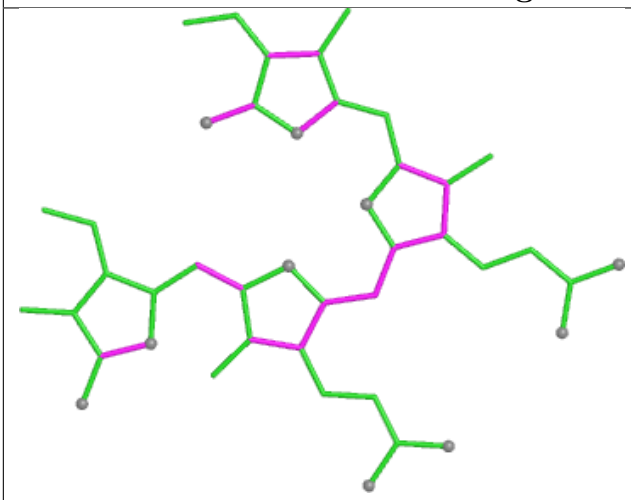


Rings

Ligand PEB w8 201



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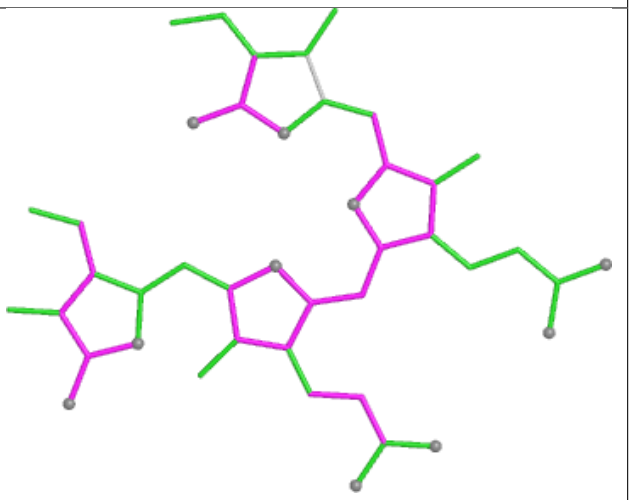
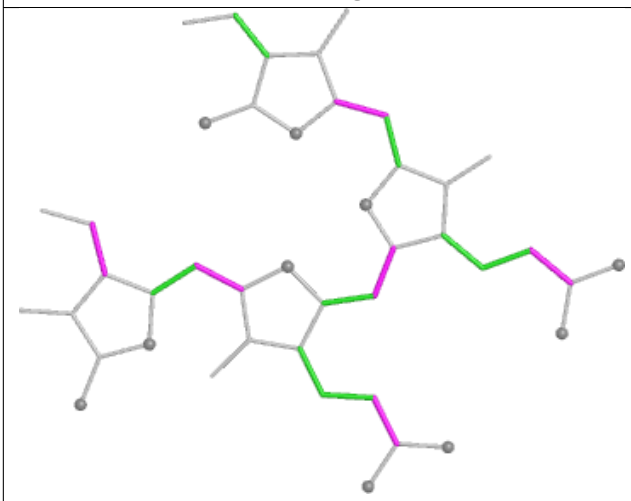


Bond angles



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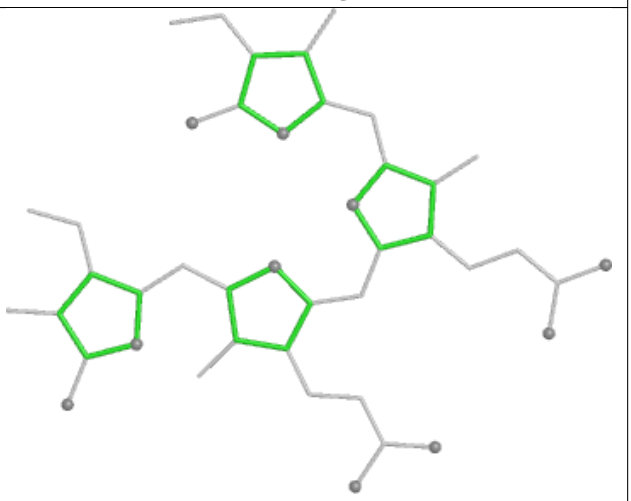
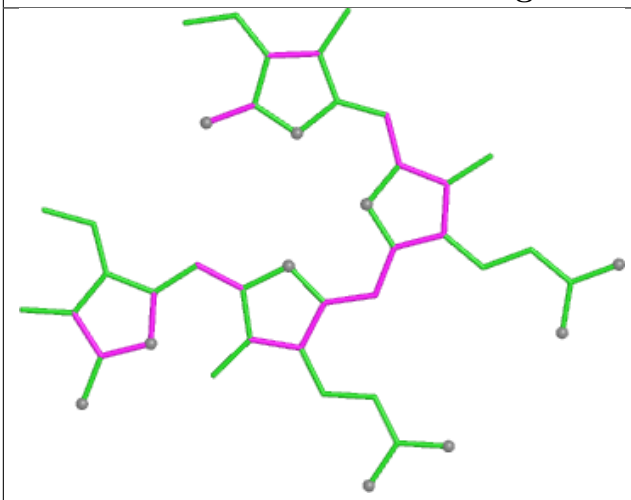


Rings

Ligand PEB 1C 202



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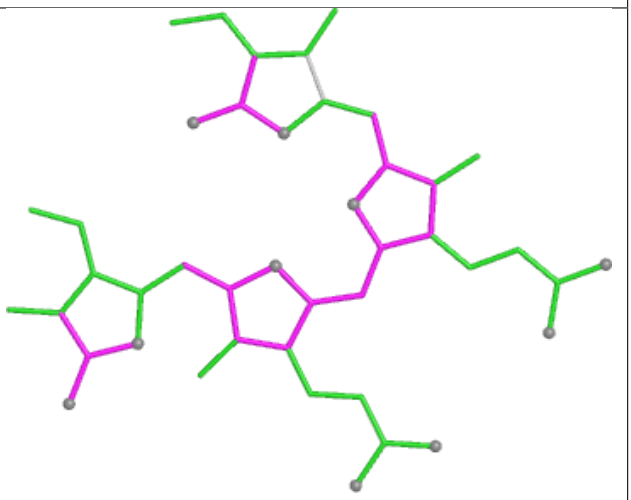

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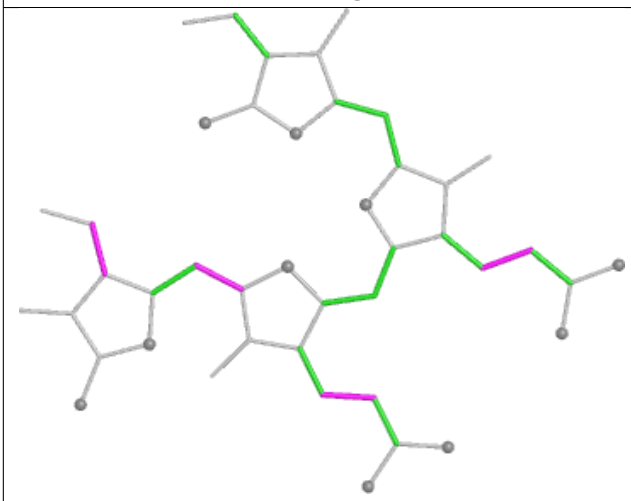

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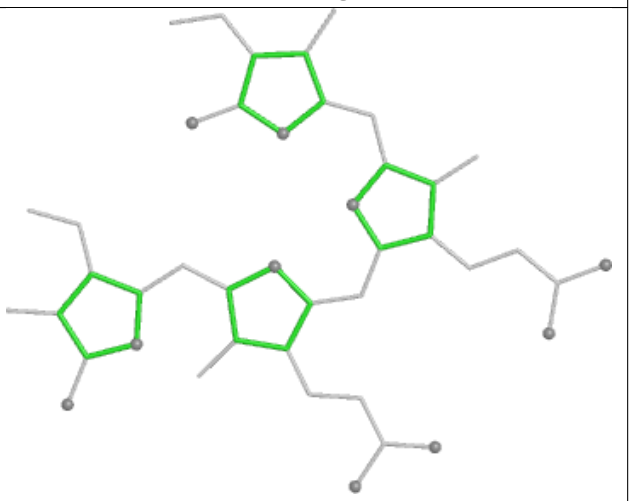
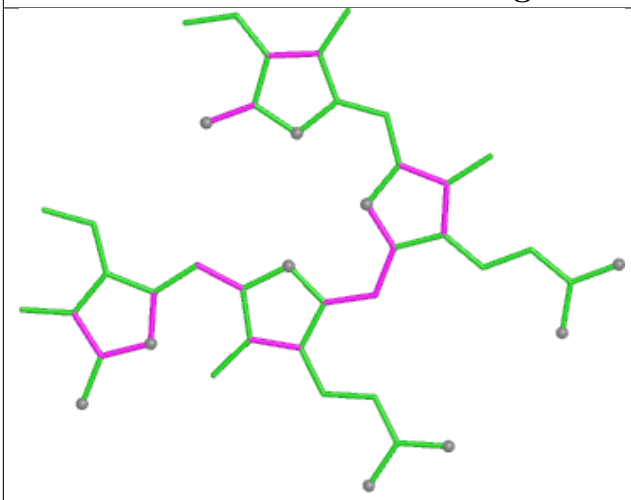


Rings

Ligand PEB PE 202



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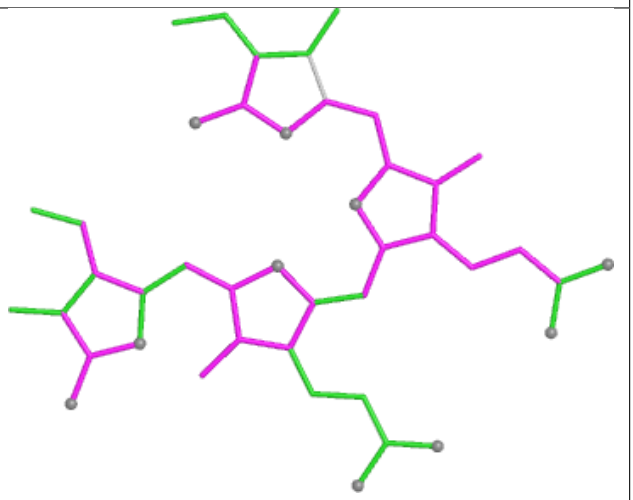

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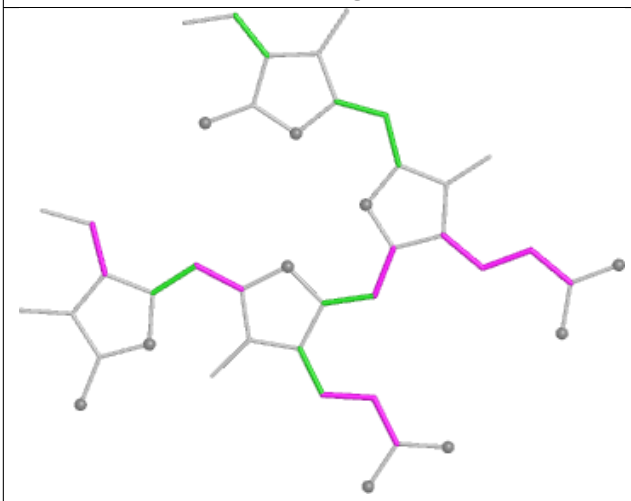

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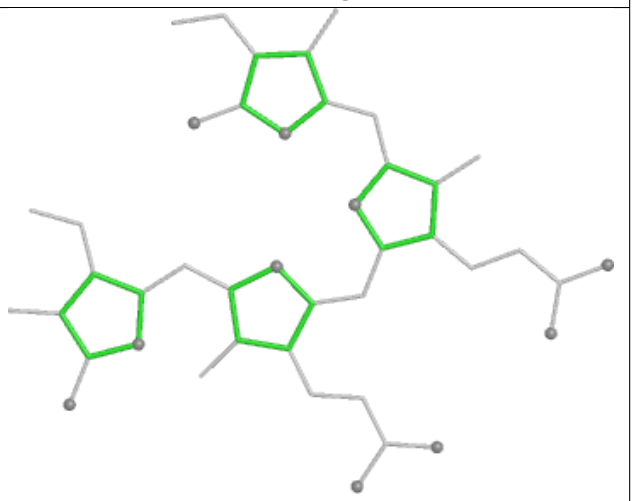
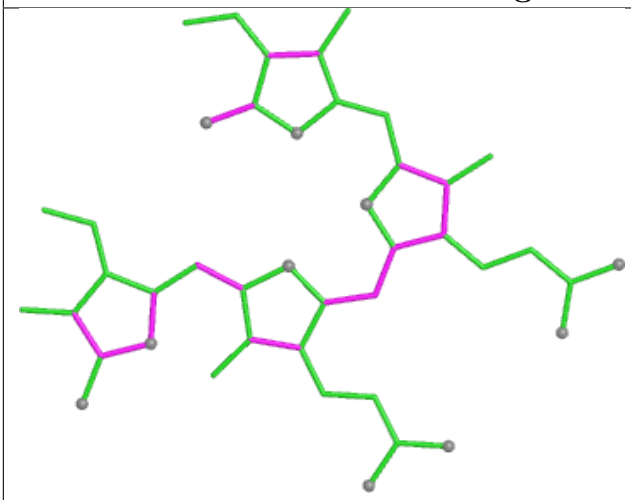


Rings

Ligand PEB hO 202



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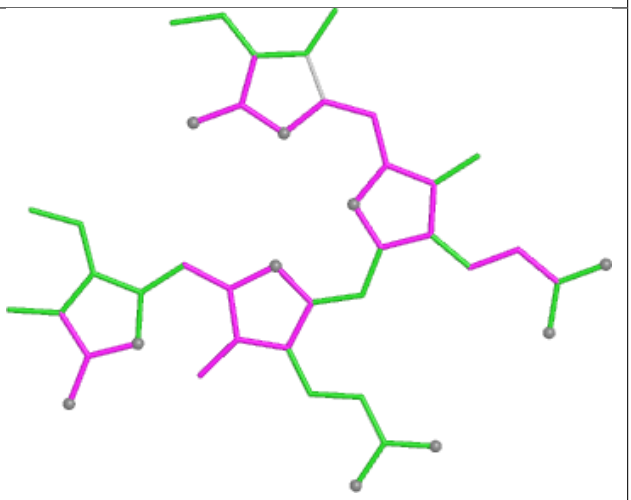

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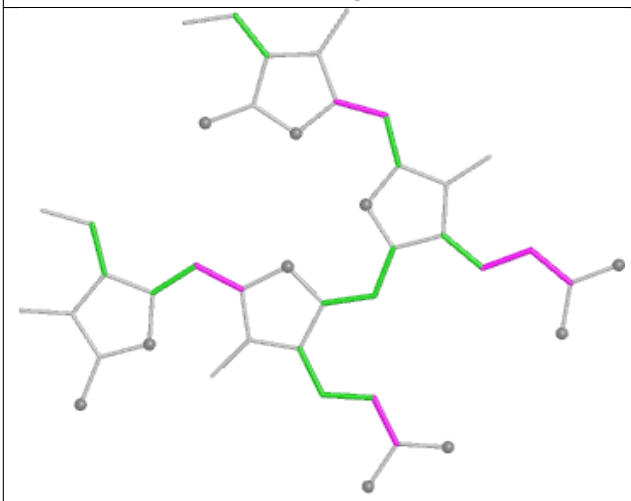

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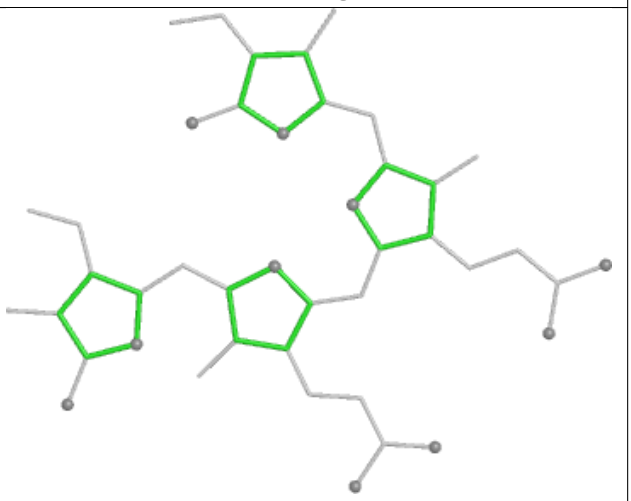

Rings

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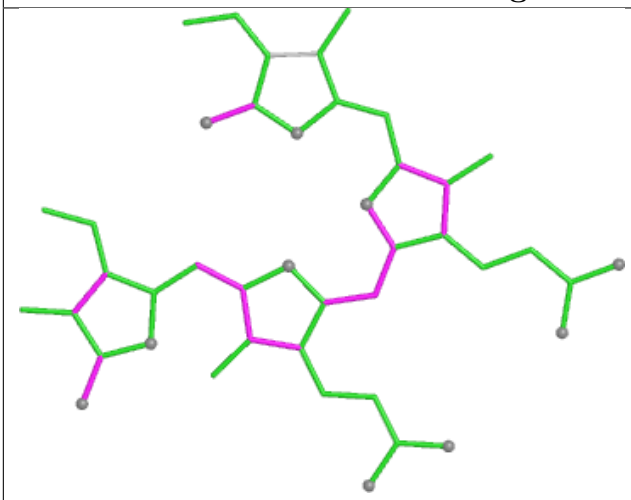

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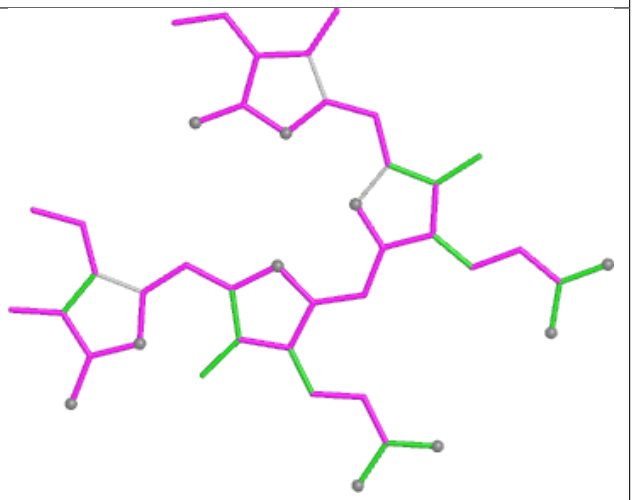

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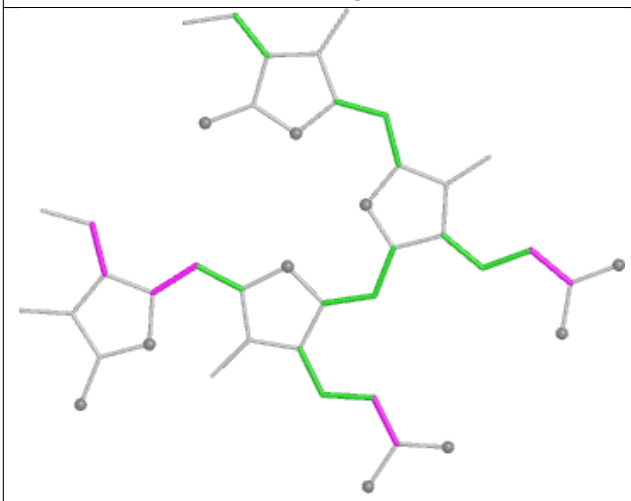

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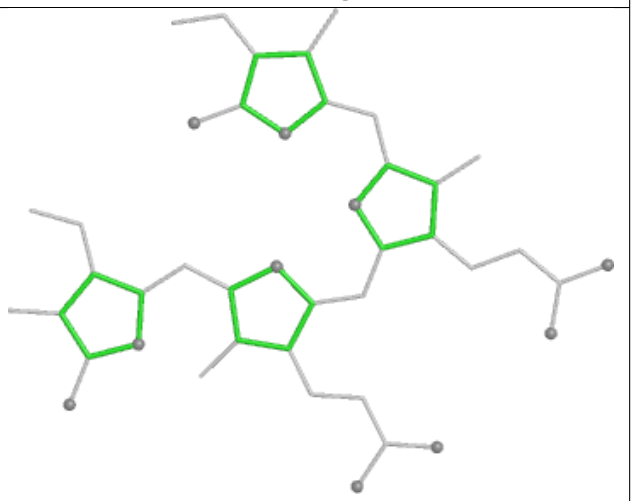
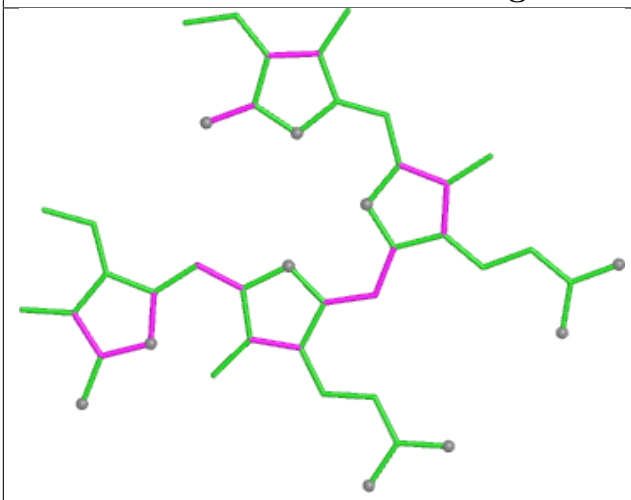


Rings

Ligand PEB mK 201



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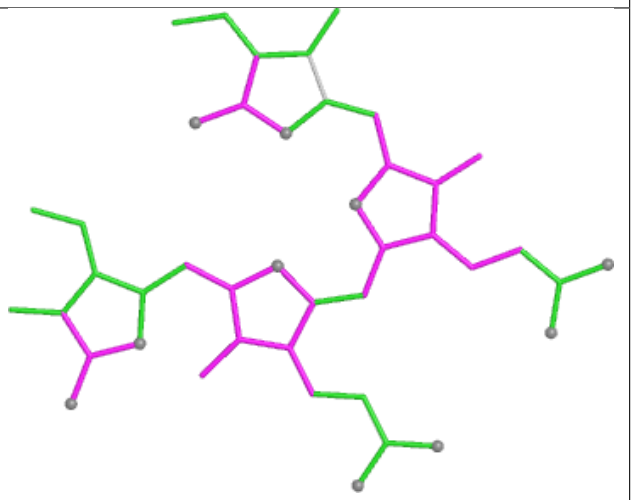

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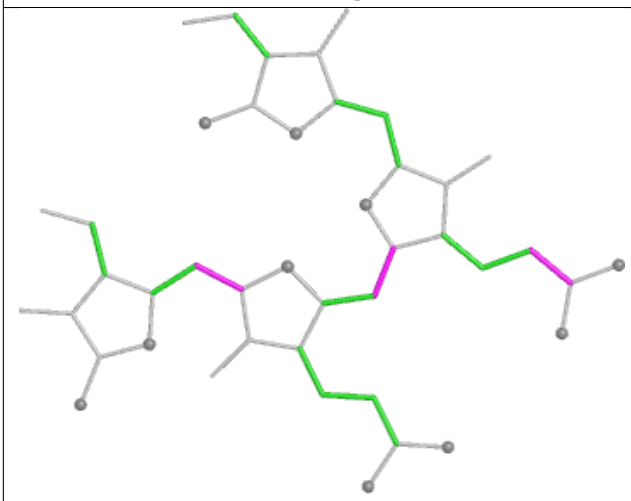

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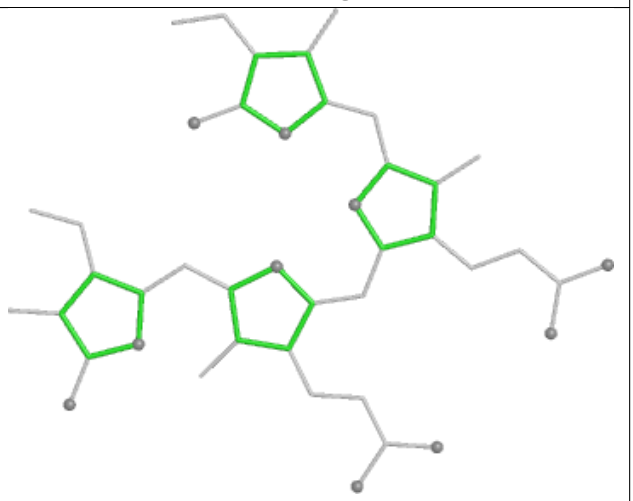

Rings

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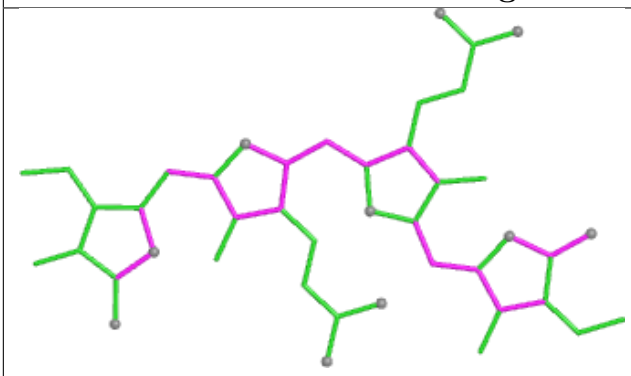

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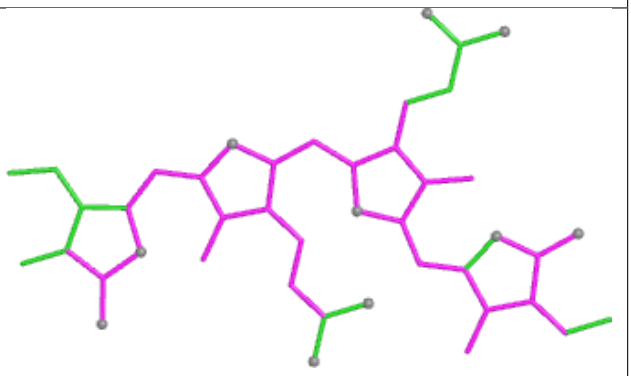

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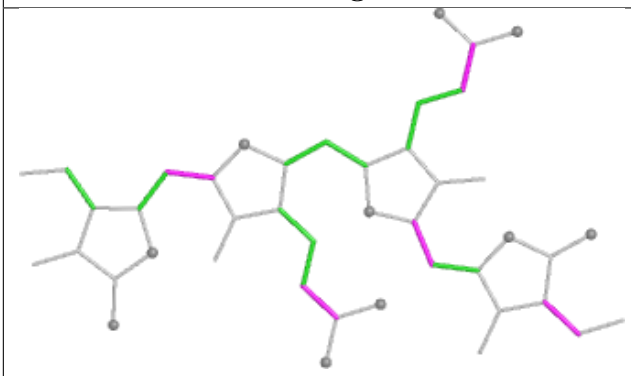

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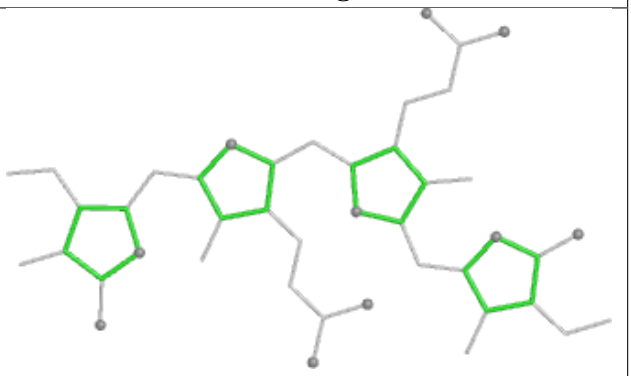
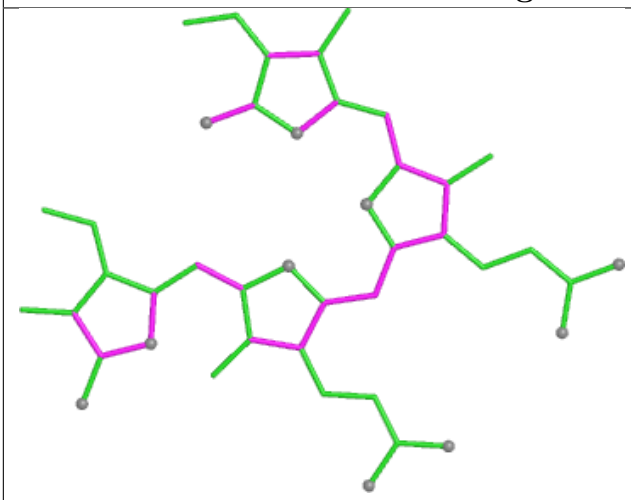


Rings

Ligand PEB hE 201



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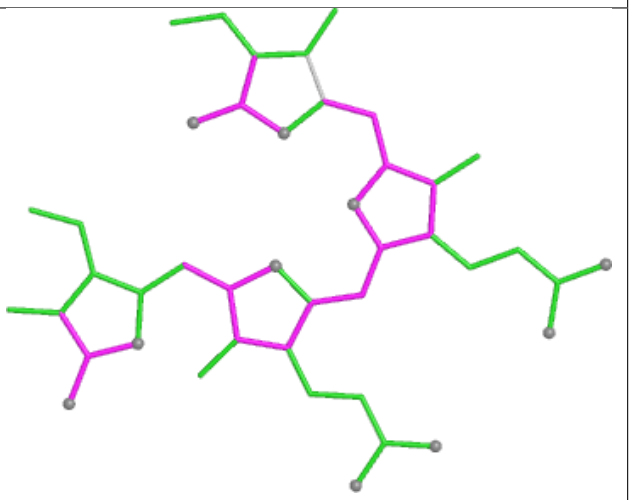

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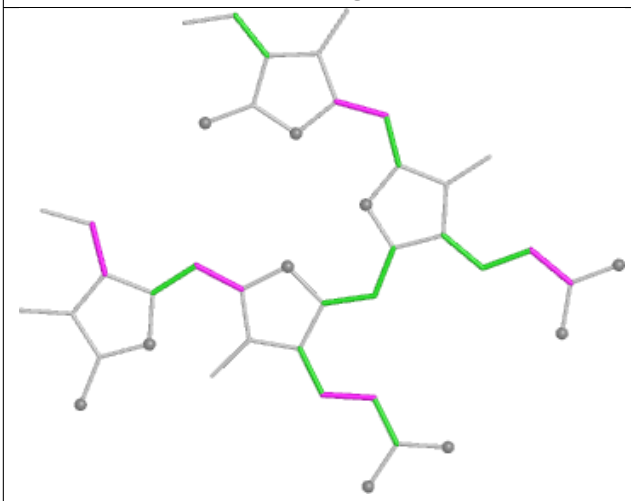

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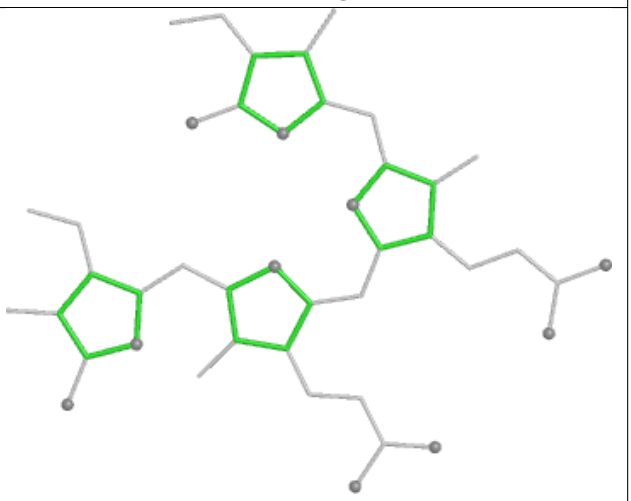

Rings

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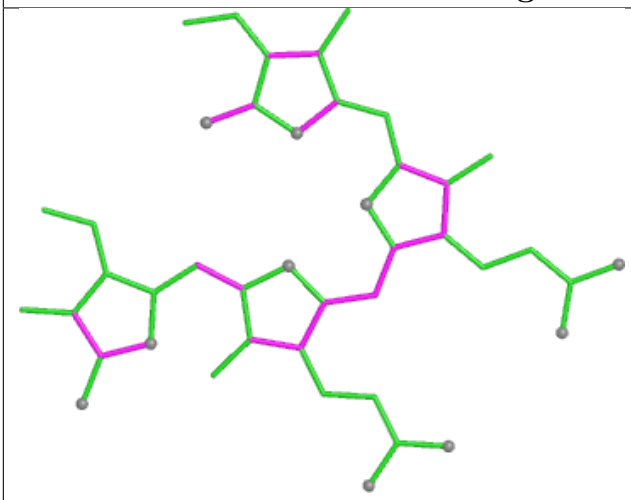

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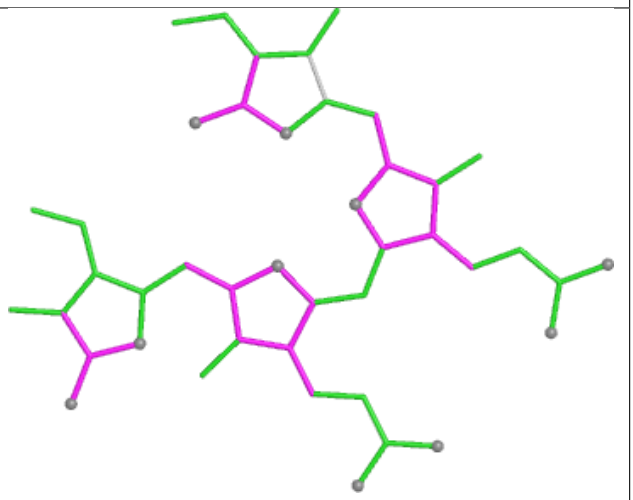

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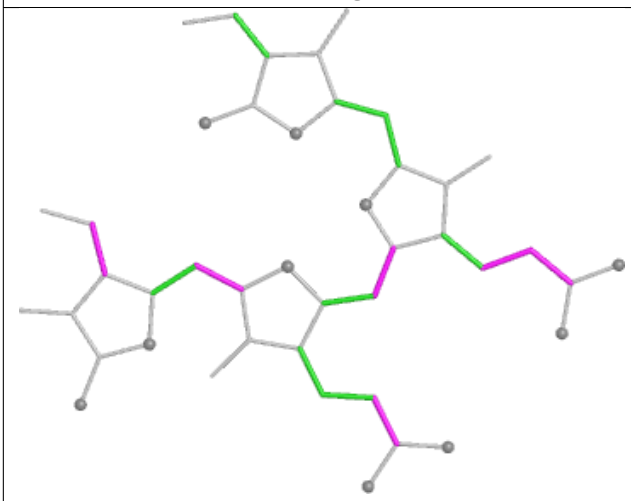

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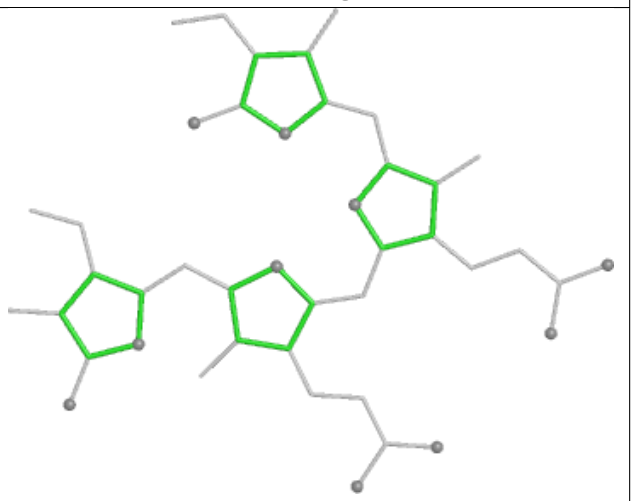

Rings

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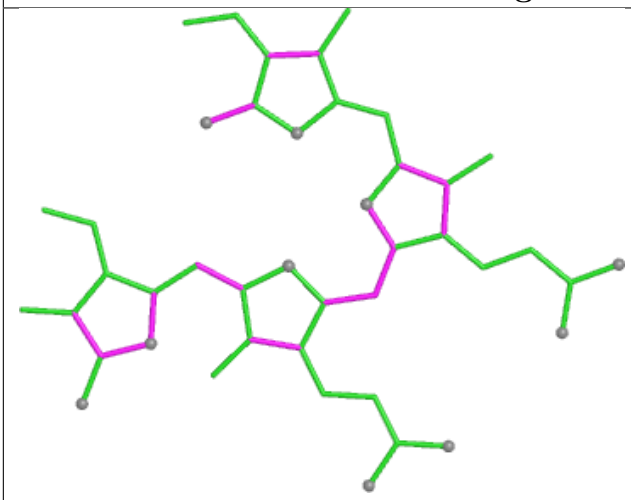

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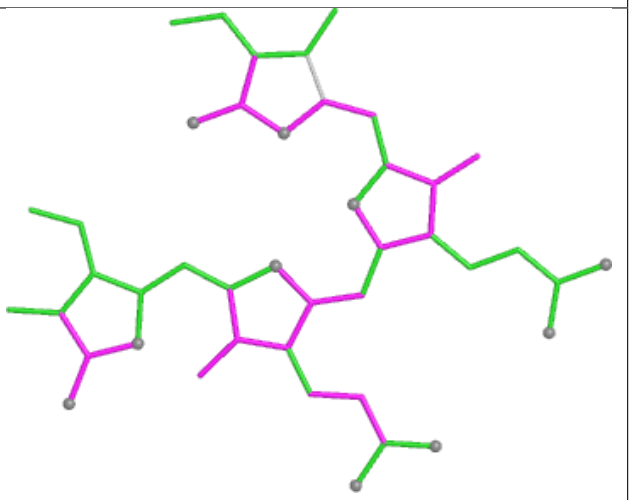

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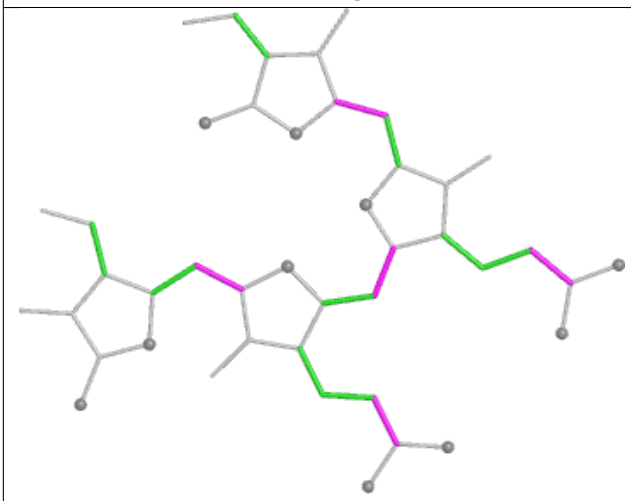

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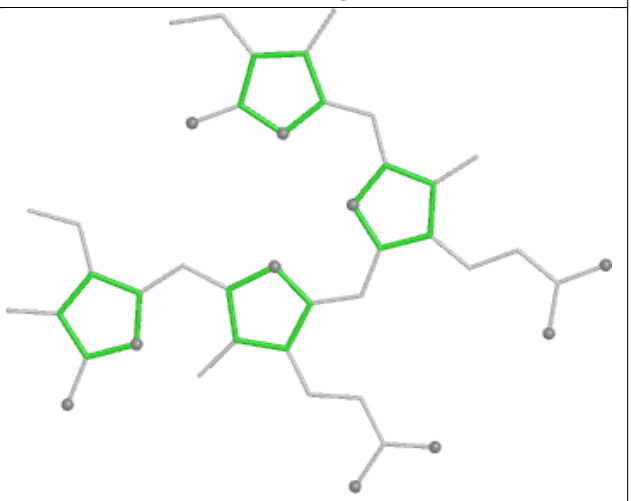

Rings

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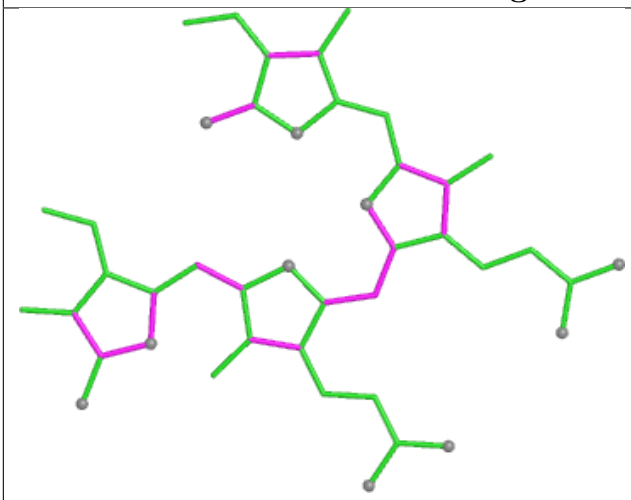

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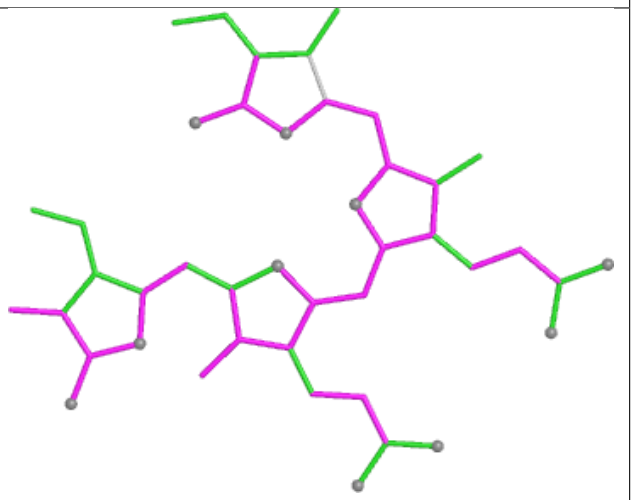

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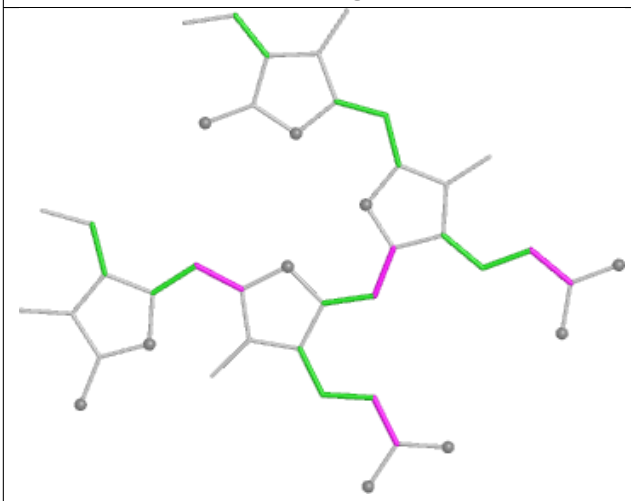

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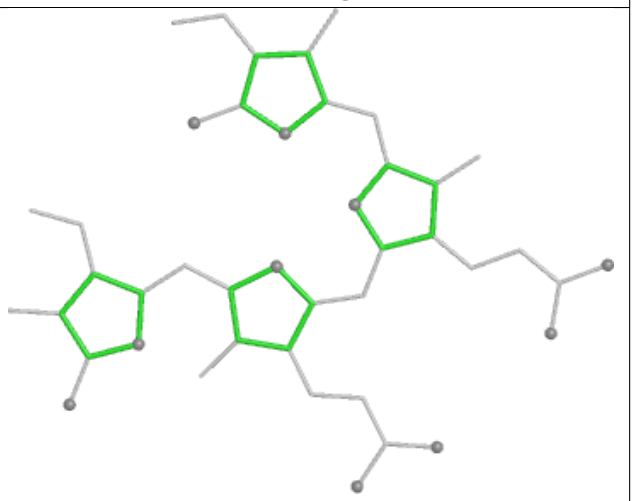

Rings

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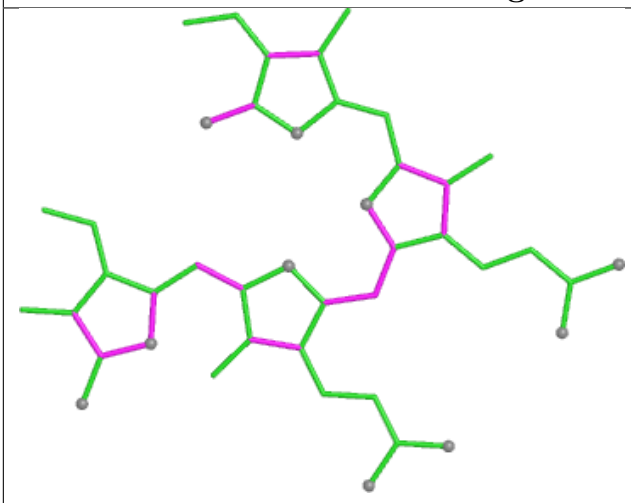

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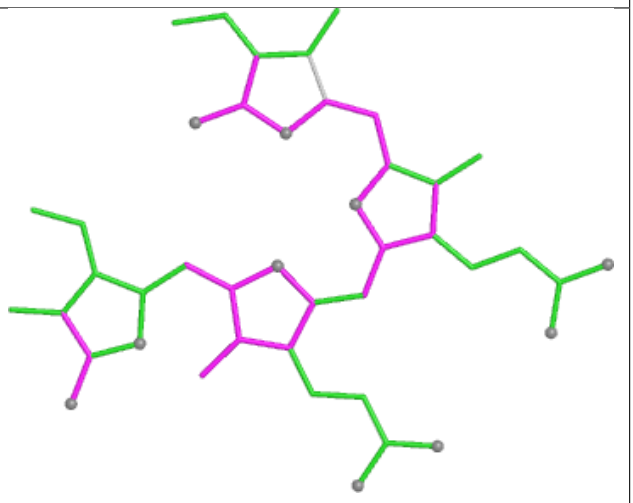

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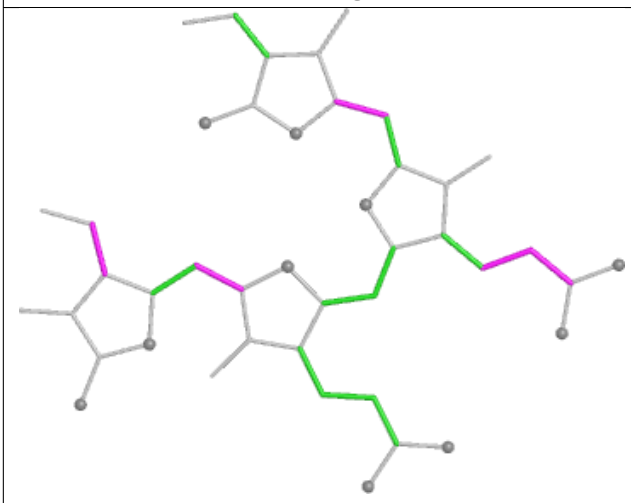

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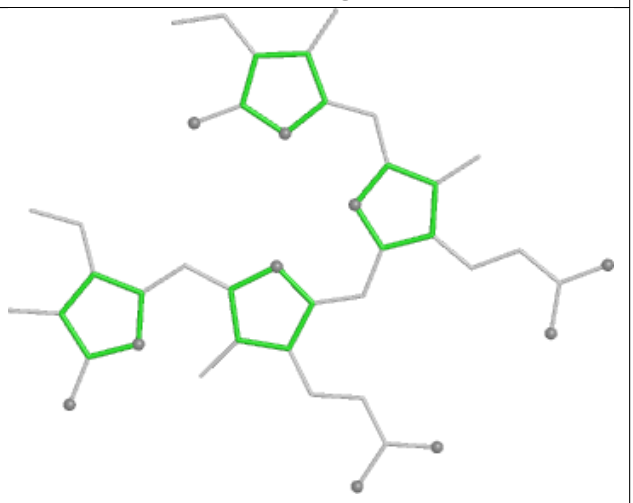
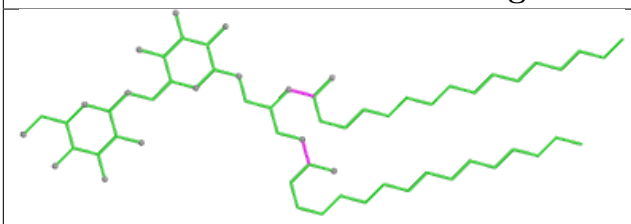


Rings

Ligand DGD DL 408



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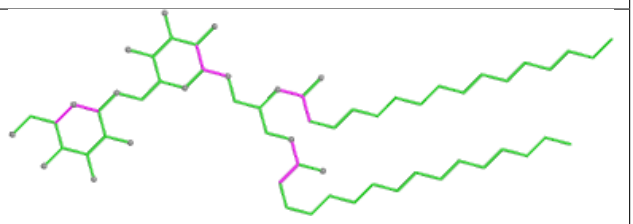
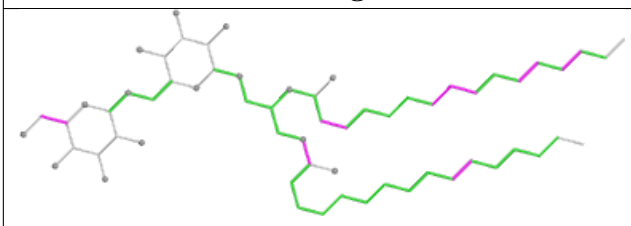


Bond angles



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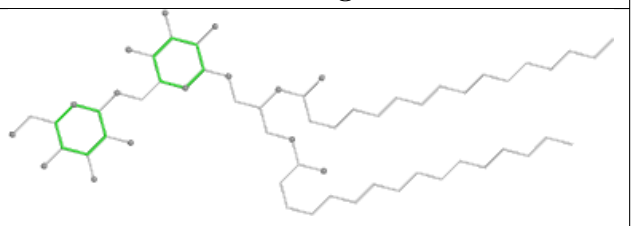
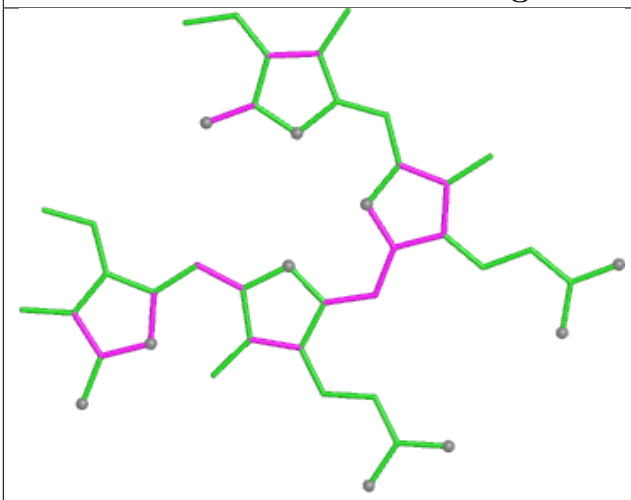


Rings

Ligand PEB DB 202



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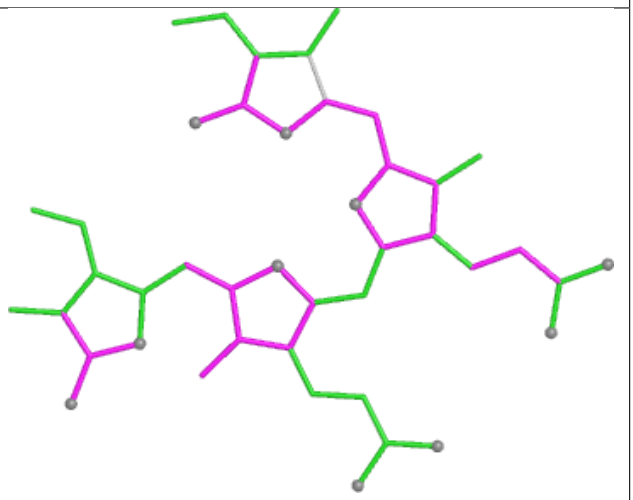

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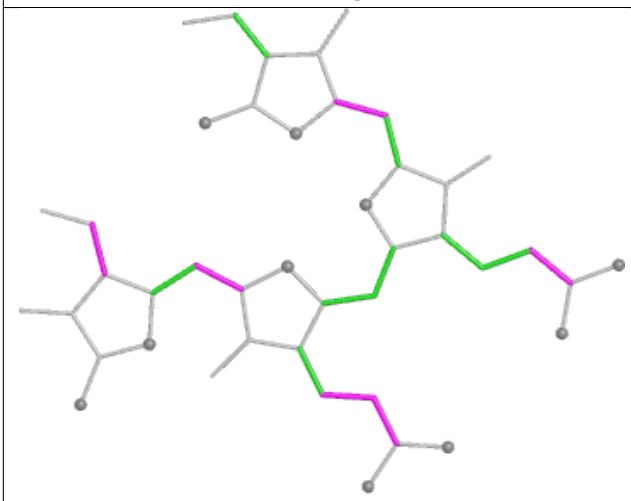

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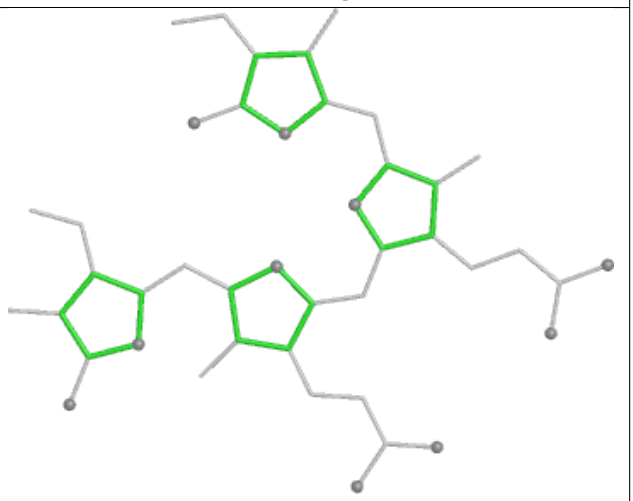
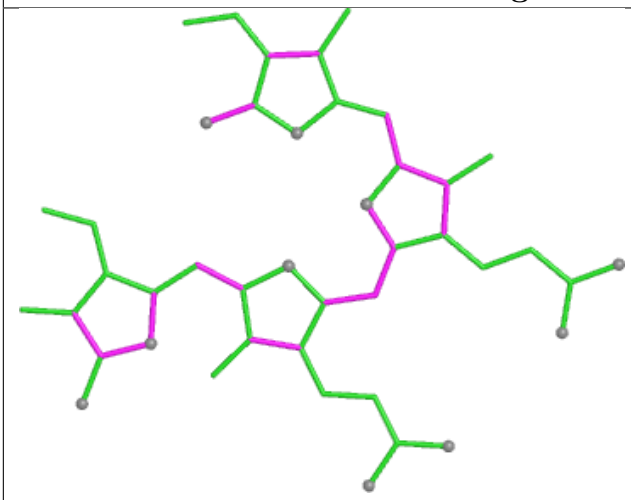


Rings

Ligand PEB HB 201



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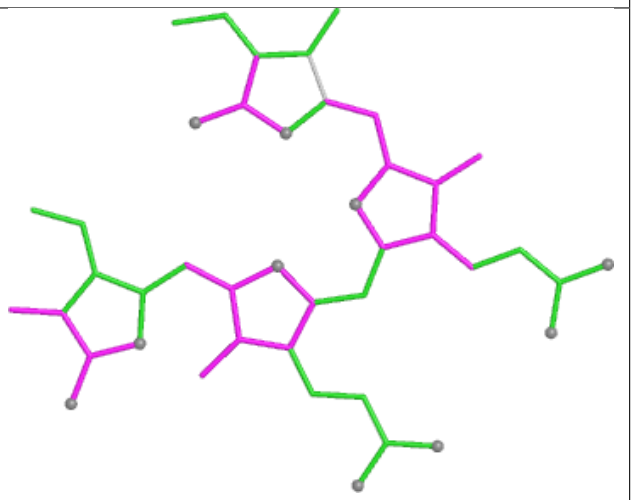
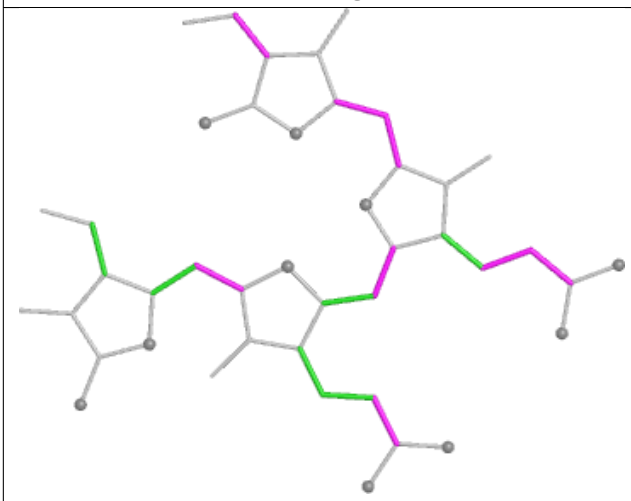


Bond angles



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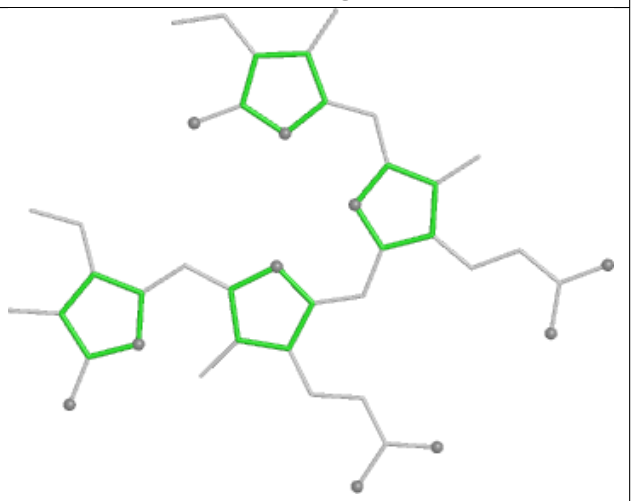

Rings

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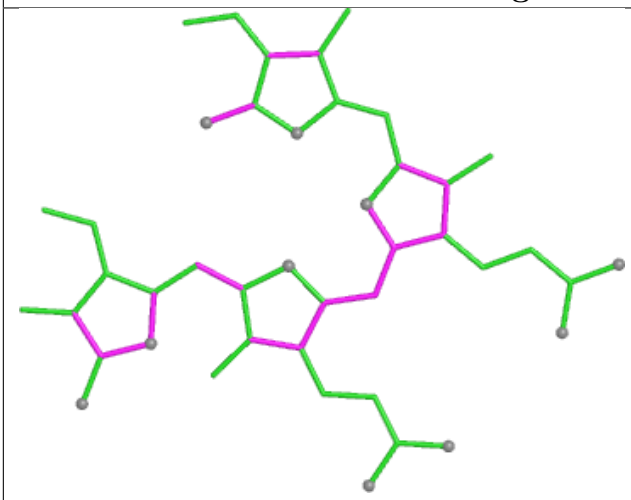

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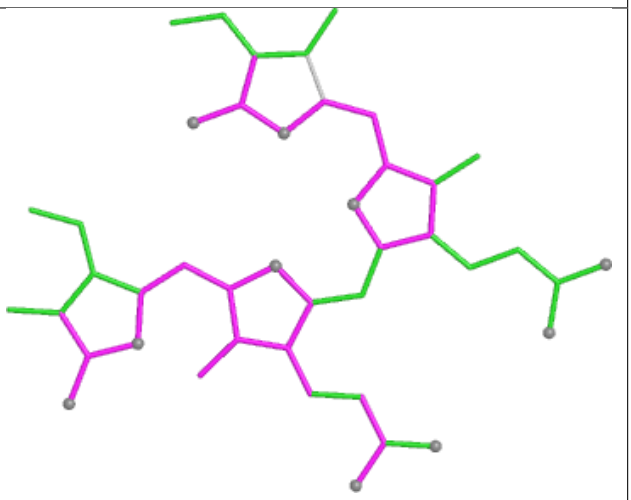
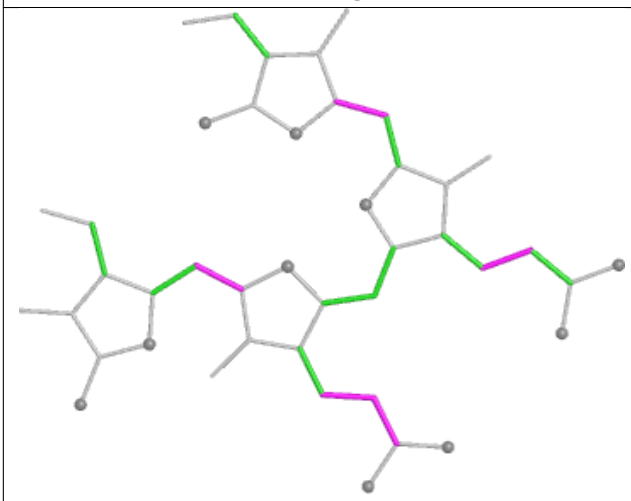


Bond angles



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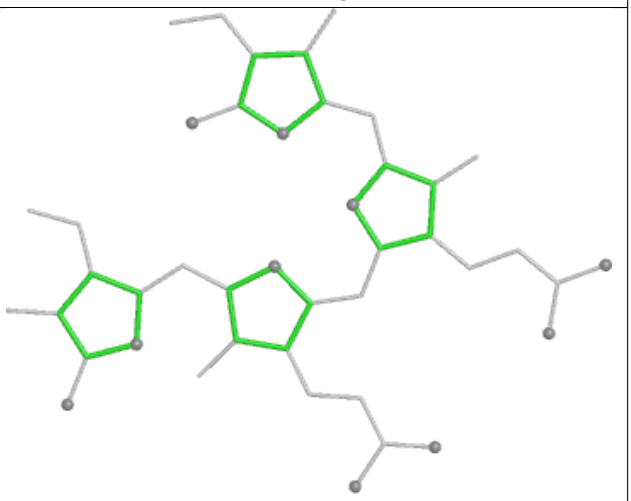
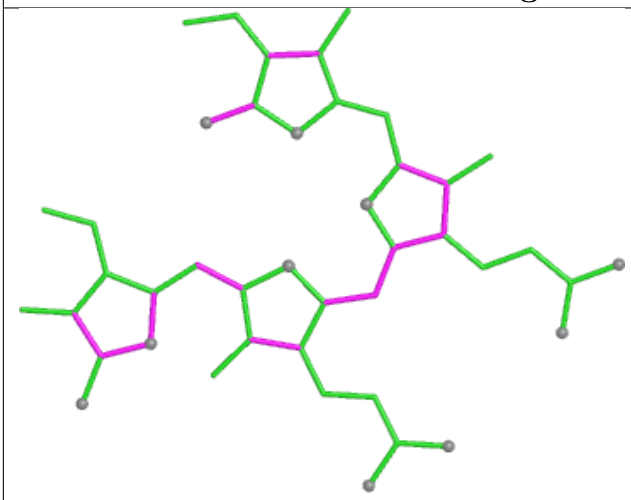


Rings

Ligand PEB eJ 202



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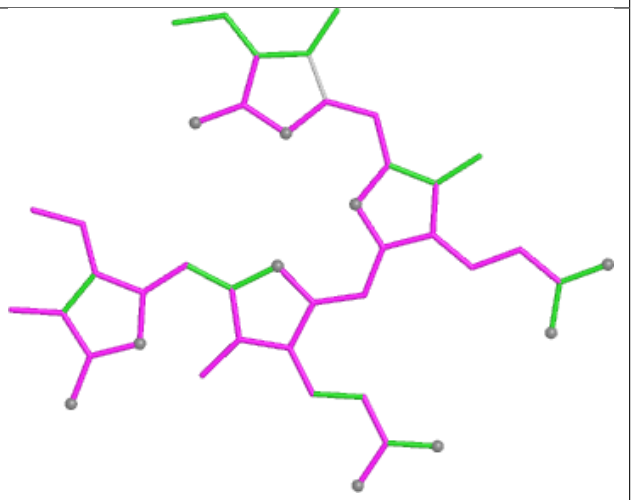

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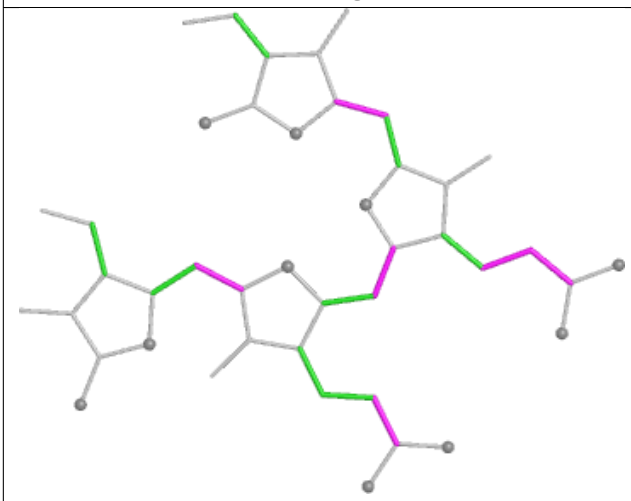

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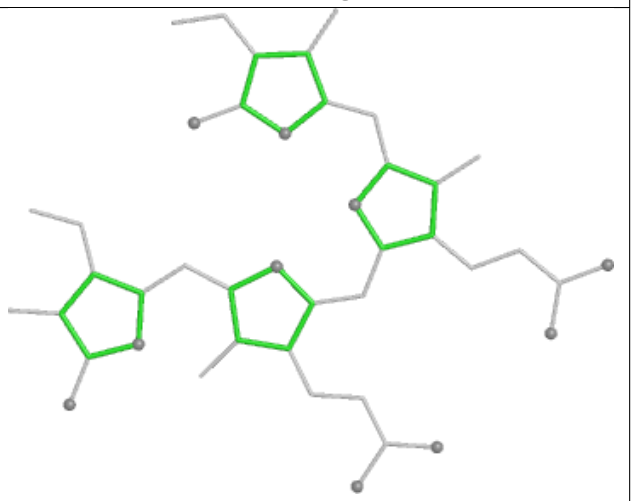
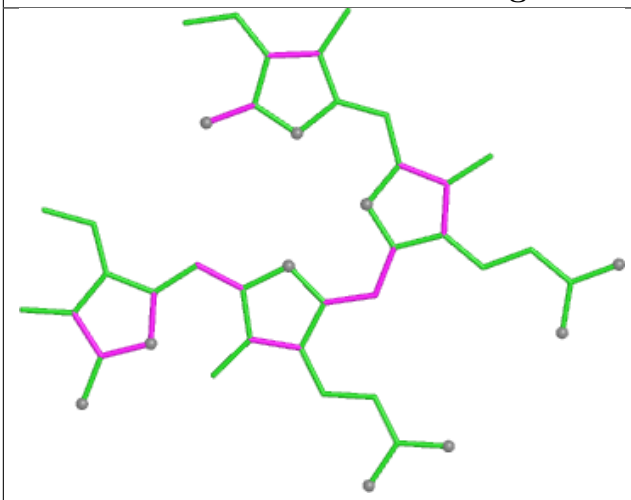


Rings

Ligand PEB MF 201



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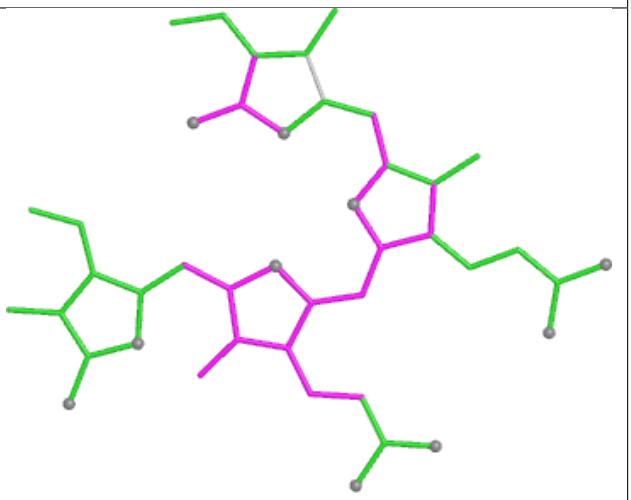

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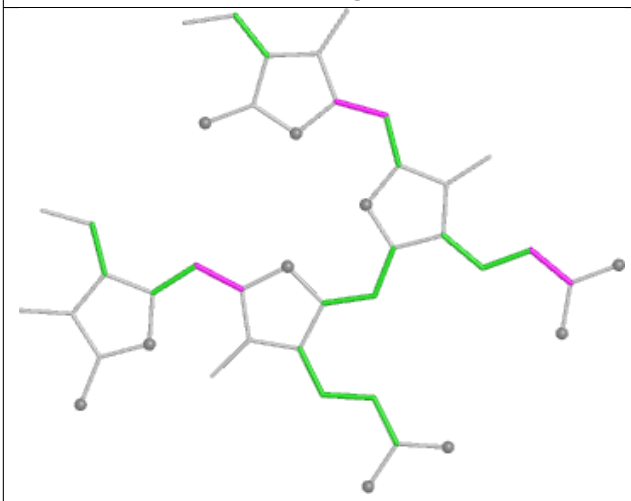

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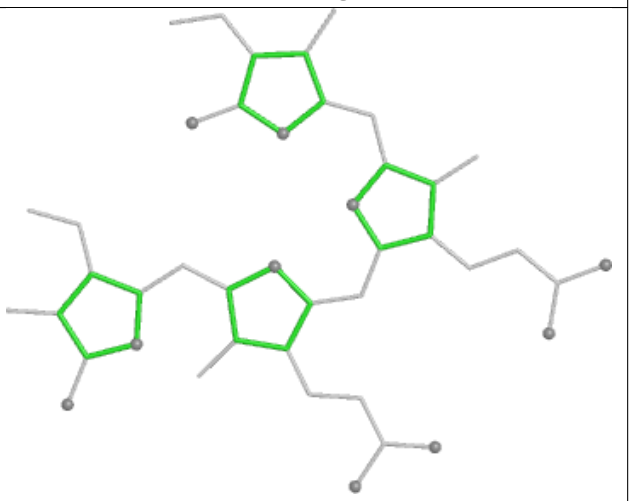
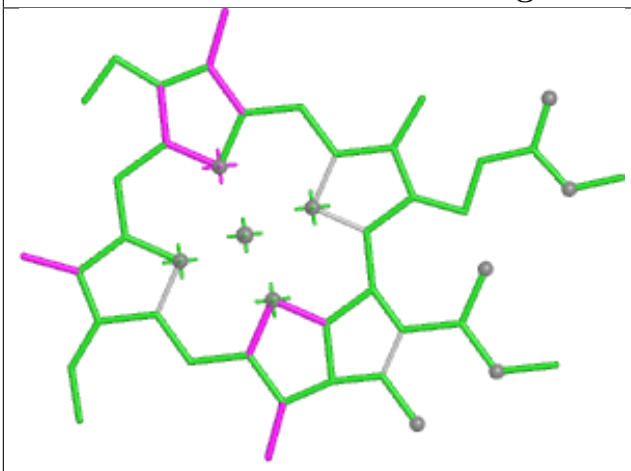
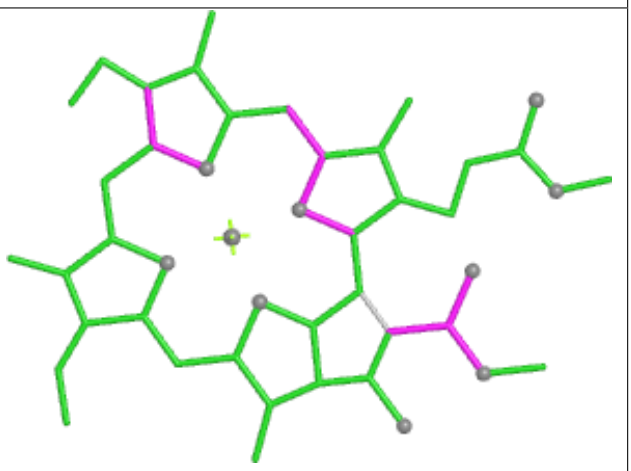
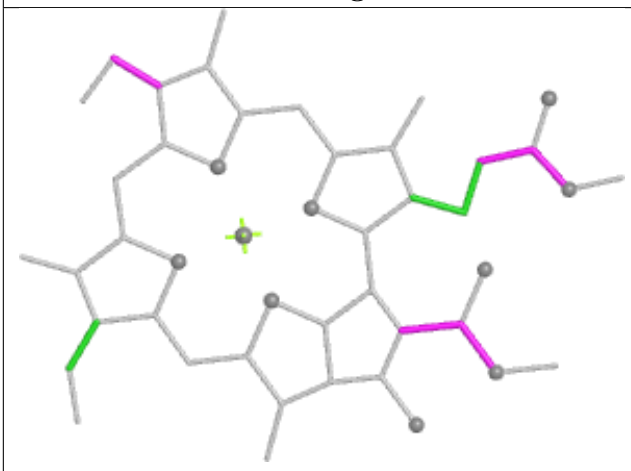
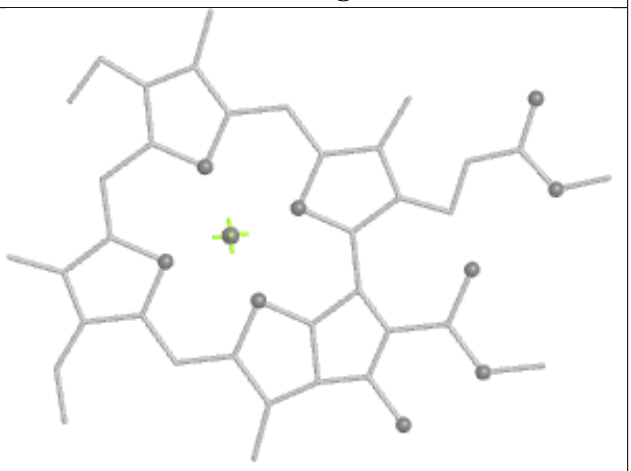
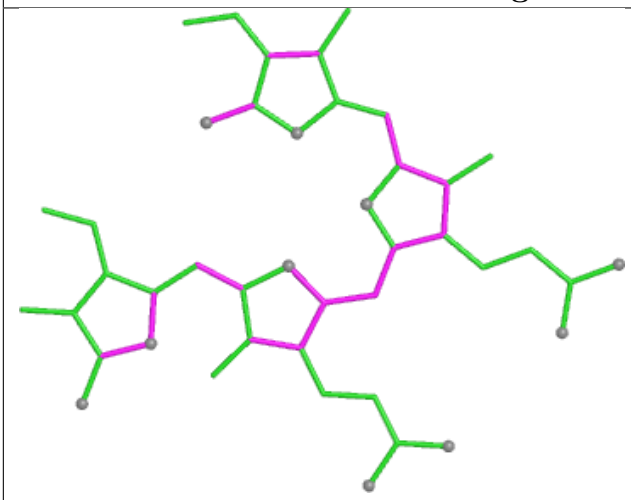


Rings

Ligand CLA bL 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEB RQ 203



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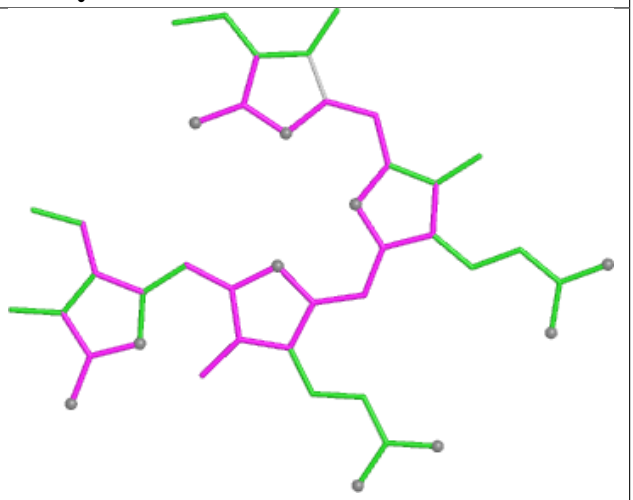

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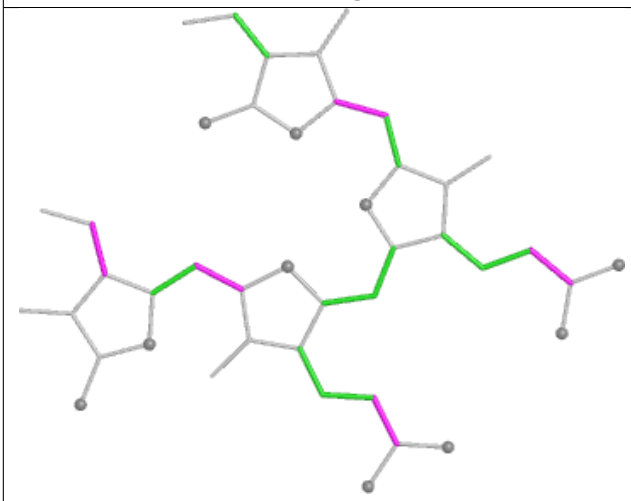

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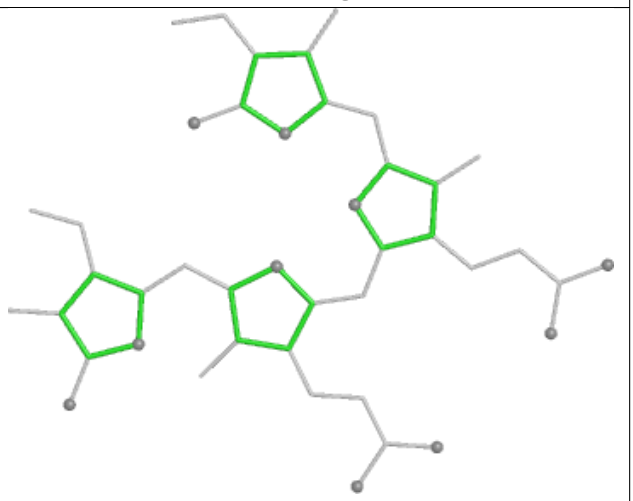

Rings

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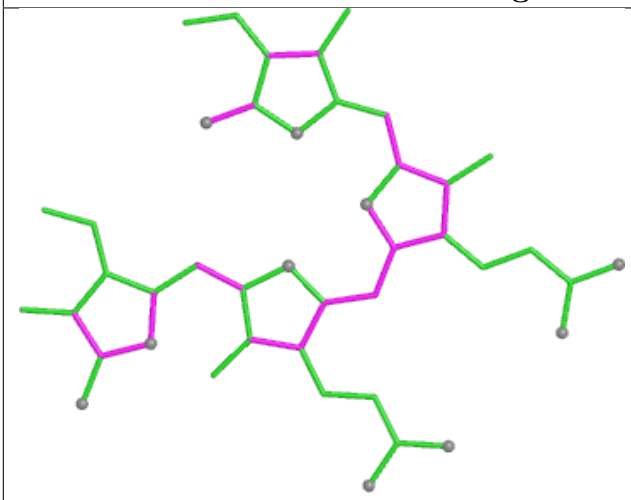

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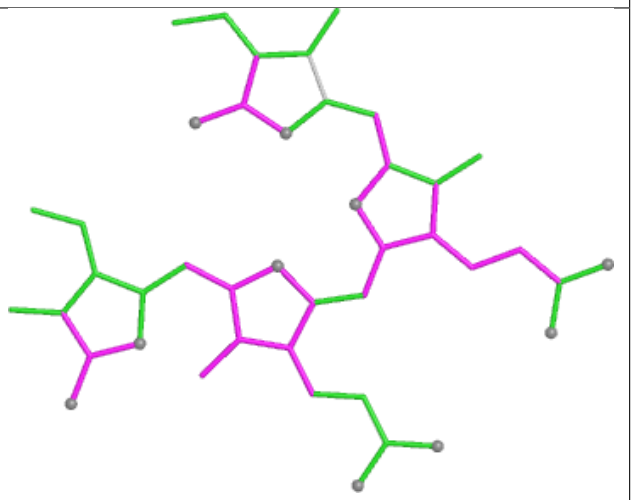

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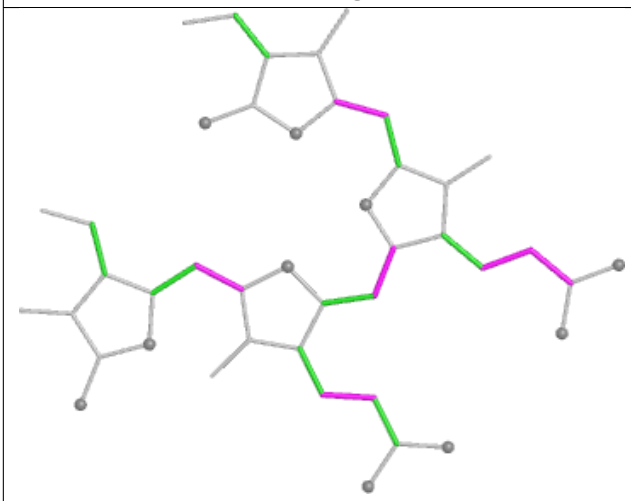

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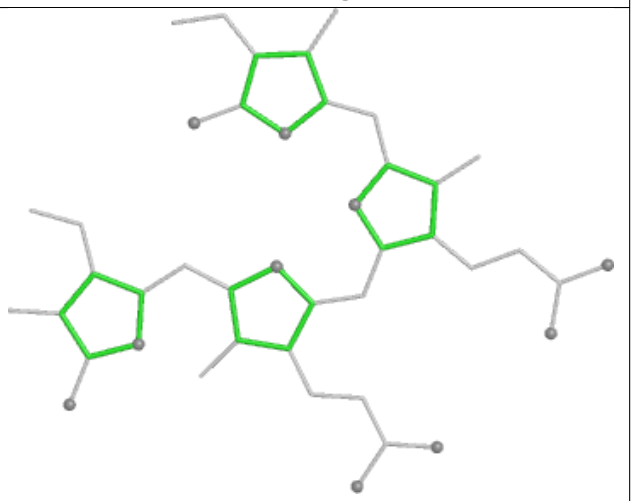

Rings

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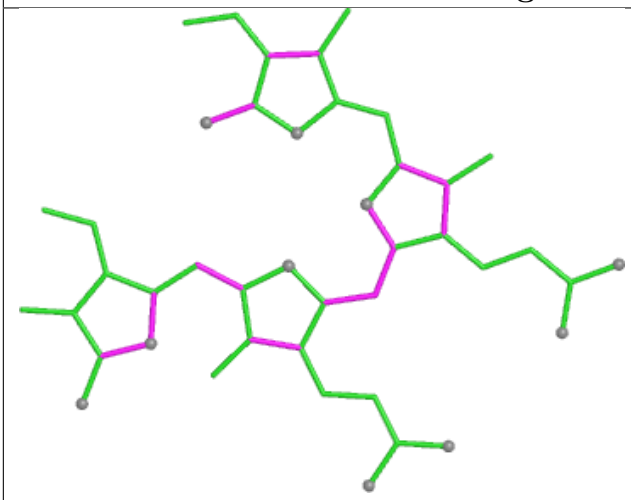

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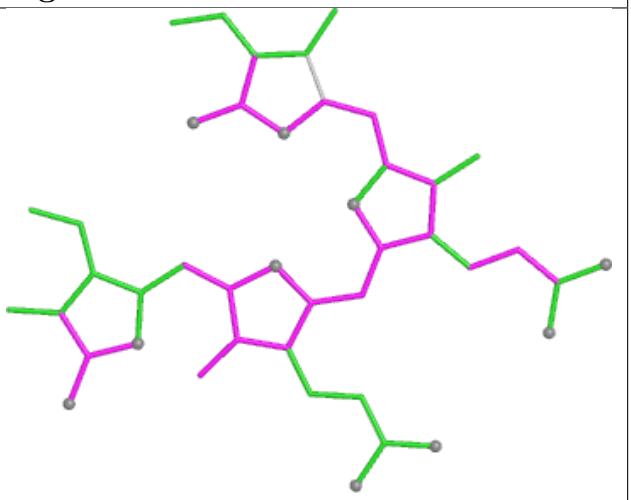

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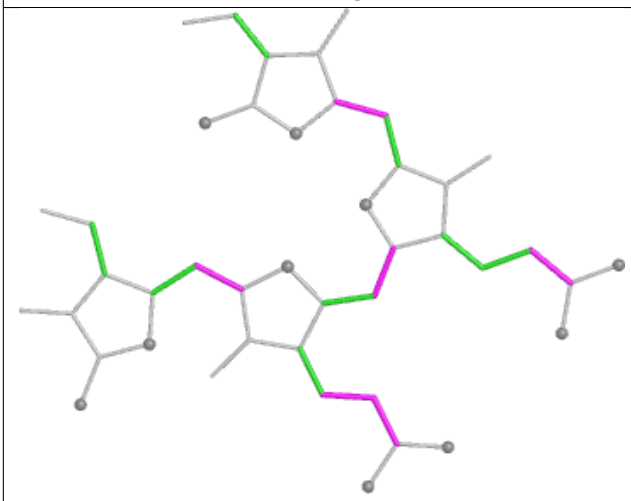

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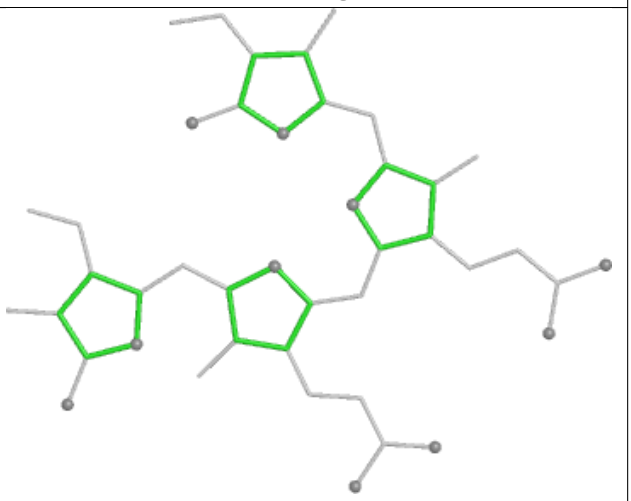
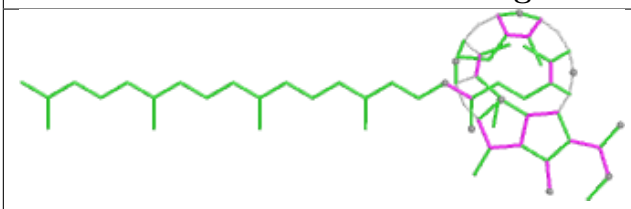


Rings

Ligand PHO dL 403



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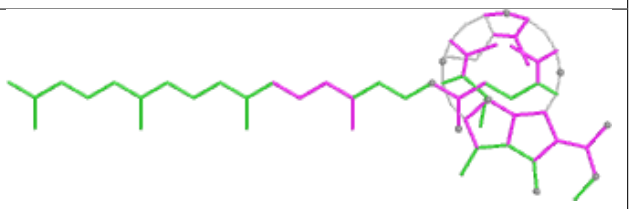

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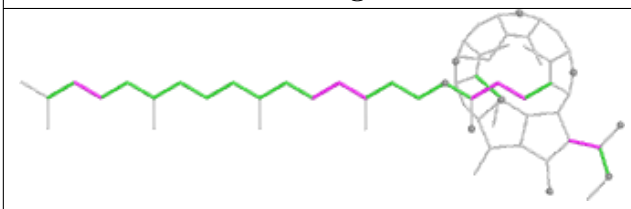

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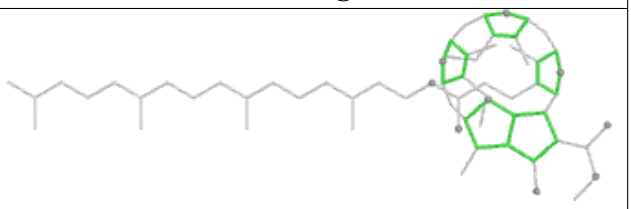
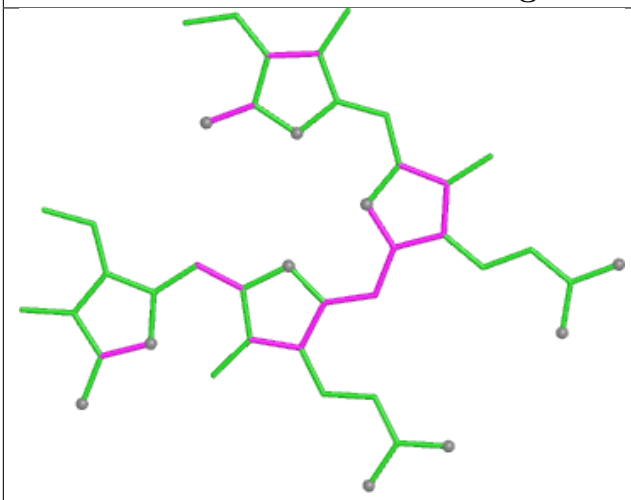


Rings

Ligand PEB q8 203



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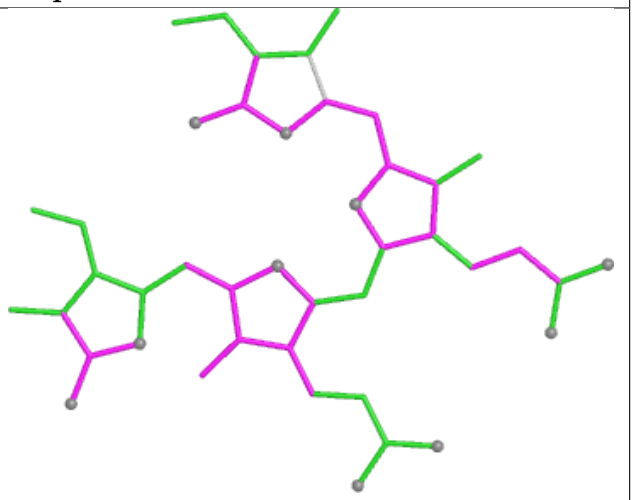

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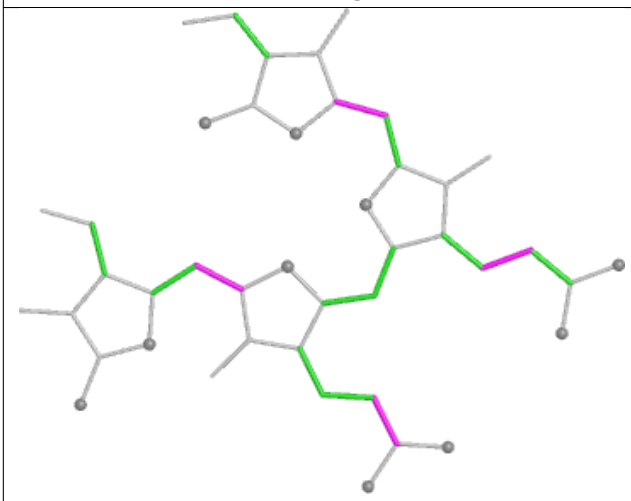

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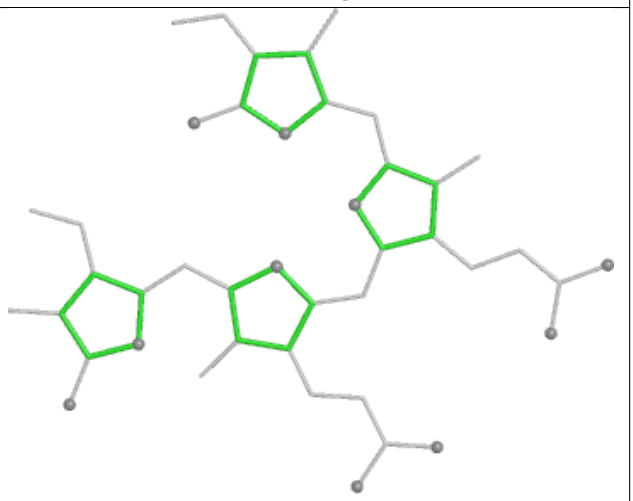
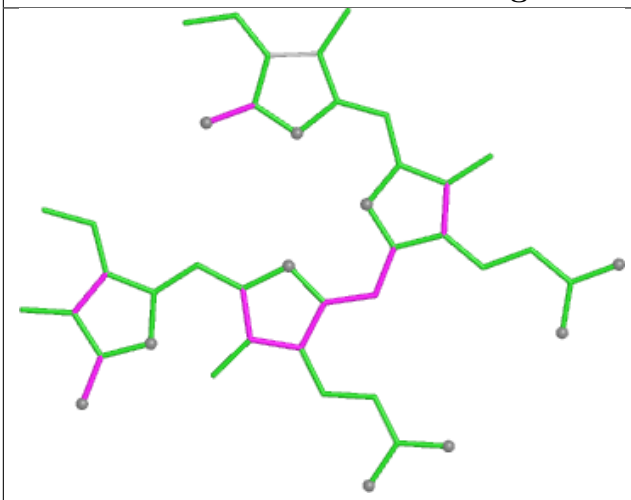


Rings

Ligand PUB AE 303



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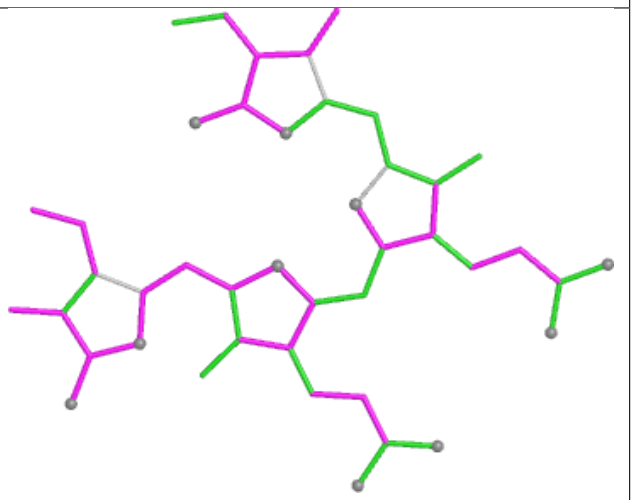

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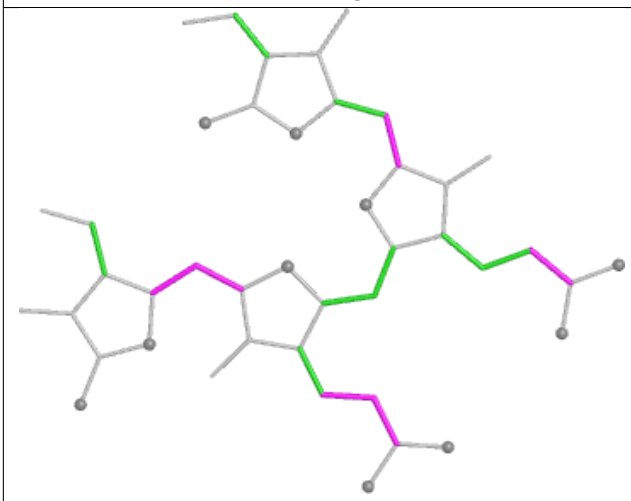

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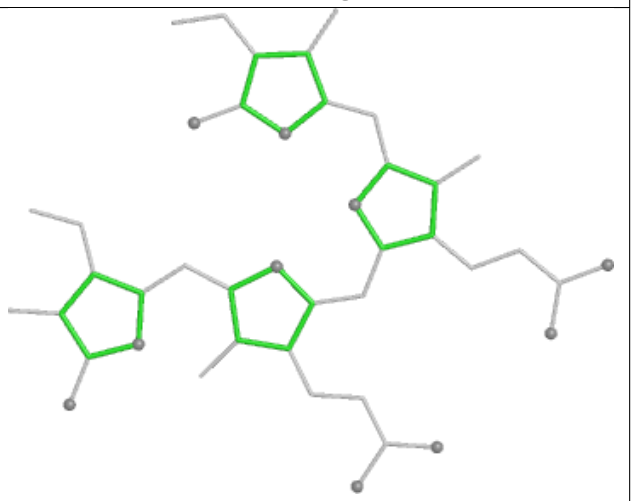
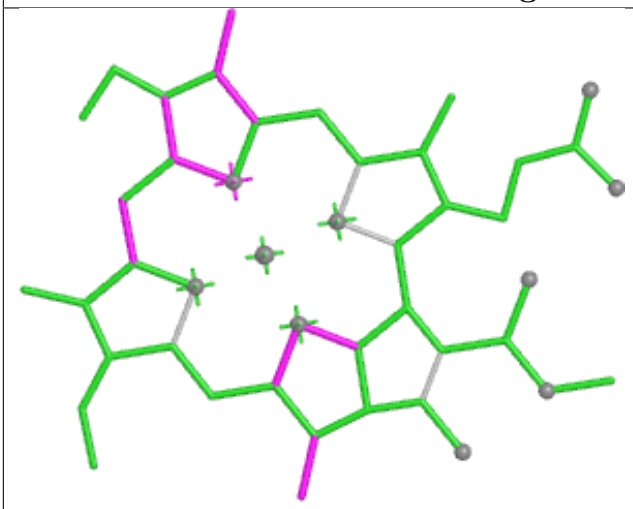


Rings

Ligand CLA 62 304



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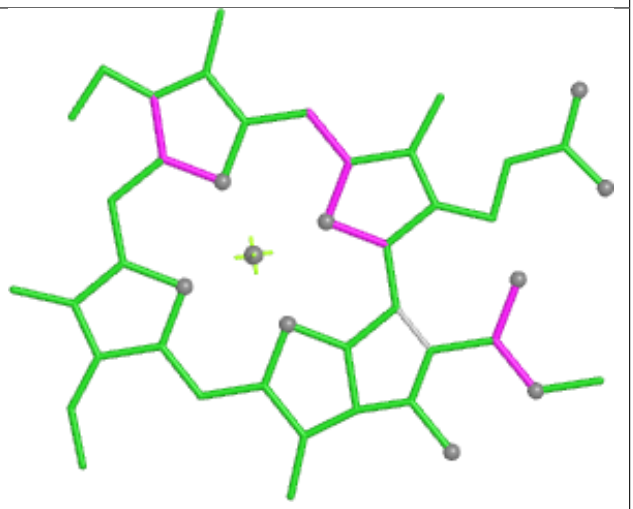

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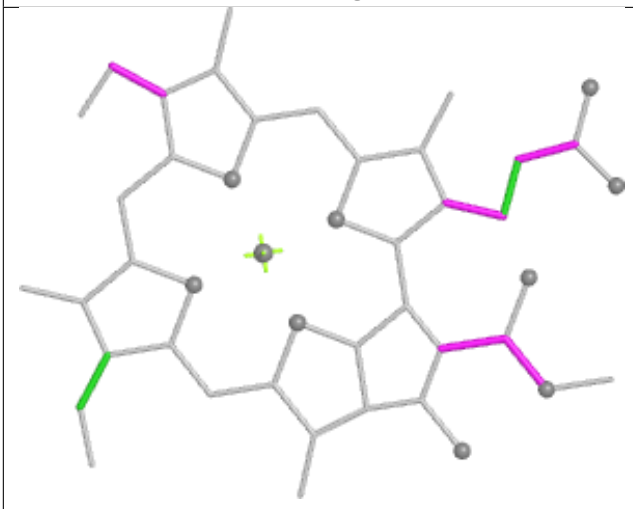
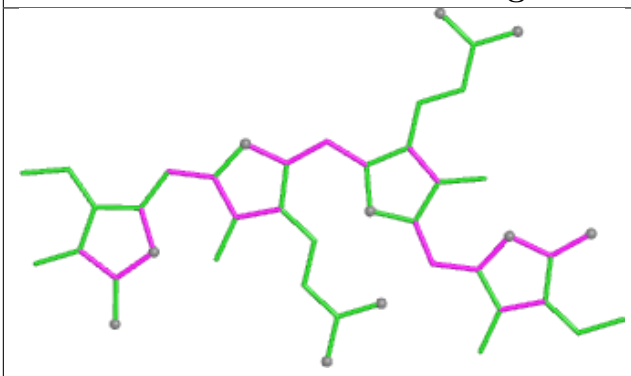


Torsions



Rings

Ligand CYC IE 1001



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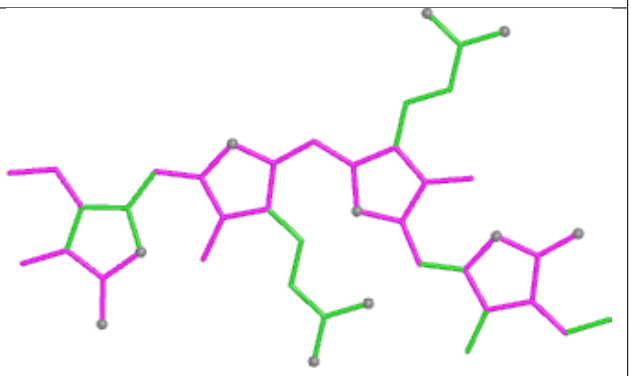

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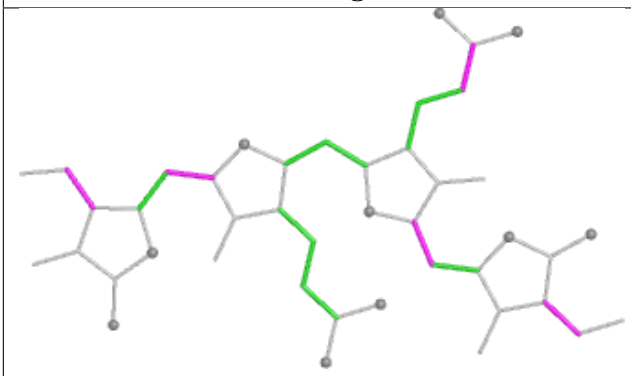

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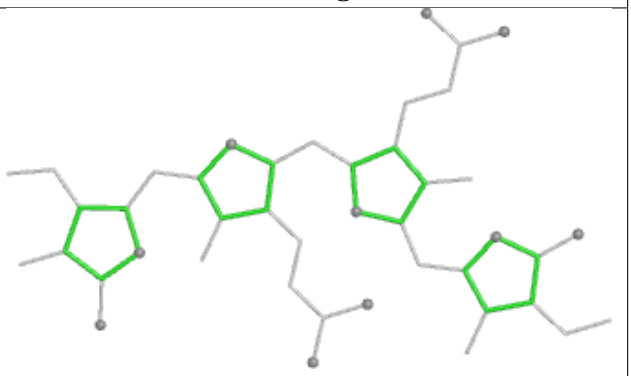
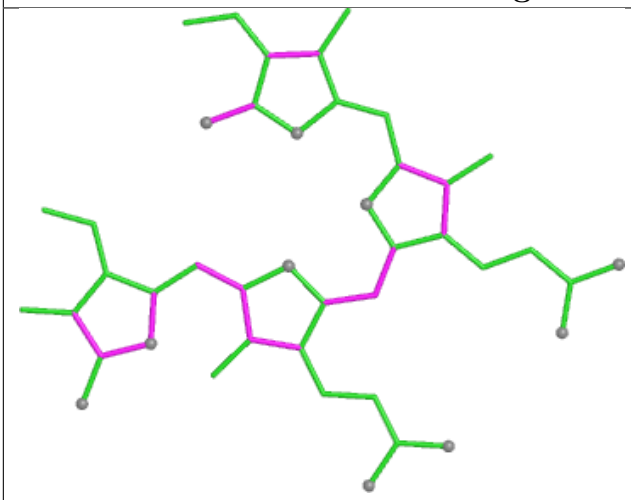


Rings

Ligand PEB LD 202



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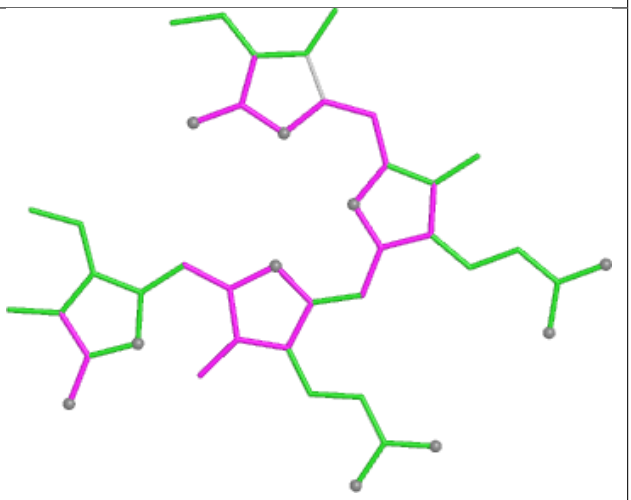
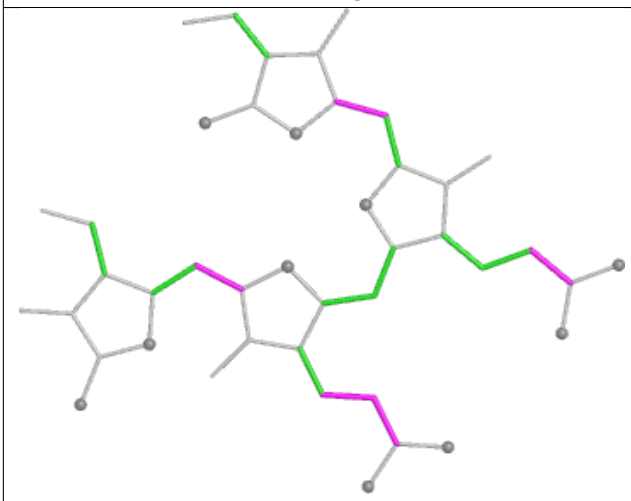


Bond angles



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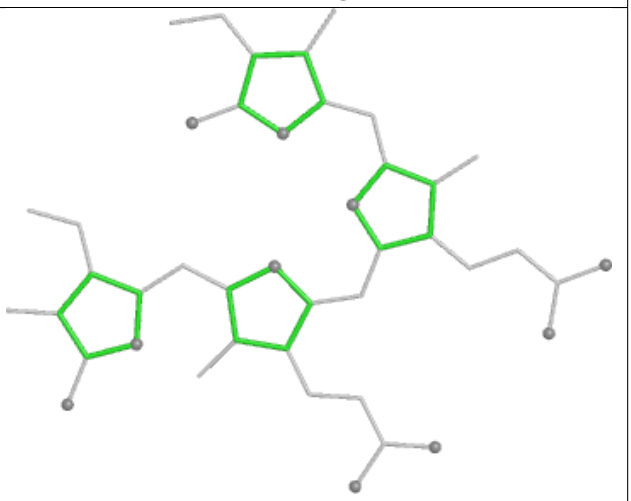
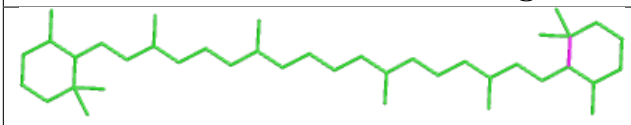


Rings

Ligand BCR a6 605



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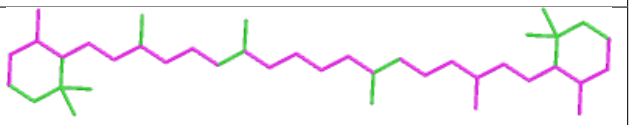
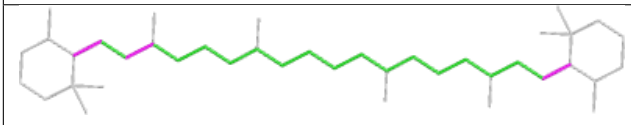


Bond angles



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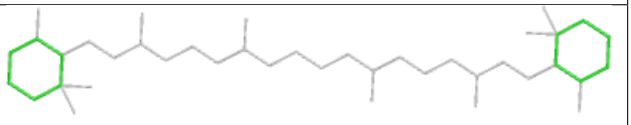
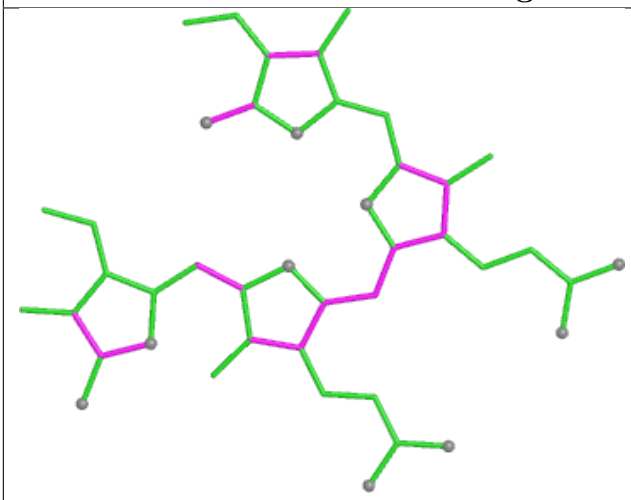


Rings

Ligand PEB B9 201



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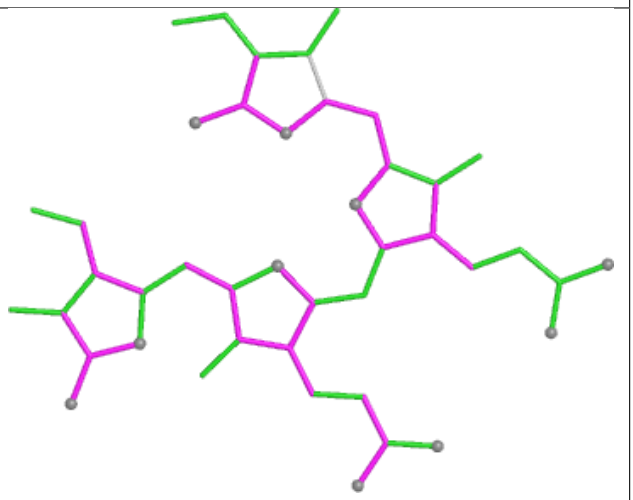
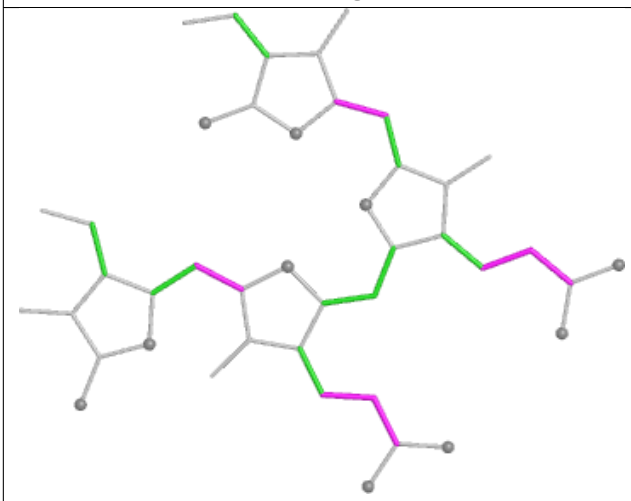


Bond angles



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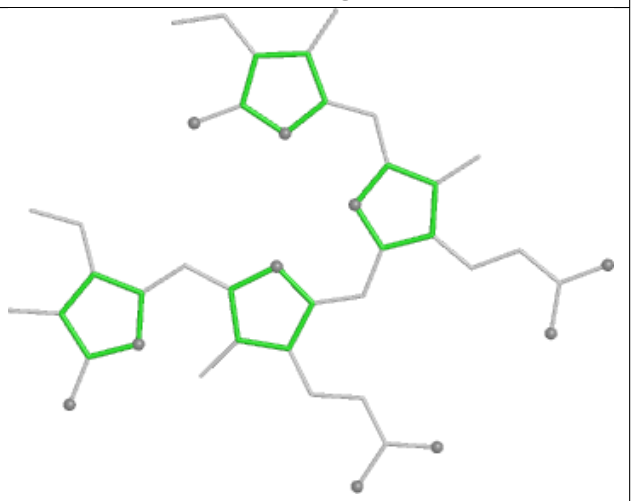
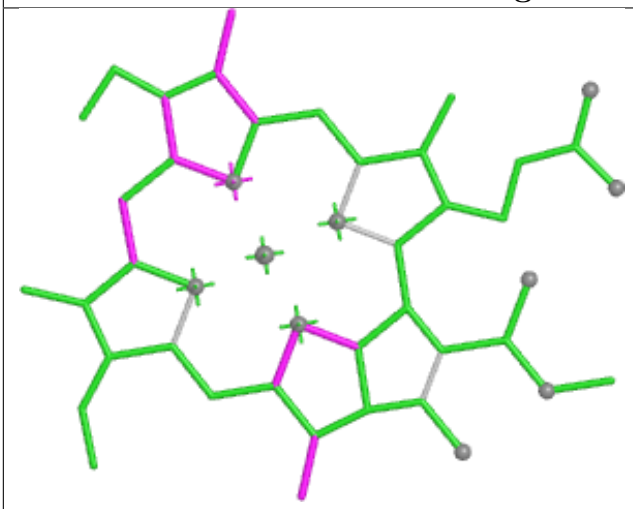
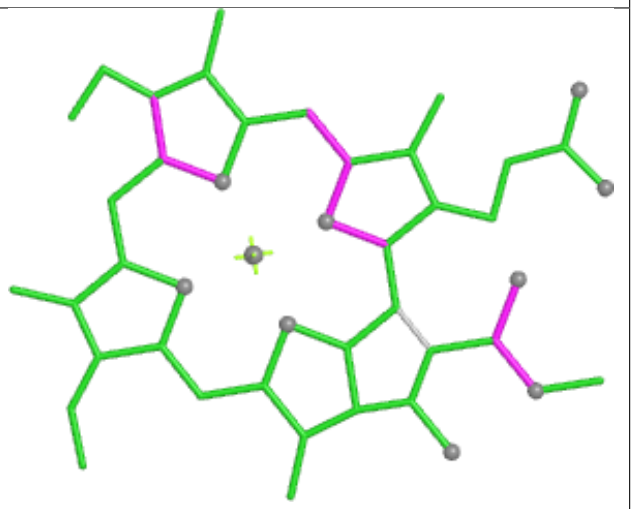


Rings

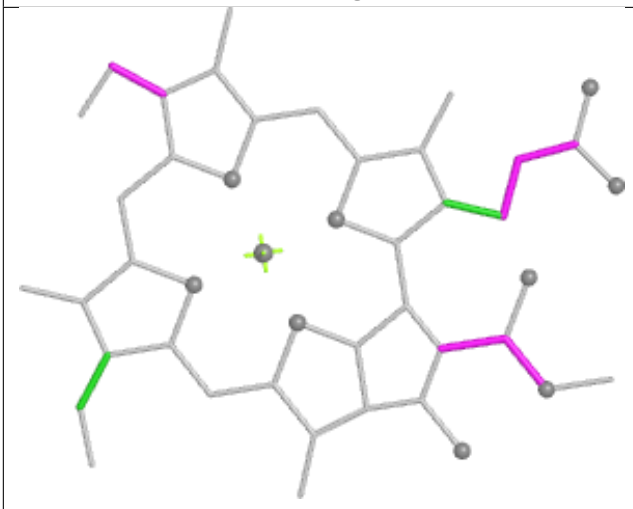
Ligand CLA 5N 603



Bond lengths



Bond angles

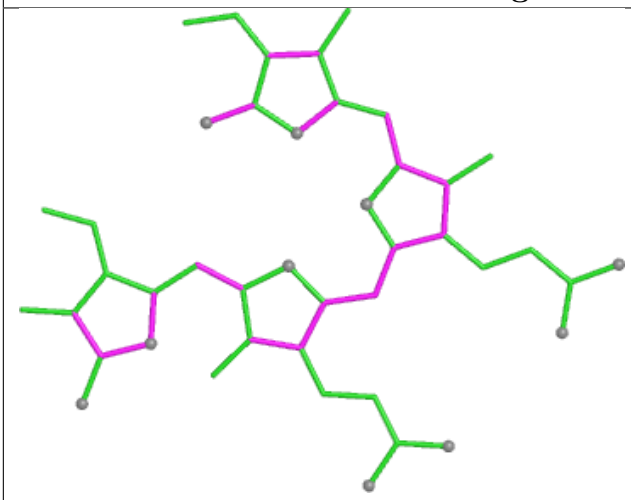


Torsions



Rings

Ligand PEB TD 201



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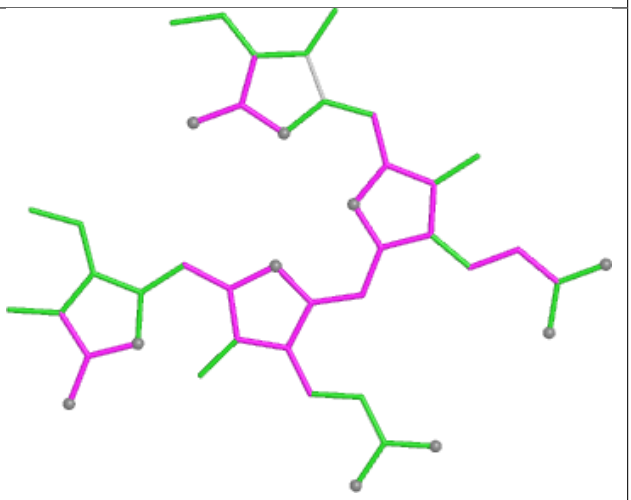

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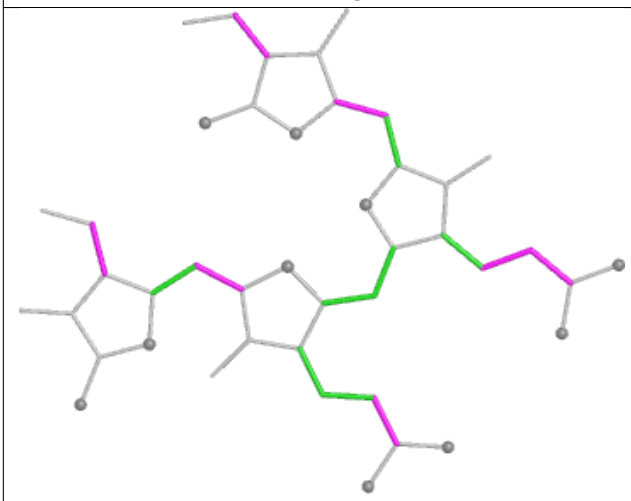

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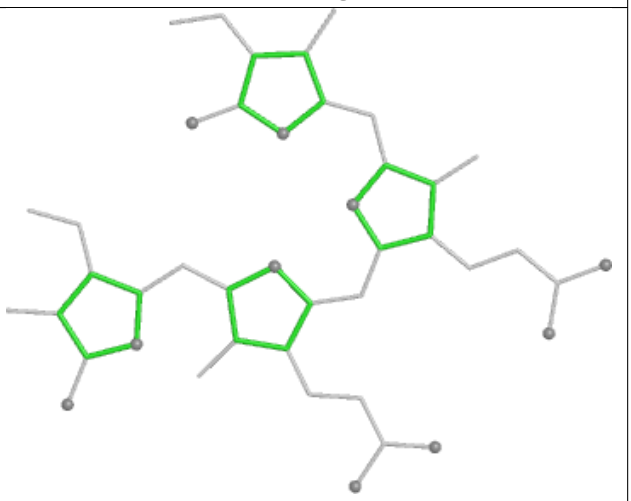
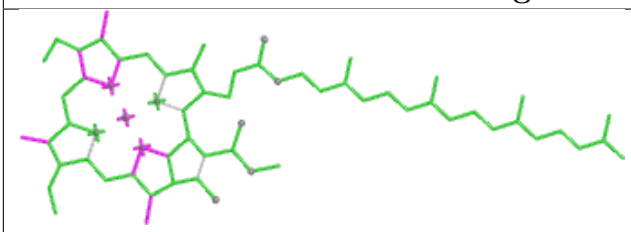


Rings

Ligand CLA CL 504



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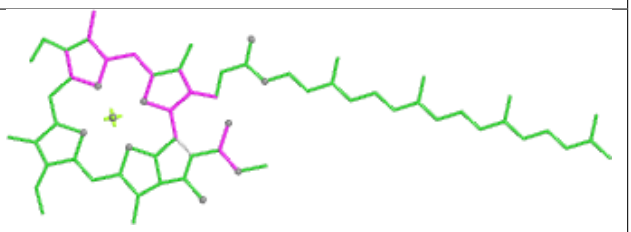

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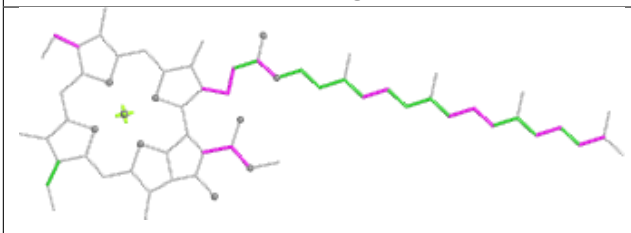

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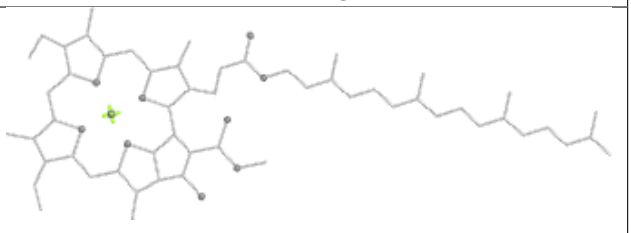
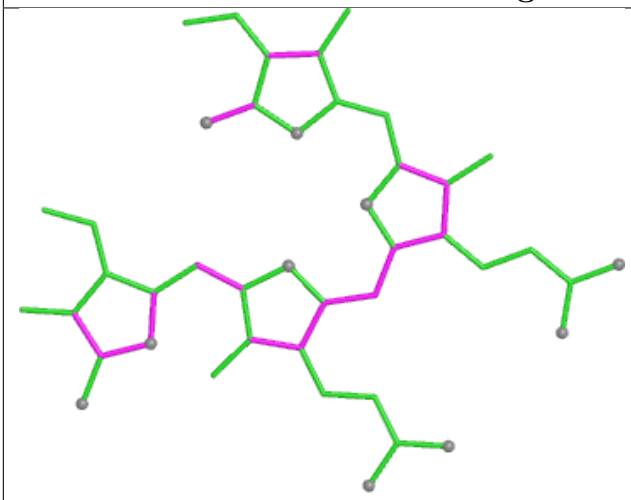


Rings

Ligand PEB F7 203



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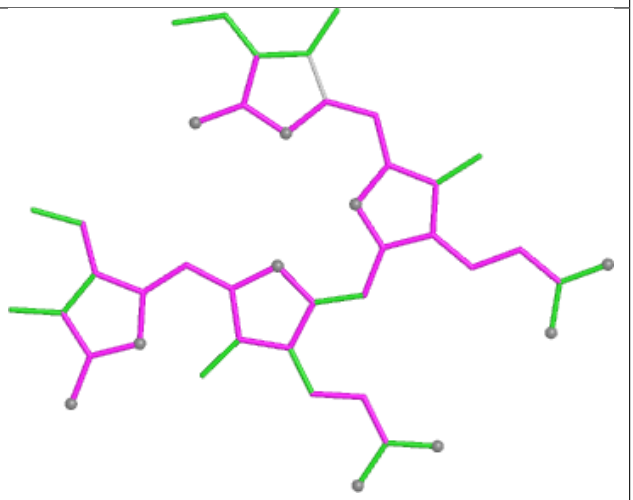

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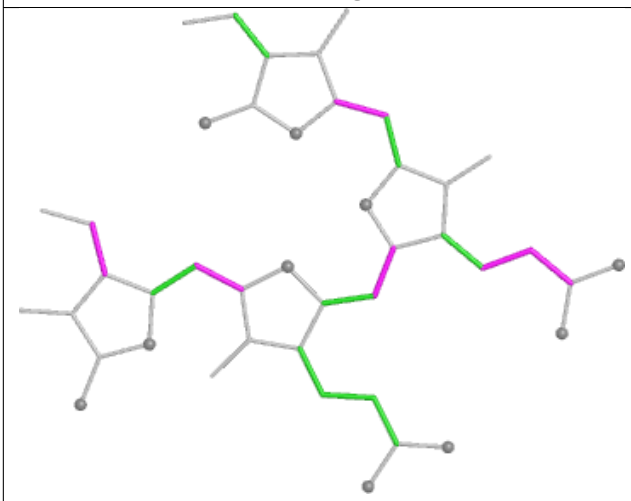

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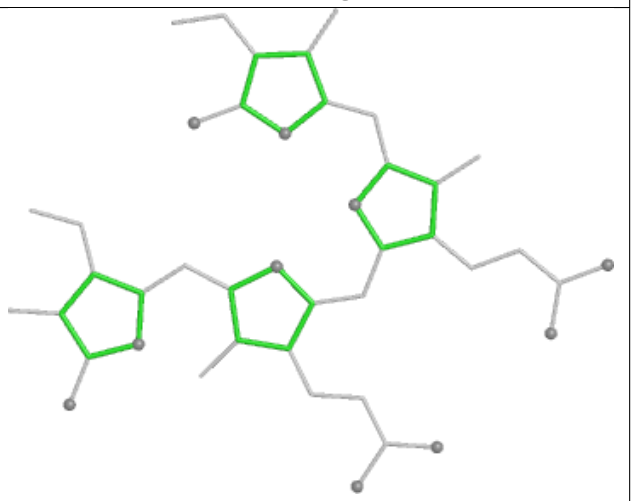
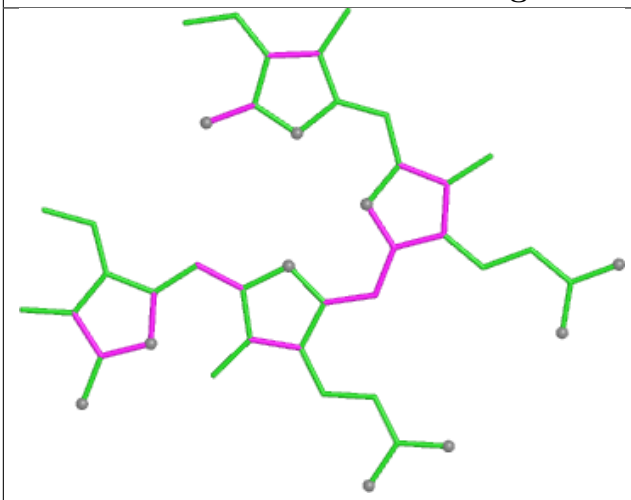


Rings

Ligand PEB QG 202



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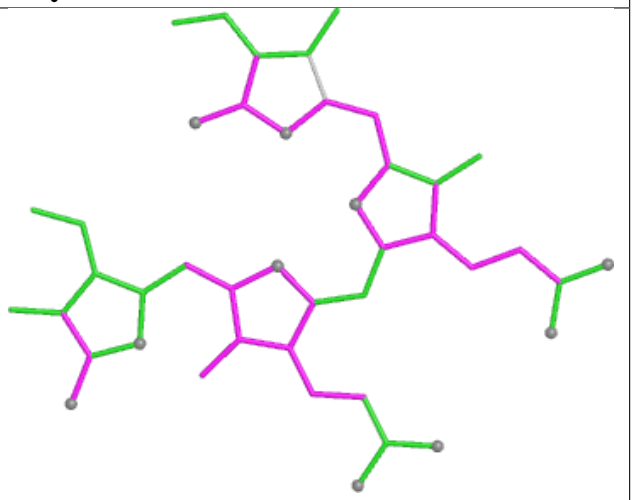

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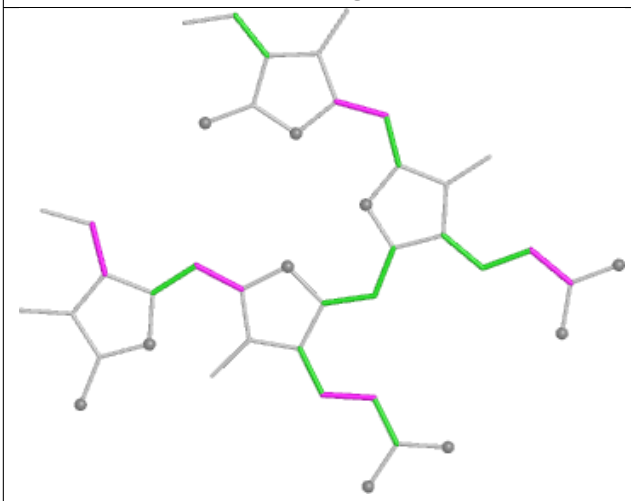

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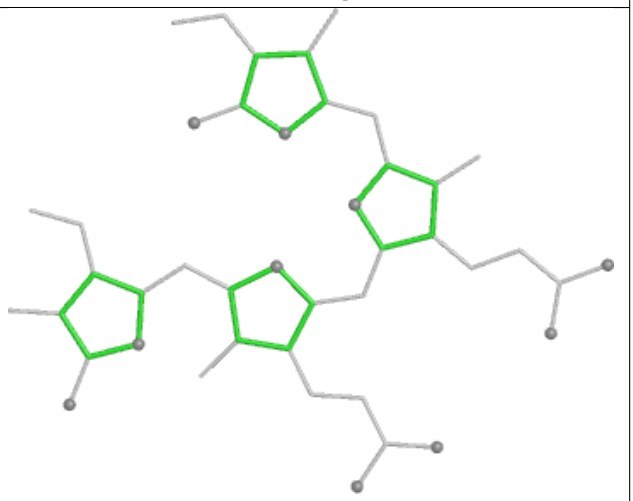

Rings

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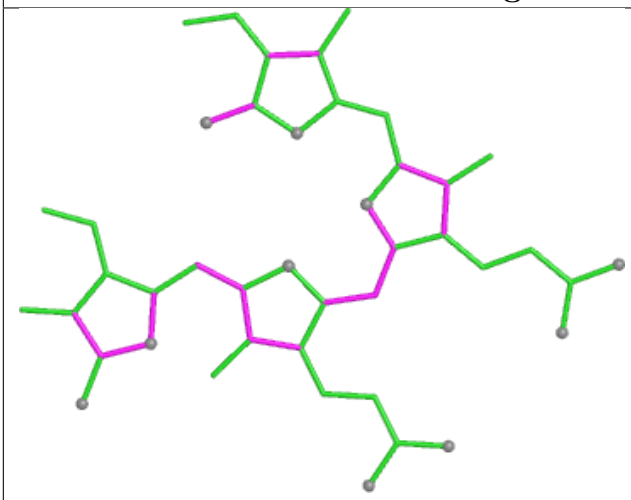

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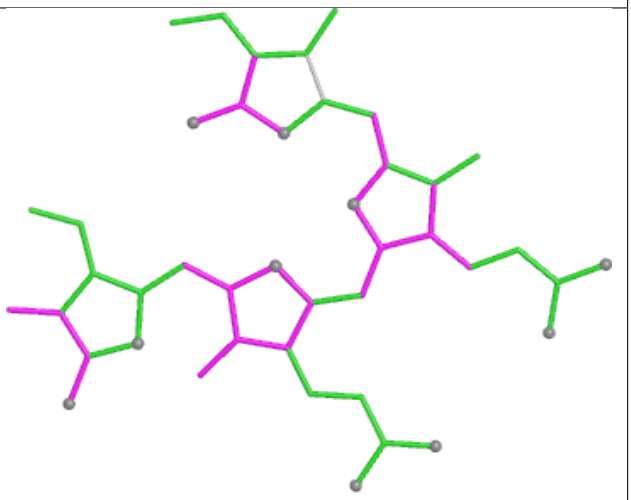

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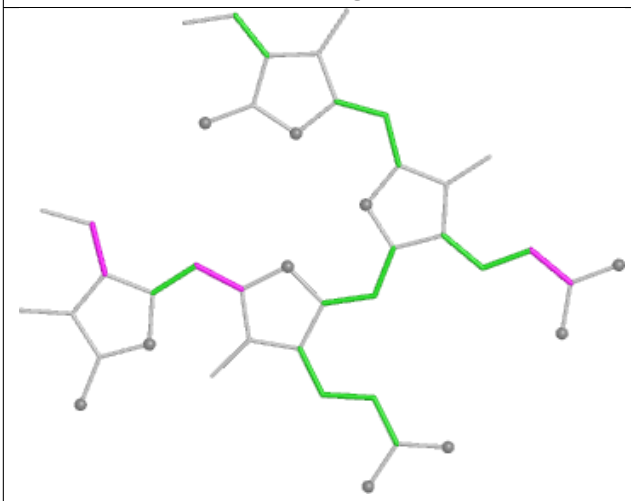

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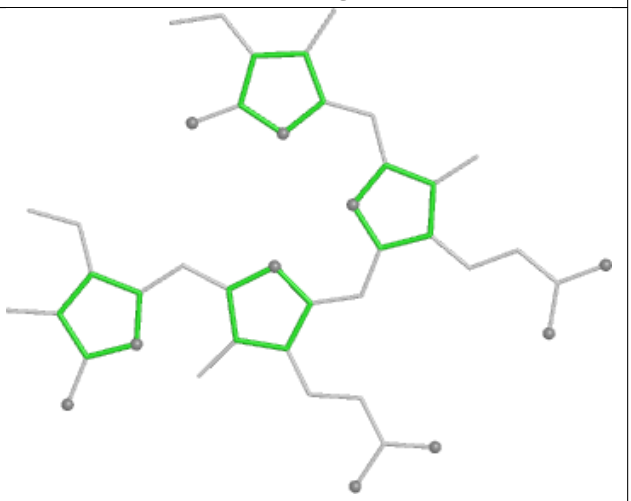

Rings

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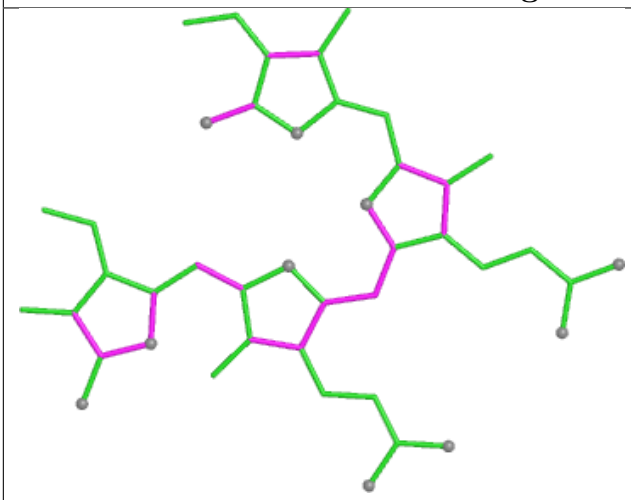

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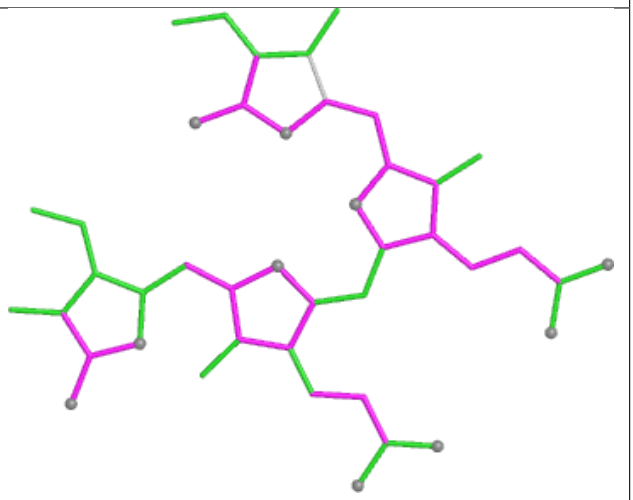

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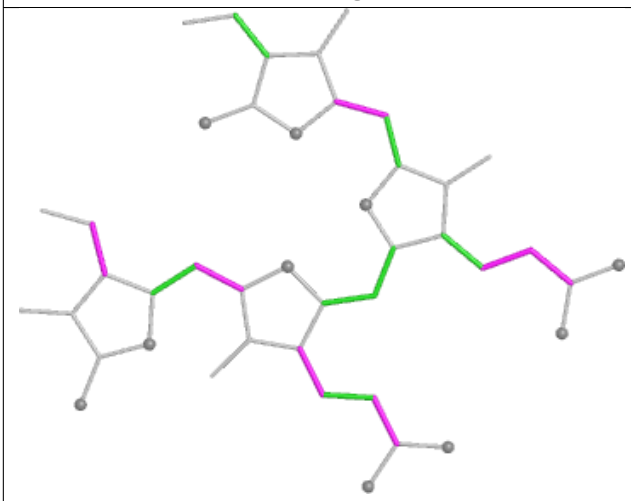

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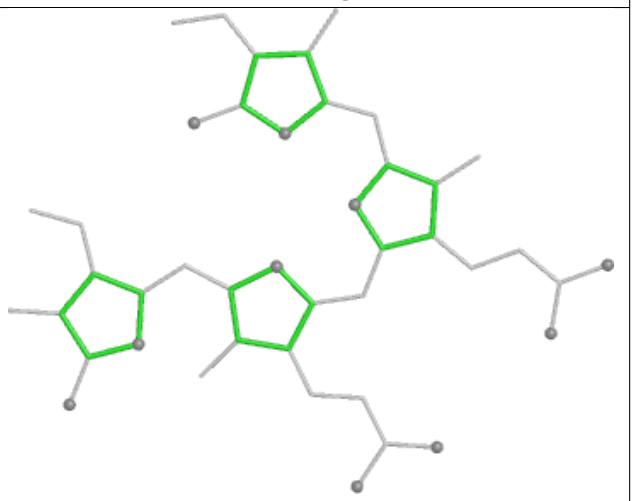

Rings

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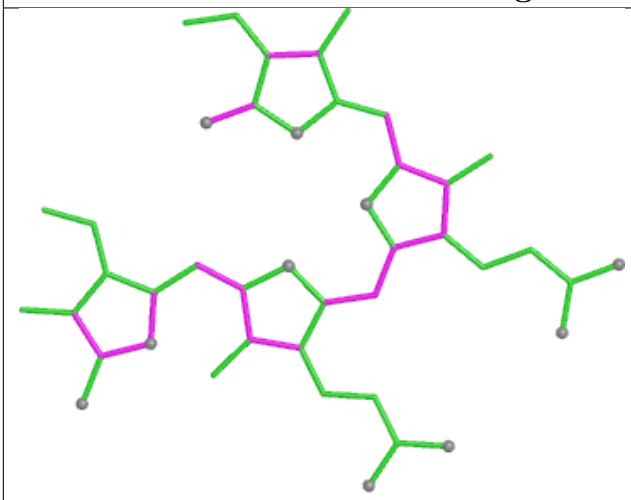

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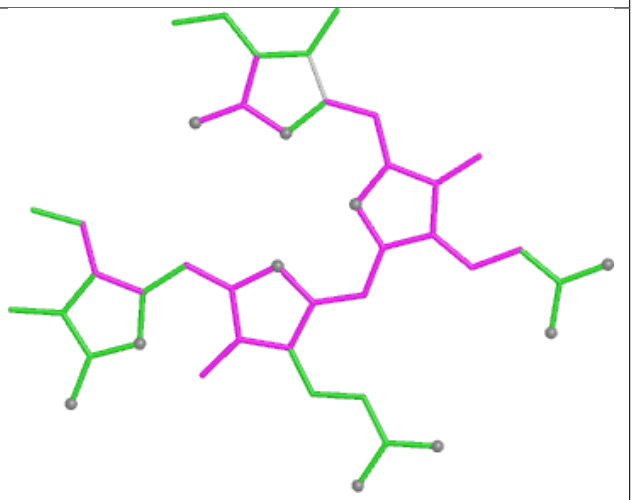

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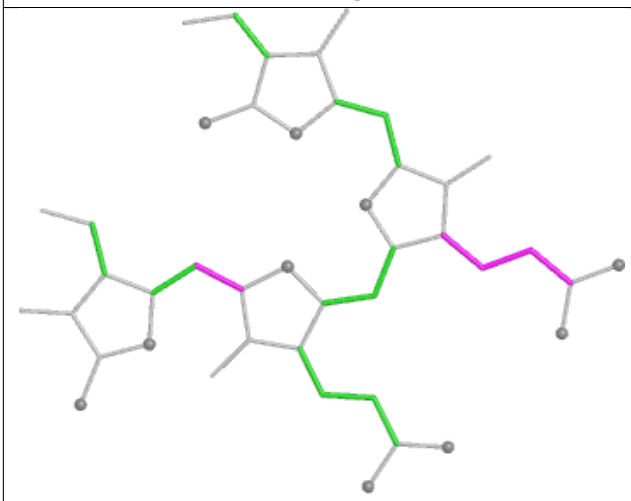

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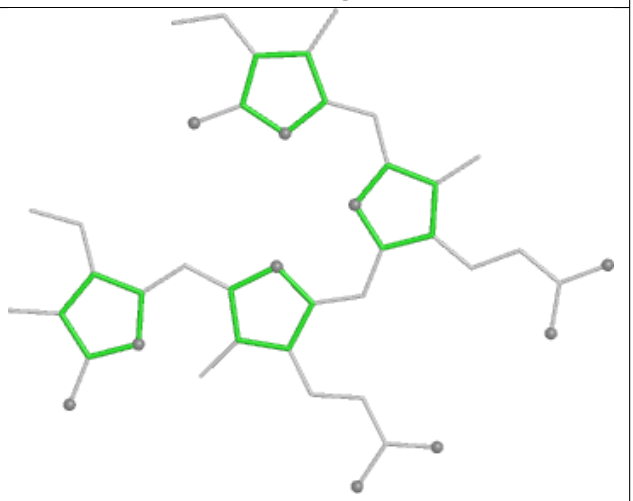

Rings

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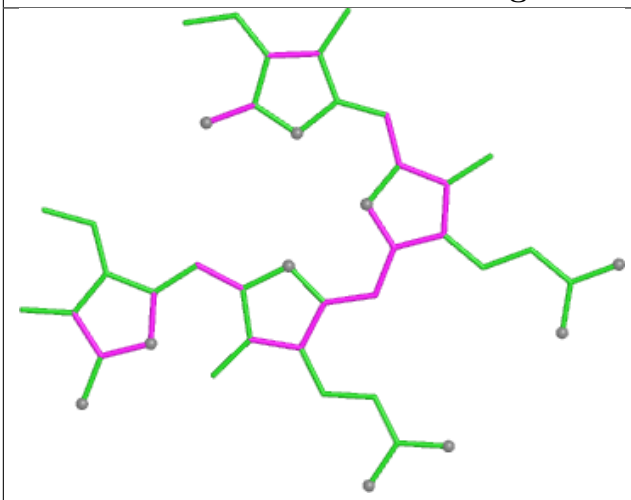

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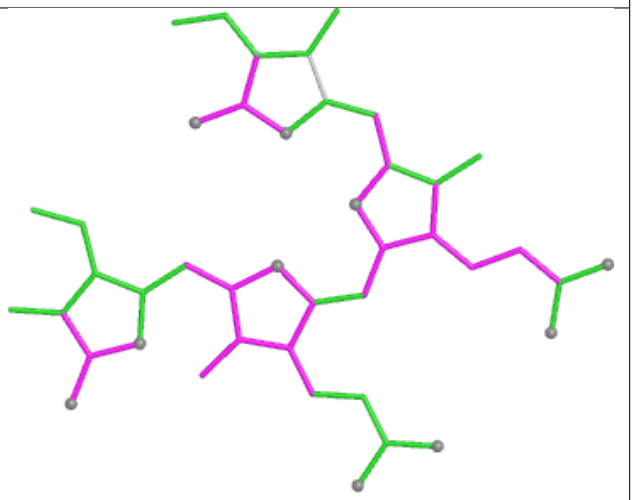

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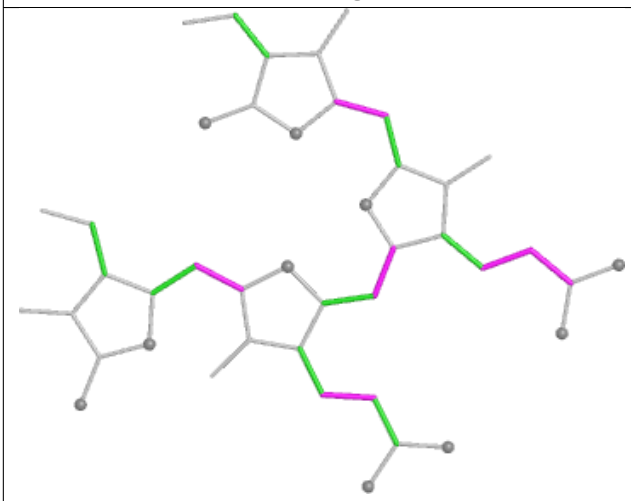

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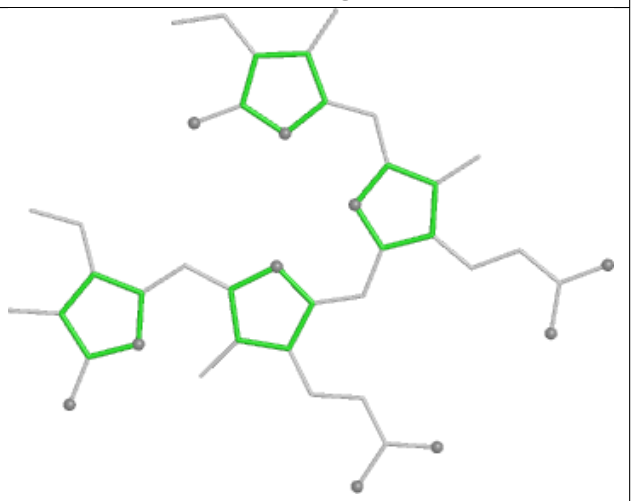
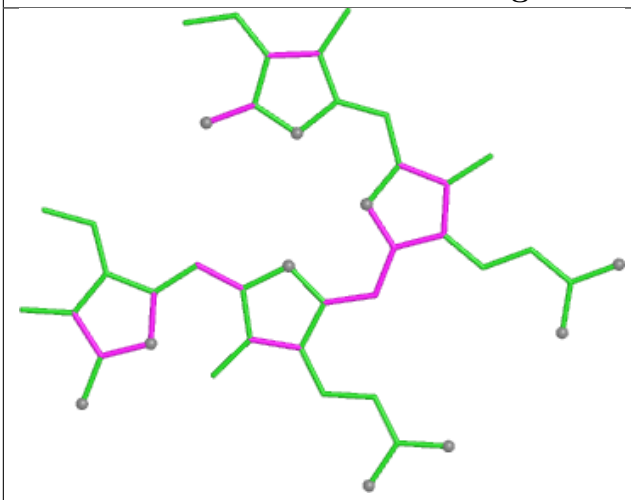


Rings

Ligand PEB MJ 203



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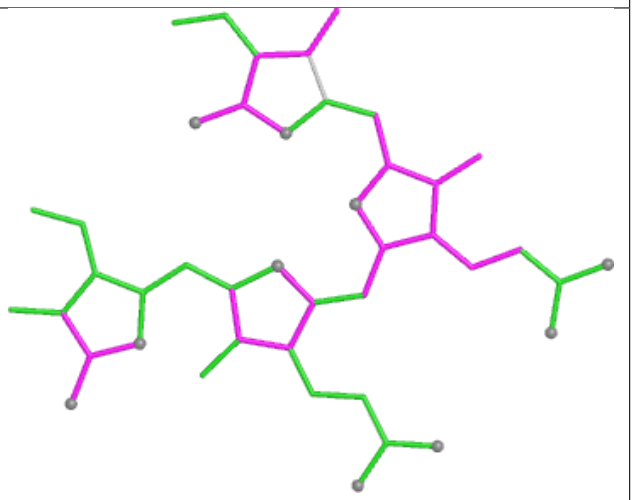

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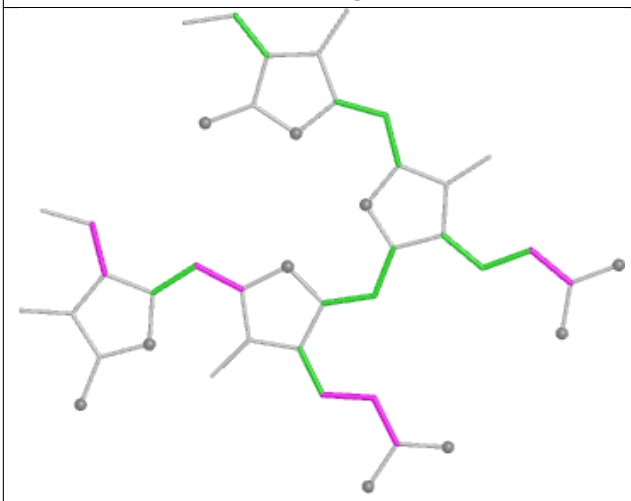

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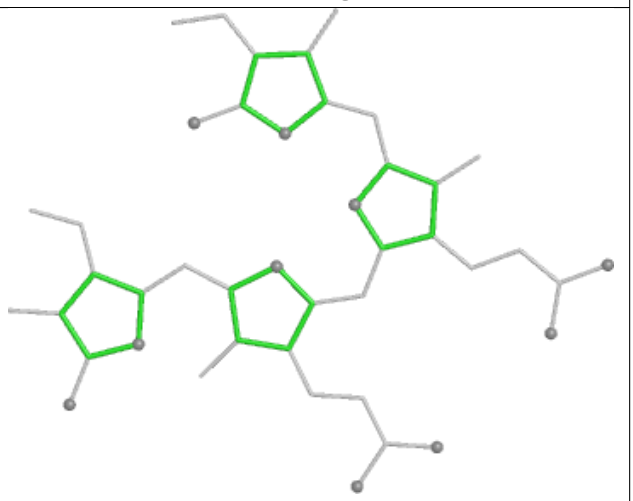
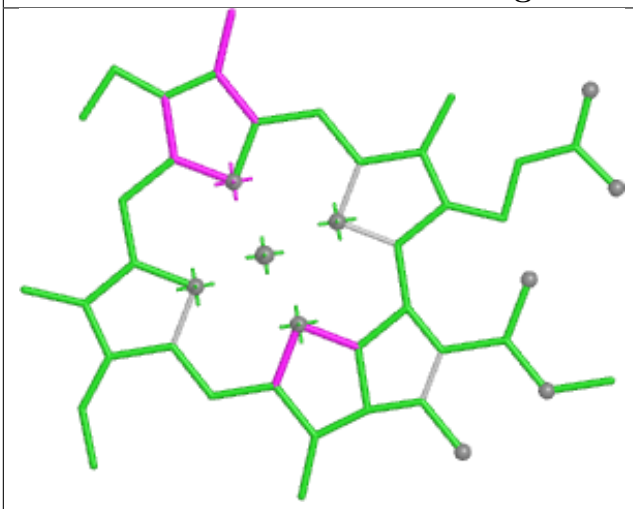


Rings

Ligand CLA 1N 605



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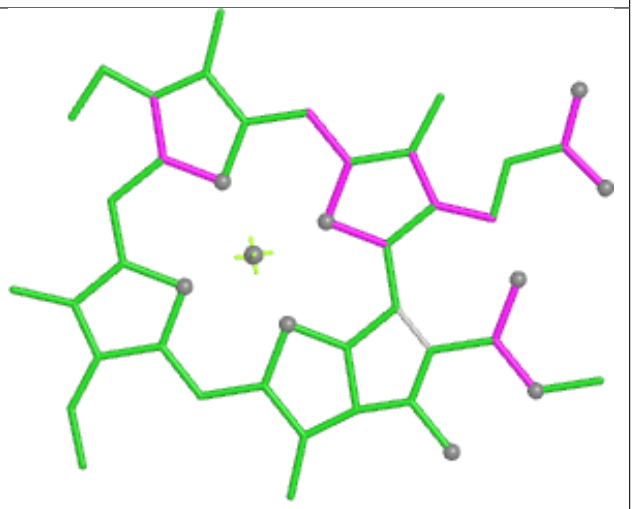

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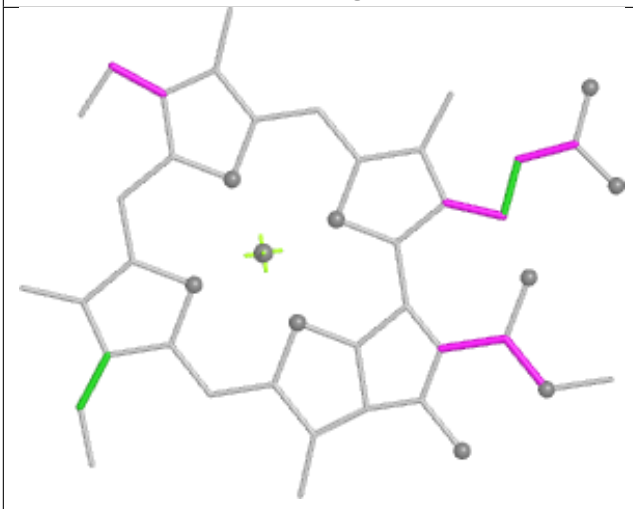
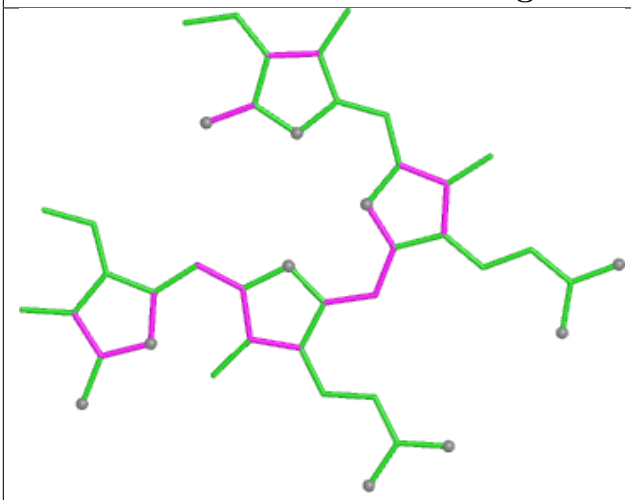


Torsions



Rings

Ligand PEB T5 201



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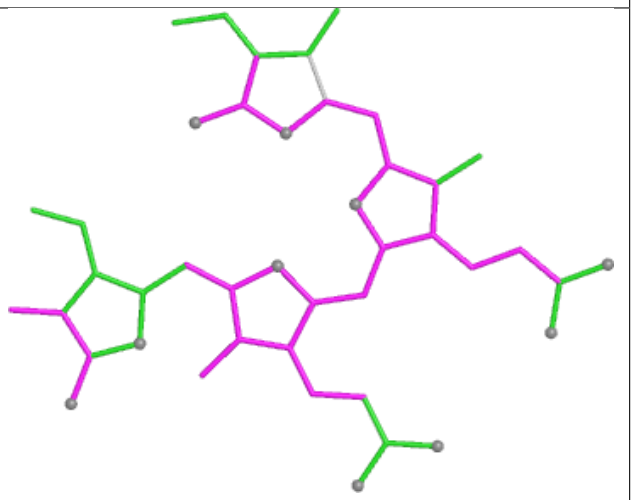
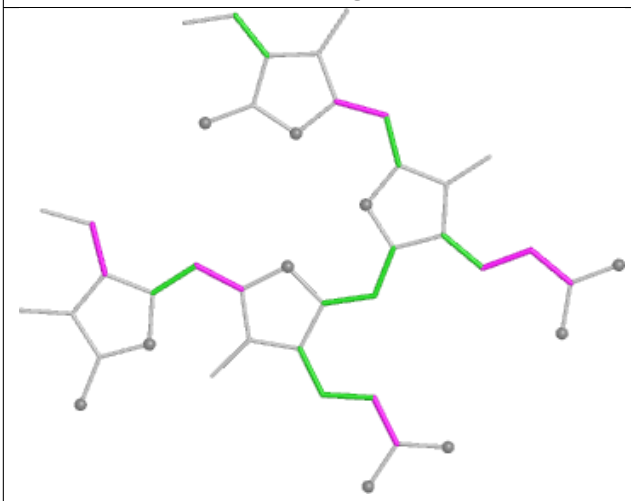


Bond angles



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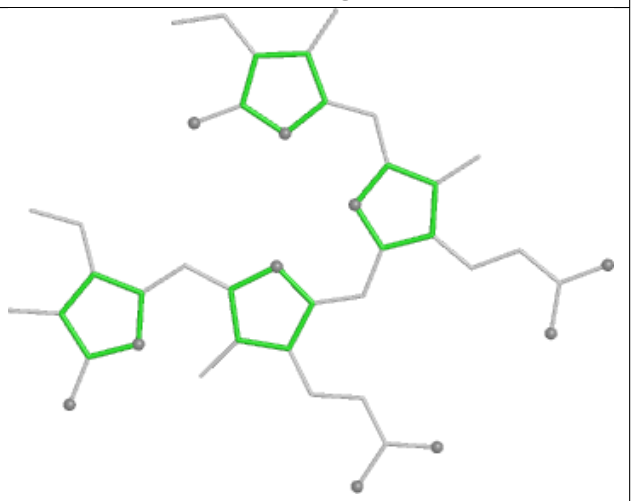
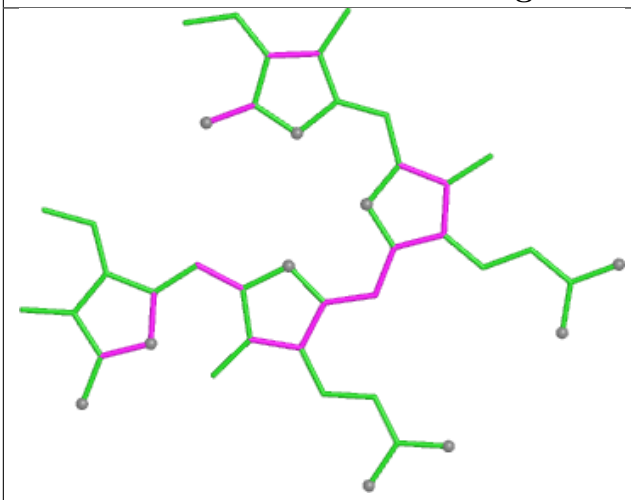


Rings

Ligand PEB Q9 203



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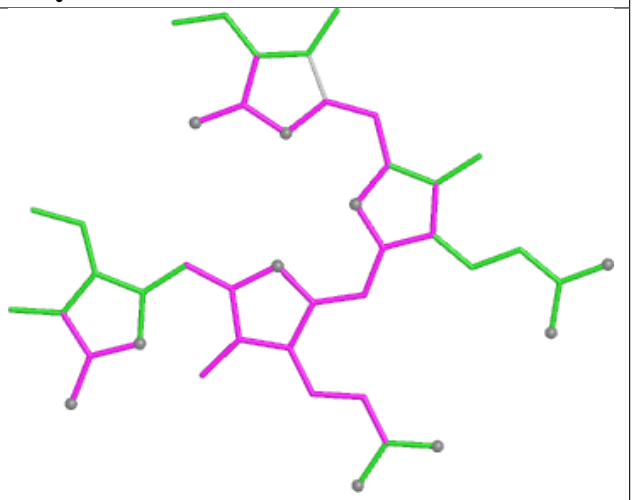
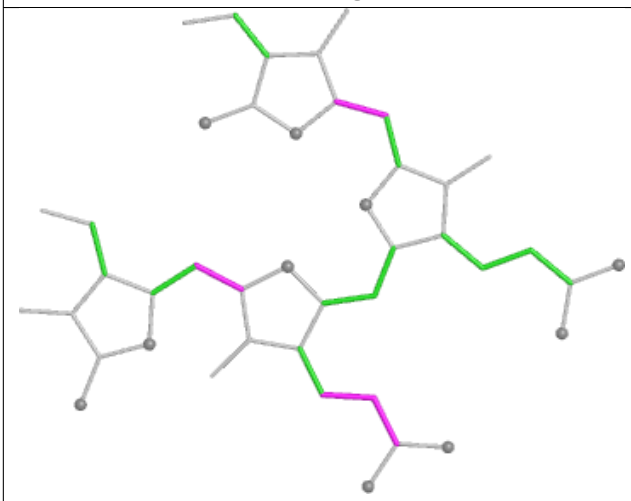


Bond angles



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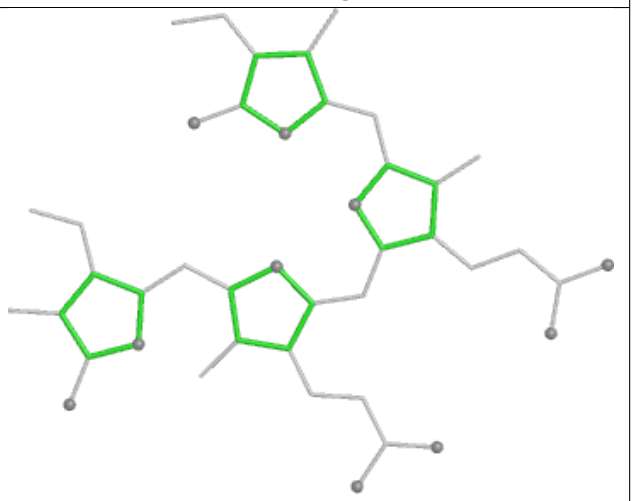

Rings

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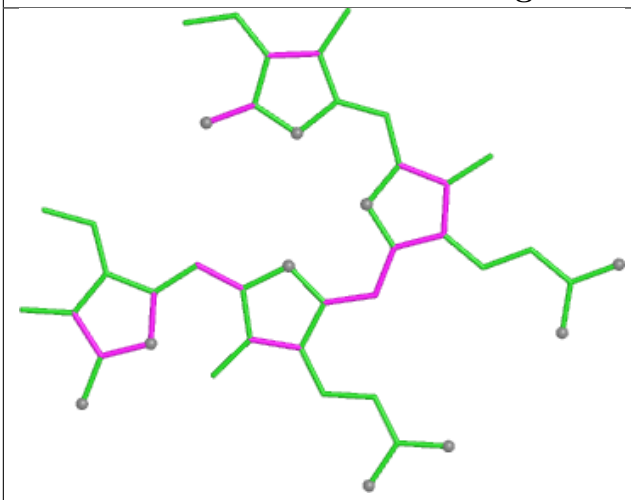

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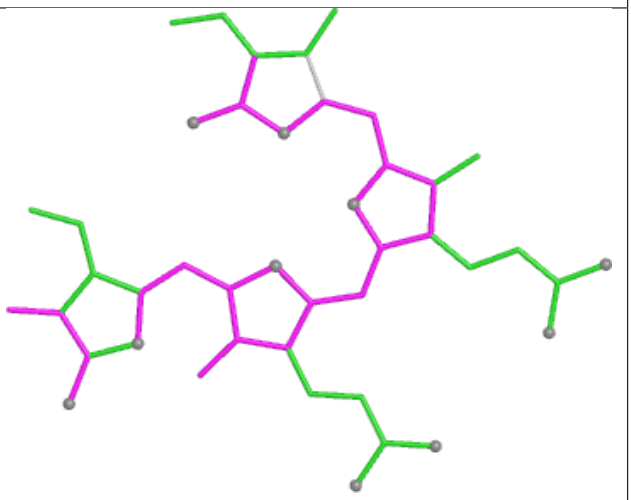
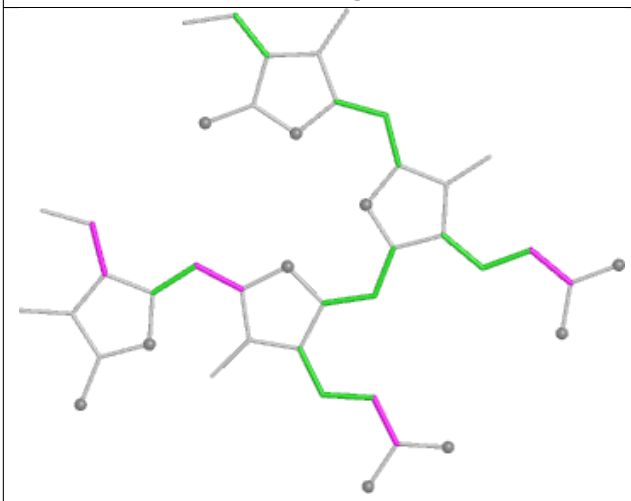


Bond angles



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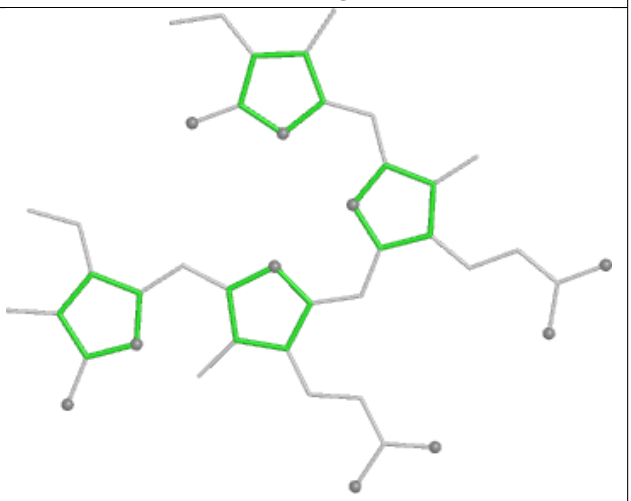
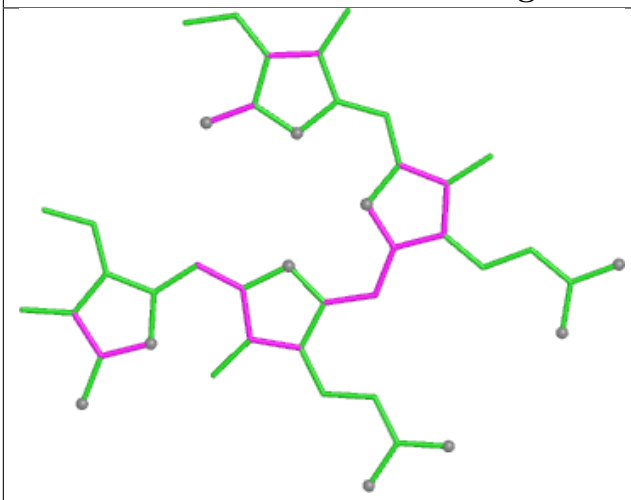


Rings

Ligand PEB Z9 303



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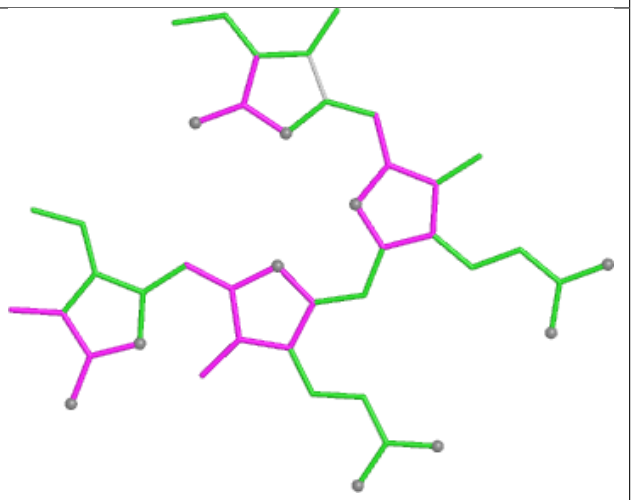
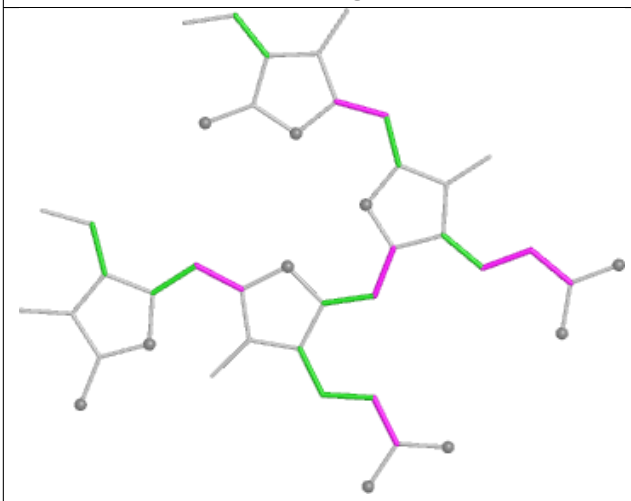


Bond angles



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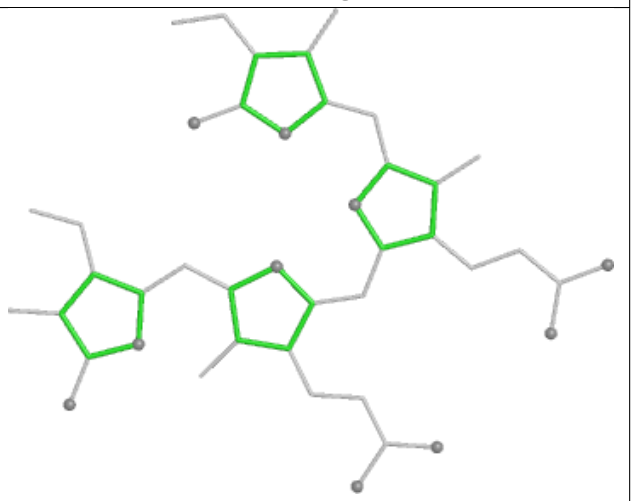
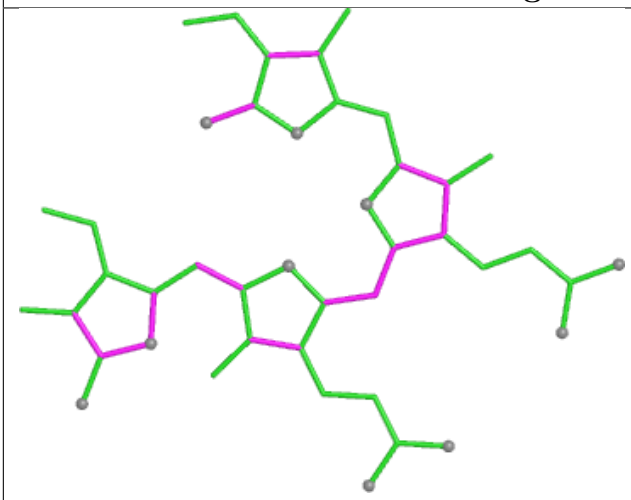
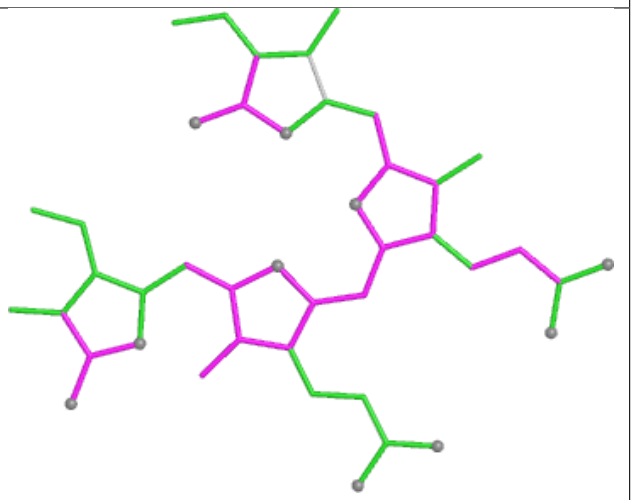


Rings

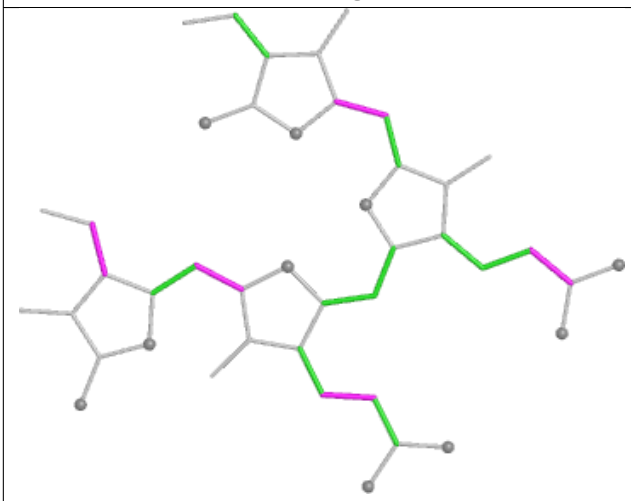
Ligand PEB i4 202



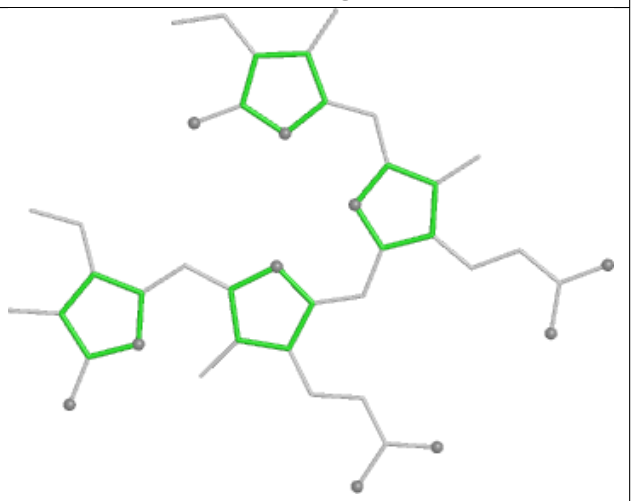
Bond lengths



Bond angles

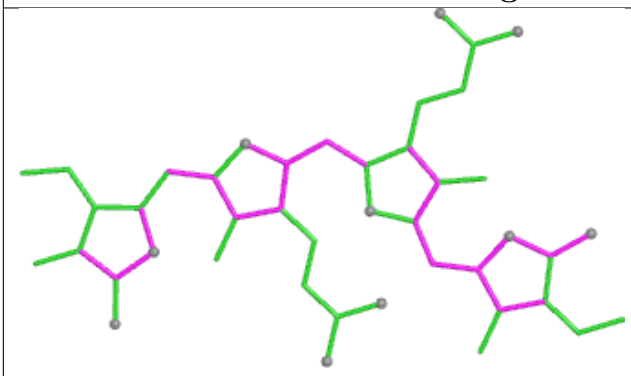


Torsions



Rings

Ligand CYC EG 1001



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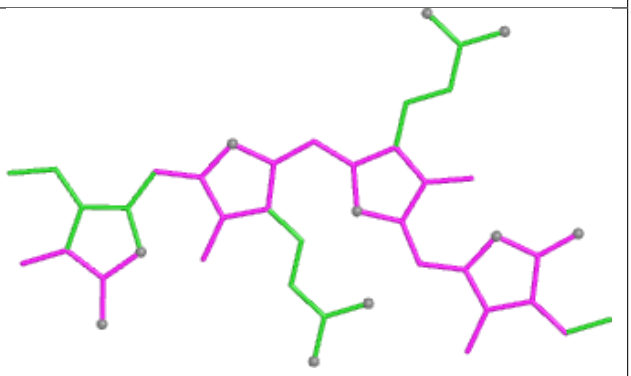

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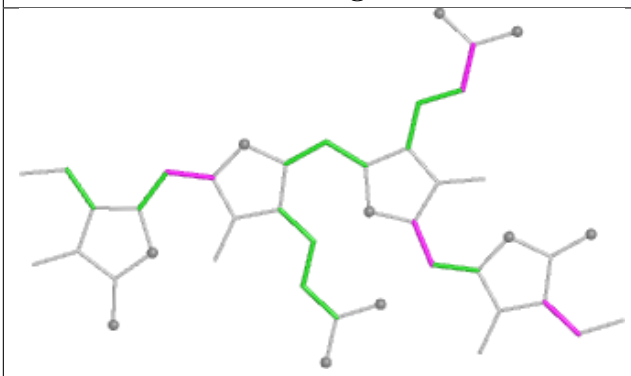

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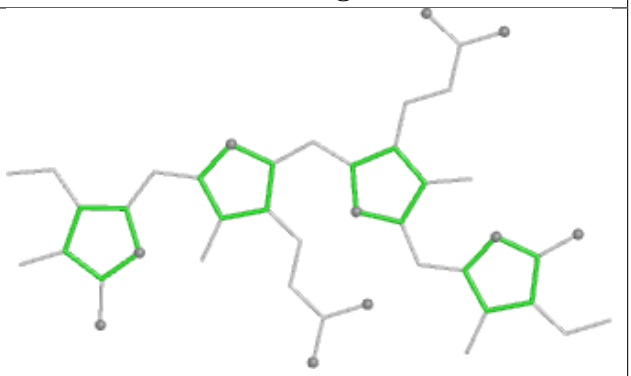
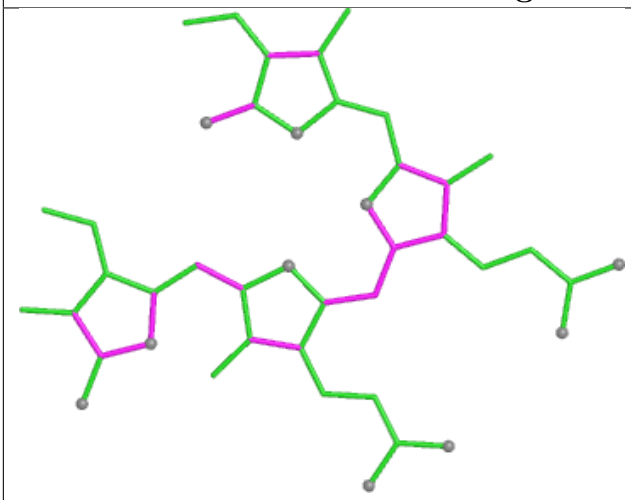


Rings

Ligand PEB BJ 301



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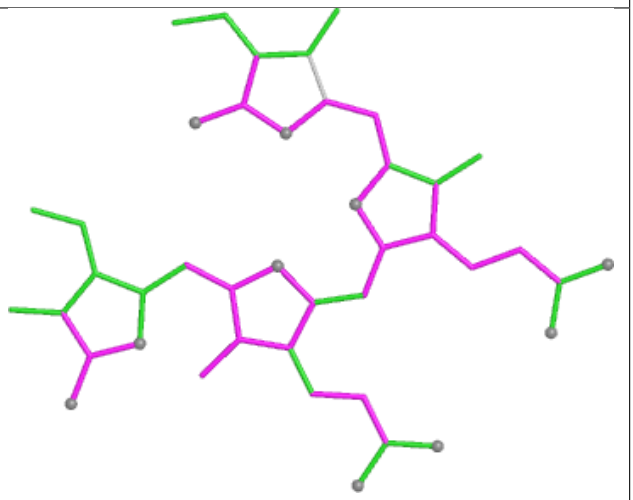

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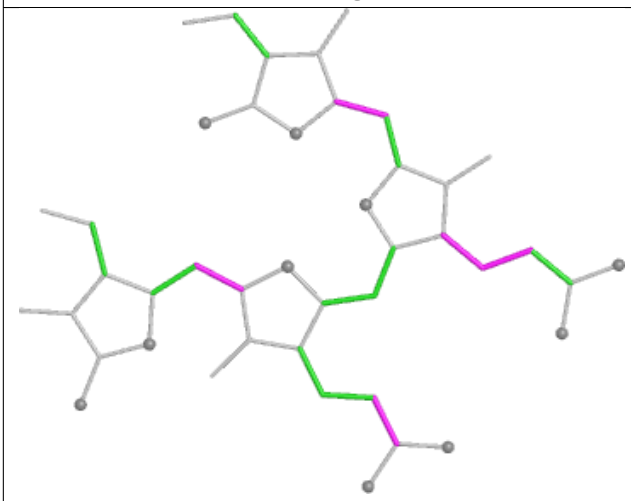

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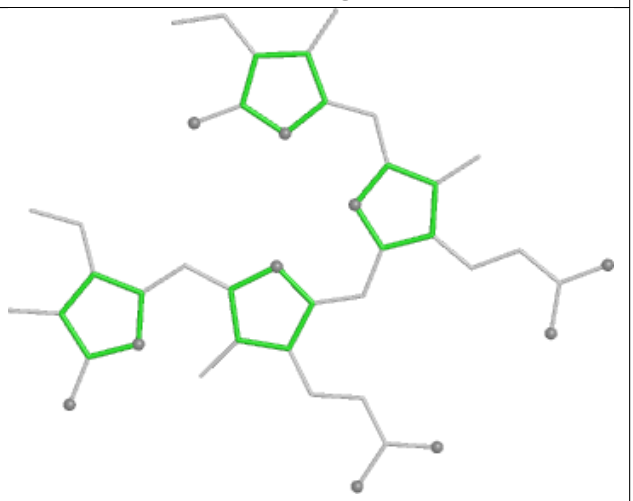
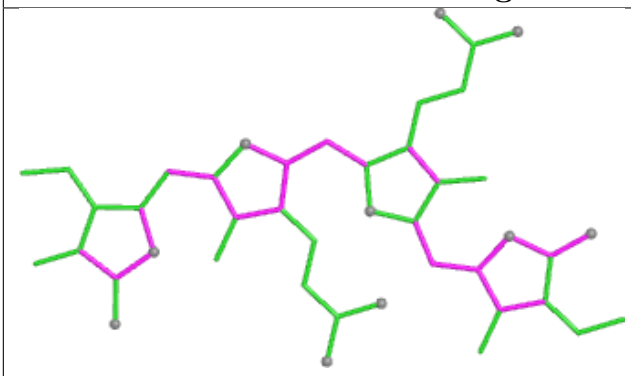


Rings

Ligand CYC MG 1001



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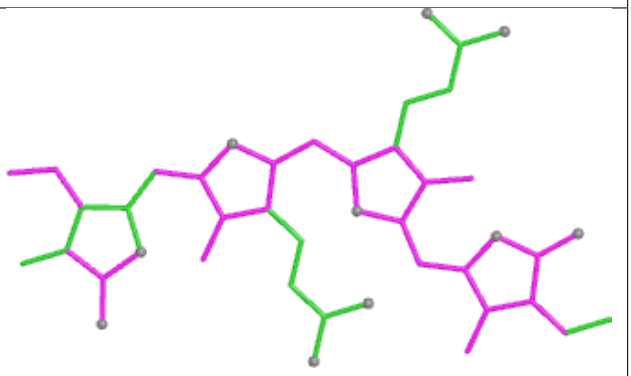

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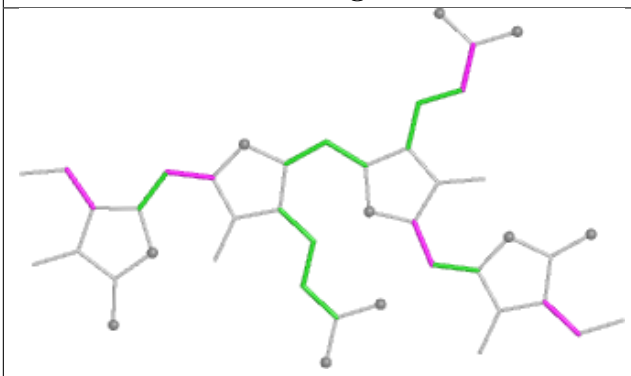

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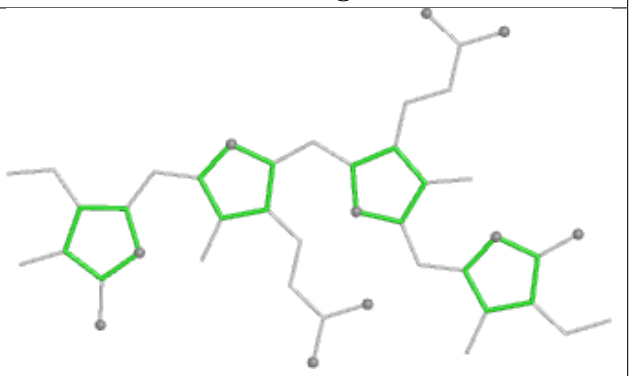
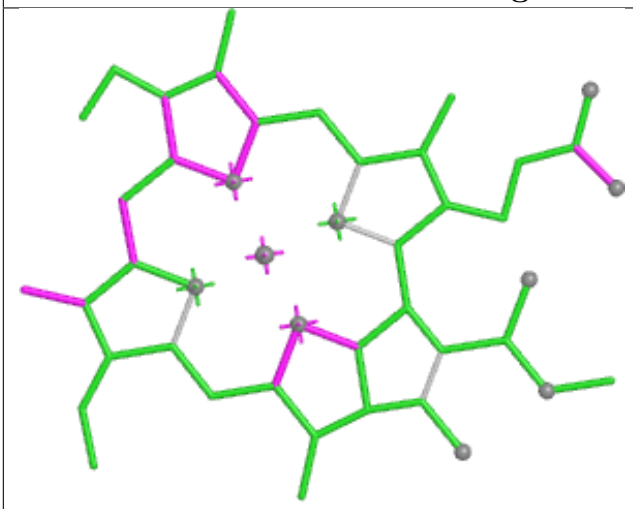


Rings

Ligand CLA M2 101



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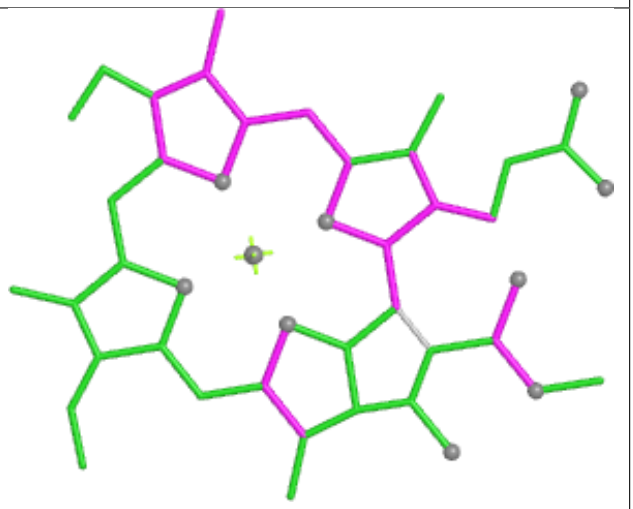

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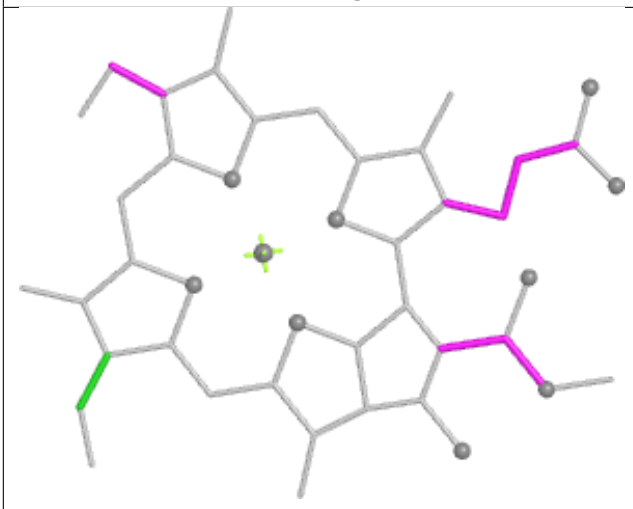
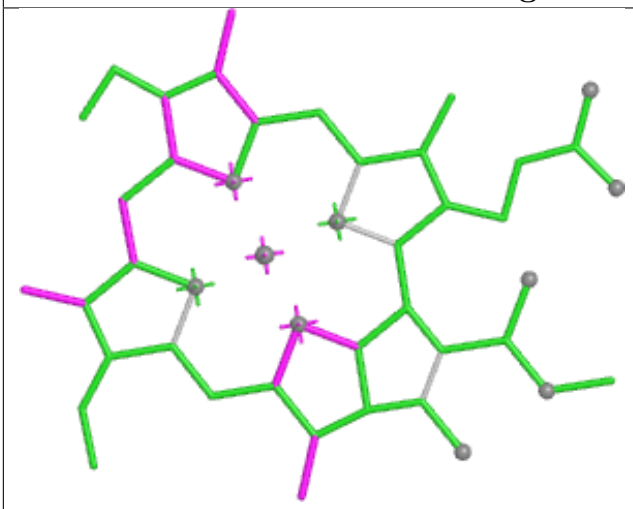


Torsions



Rings

Ligand CLA 82 301



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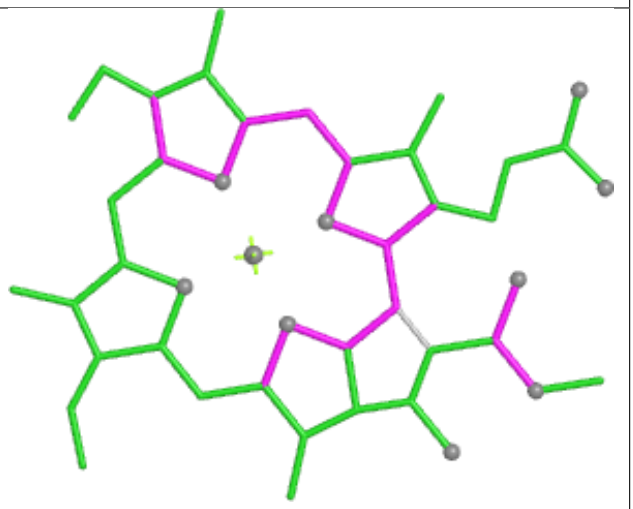
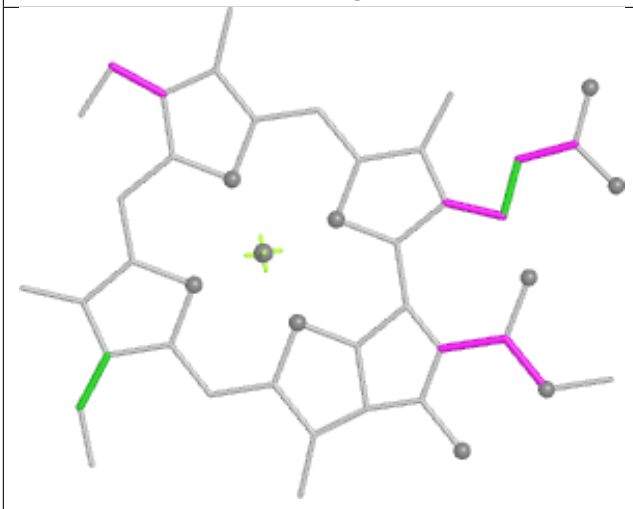


Bond angles

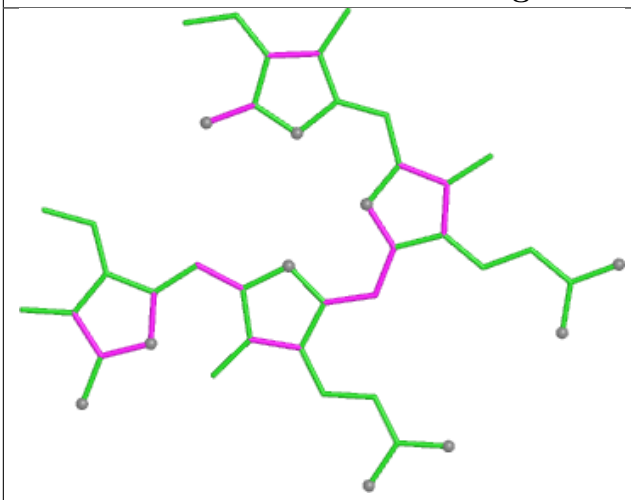


Torsions



Rings

Ligand PEB EQ 202



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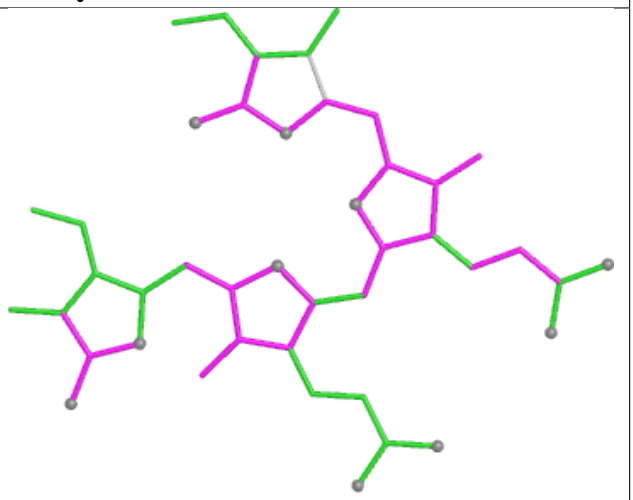

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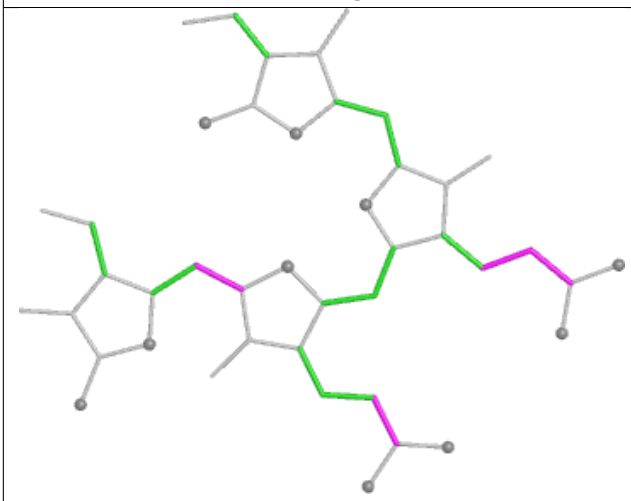

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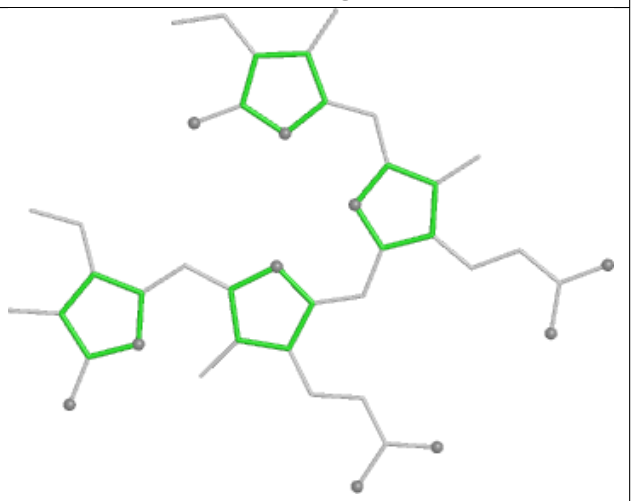
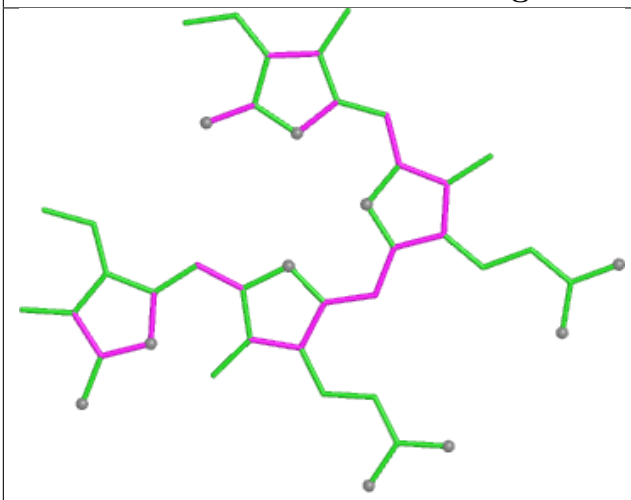


Rings

Ligand PEB TQ 201



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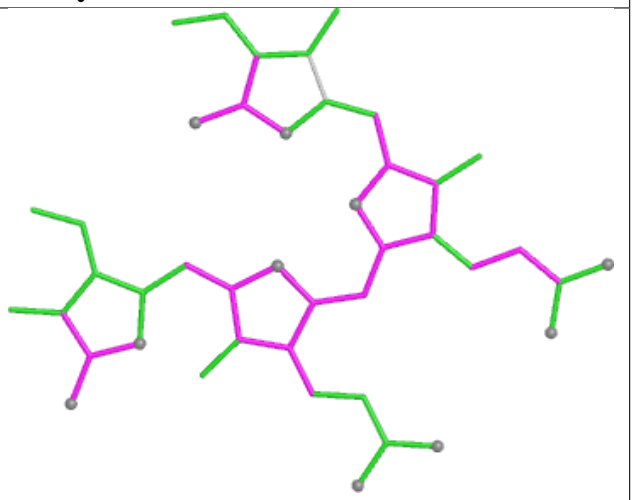
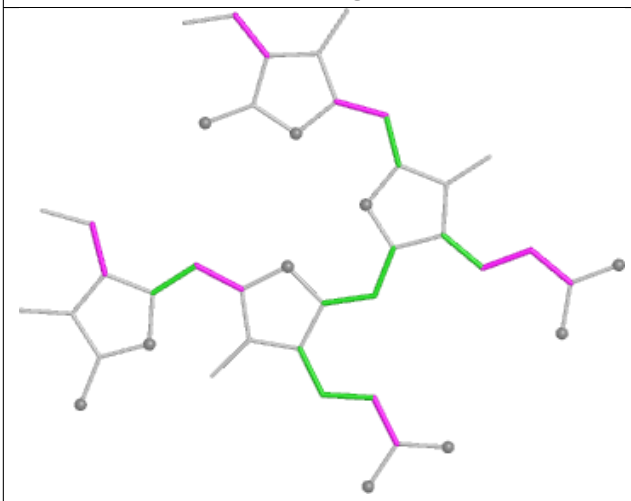


Bond angles



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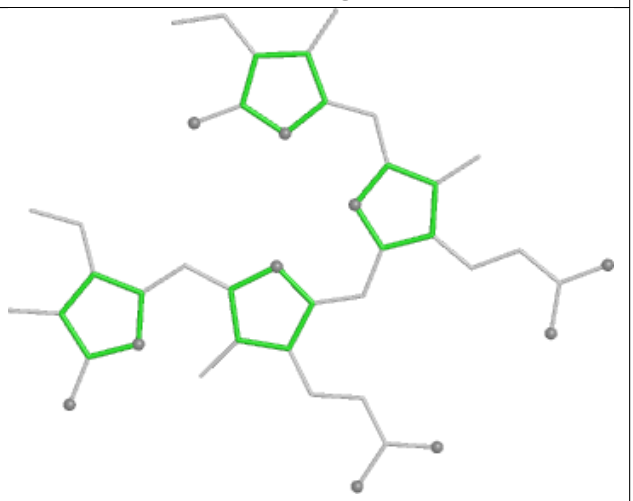
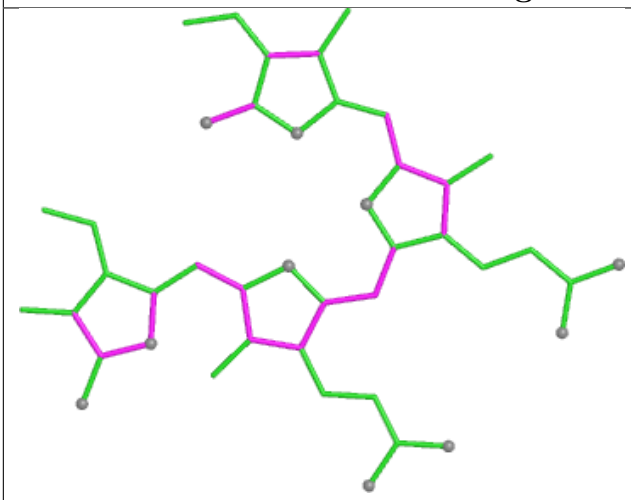


Rings

Ligand PEB D7 201



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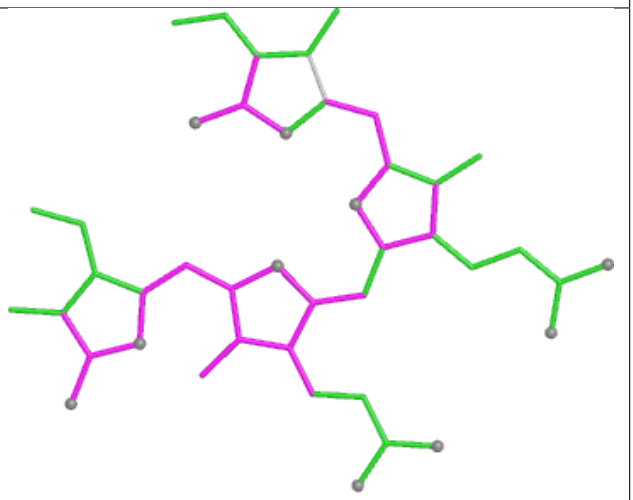
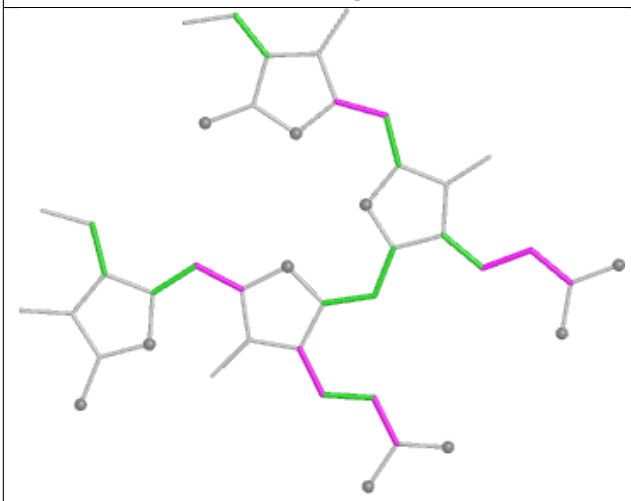


Bond angles



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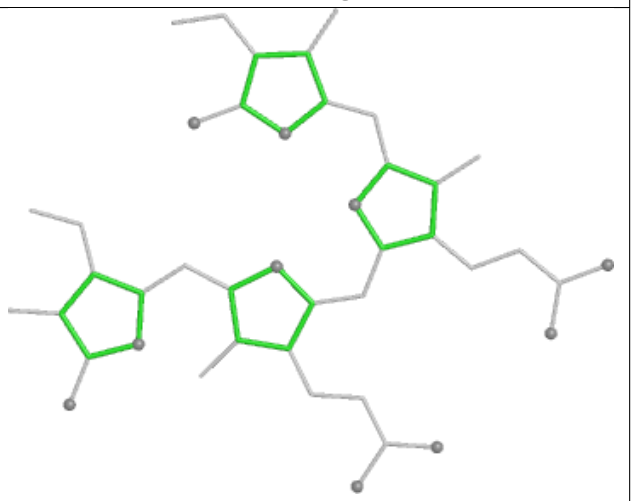
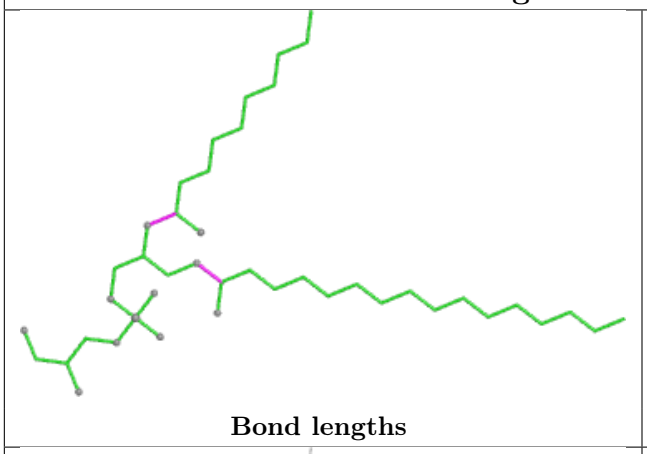


Rings

Ligand LHG AL 407



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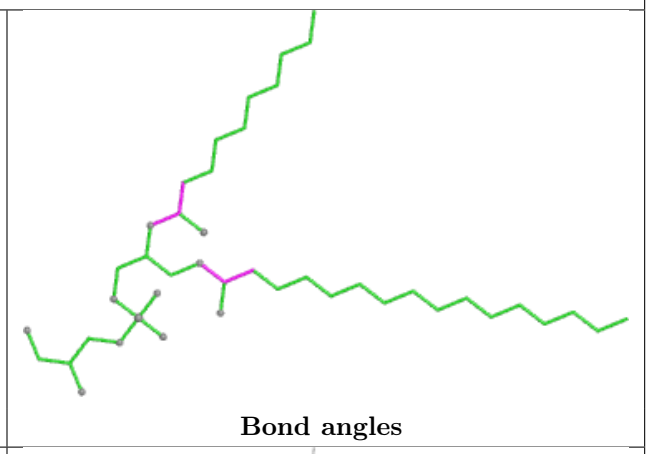
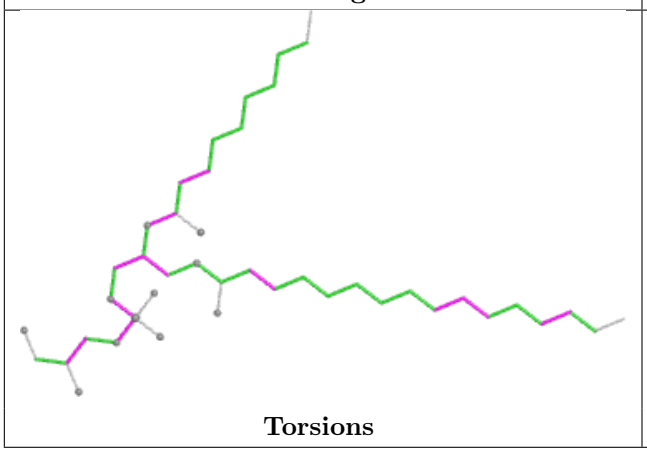


Bond angles



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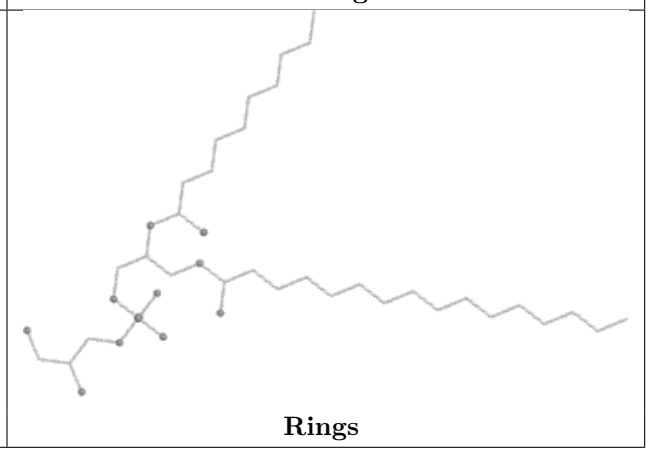
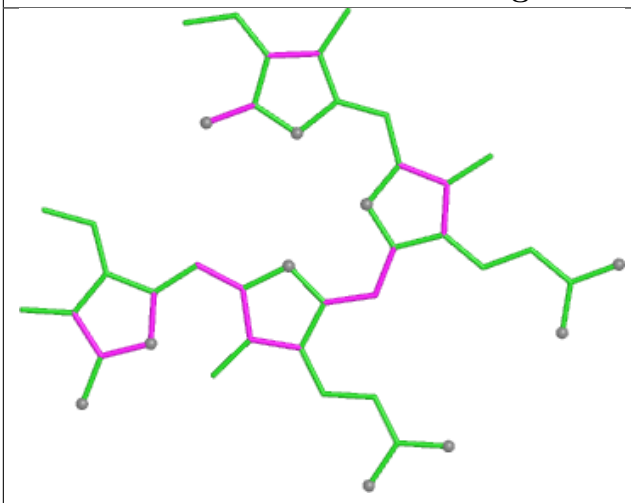


Rings

Ligand PEB PD 202



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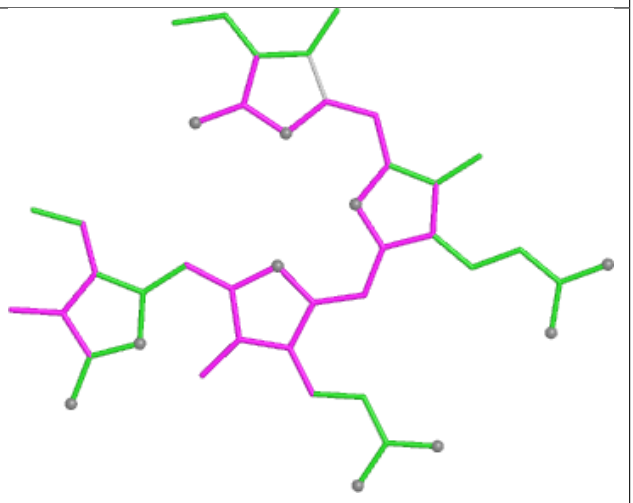

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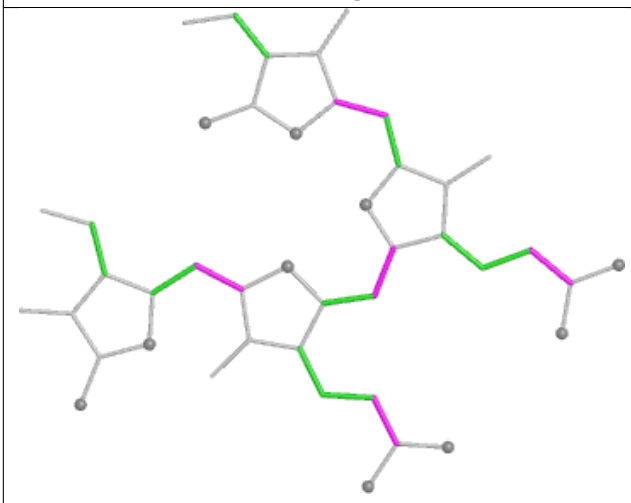

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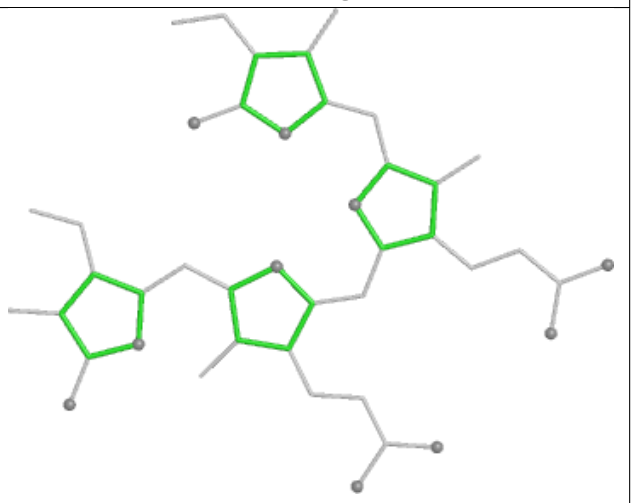
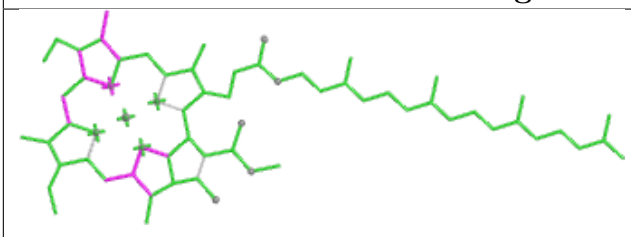


Rings

Ligand CLA 7N 602



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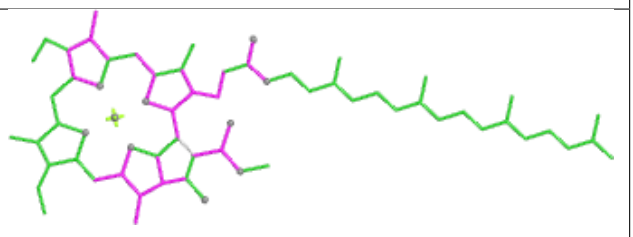
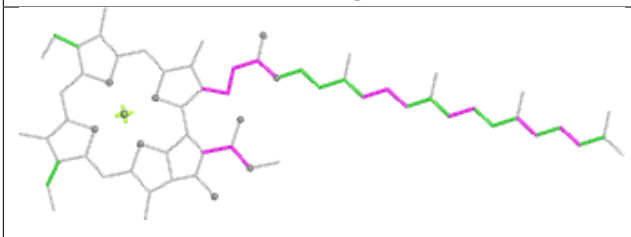


Bond angles



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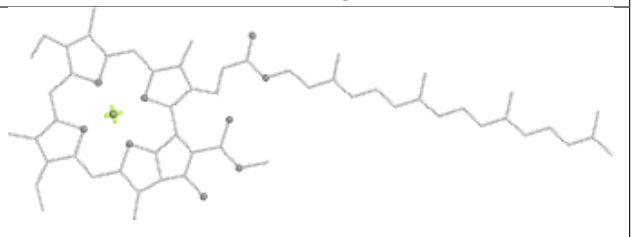
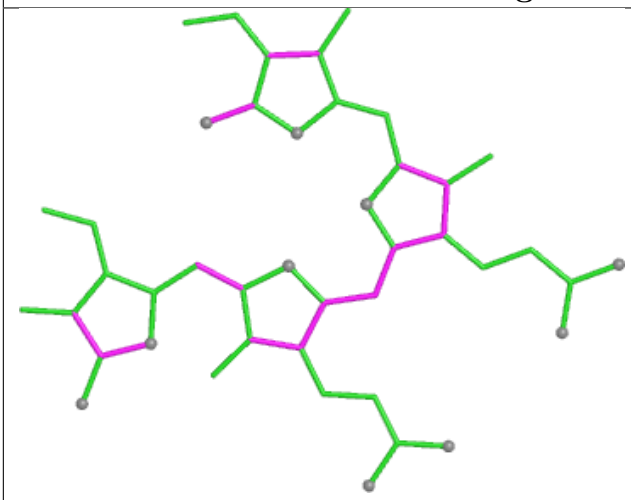


Rings

Ligand PEB w8 203



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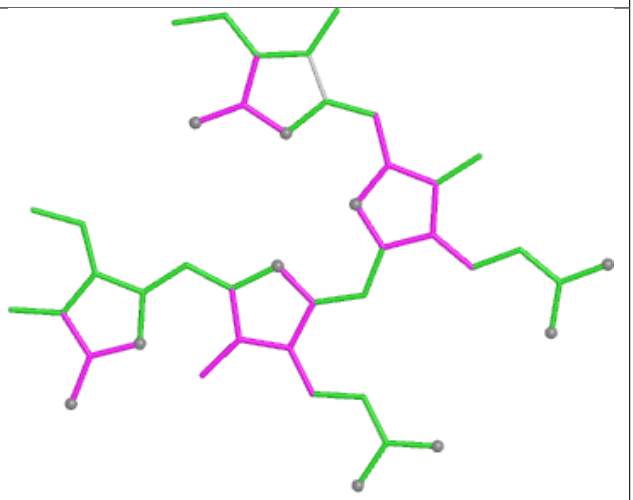
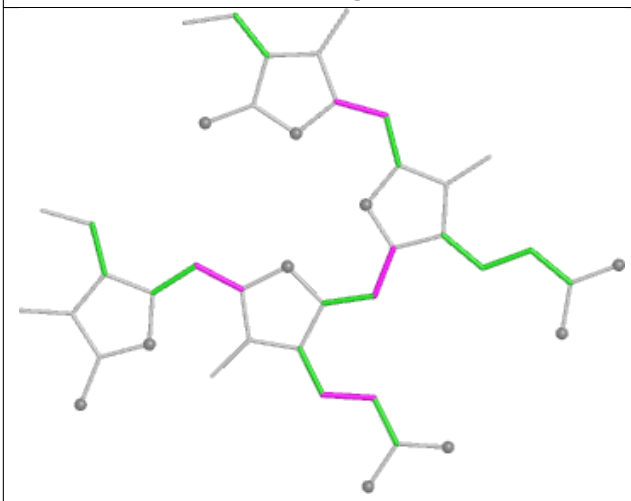


Bond angles



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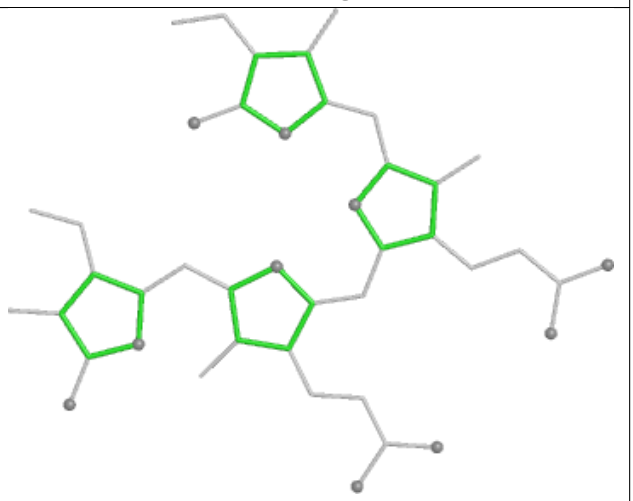
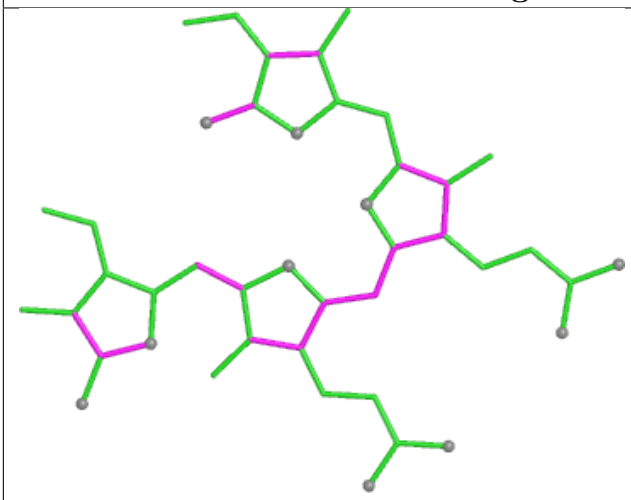


Rings

Ligand PEB PH 202



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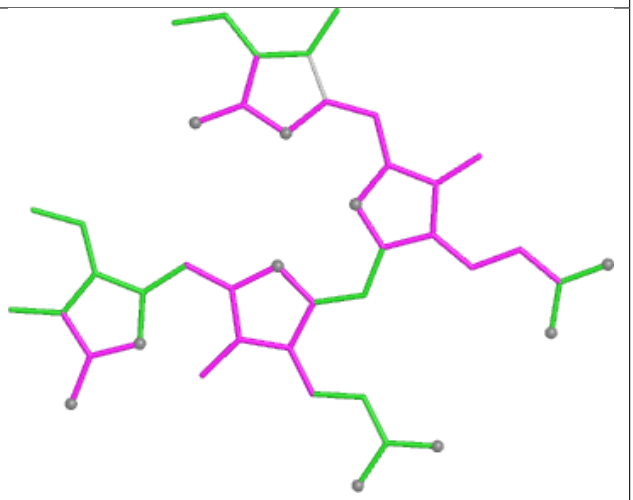
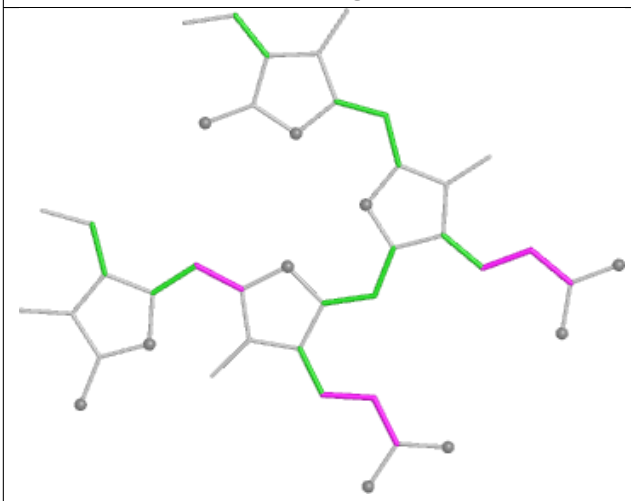


Bond angles



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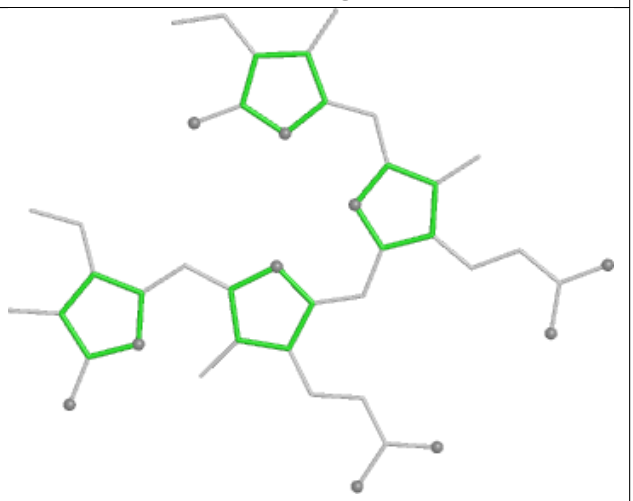
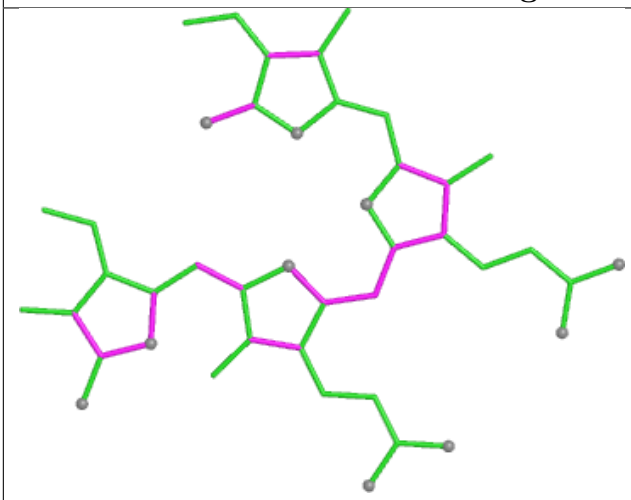


Rings

Ligand PEB a4 202



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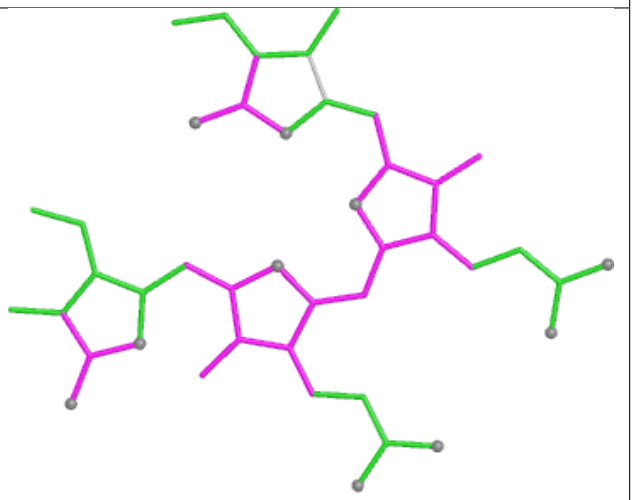
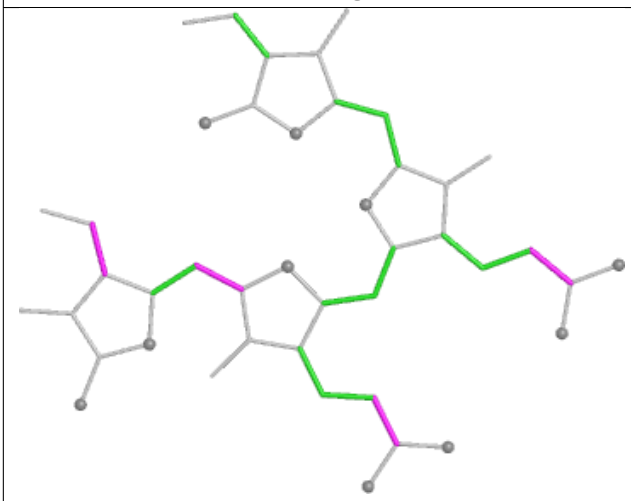


Bond angles



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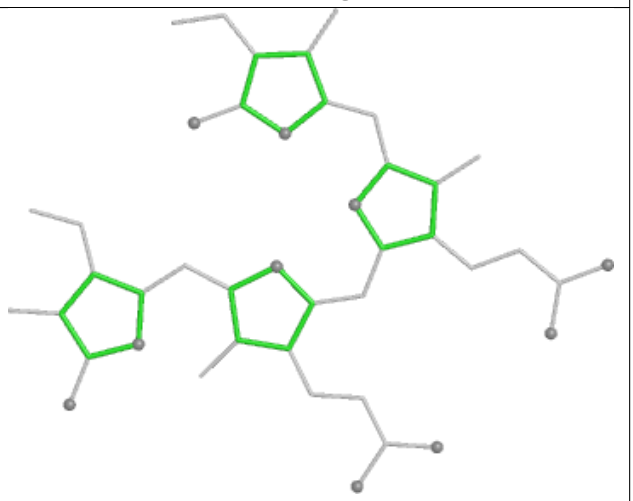
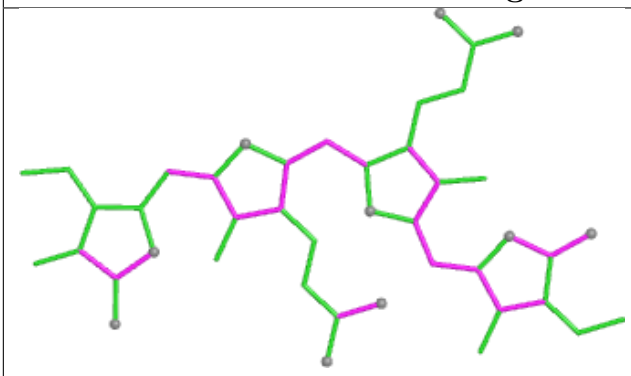
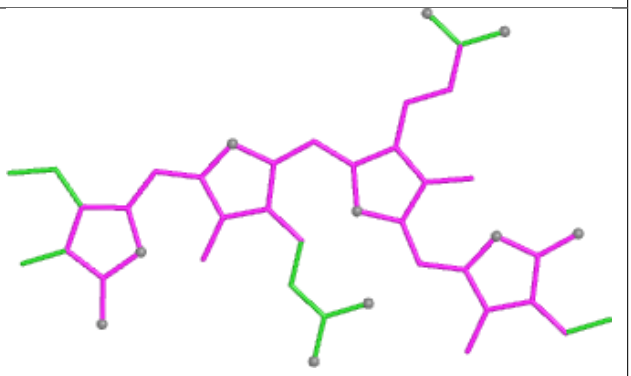


Rings

Ligand CYC L3 1001



Bond lengths



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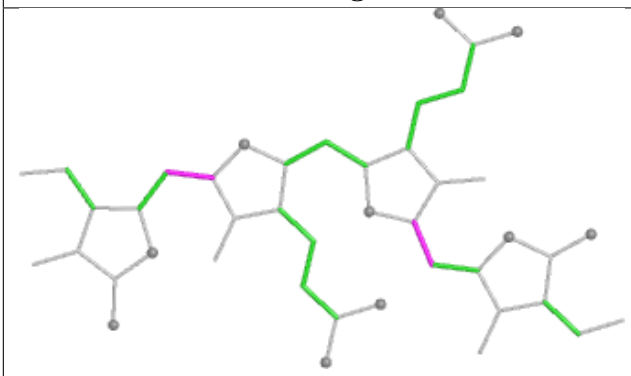

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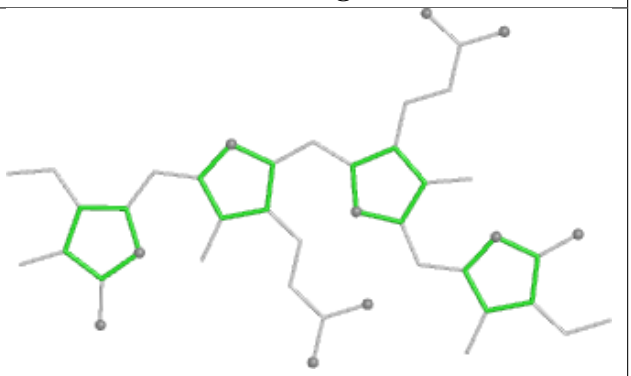
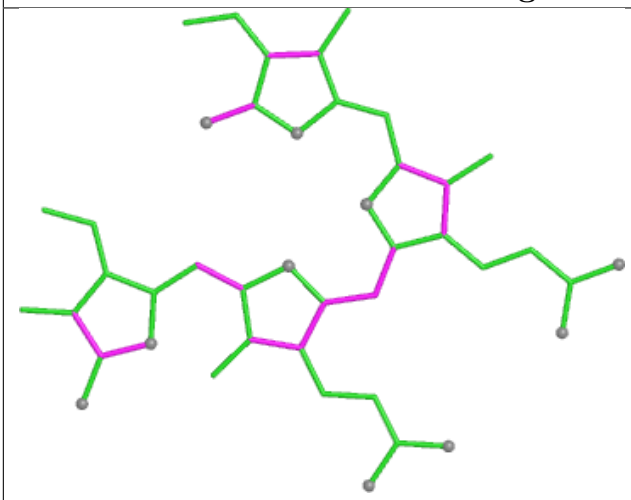


Rings

Ligand PEB jK 201



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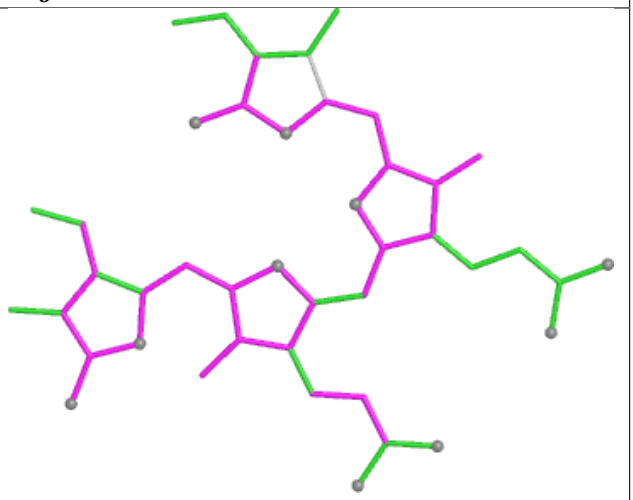

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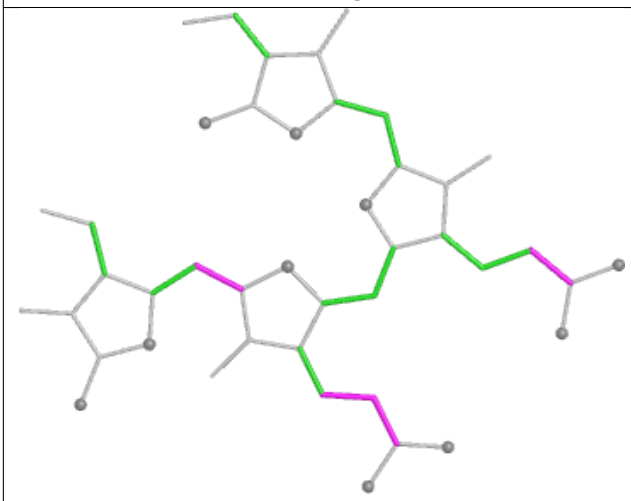

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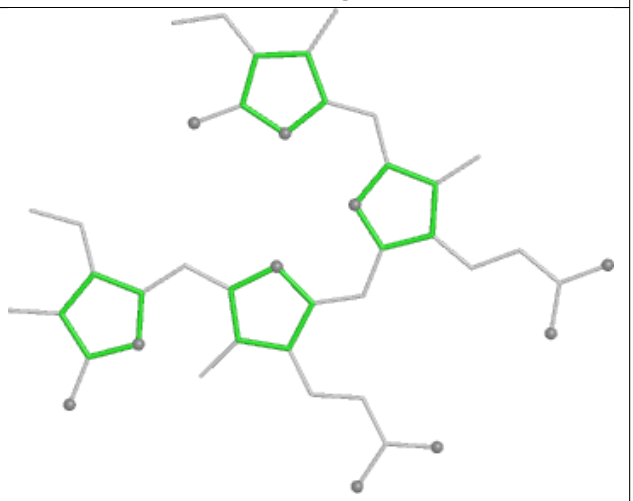
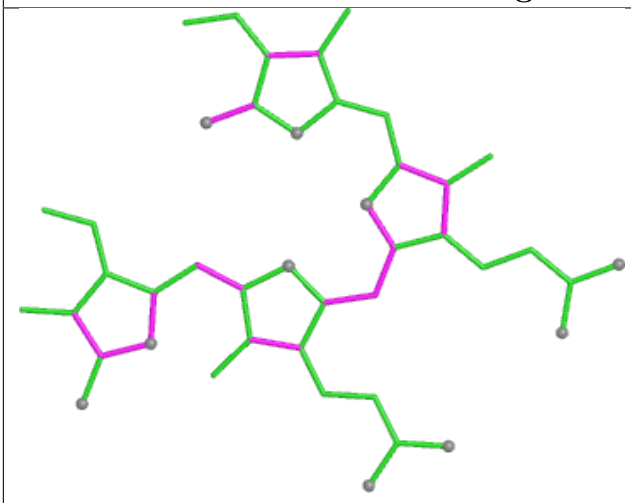


Rings

Ligand PEB Q7 202



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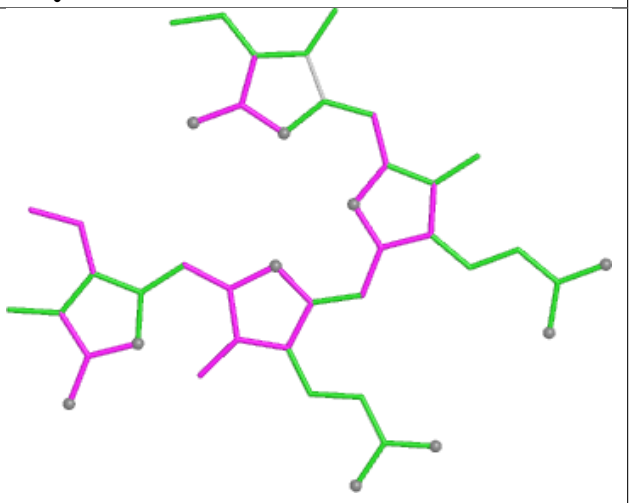

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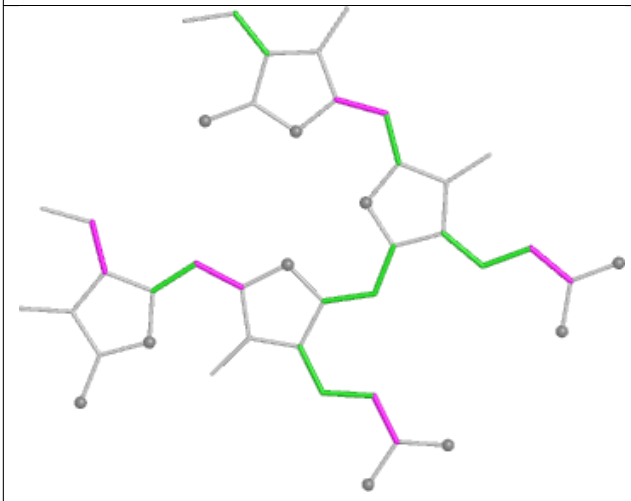

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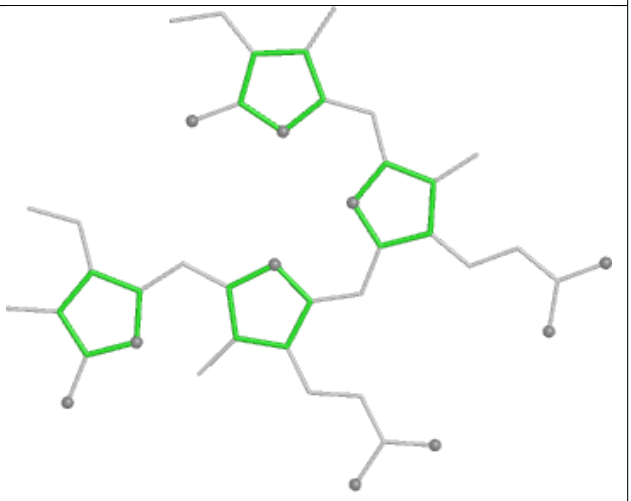
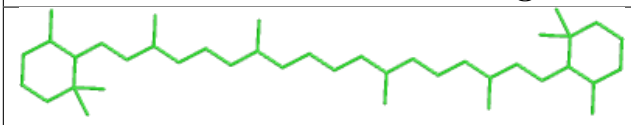


Rings

Ligand BCR h6 102



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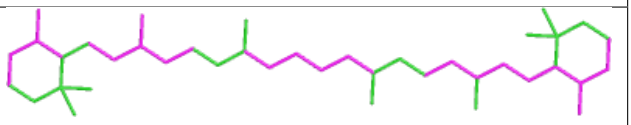

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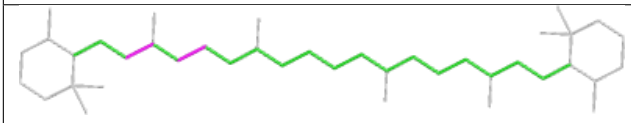

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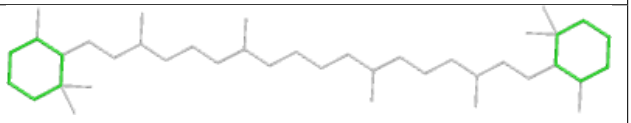
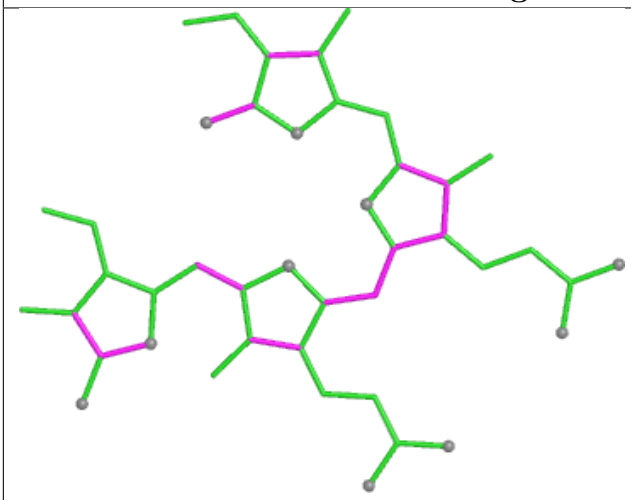


Rings

Ligand PEB QH 203



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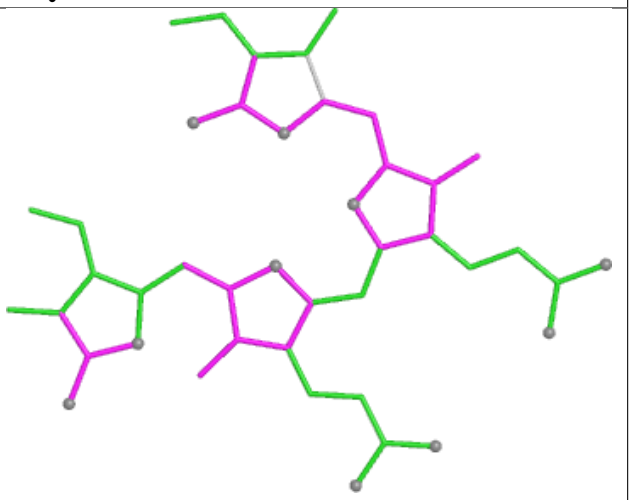

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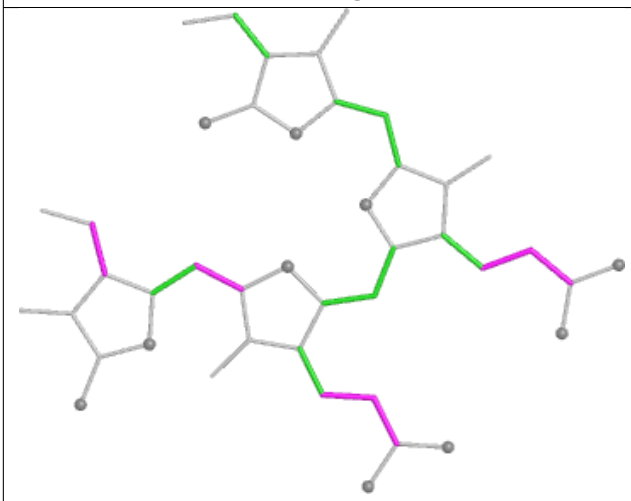

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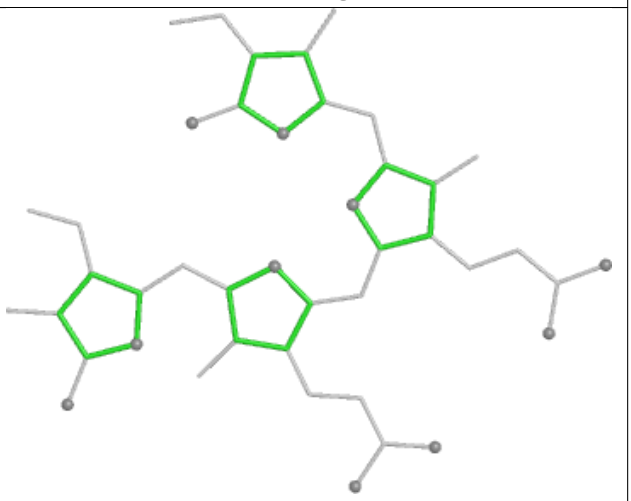

Rings

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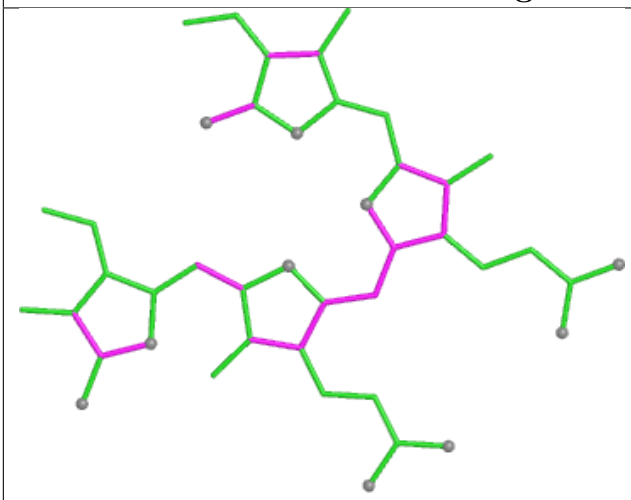

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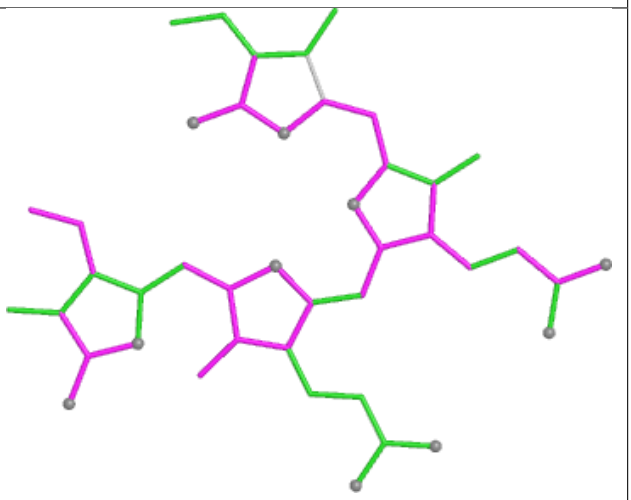

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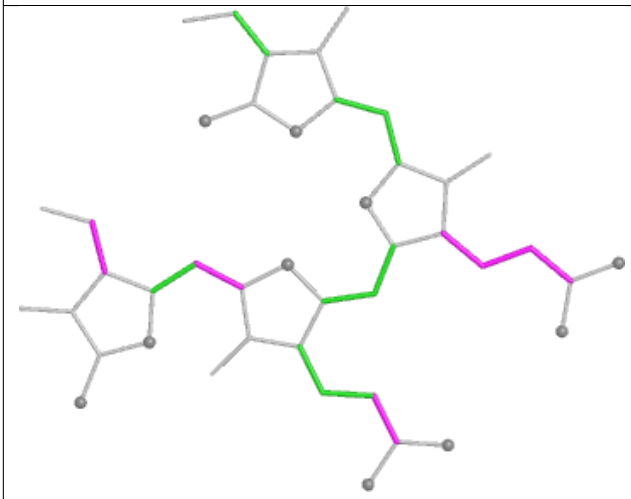

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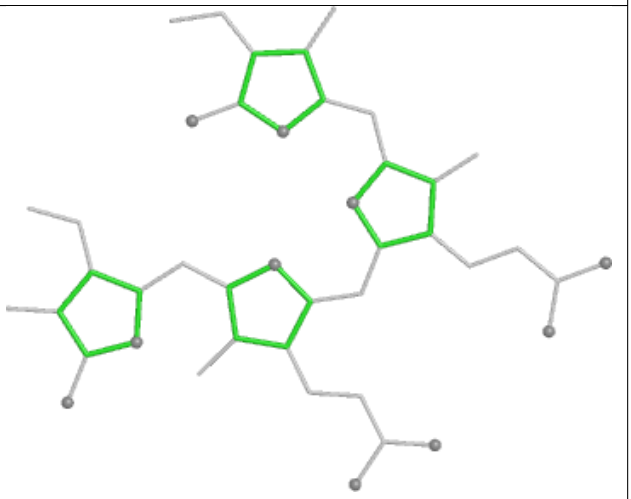
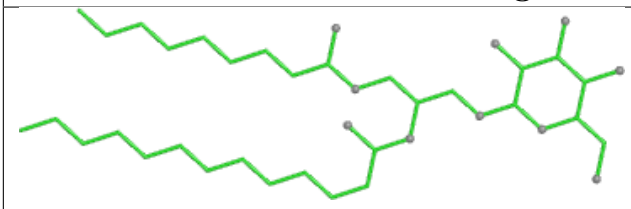


Rings

Ligand LMG b6 623



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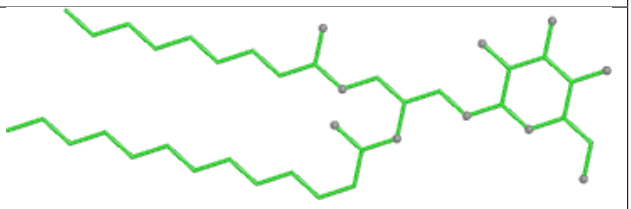
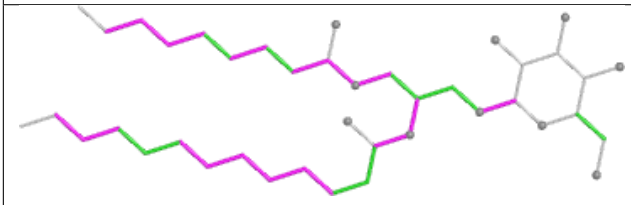


Bond angles



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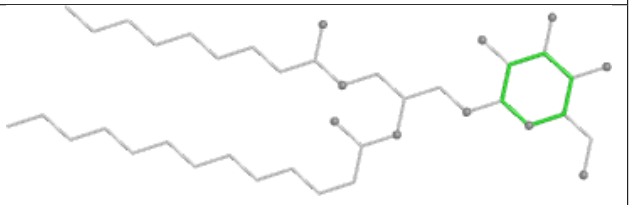
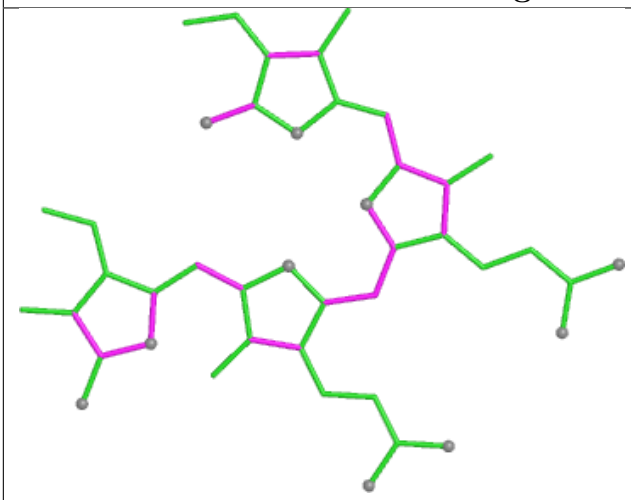


Rings

Ligand PEB BF 202



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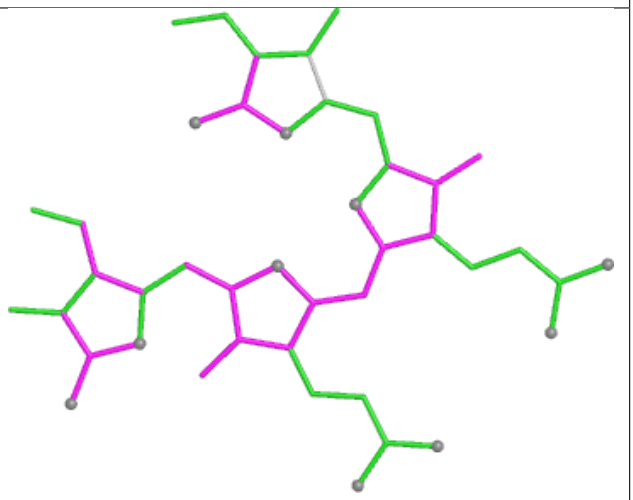

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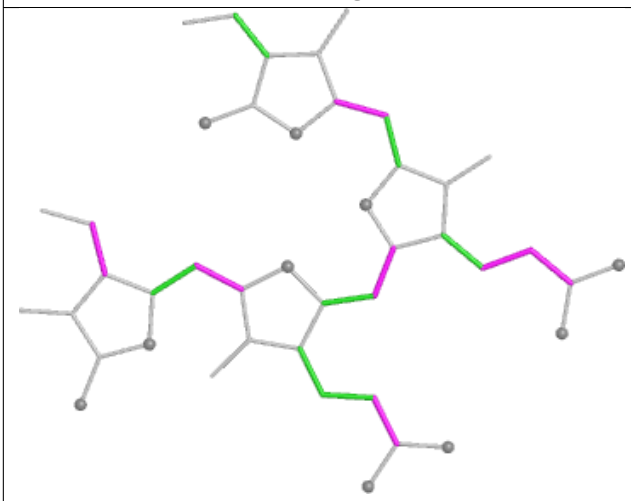

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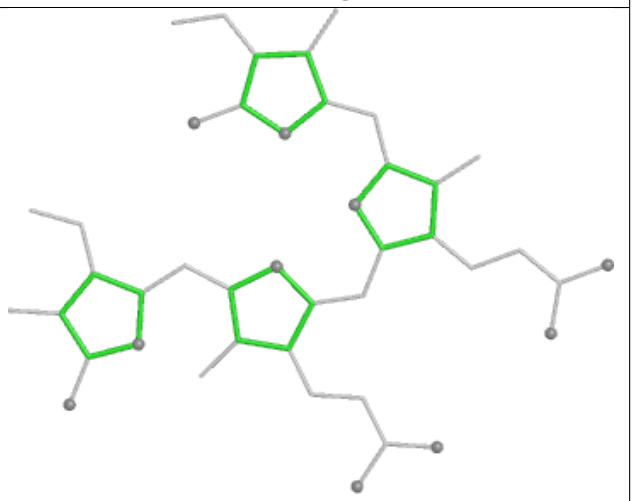
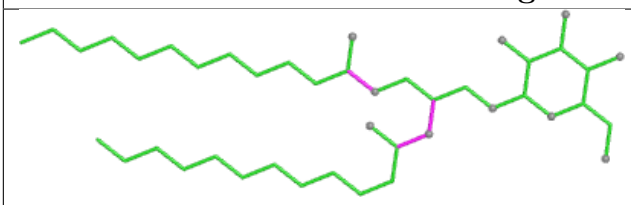


Rings

Ligand LMG j6 101



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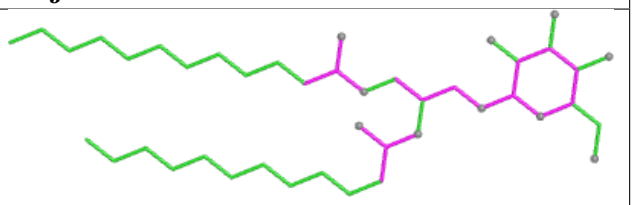

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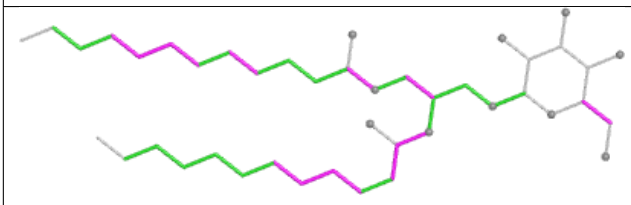

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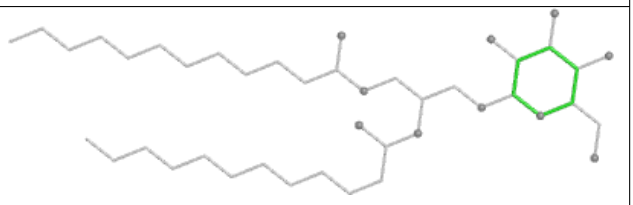
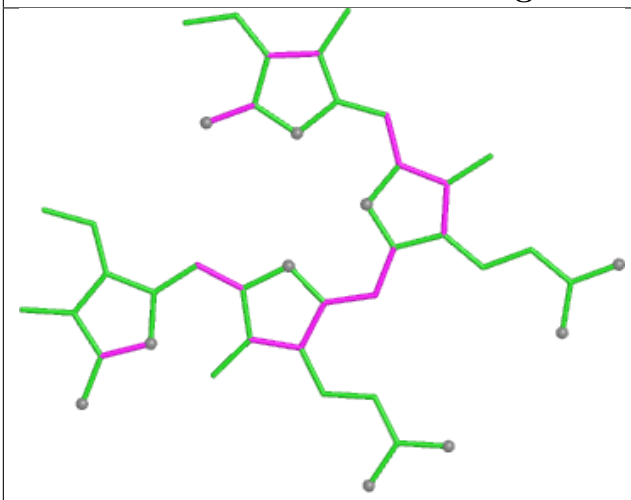


Rings

Ligand PEB yC 202



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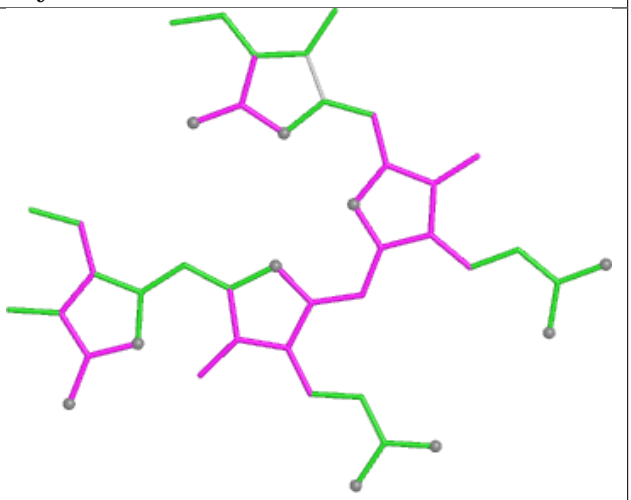

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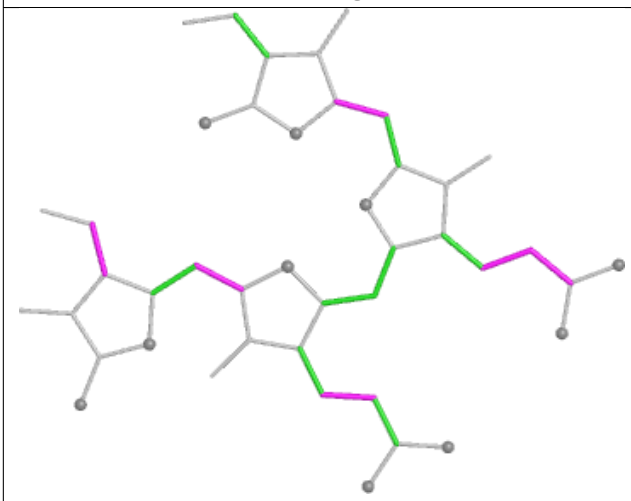

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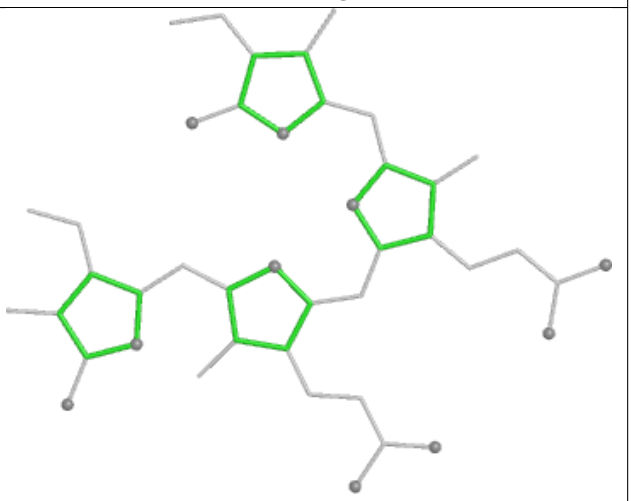
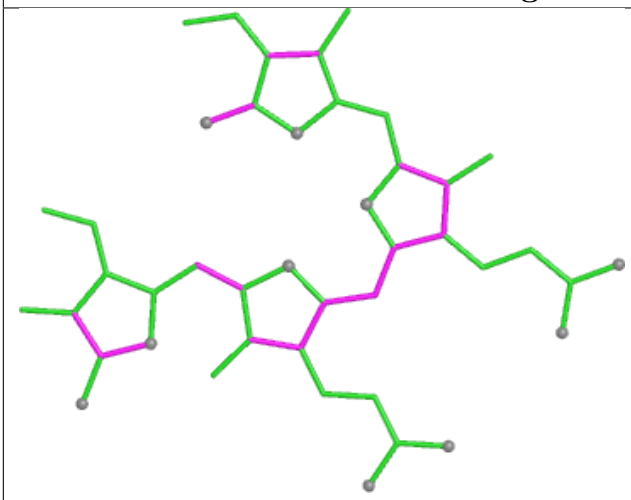


Rings

Ligand PEB iE 202



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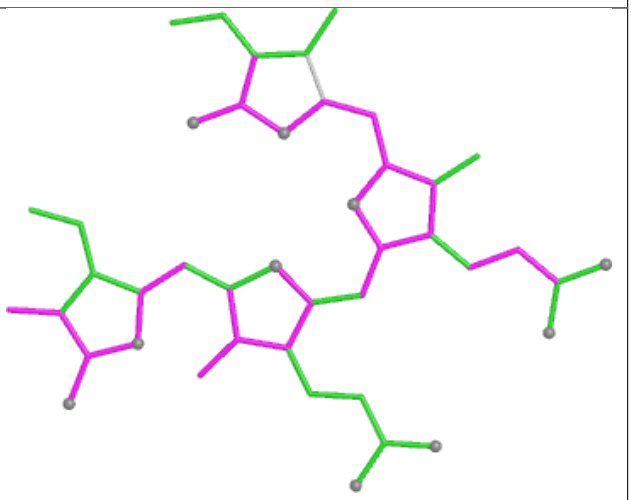

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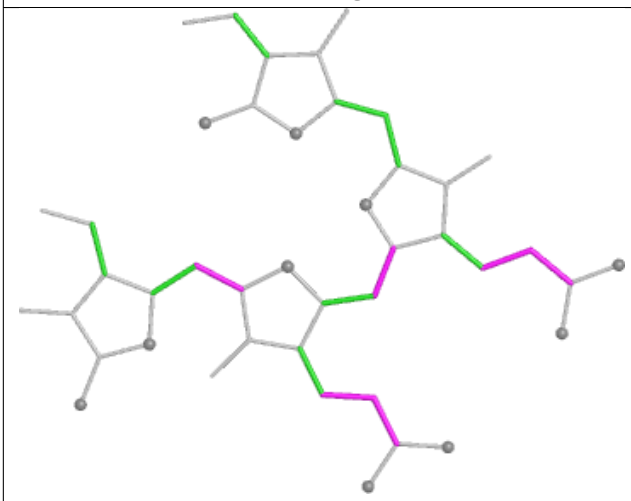

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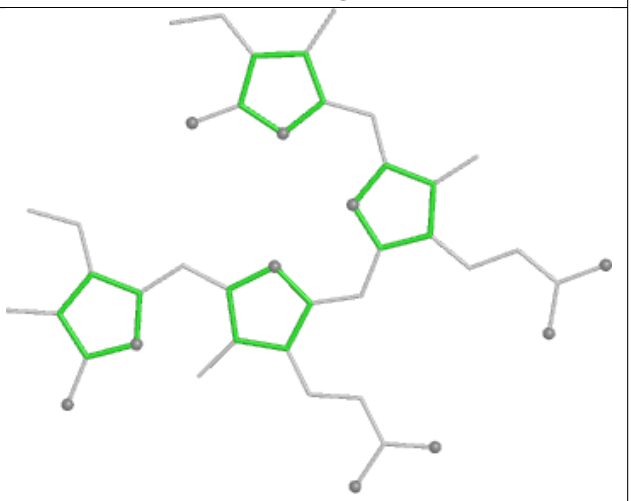
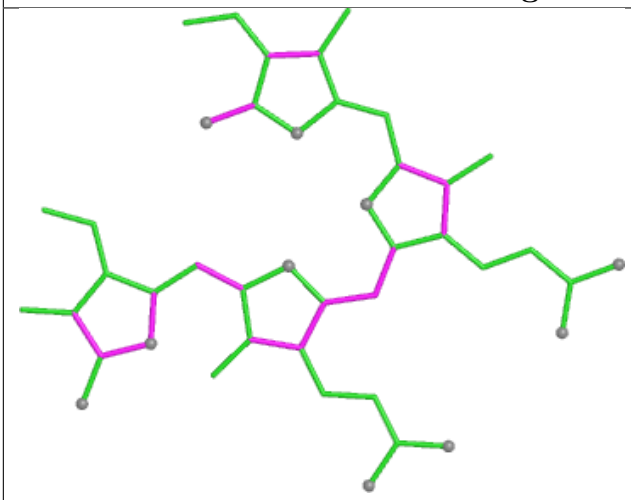


Rings

Ligand PEB iF 203



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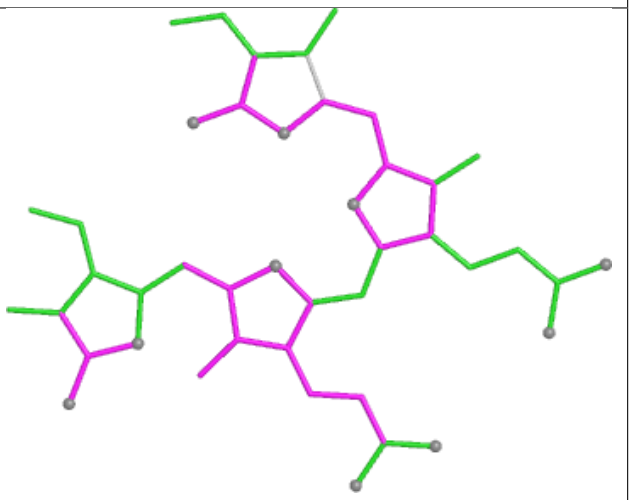

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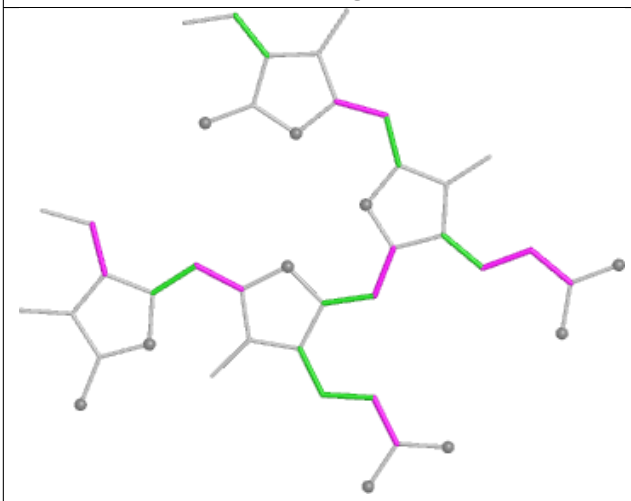

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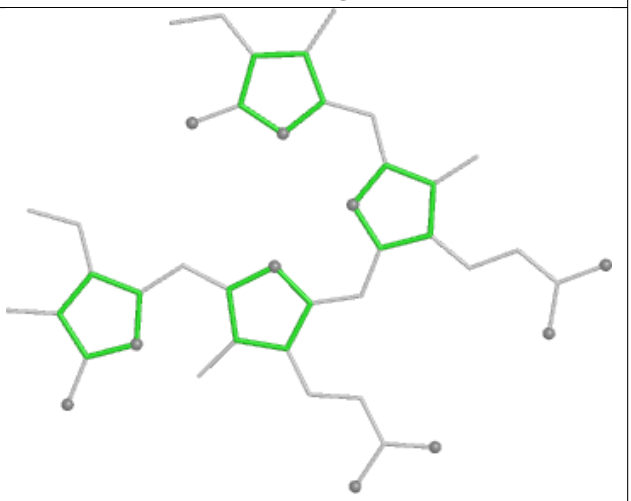
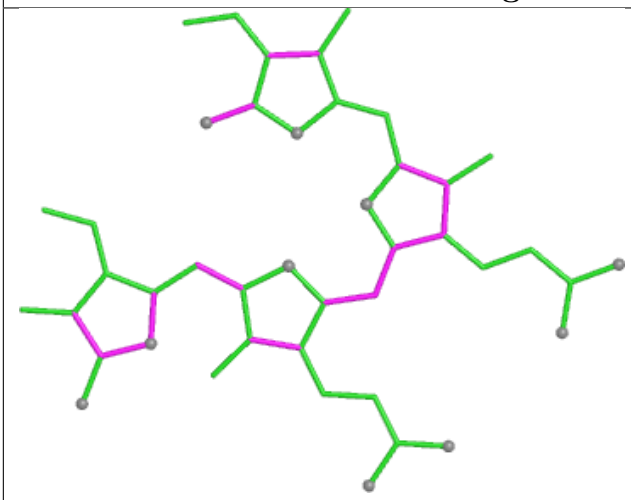


Rings

Ligand PEB WM 202



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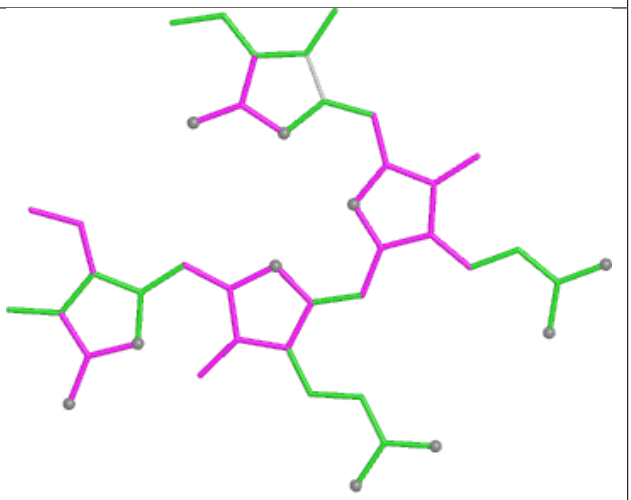

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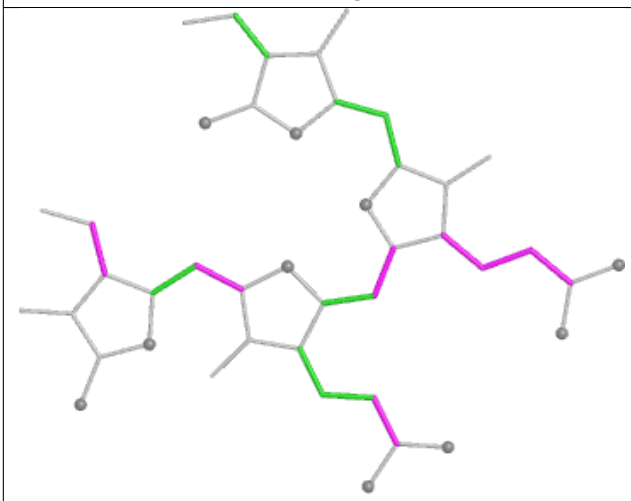

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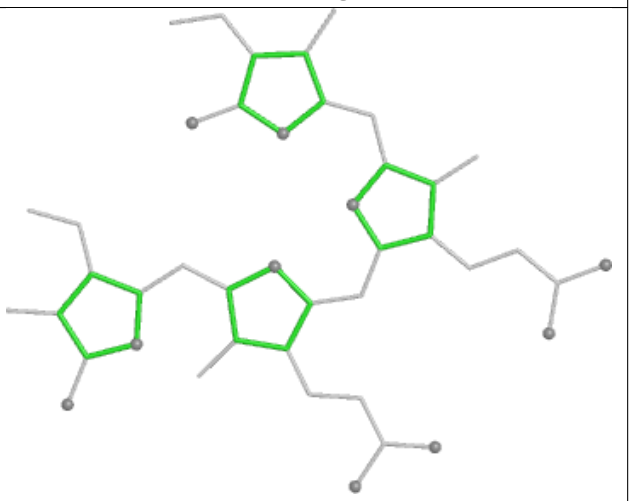
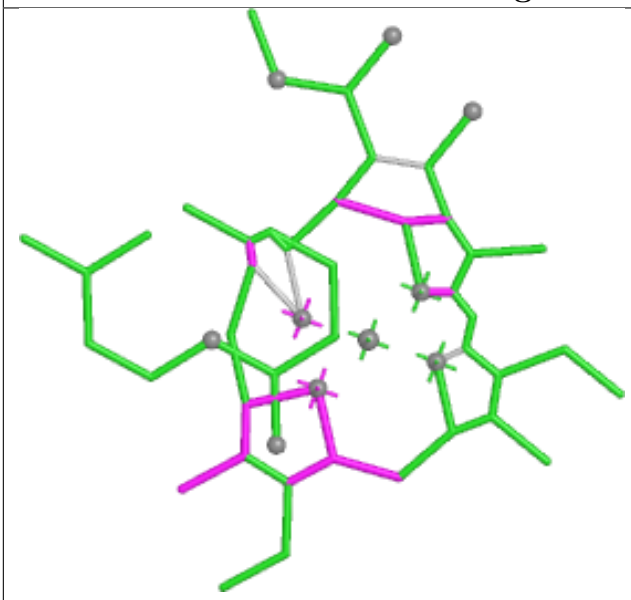


Rings

Ligand CLA 6N 608



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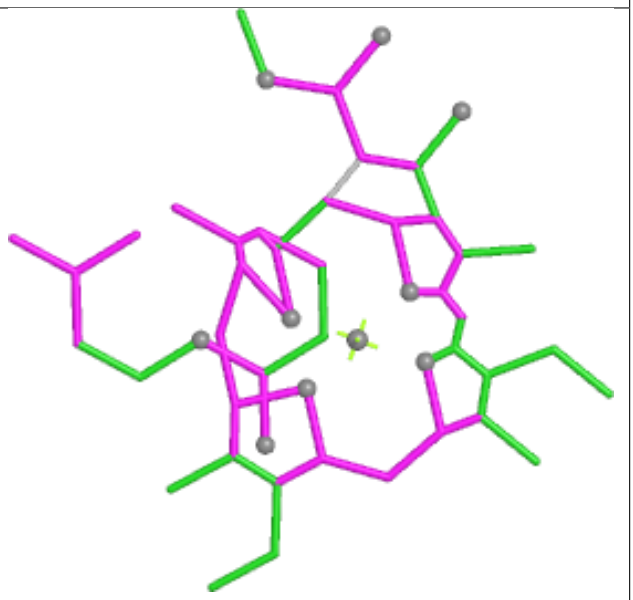
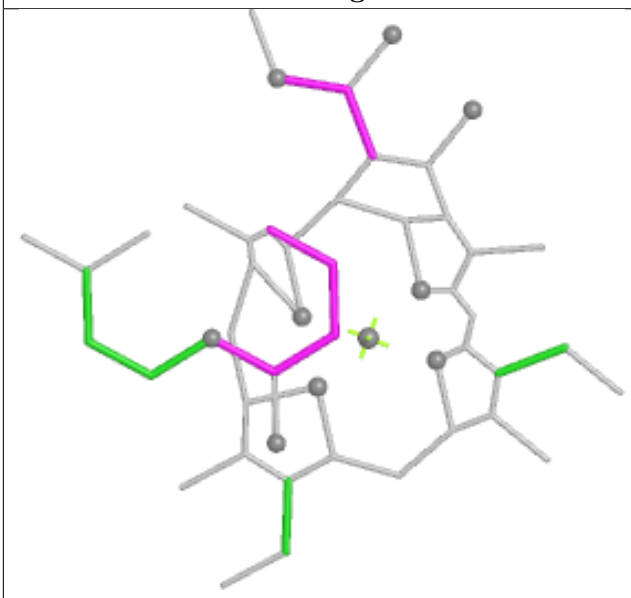


Bond angles



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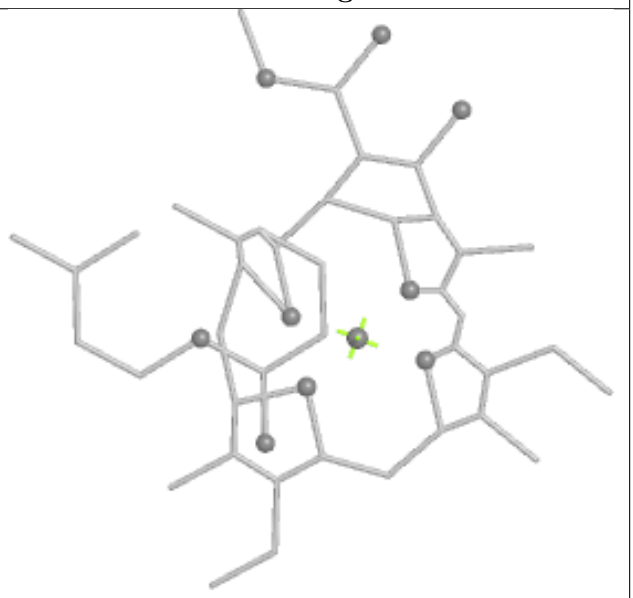

Rings

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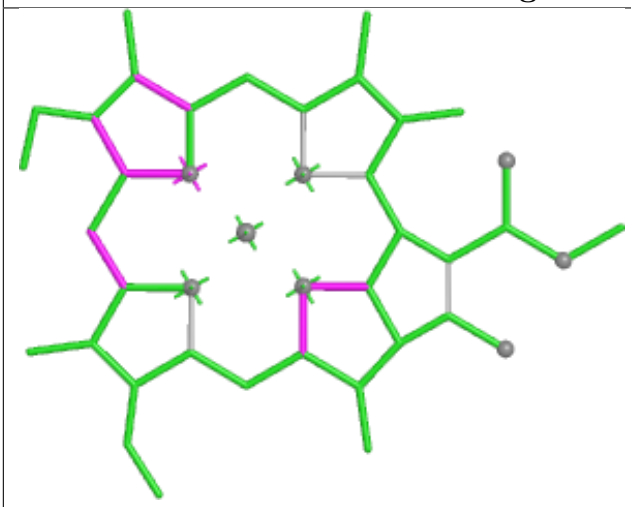

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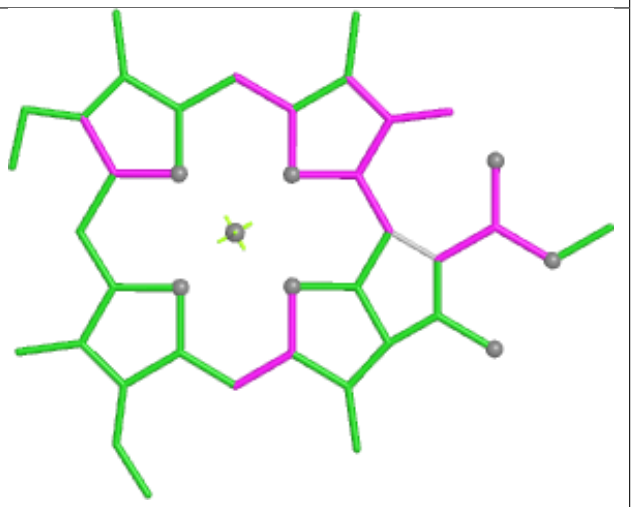
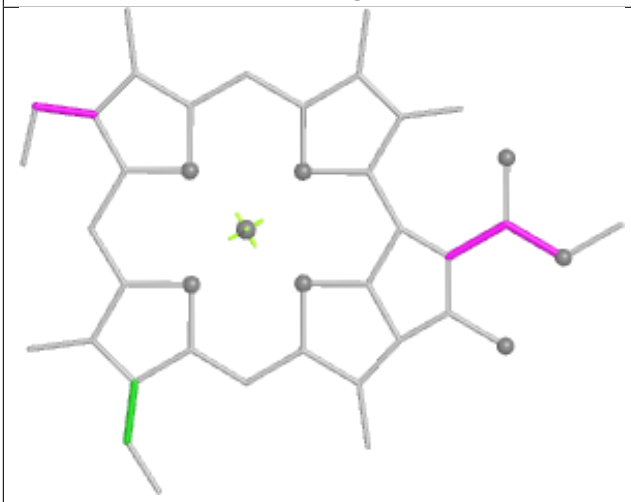
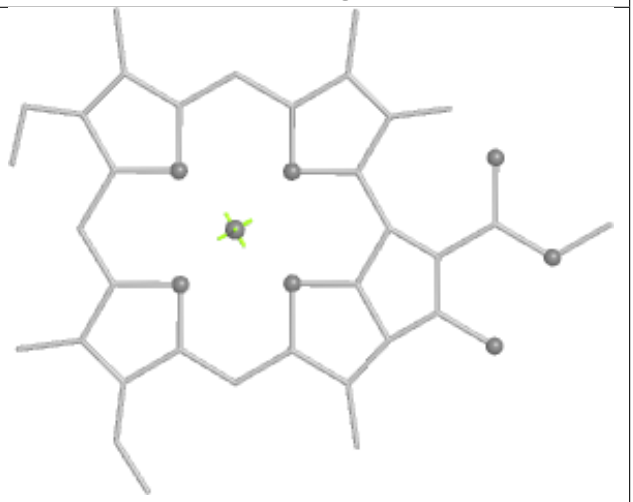


Bond angles

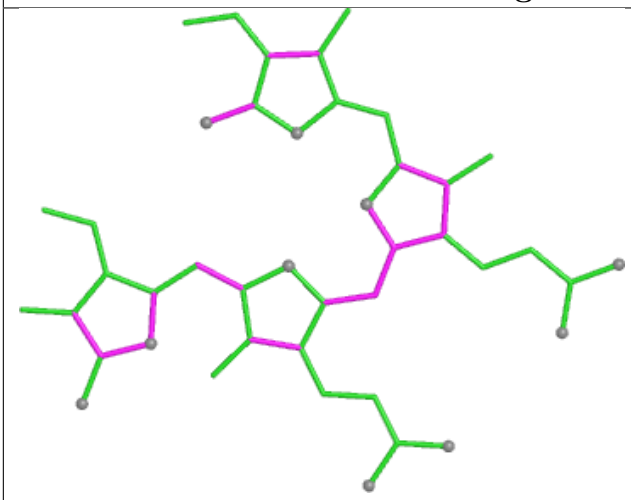


Torsions



Rings

Ligand PEB YJ 203



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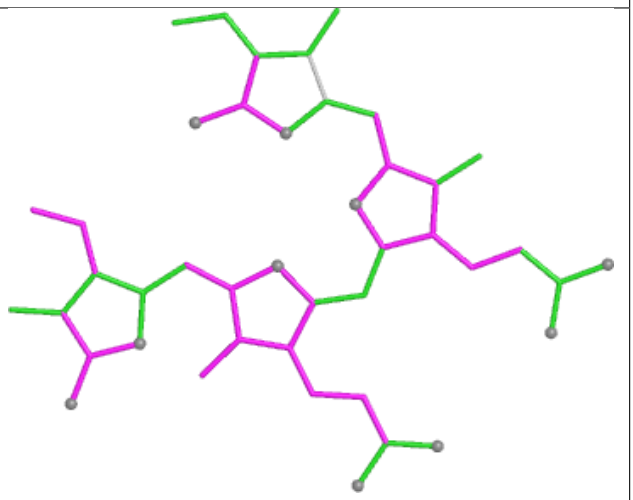
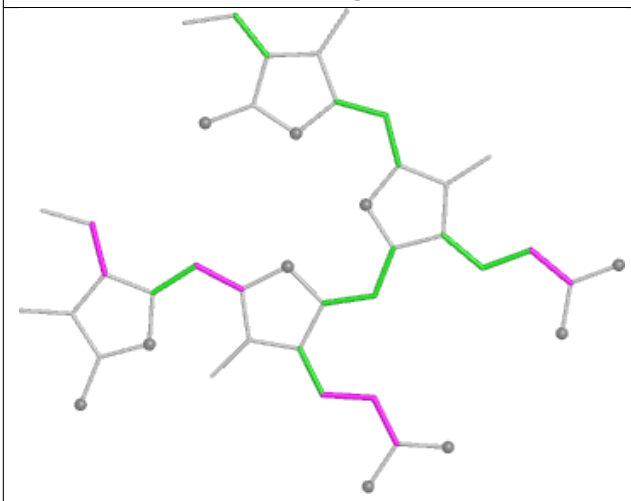


Bond angles



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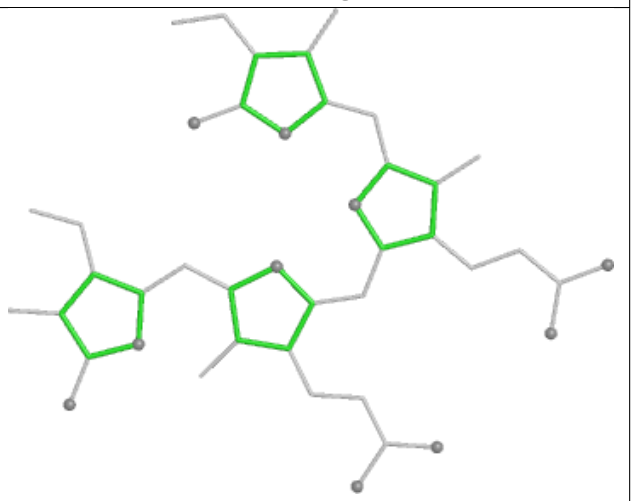
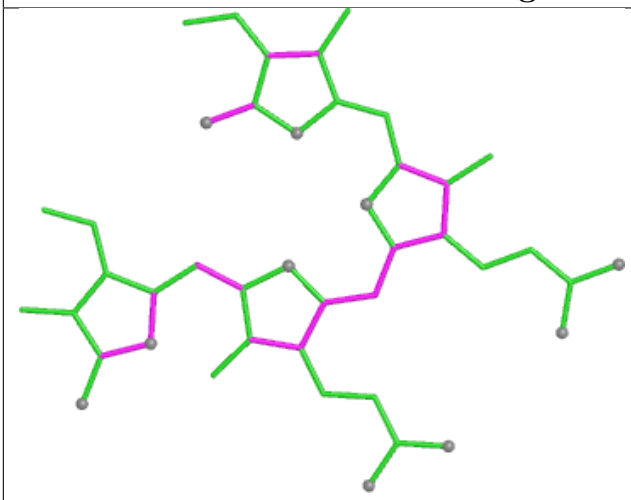


Rings

Ligand PEB b4 202



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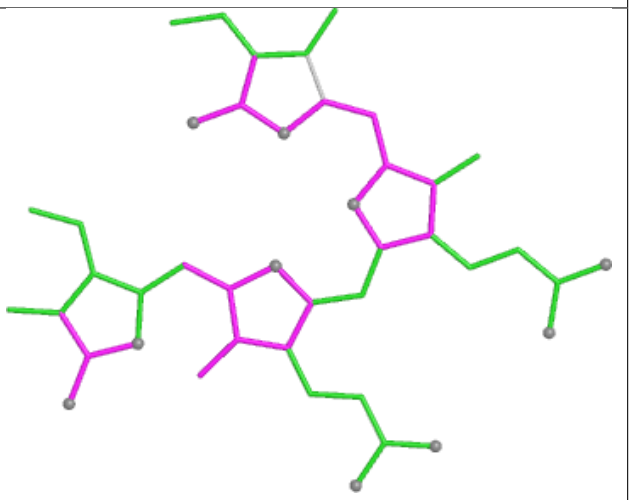

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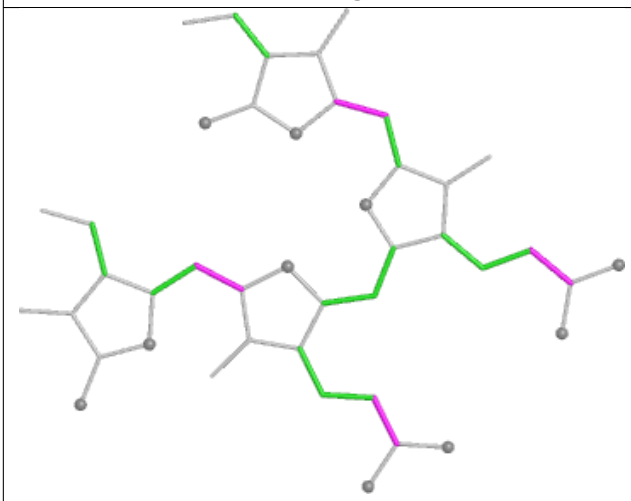

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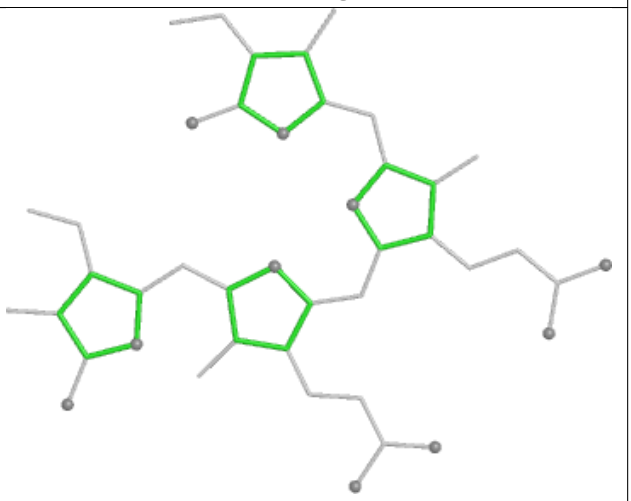
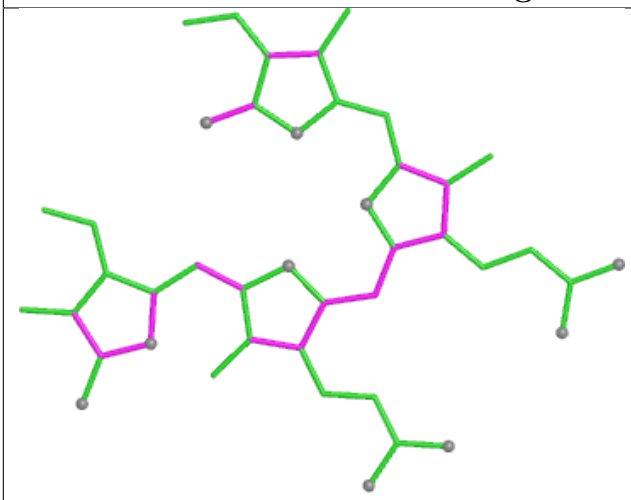


Rings

Ligand PEB H9 203



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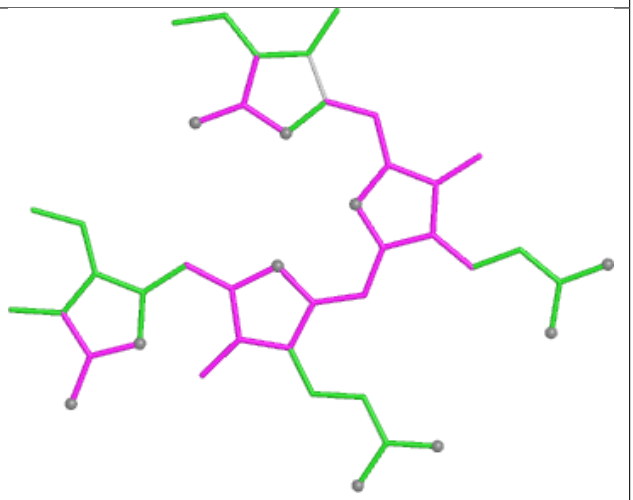

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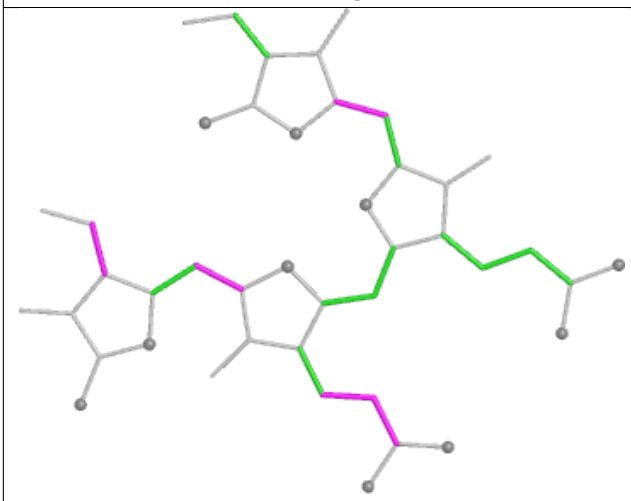

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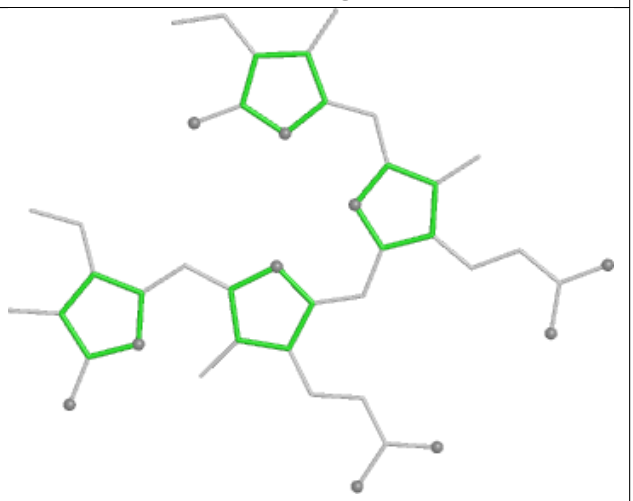
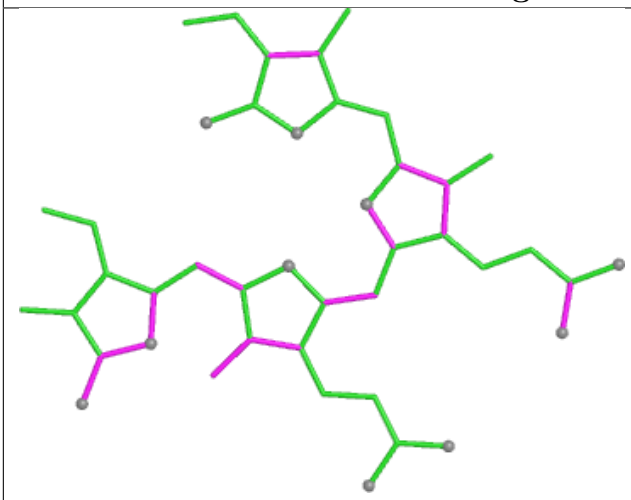


Rings

Ligand PEB GF 202



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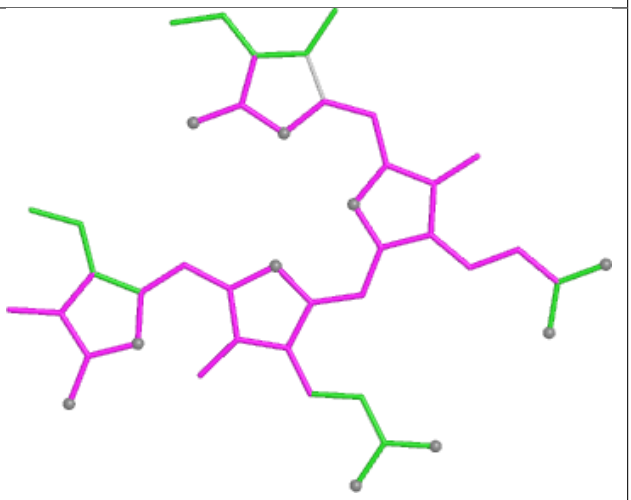

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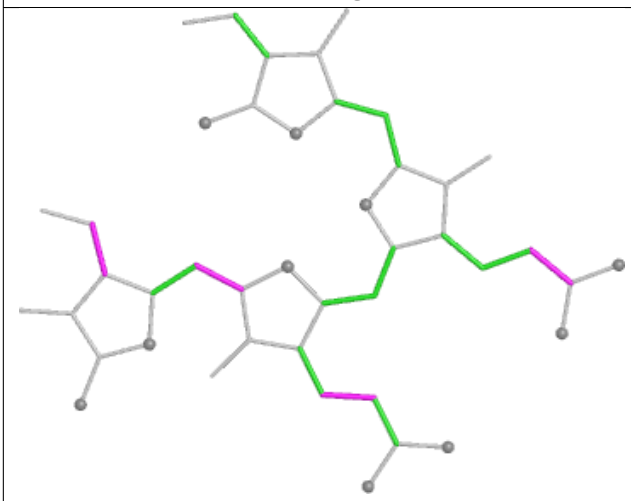

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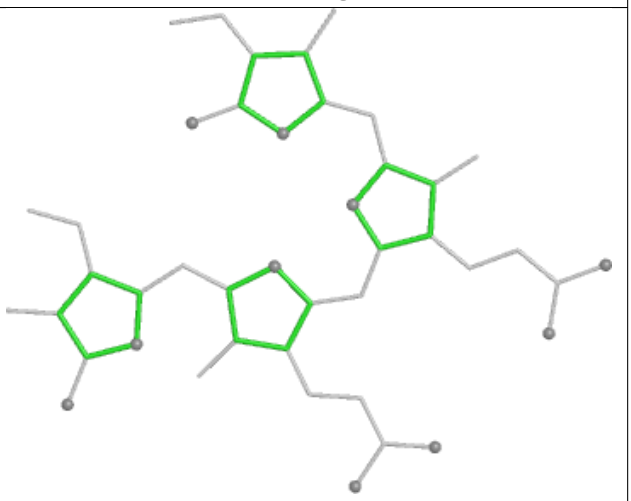
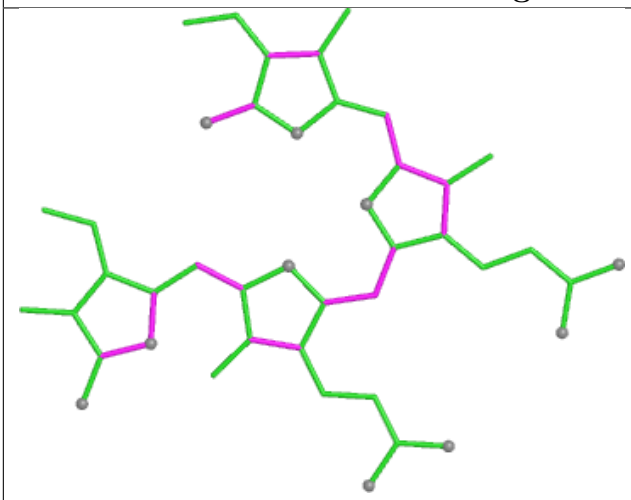


Rings

Ligand PEB YF 201



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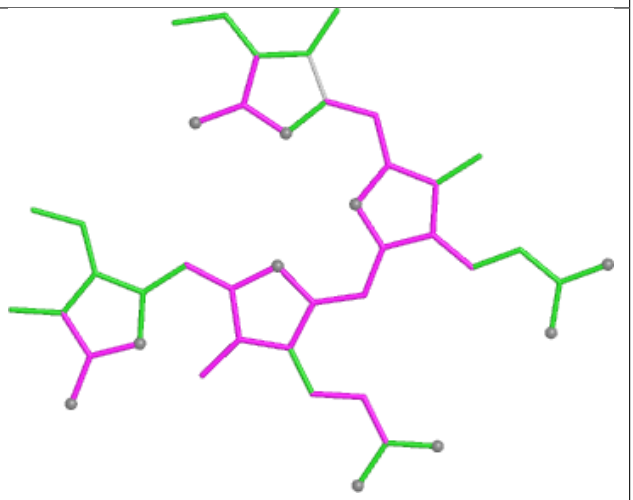

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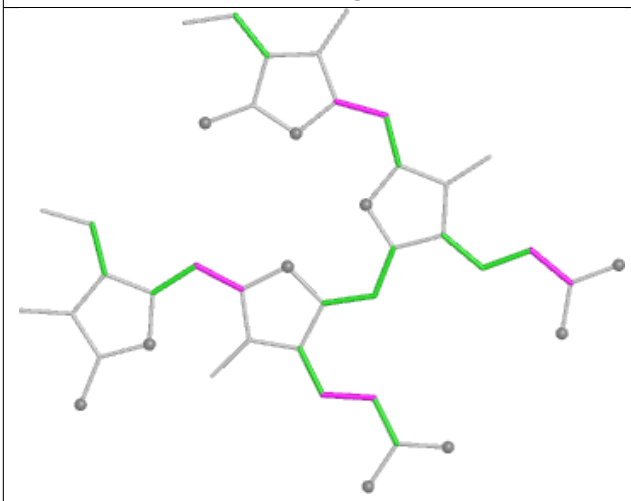

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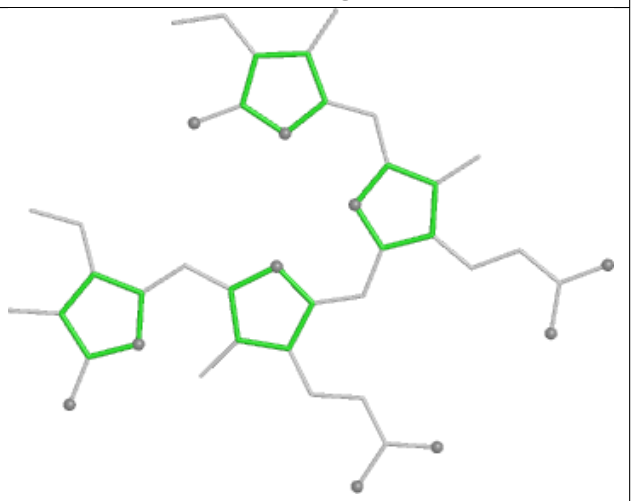
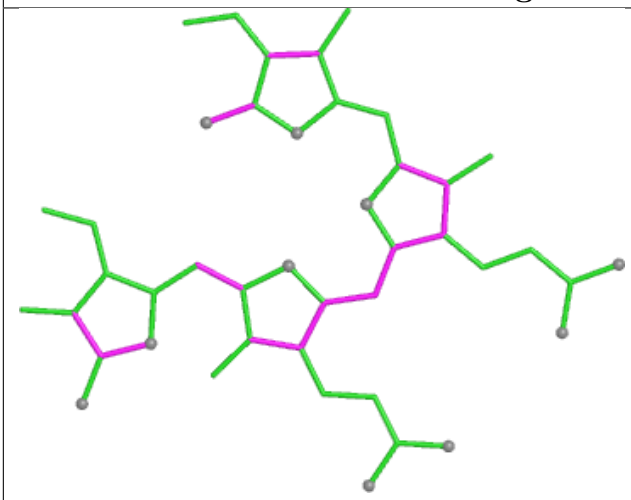


Rings

Ligand PEB V1 202



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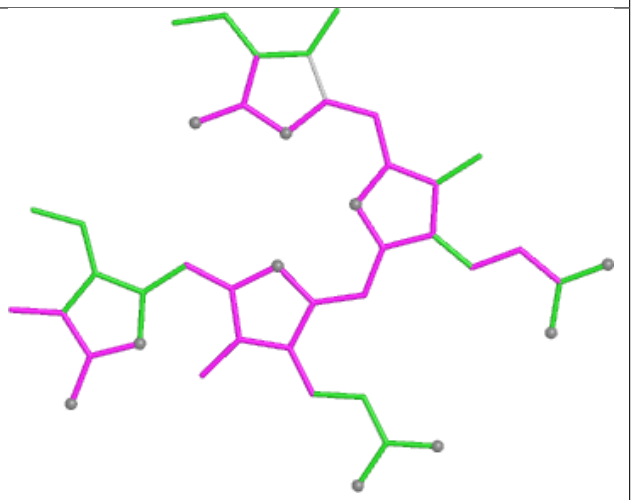

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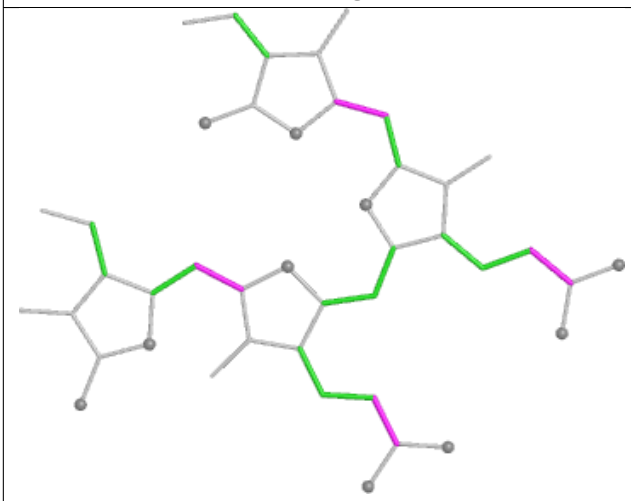

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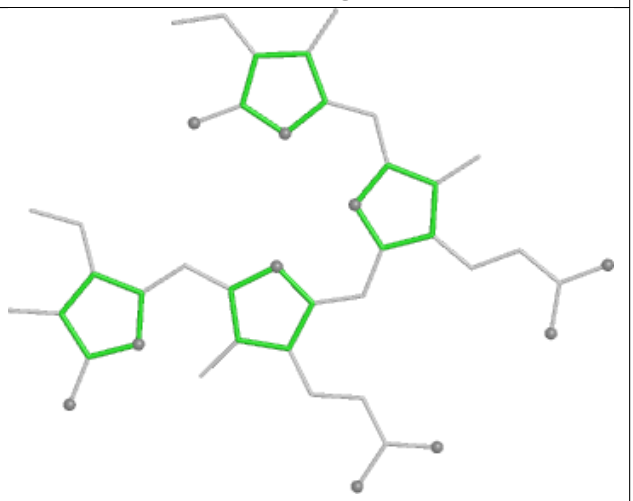
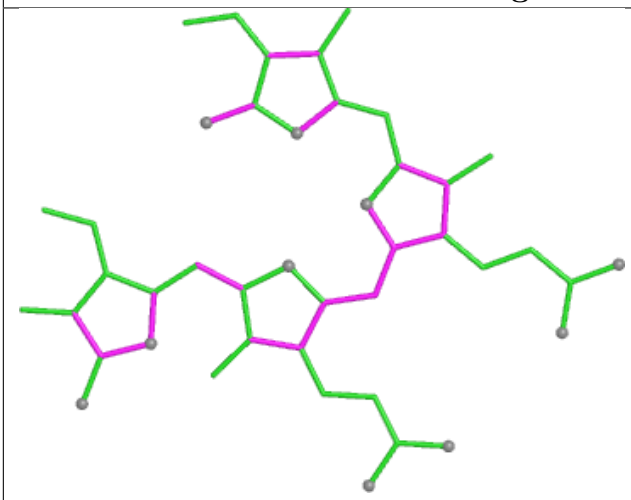


Rings

Ligand PEB TH 201



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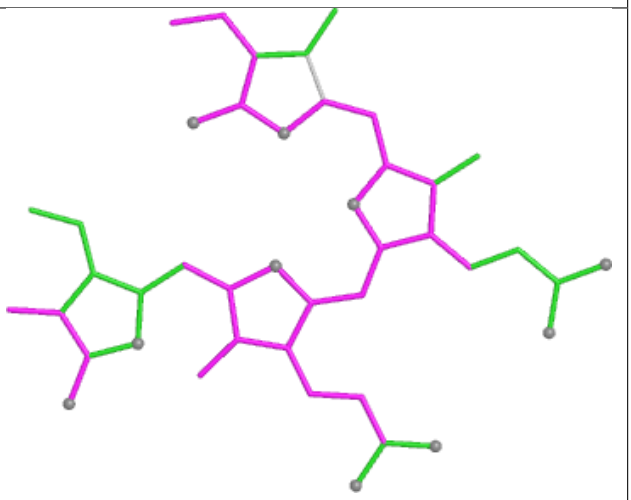

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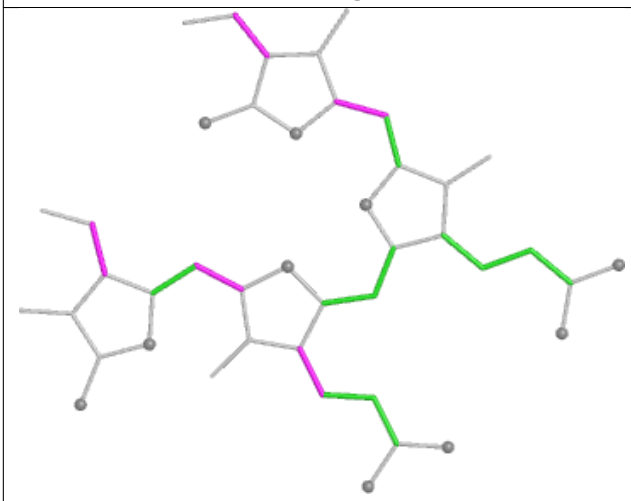

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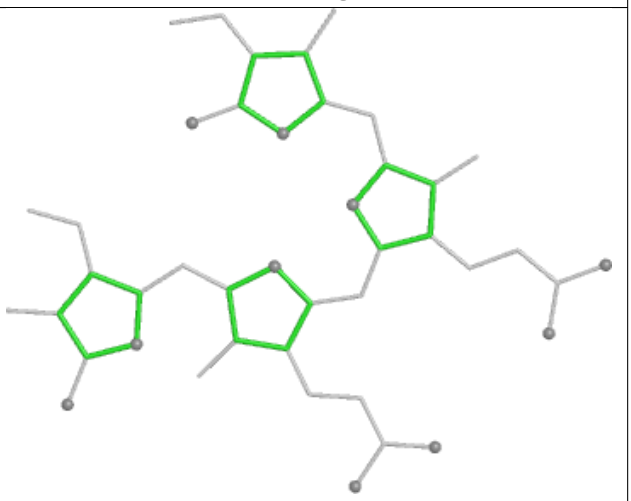

Rings

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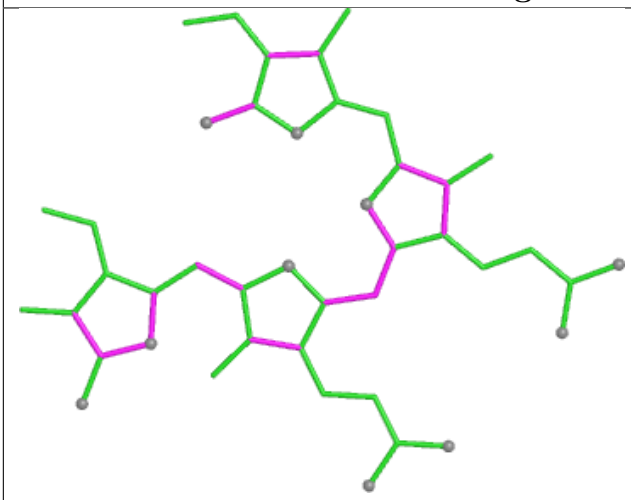

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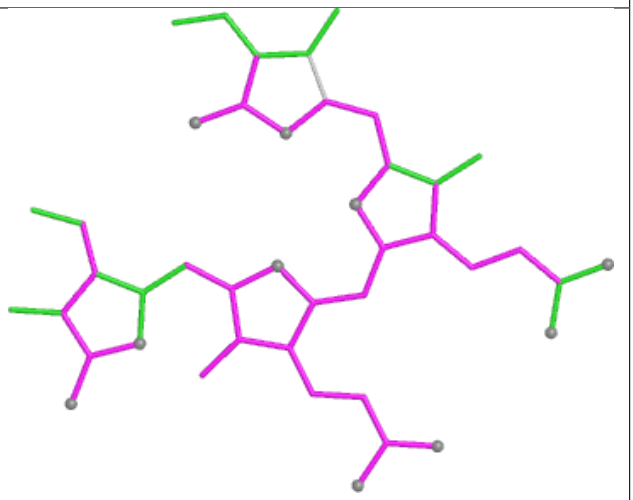

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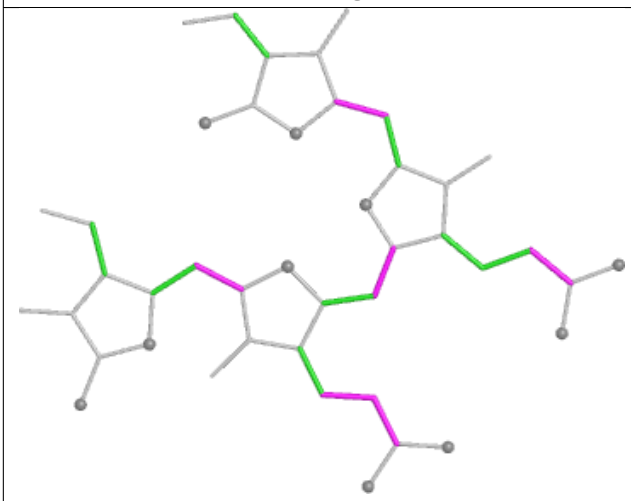

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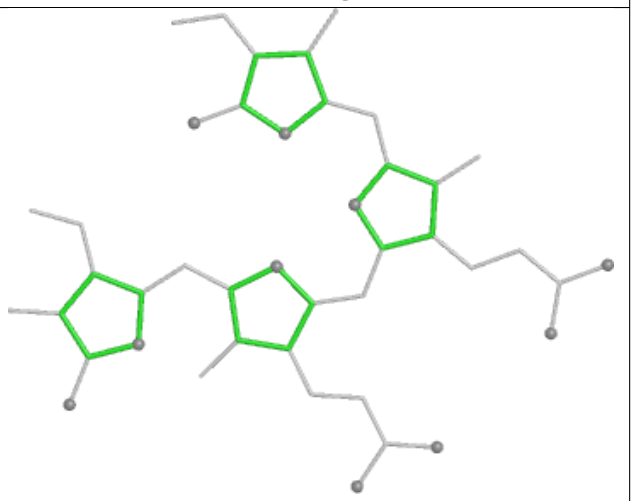
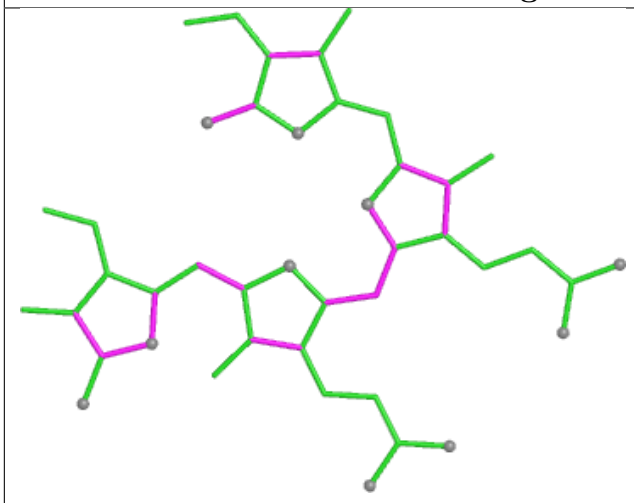


Rings

Ligand PEB J5 201



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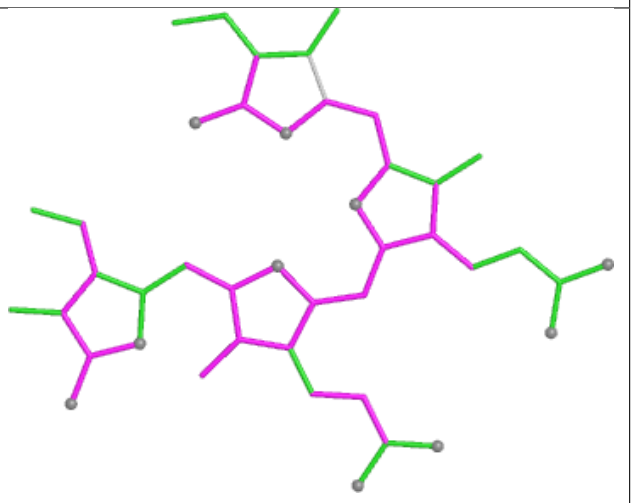

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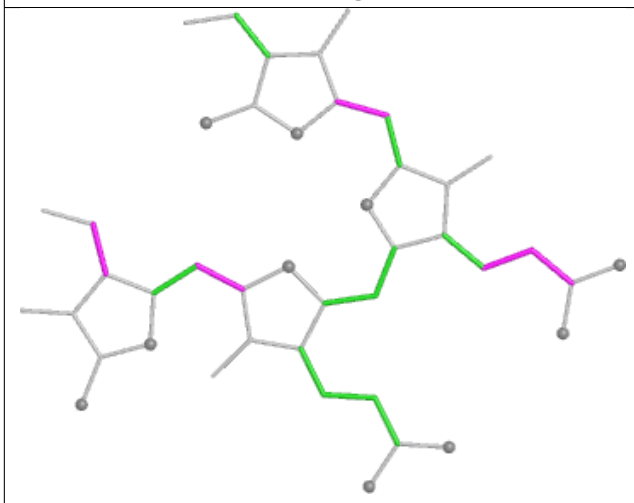

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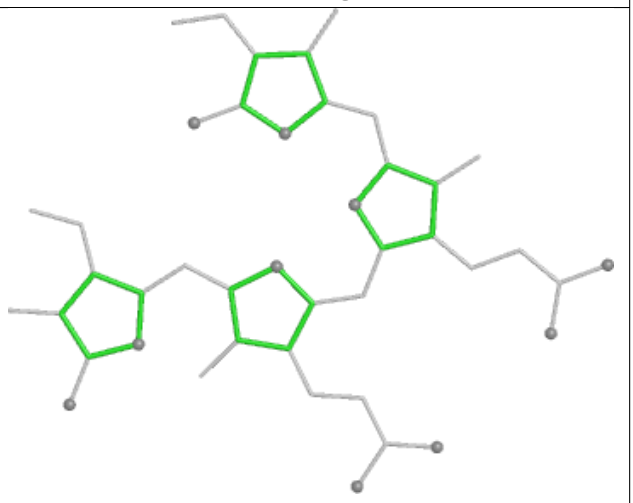
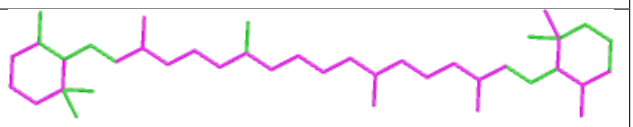


Rings

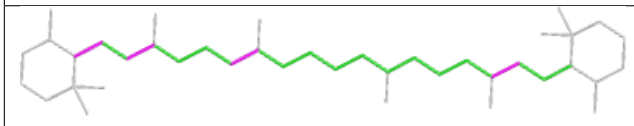
Ligand BCR AN 847



Bond lengths



Bond angles



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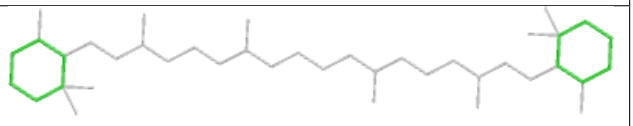
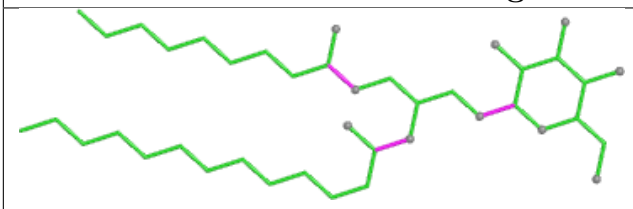


Rings

Ligand LMG mL 101



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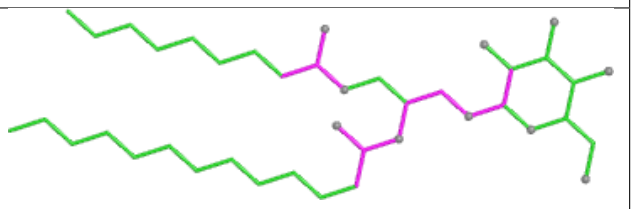
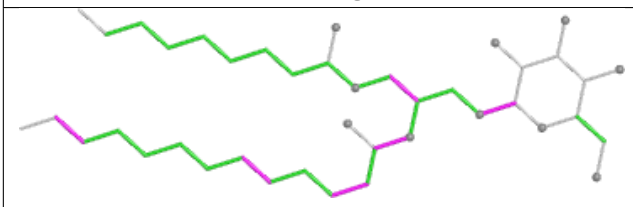


Bond angles



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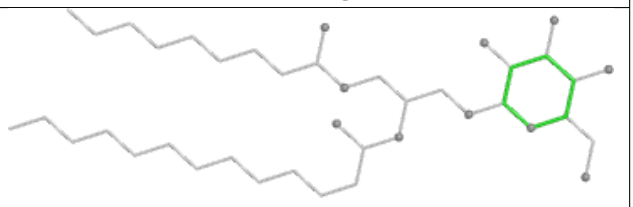
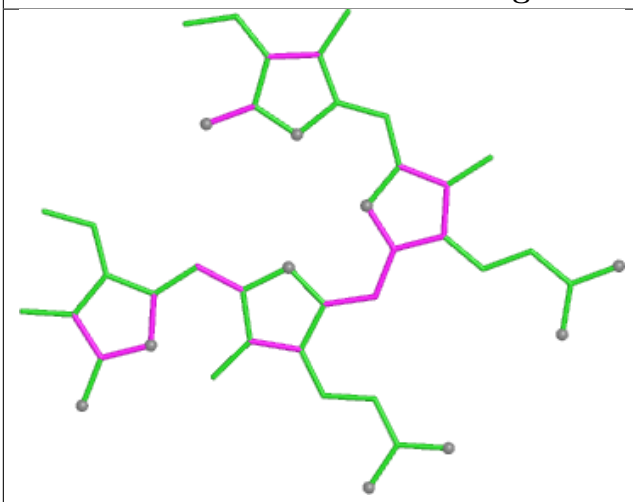


Rings

Ligand PEB RE 201



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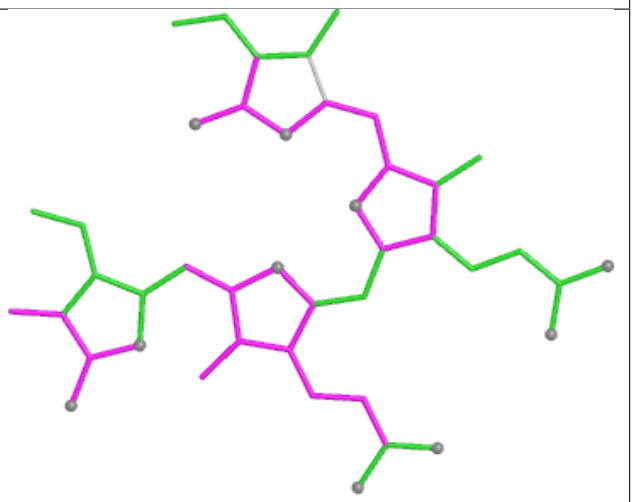
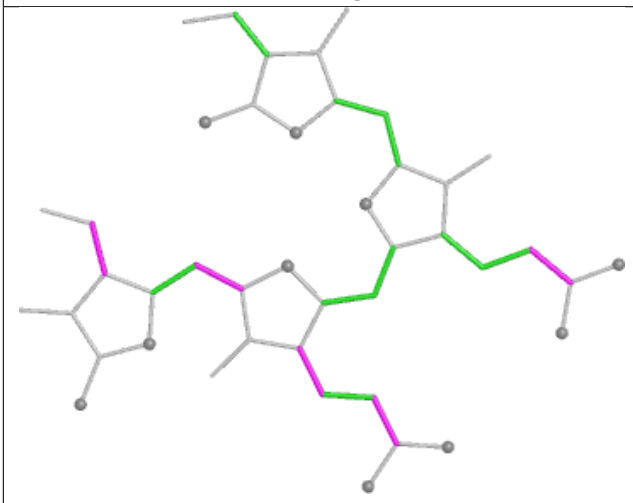


Bond angles



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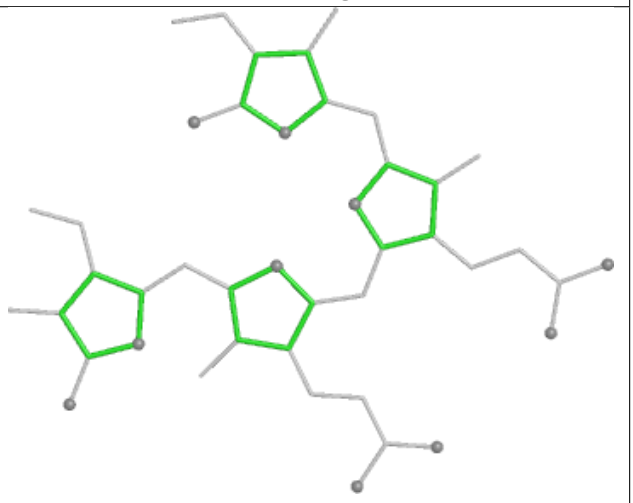
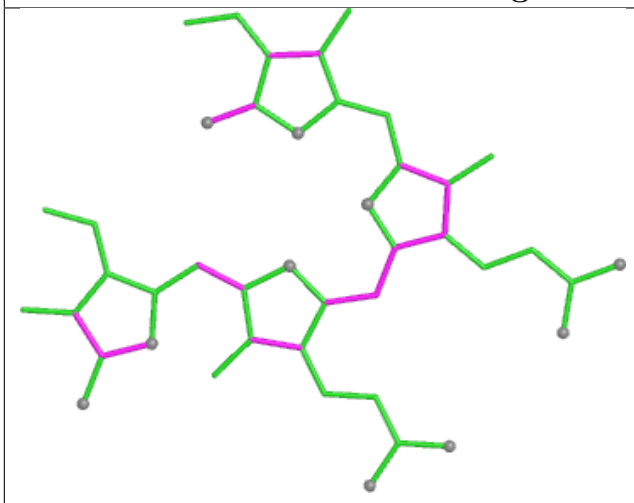


Rings

Ligand PEB QD 201



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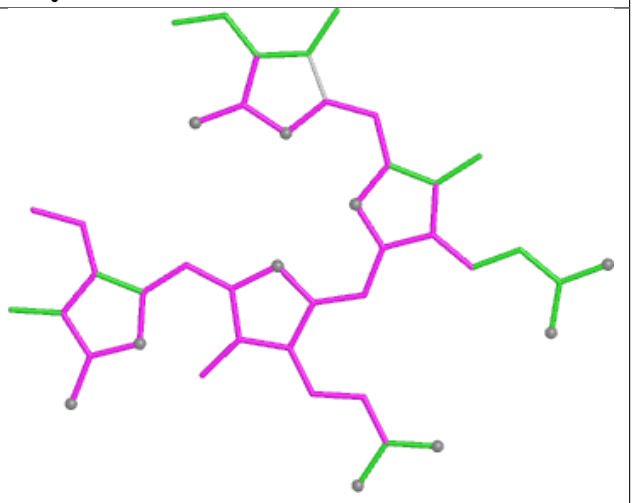
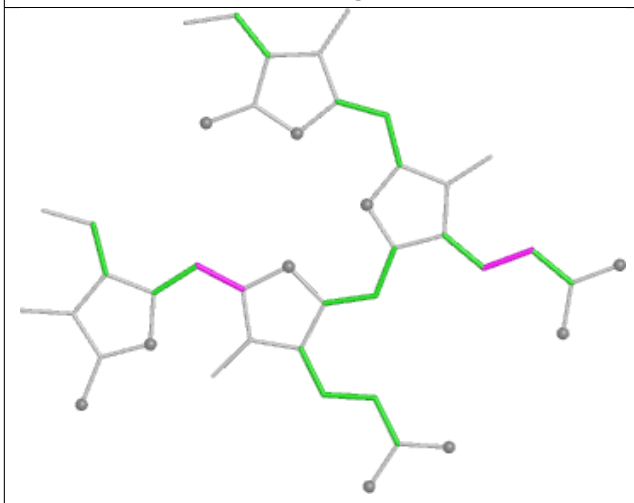


Bond angles



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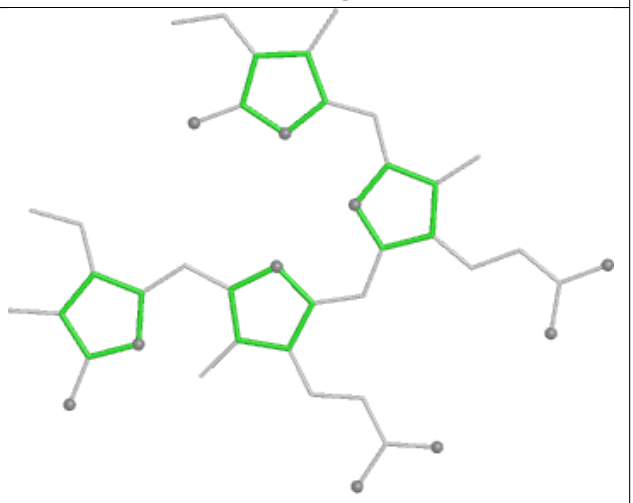
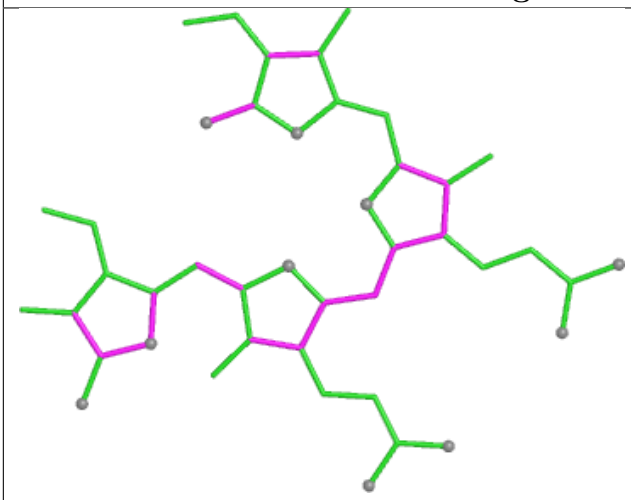


Rings

Ligand PEB eM 202



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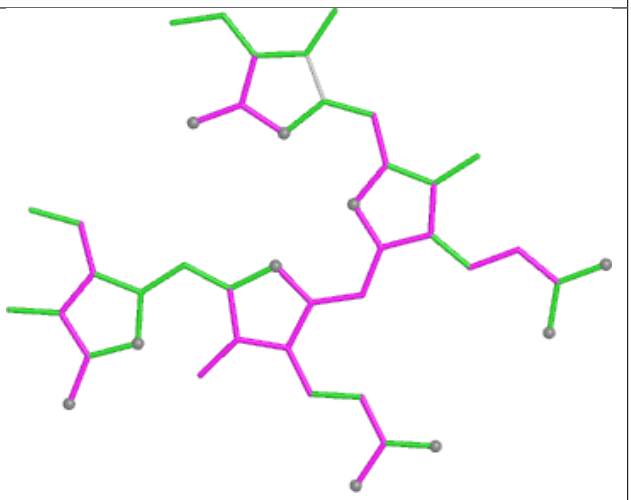
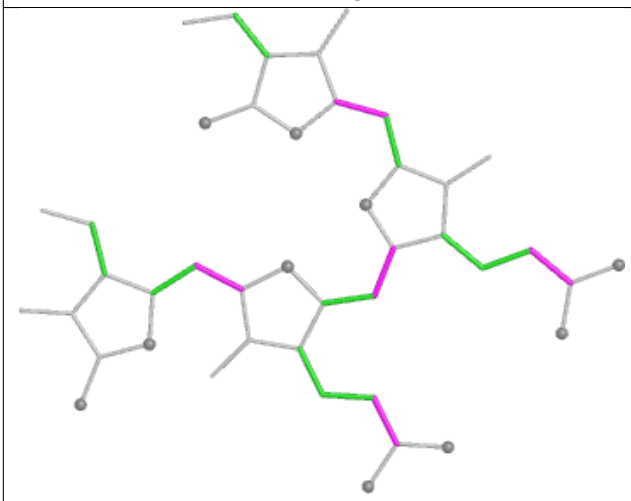


Bond angles



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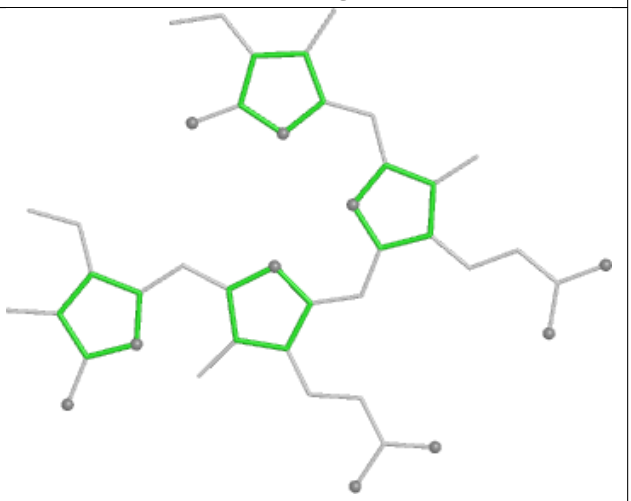
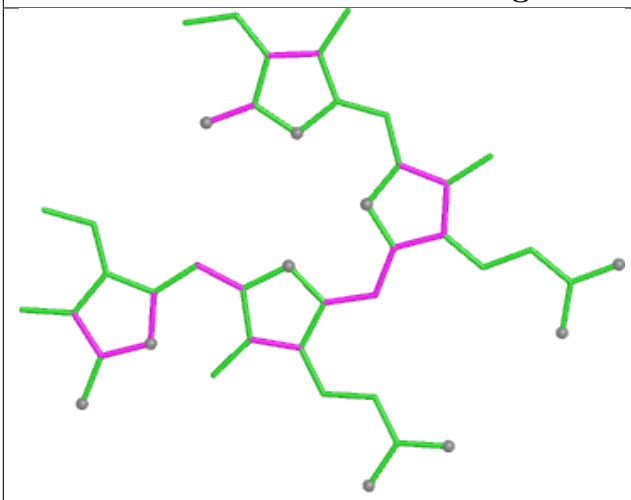


Rings

Ligand PEB aM 203



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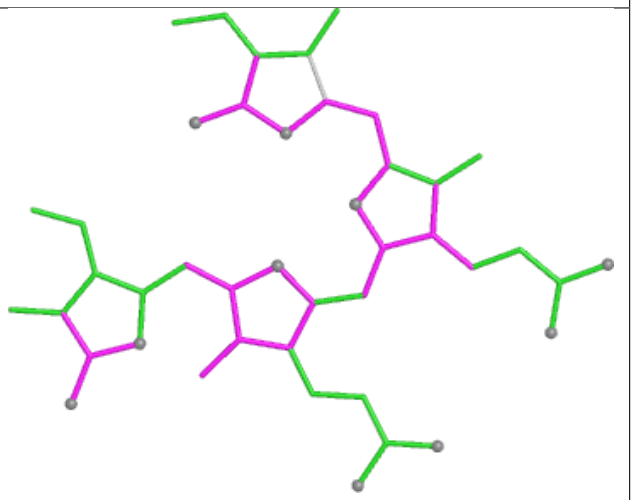
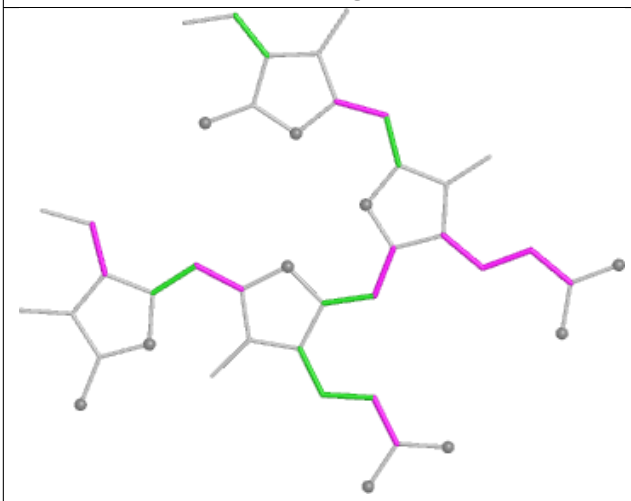
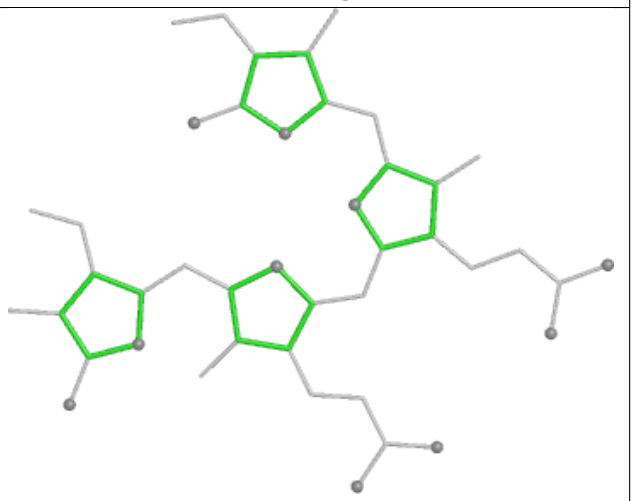


Bond angles

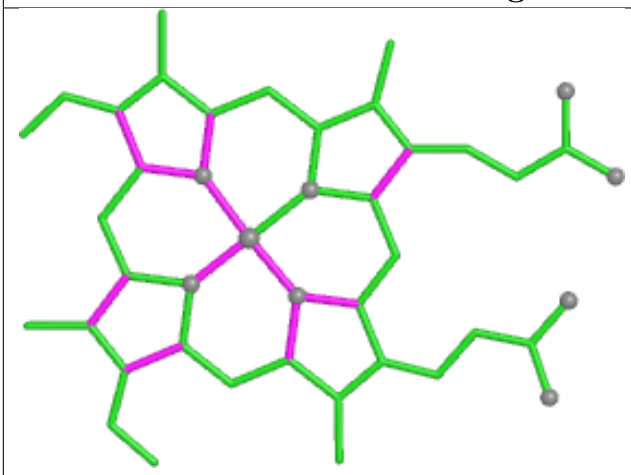


Torsions



Rings

Ligand HEM VL 201



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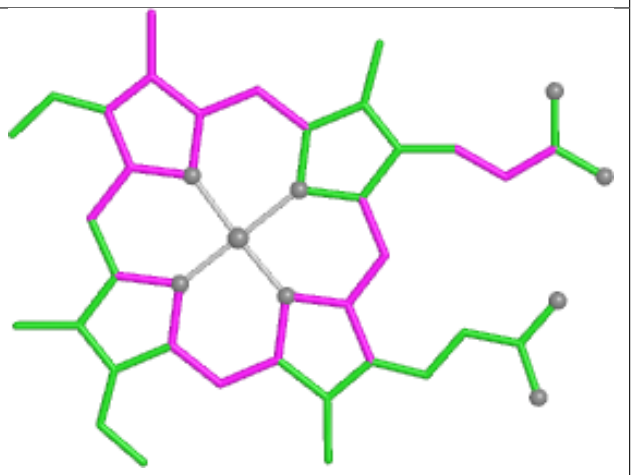

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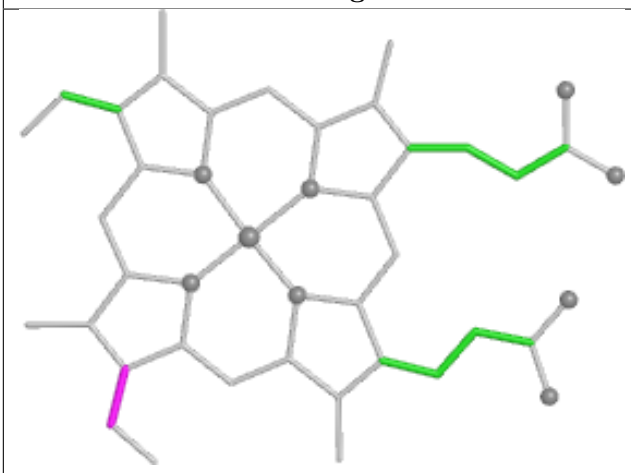

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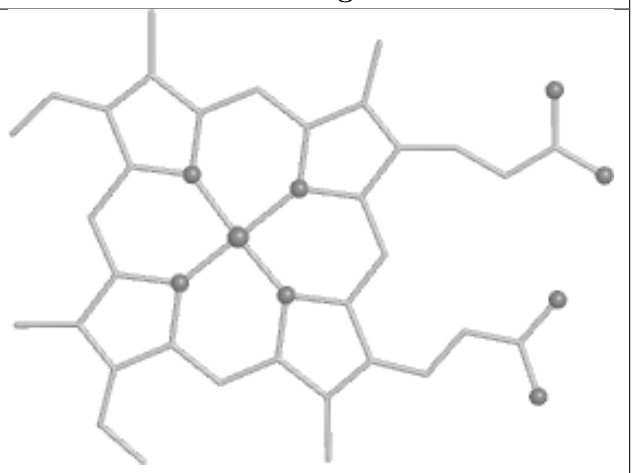
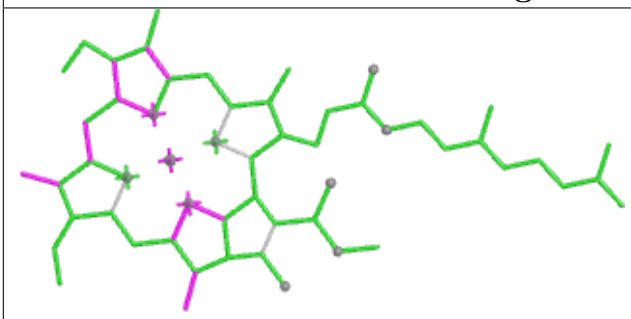


Rings

Ligand CLA A2 827



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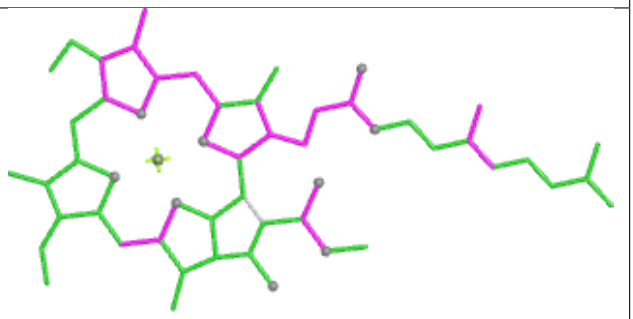

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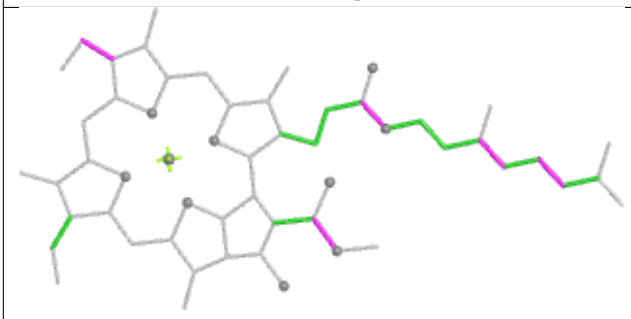

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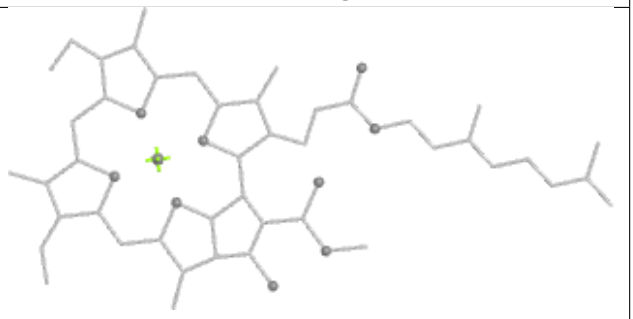
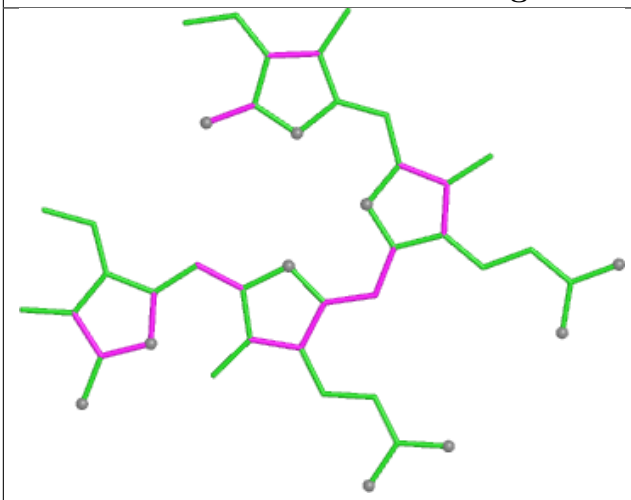


Rings

Ligand PEB HQ 201



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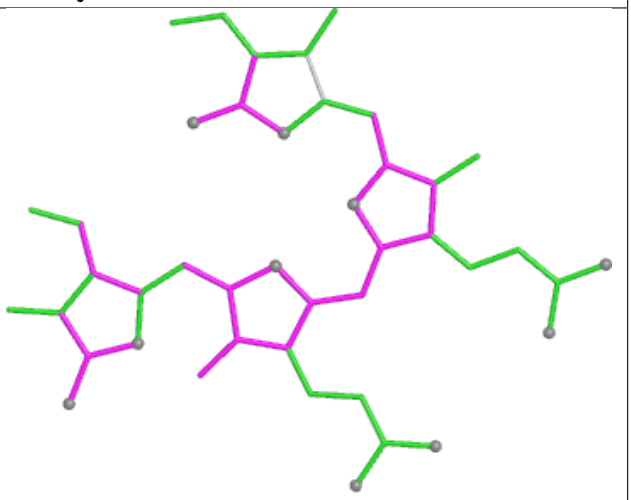

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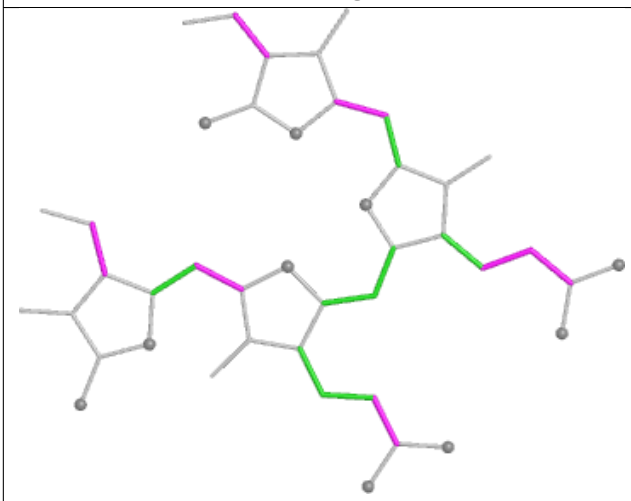

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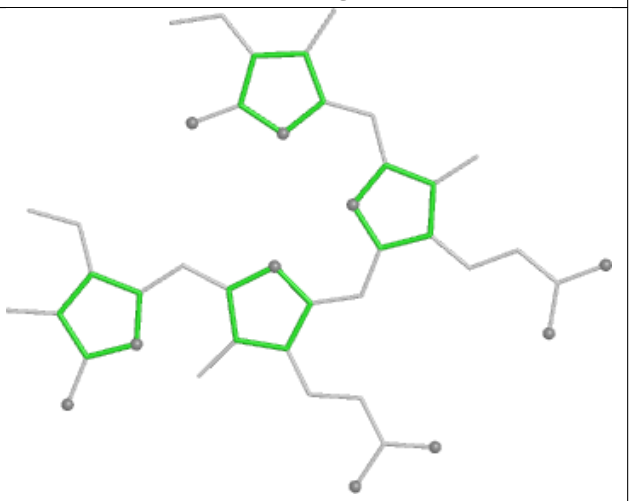
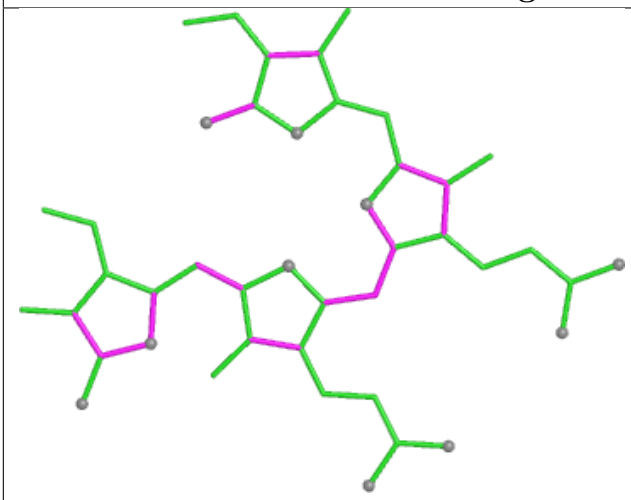


Rings

Ligand PEB IB 201



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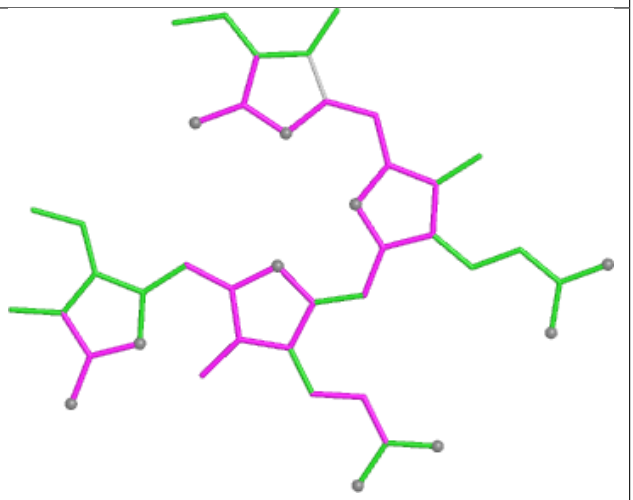

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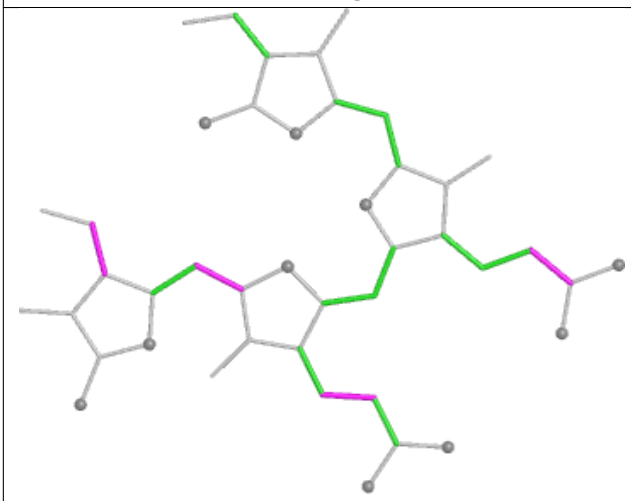

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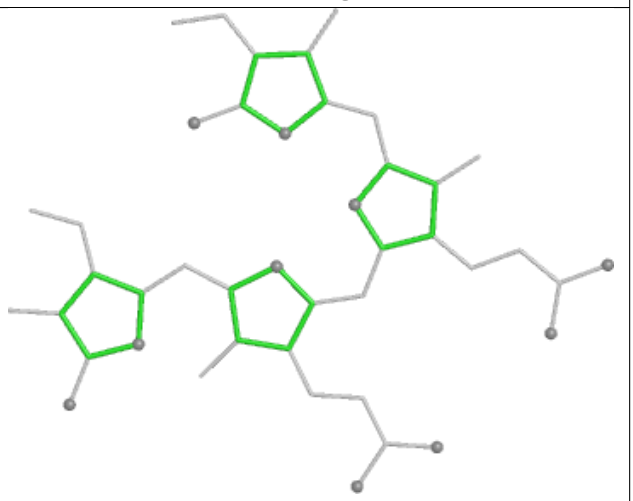
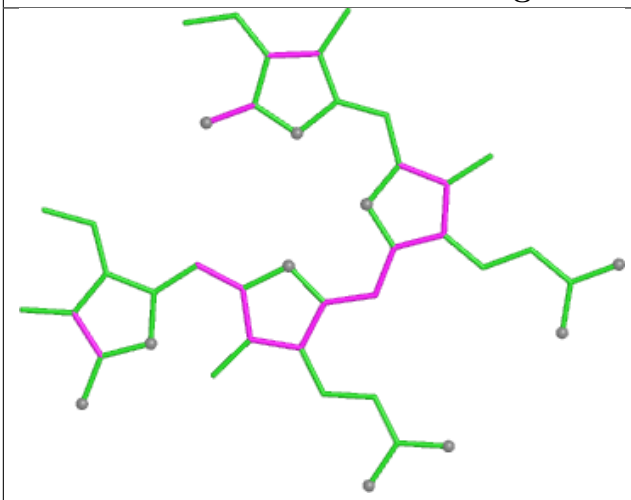


Rings

Ligand PEB m1 202



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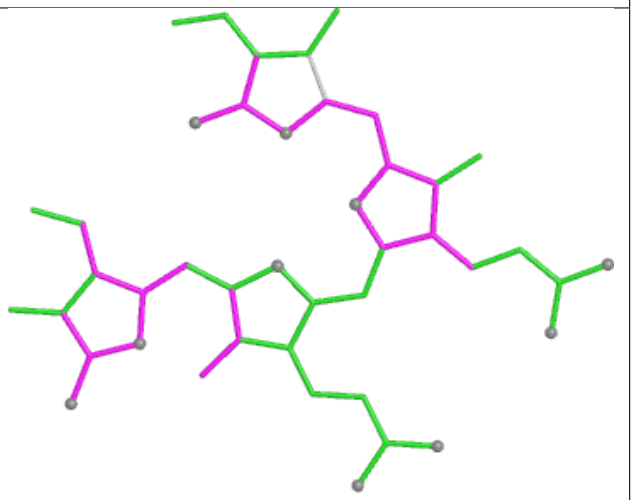

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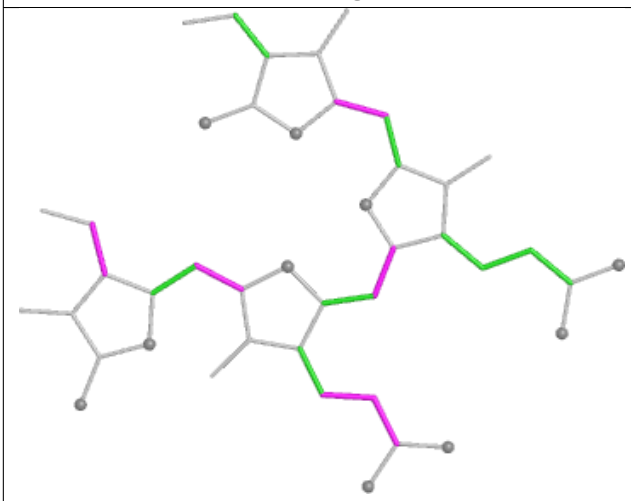

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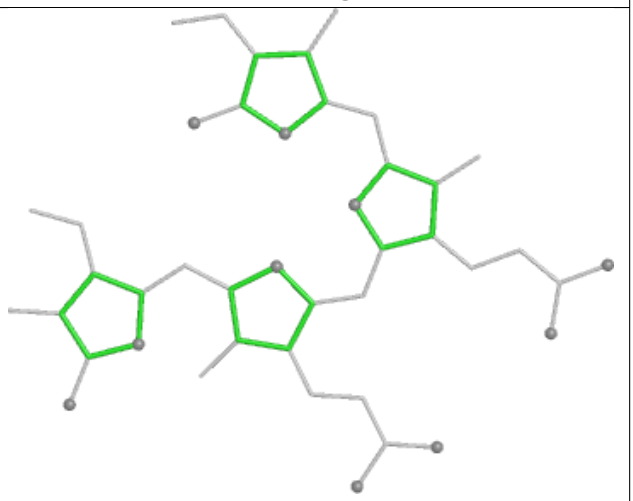
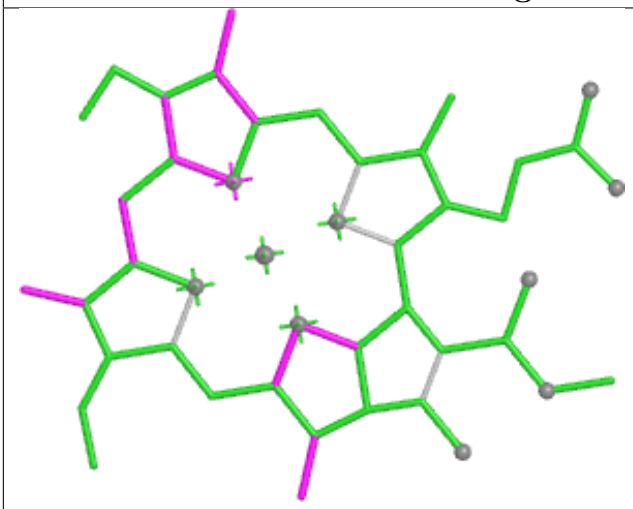


Rings

Ligand CLA 4N 611



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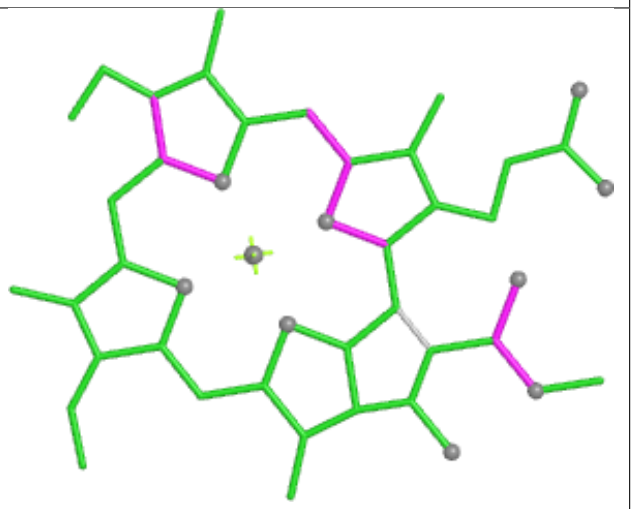
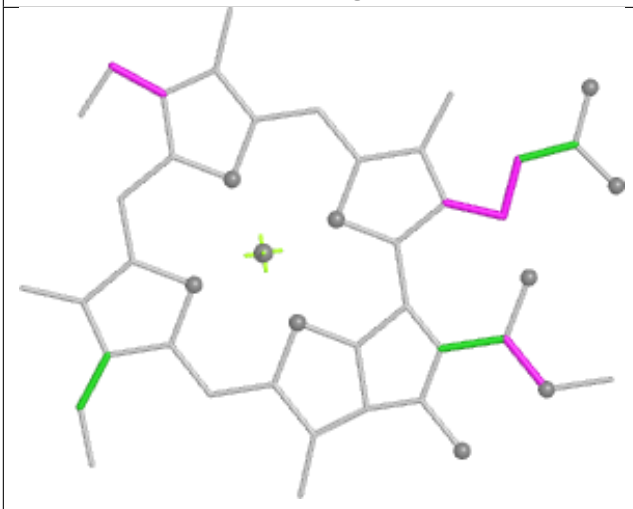


Bond angles

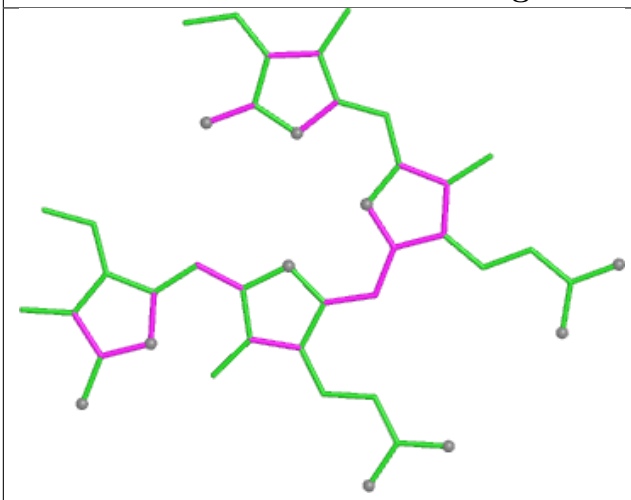


Torsions



Rings

Ligand PEB UE 203



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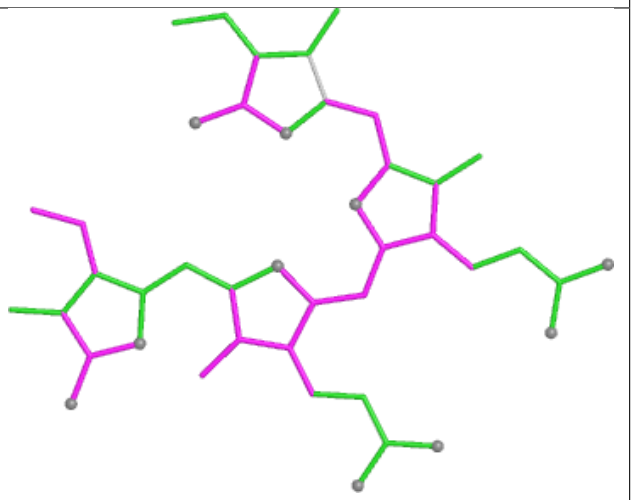

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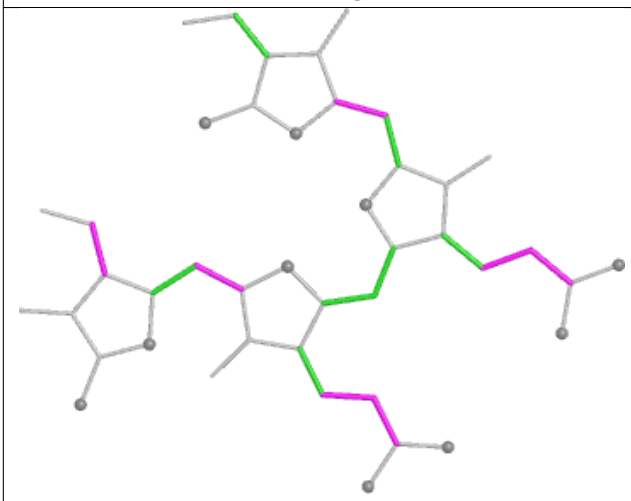

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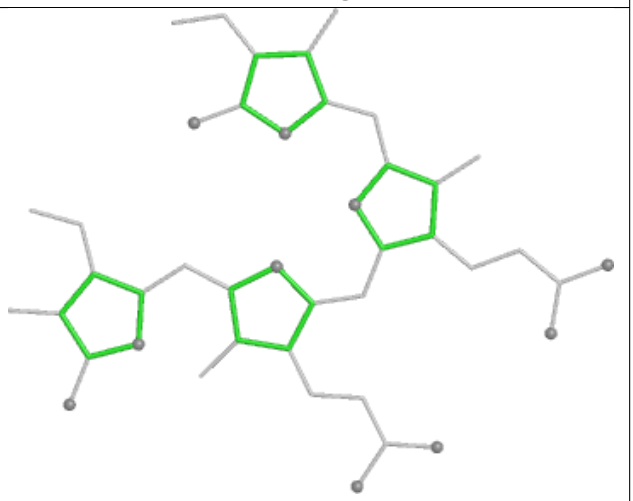
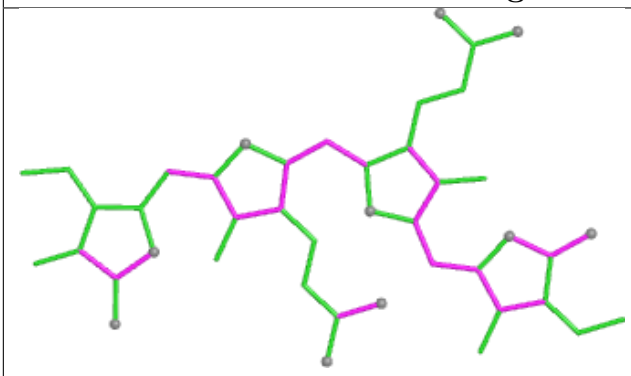


Rings

Ligand CYC h3 1001



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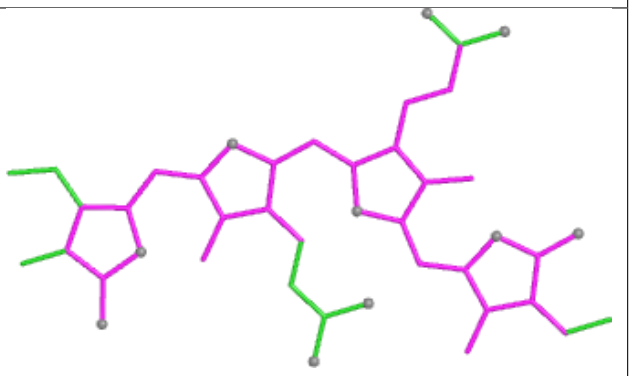

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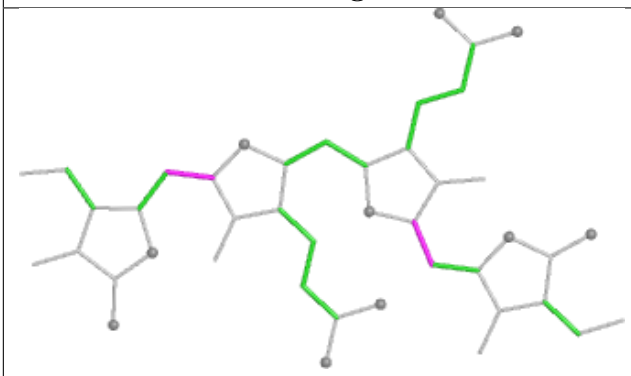

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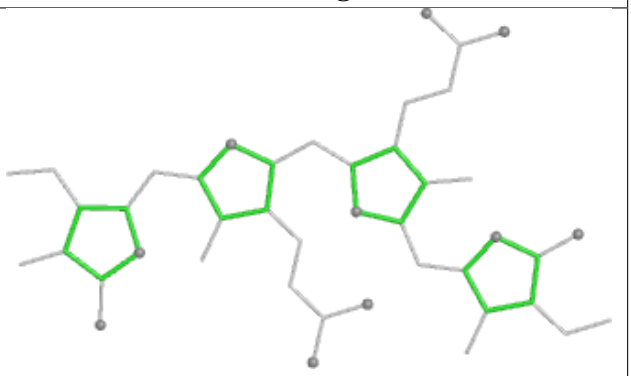
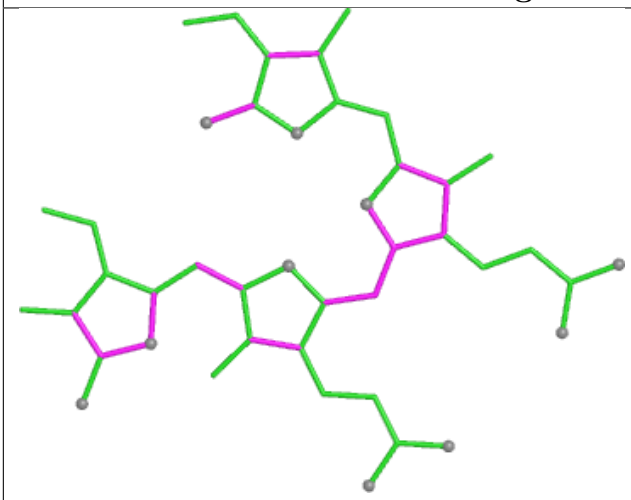


Rings

Ligand PEB aG 201



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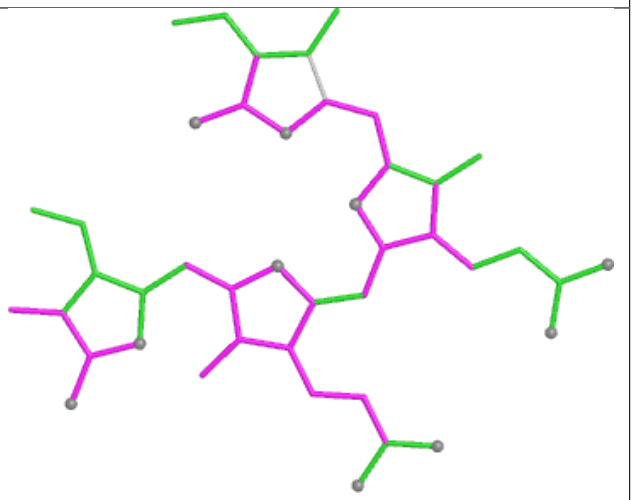

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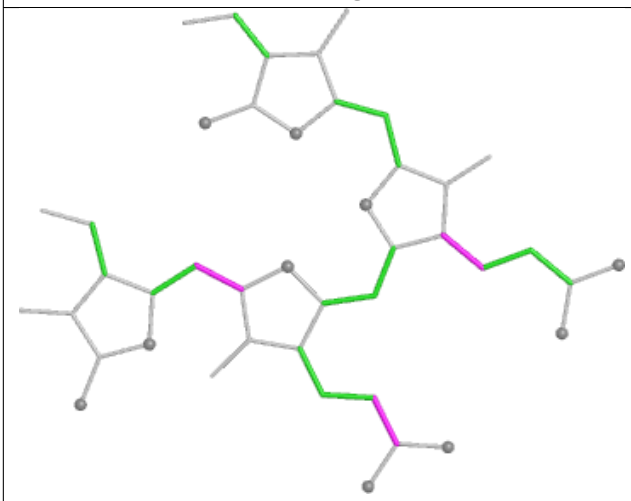

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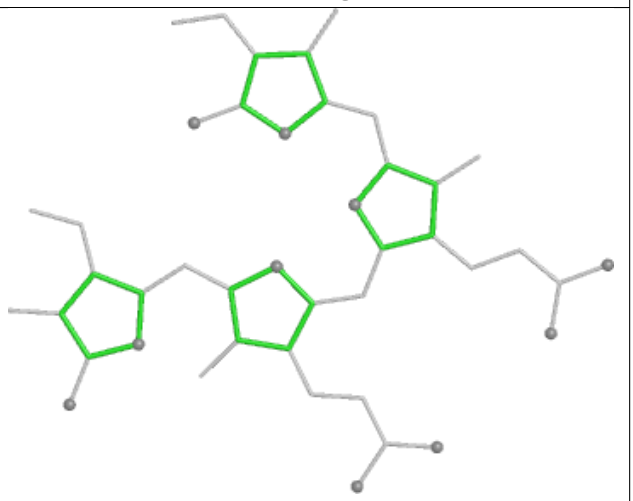

Rings

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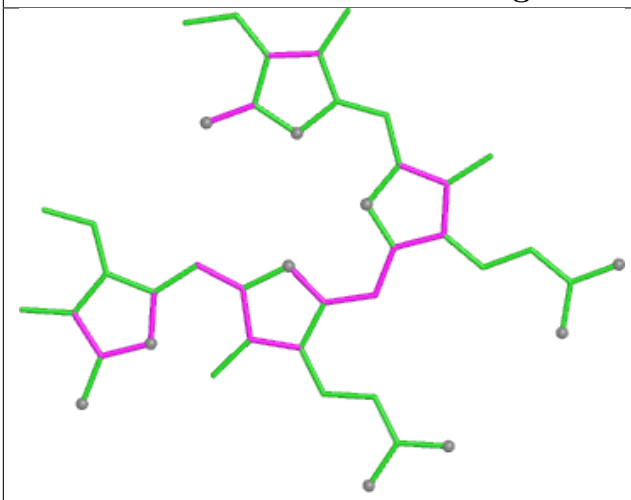

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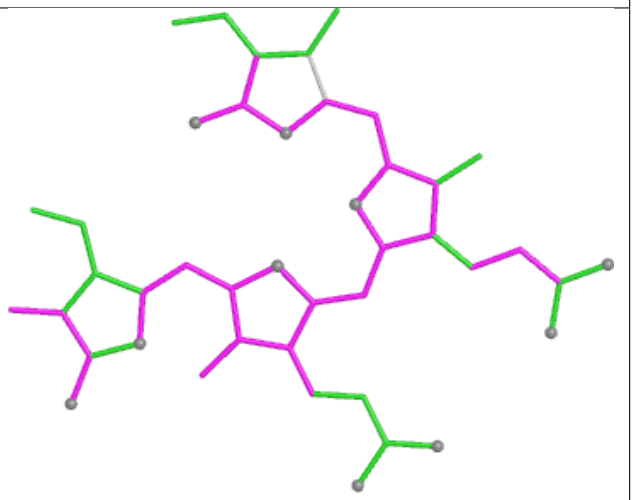

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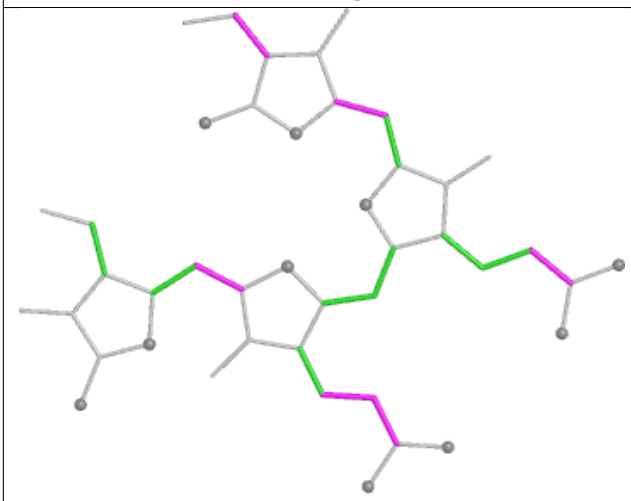

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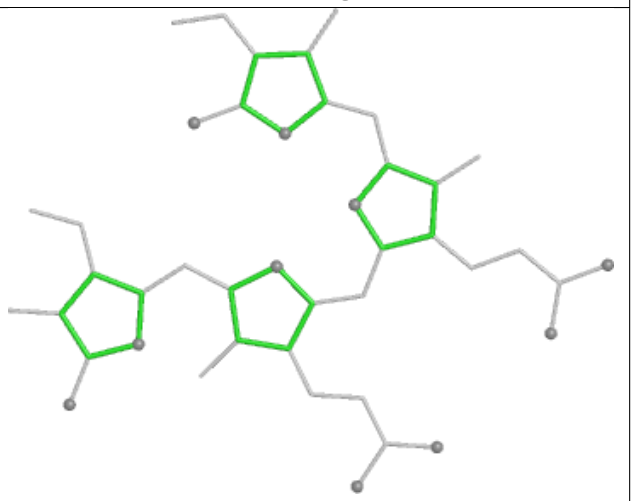
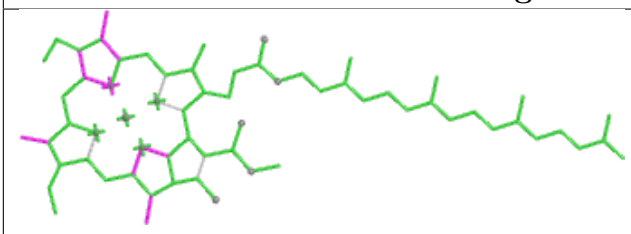


Rings

Ligand CLA A2 809



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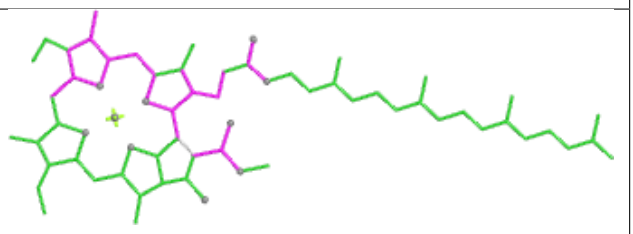

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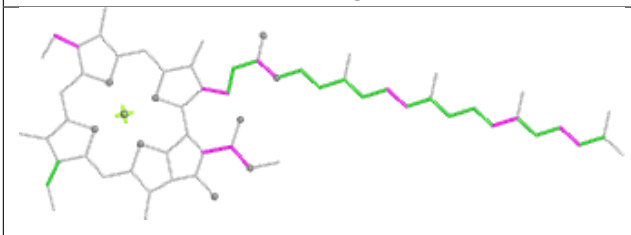

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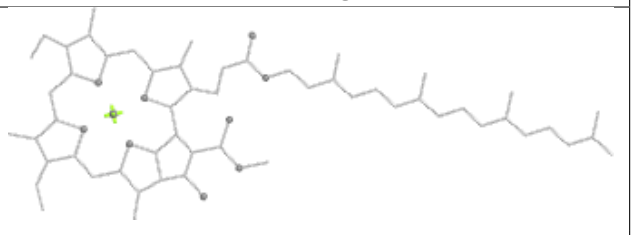
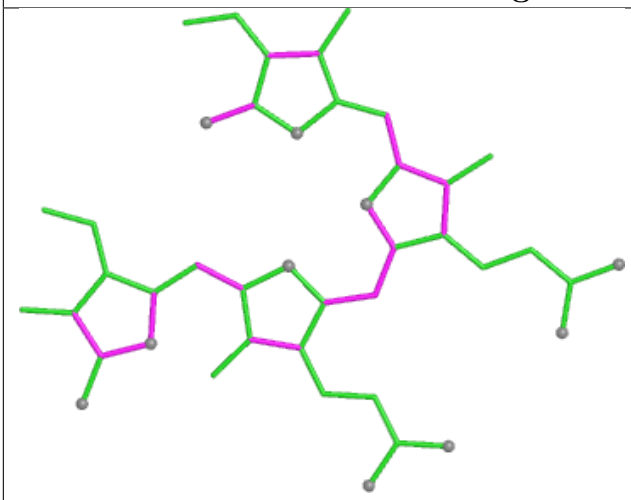


Rings

Ligand PEB TB 202



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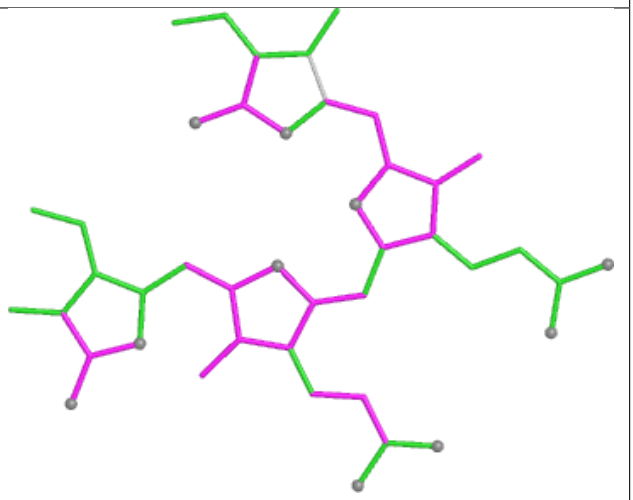
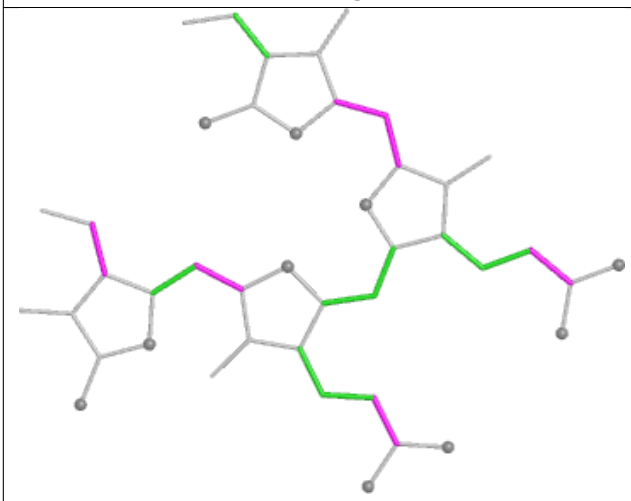


Bond angles



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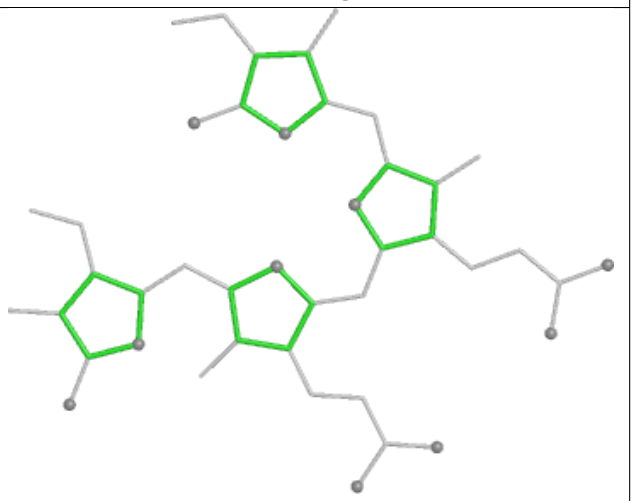
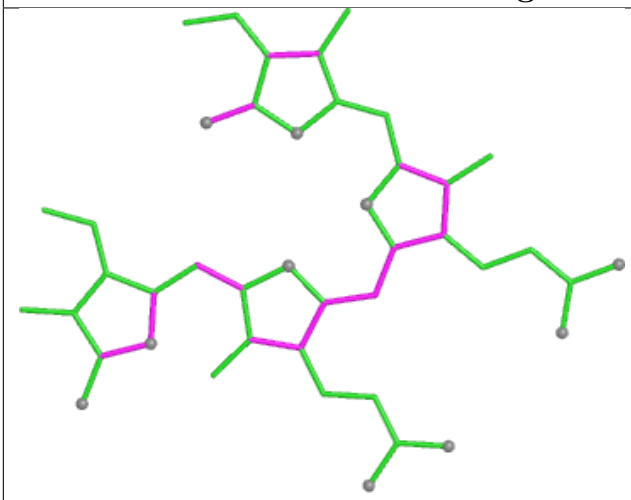


Rings

Ligand PEB kF 203



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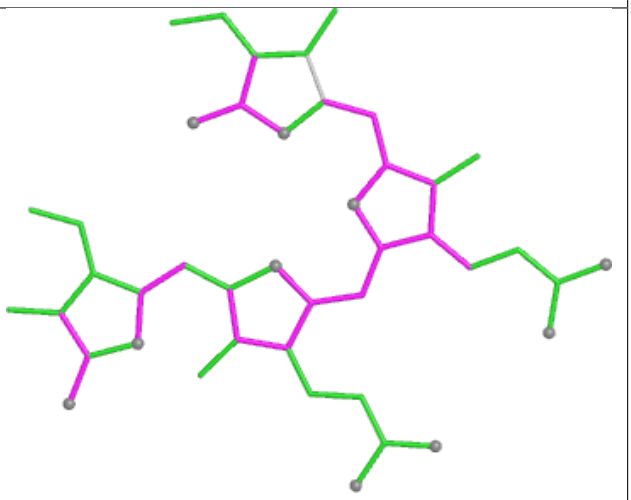
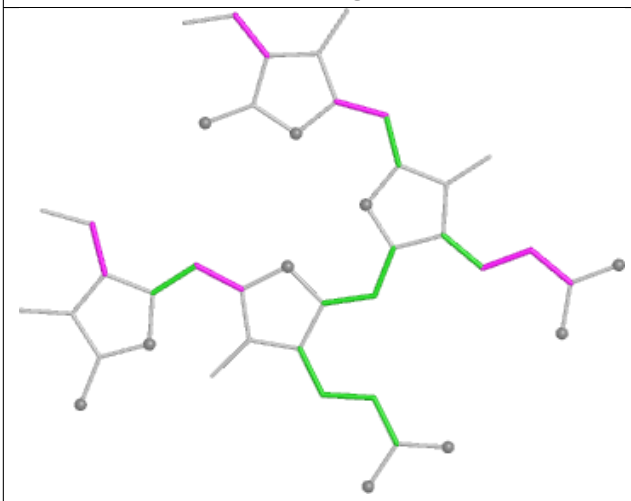


Bond angles



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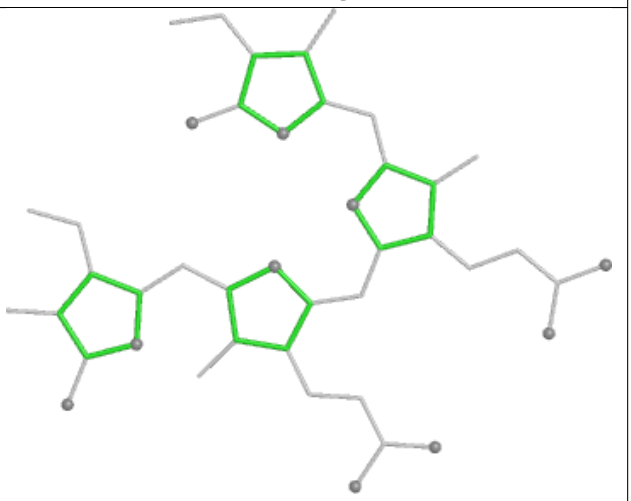
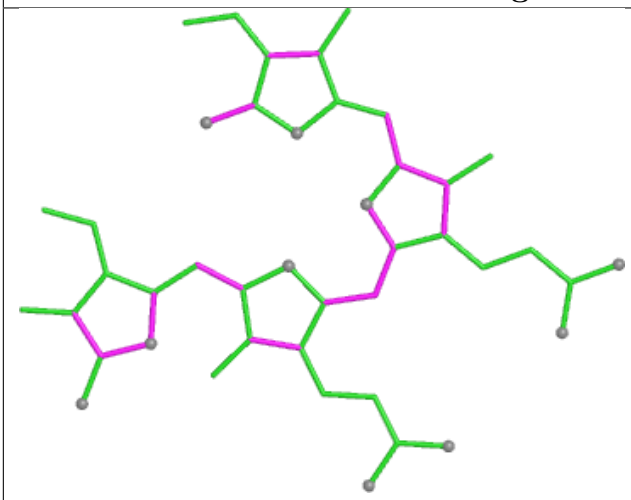


Rings

Ligand PEB UB 301



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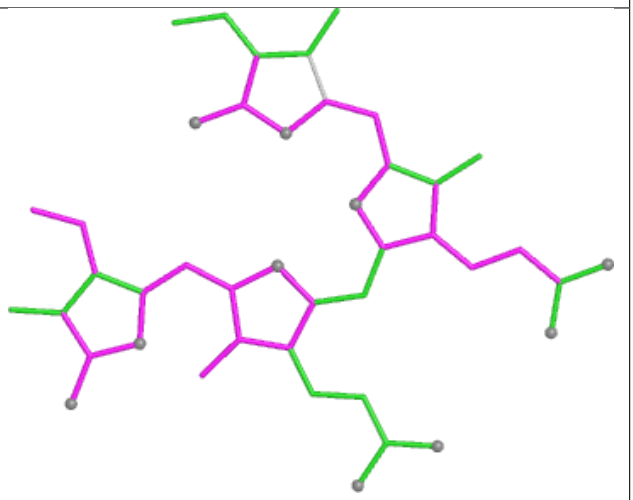
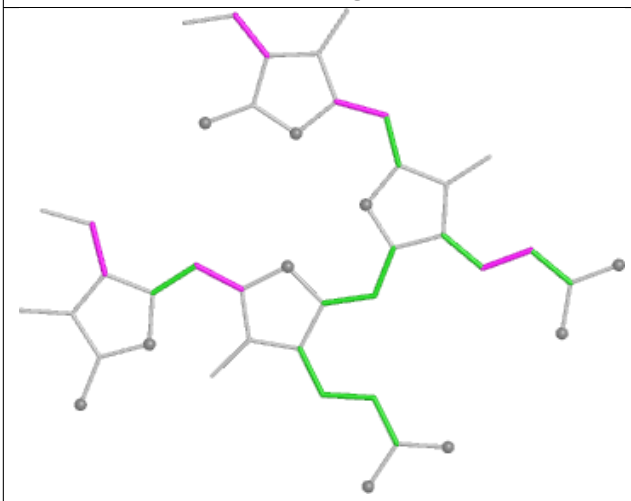


Bond angles



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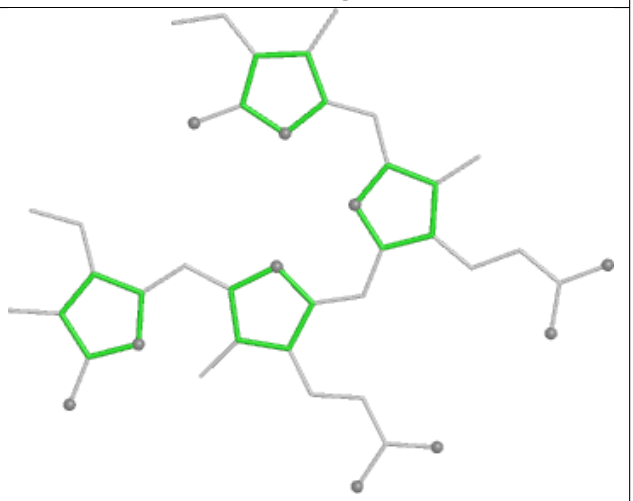
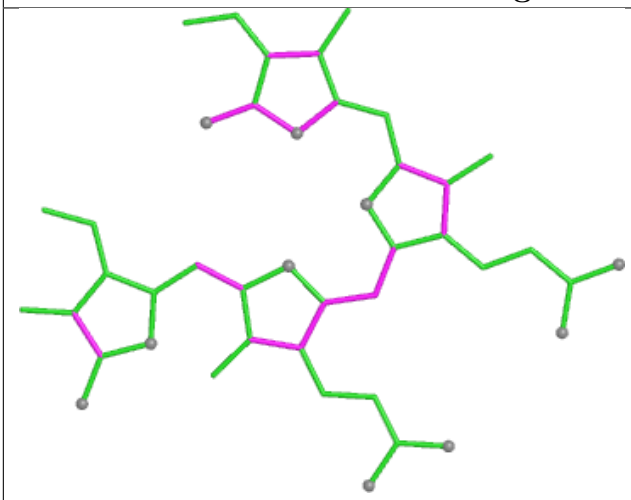
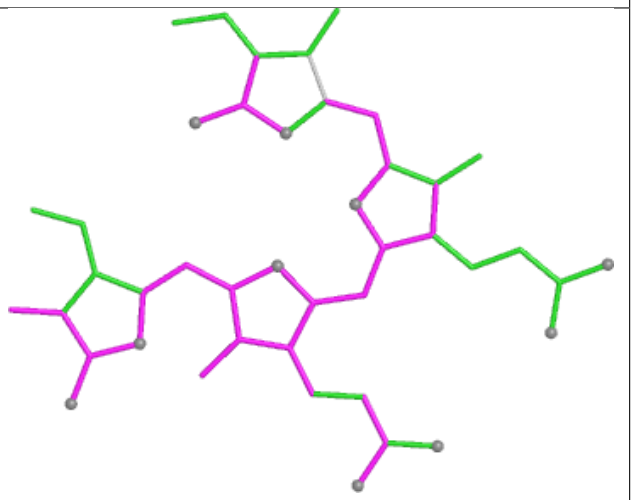


Rings

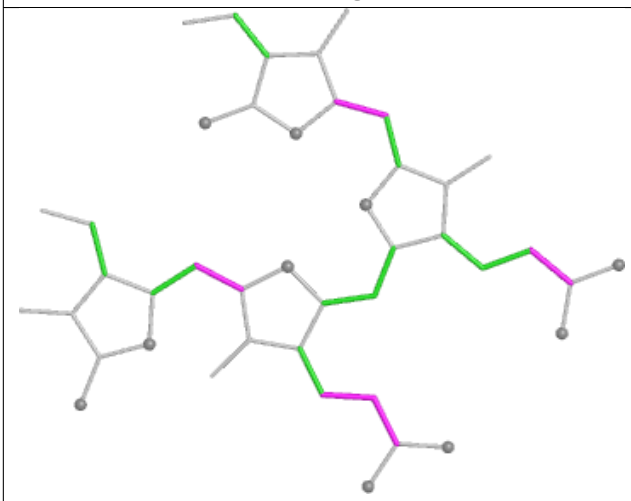
Ligand PEB BF 201



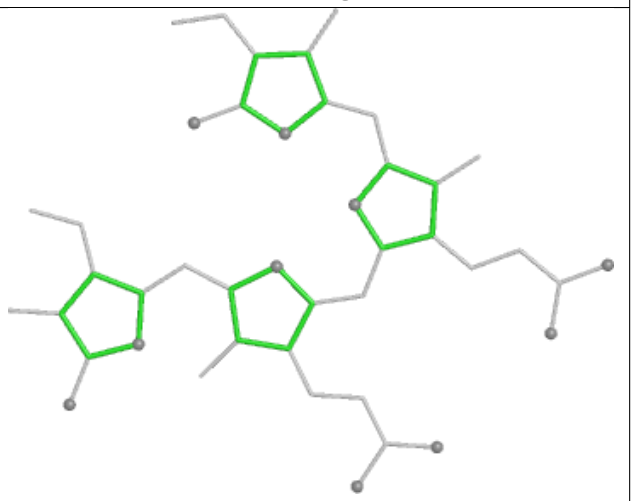
Bond lengths



Bond angles

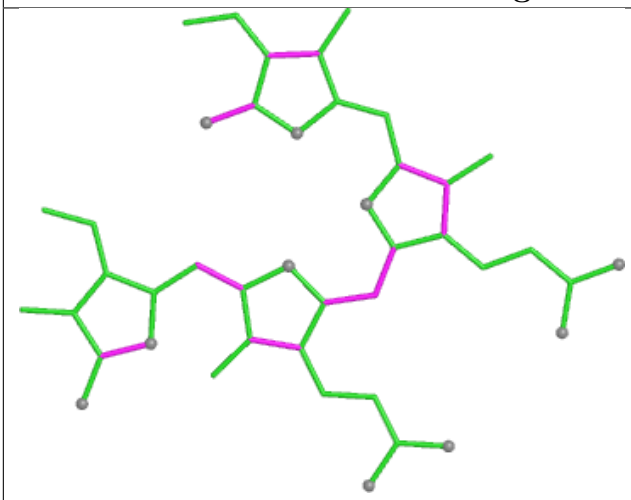


Torsions



Rings

Ligand PEB CF 202



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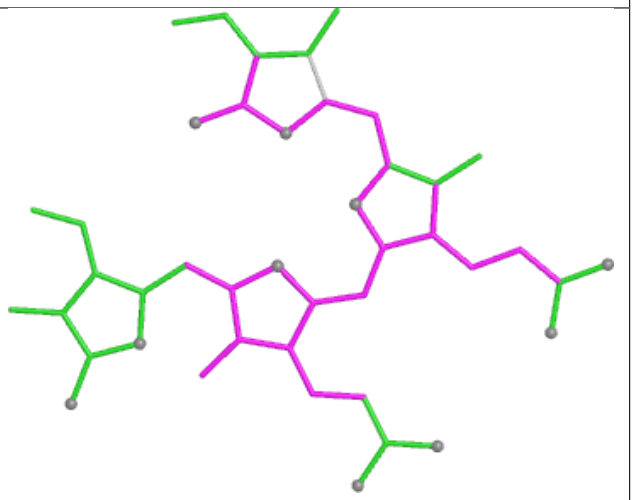

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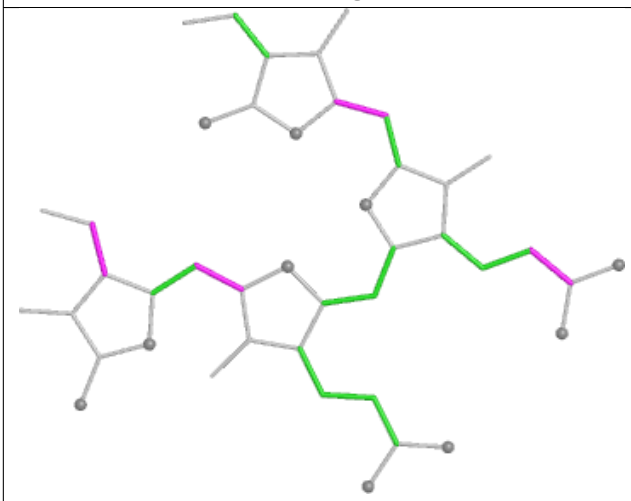

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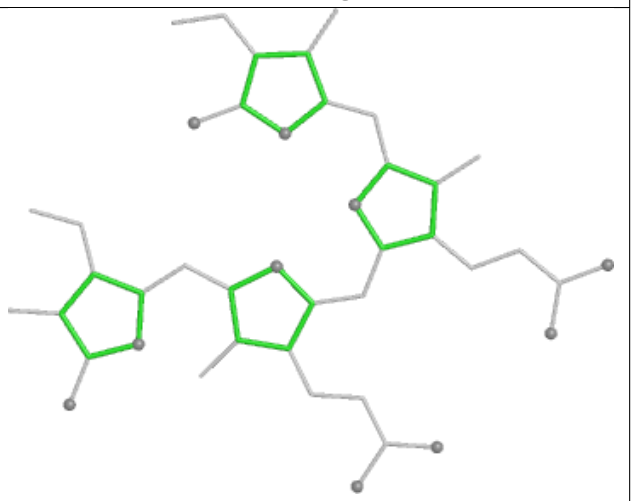
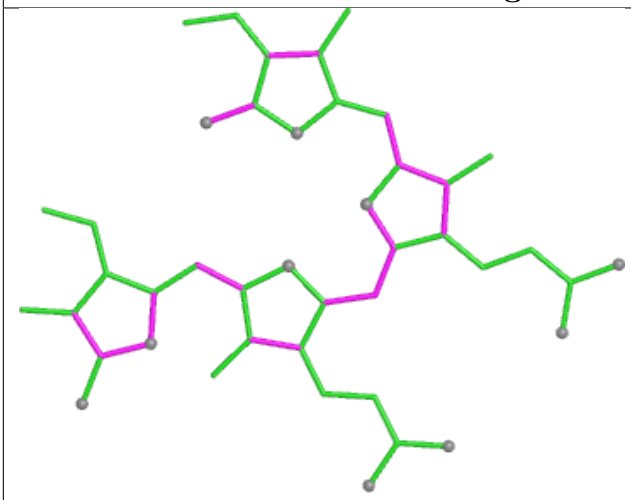


Rings

Ligand PEB LG 1002



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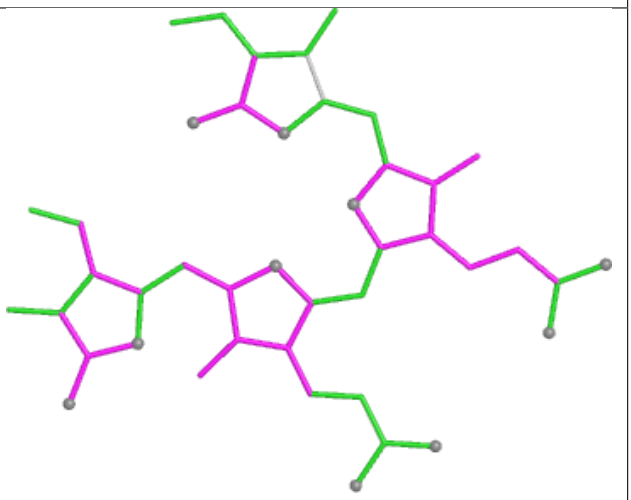

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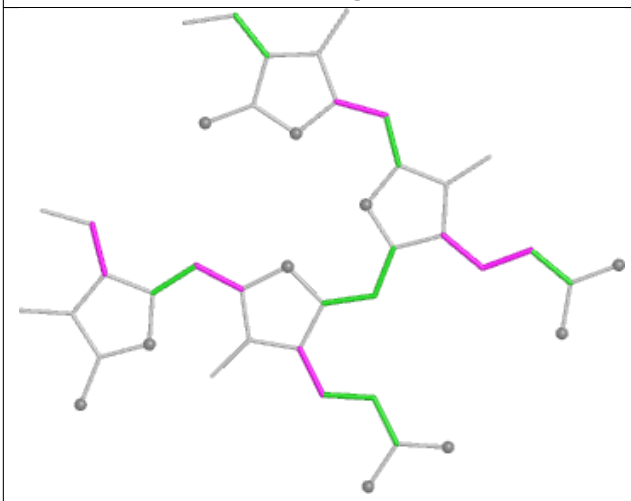

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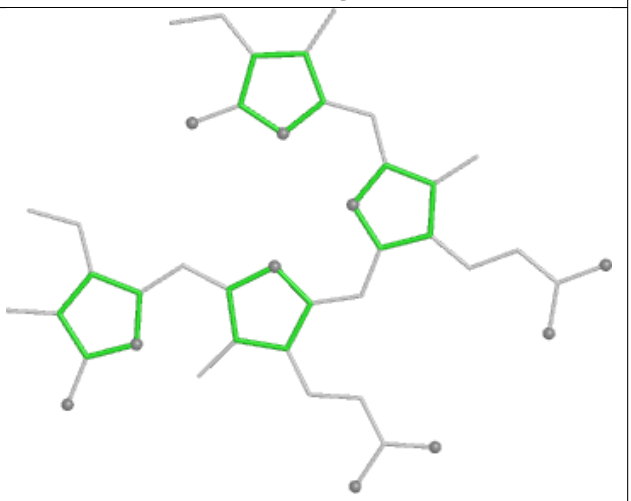
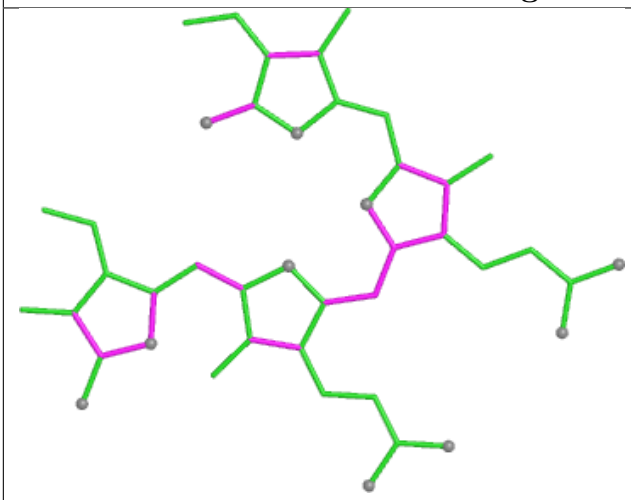


Rings

Ligand PEB iE 201



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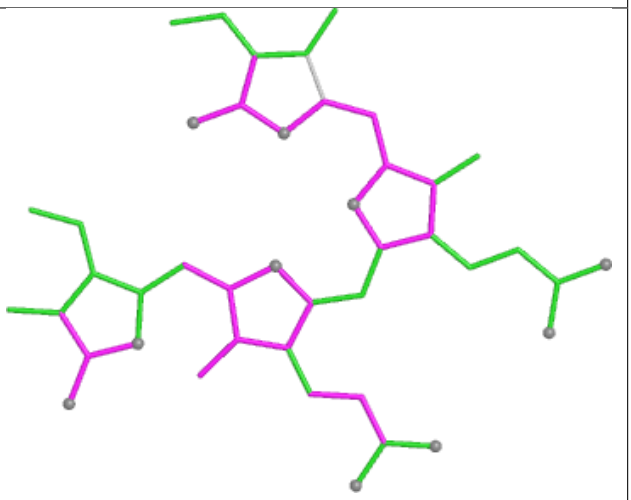

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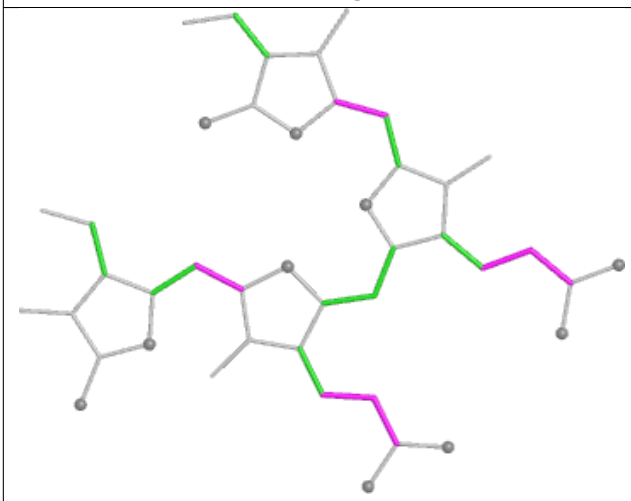

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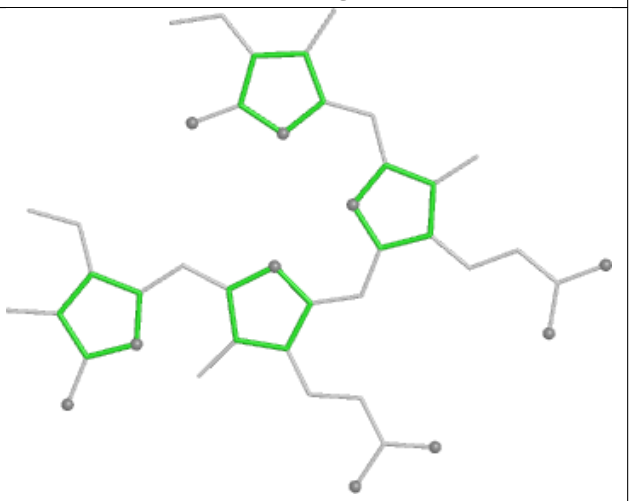
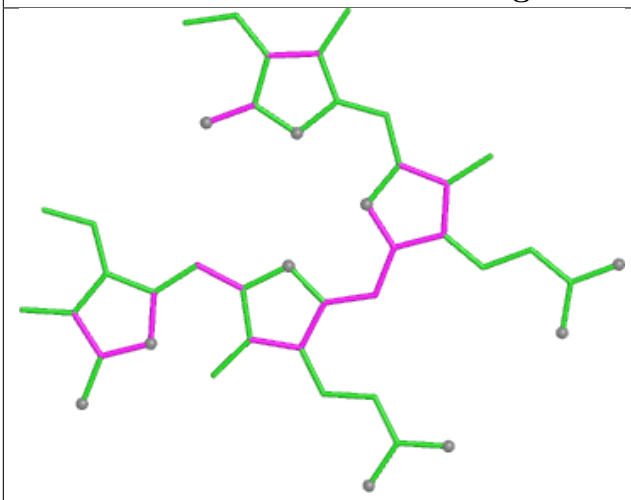


Rings

Ligand PEB WI 201



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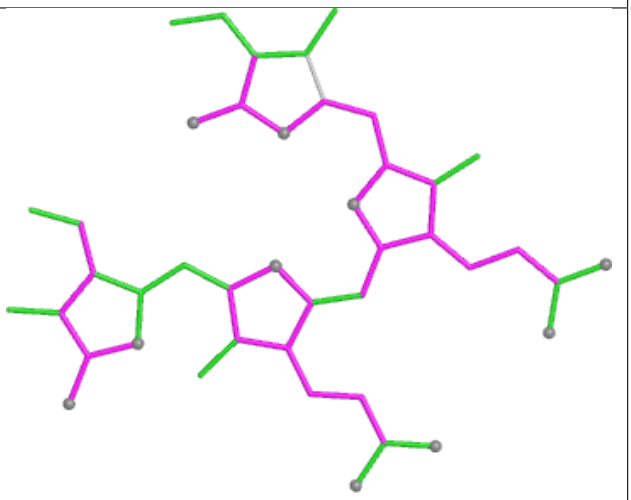

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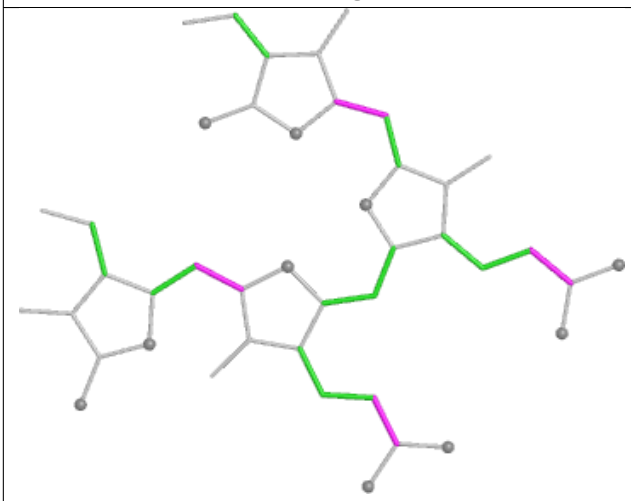

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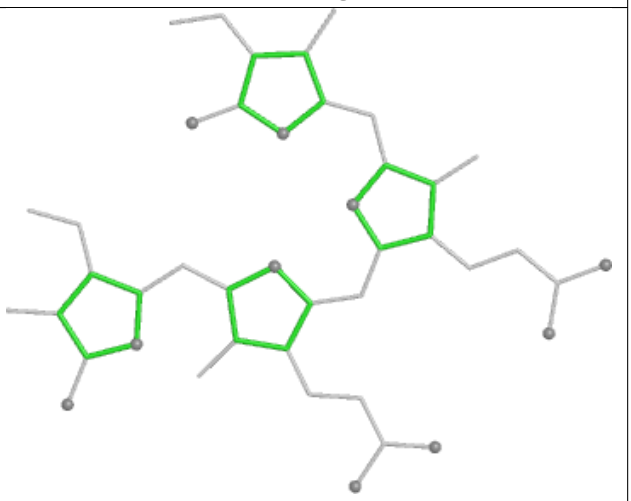
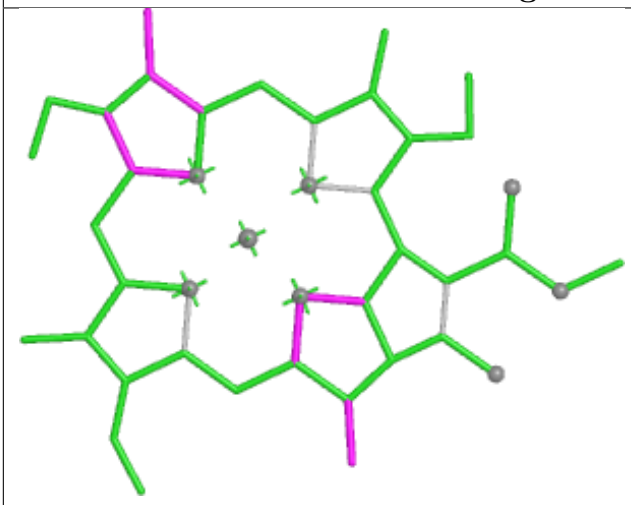


Rings

Ligand CLA 42 610



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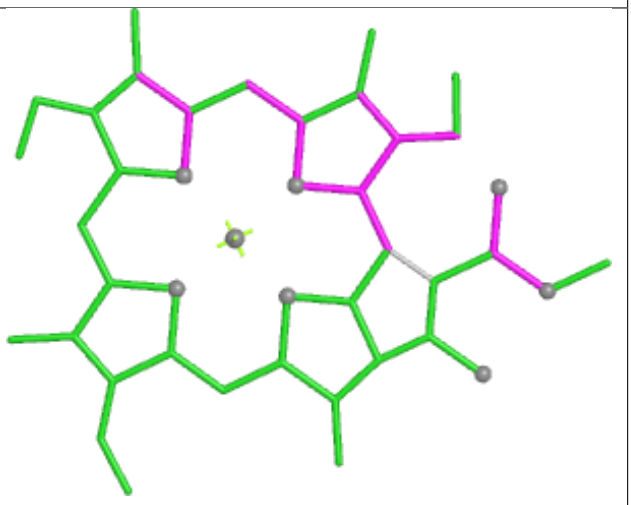

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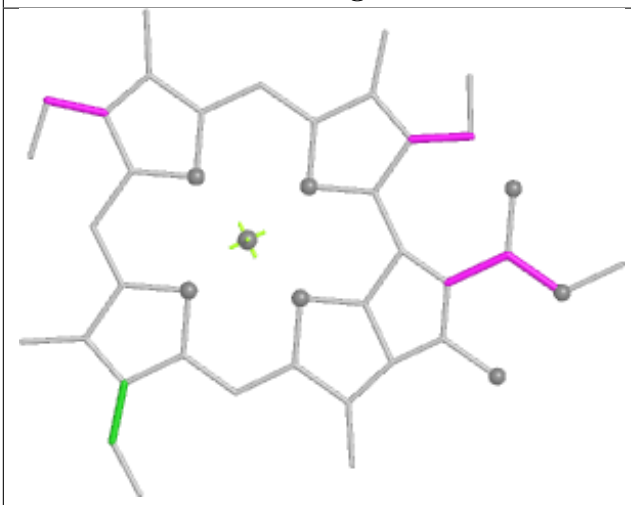
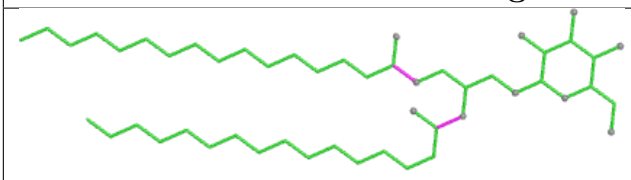


Torsions



Rings

Ligand LMG AL 411



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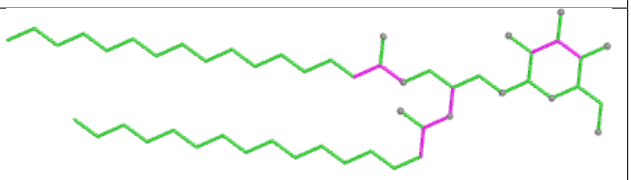

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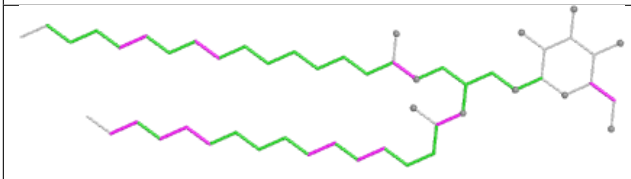

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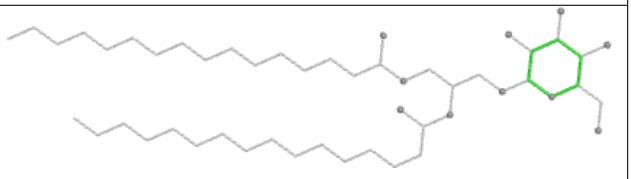
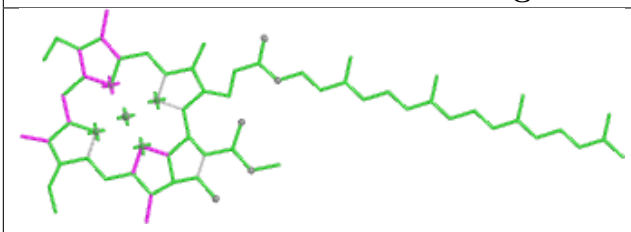


Rings

Ligand CLA BL 609



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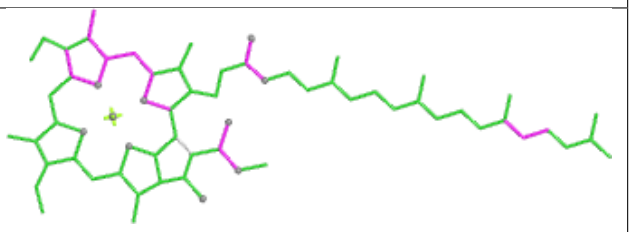

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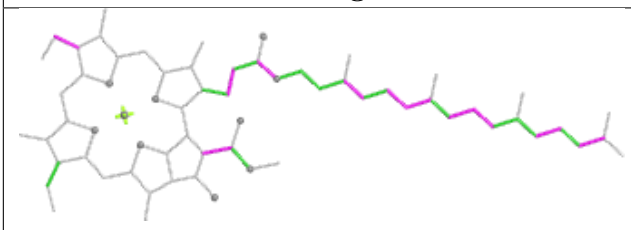

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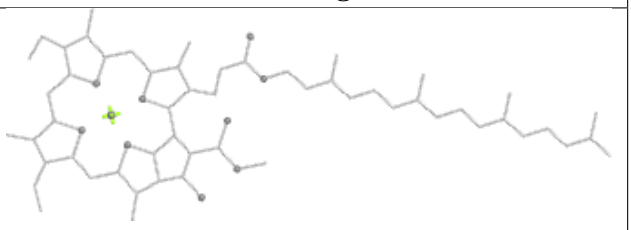
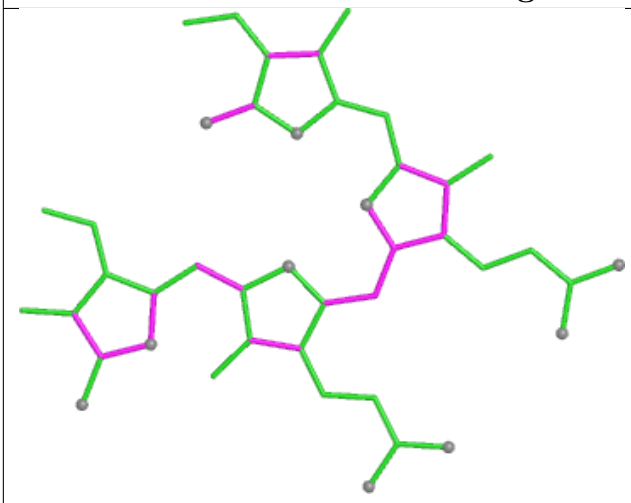


Rings

Ligand PEB aE 201



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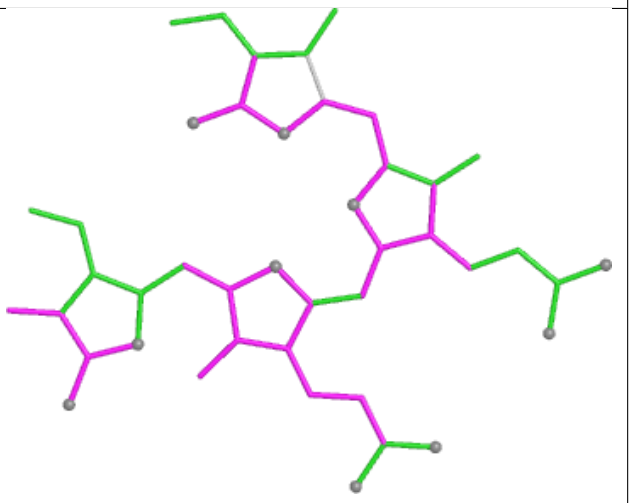

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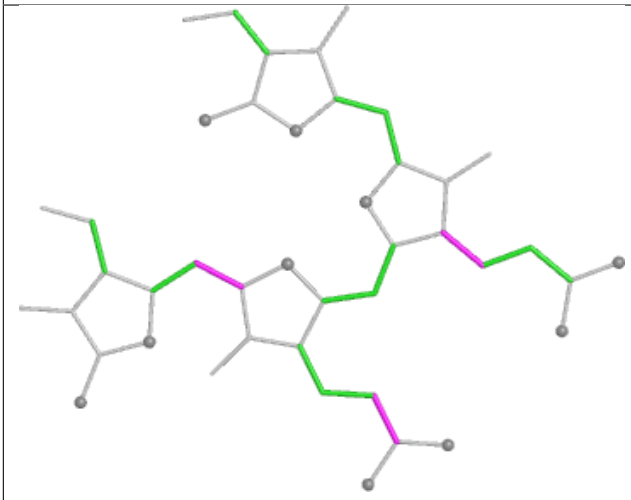

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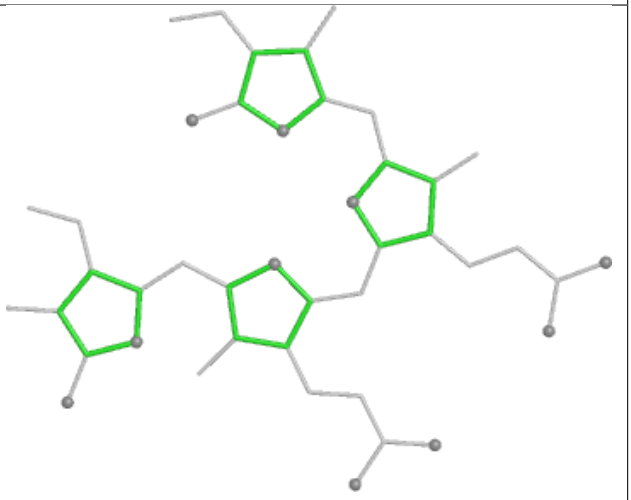
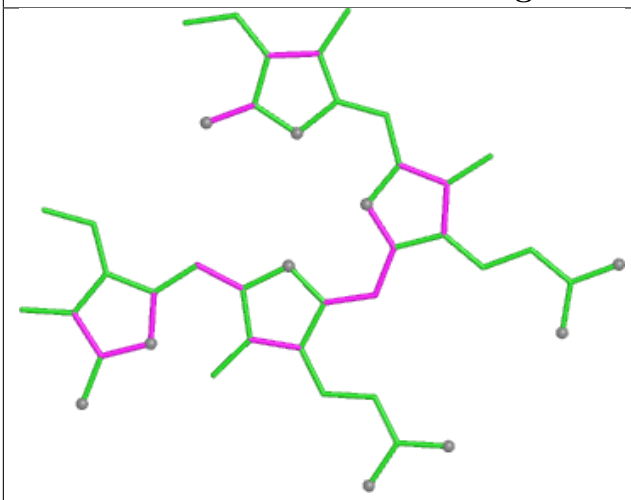


Rings

Ligand PEB YJ 202



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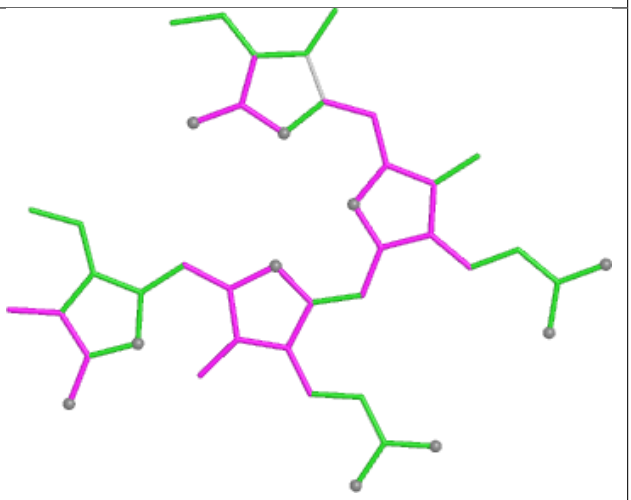

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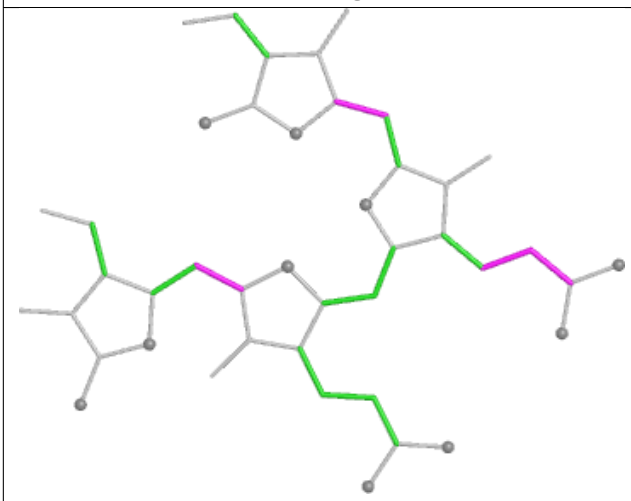

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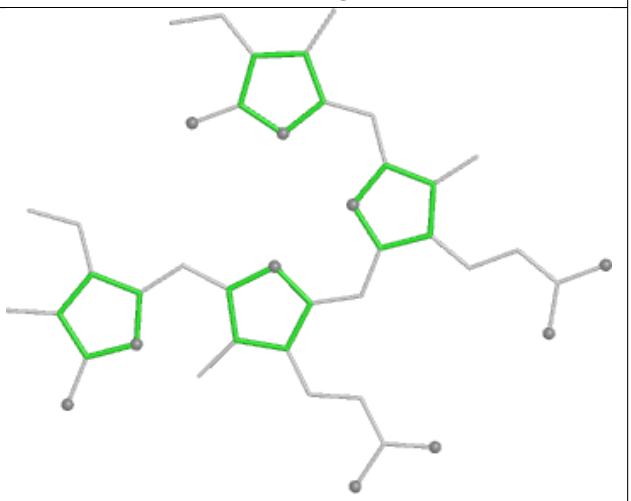
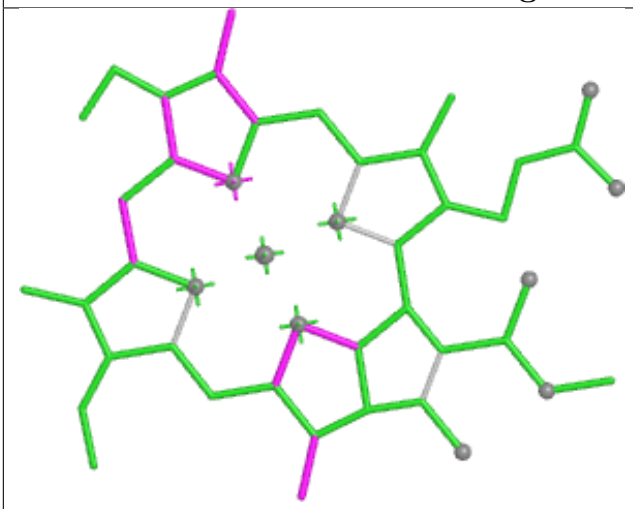


Rings

Ligand CLA 52 603



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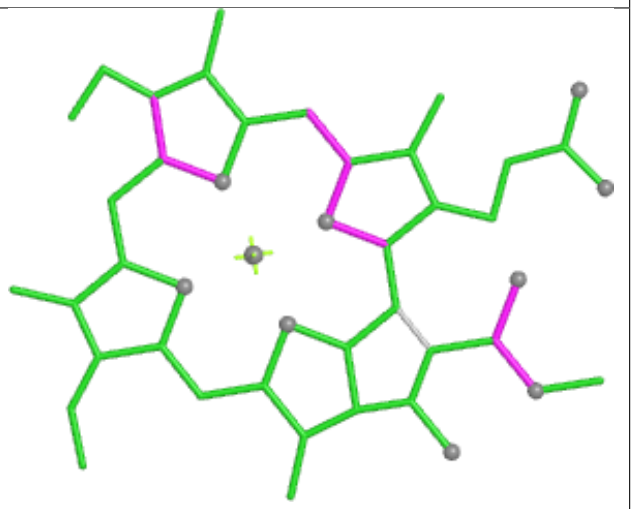

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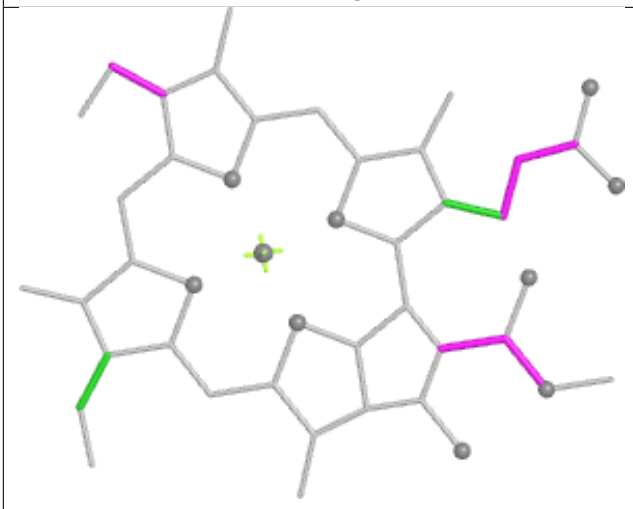
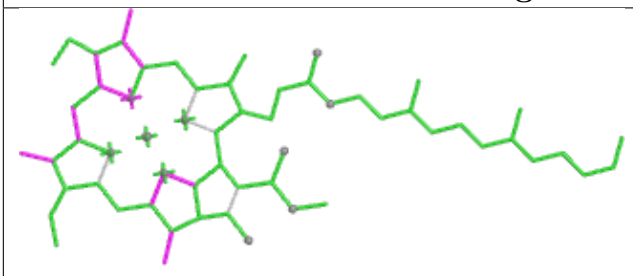


Torsions



Rings

Ligand CLA B6 612



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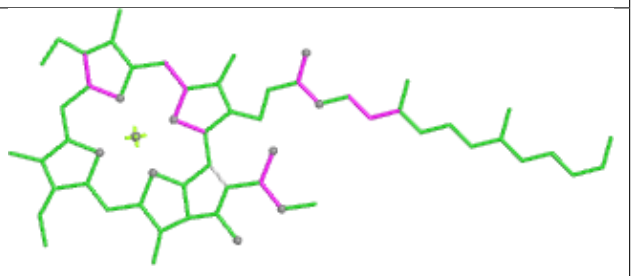

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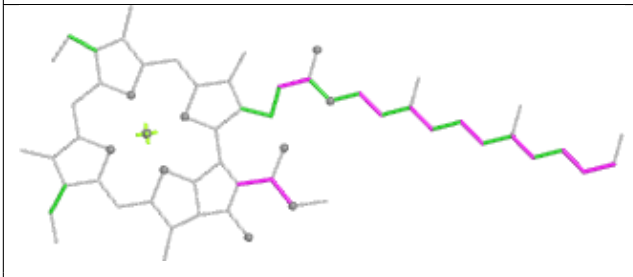

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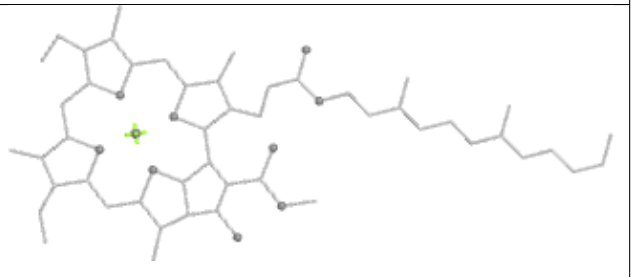
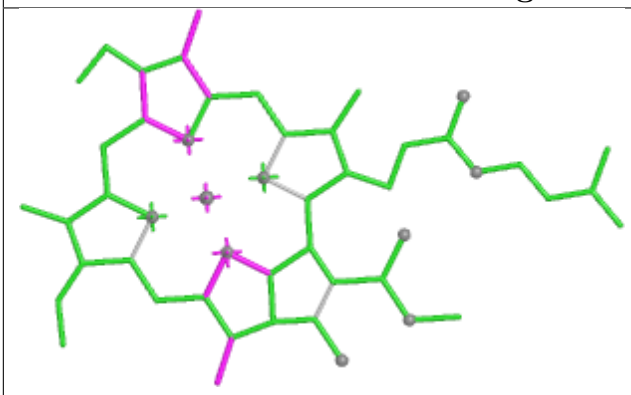


Rings

Ligand CLA dL 409



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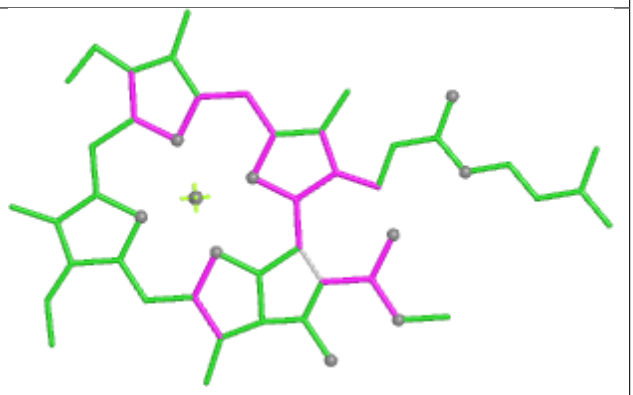
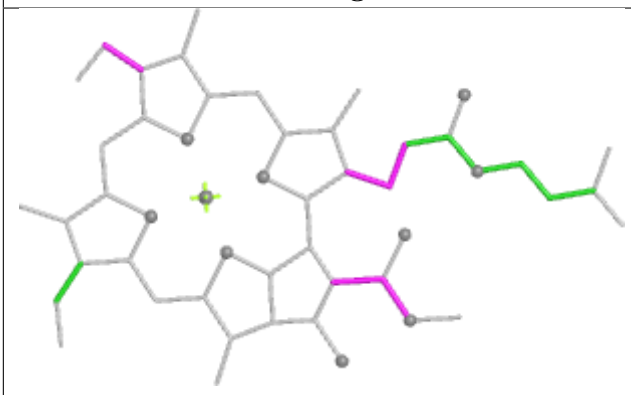


Bond angles



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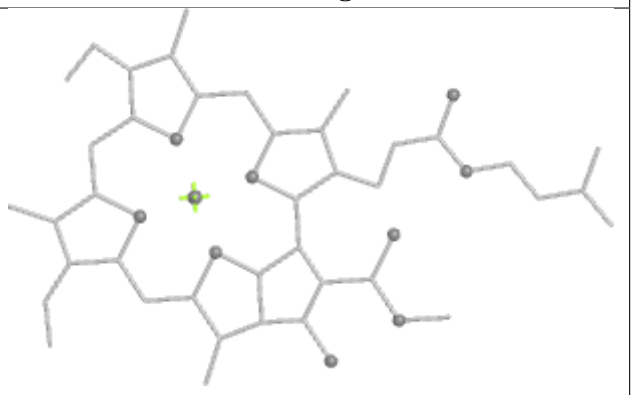
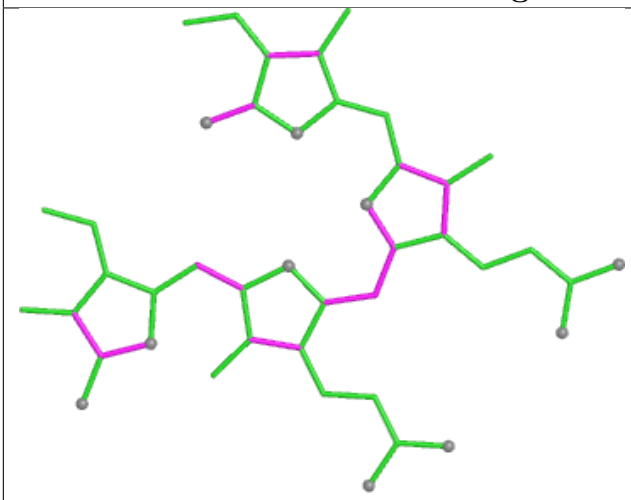


Rings

Ligand PEB BD 202



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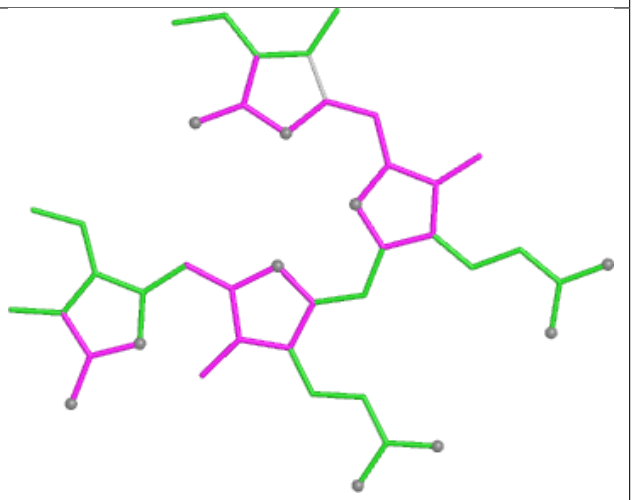
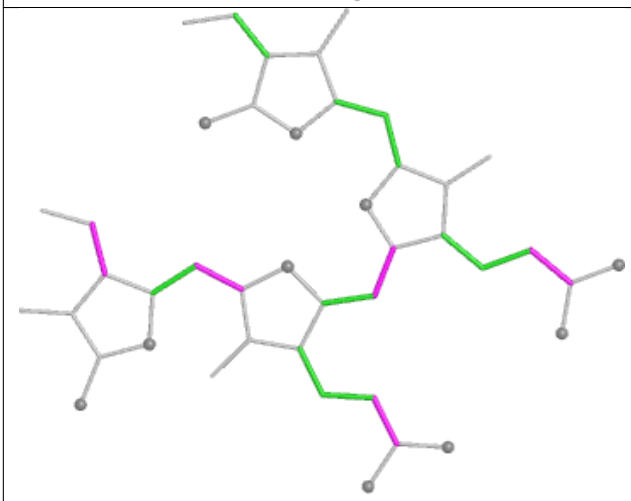


Bond angles



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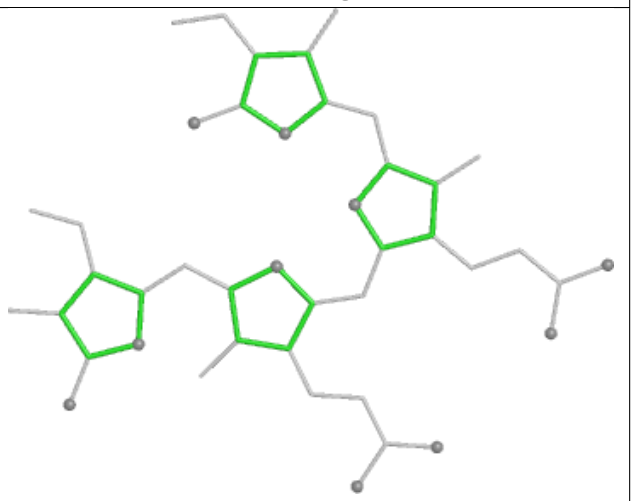
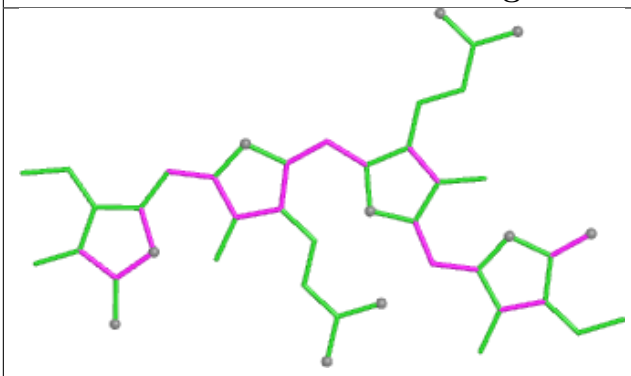


Rings

Ligand CYC K1 1001



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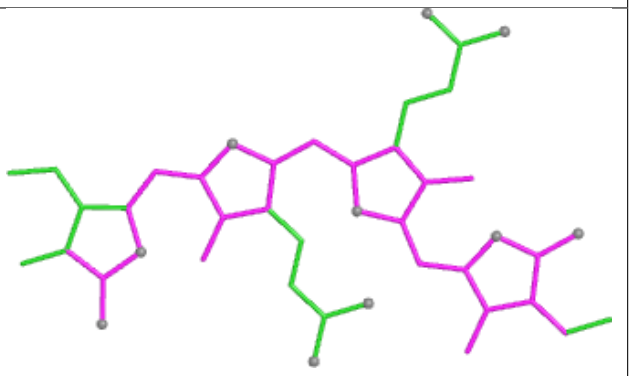
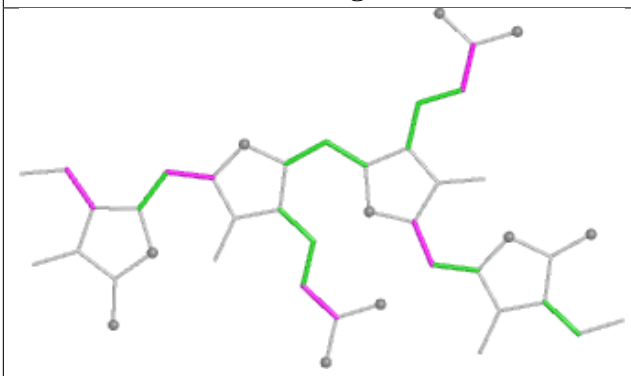


Bond angles



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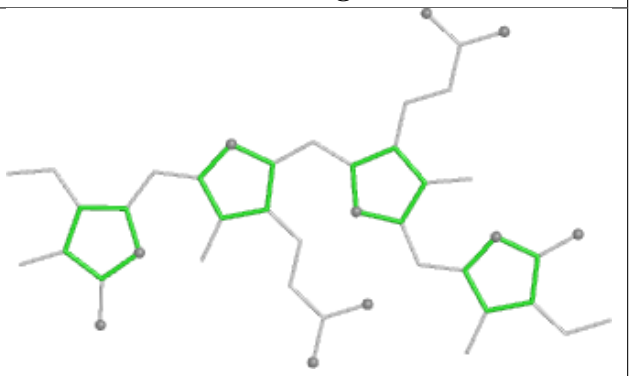
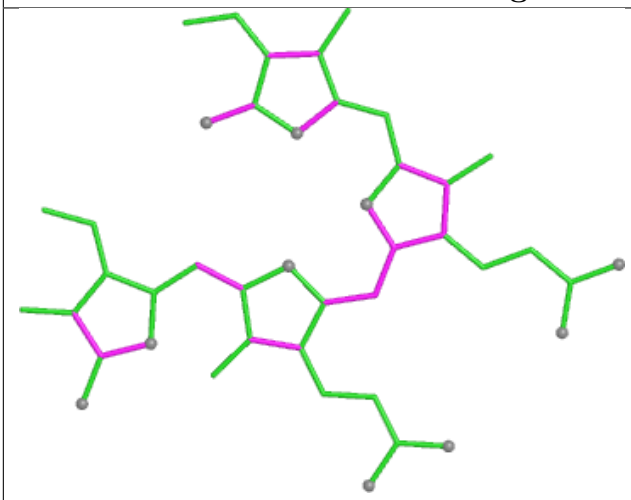
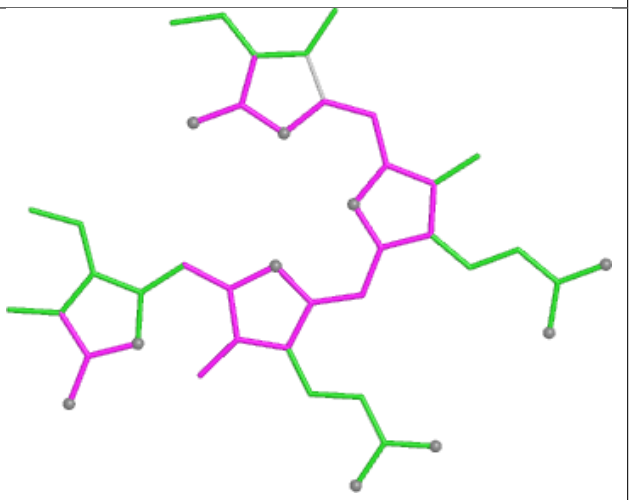


Rings

Ligand PEB KD 202



Bond lengths



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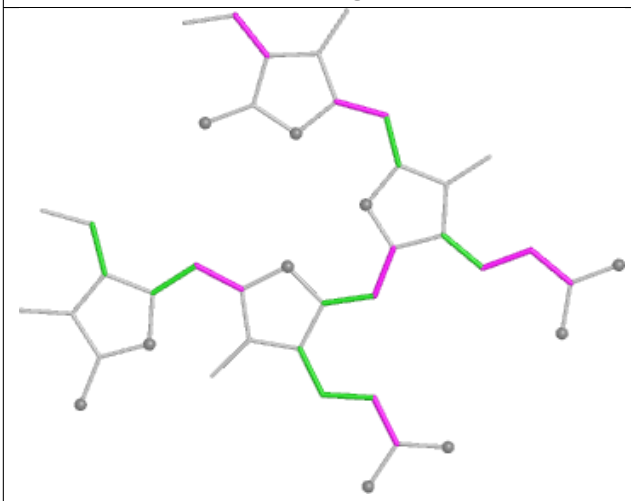

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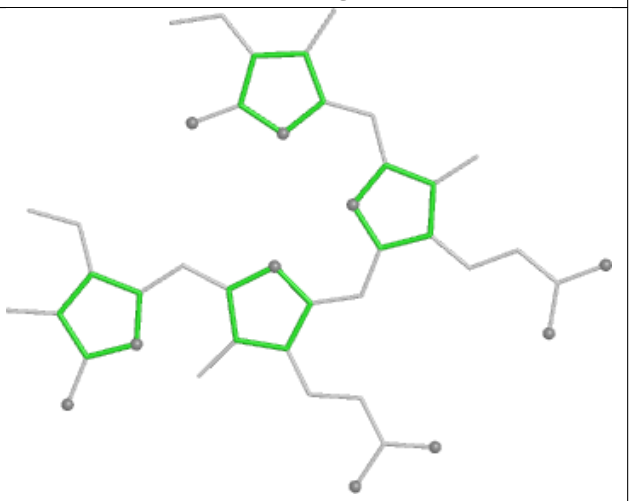
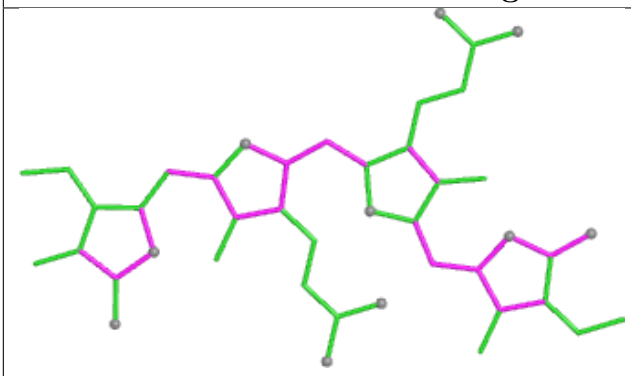


Rings

Ligand CYC BE 1001



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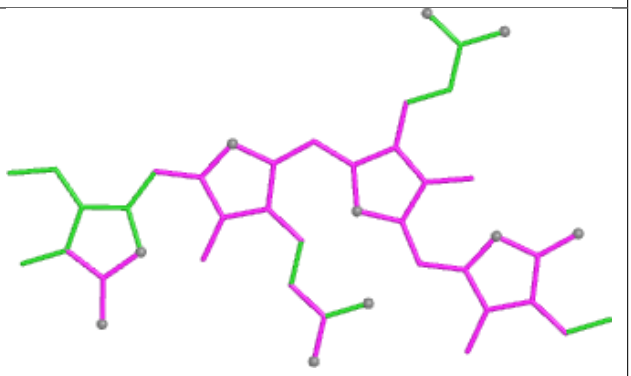

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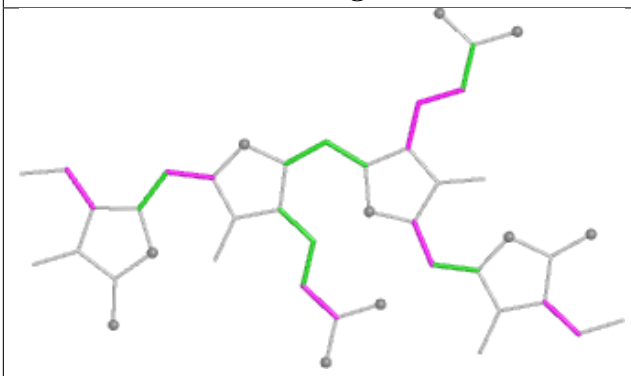

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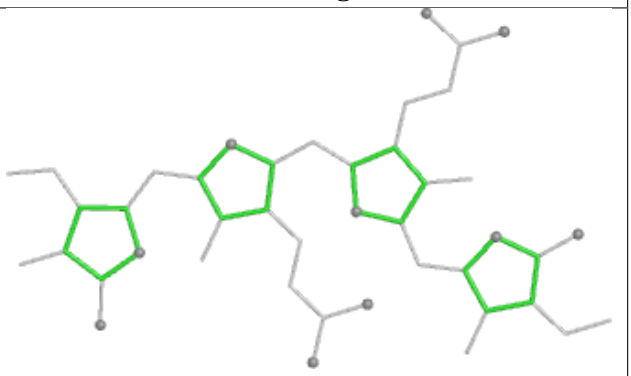
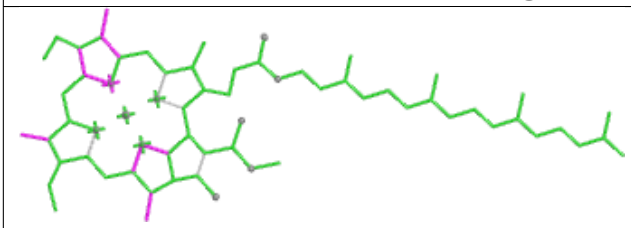


Rings

Ligand CLA c6 611



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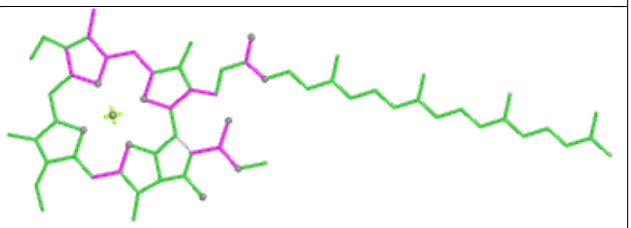

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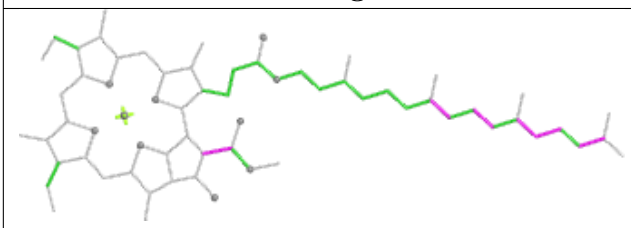

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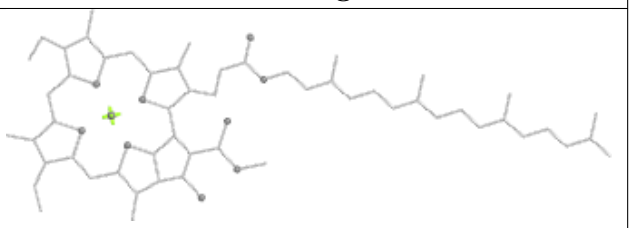
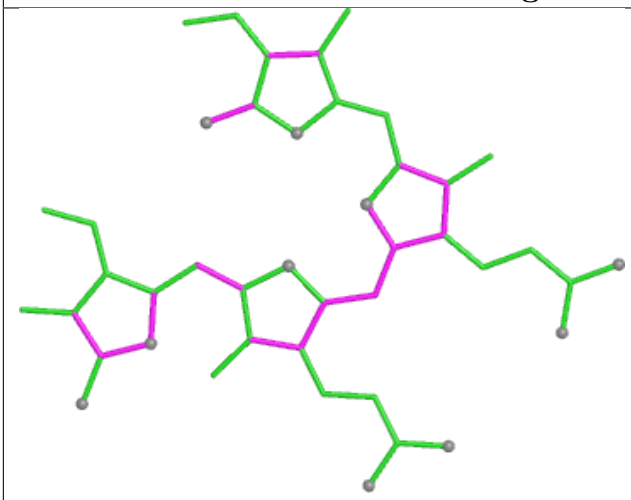


Rings

Ligand PEB JI 201



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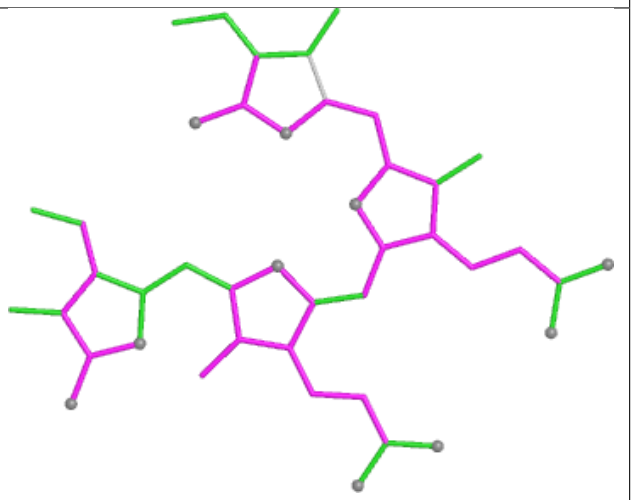

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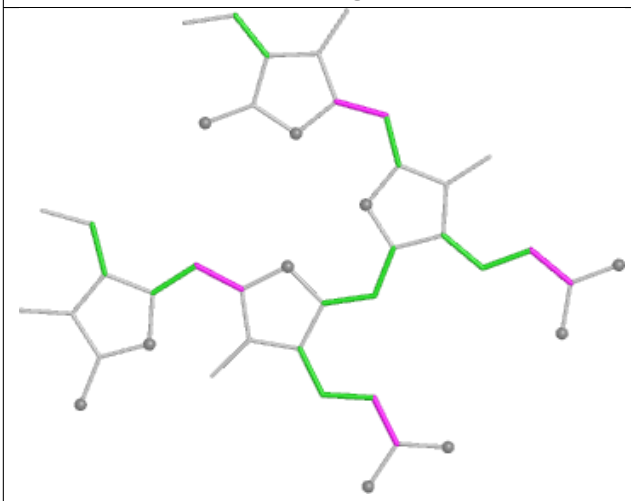

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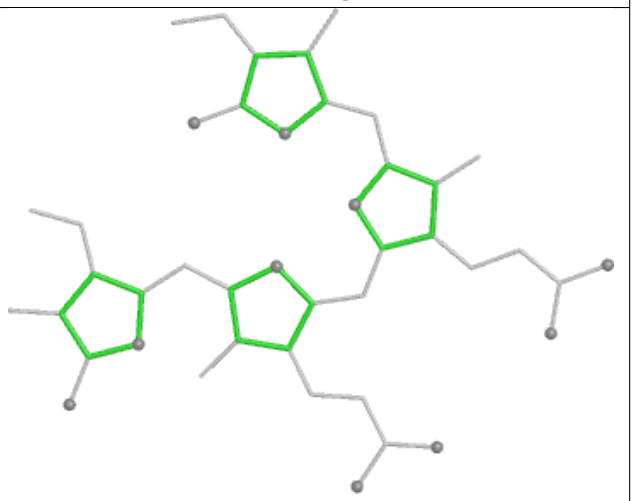

Rings

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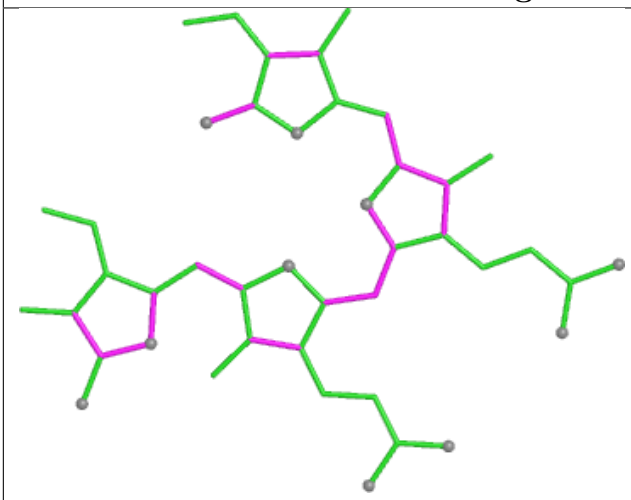

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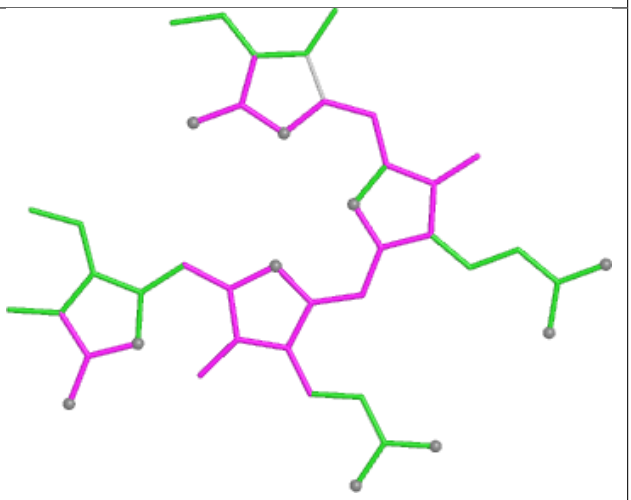

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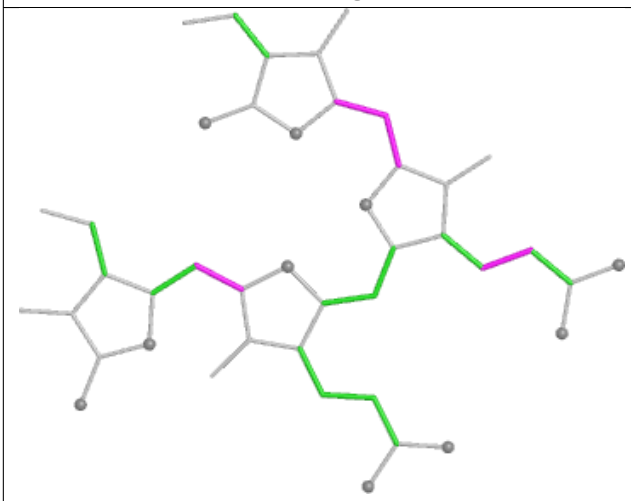

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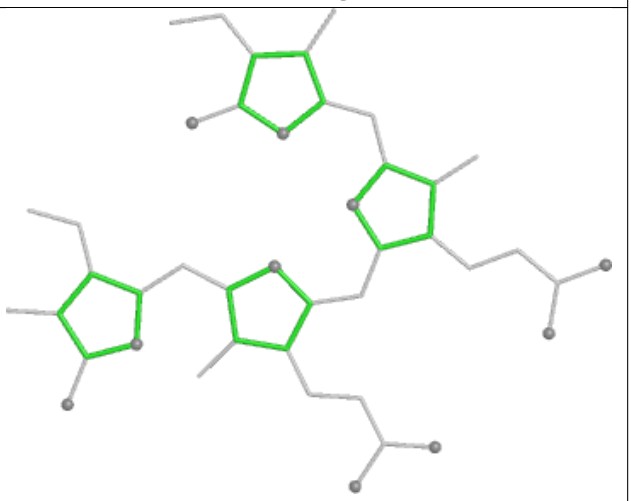

Rings

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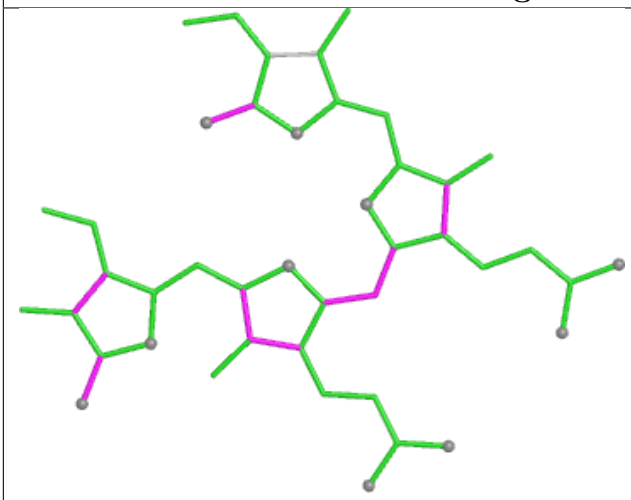

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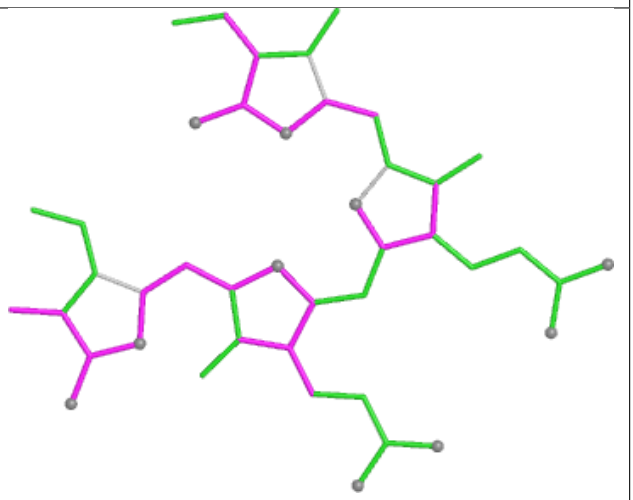

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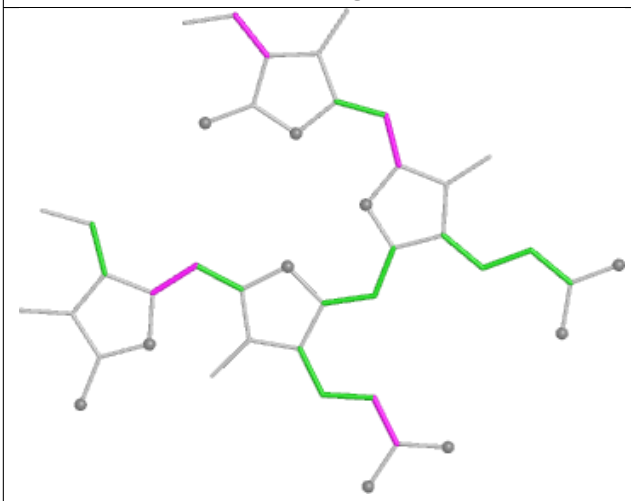

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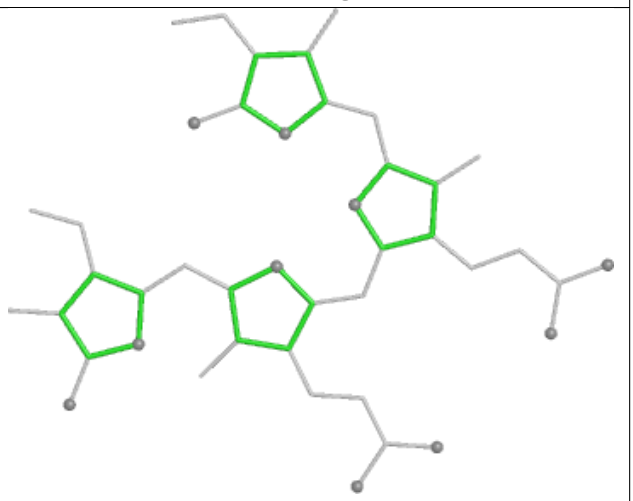
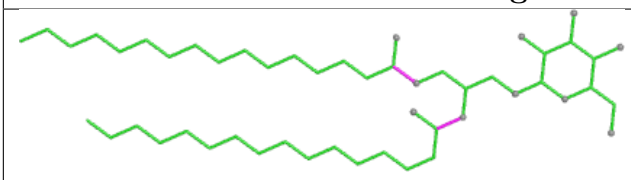


Rings

Ligand LMG A6 408



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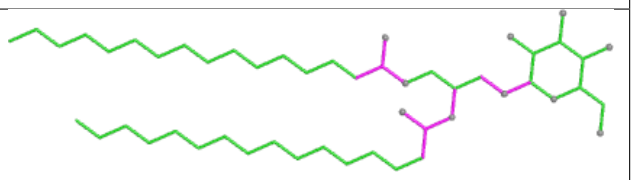

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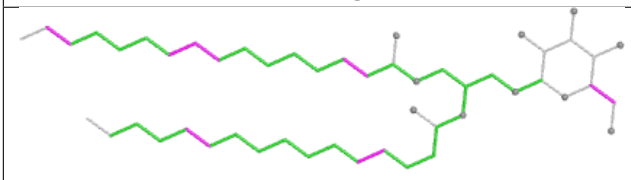

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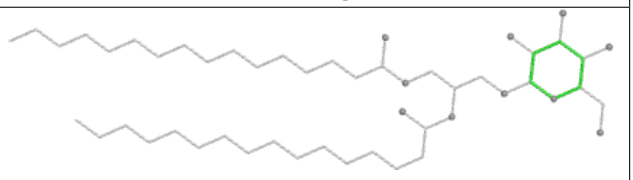
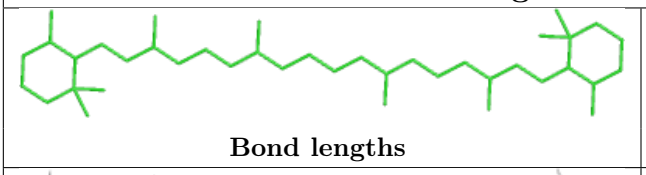


Rings

Ligand BCR CL 501



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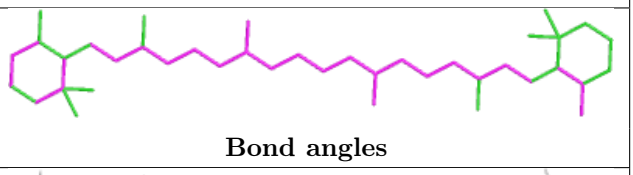

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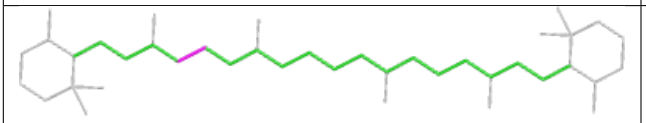

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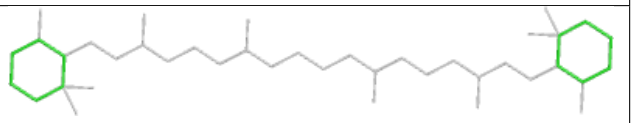
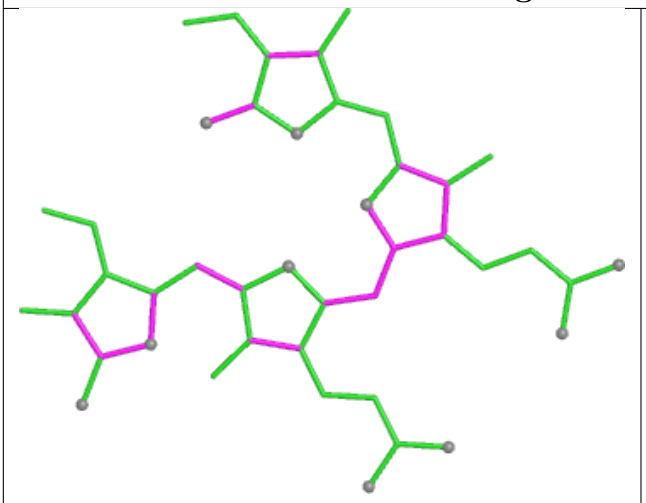


Rings

Ligand PEB VJ 202



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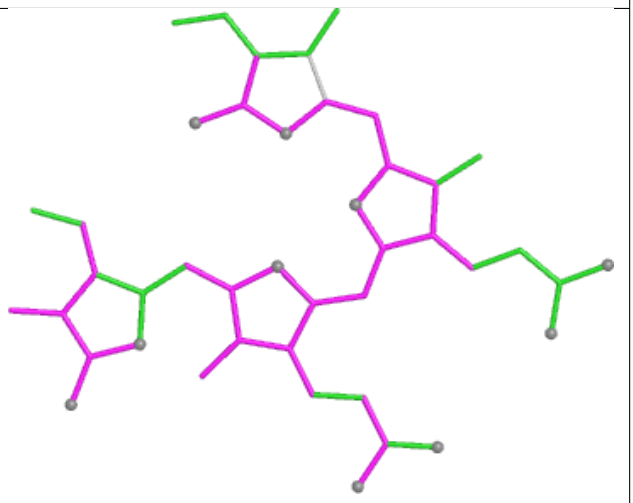

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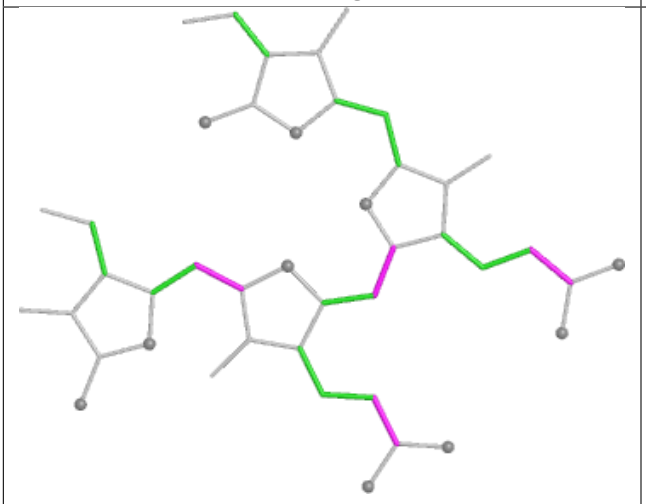

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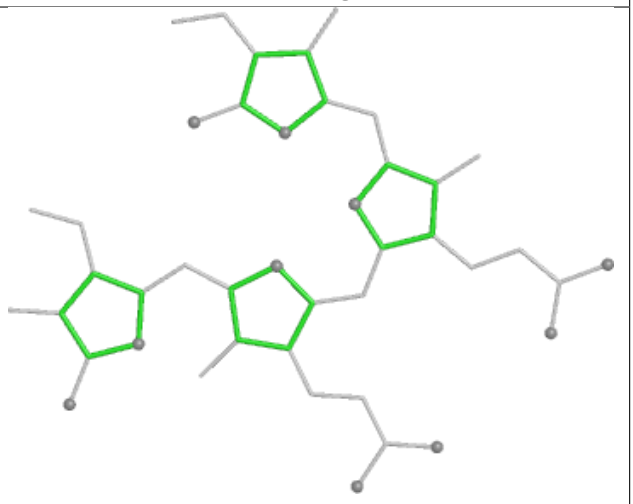
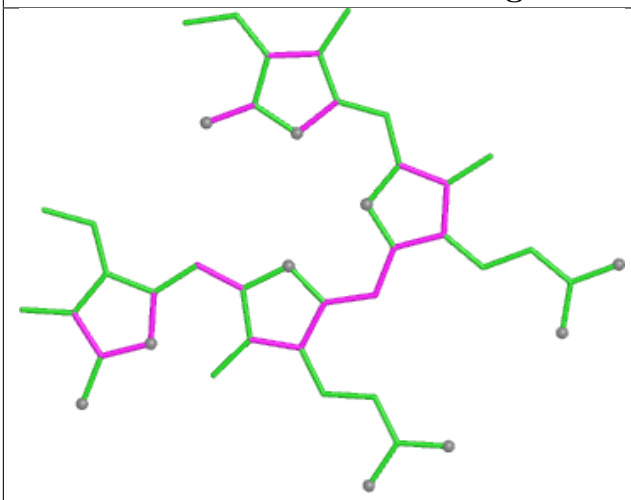


Rings

Ligand PEB N1 1002



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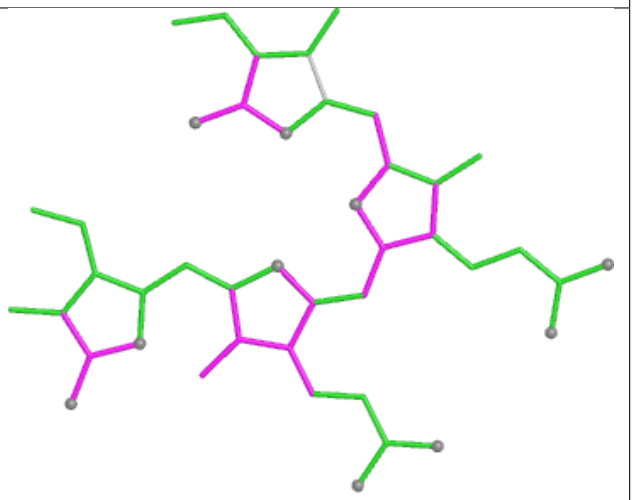

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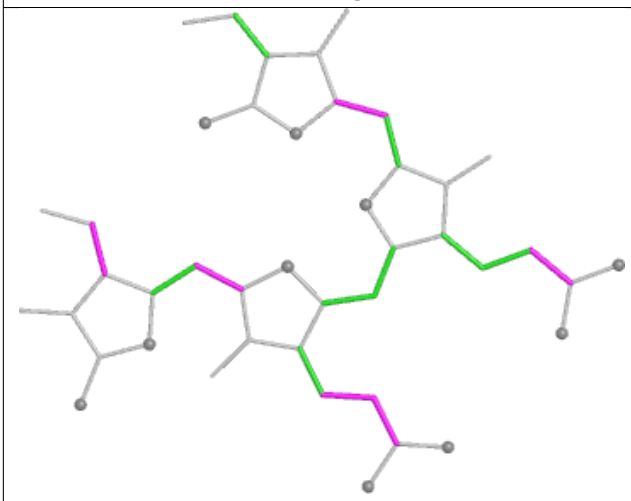

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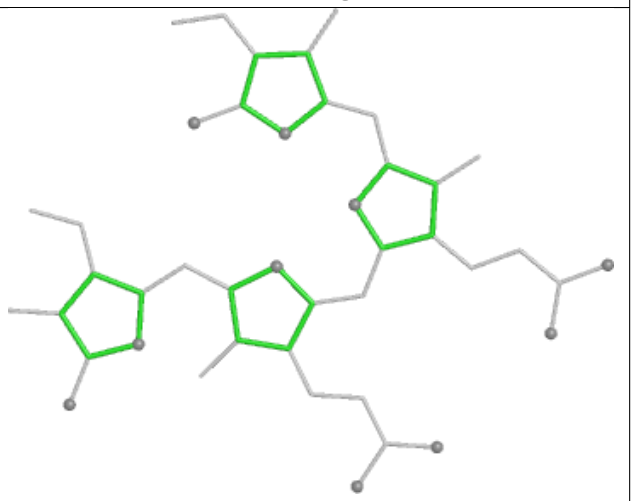

Rings

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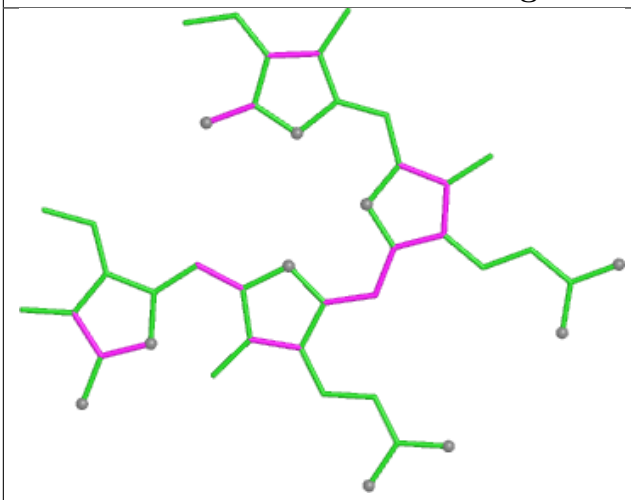

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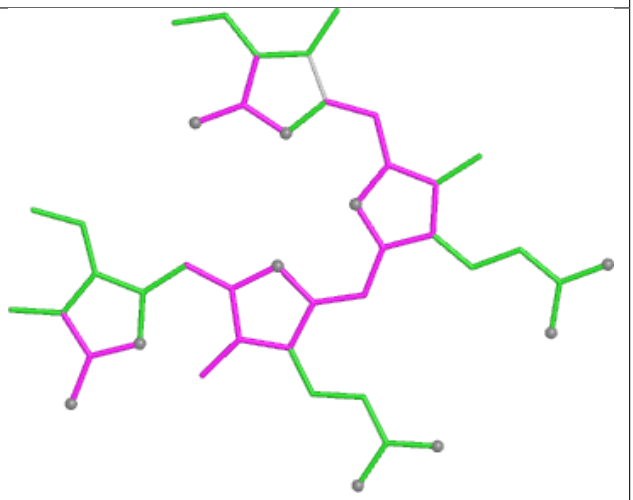

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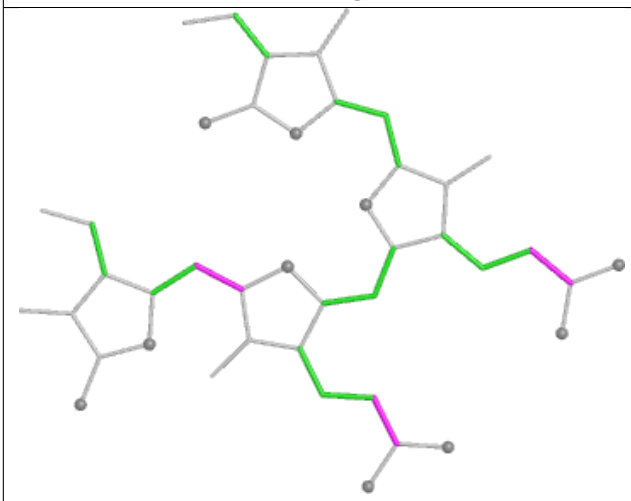

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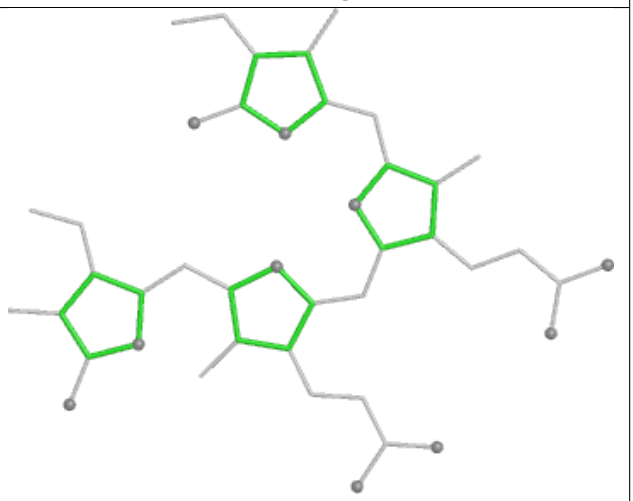
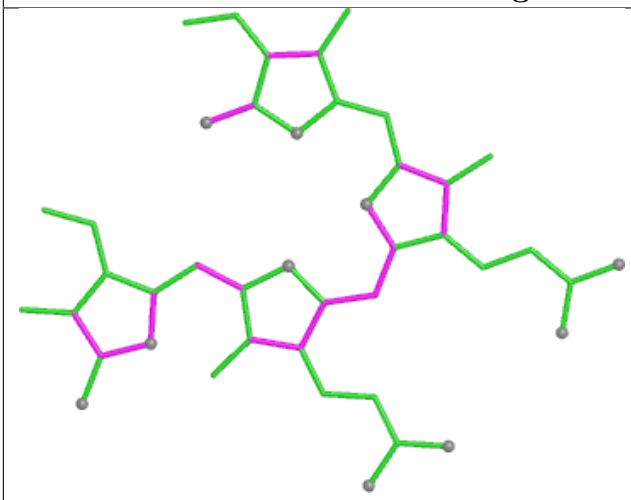


Rings

Ligand PEB XP 201



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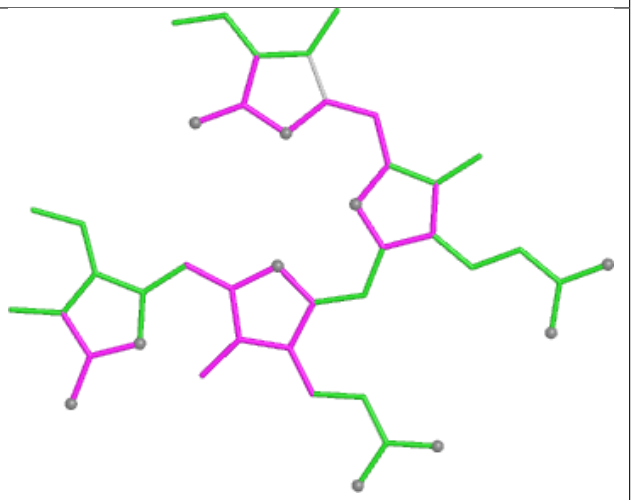

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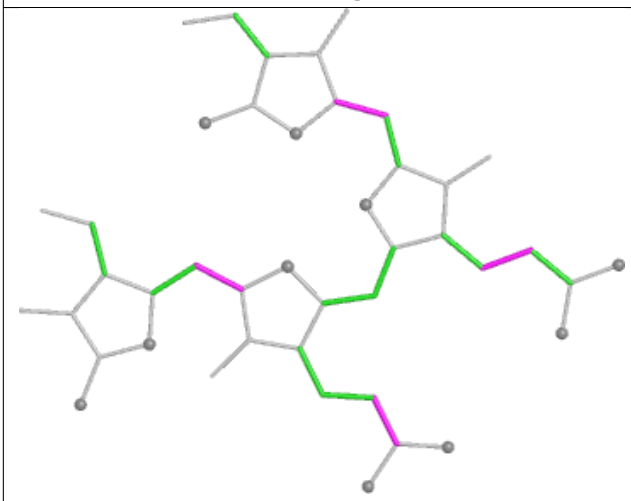

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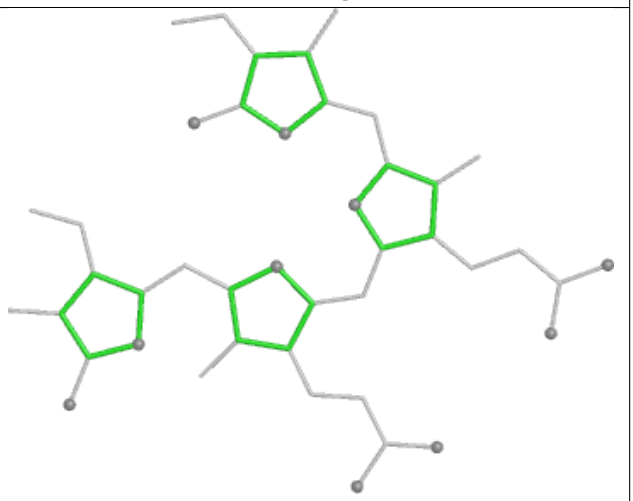
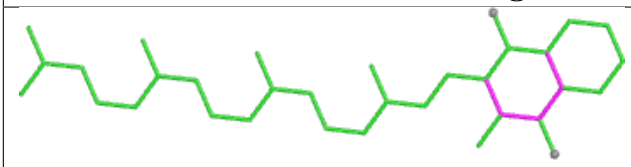


Rings

Ligand PQN BN 837



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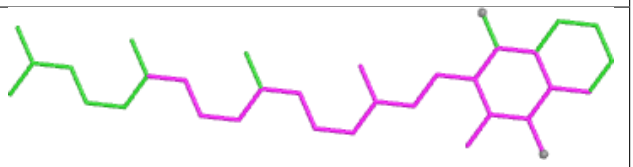
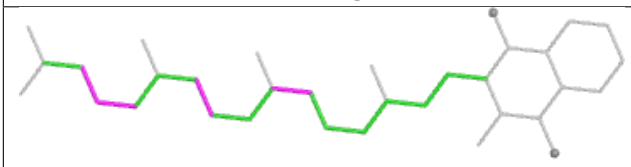


Bond angles



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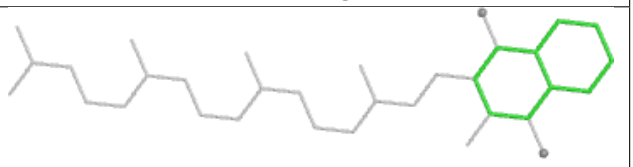
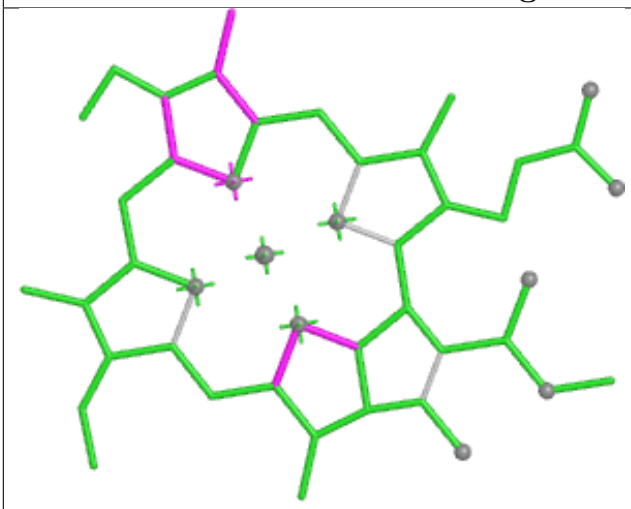


Rings

Ligand CLA 22 606



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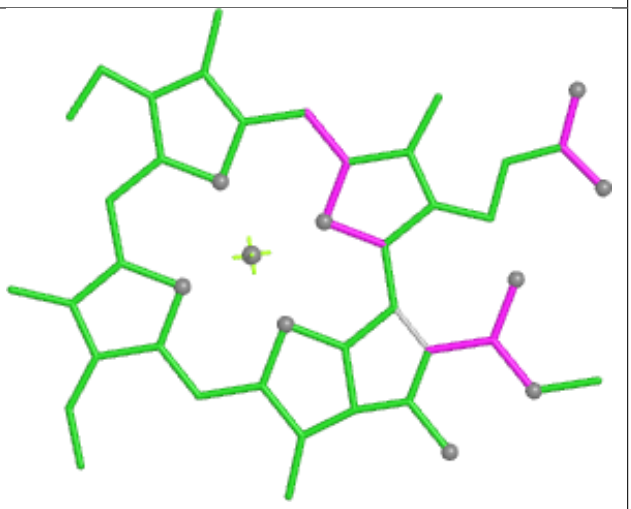

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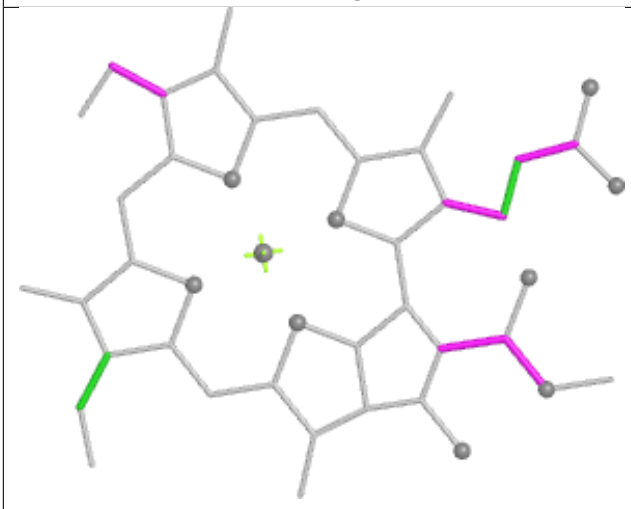
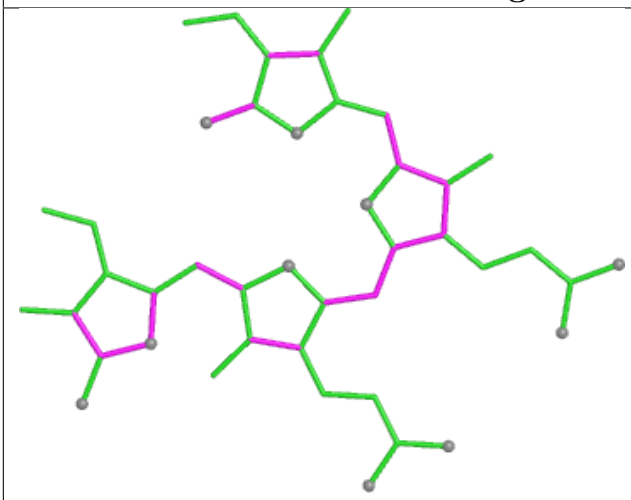


Torsions



Rings

Ligand PEB mG 202



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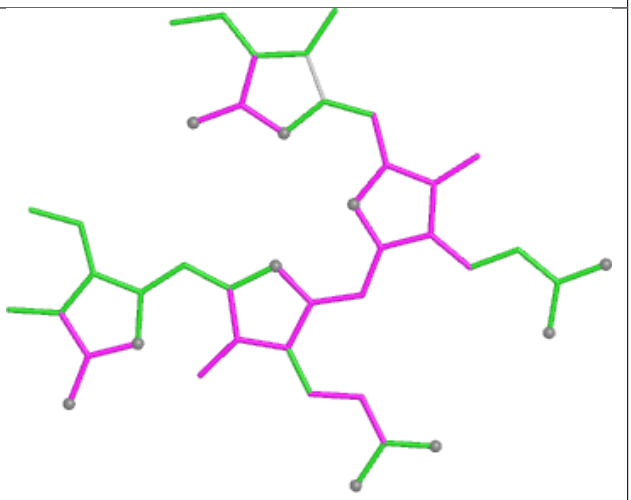
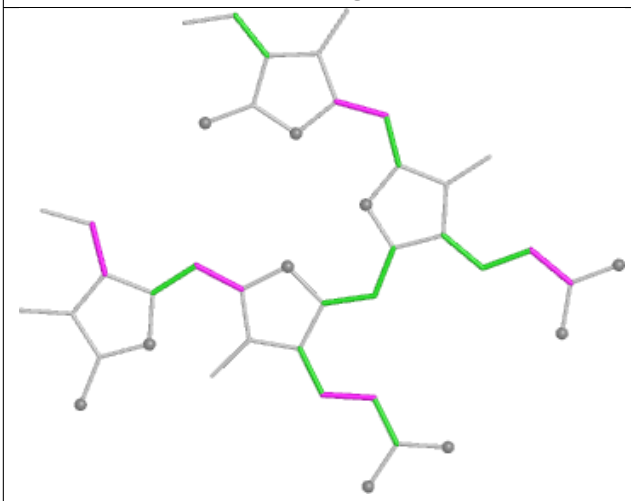


Bond angles



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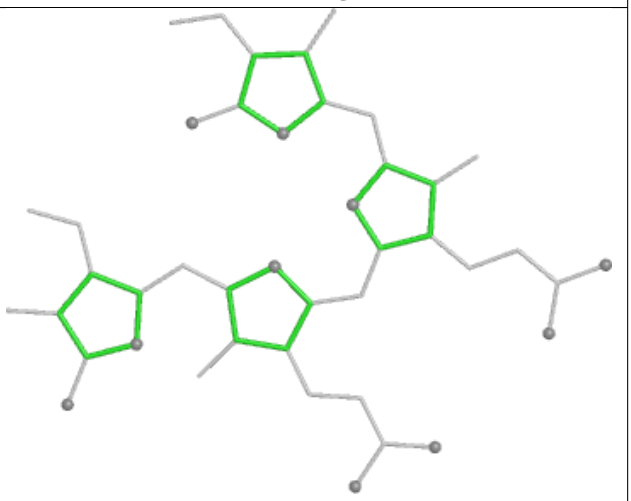
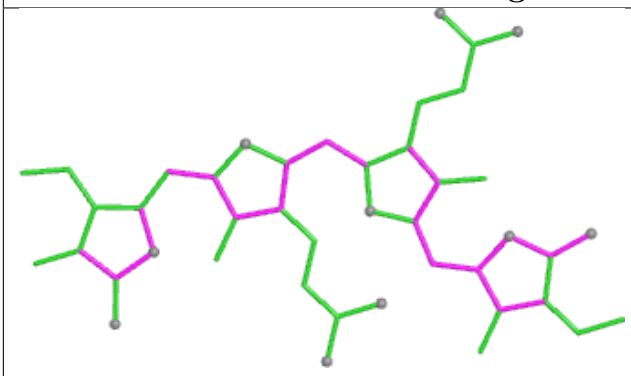


Rings

Ligand CYC J1 1001



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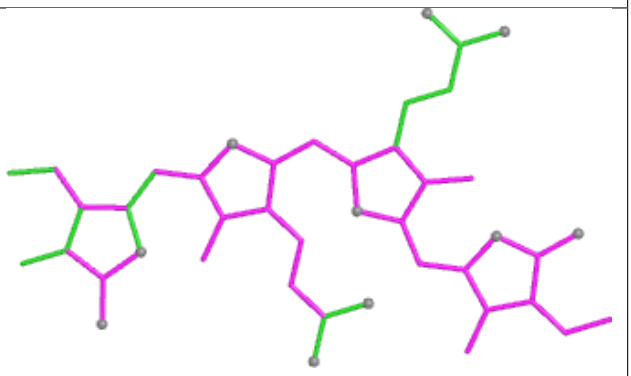

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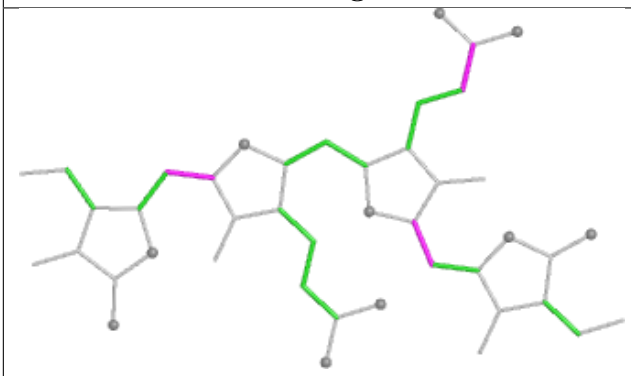
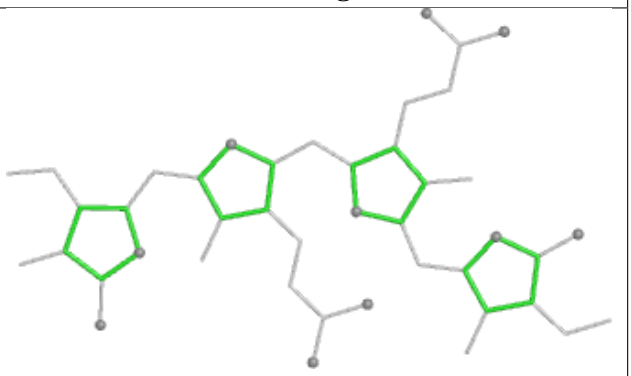
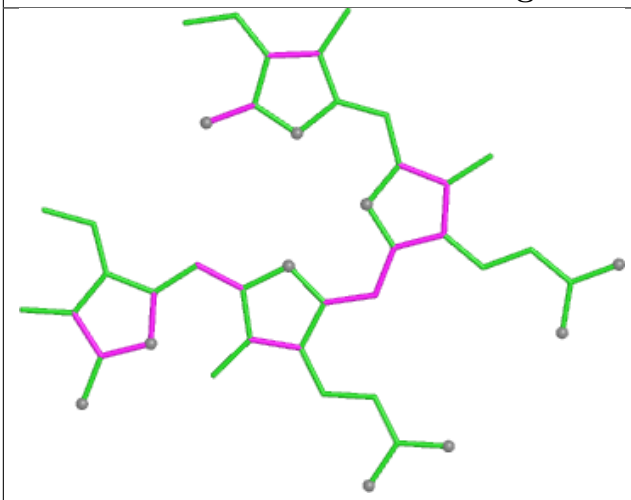


Torsions



Rings

Ligand PEB EJ 201



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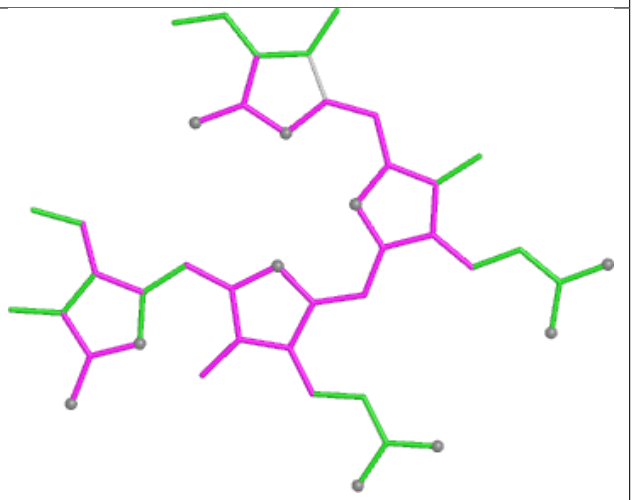

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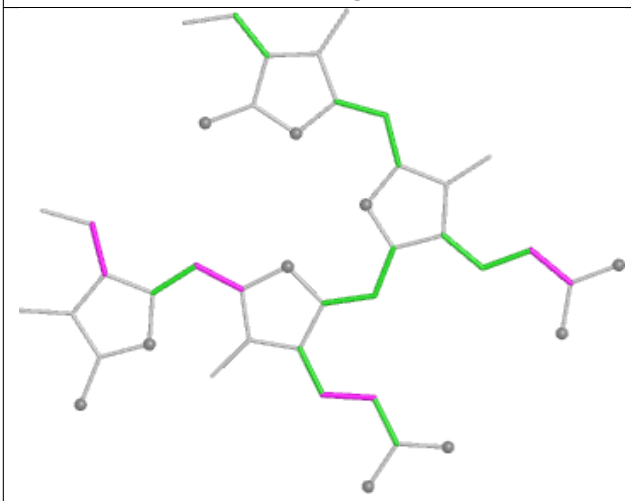

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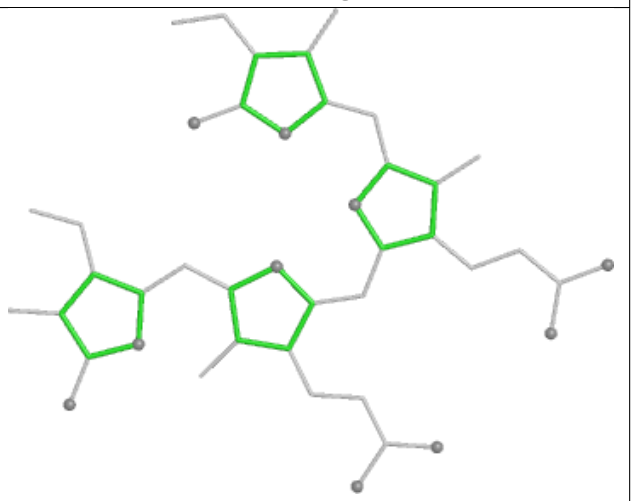
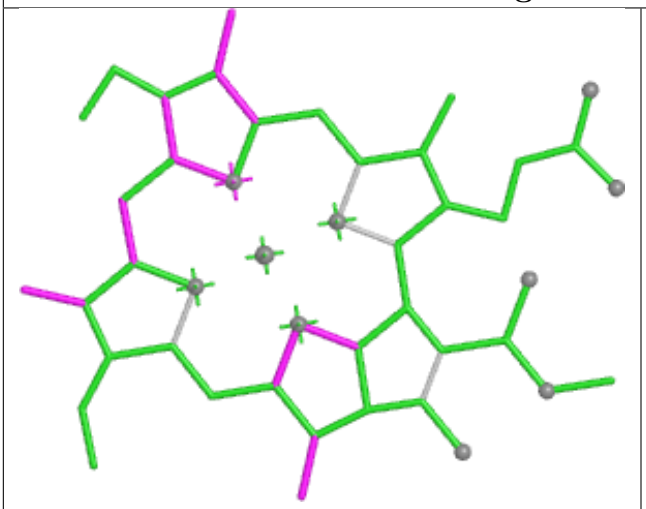


Rings

Ligand CLA R2 204



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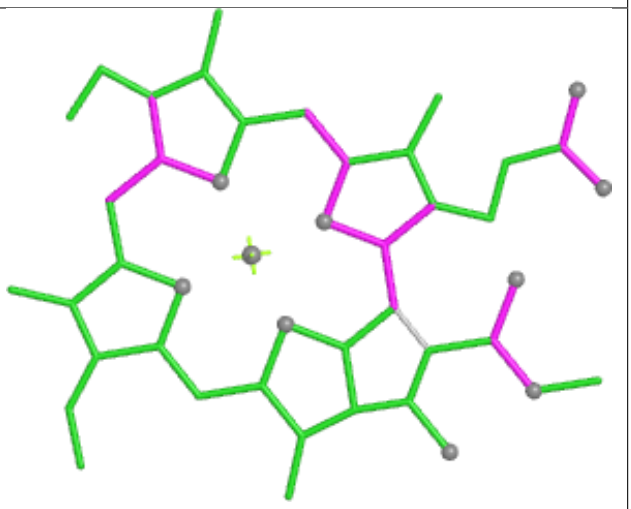

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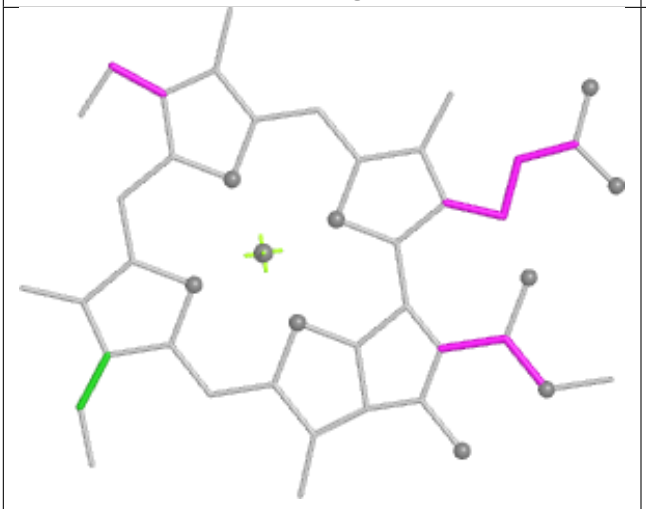
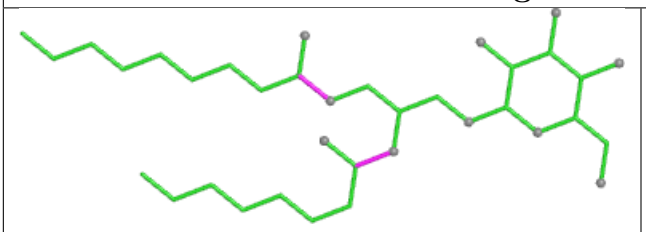


Torsions



Rings

Ligand LMG b6 624



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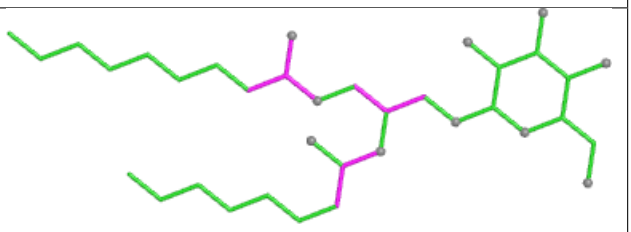

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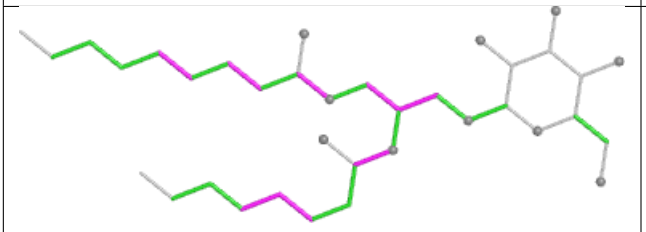

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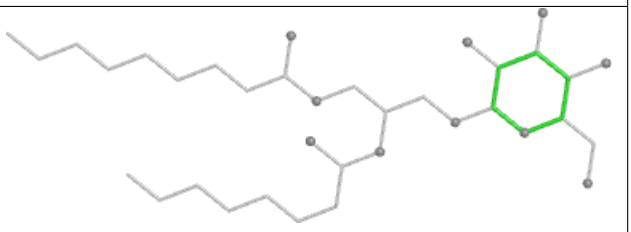
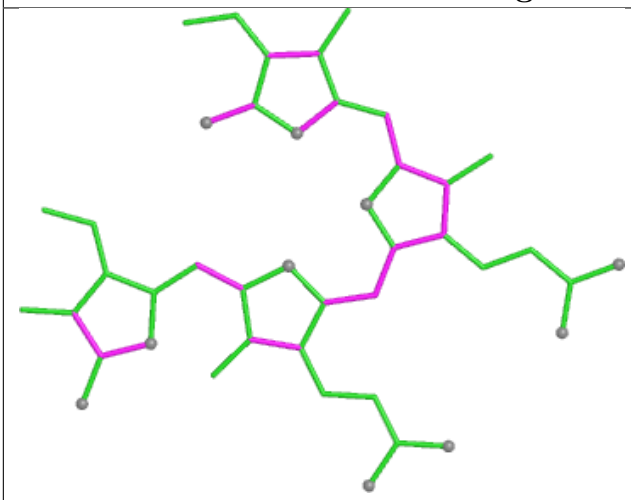


Rings

Ligand PEB eH 202



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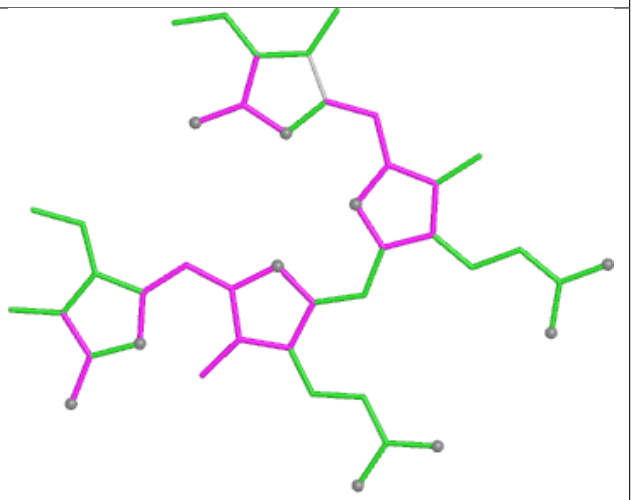

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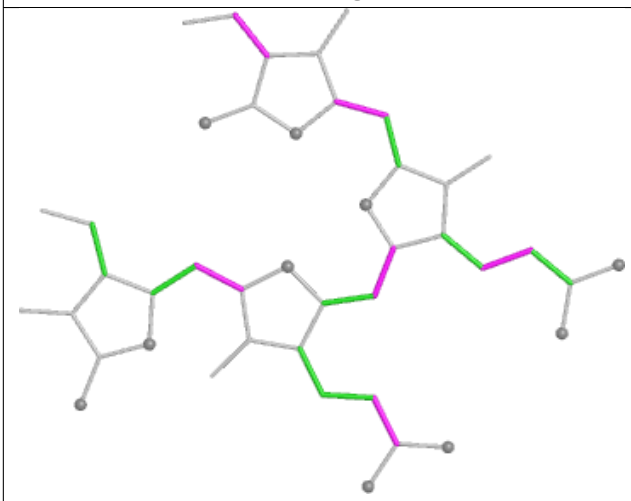

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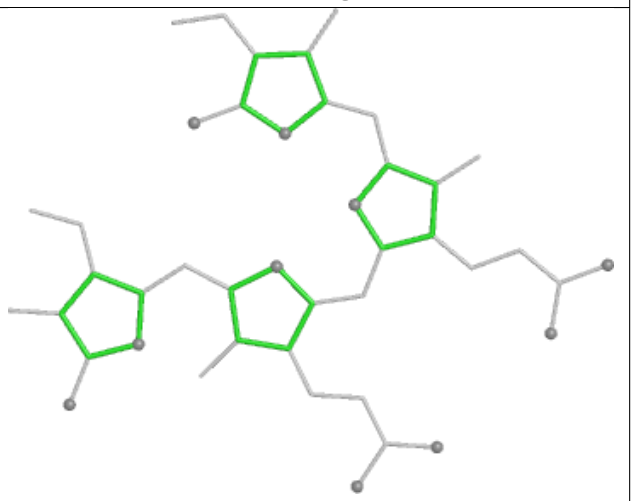
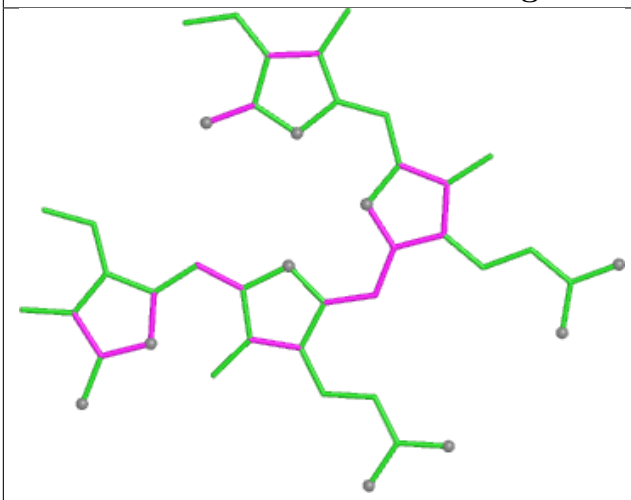


Rings

Ligand PEB jF 202



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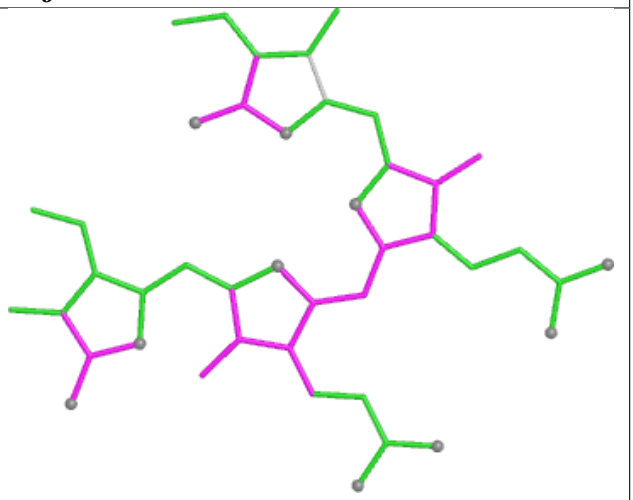

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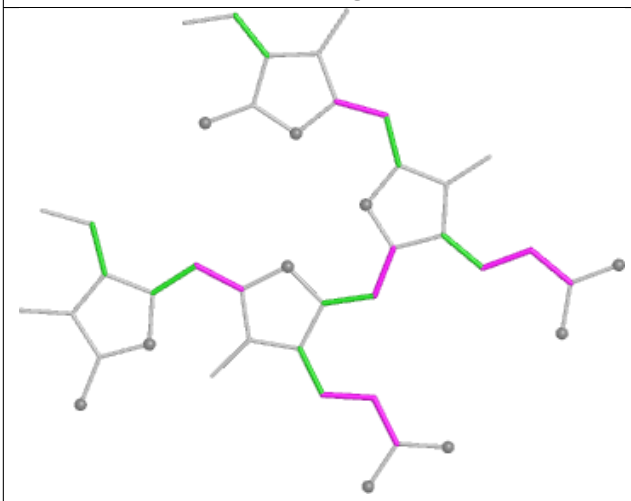

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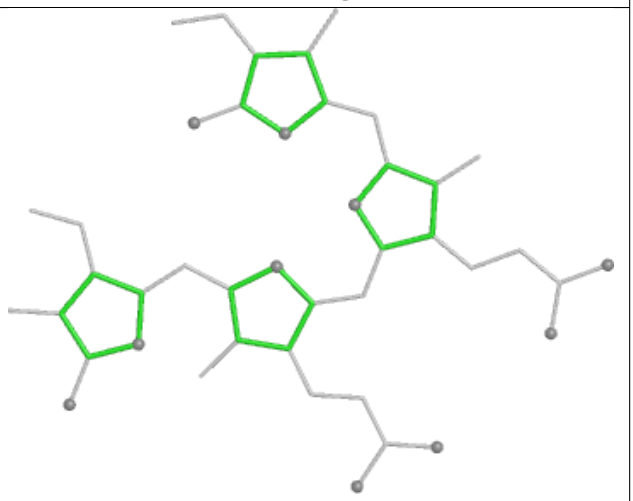
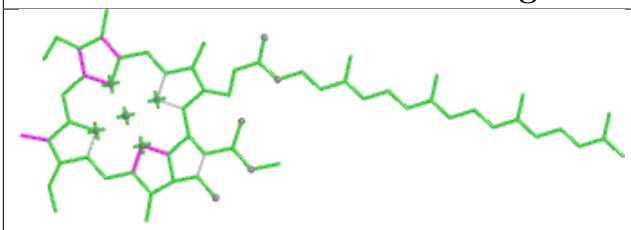


Rings

Ligand CLA 12 602



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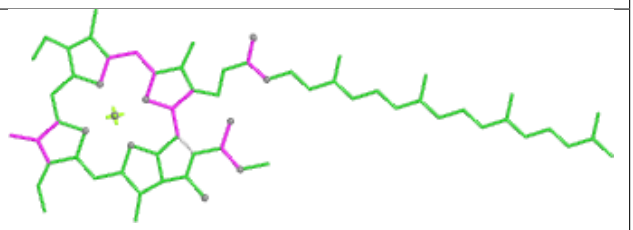

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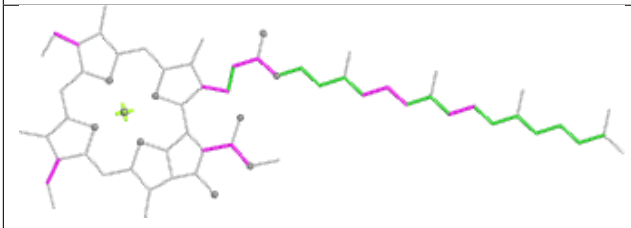

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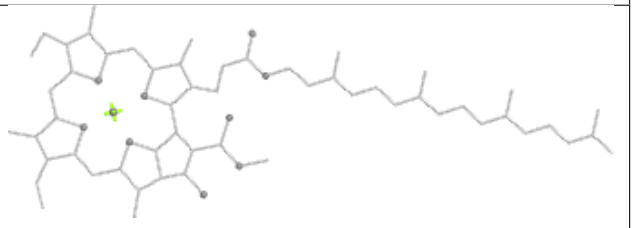
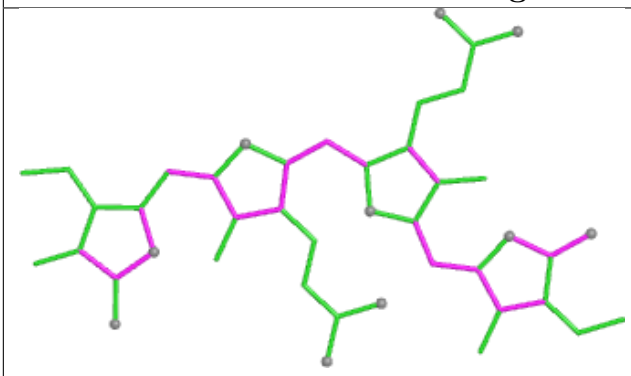


Rings

Ligand CYC e3 1001



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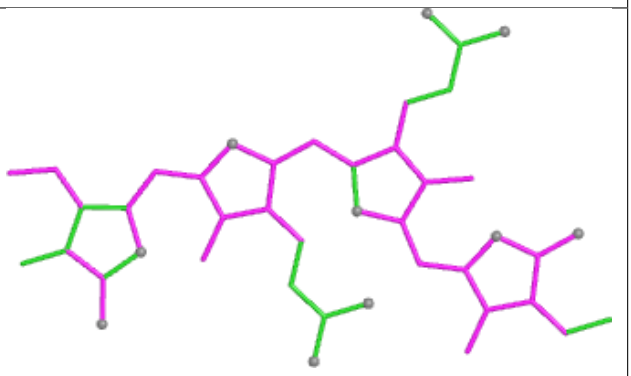

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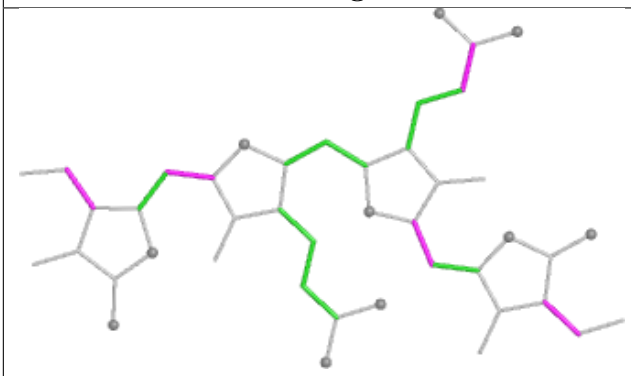

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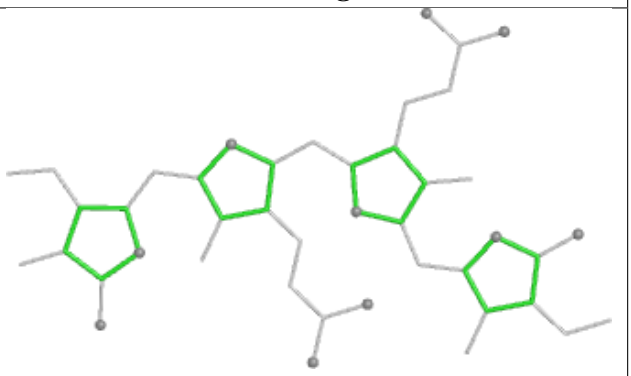
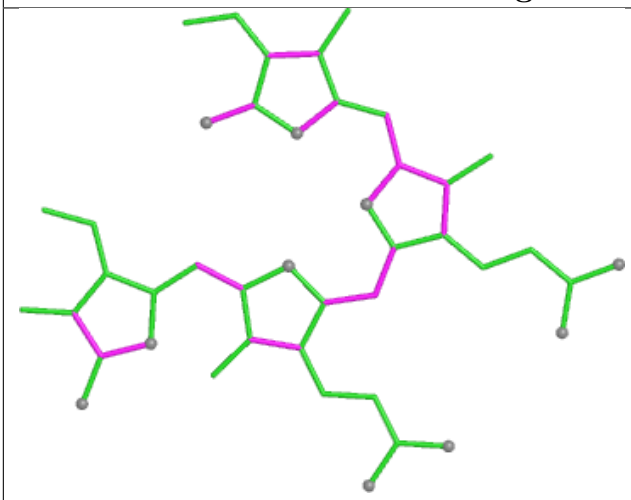


Rings

Ligand PEB O9 202



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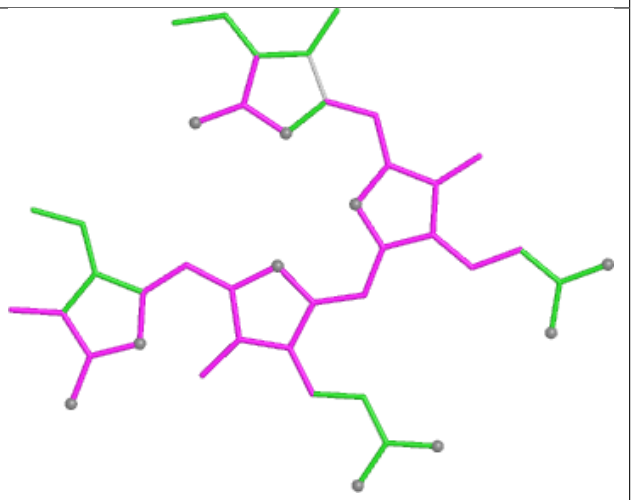

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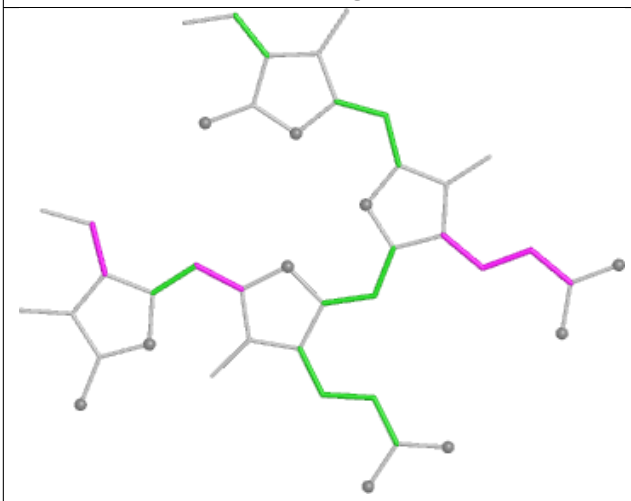

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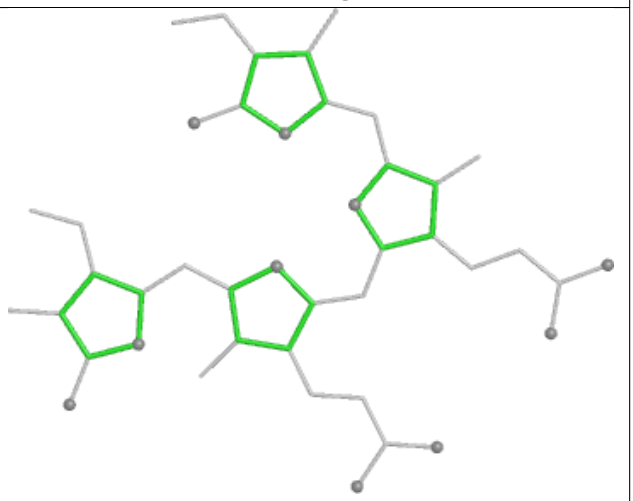
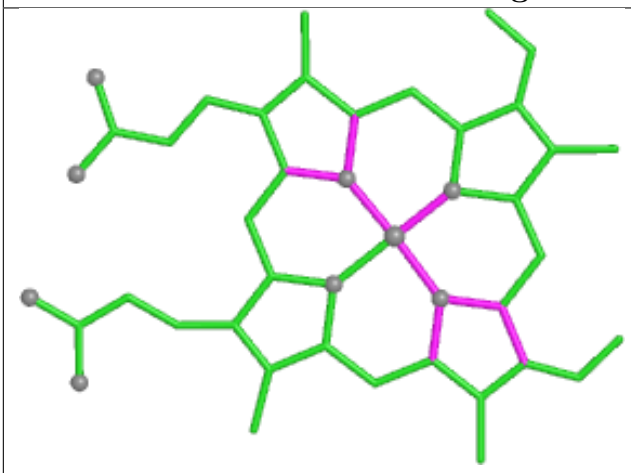


Rings

Ligand HEM E6 101



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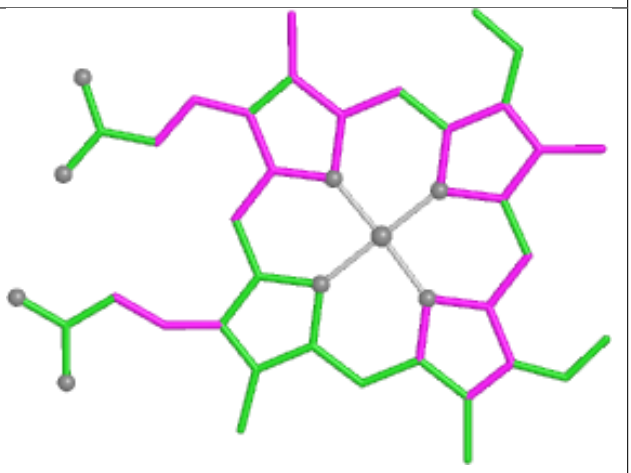

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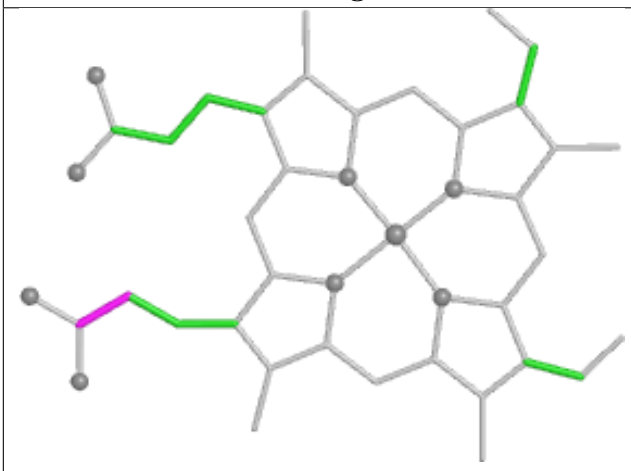

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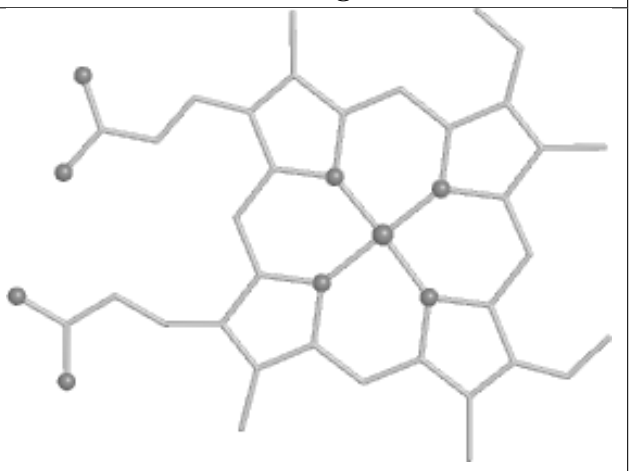
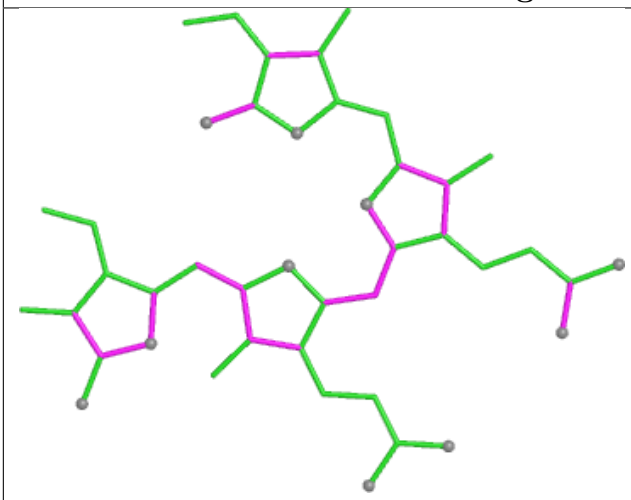


Rings

Ligand PEB SF 202



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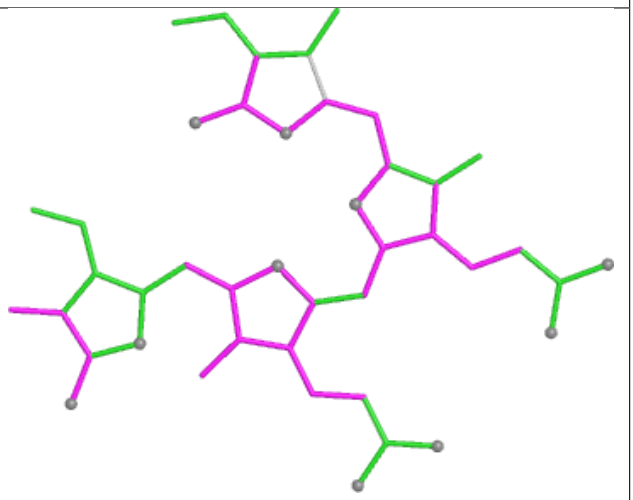

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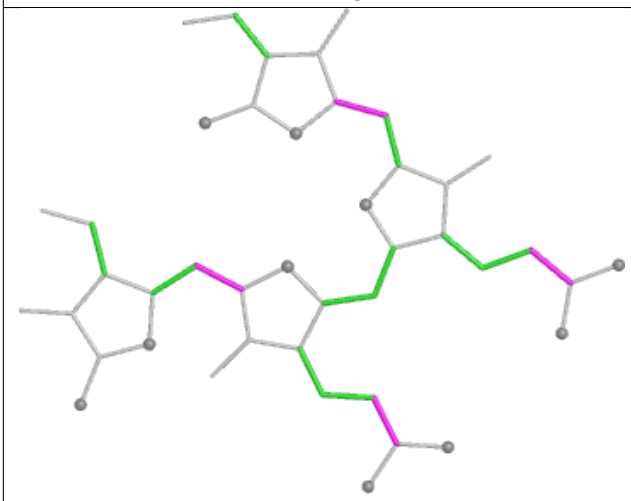

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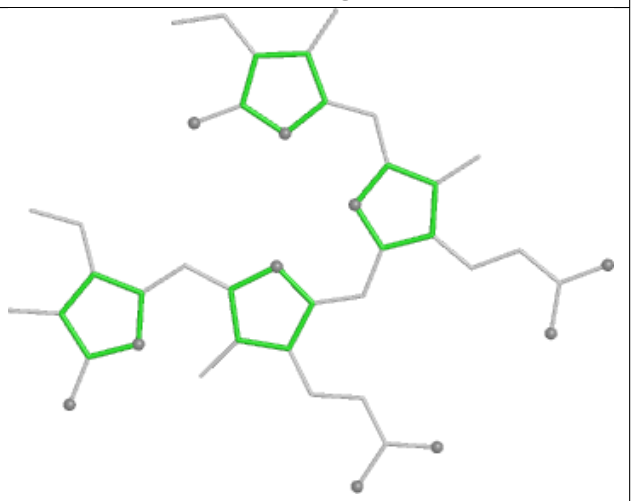
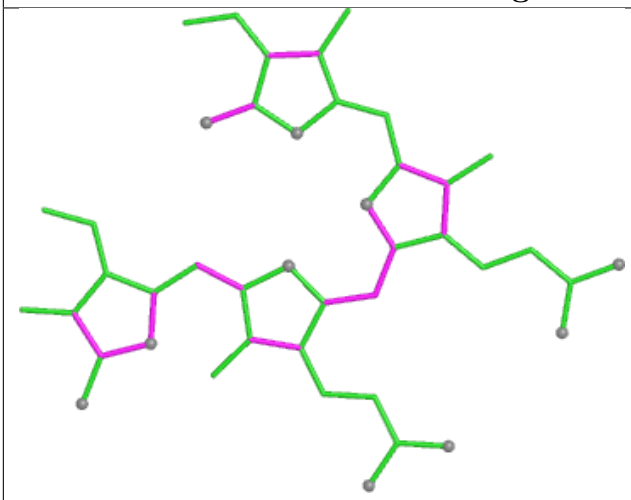


Rings

Ligand PEB PO 201



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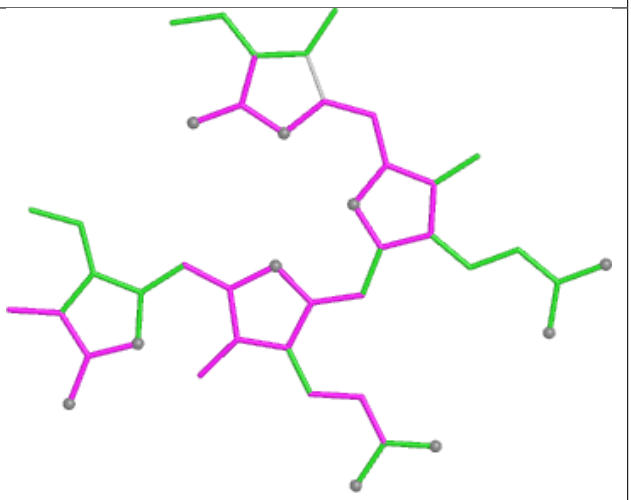

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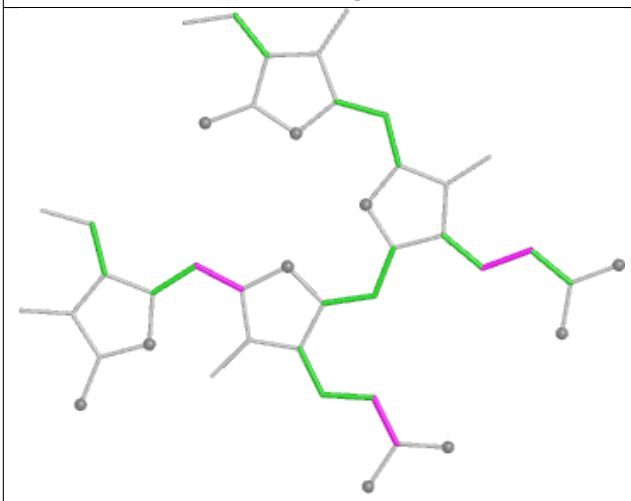

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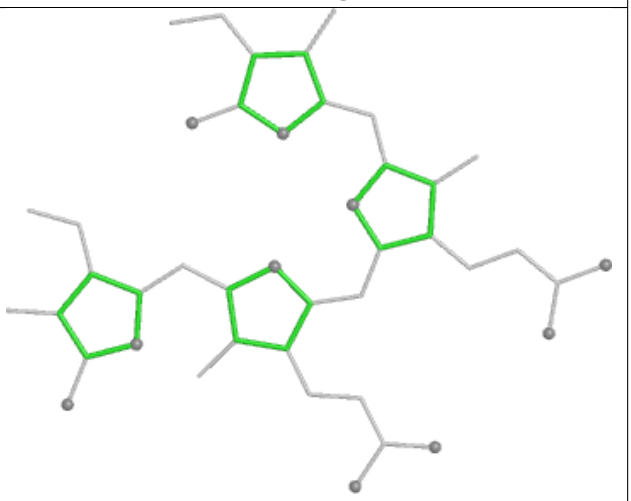
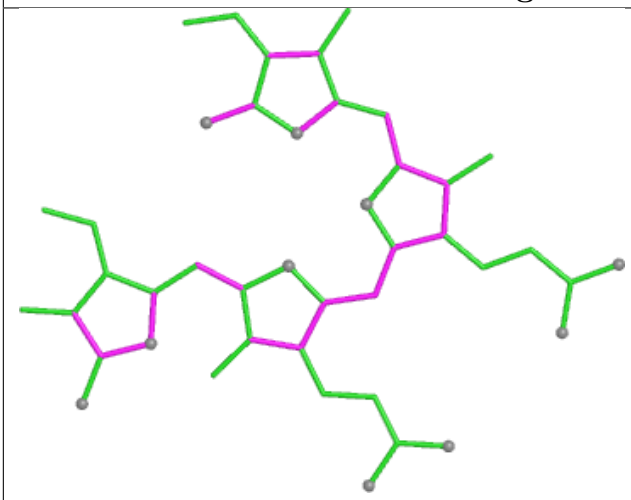


Rings

Ligand PEB nF 202



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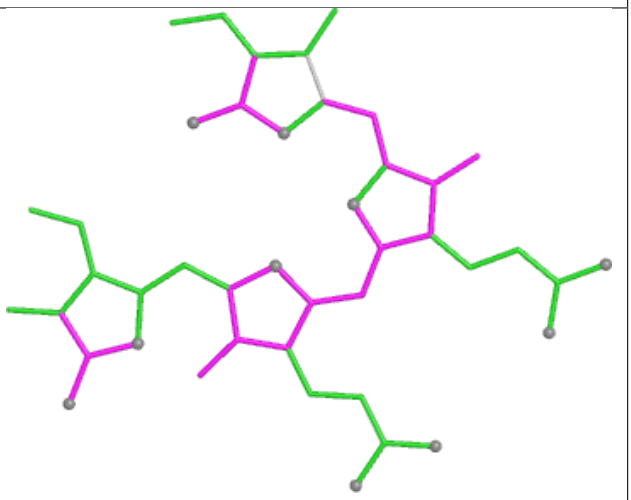
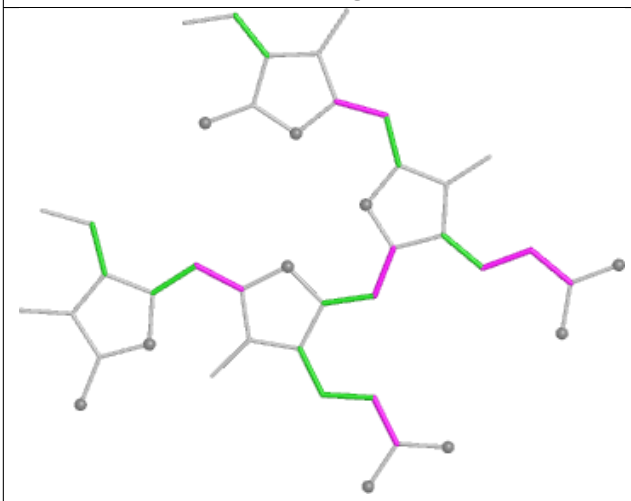


Bond angles



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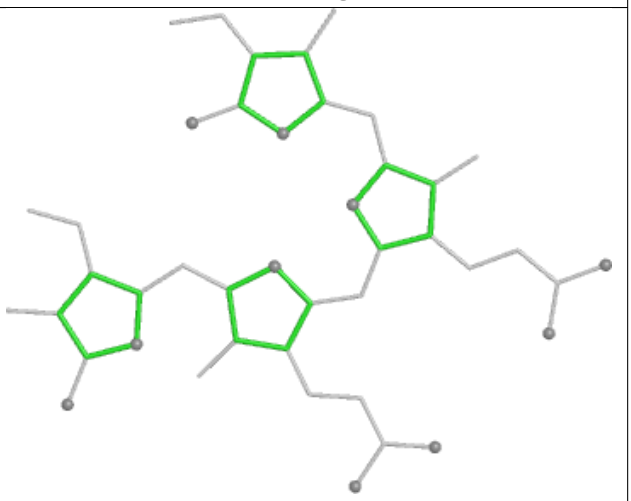
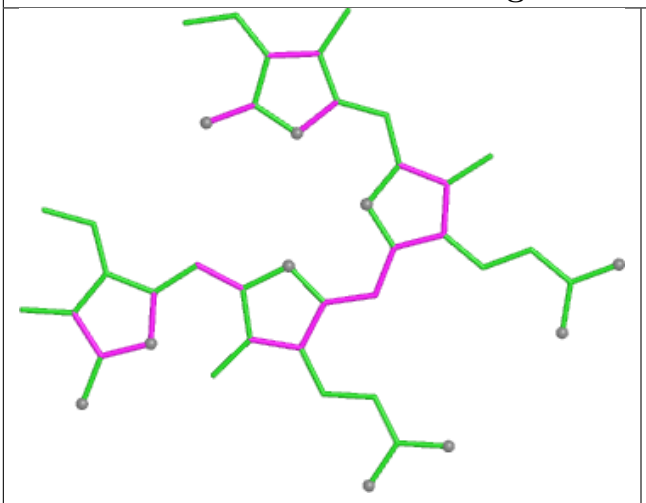


Rings

Ligand PEB YM 203



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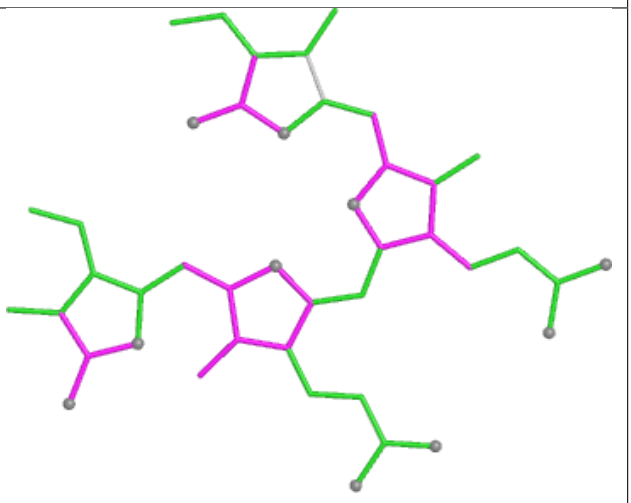

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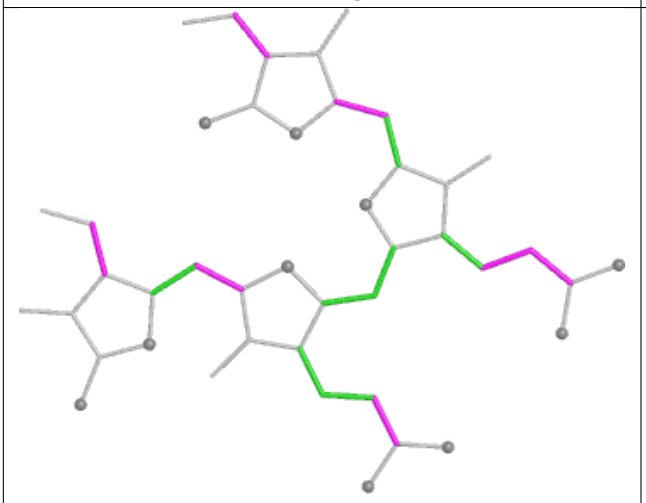

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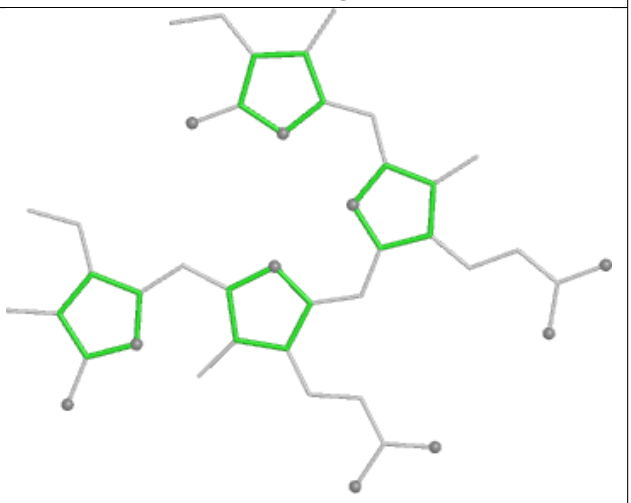
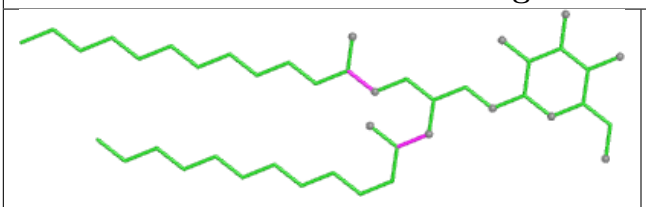


Rings

Ligand LMG JL 102



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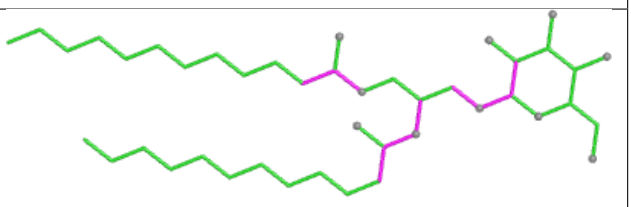
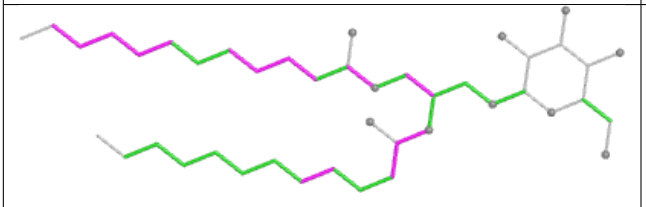


Bond angles



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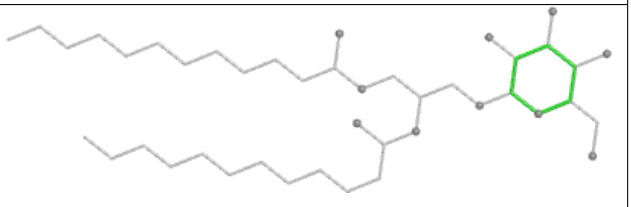
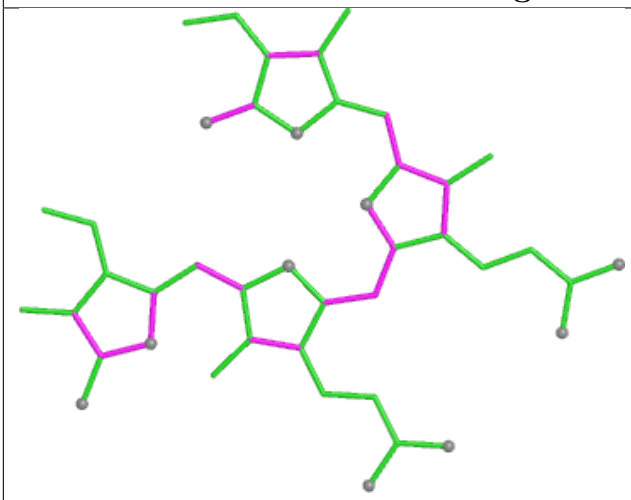


Rings

Ligand PEB EP 203



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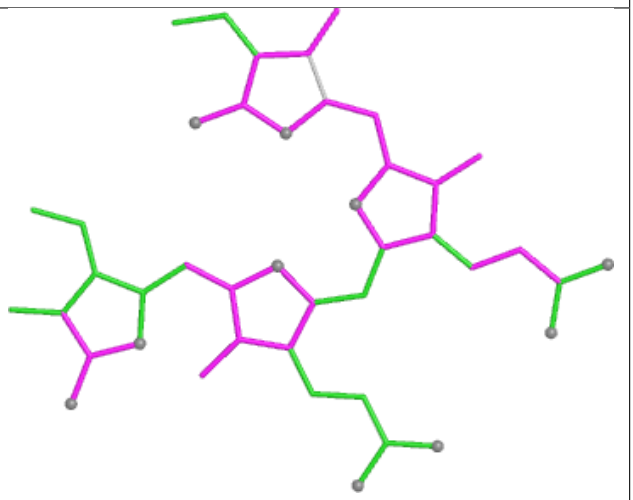

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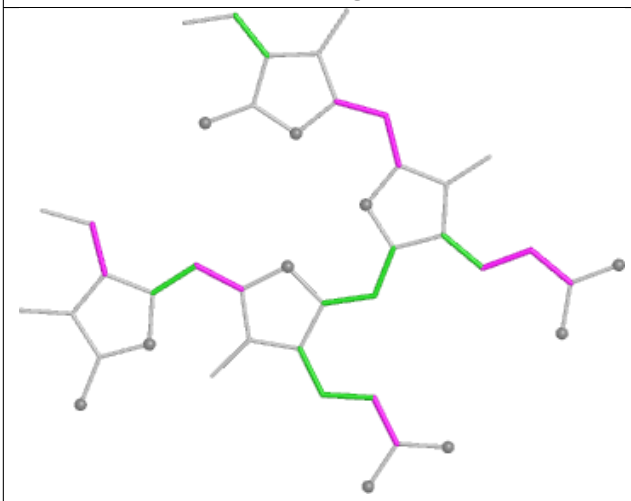
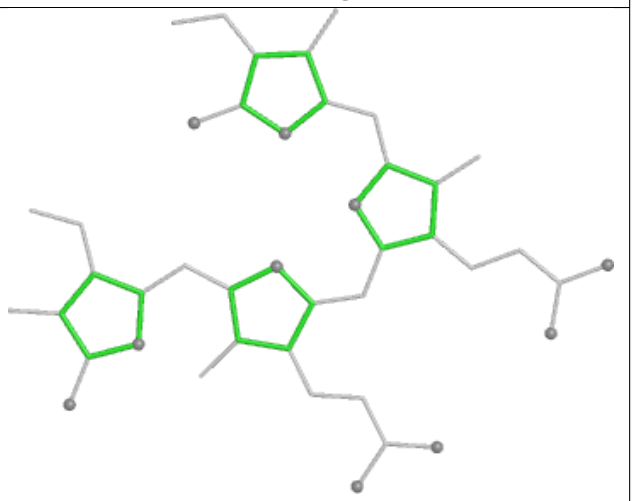
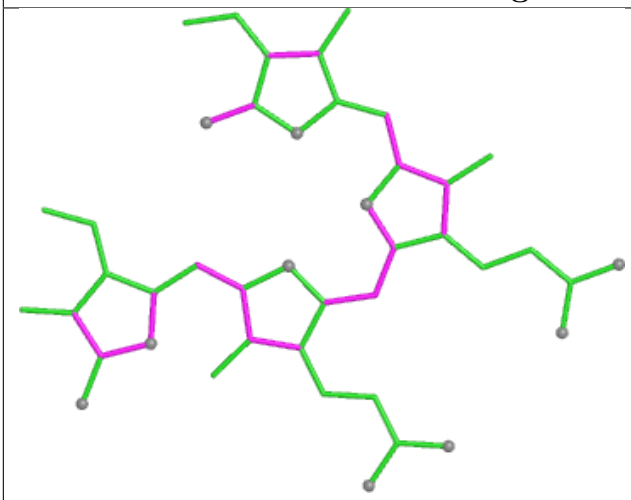


Torsions



Rings

Ligand PEB VB 201



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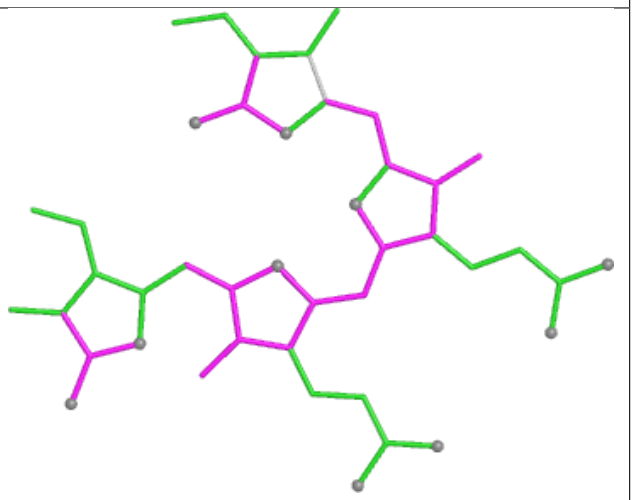

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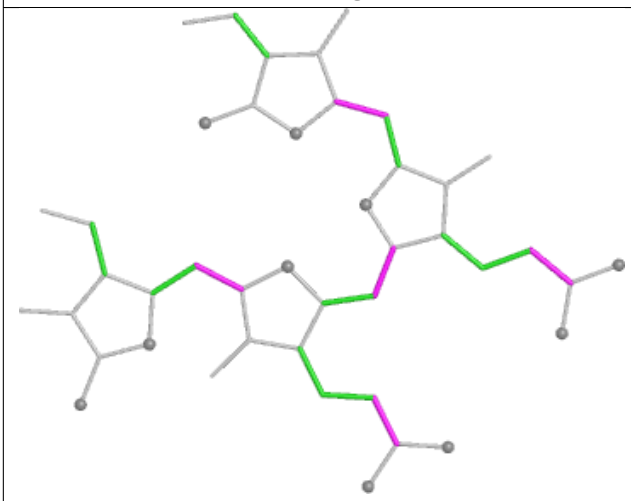

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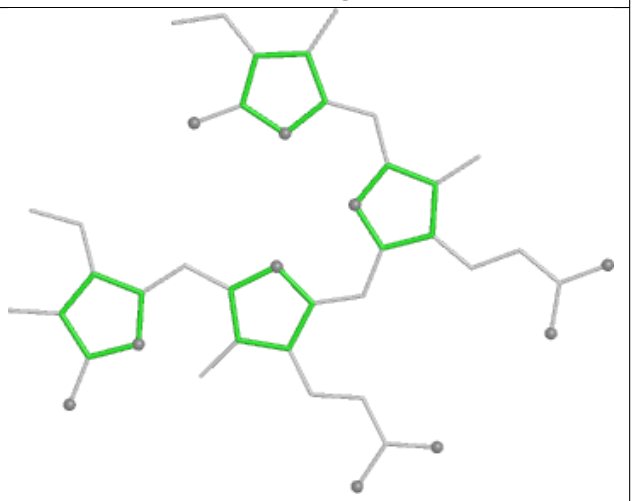
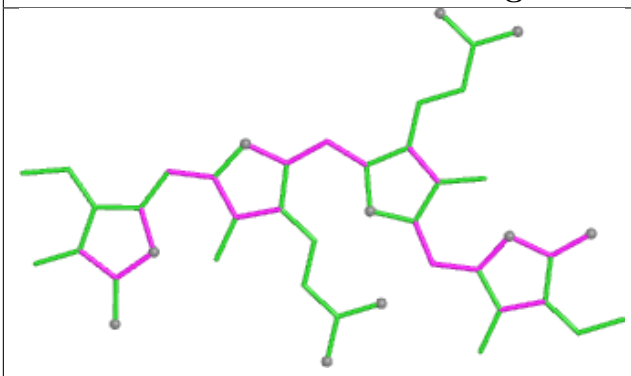


Rings

Ligand CYC IG 1001



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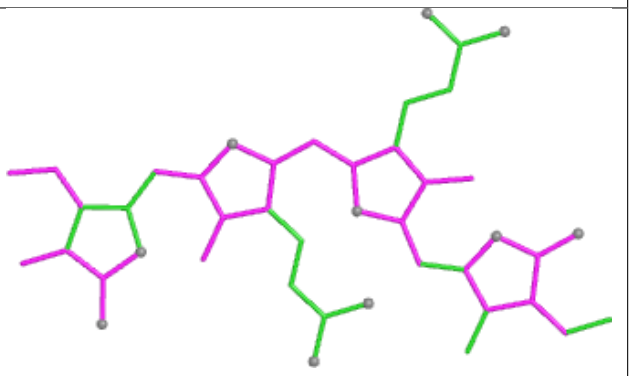

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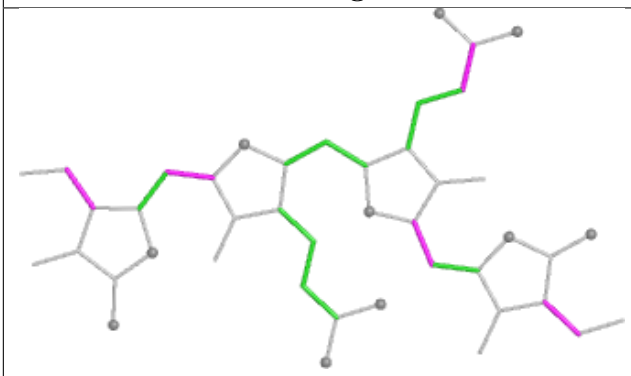

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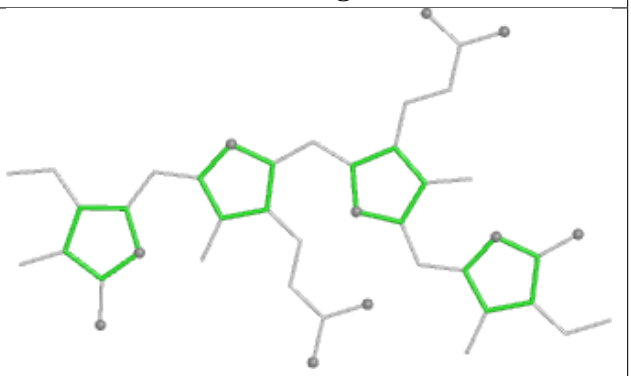
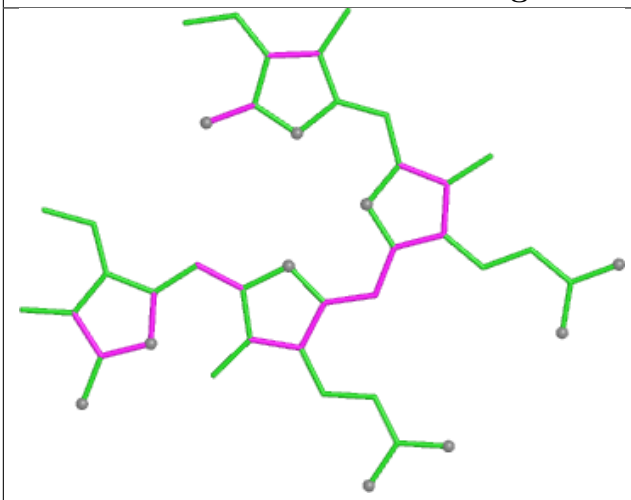


Rings

Ligand PEB dM 201



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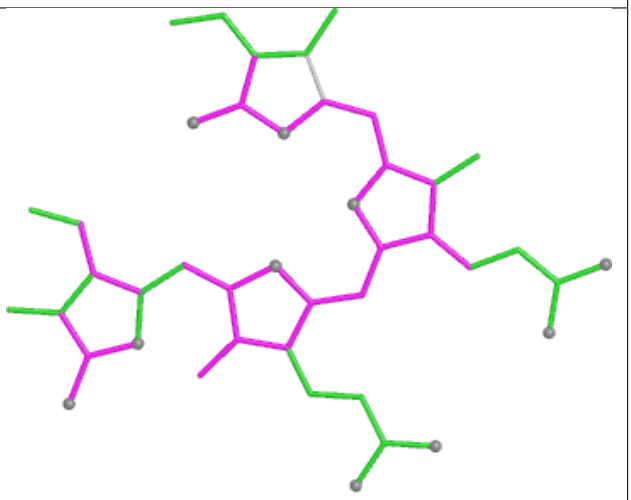

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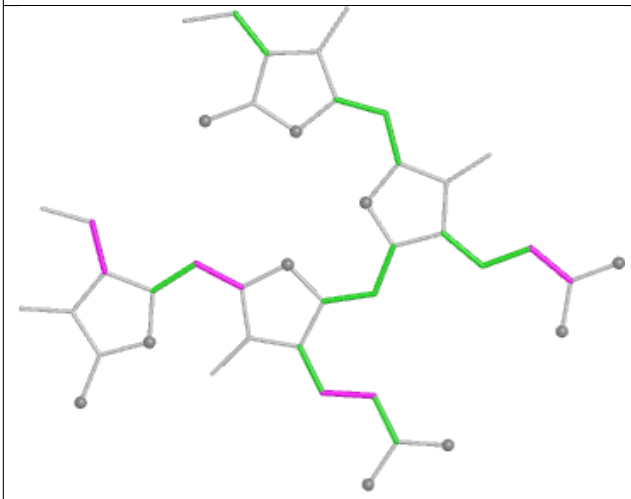

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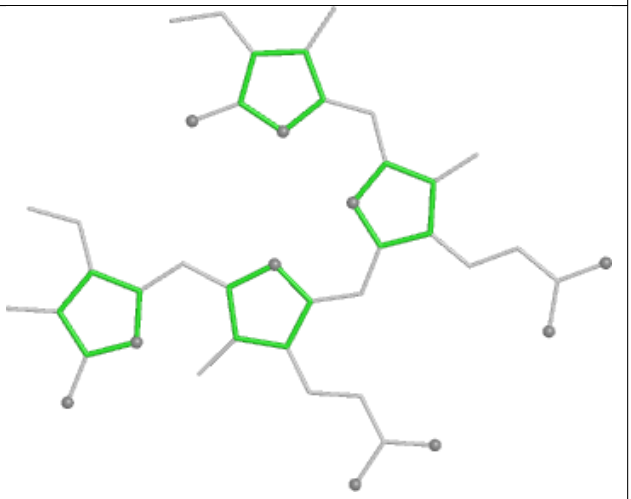
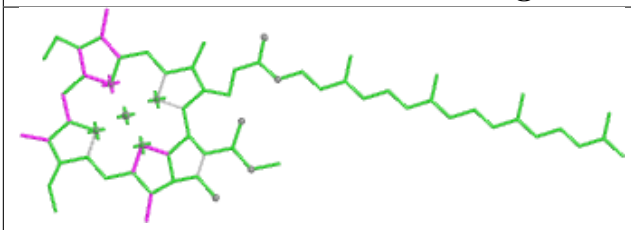


Rings

Ligand CLA C6 515



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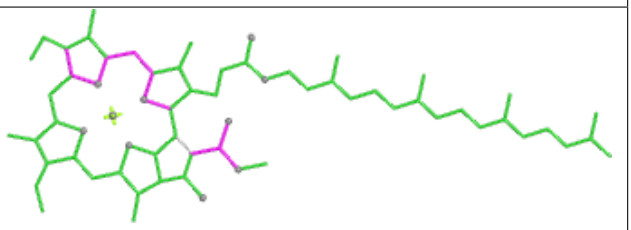

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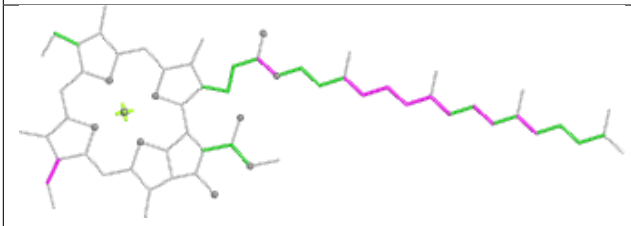

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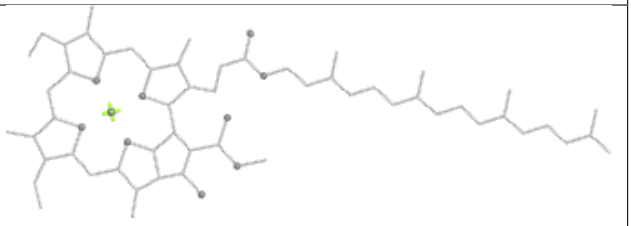
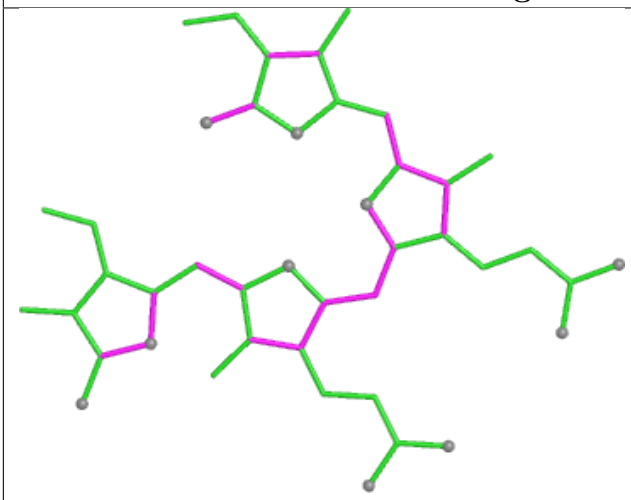


Rings

Ligand PEB hK 202



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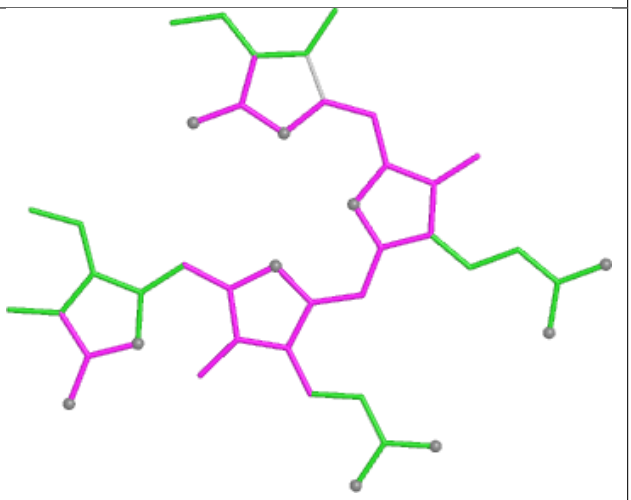

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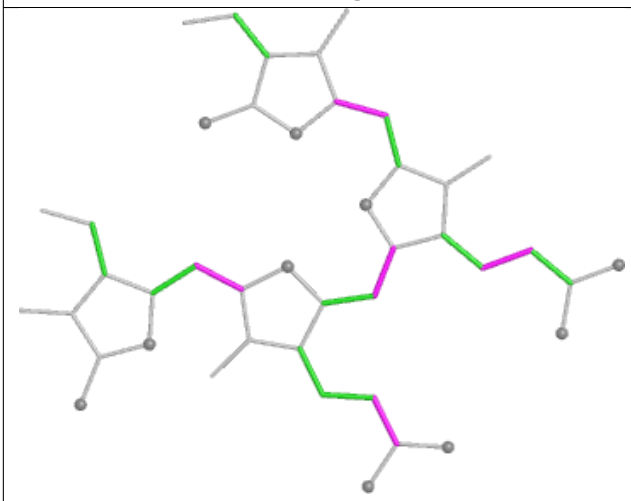

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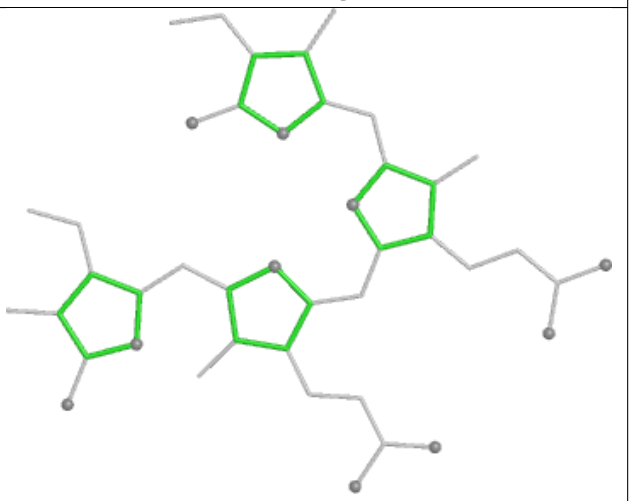
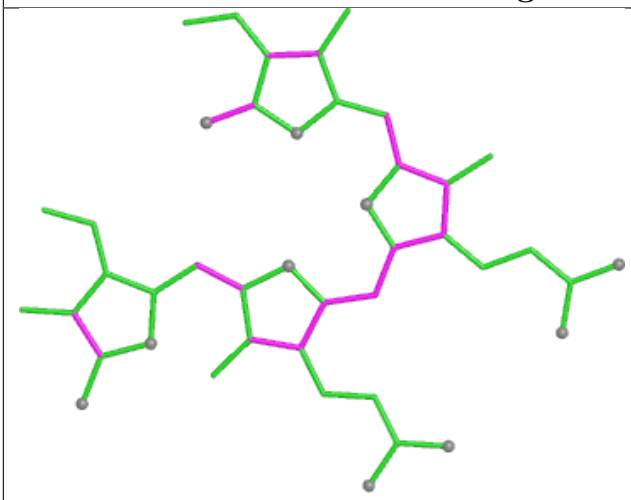


Rings

Ligand PEB vF 201



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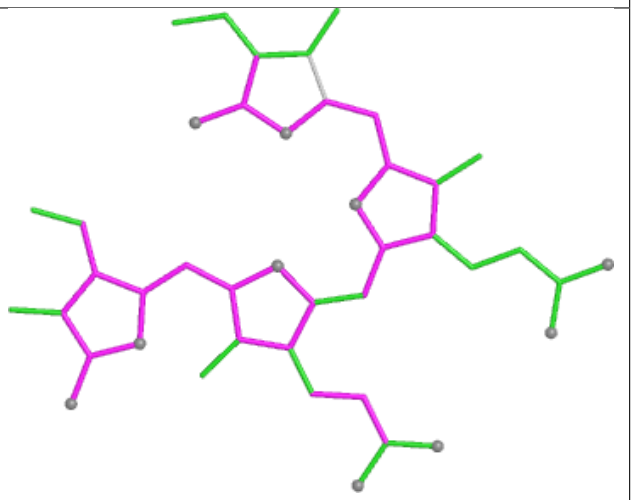

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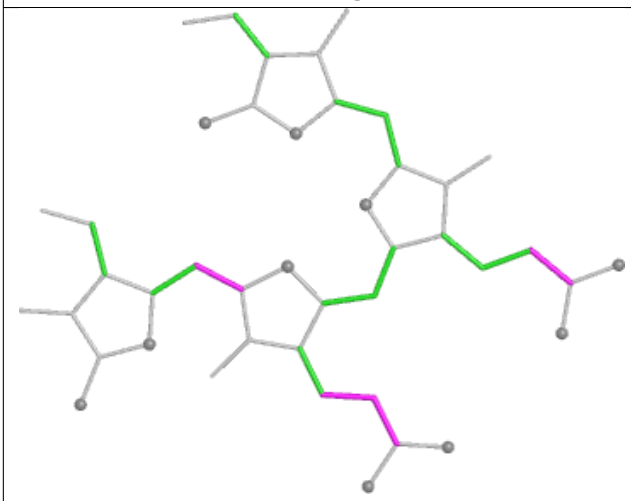

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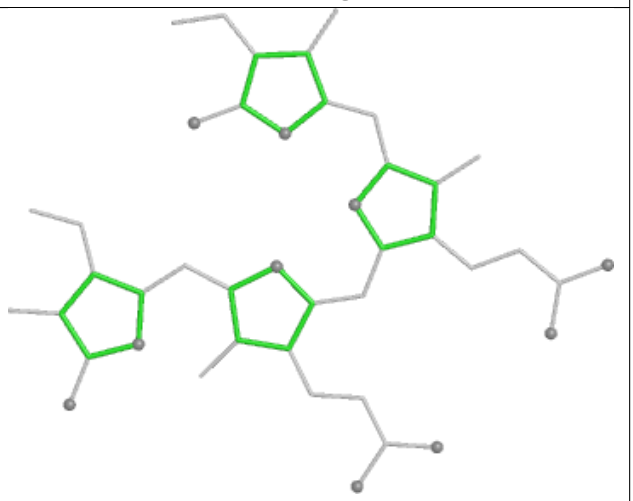
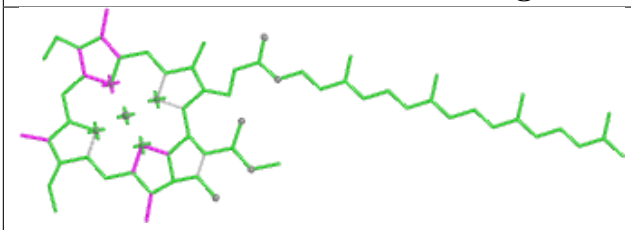


Rings

Ligand CLA C6 516



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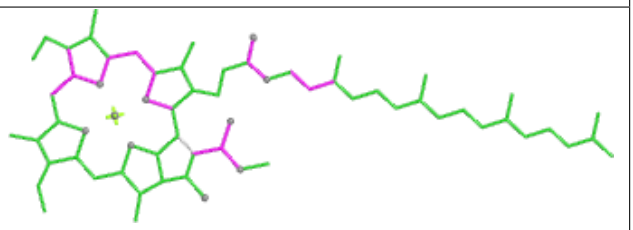

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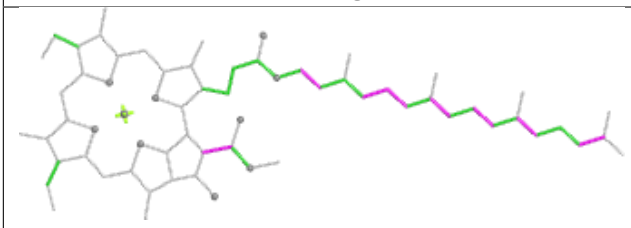

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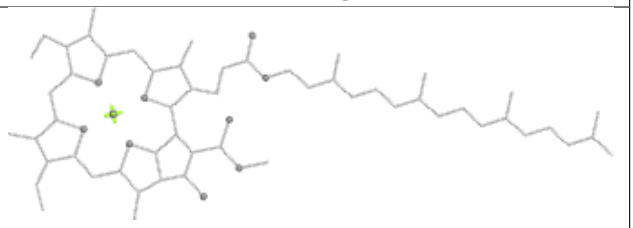
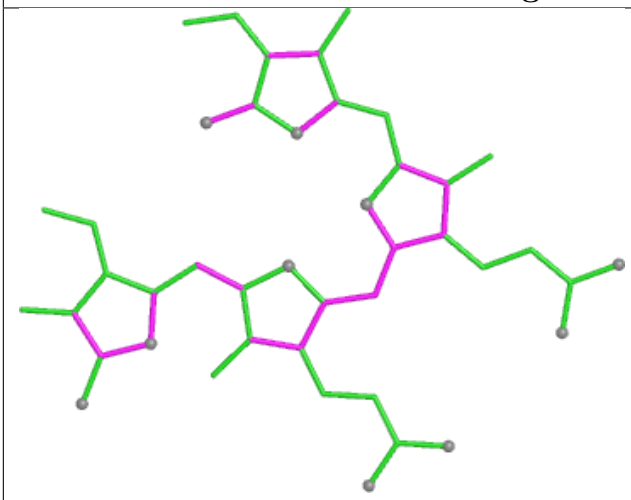


Rings

Ligand PEB I9 201



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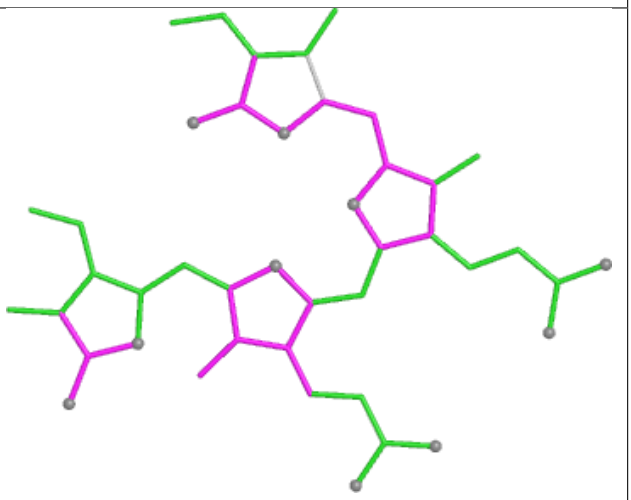

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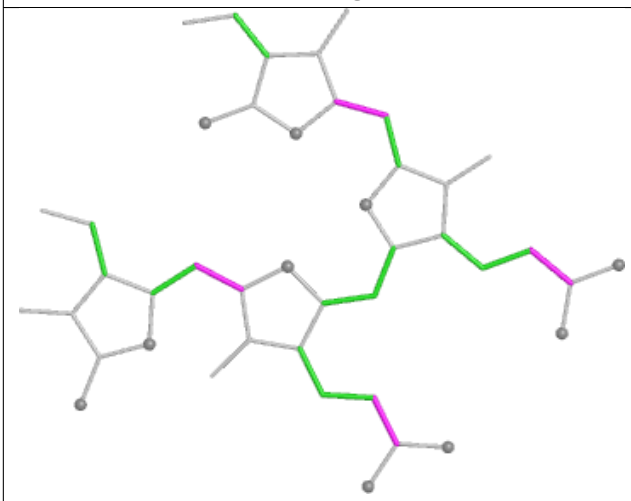

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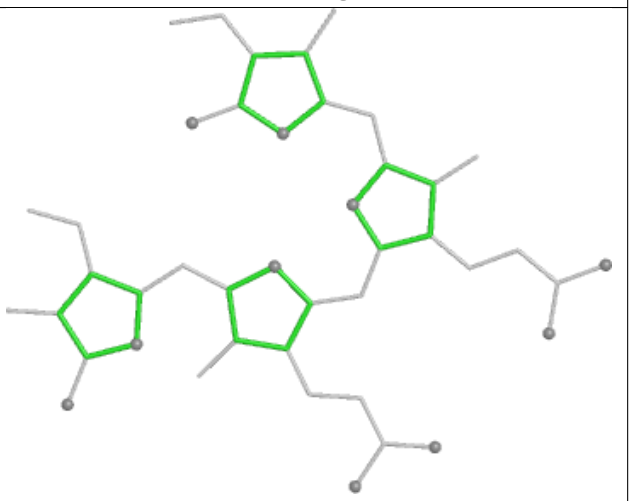
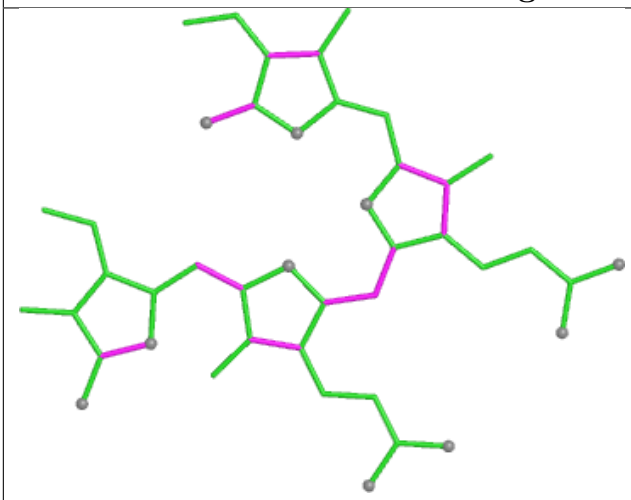


Rings

Ligand PEB zF 501



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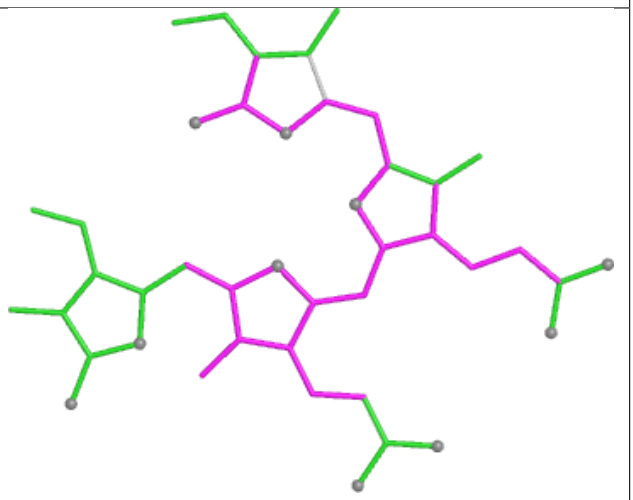

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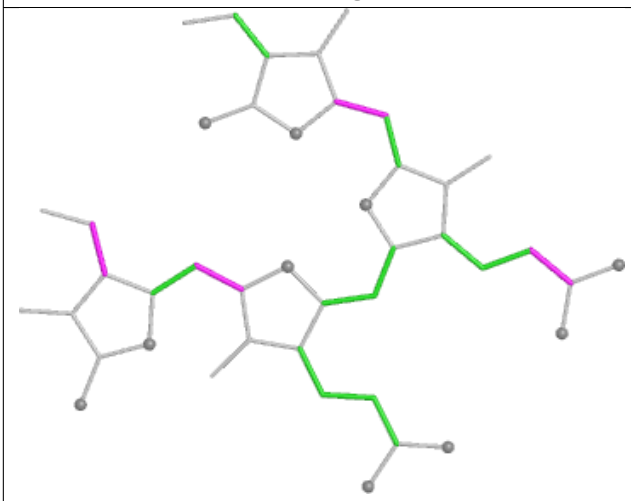

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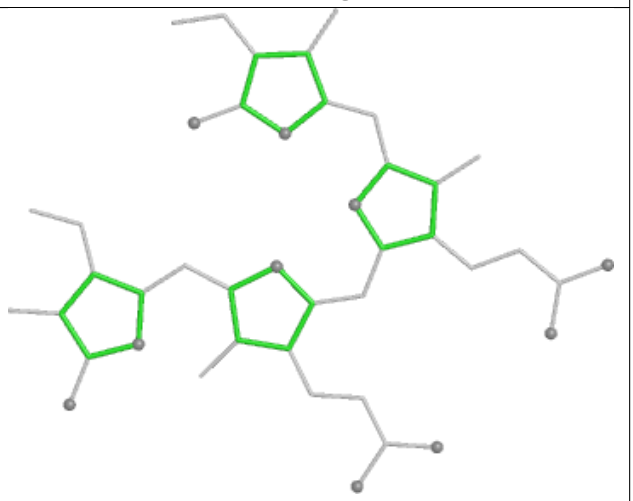
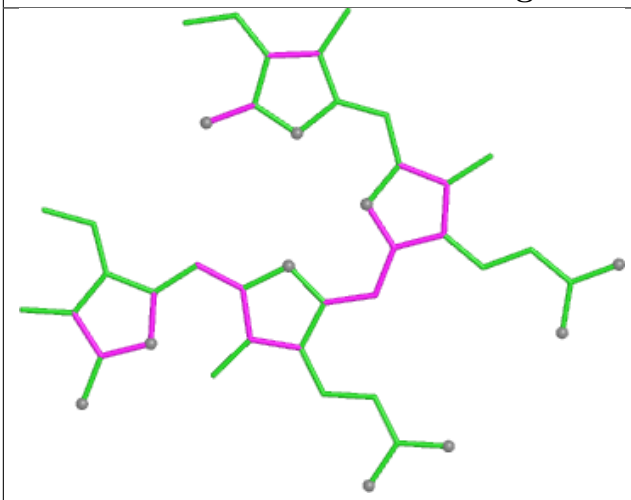


Rings

Ligand PEB eO 201



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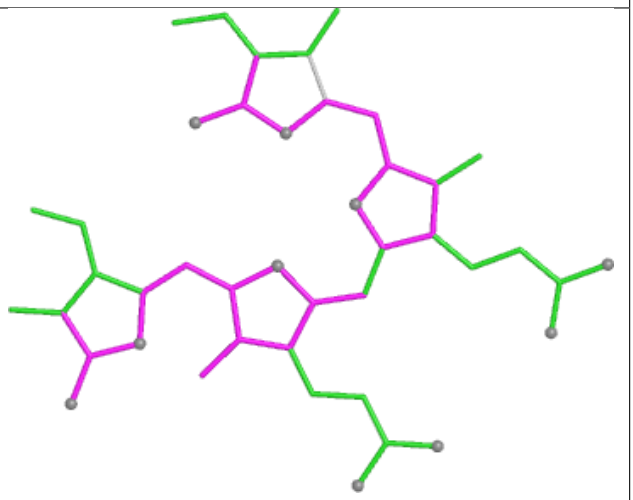

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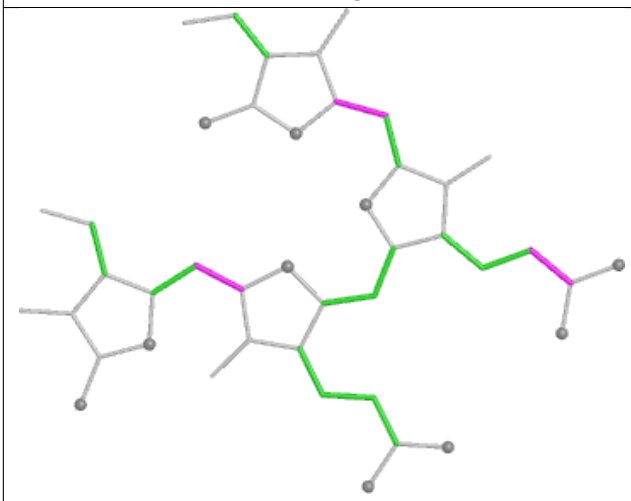

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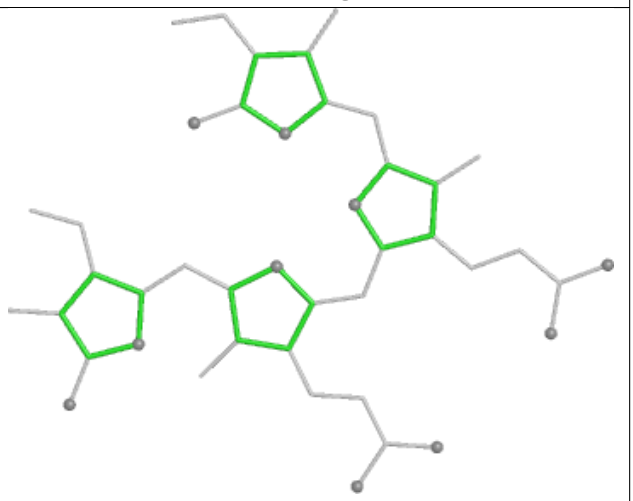
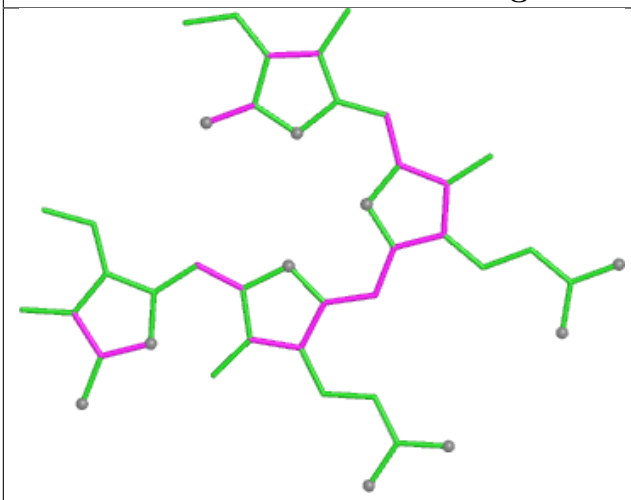


Rings

Ligand PEB XD 202



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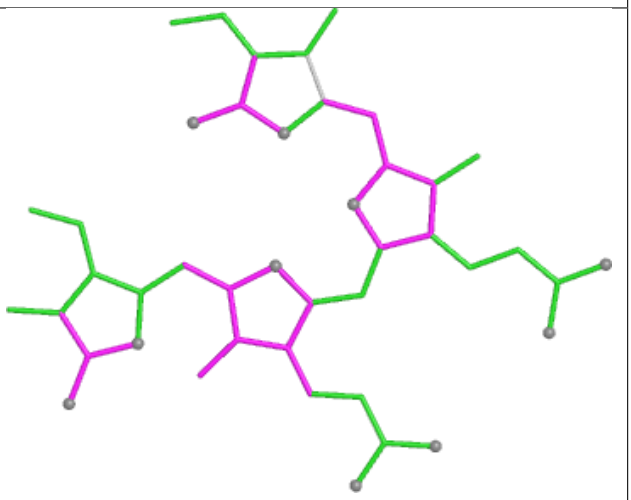

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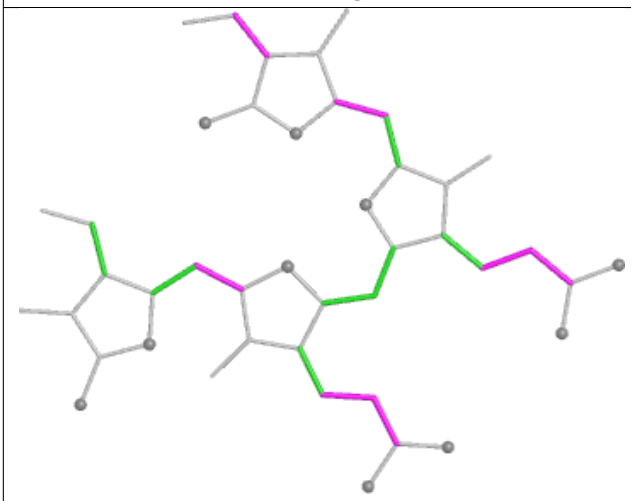

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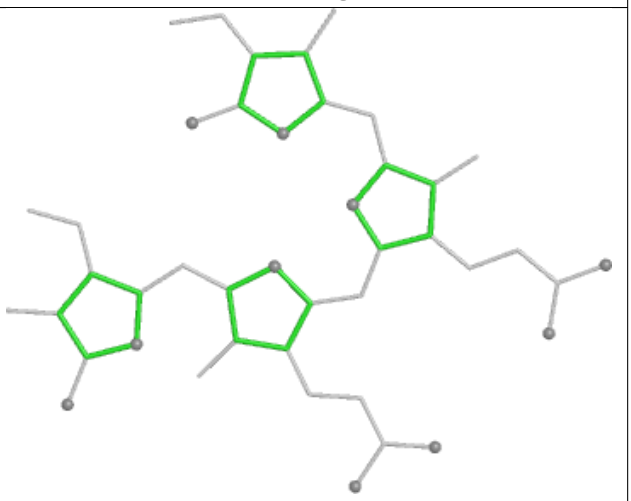
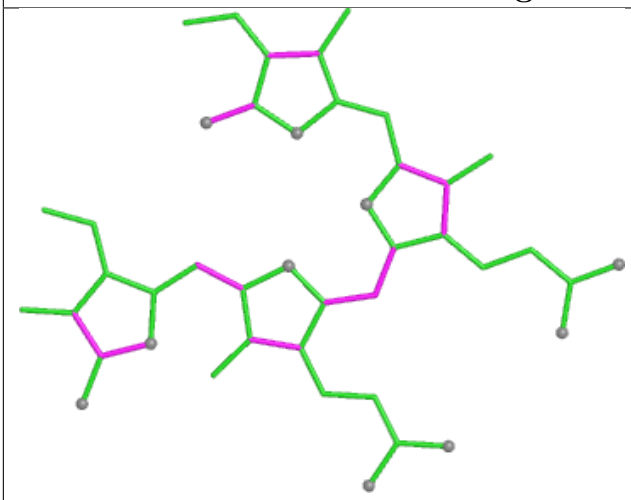


Rings

Ligand PEB X7 202



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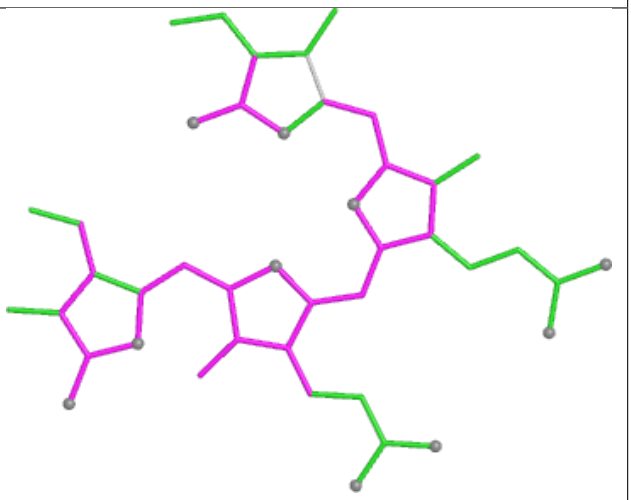
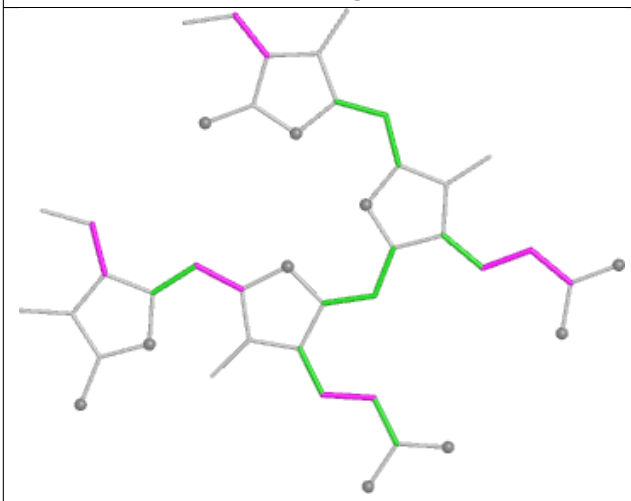


Bond angles



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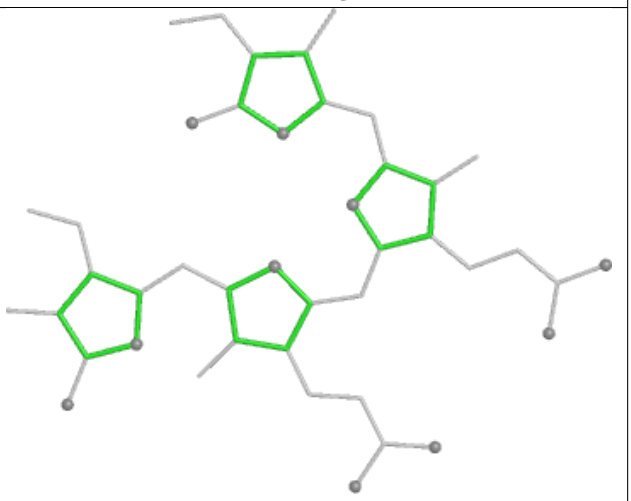
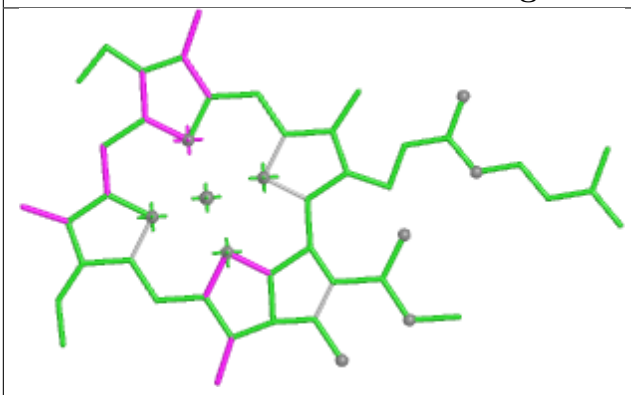


Rings

Ligand CLA a6 609



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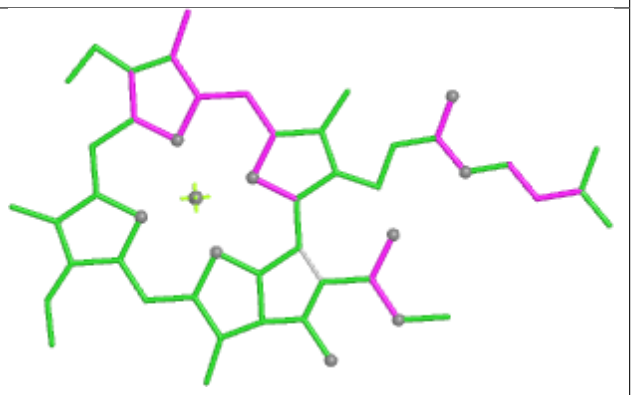
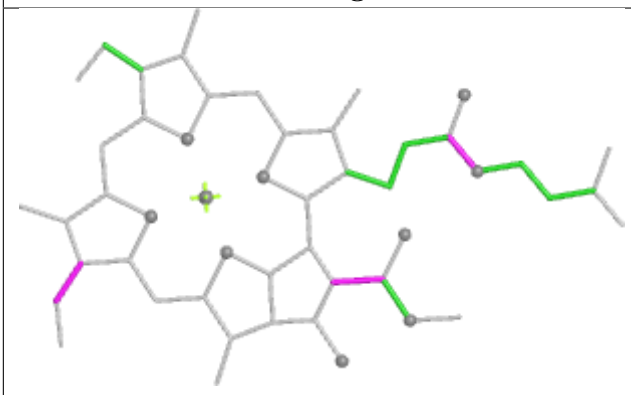


Bond angles



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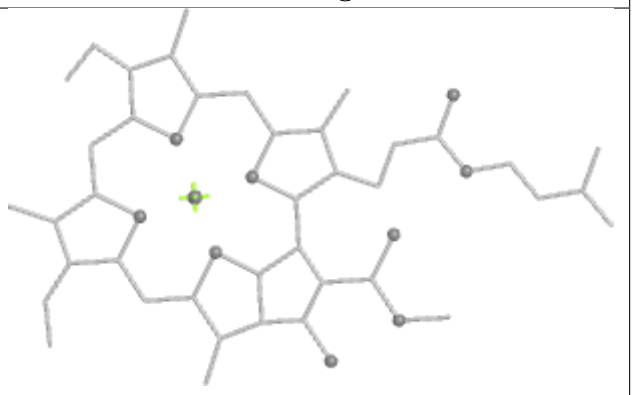
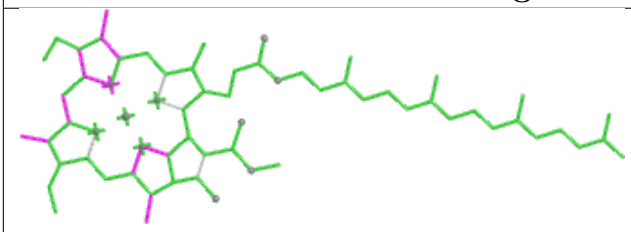
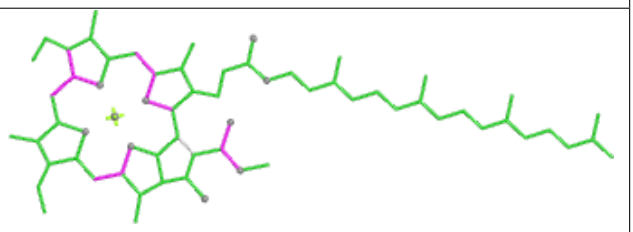


Rings

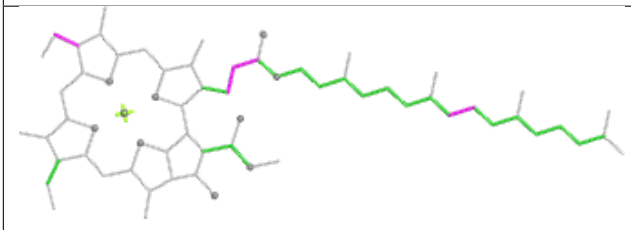
Ligand CLA CL 512



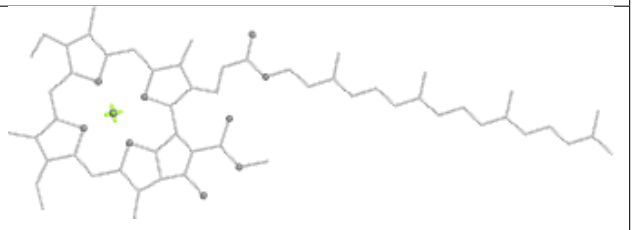
Bond lengths



Bond angles

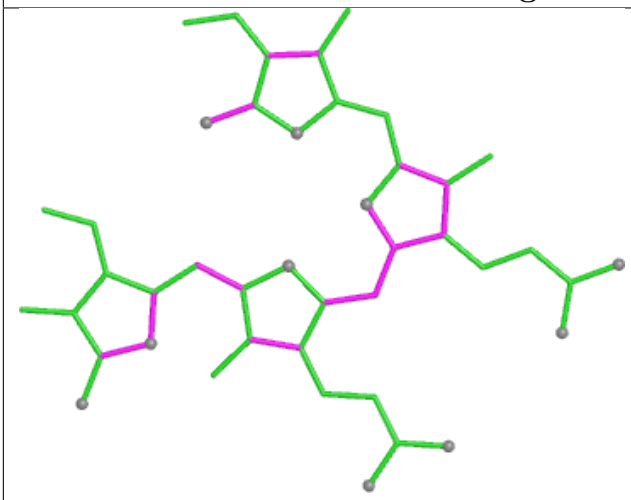


Torsions



Rings

Ligand PEB EI 201



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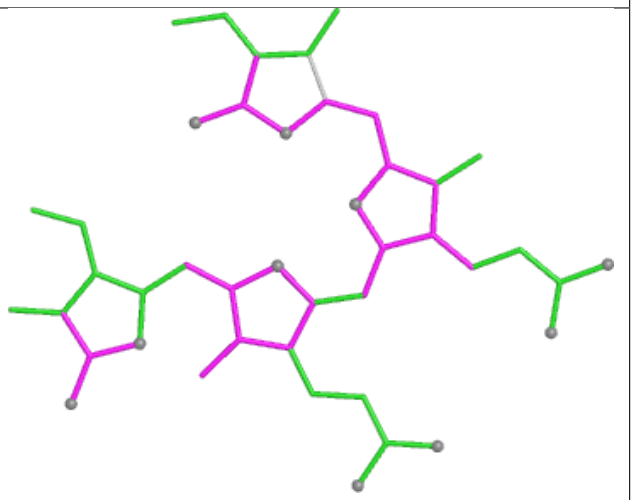
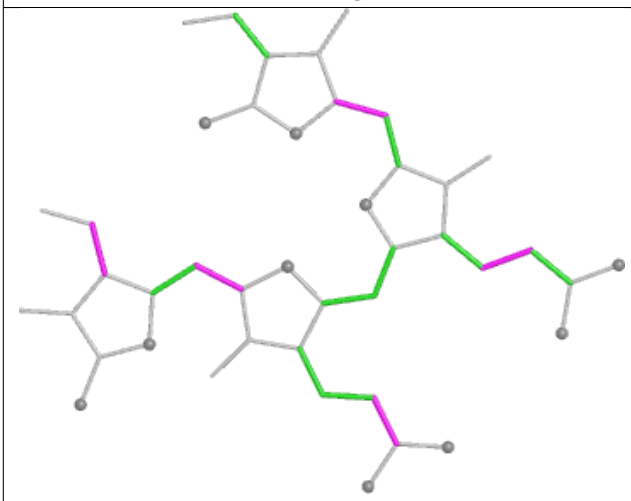


Bond angles



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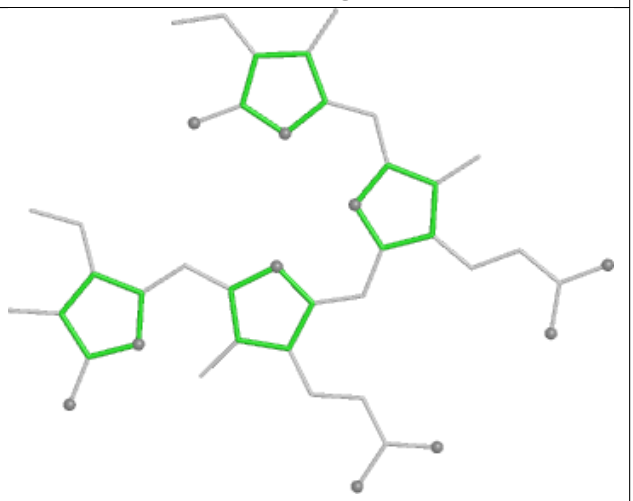
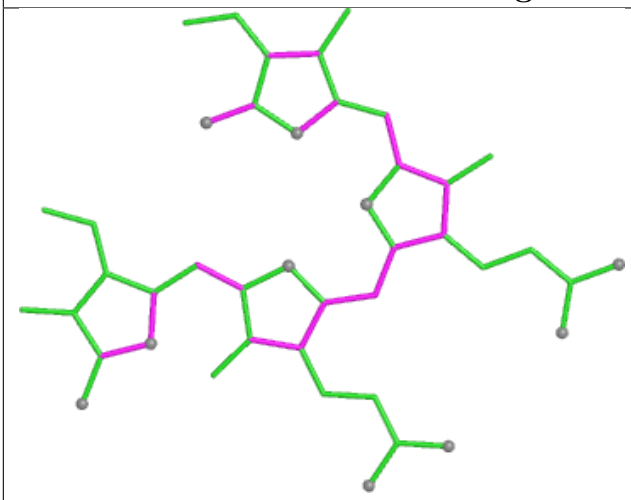


Rings

Ligand PEB aK 201



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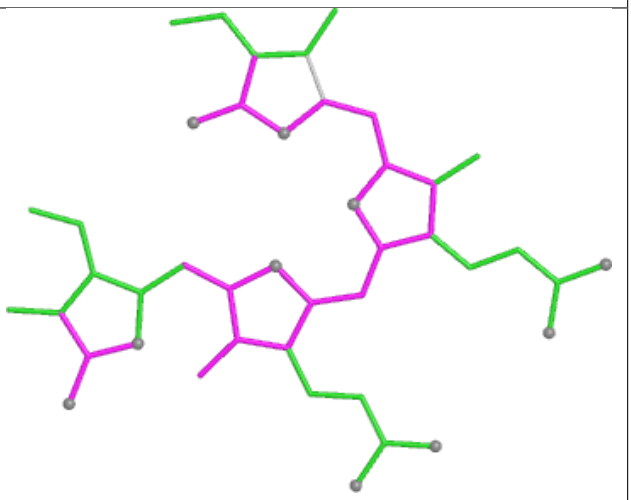

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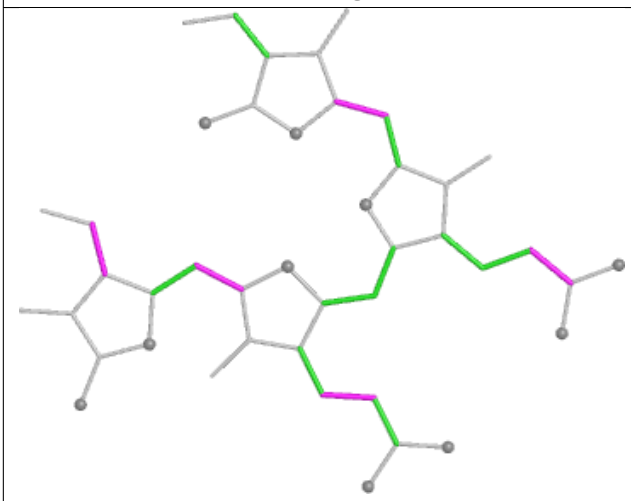

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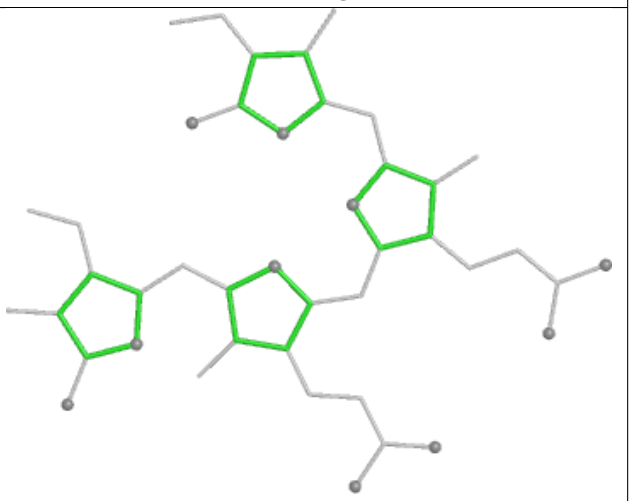
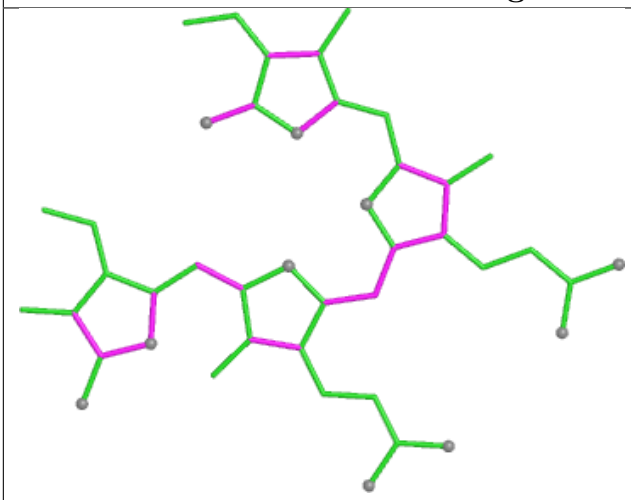


Rings

Ligand PEB QM 204



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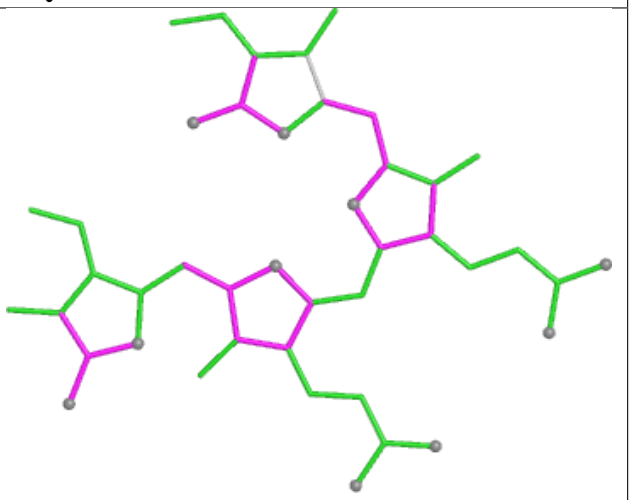

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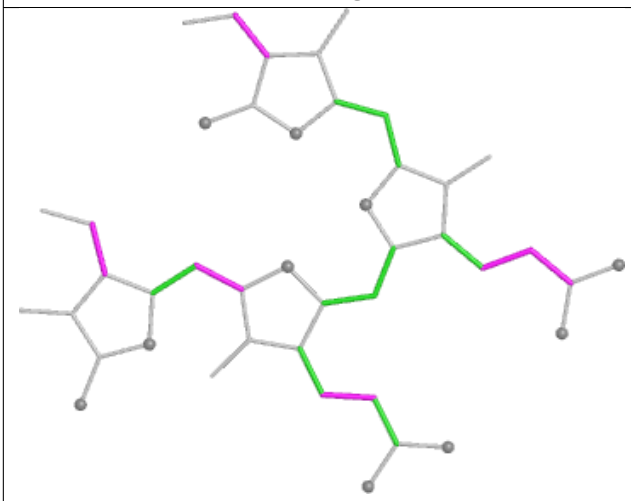

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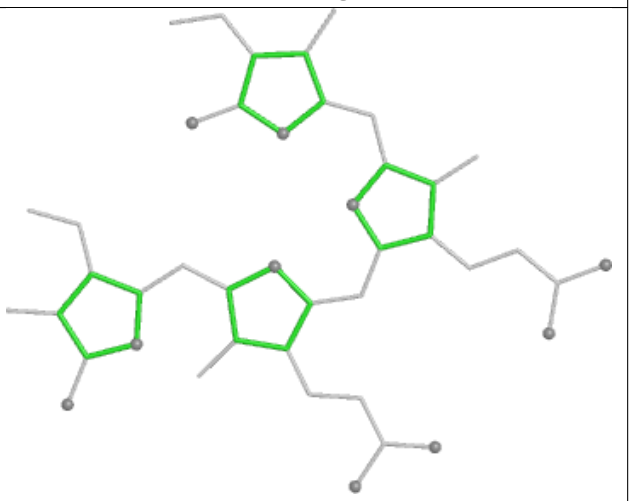
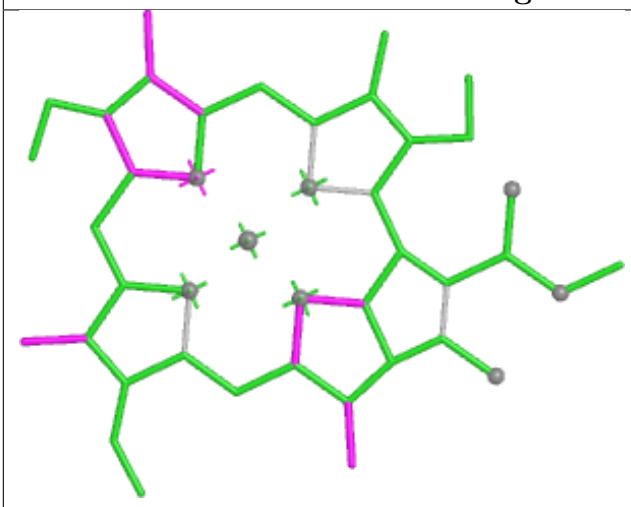


Rings

Ligand CLA 3N 307



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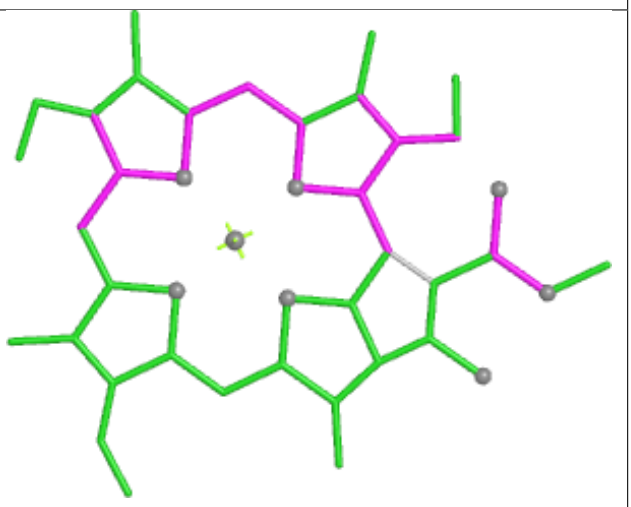
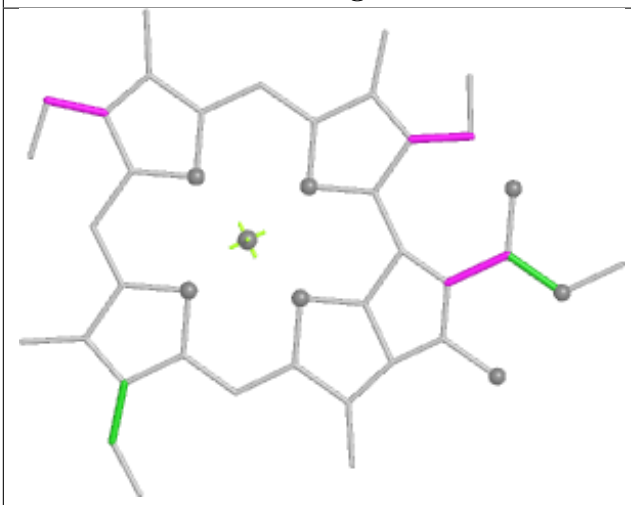


Bond angles

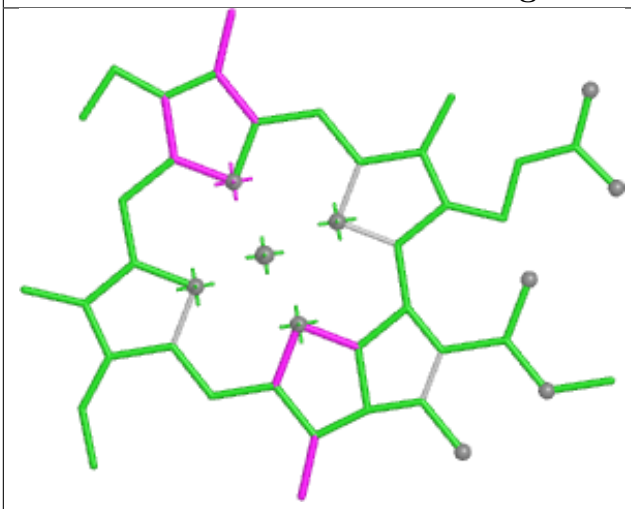


Torsions



Rings

Ligand CLA 22 603



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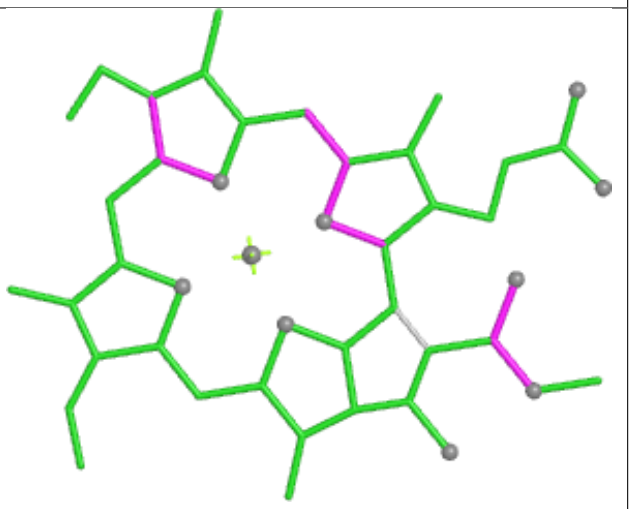

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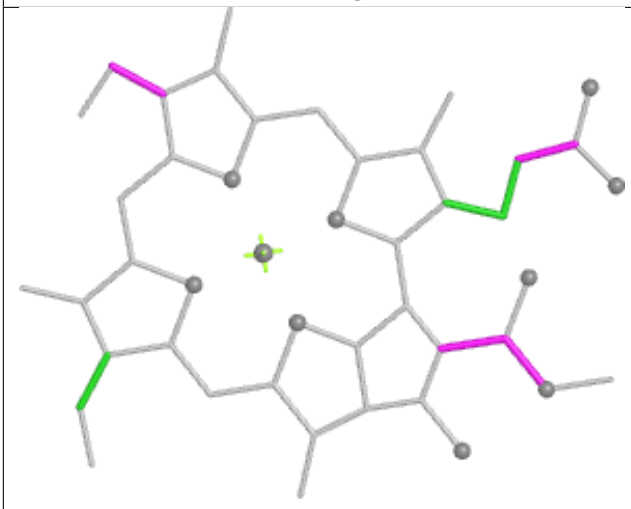
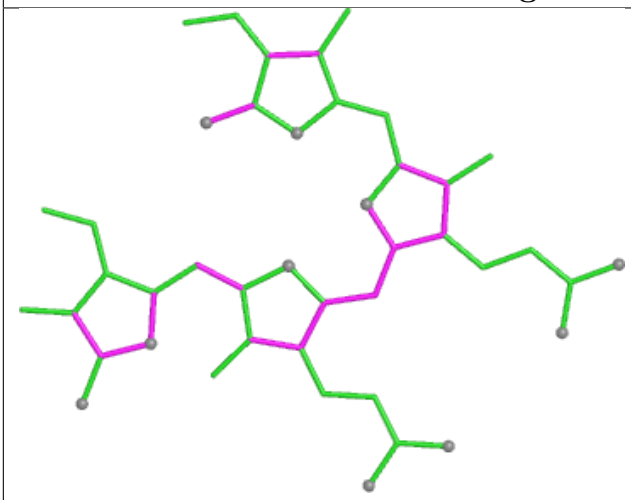


Torsions



Rings

Ligand PEB v8 201



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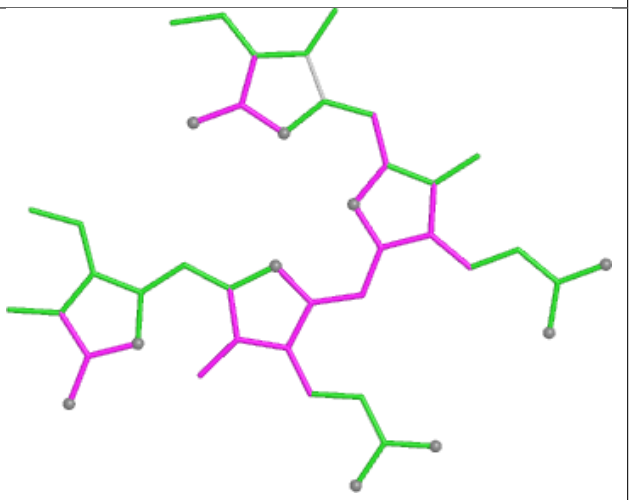

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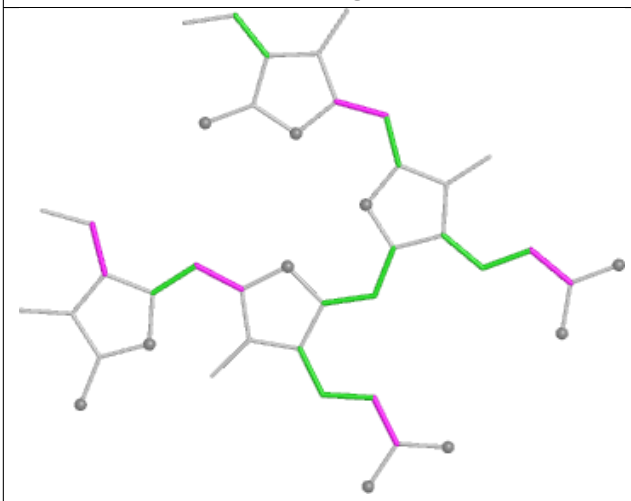

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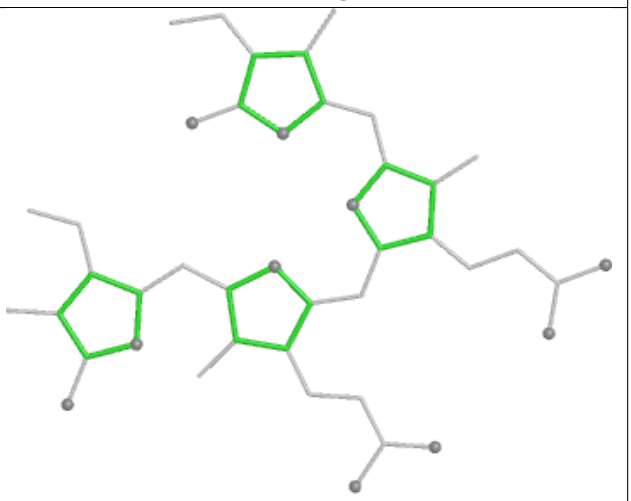

Rings

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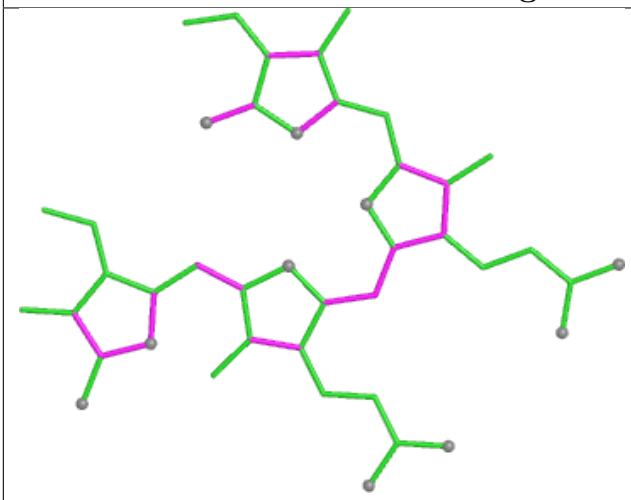

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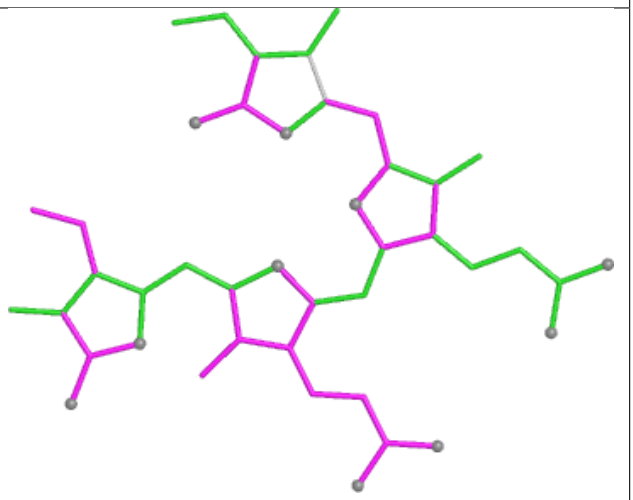

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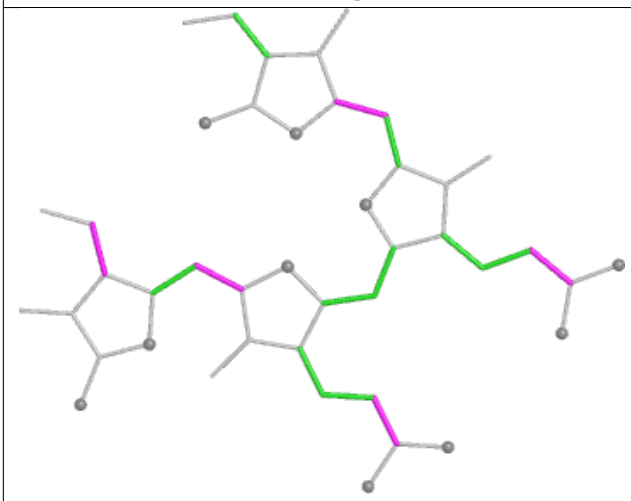

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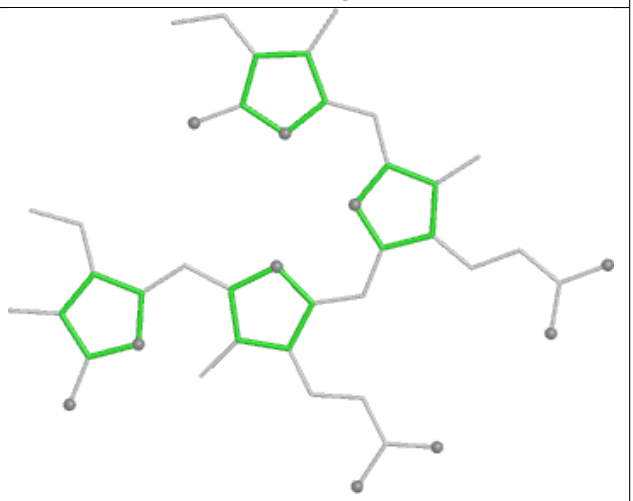
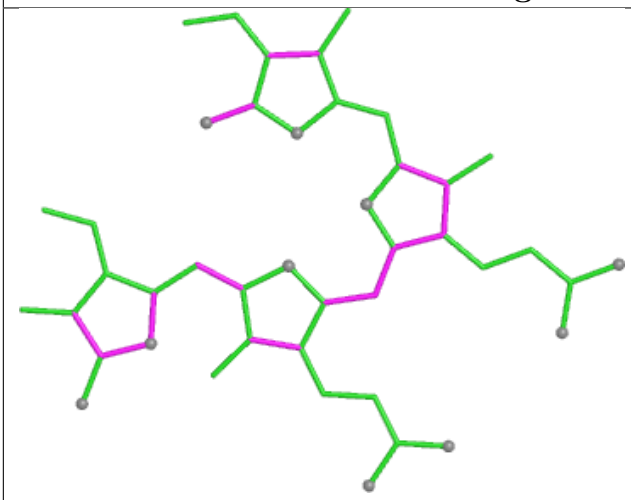


Rings

Ligand PEB GJ 202



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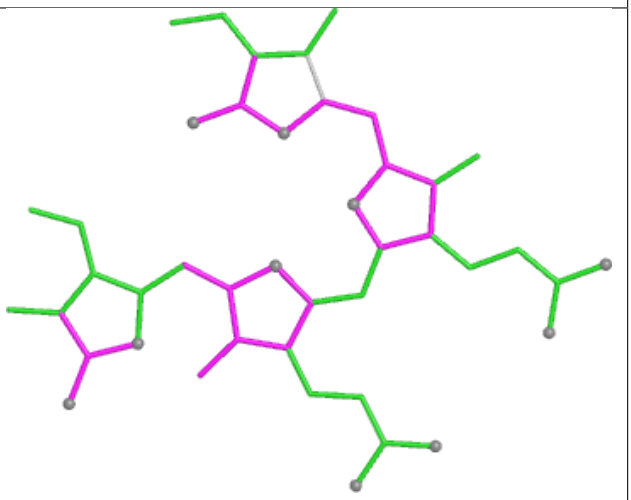

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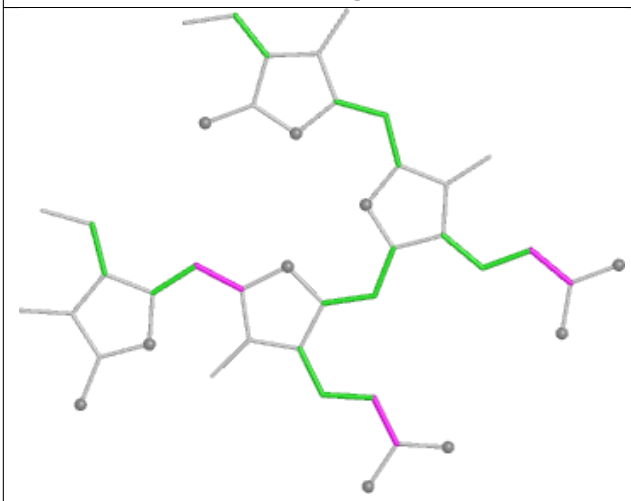

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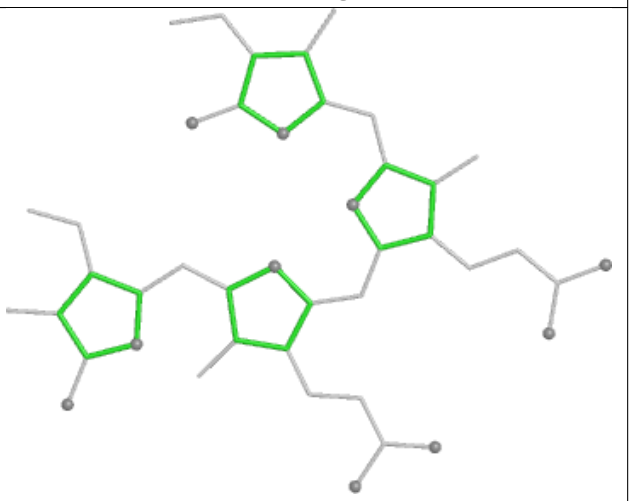
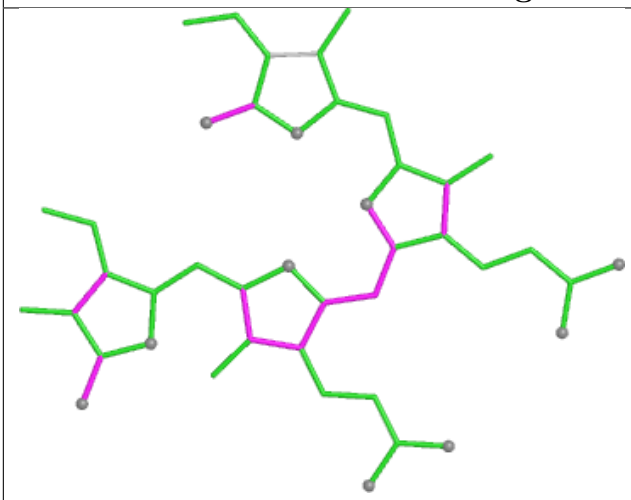


Rings

Ligand PUB xF 301



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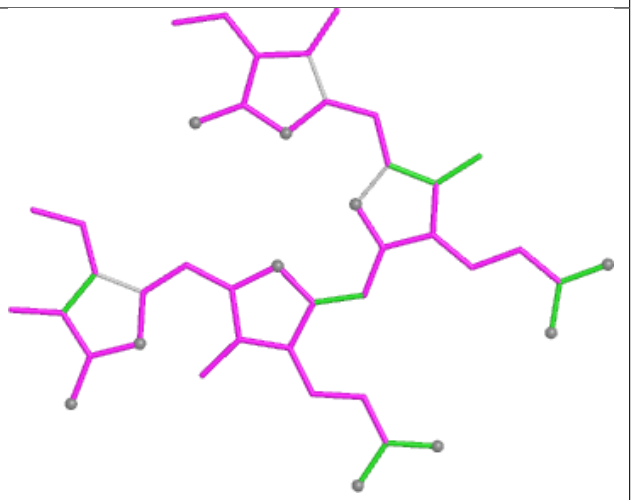

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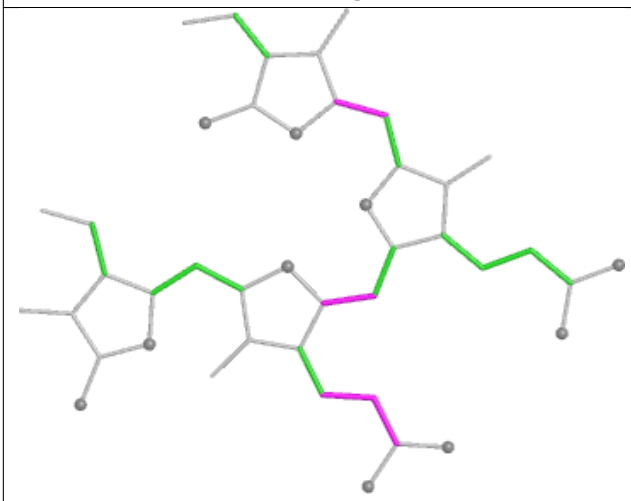

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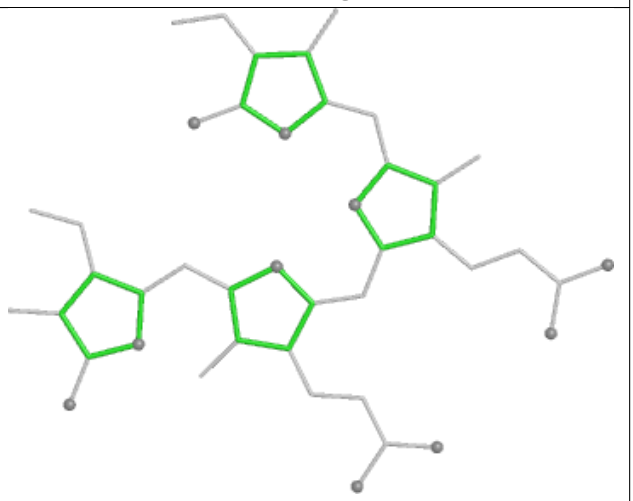
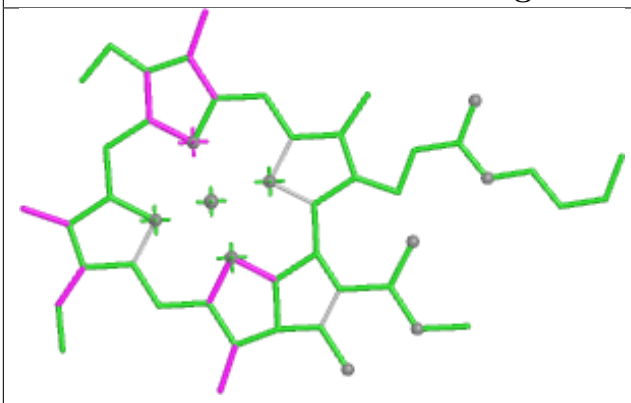


Rings

Ligand CLA K2 106



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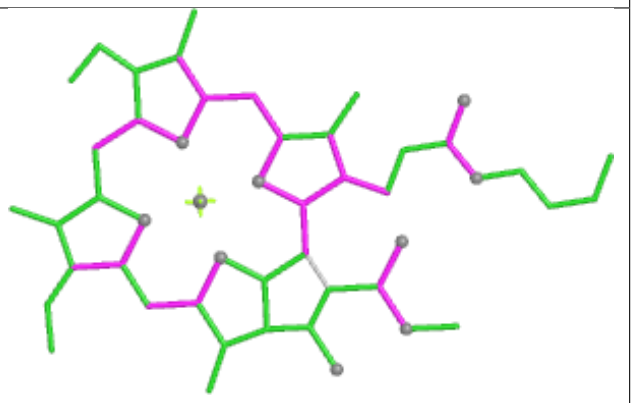

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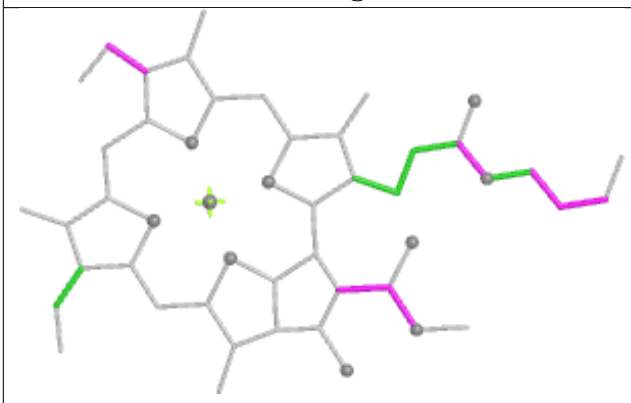

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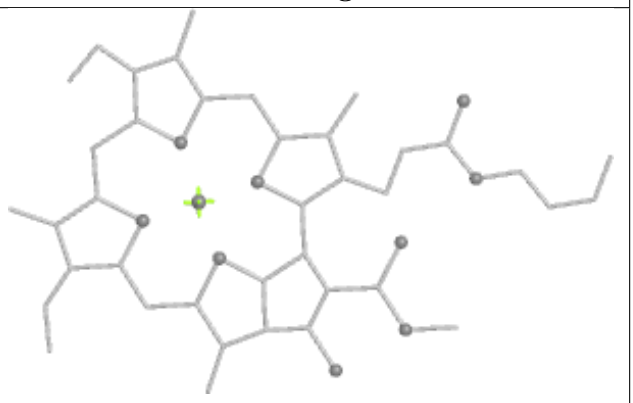
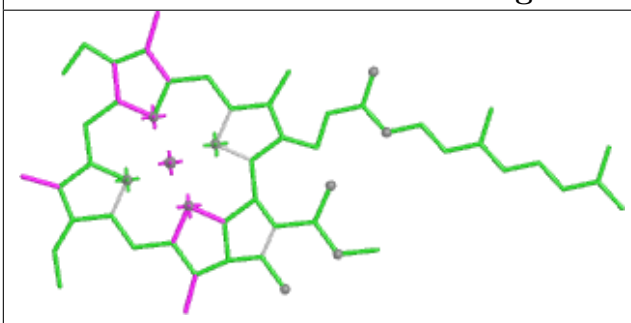


Rings

Ligand CLA B2 811



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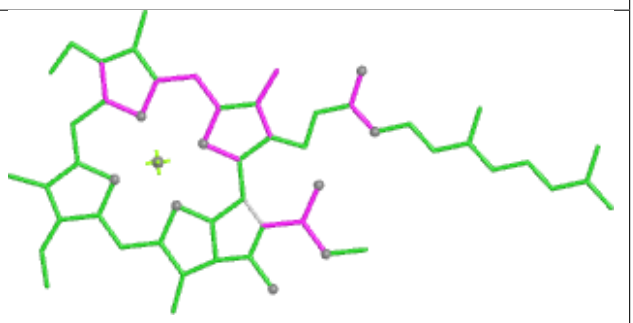

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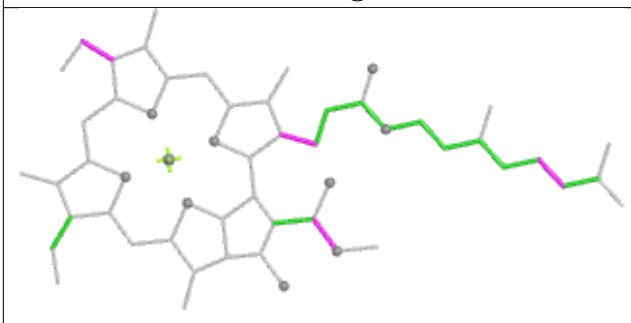

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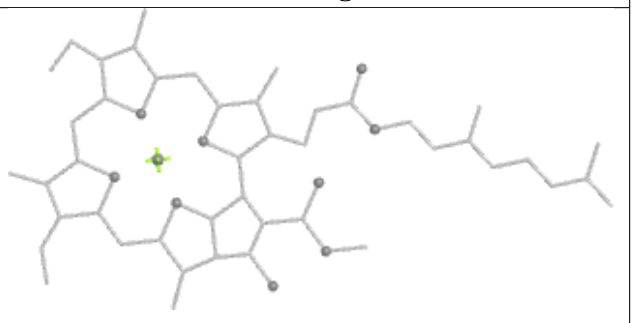
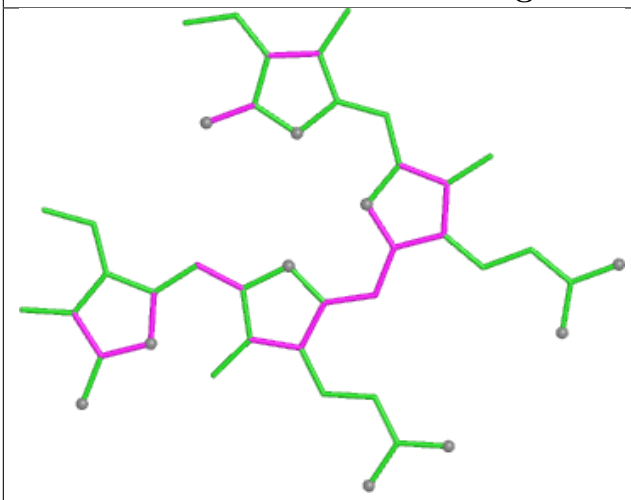


Rings

Ligand PEB eH 201



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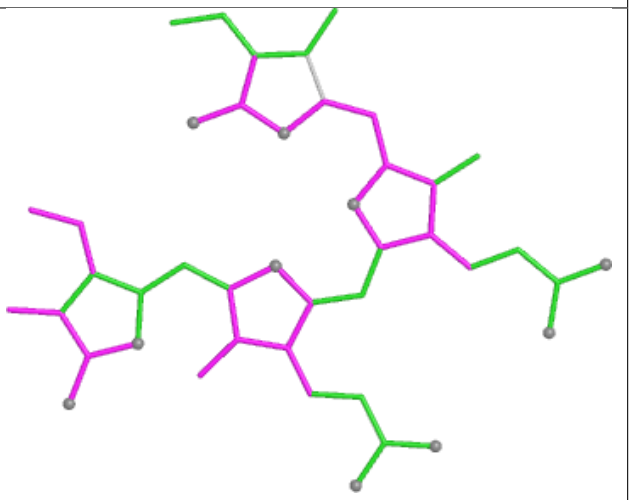

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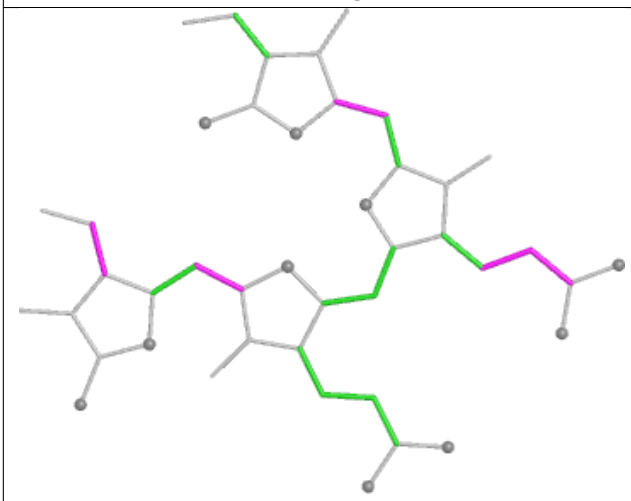

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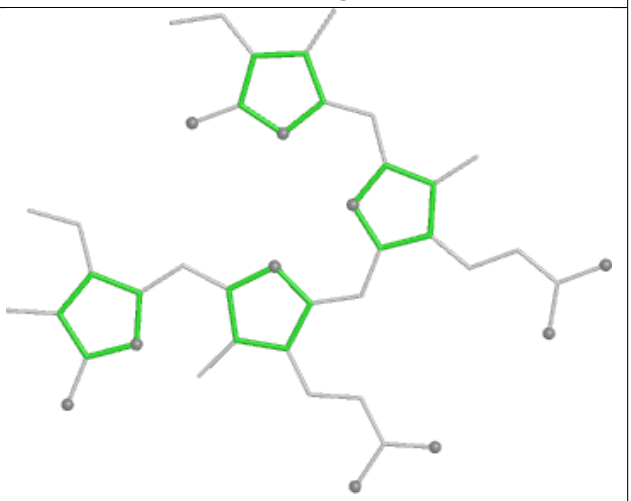
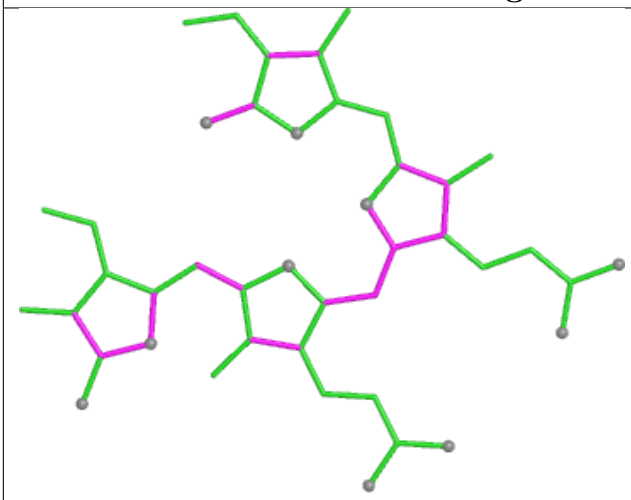


Rings

Ligand PEB WG 202



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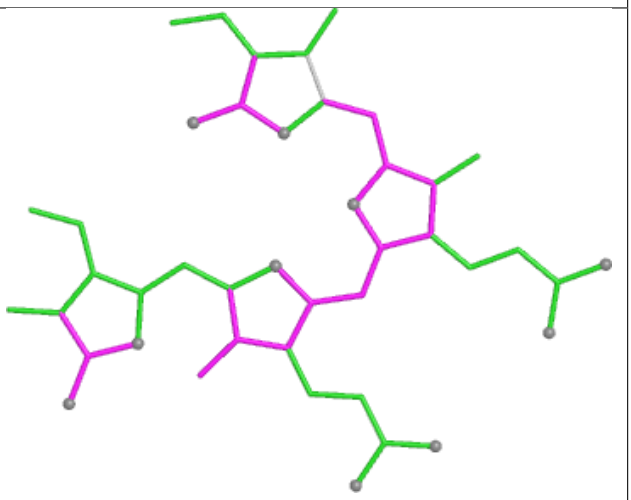
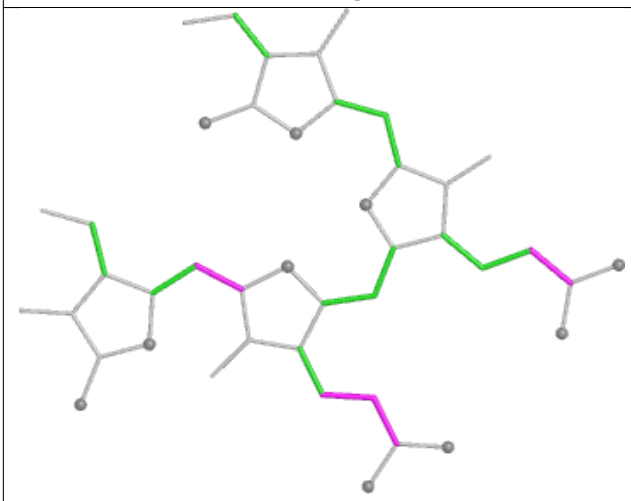


Bond angles



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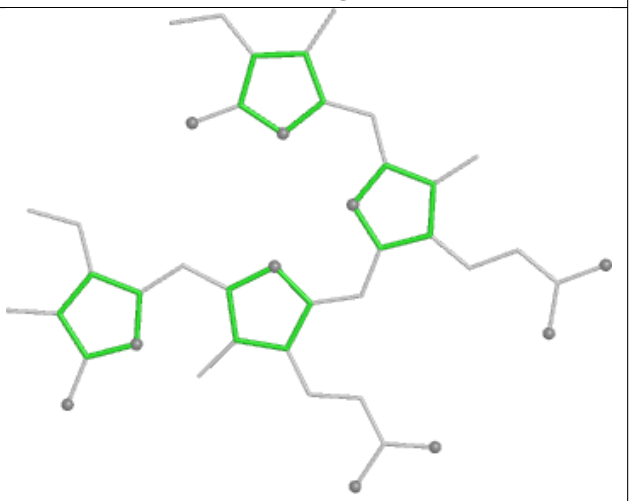
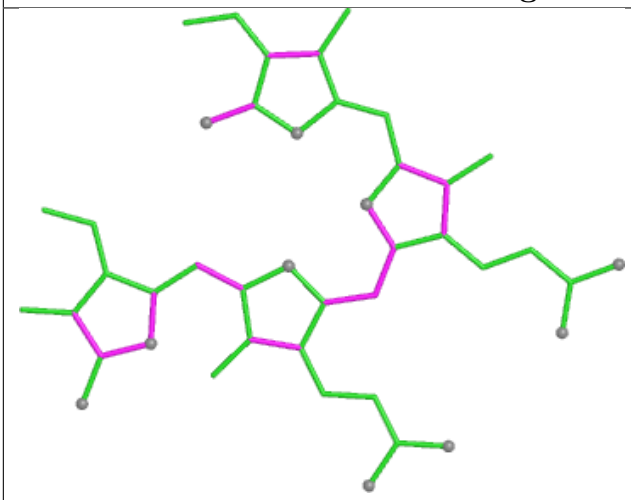


Rings

Ligand PEB aJ 202



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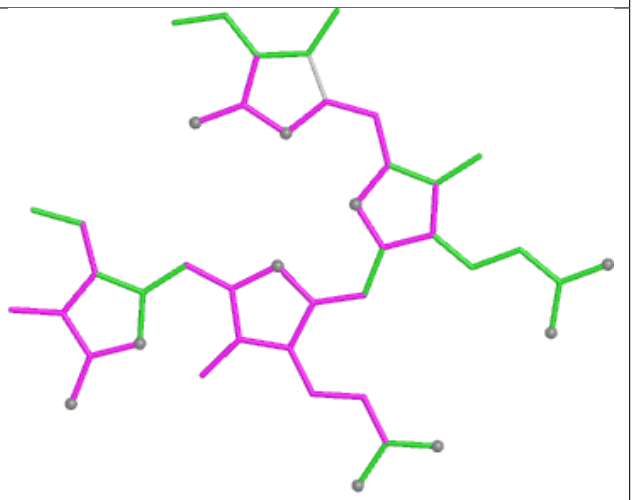
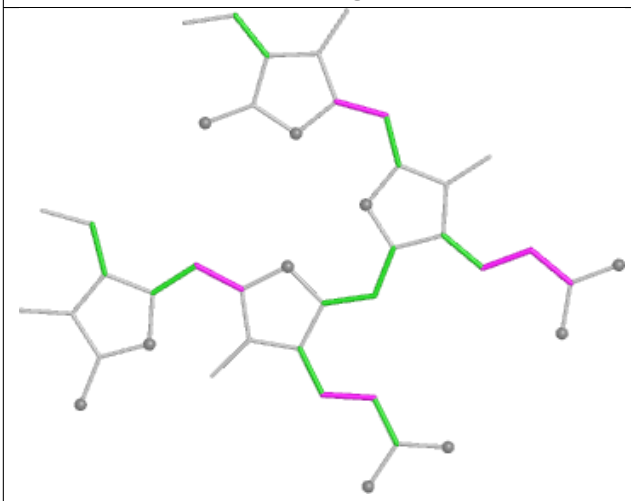


Bond angles



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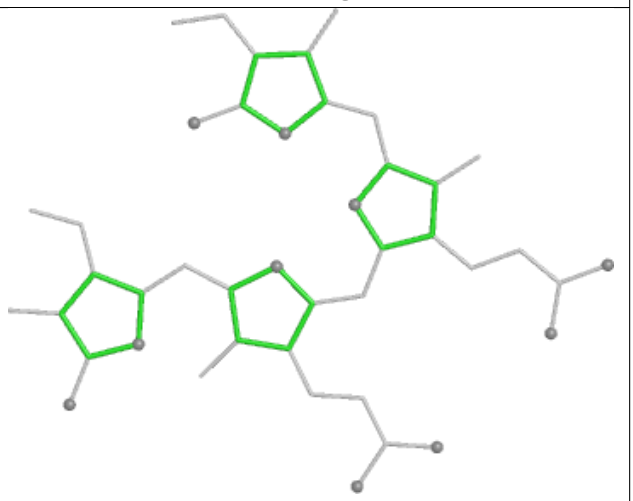
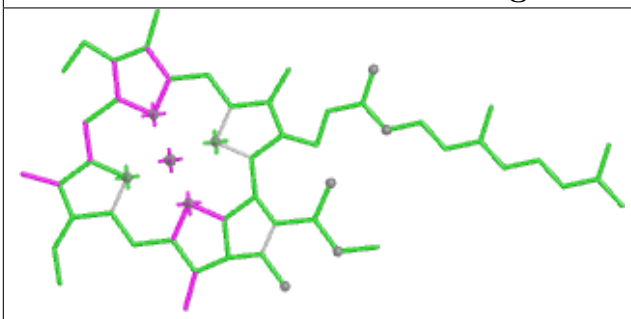
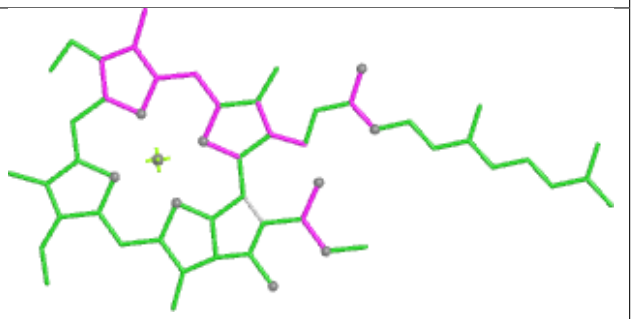


Rings

Ligand CLA AN 825	
	
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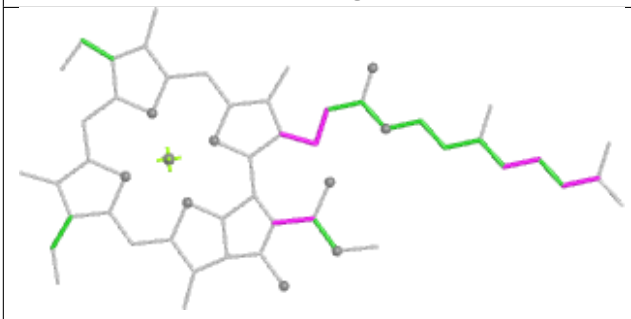
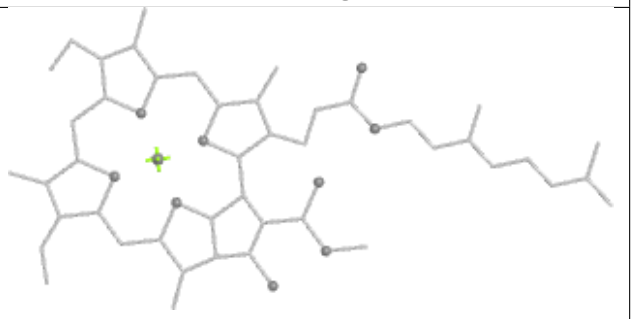
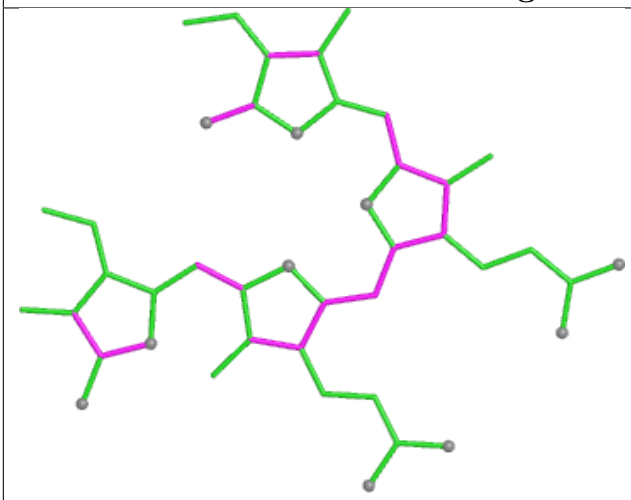
	
Torsions	**Rings**

Ligand PEB sC 202



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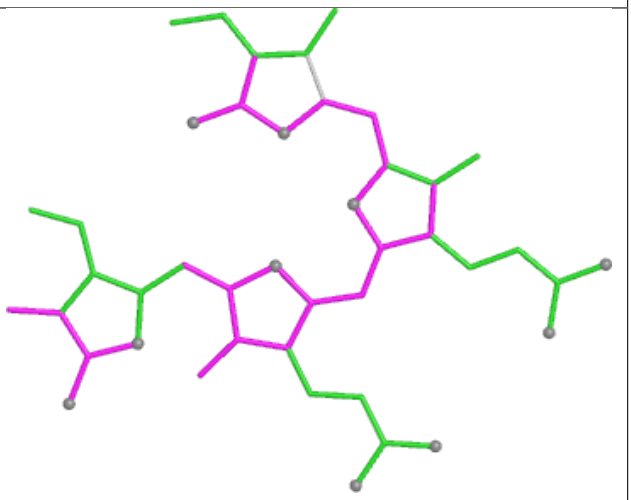

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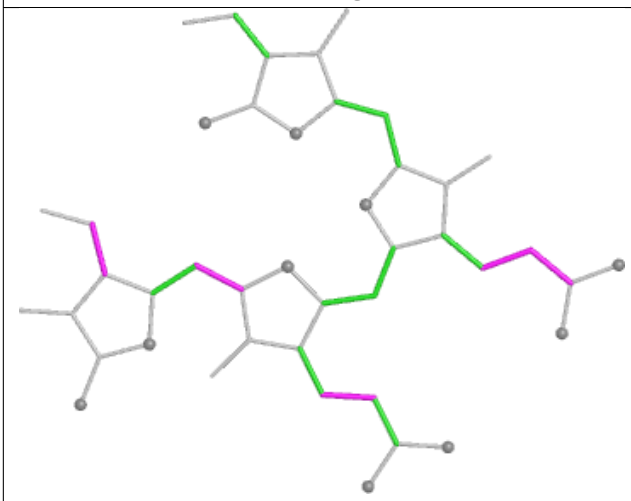

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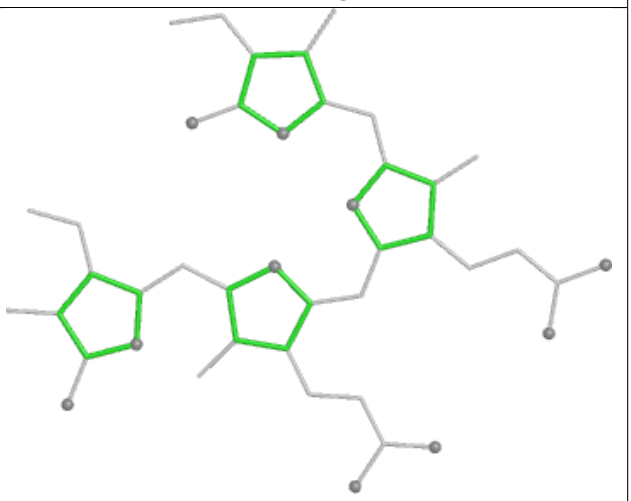
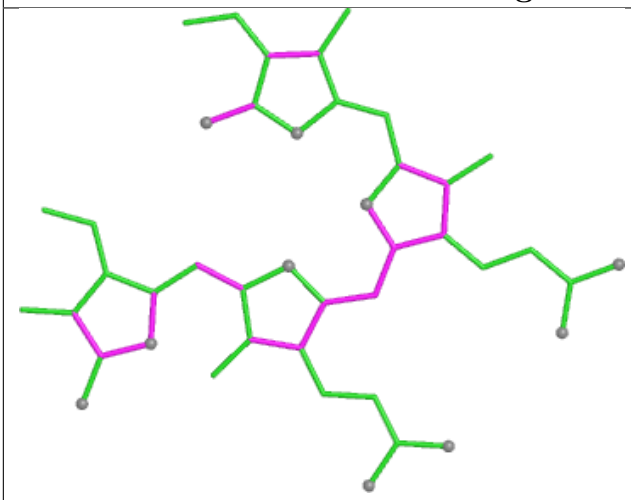


Rings

Ligand PEB O9 201



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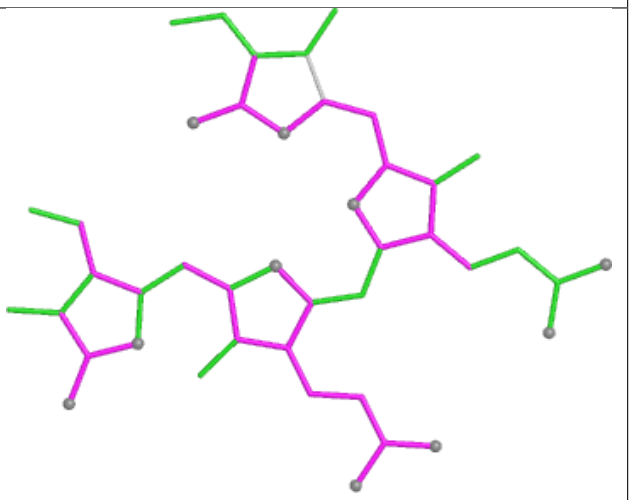

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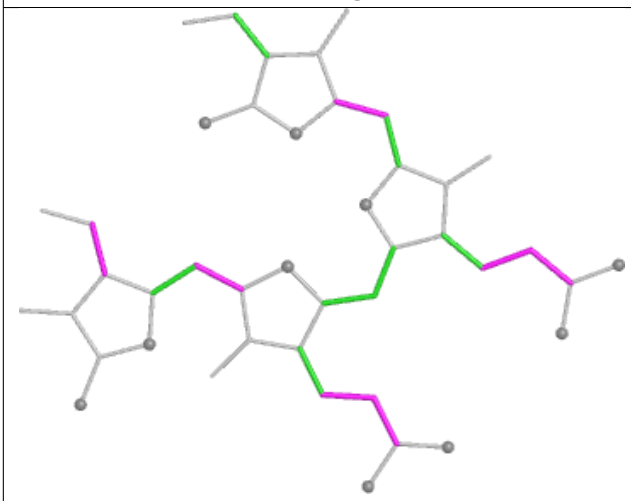

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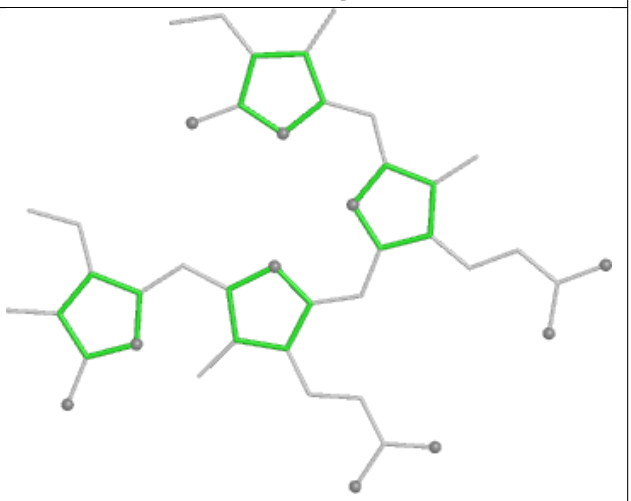

Rings

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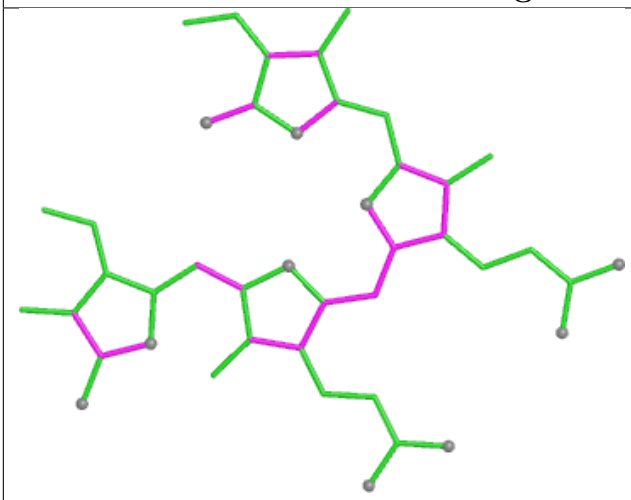

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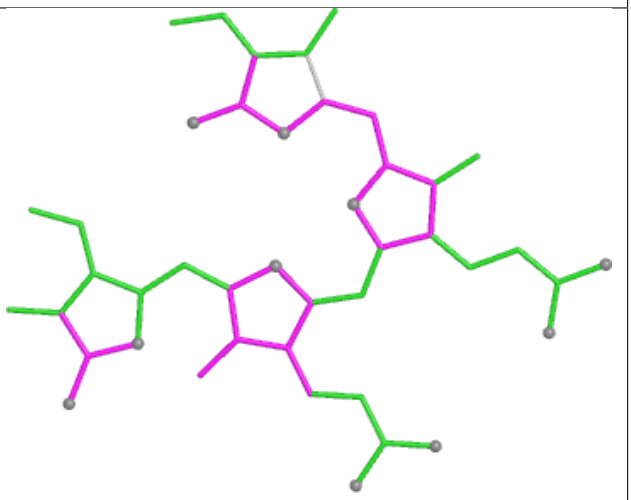

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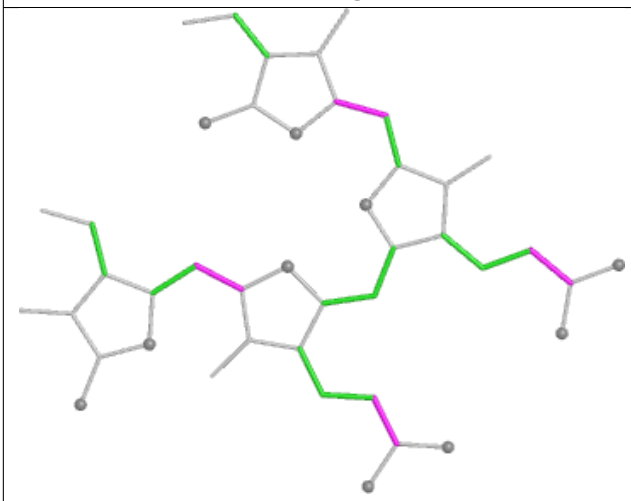

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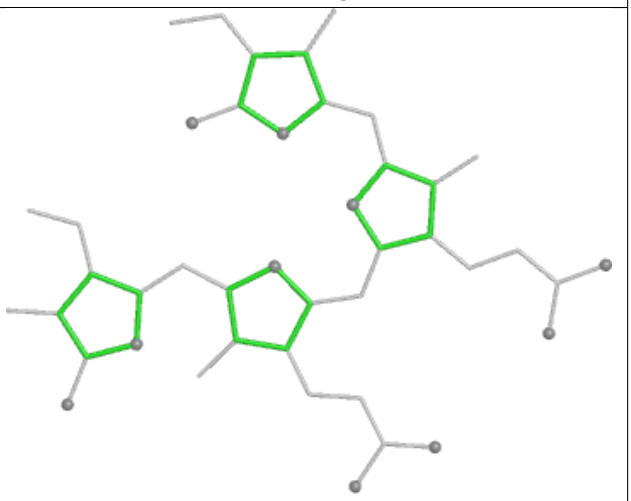
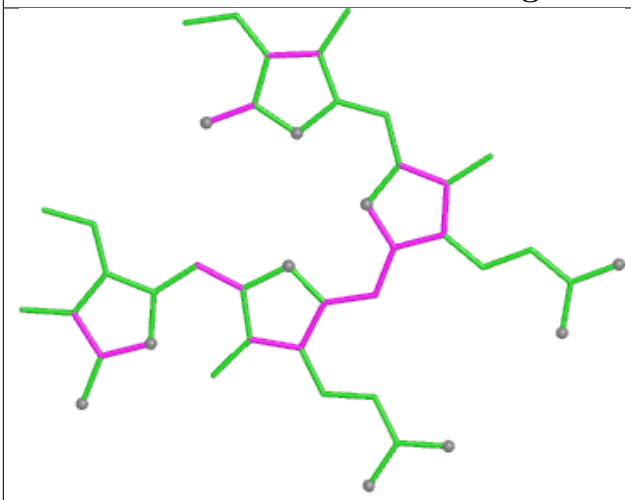


Rings

Ligand PEB t8 202



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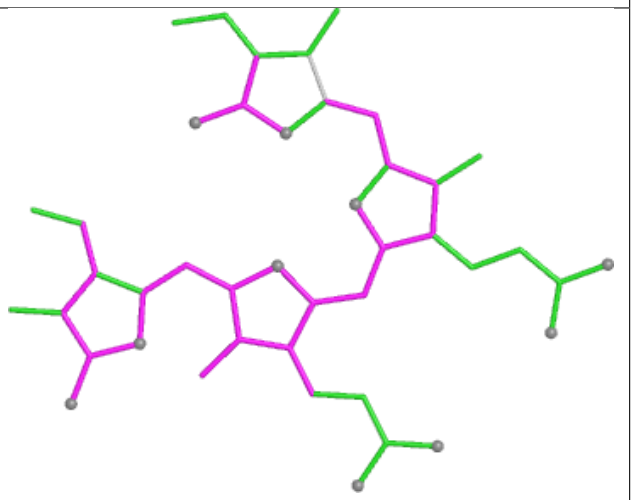

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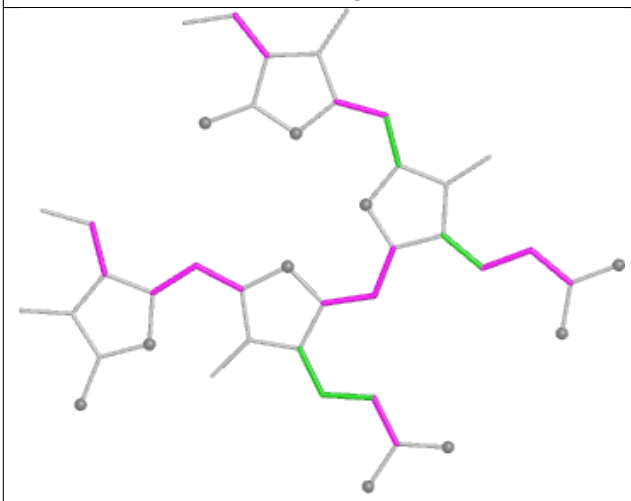

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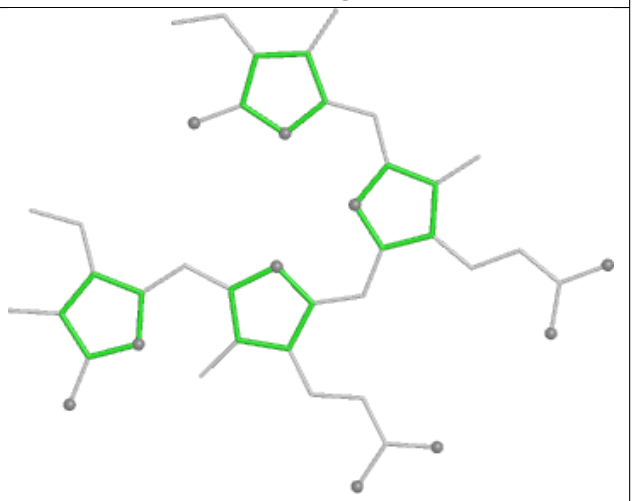

Rings

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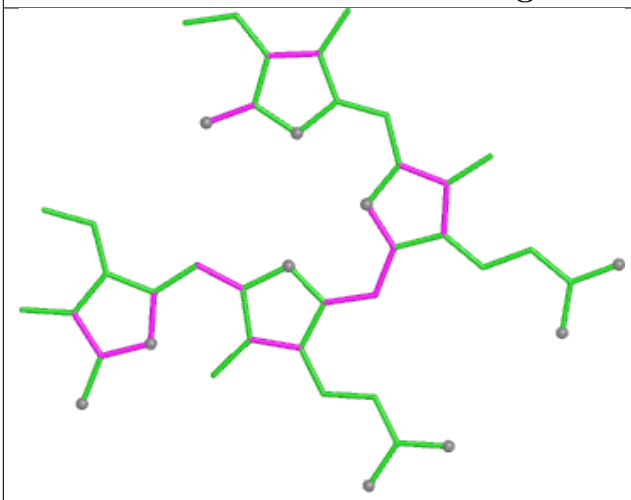

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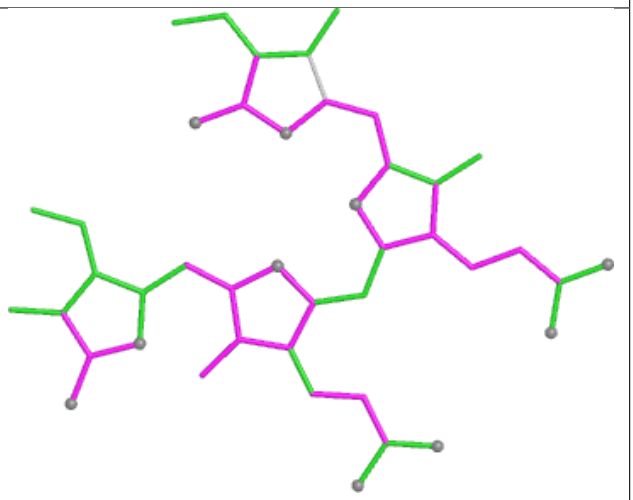

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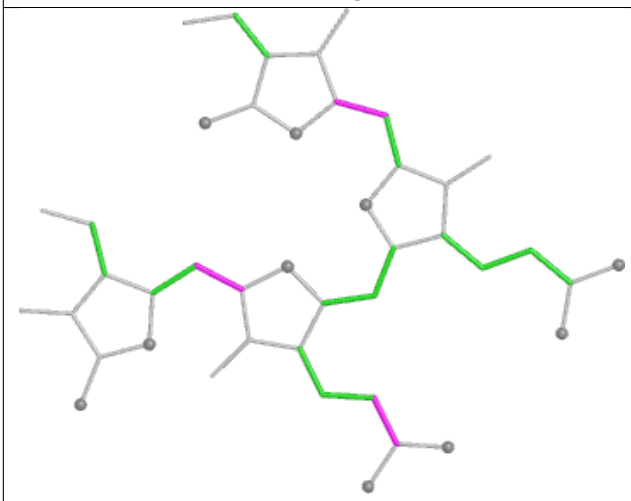

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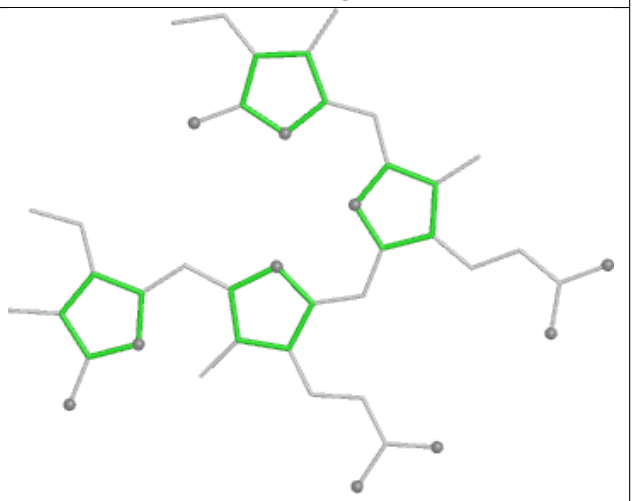

Rings

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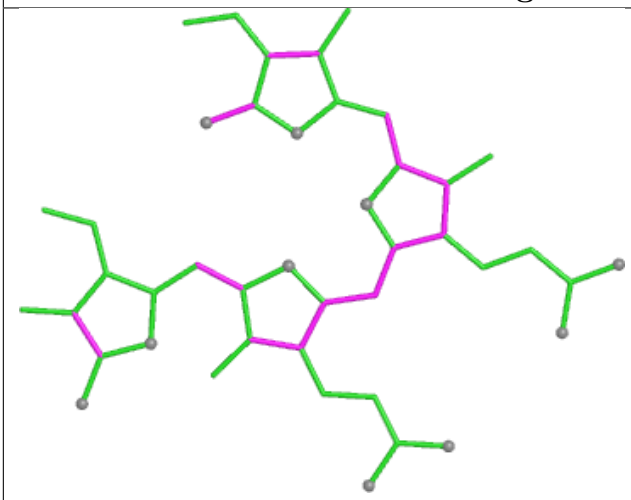

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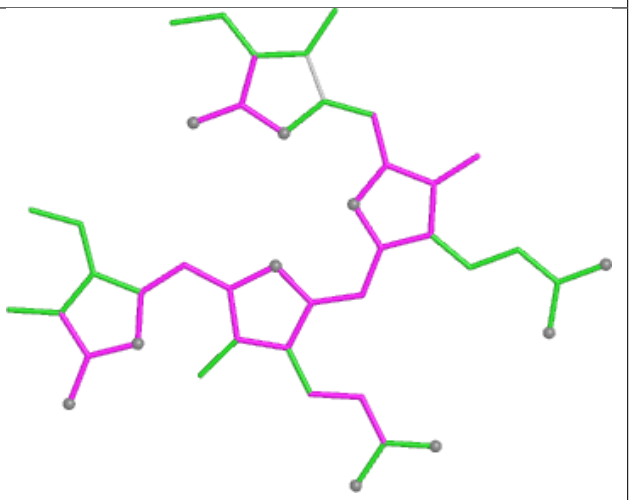

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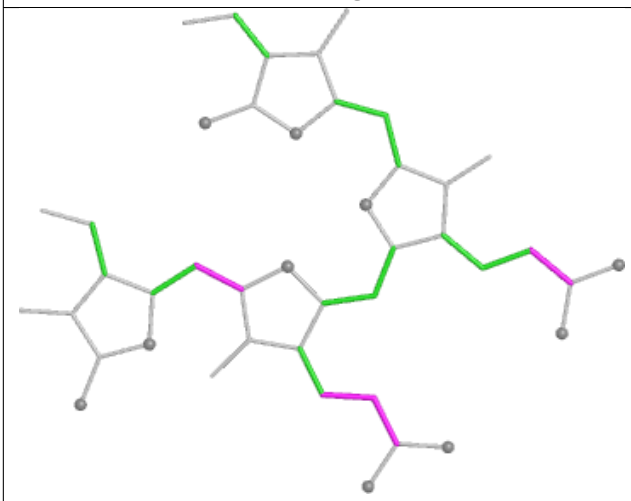

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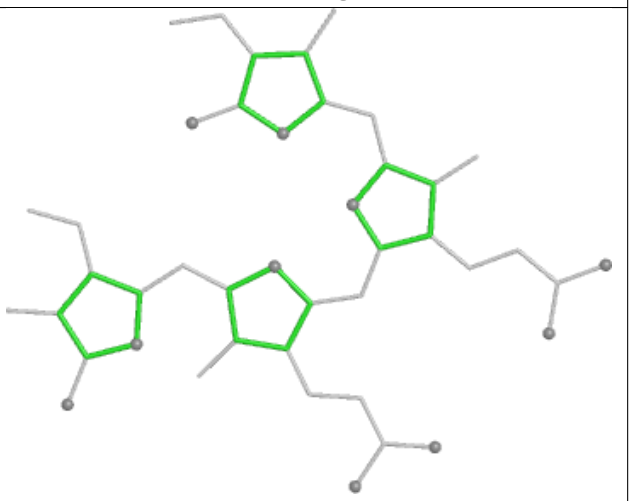
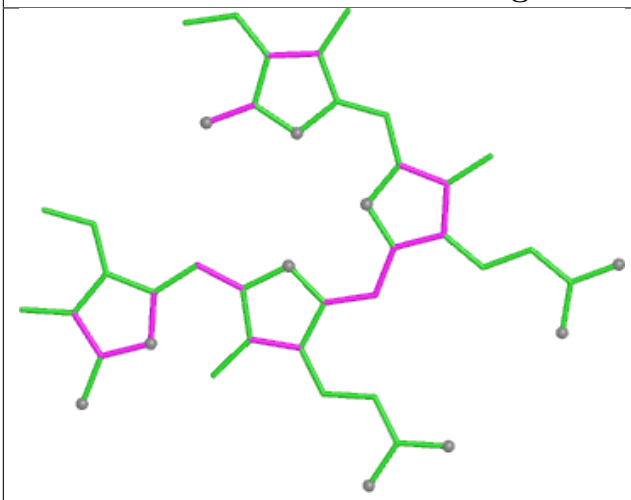


Rings

Ligand PEB UB 303



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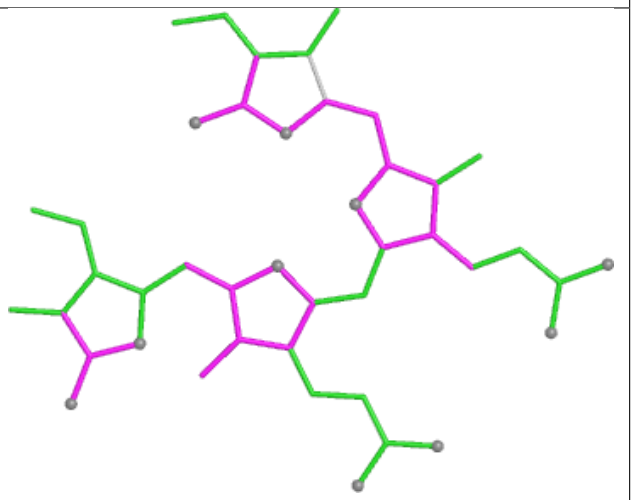

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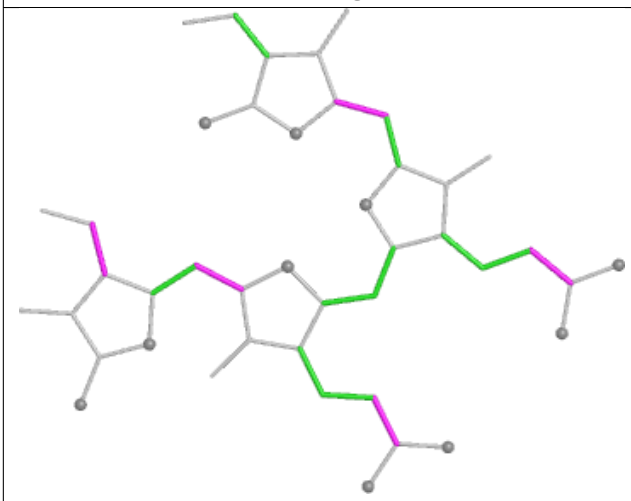

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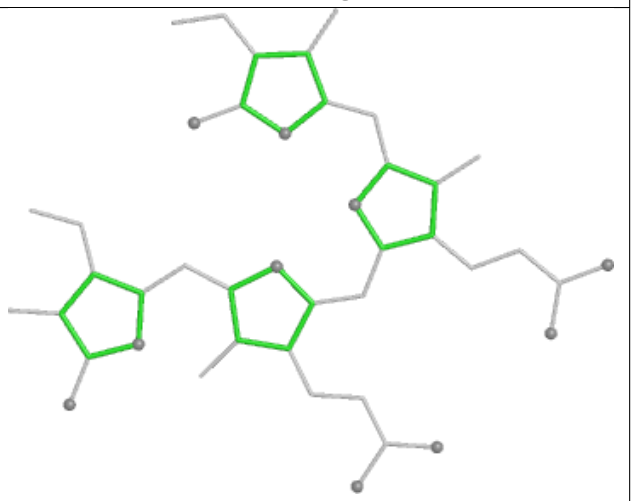

Rings

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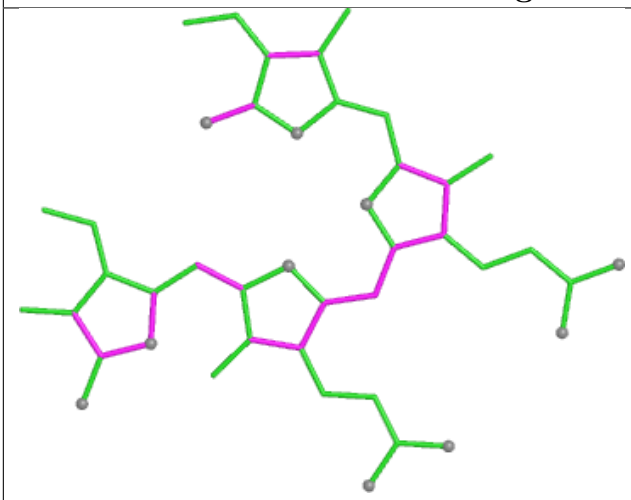

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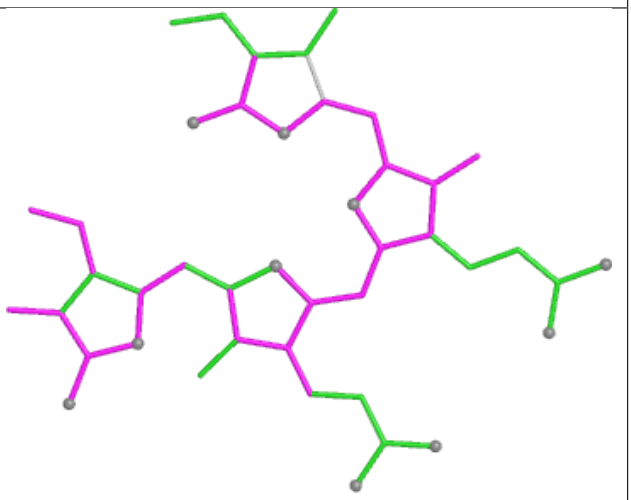

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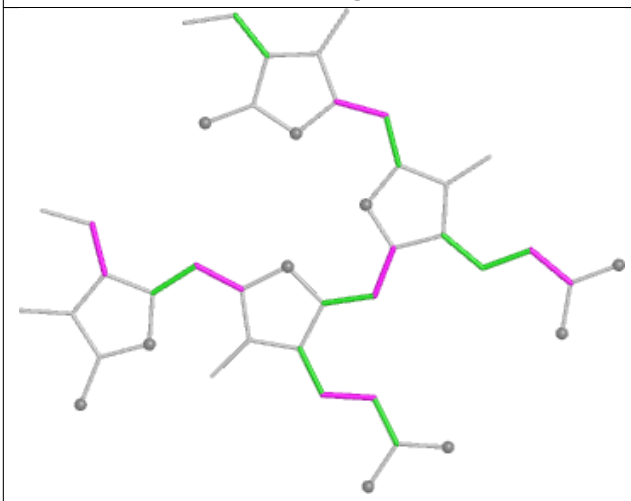

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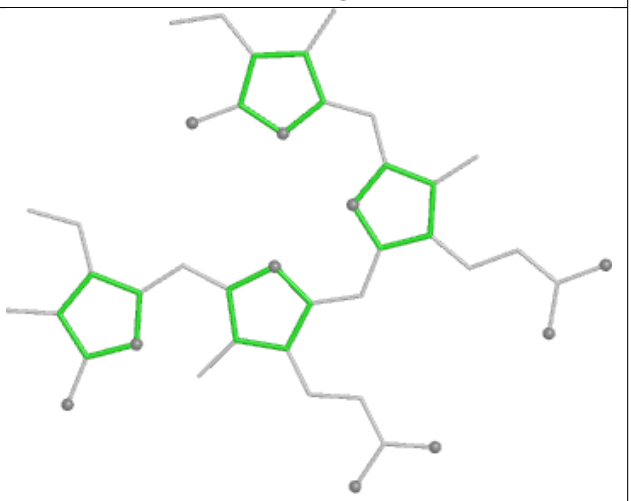
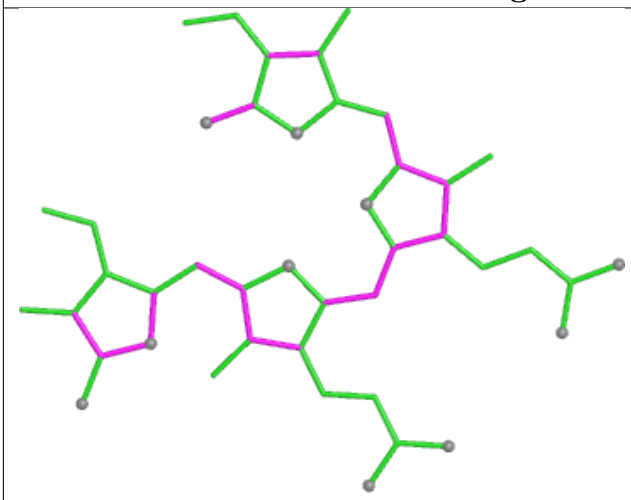


Rings

Ligand PEB HD 202



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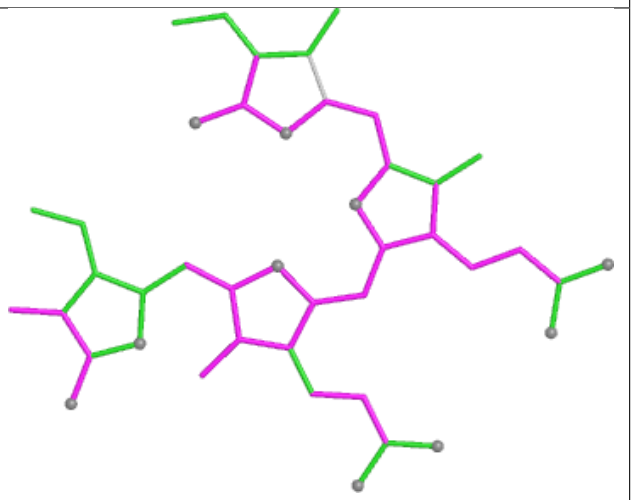

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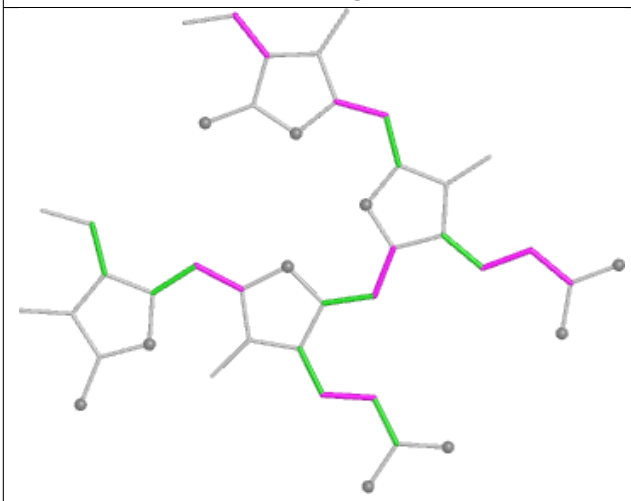

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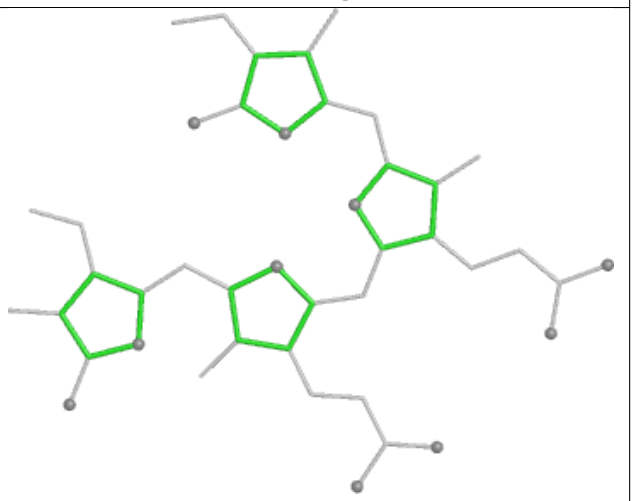
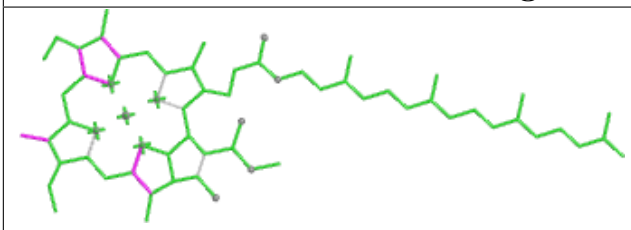


Rings

Ligand CLA 22 602



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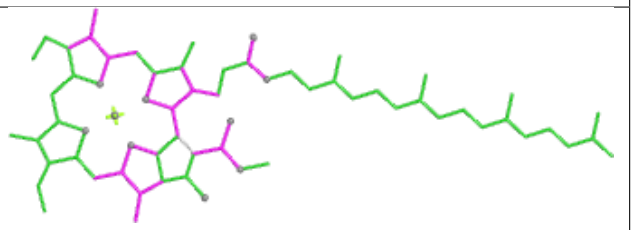

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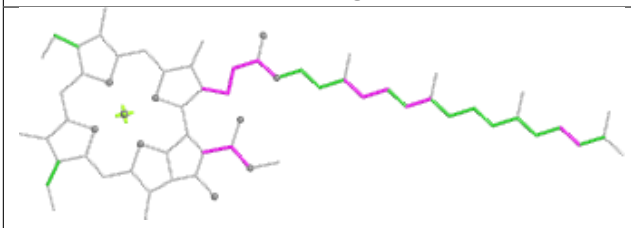

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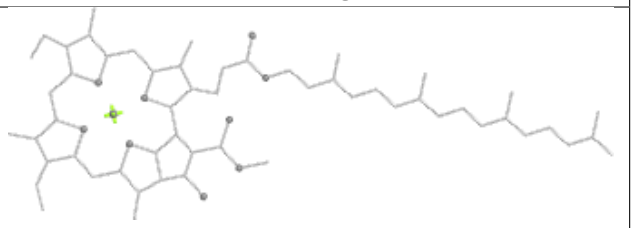
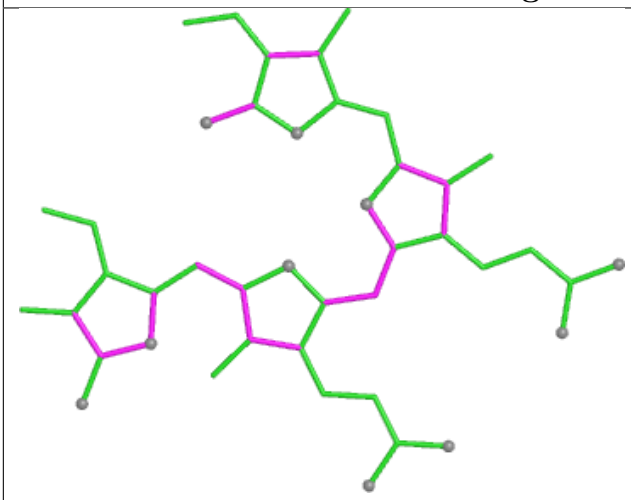


Rings

Ligand PEB I5 201



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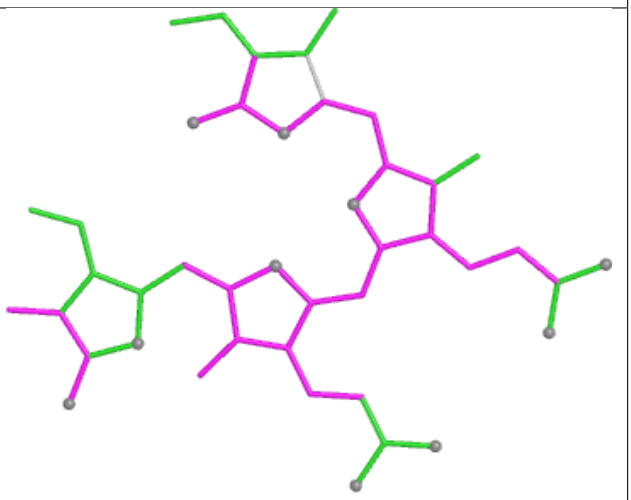

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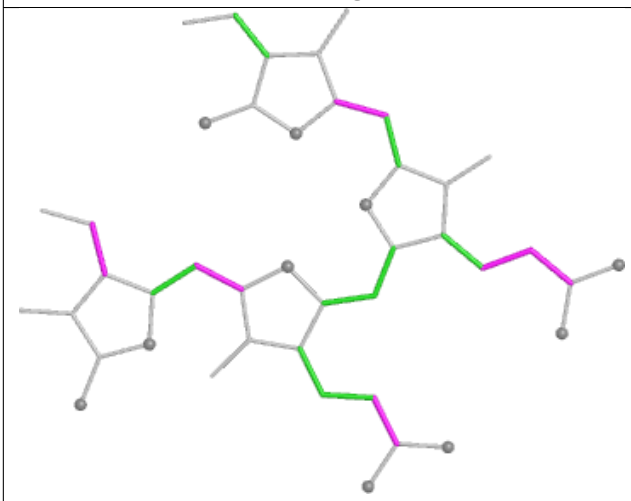

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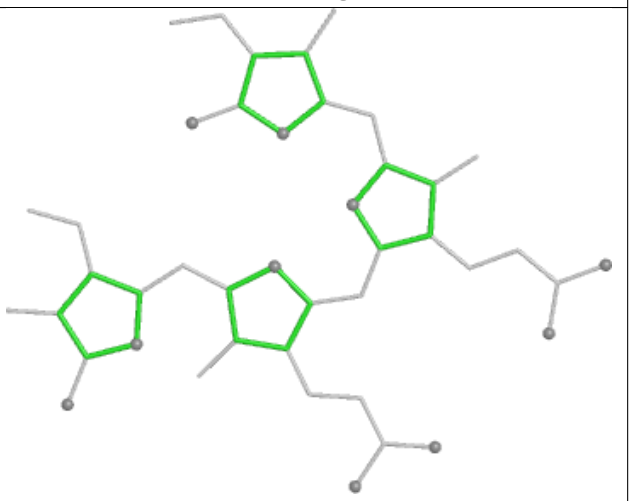
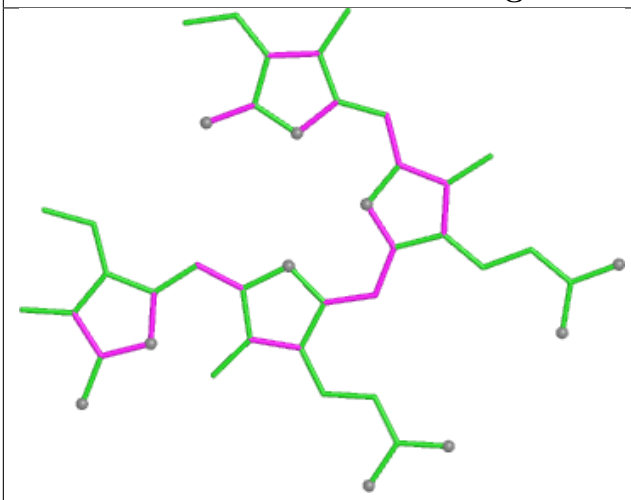


Rings

Ligand PEB mM 201



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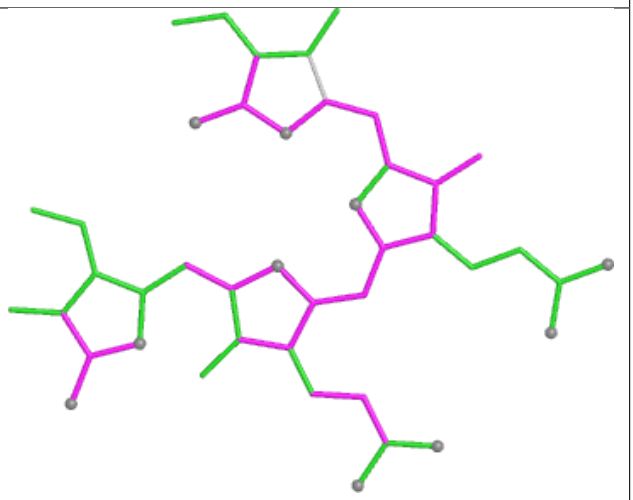

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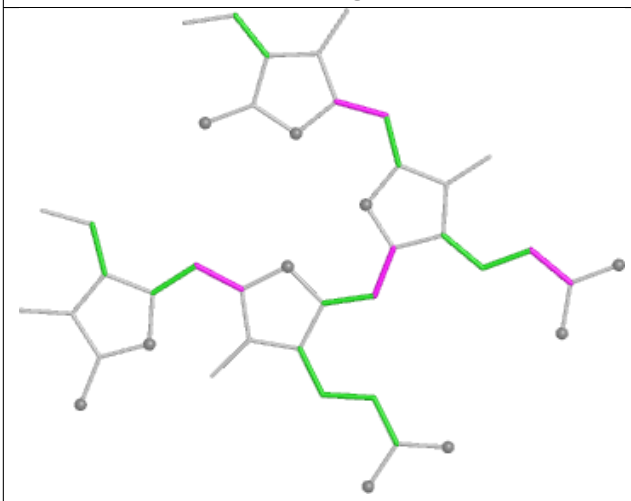

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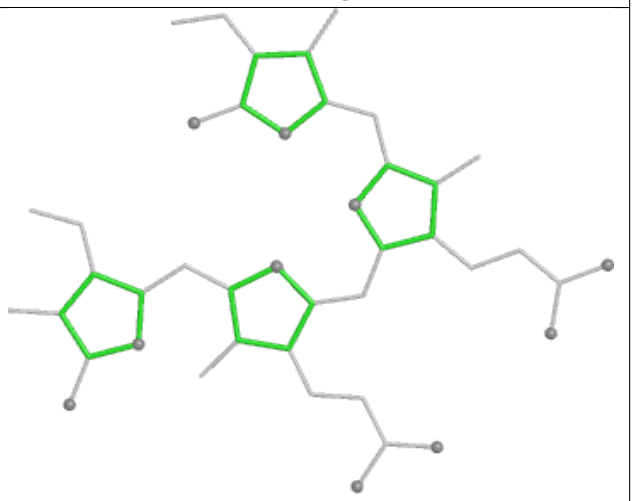
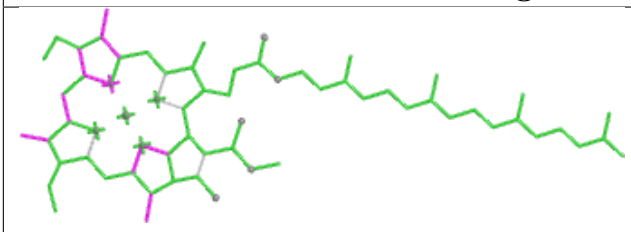


Rings

Ligand CLA B6 607



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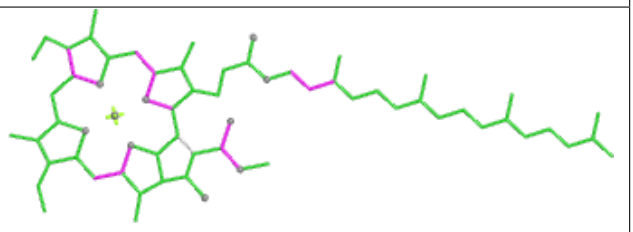
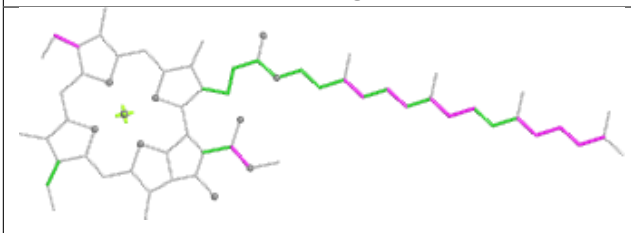


Bond angles



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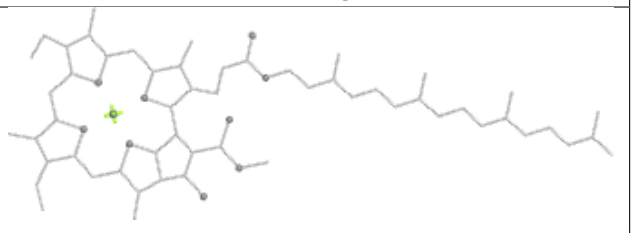
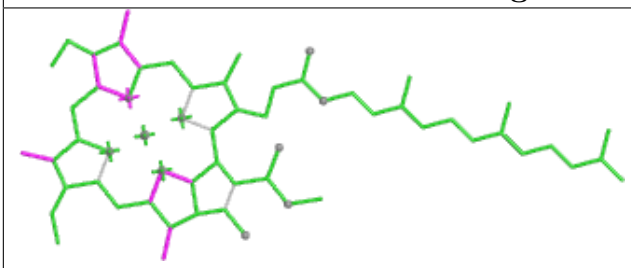


Rings

Ligand CLA BN 818



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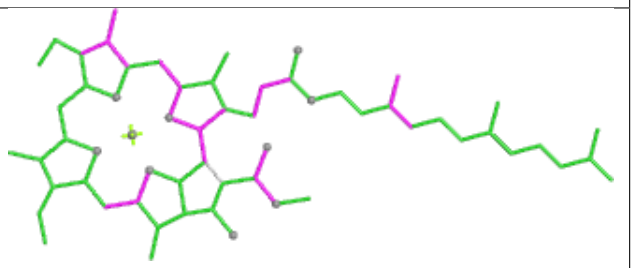
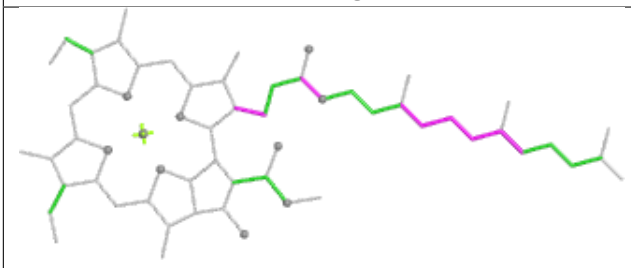


Bond angles



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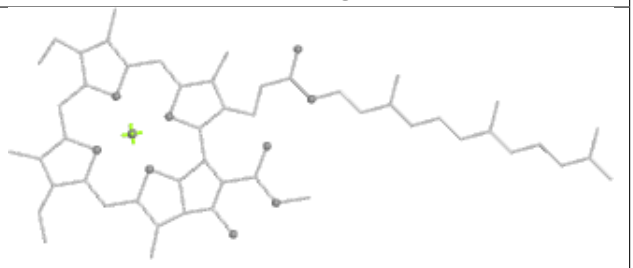
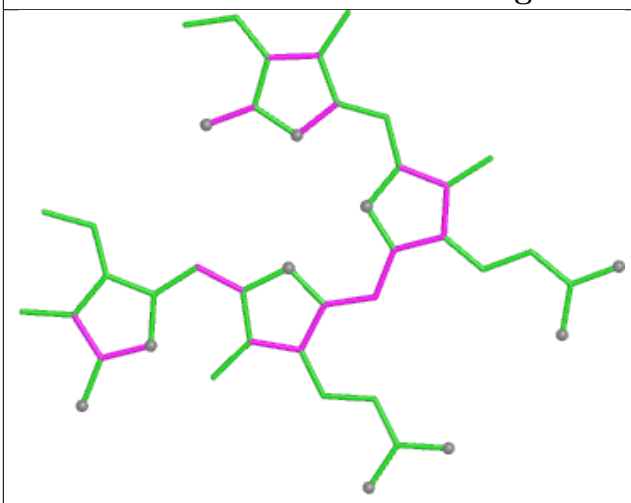


Rings

Ligand PEB oK 203



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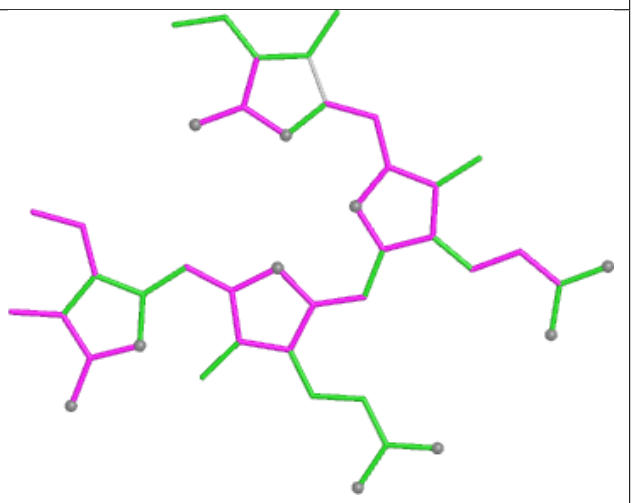

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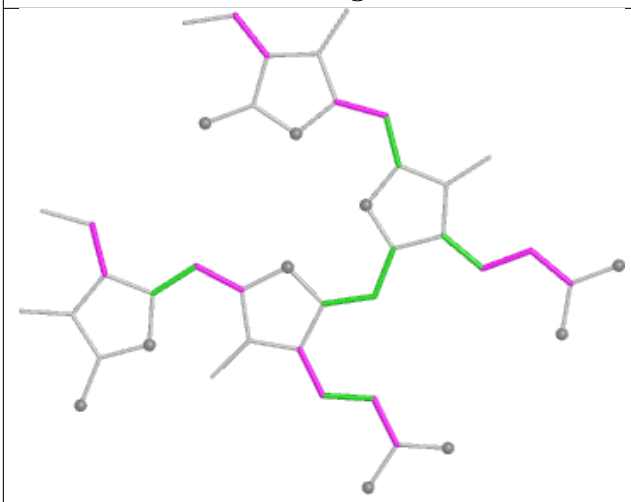

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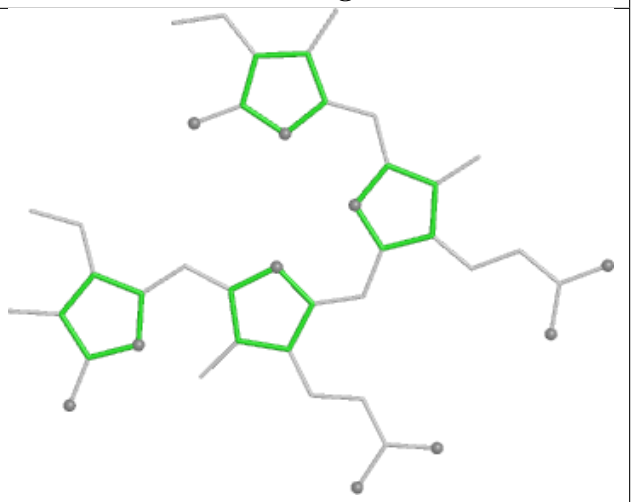
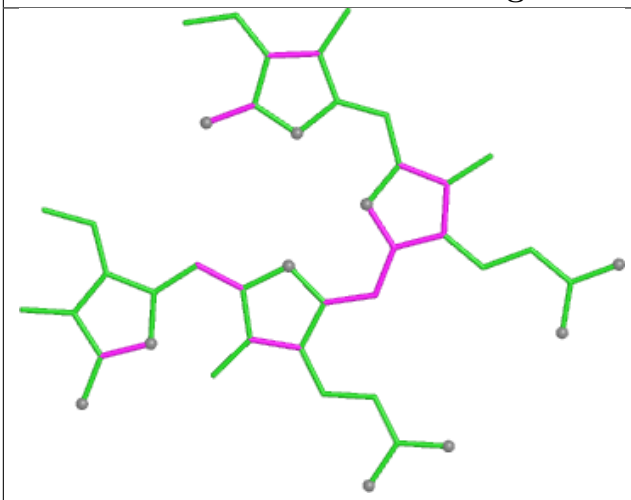


Rings

Ligand PEB AM 302



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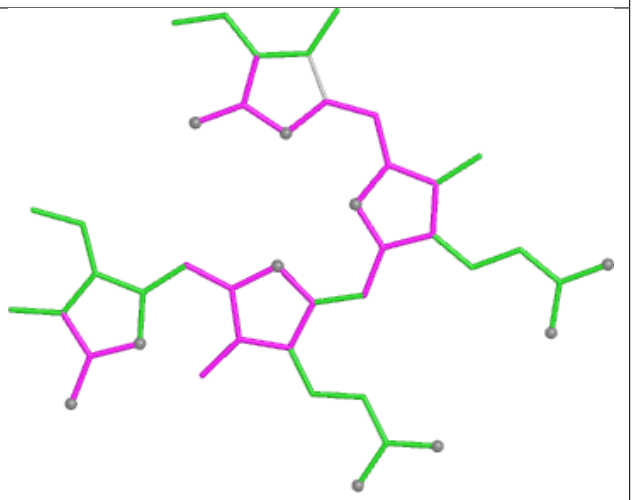

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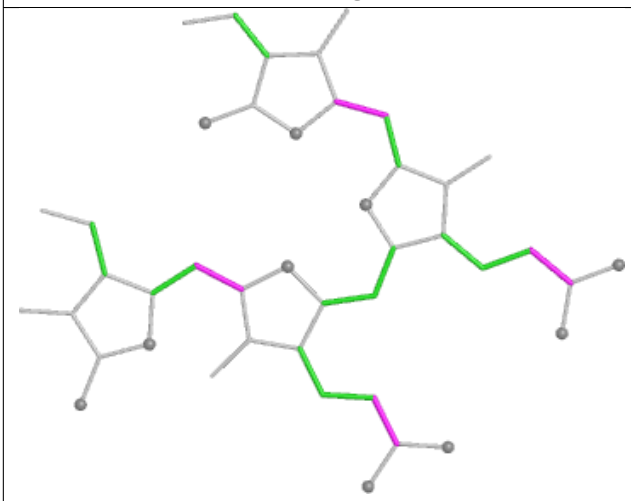

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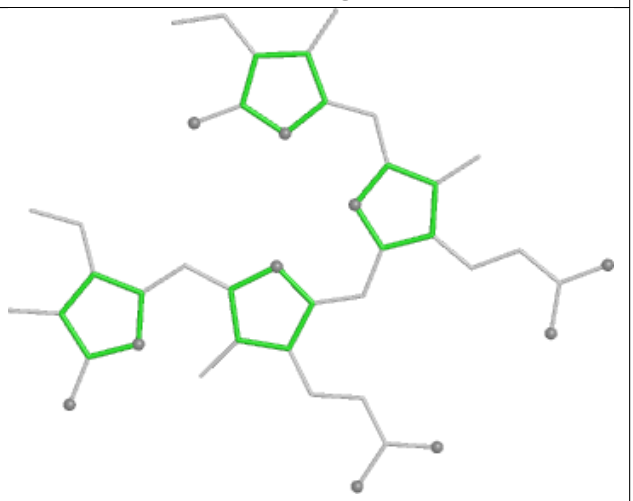
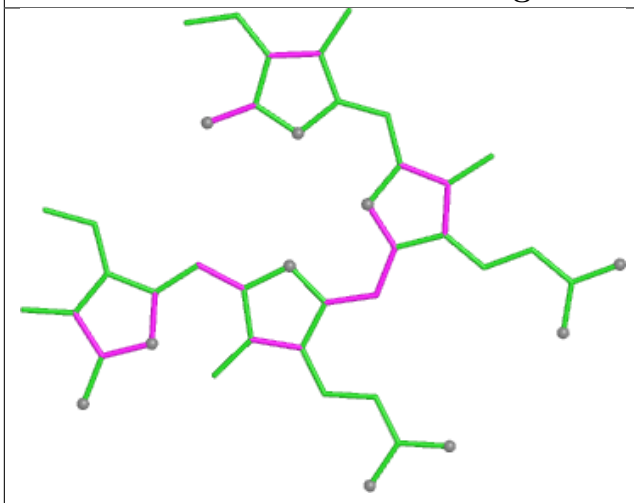


Rings

Ligand PEB QE 203



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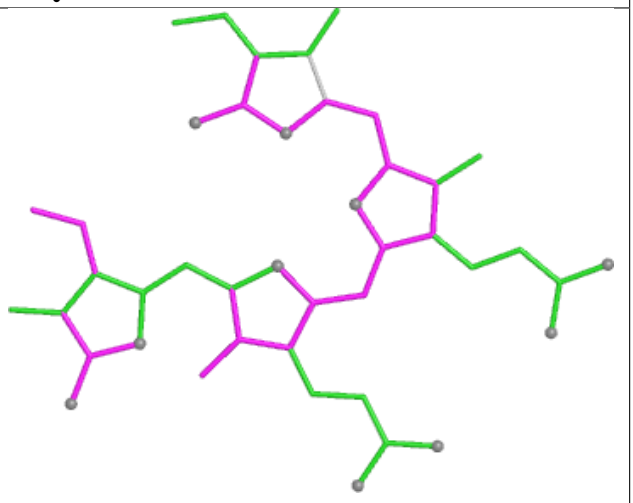

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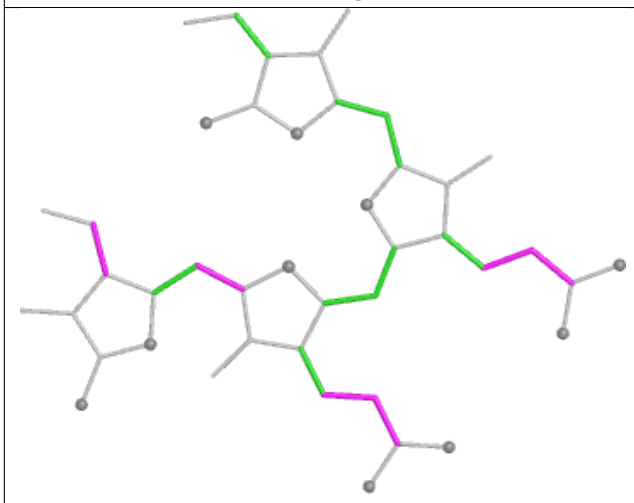

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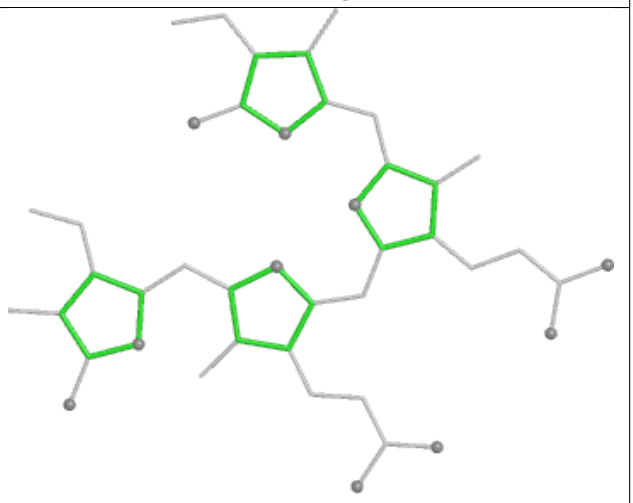

Rings

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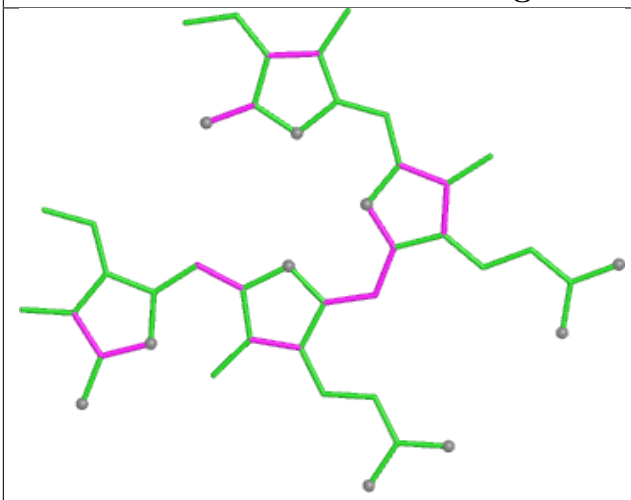

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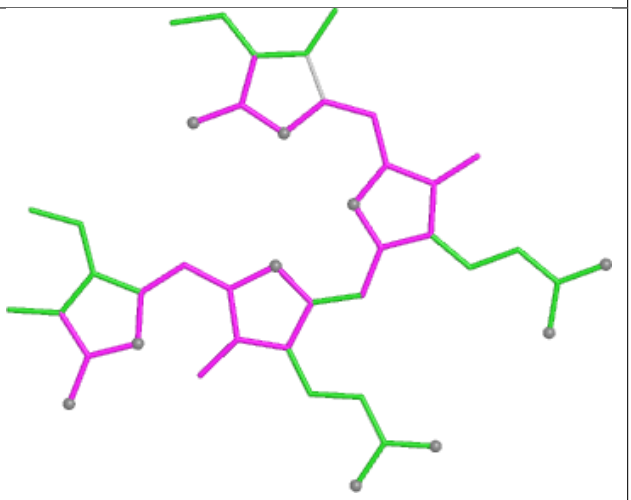

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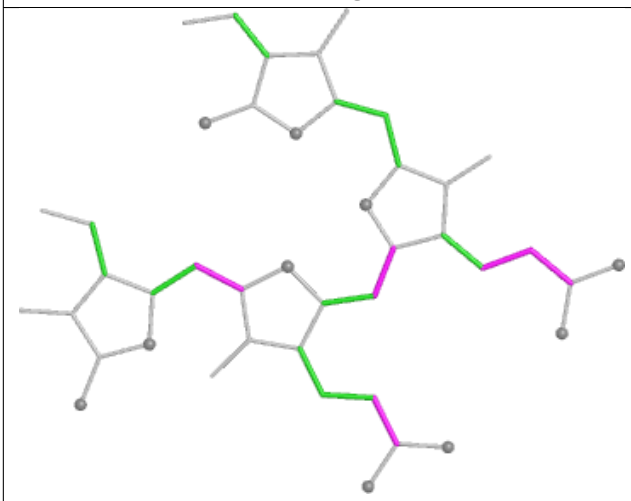

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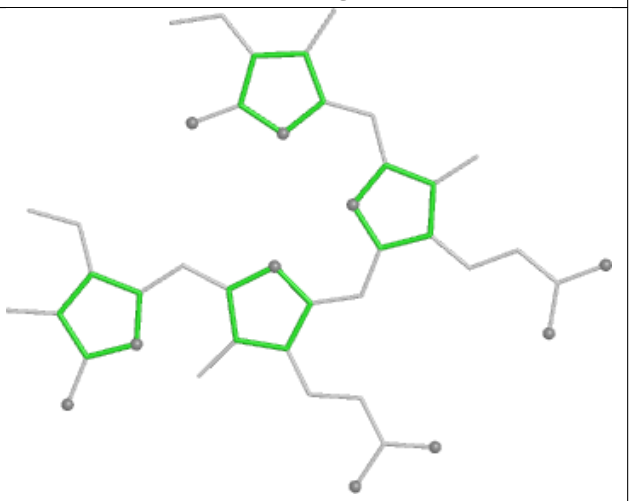
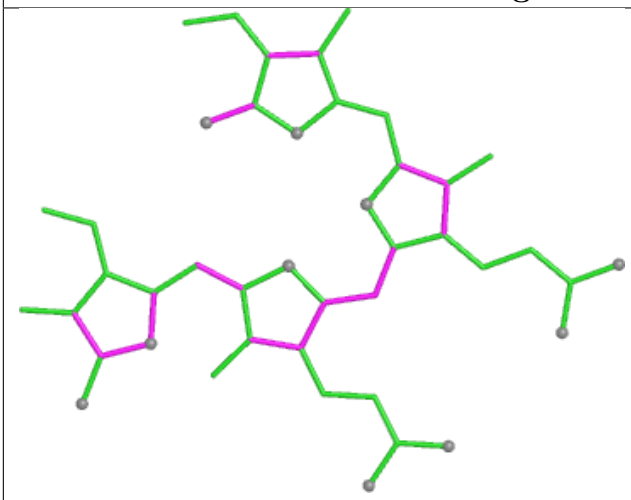


Rings

Ligand PEB ZK 201



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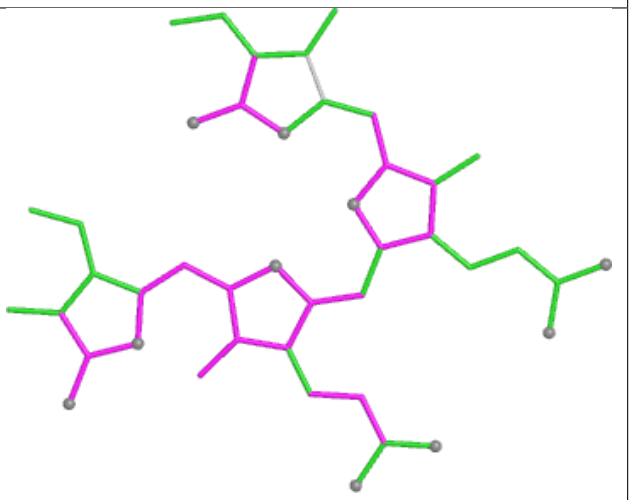

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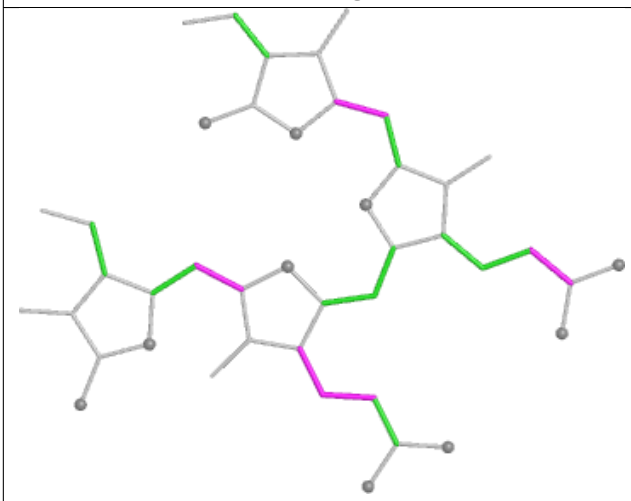

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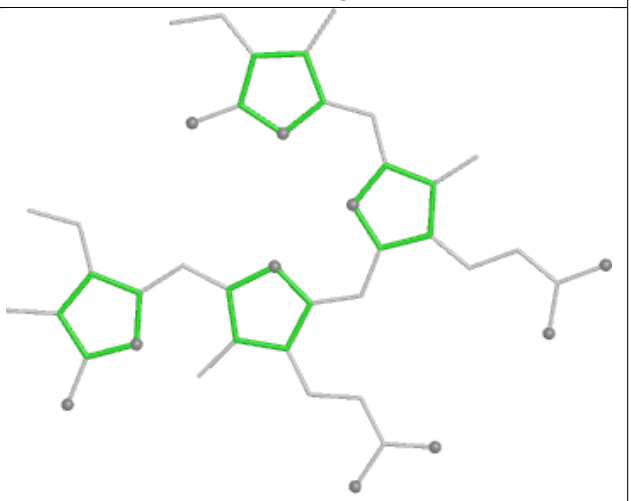
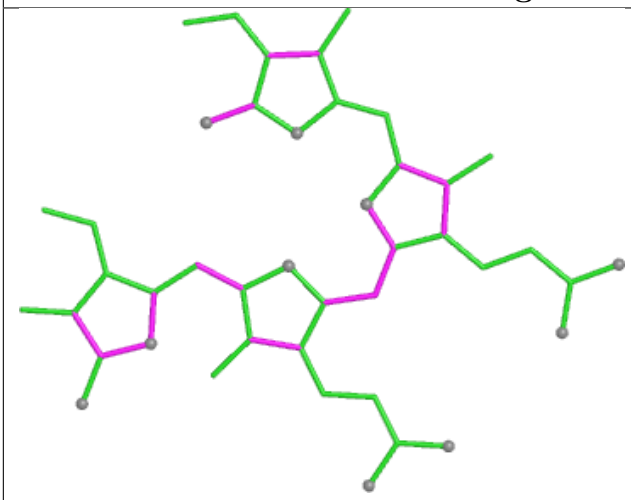


Rings

Ligand PEB U4 202



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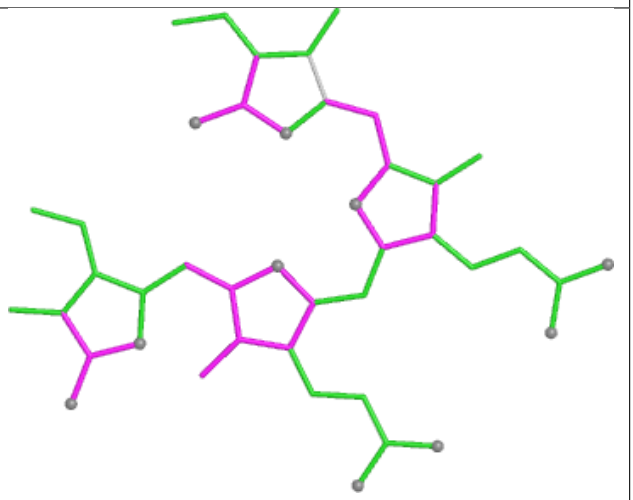

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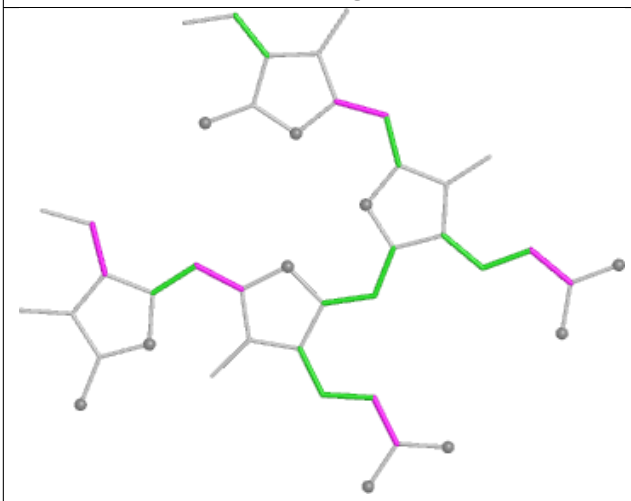

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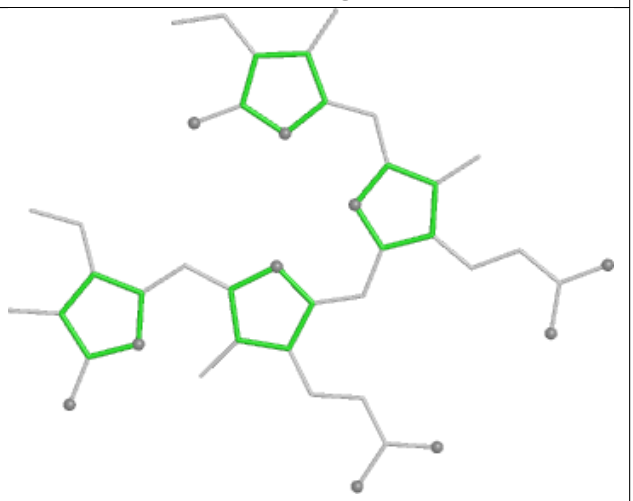
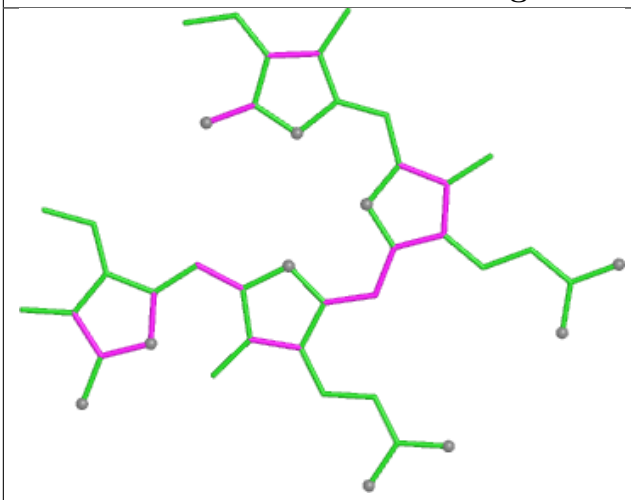


Rings

Ligand PEB AH 302



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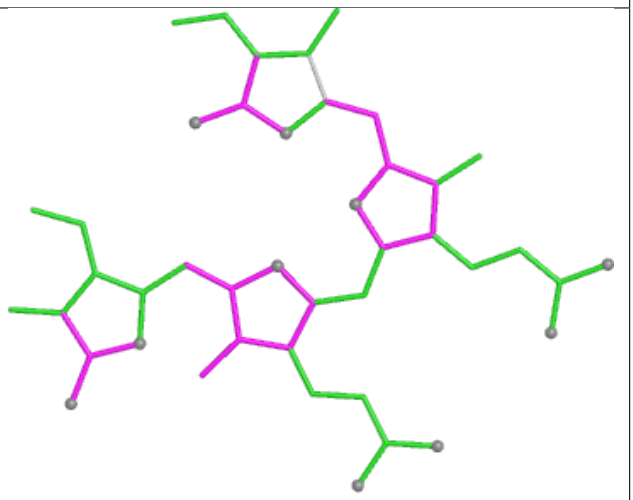

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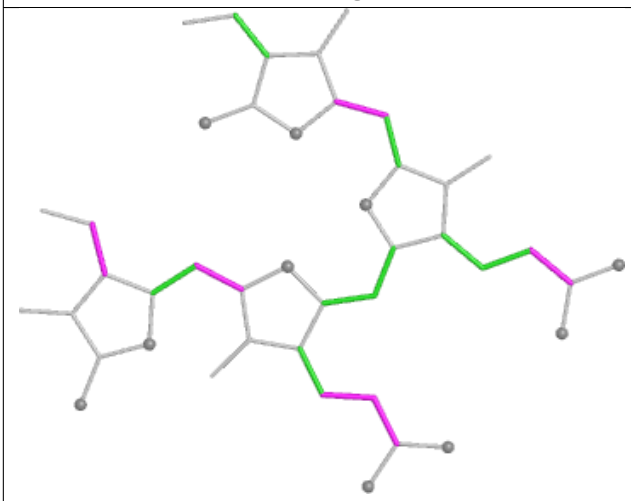

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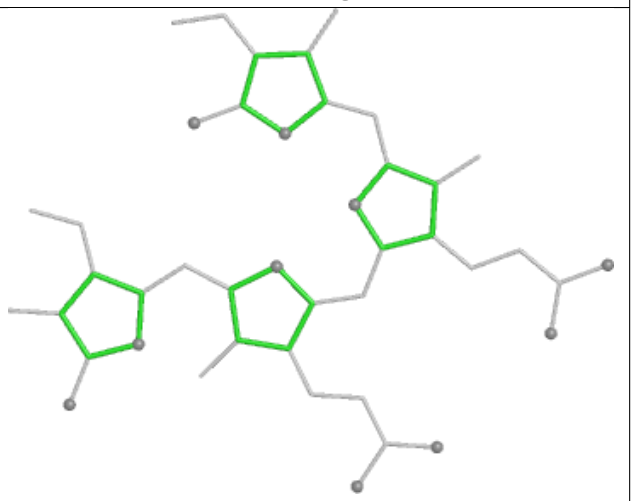
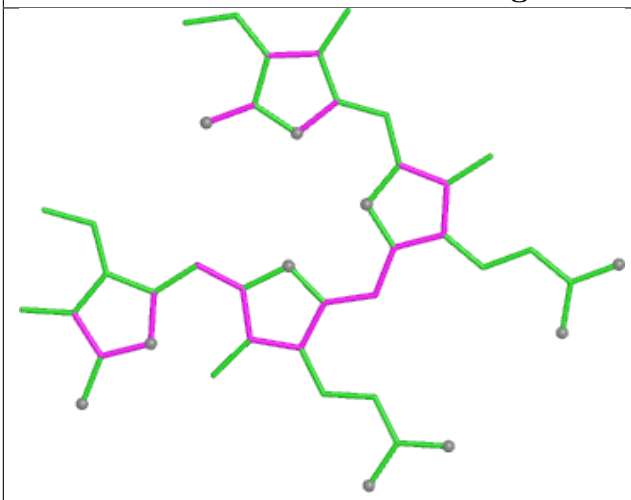


Rings

Ligand PEB OQ 202



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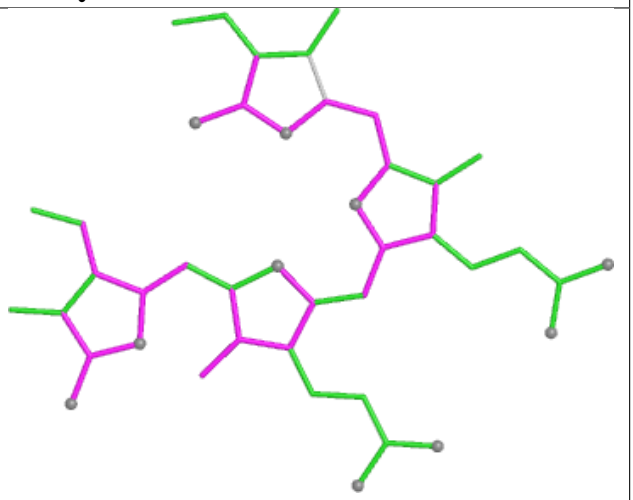

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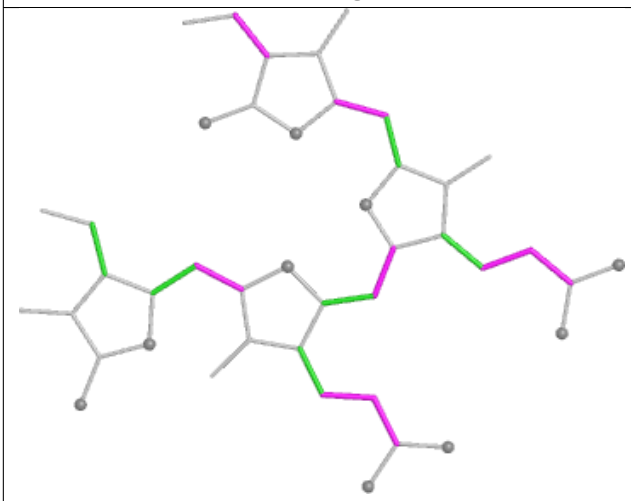

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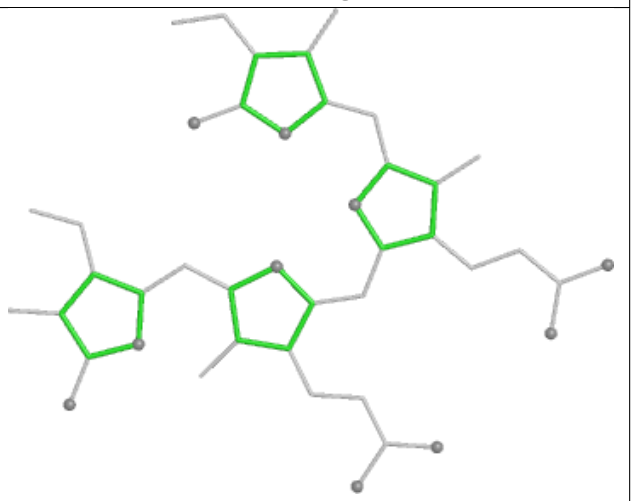
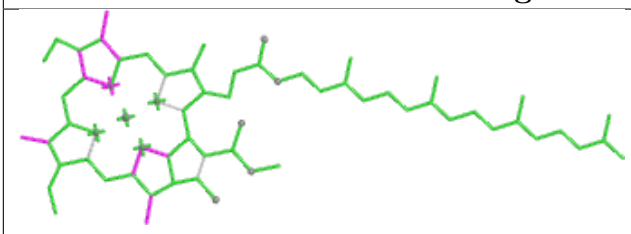


Rings

Ligand CLA K6 101



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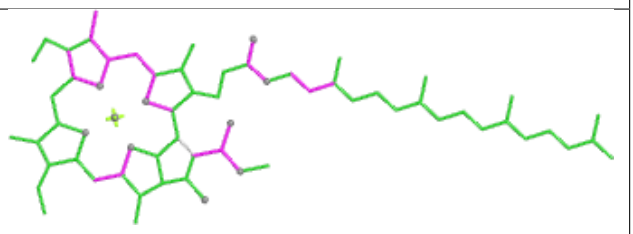

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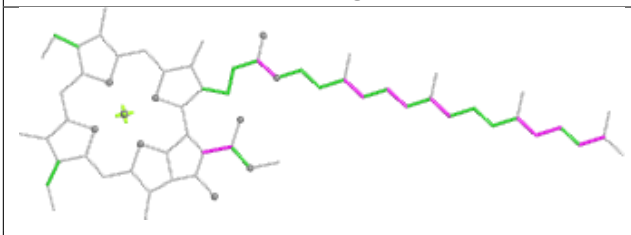

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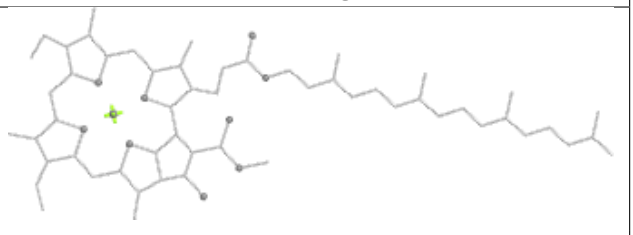
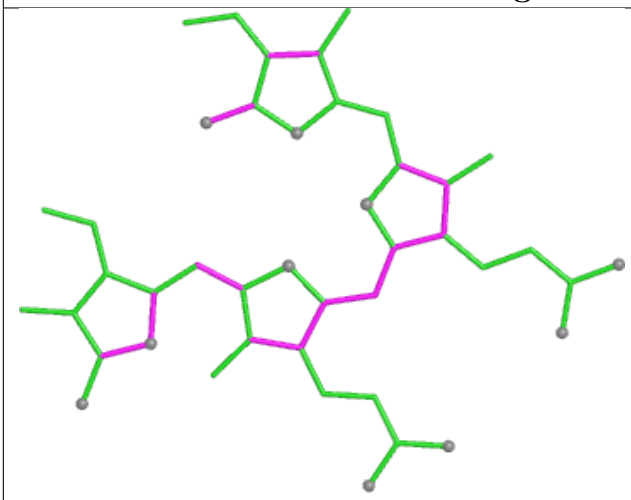


Rings

Ligand PEB bH 202



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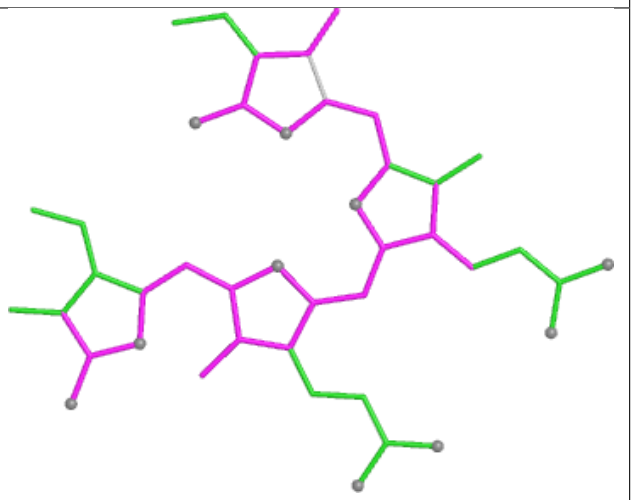

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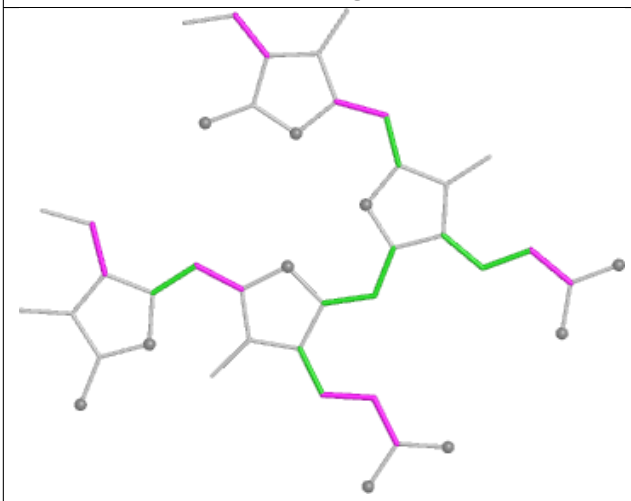

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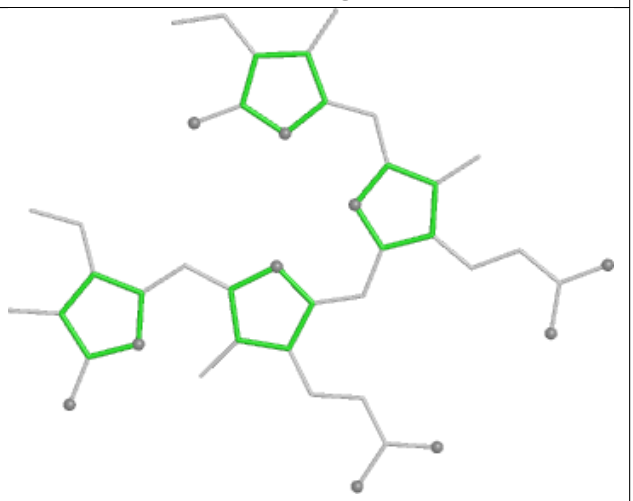
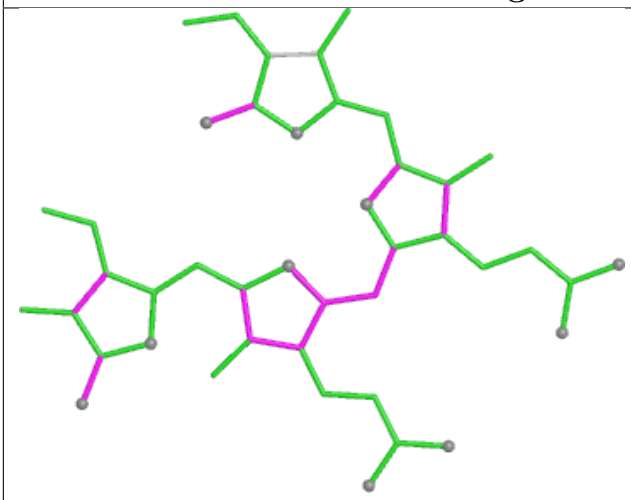


Rings

Ligand PUB ND 201



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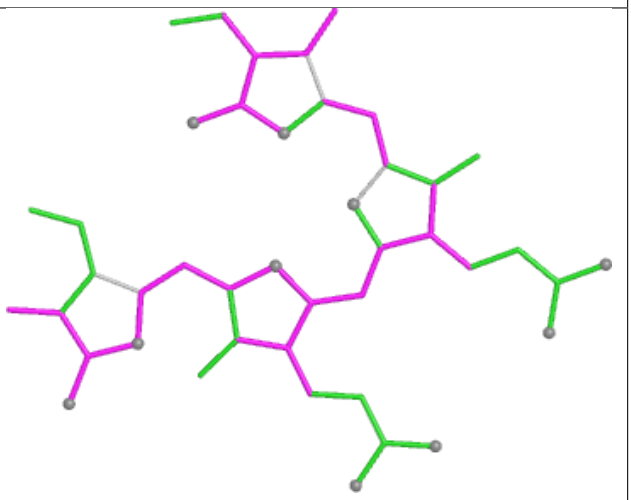

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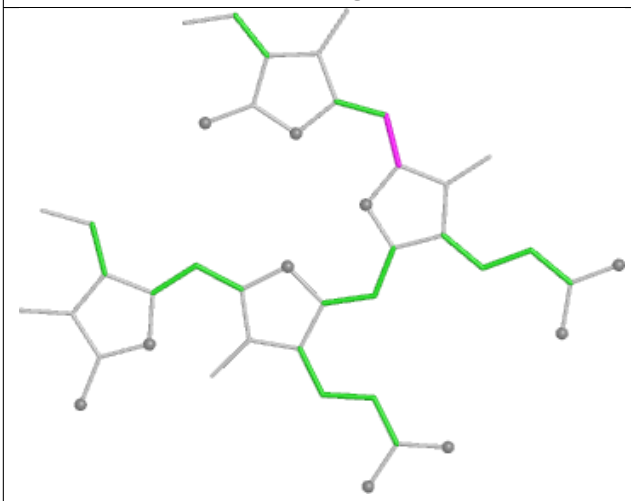

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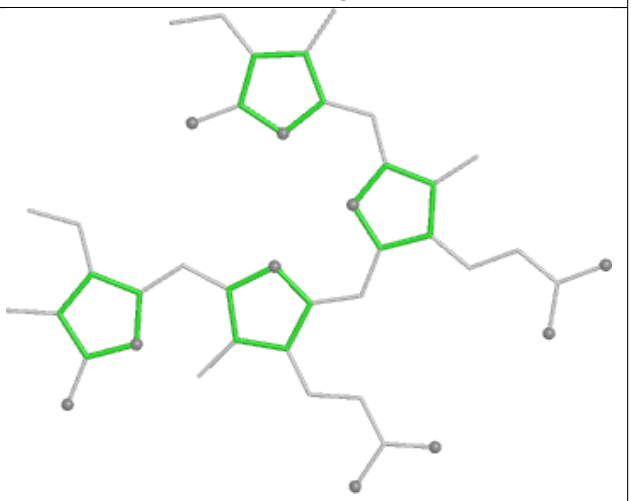
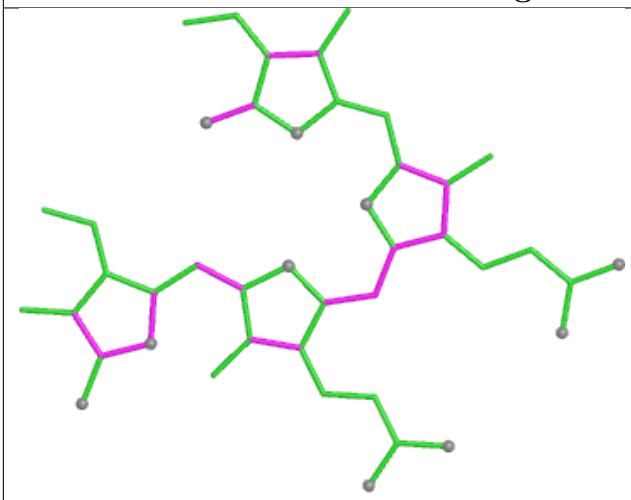


Rings

Ligand PEB HJ 202



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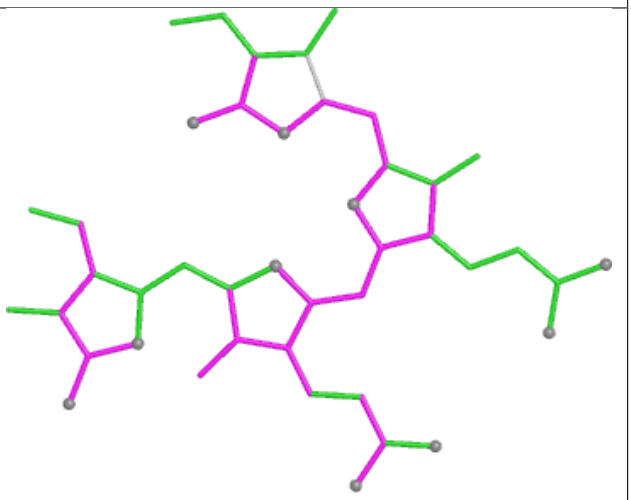

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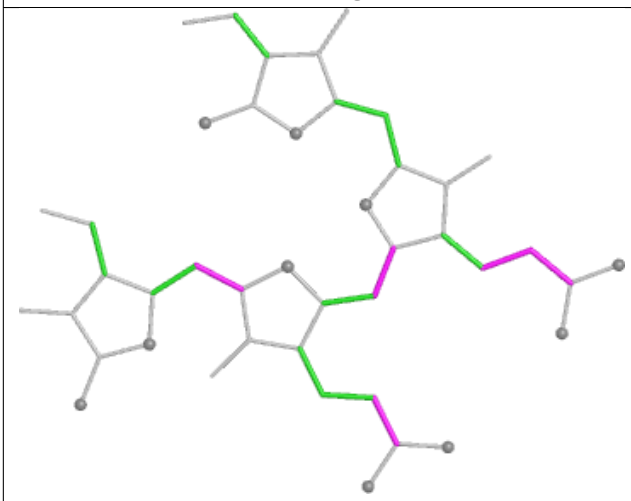

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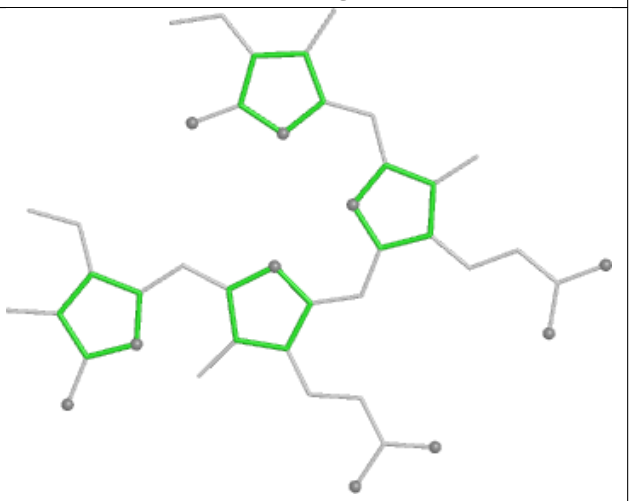
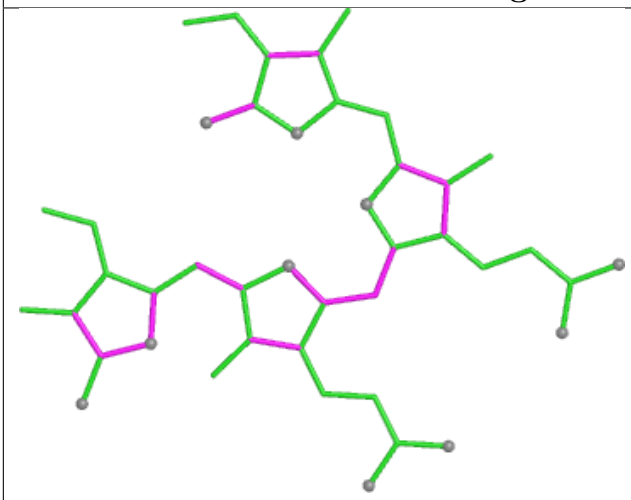


Rings

Ligand PEB WJ 201



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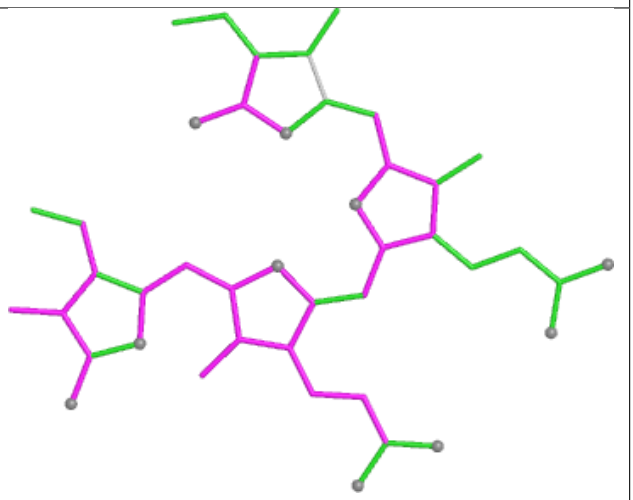
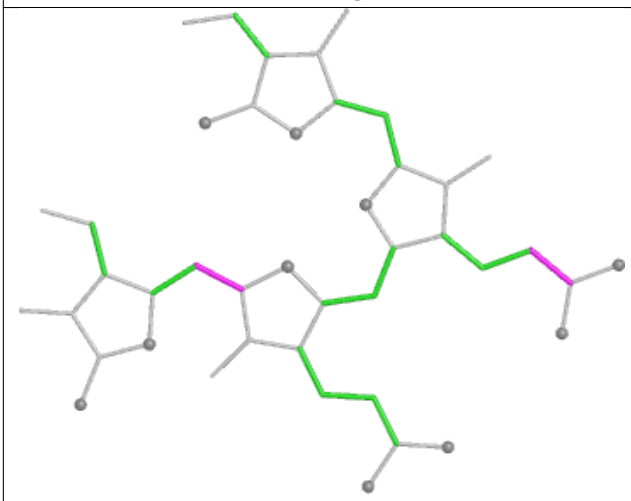


Bond angles



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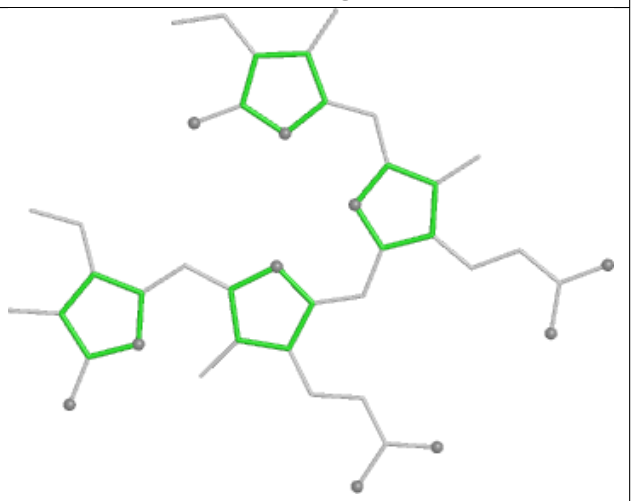
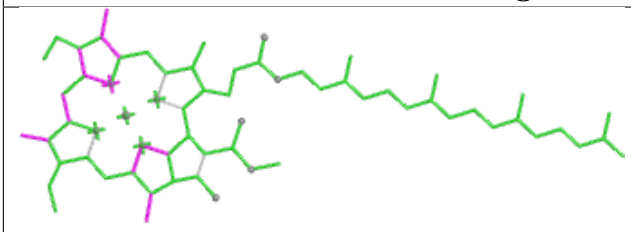


Rings

Ligand CLA A2 838



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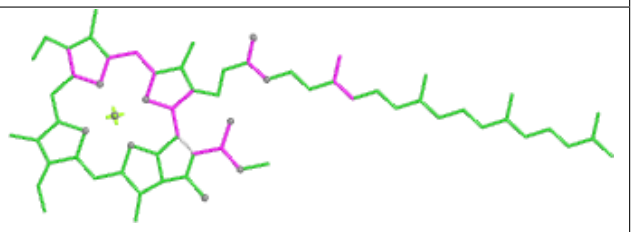
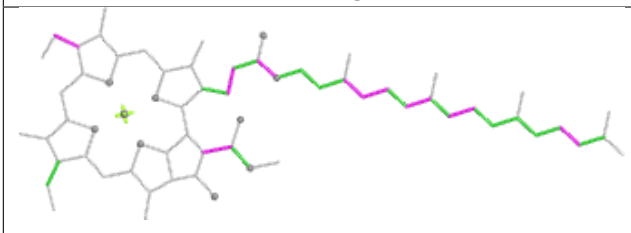


Bond angles



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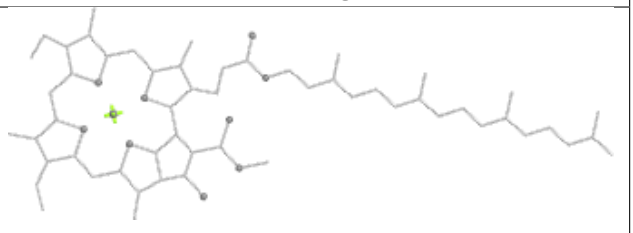
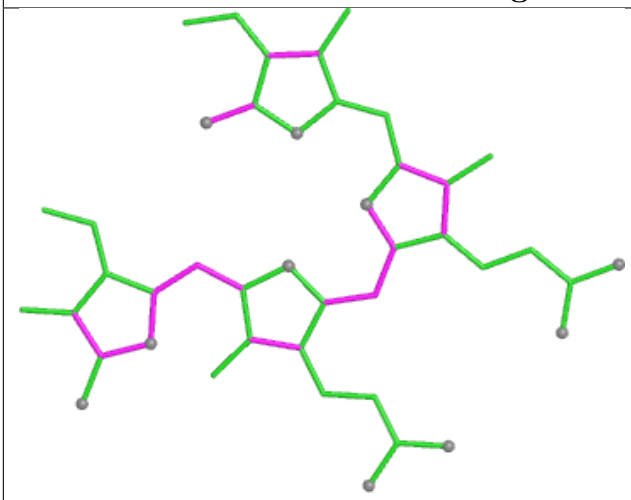


Rings

Ligand PEB QO 201



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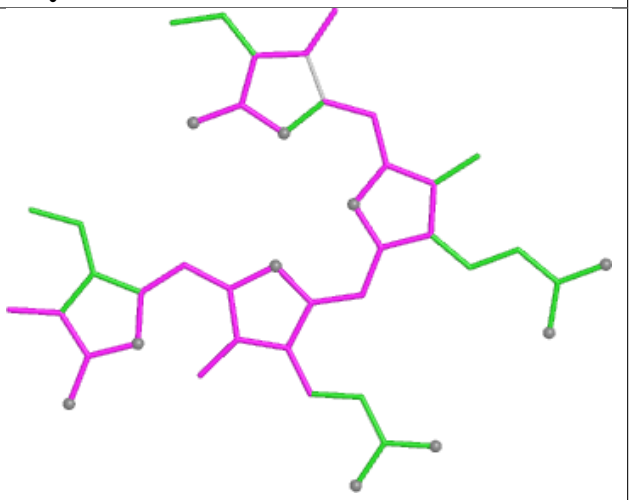
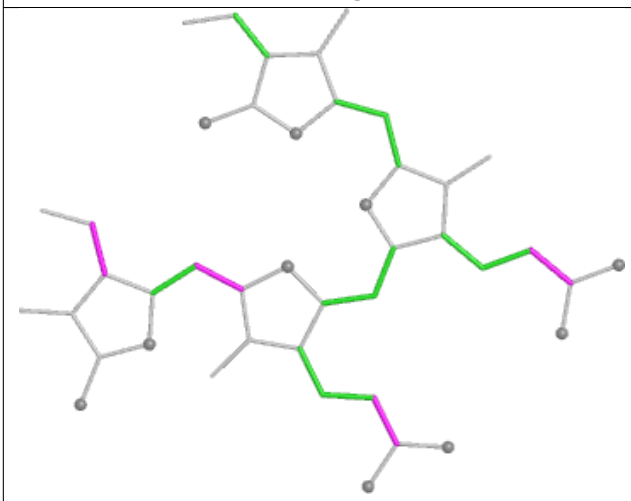


Bond angles



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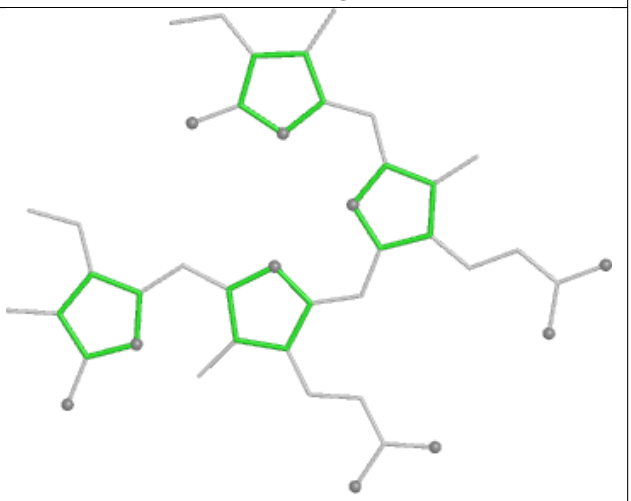
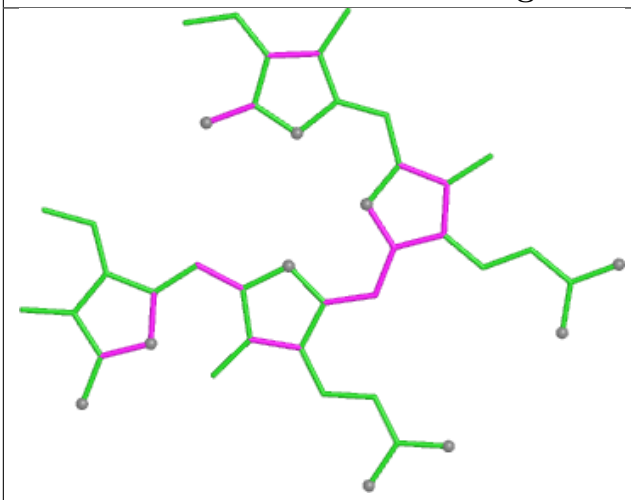


Rings

Ligand PEB NI 202



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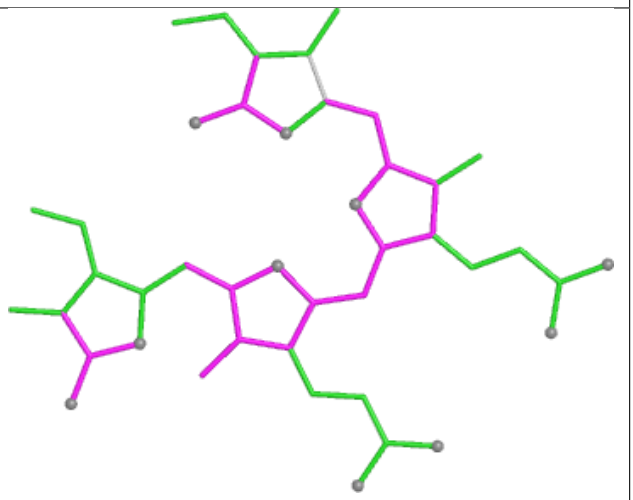

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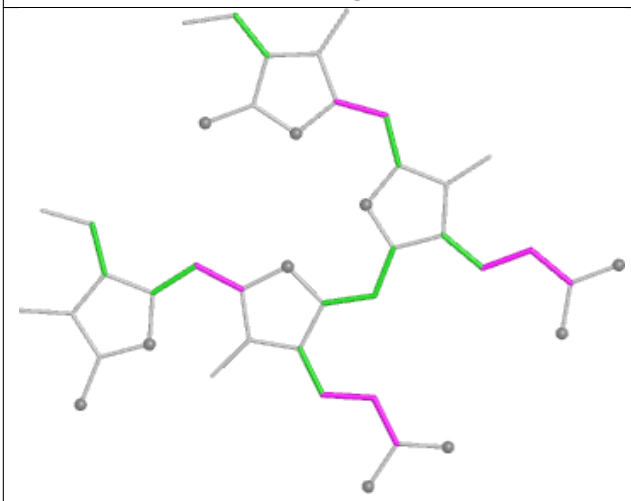

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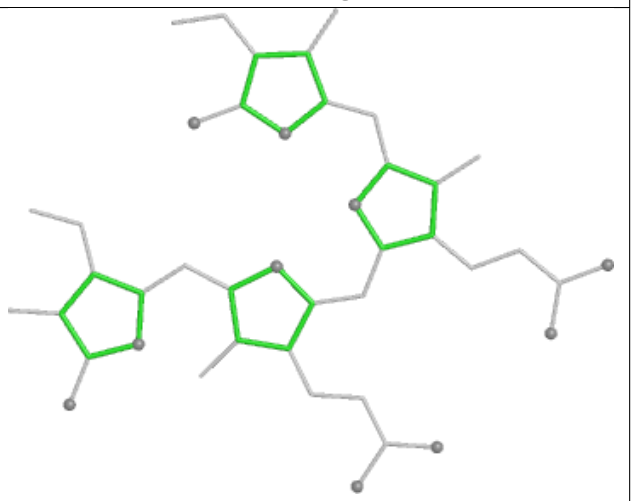
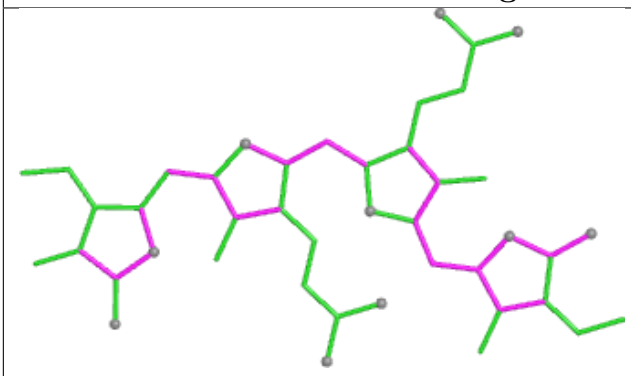


Rings

Ligand CYC BG 1002



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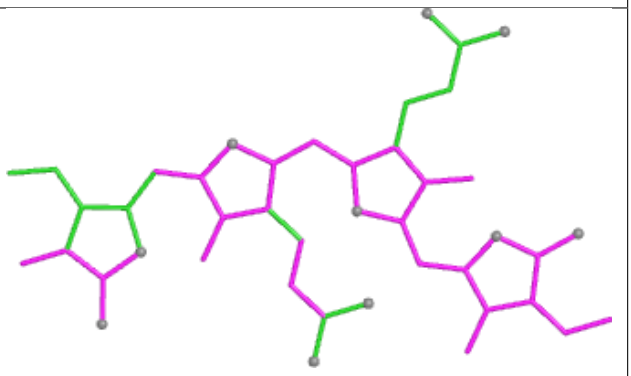

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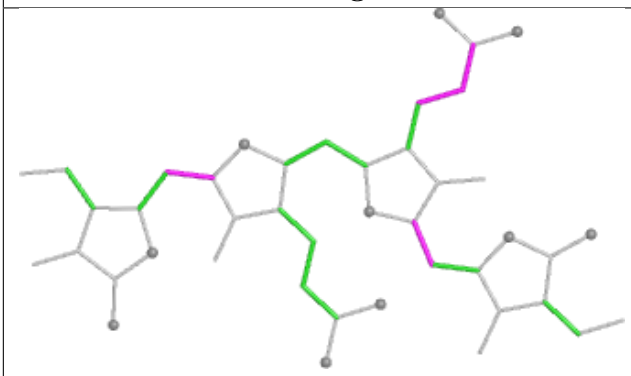

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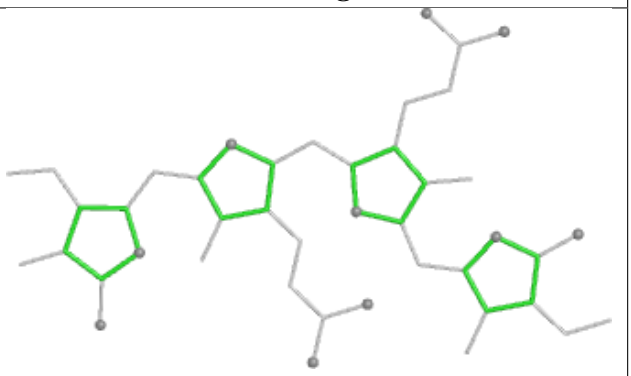
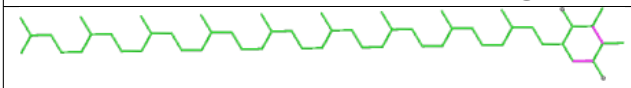


Rings

Ligand PL9 AL 413



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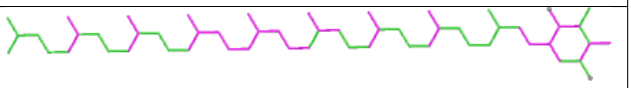

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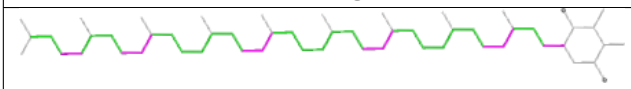

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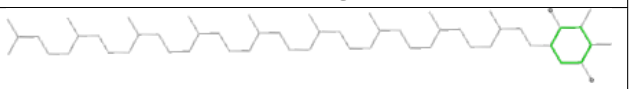
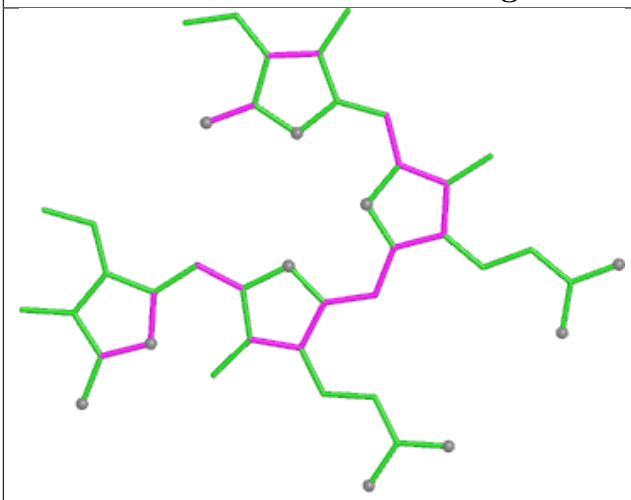


Rings

Ligand PEB HH 1002



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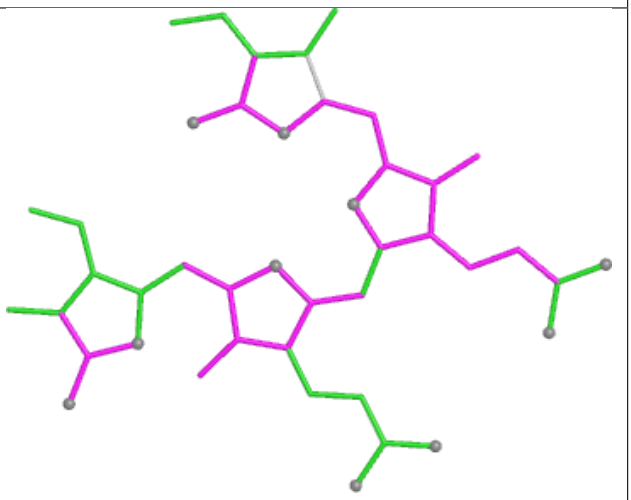
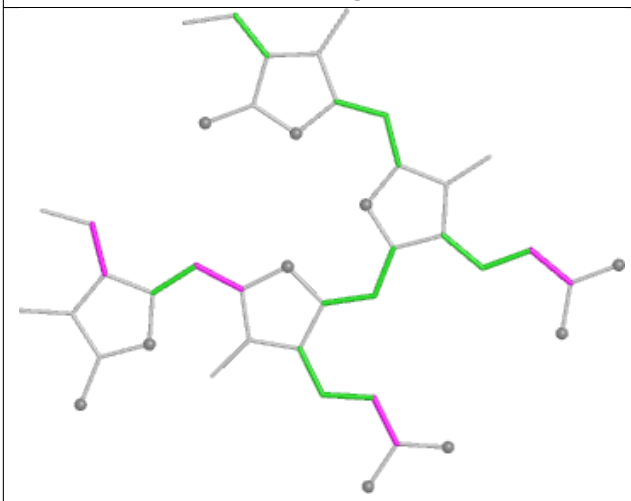


Bond angles



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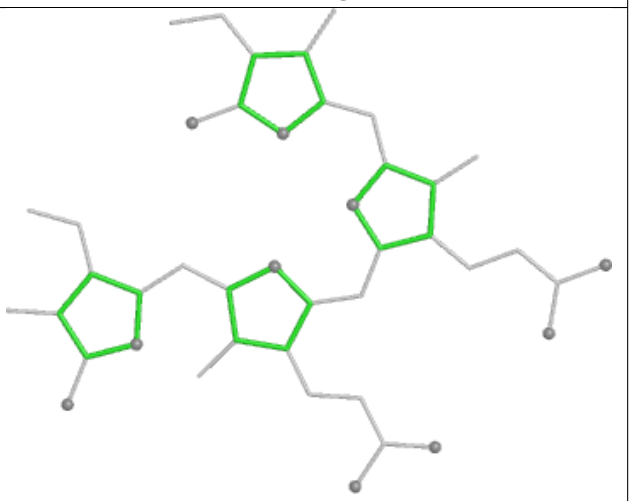
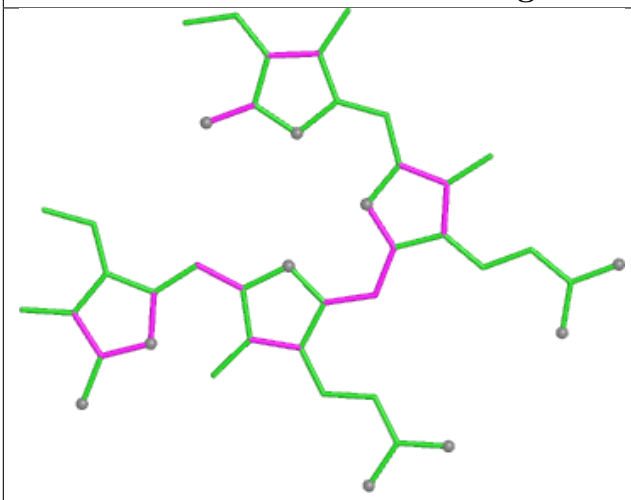


Rings

Ligand PEB UI 202



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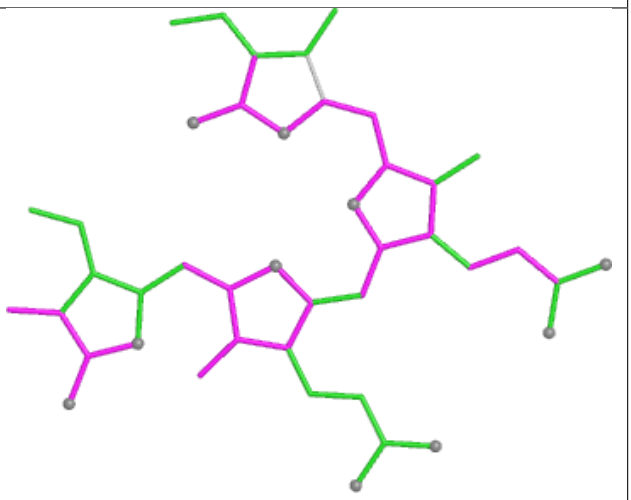

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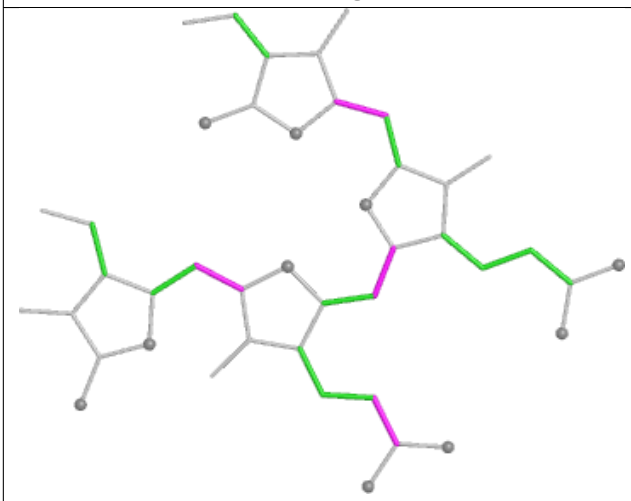

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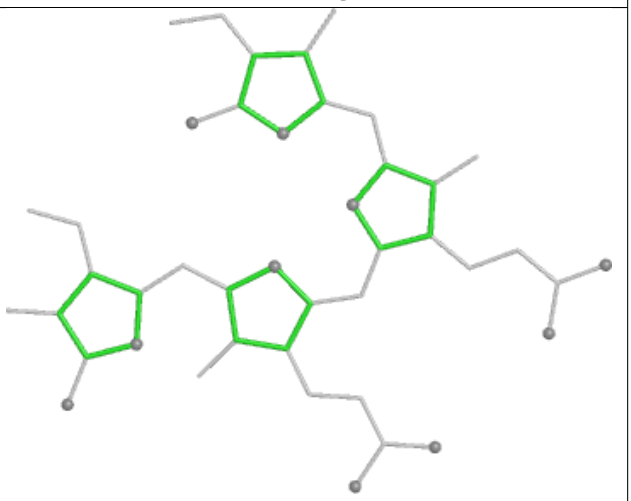
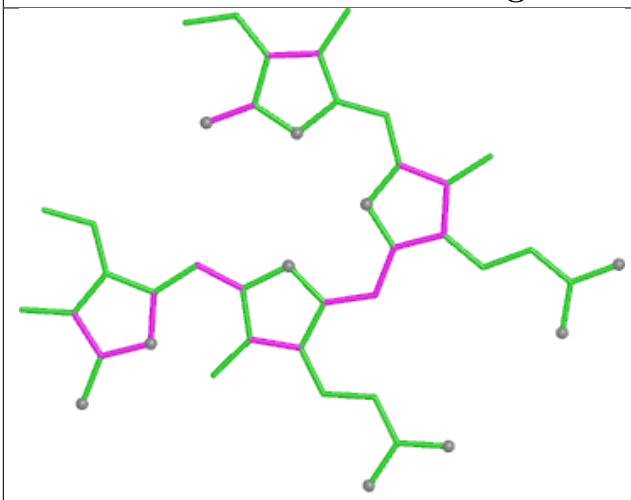


Rings

Ligand PEB RM 202



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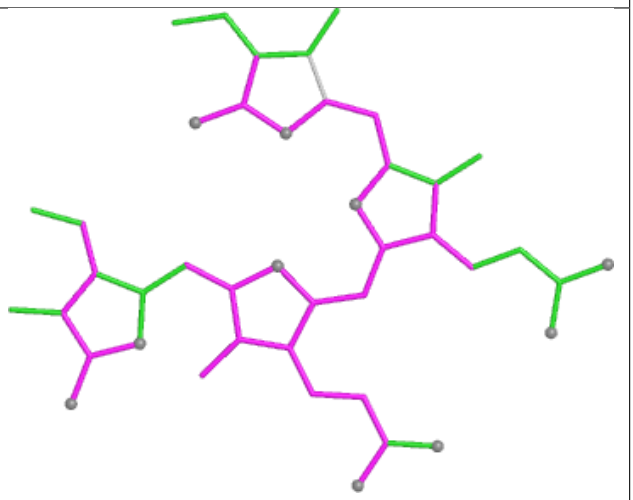
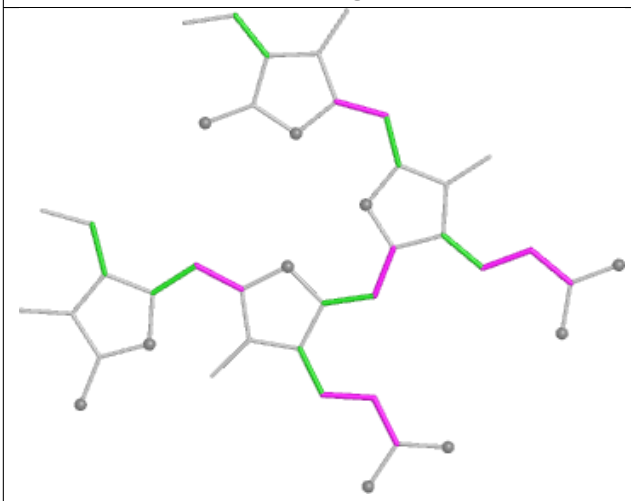


Bond angles



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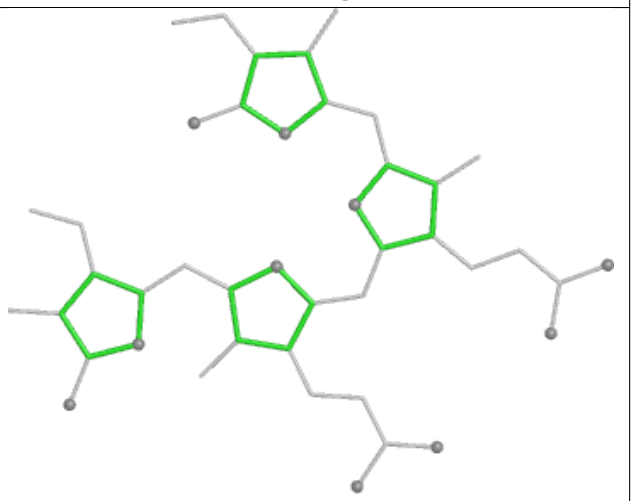
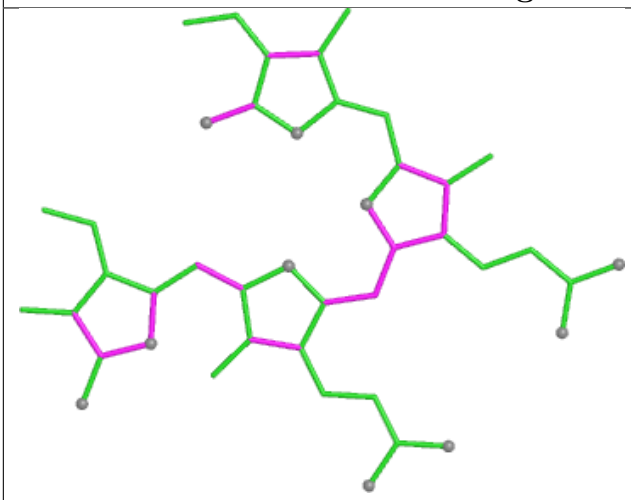


Rings

Ligand PEB T4 201



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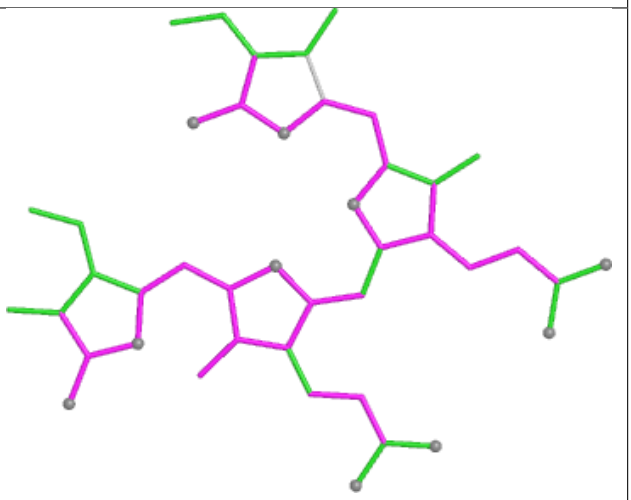

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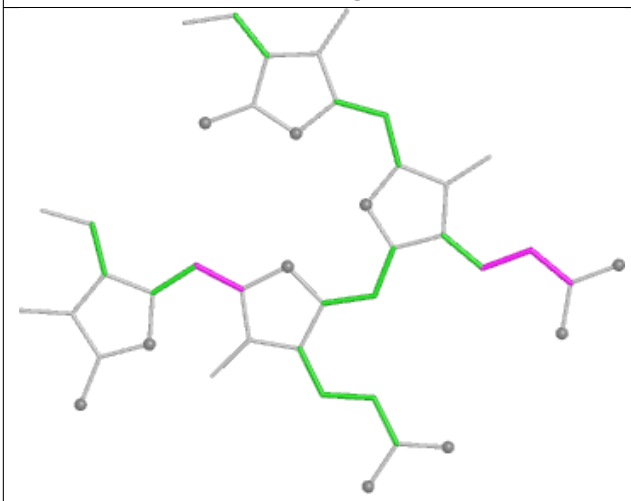

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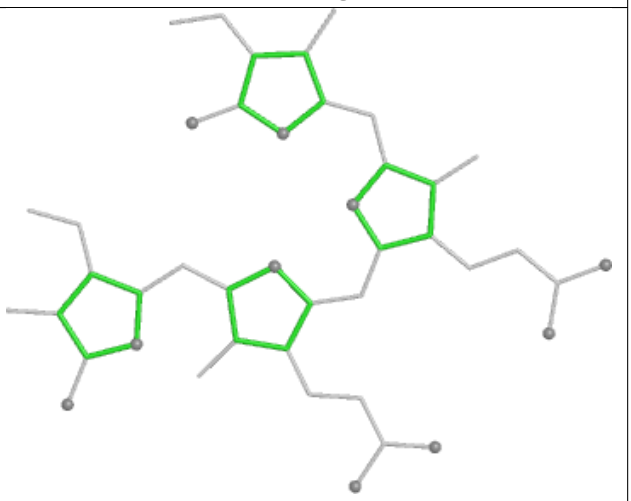
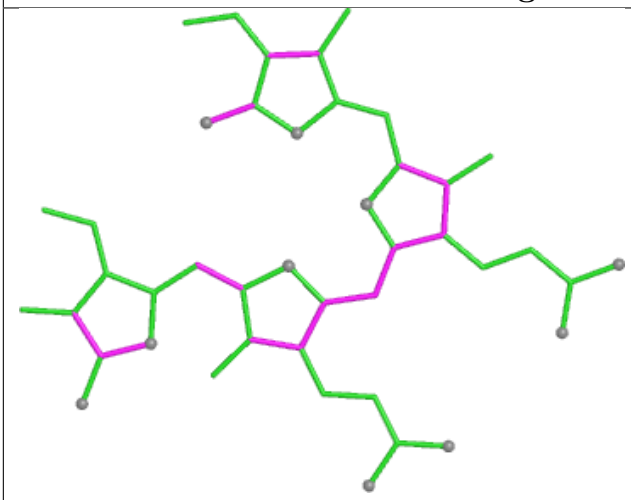


Rings

Ligand PEB L9 202



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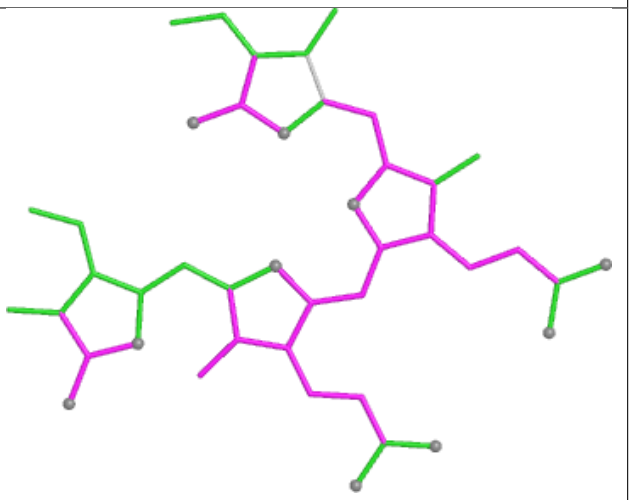

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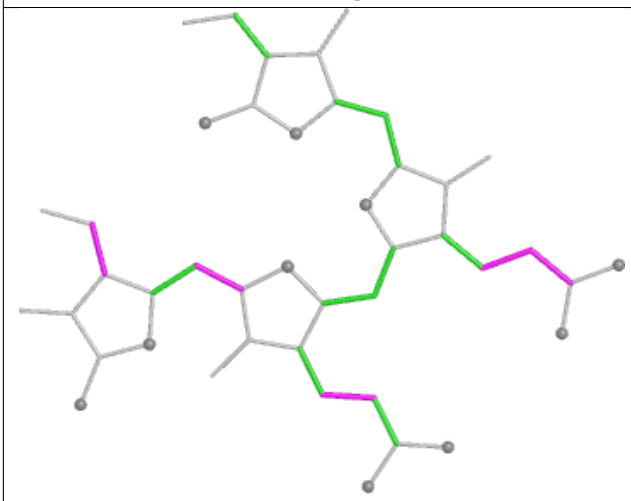

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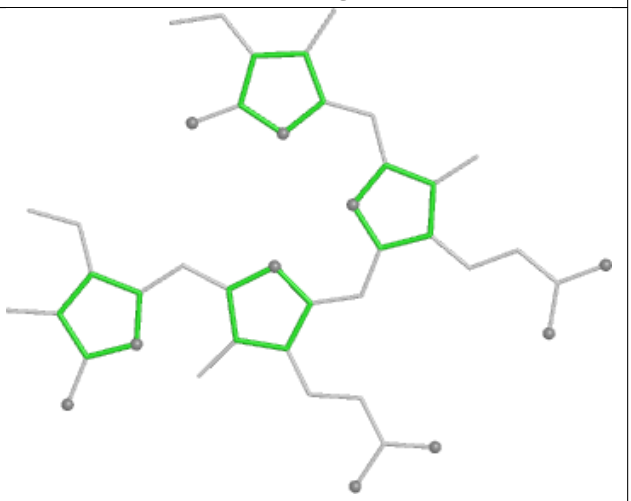
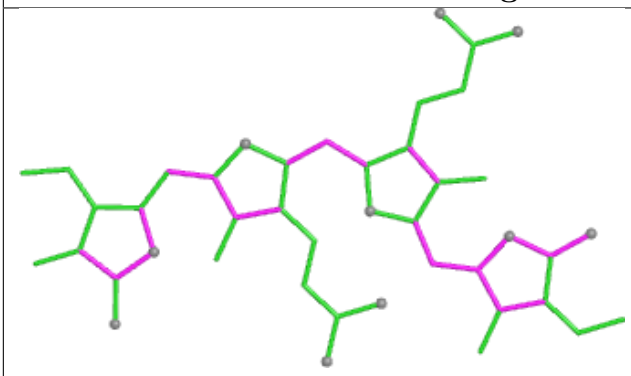


Rings

Ligand CYC GE 1001



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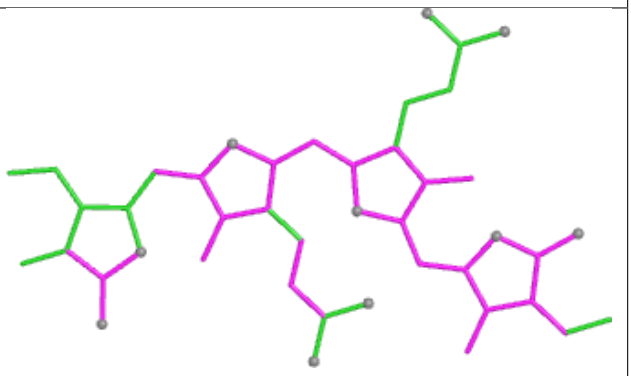

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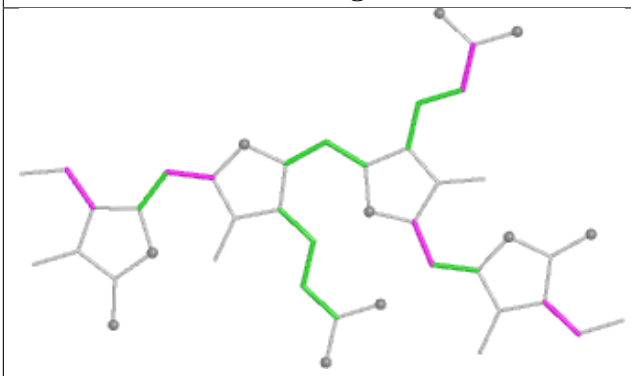

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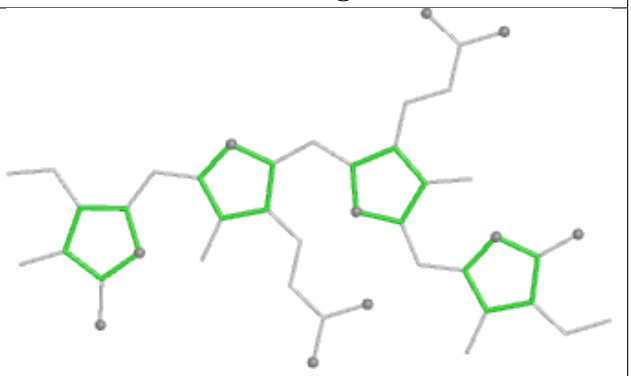
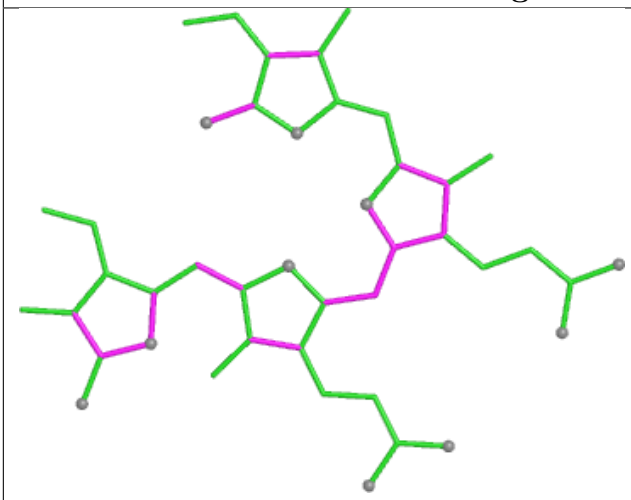


Rings

Ligand PEB BQ 202



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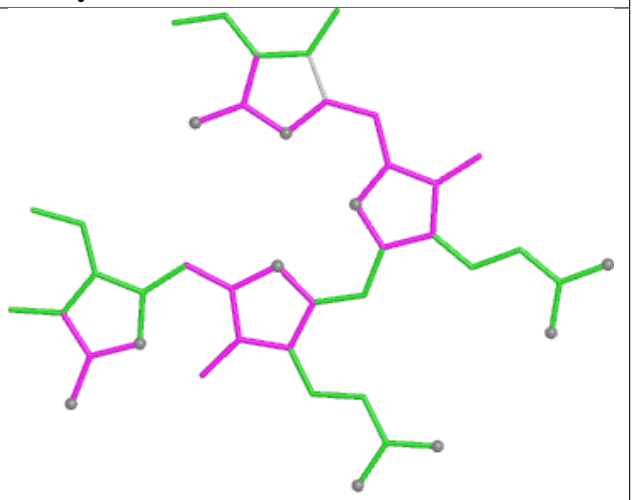

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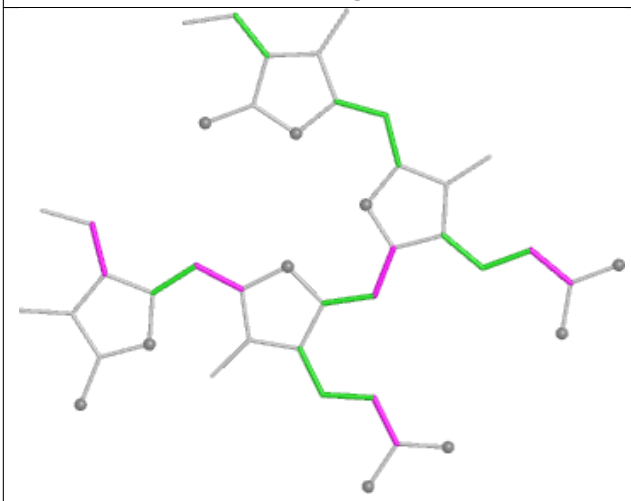

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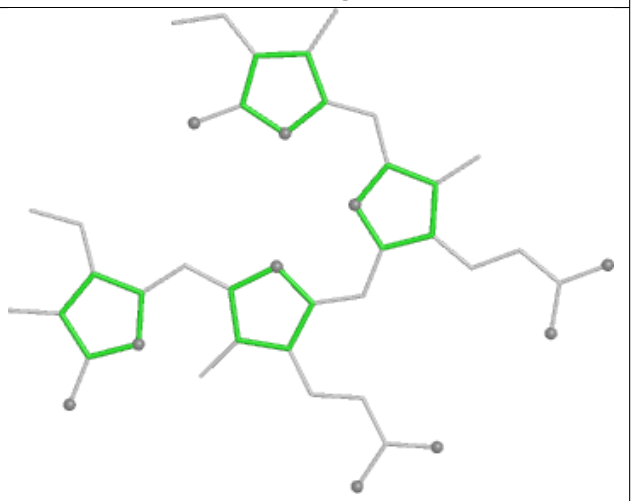
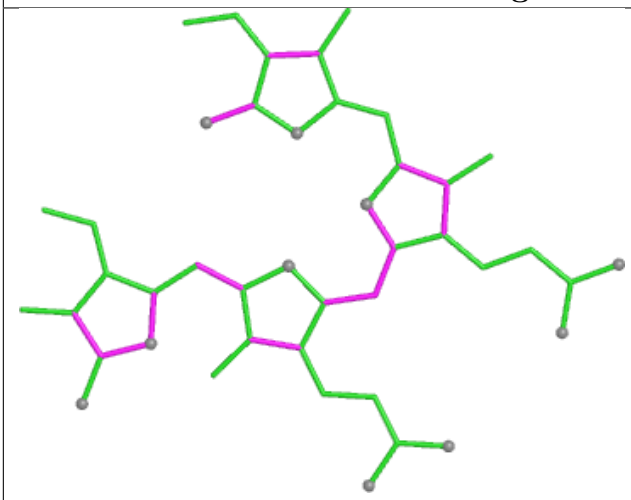


Rings

Ligand PEB OA 202



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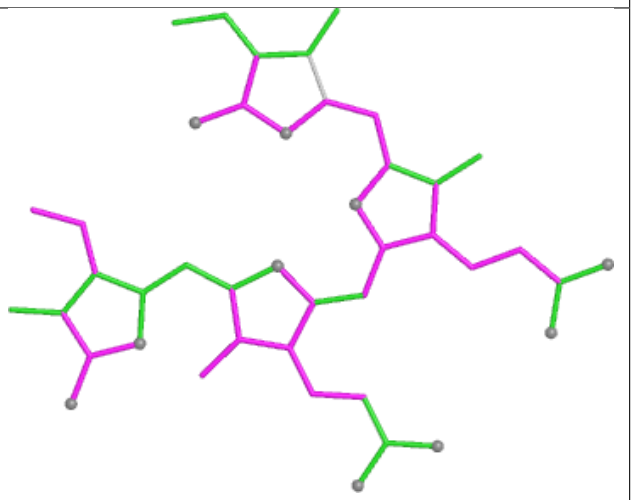

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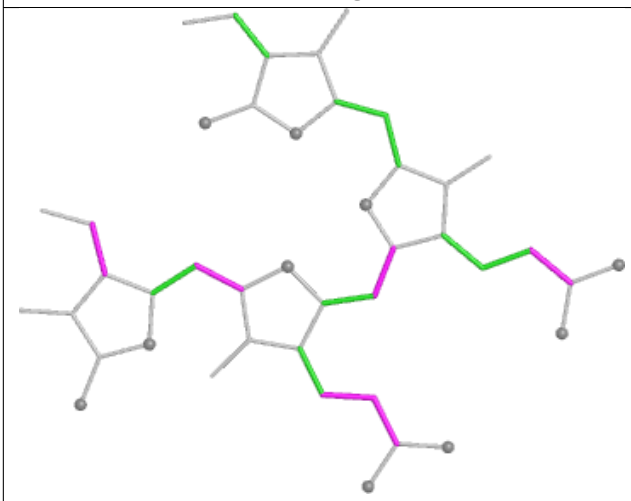

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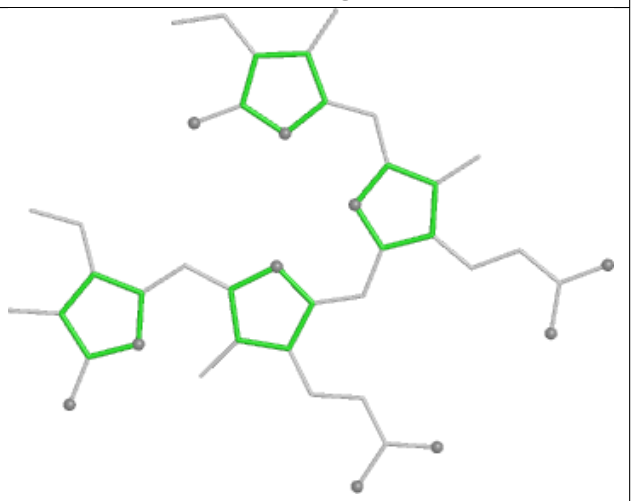
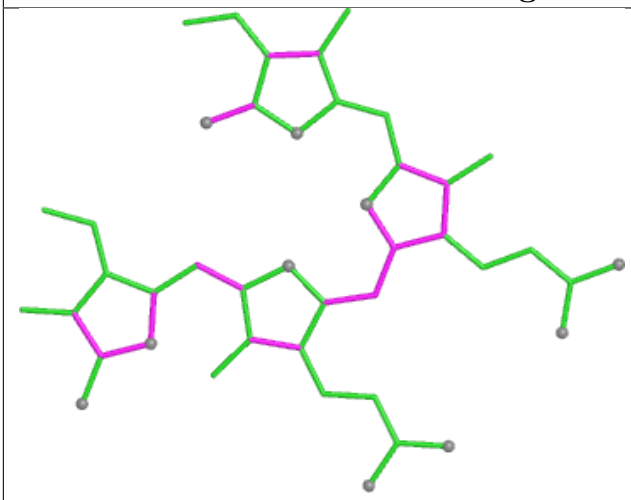


Rings

Ligand PEB kJ 202



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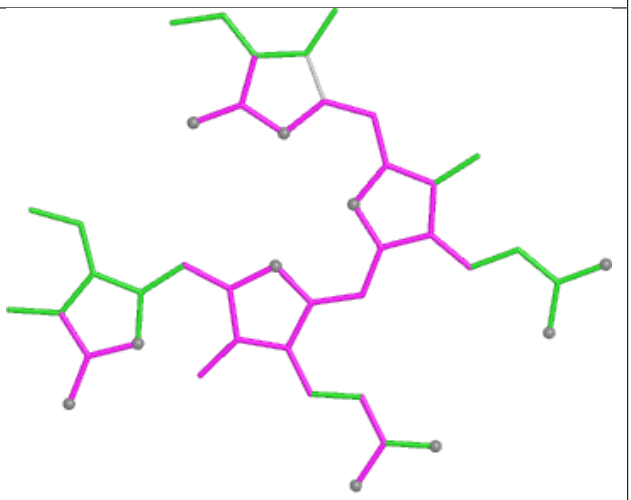
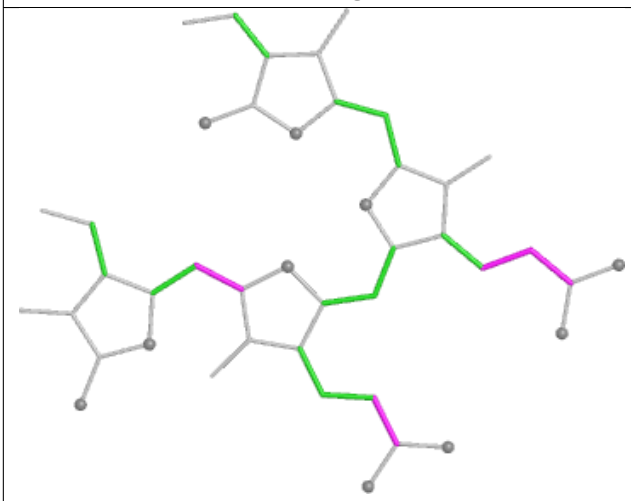


Bond angles



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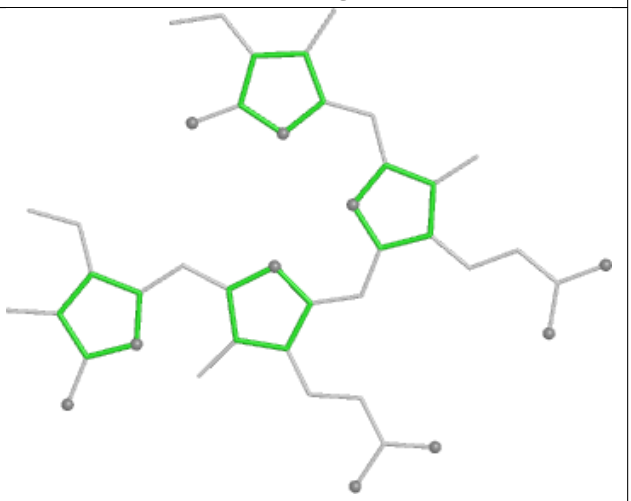
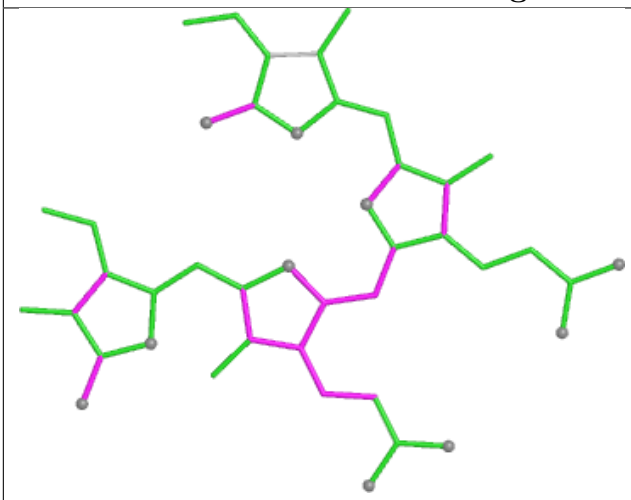


Rings

Ligand PUB M5 302



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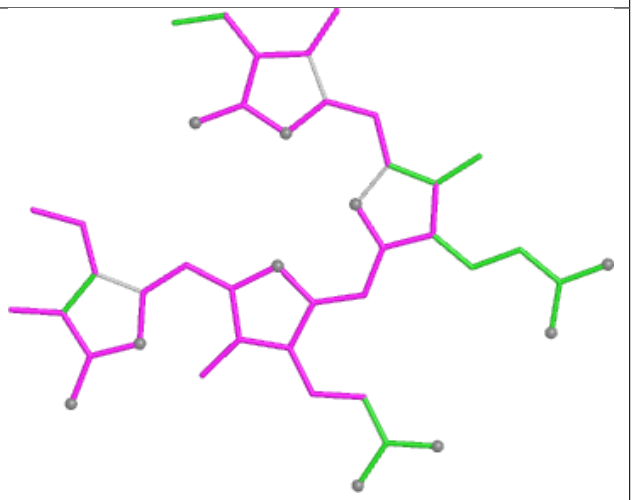
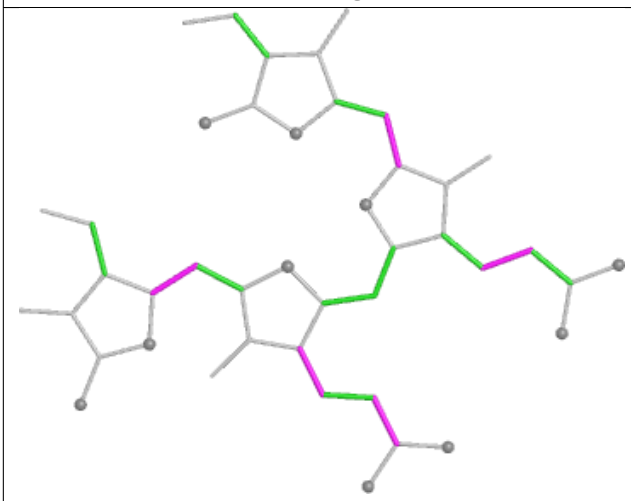


Bond angles



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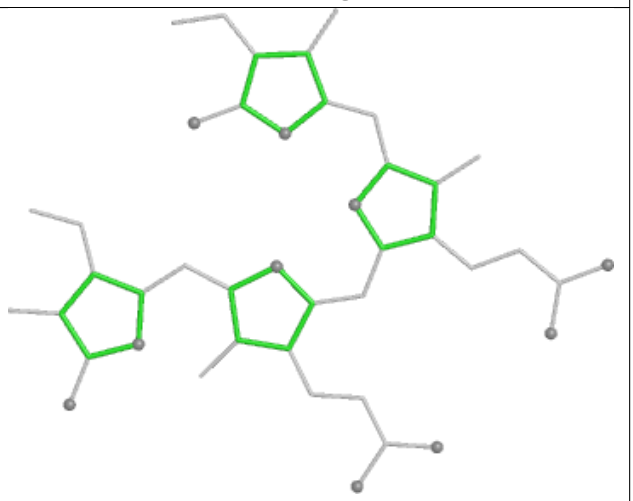
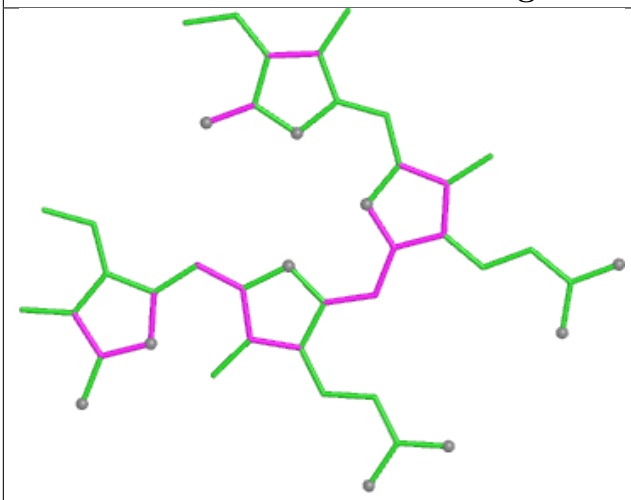


Rings

Ligand PEB sC 201



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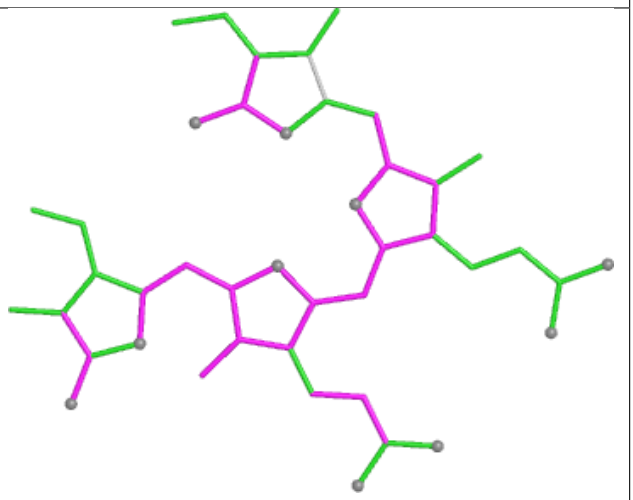
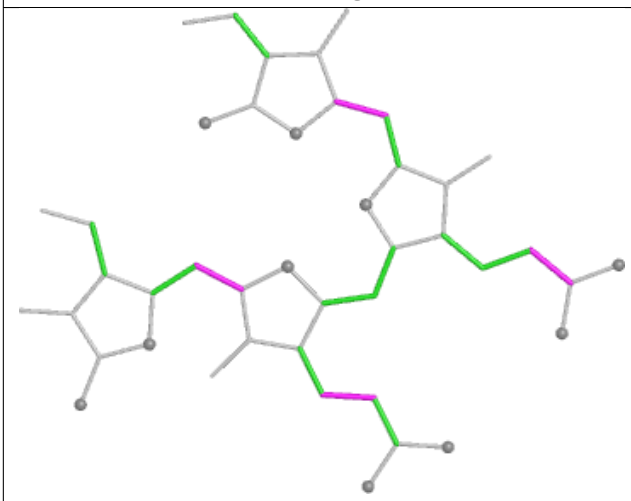


Bond angles



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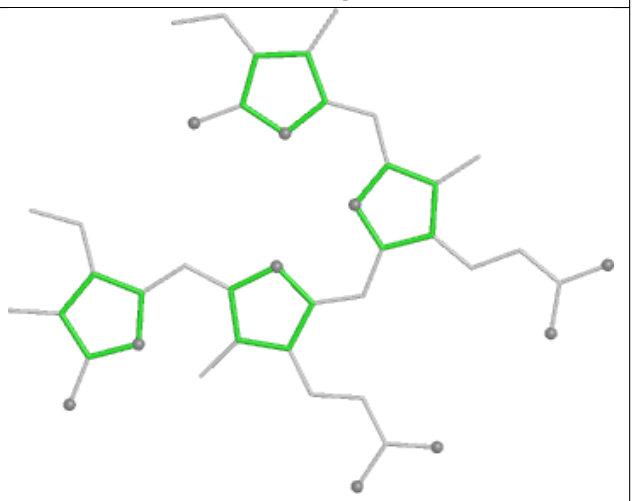
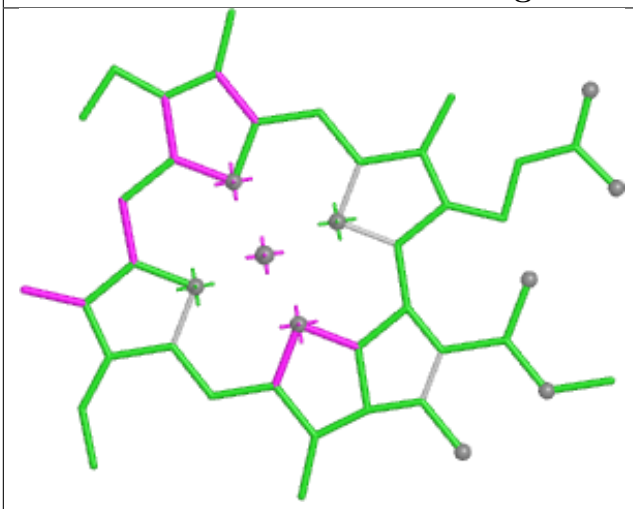


Rings

Ligand CLA 3N 301



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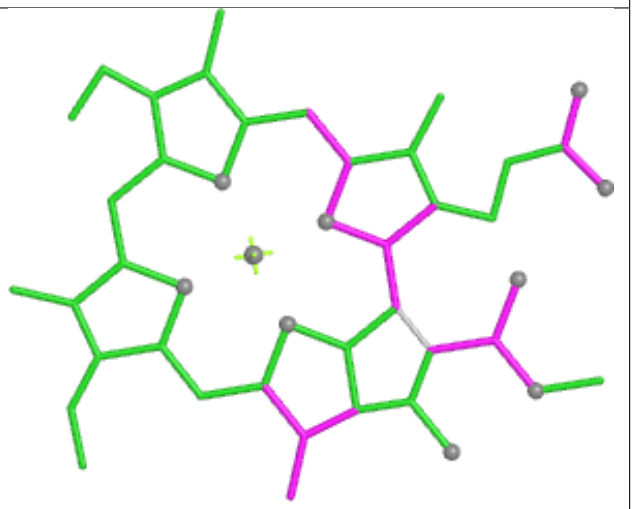
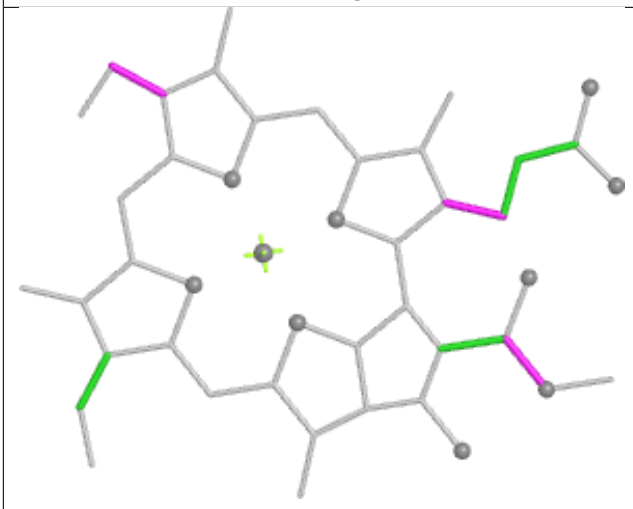


Bond angles

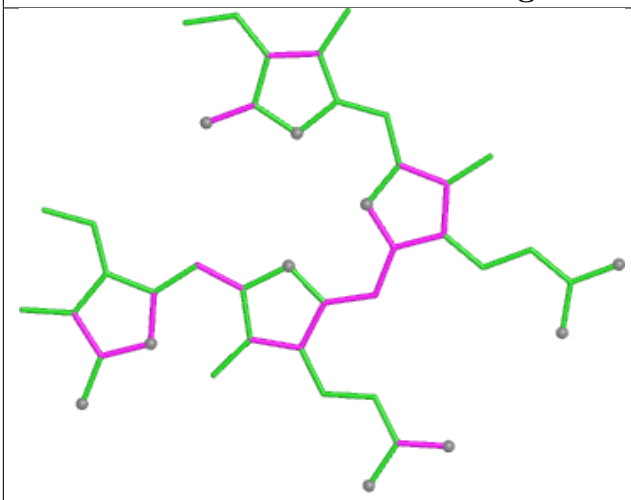


Torsions



Rings

Ligand PEB OI 201



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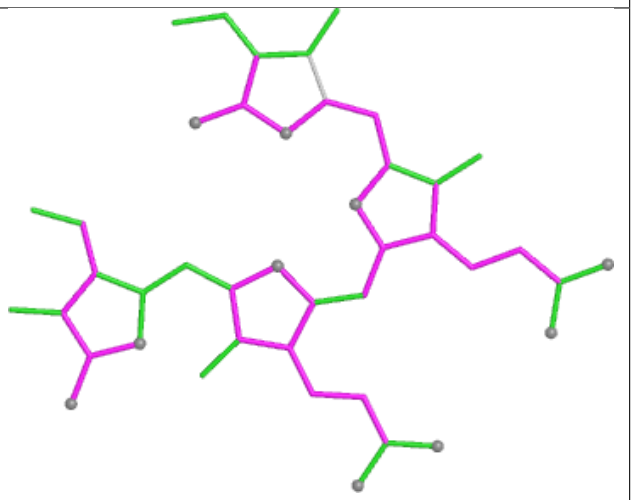

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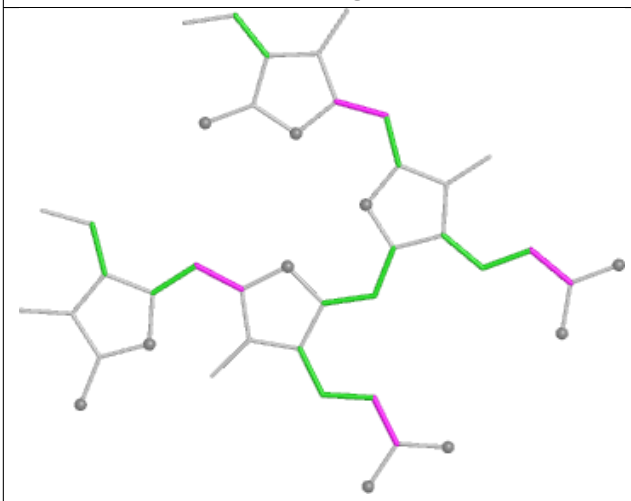

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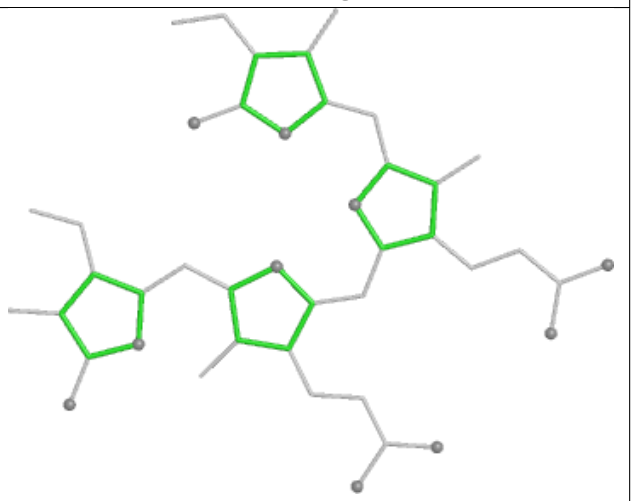
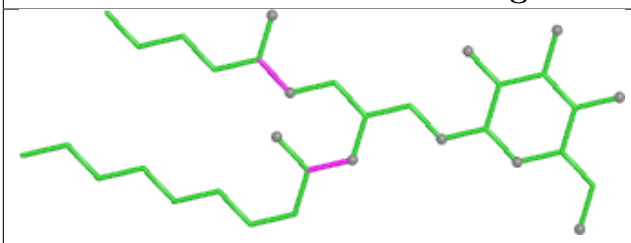


Rings

Ligand LMG D6 407



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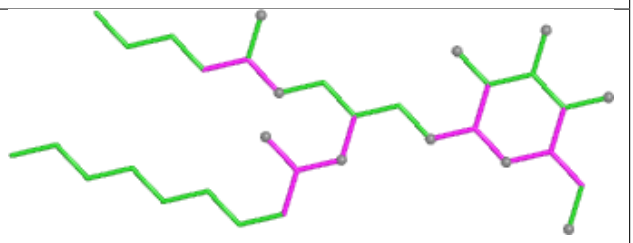

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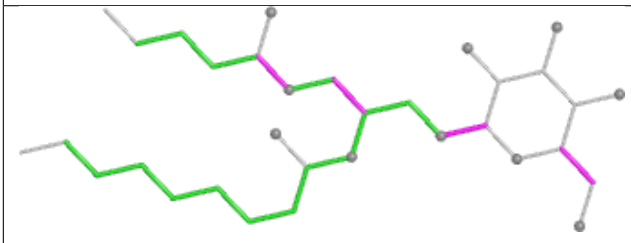

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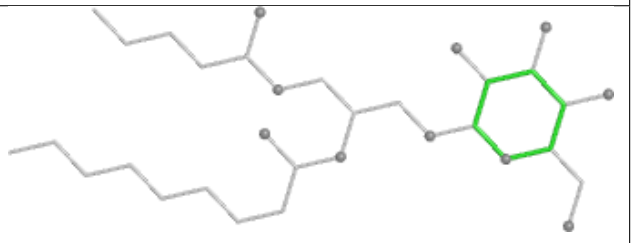
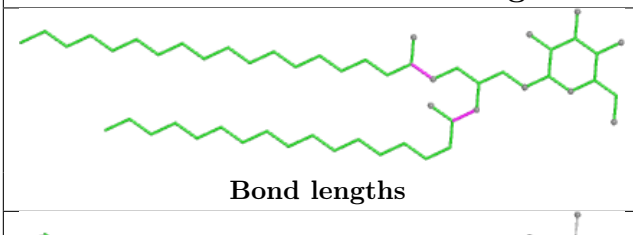


Rings

Ligand LMG DL 402



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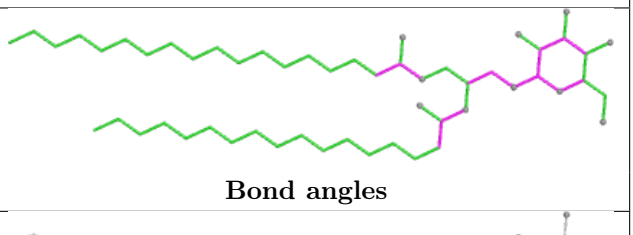

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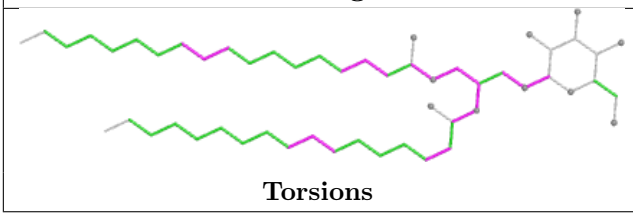

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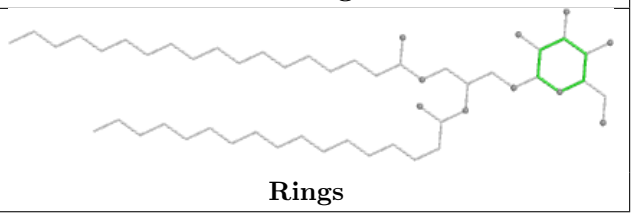
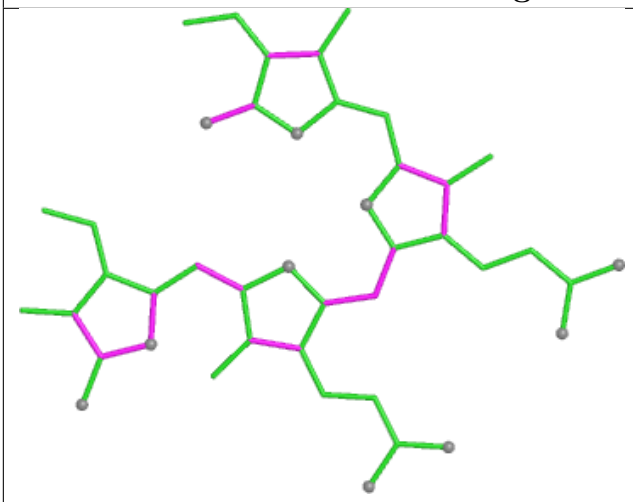


Rings

Ligand PEB EB 501



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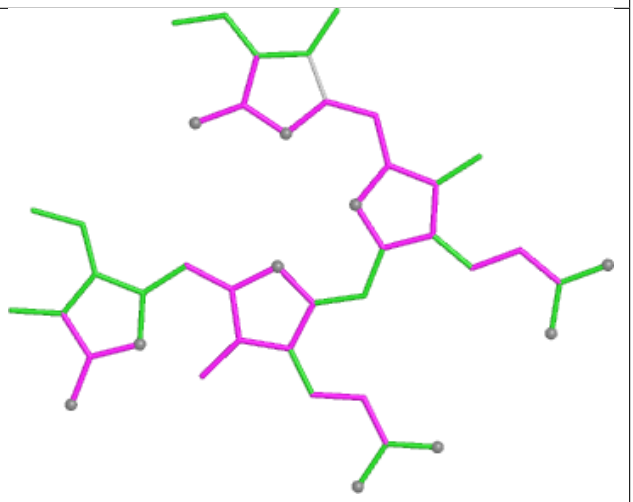
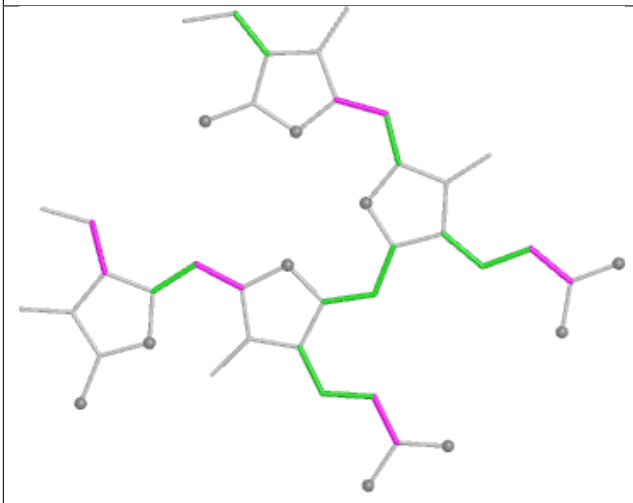


Bond angles



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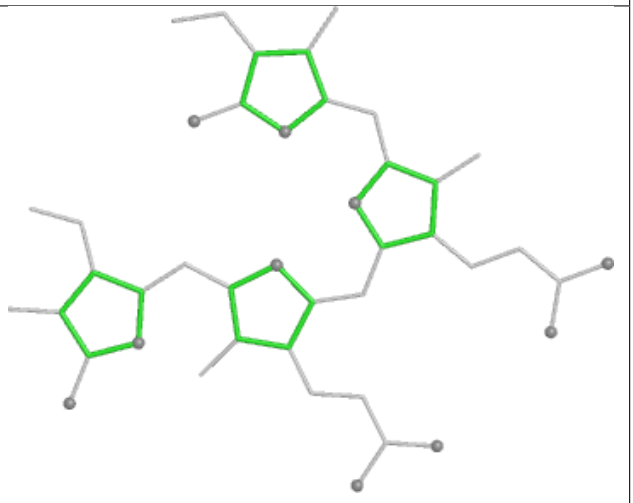
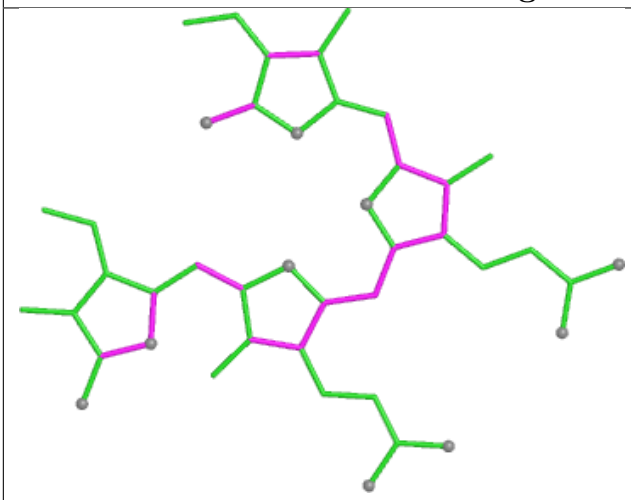


Rings

Ligand PEB h1 201



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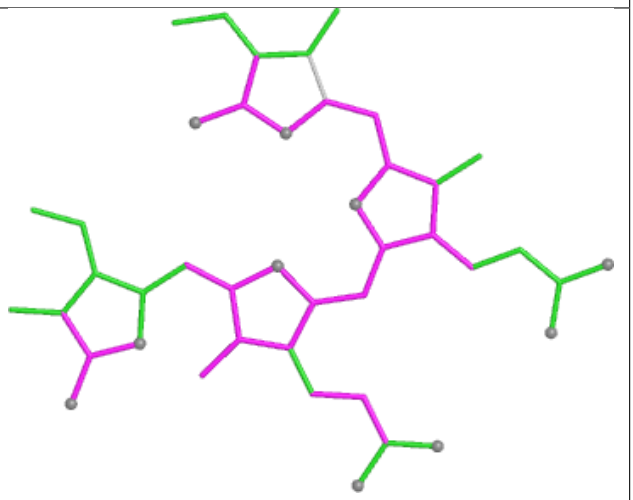

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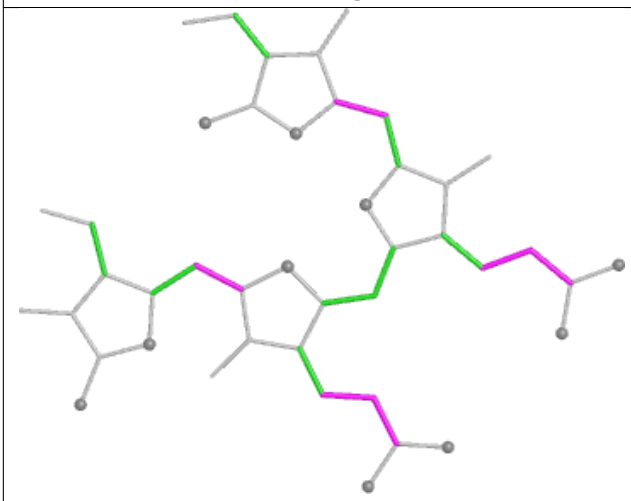

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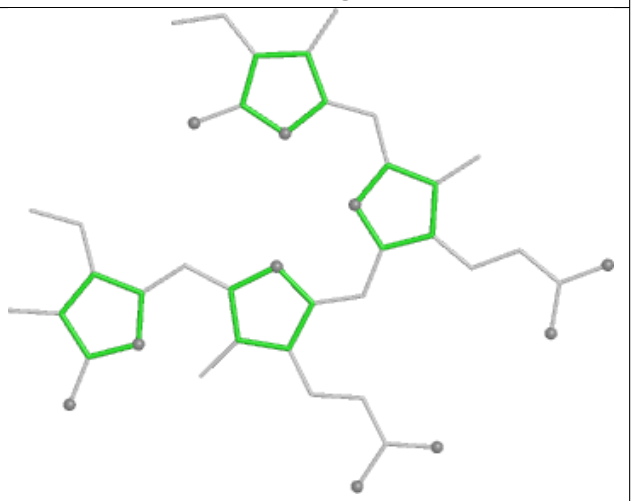
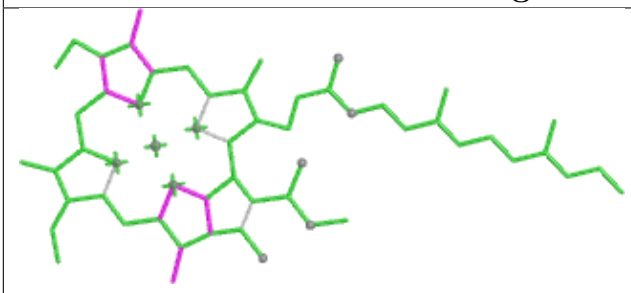
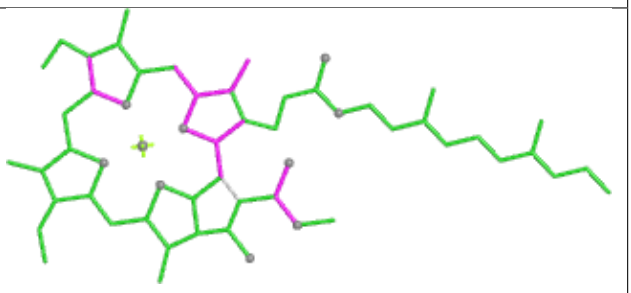


Rings

Ligand CLA LN 202	
	
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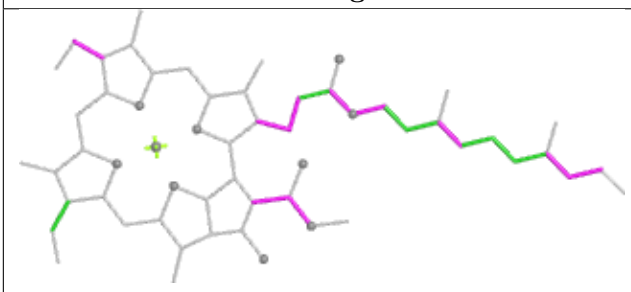
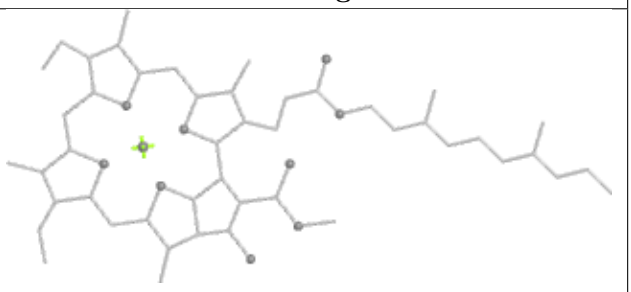
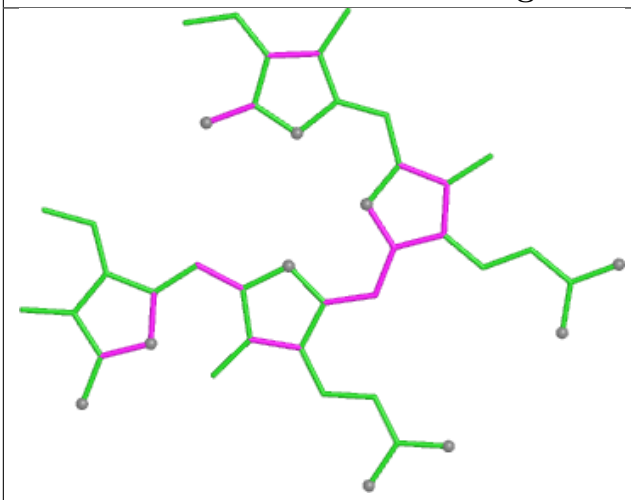
	
Torsions	**Rings**

Ligand PEB E9 201



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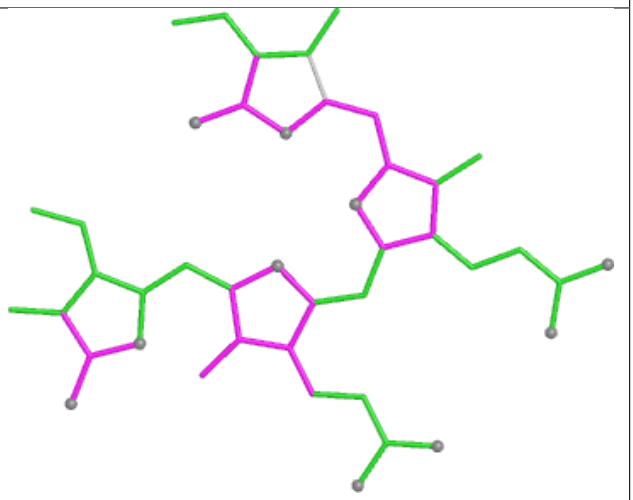
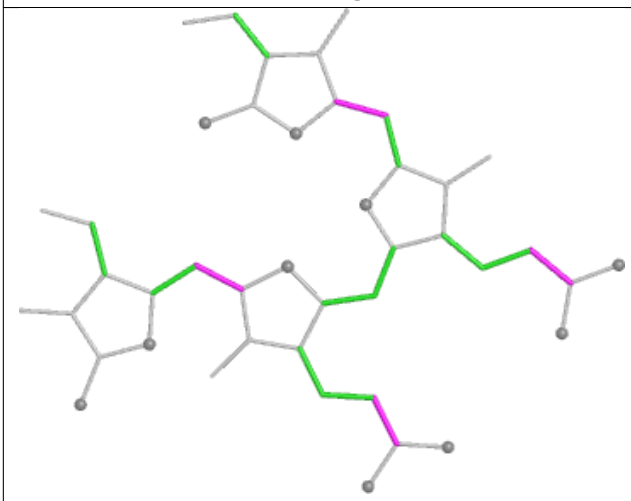


Bond angles



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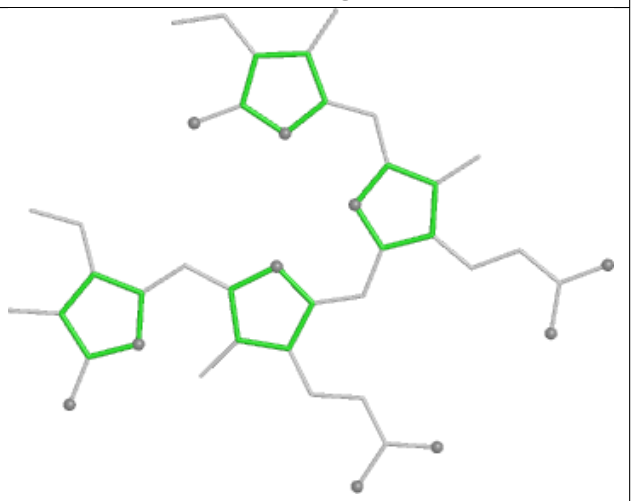
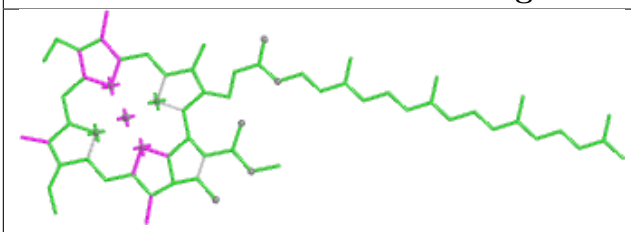


Rings

Ligand CLA B2 808



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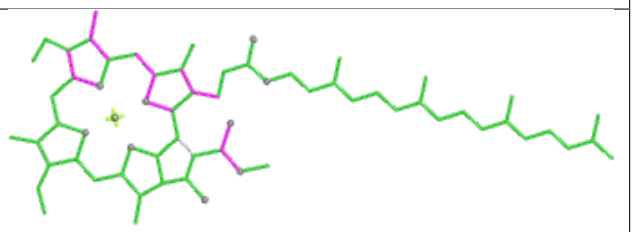

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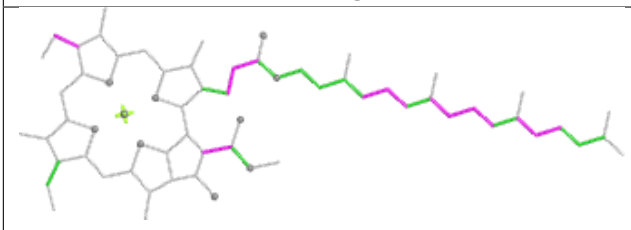

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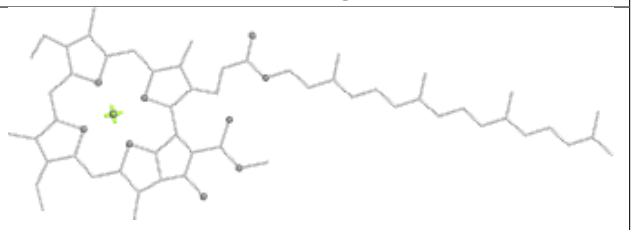
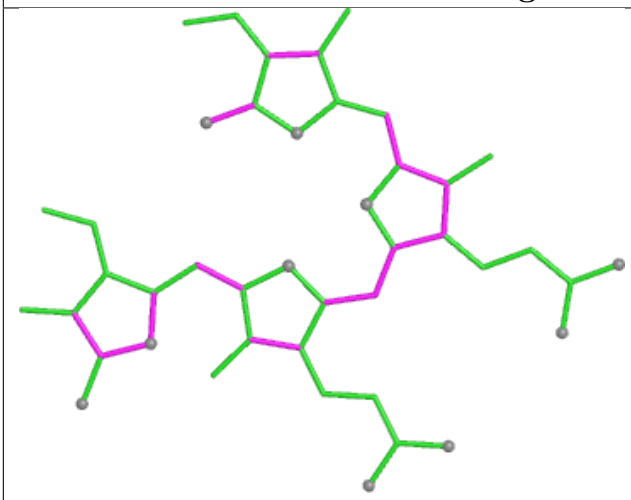


Rings

Ligand PEB dJ 202



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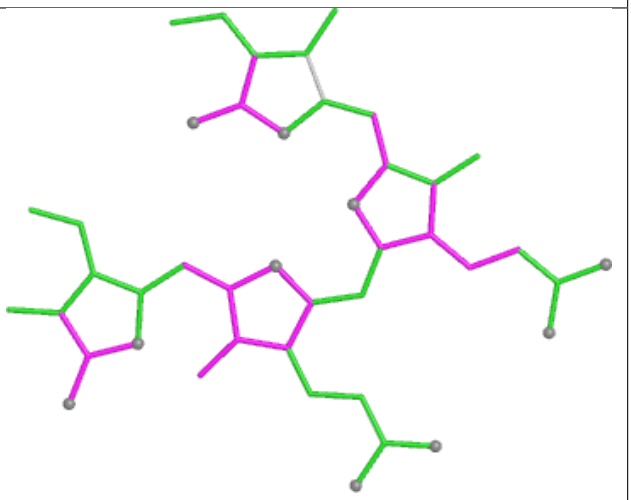

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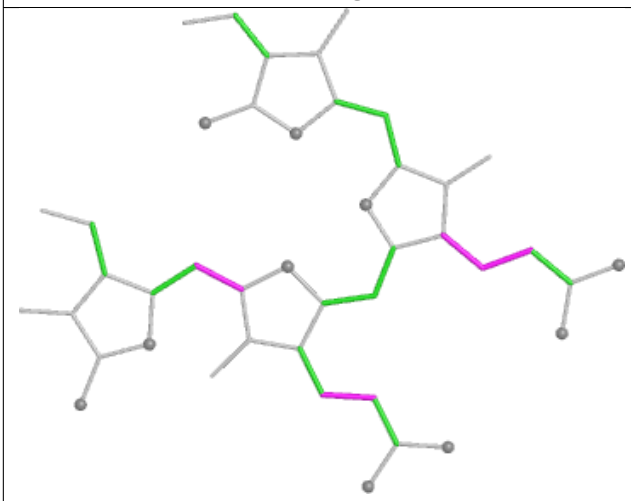

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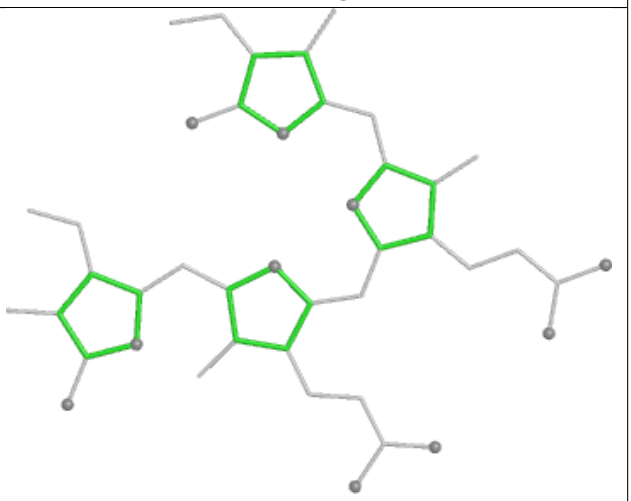
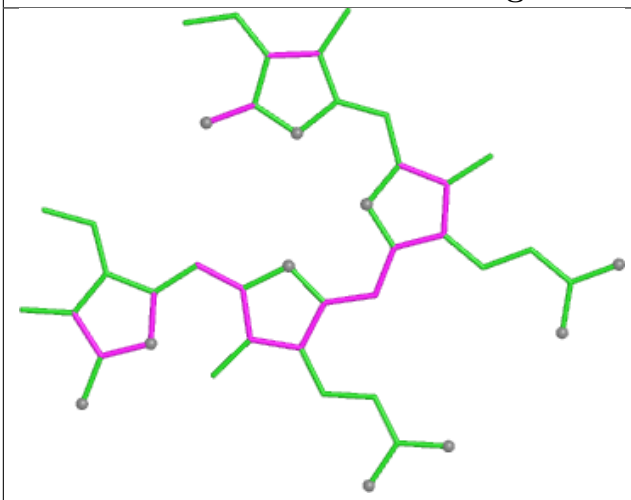


Rings

Ligand PEB HM 202



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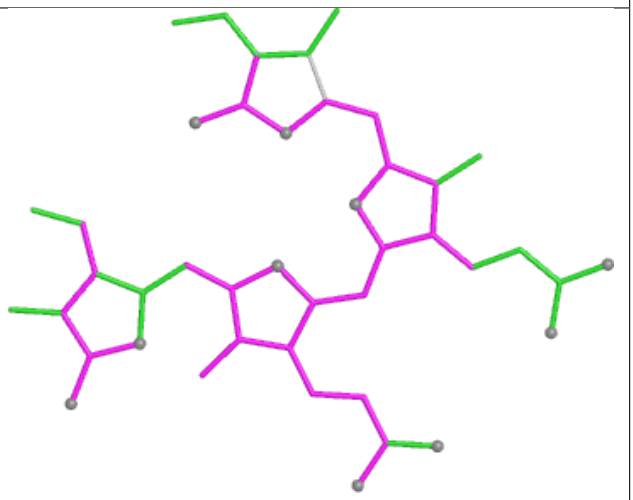

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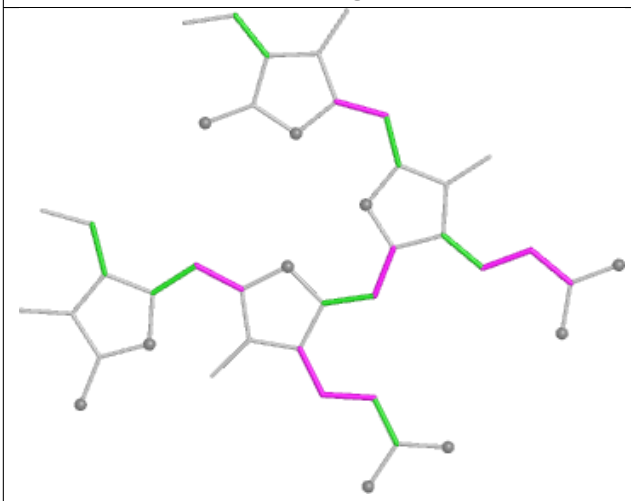

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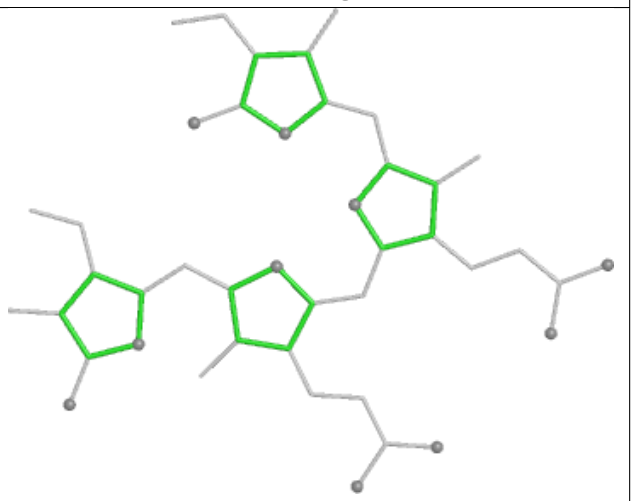
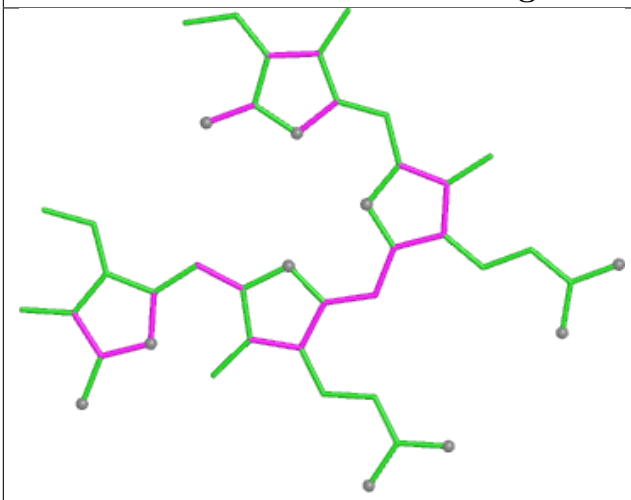


Rings

Ligand PEB fH 201



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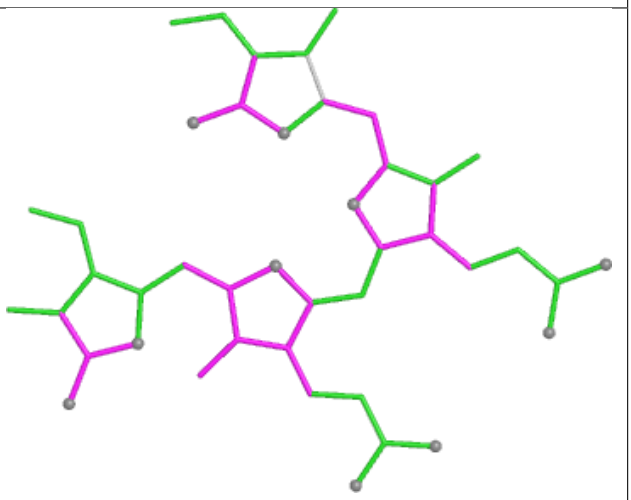
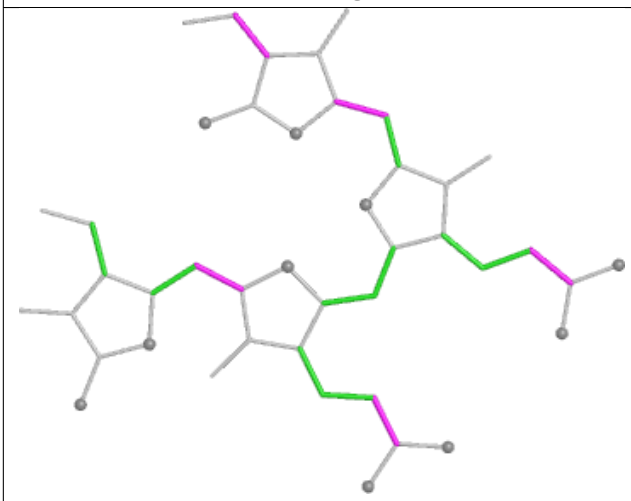


Bond angles



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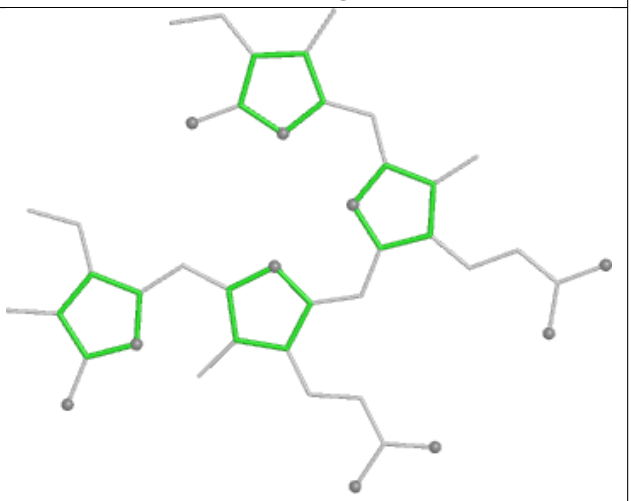
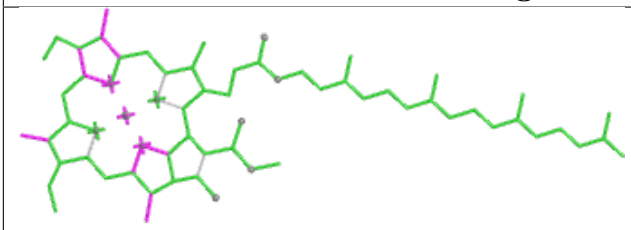


Rings

Ligand CLA B2 812



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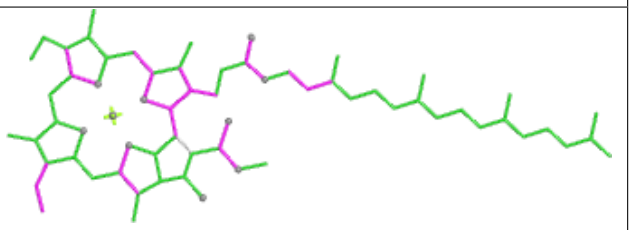
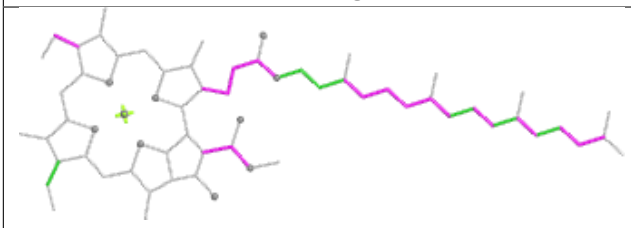


Bond angles



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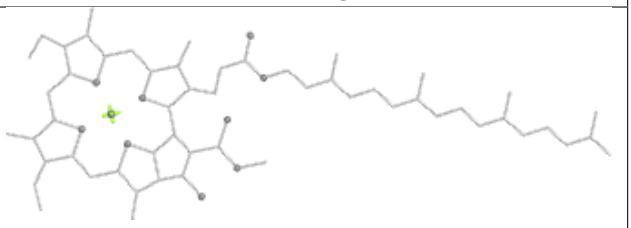
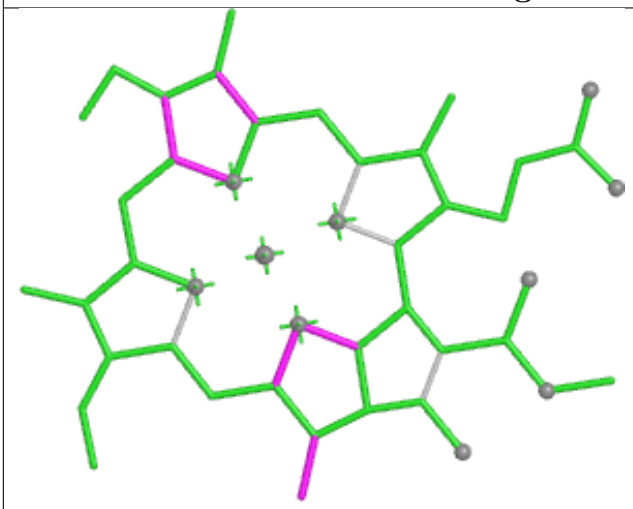


Rings

Ligand CLA 5N 606



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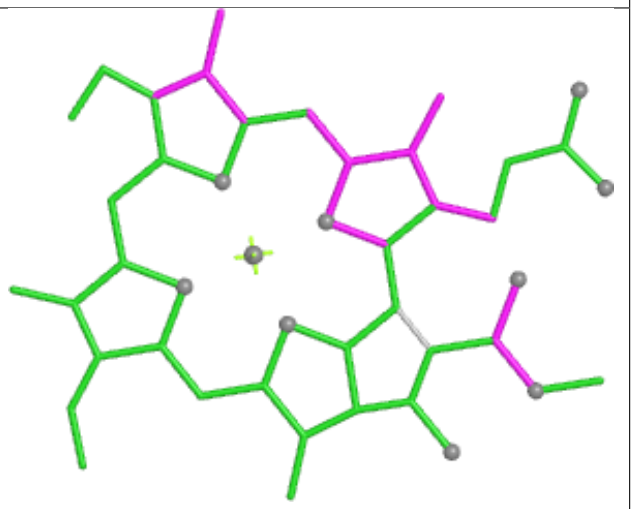
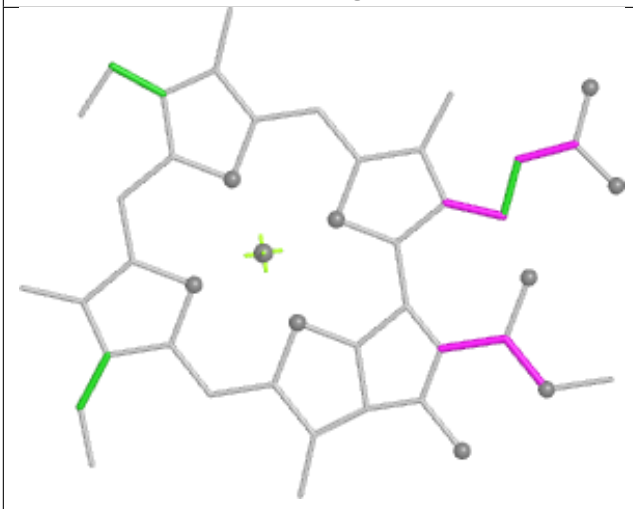


Bond angles

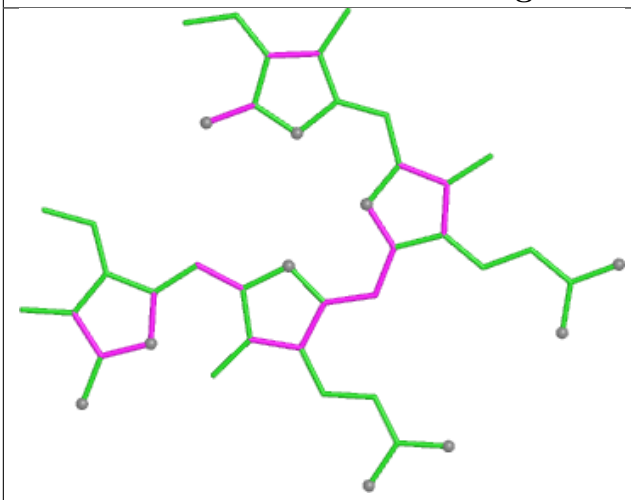


Torsions



Rings

Ligand PEB O5 201



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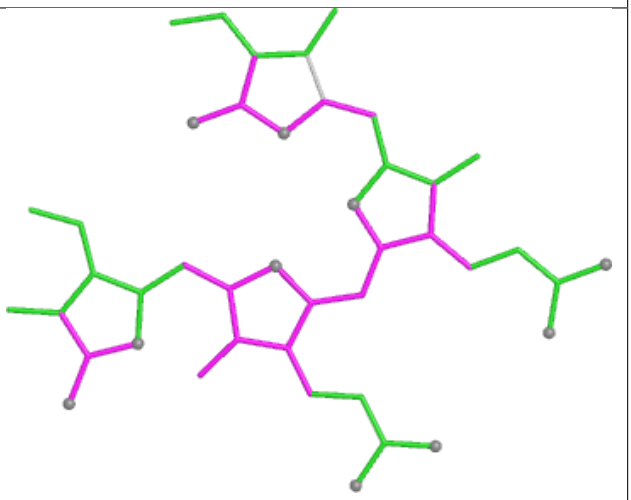
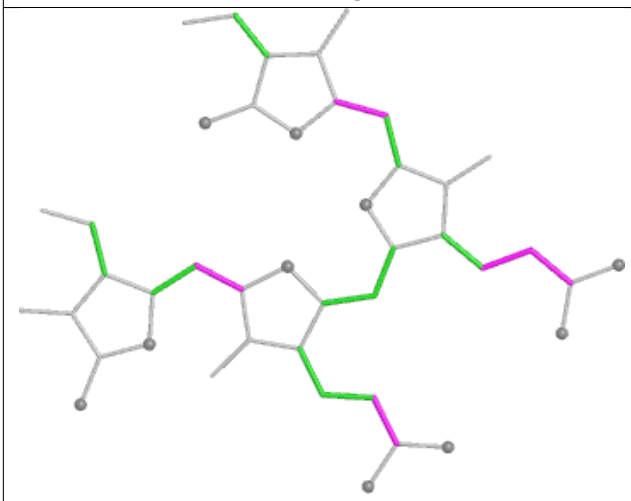
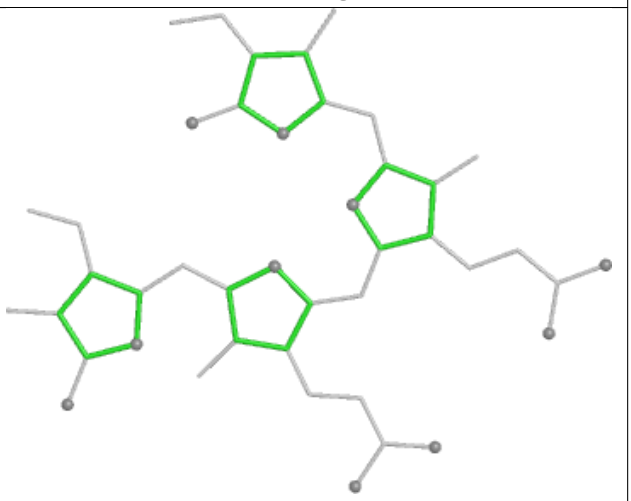


Bond angles

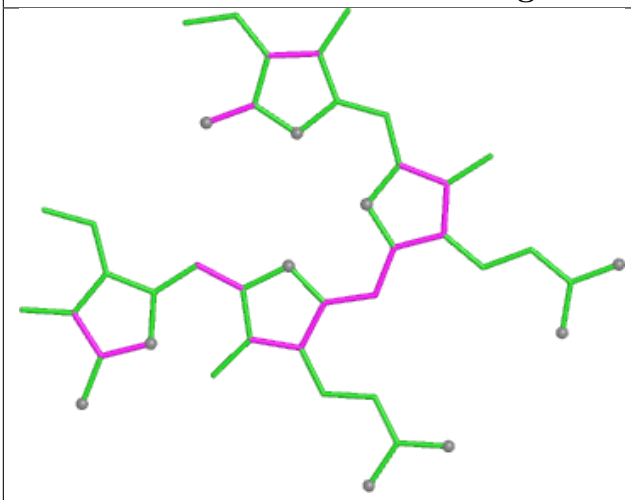


Torsions

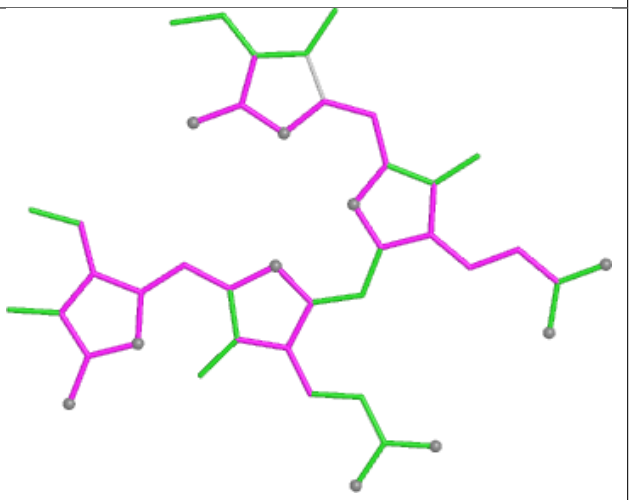


Rings

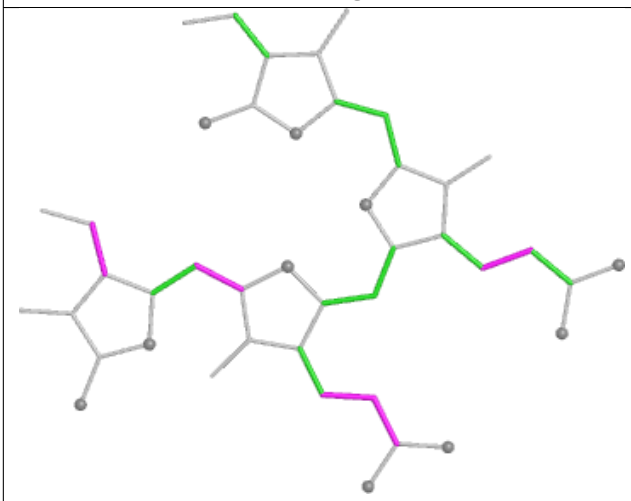
Ligand PEB JF 201



Bond lengths



Bond angles



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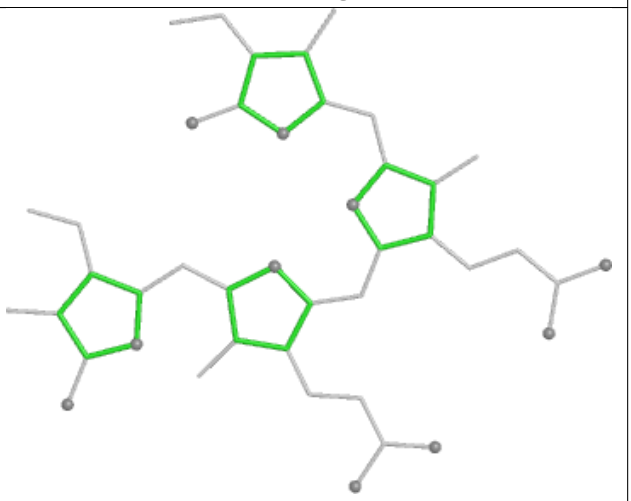
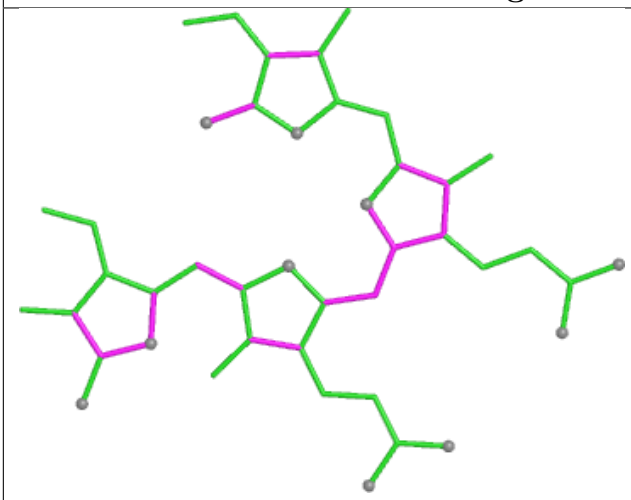


Rings

Ligand PEB DM 201



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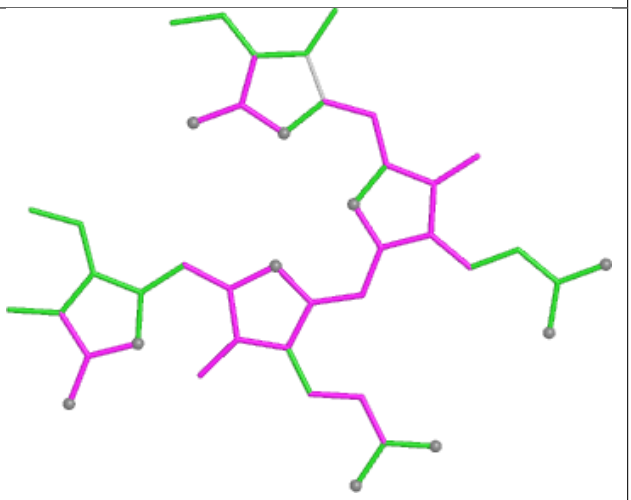

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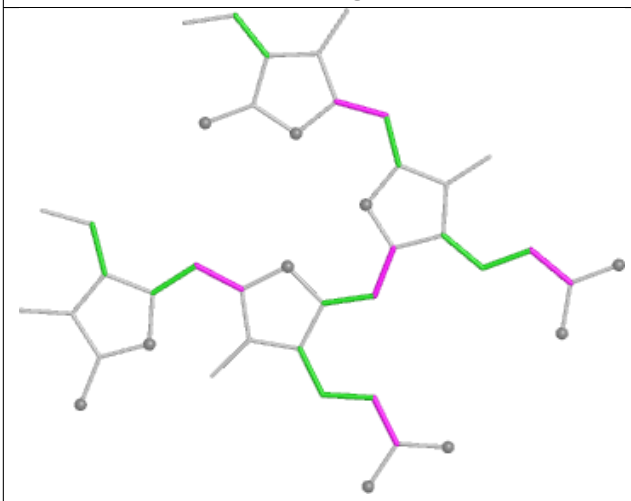

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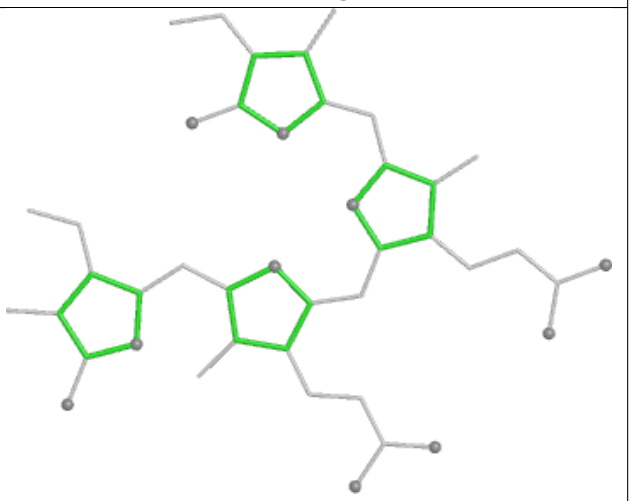
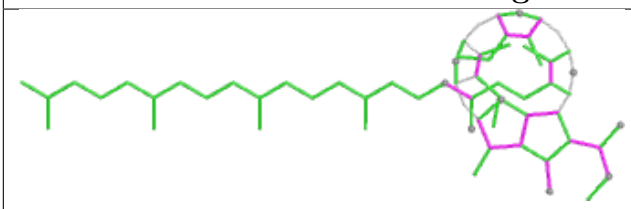


Rings

Ligand PHO D6 404



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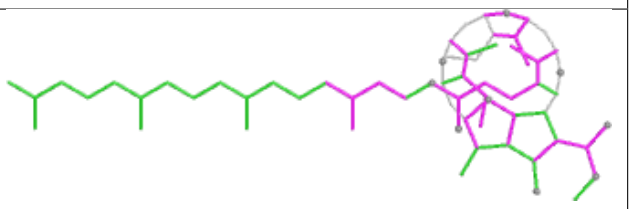

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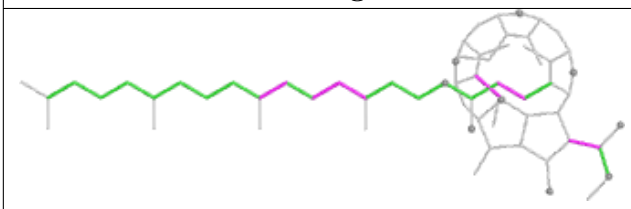

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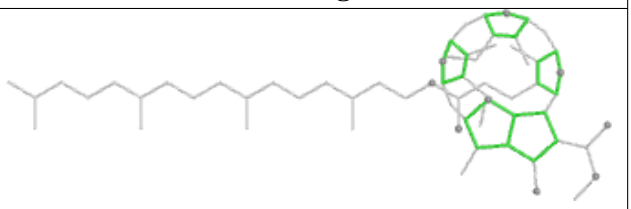
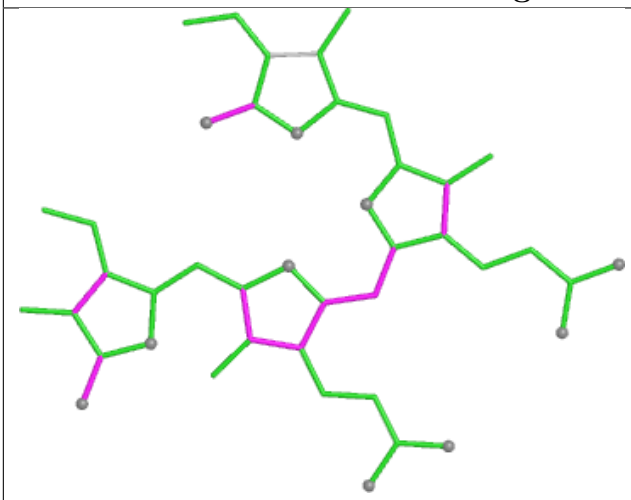


Rings

Ligand PUB A4 302



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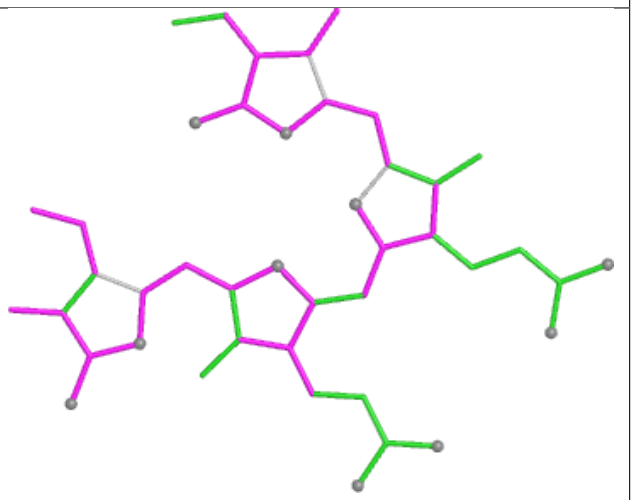

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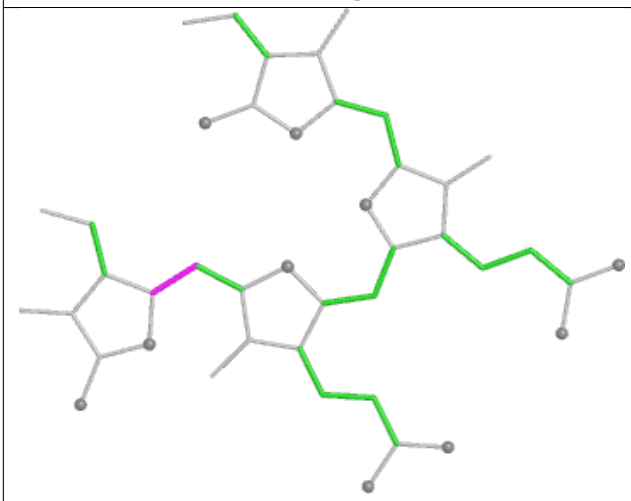

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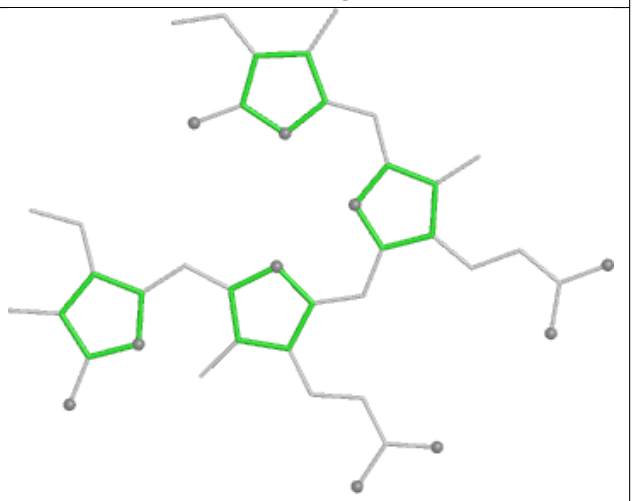
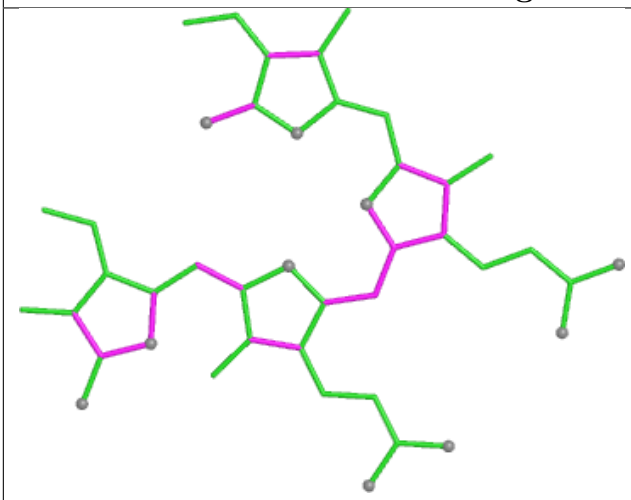


Rings

Ligand PEB cH 201



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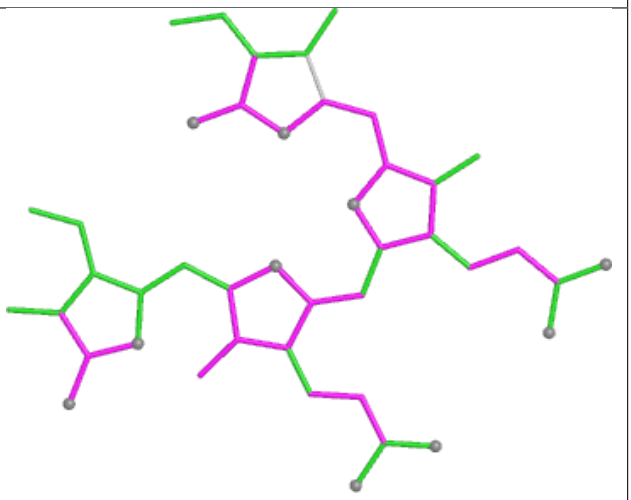

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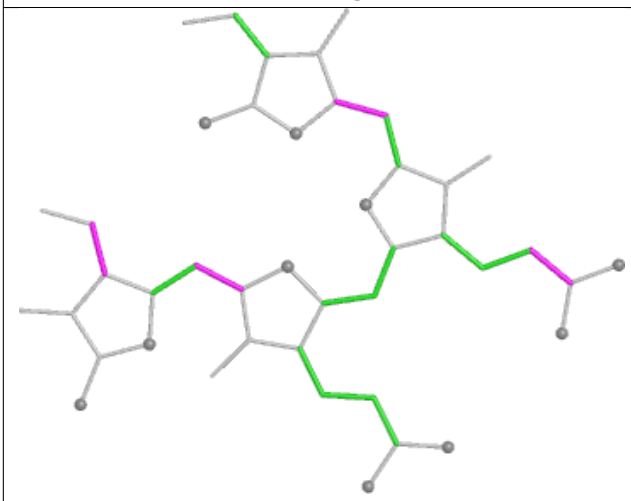

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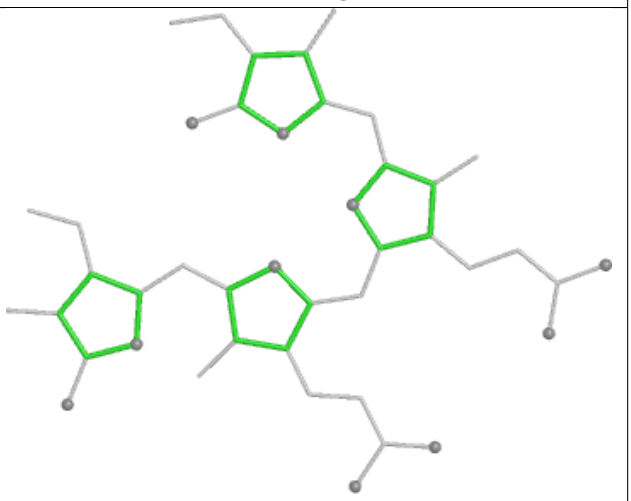
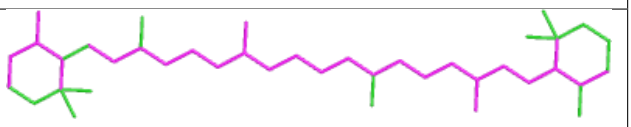


Rings

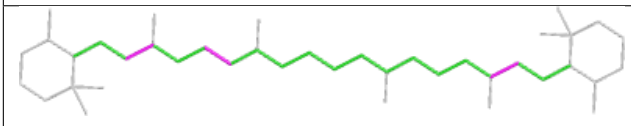
Ligand BCR B2 838



Bond lengths



Bond angles



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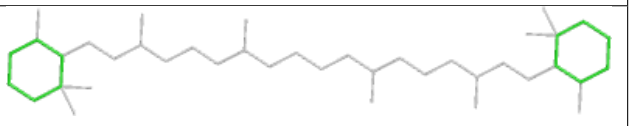
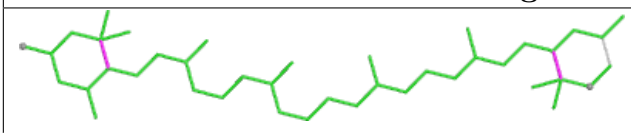


Rings

Ligand ZEX 82 309



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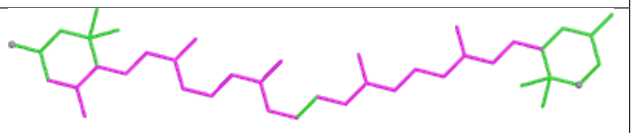

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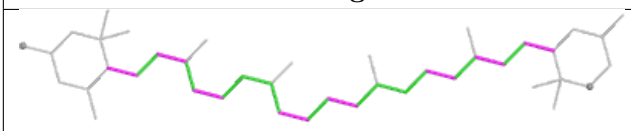

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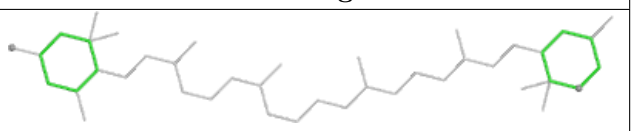
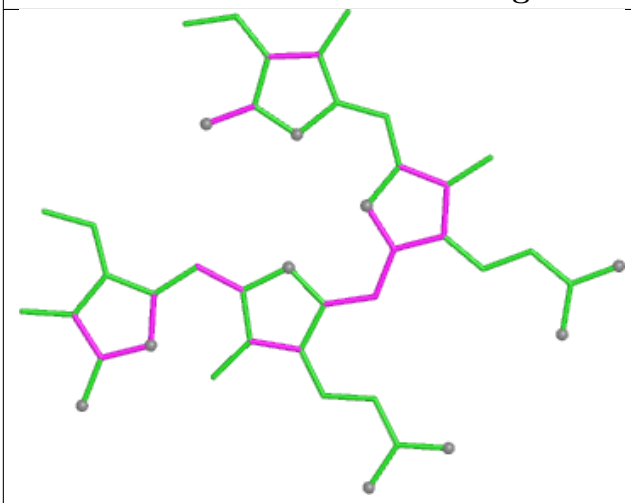


Rings

Ligand PEB FK 202



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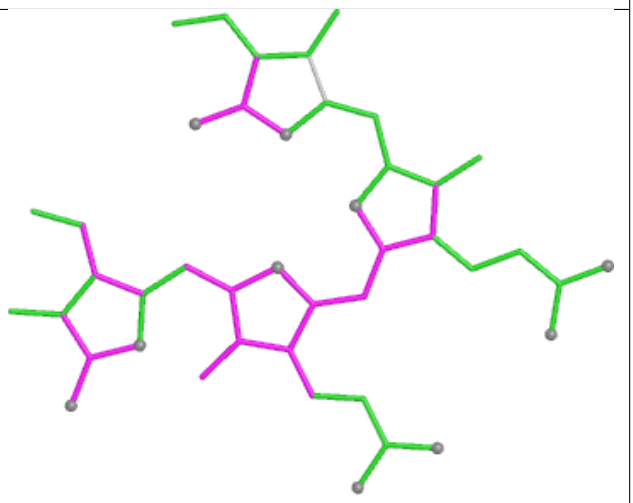

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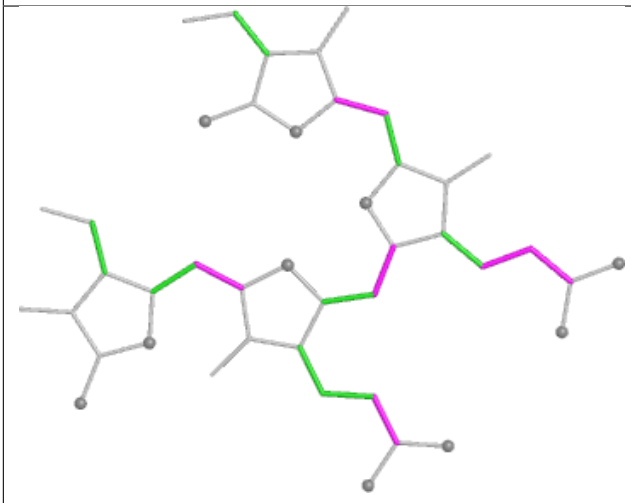

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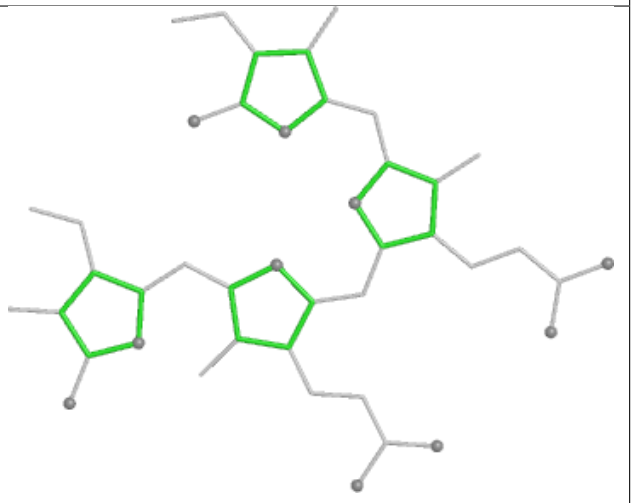
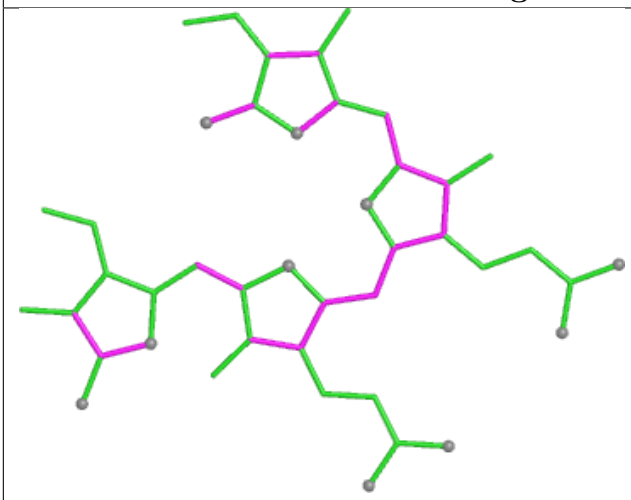


Rings

Ligand PEB NQ 202



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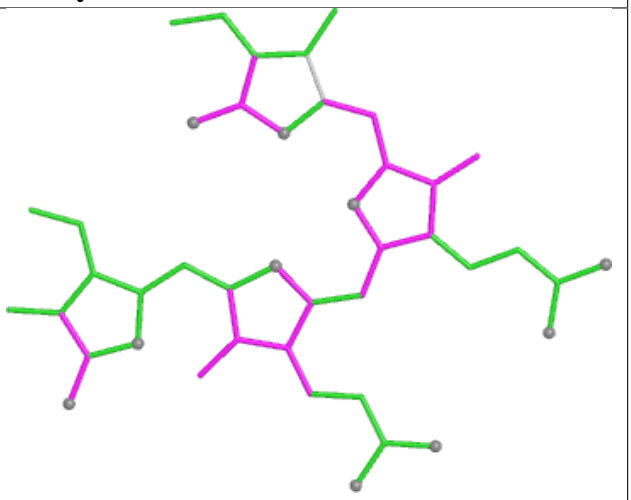

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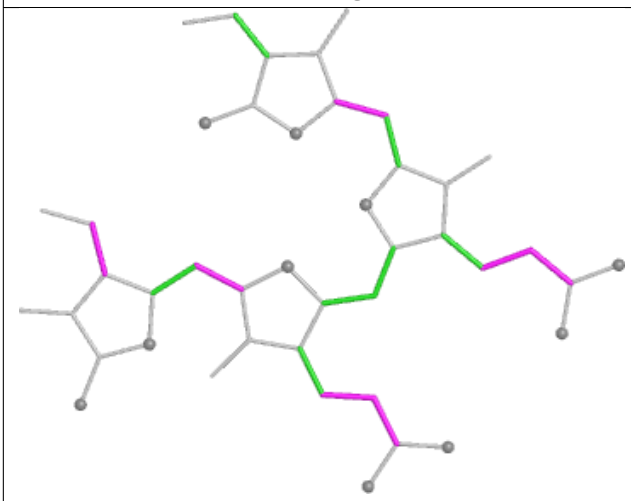

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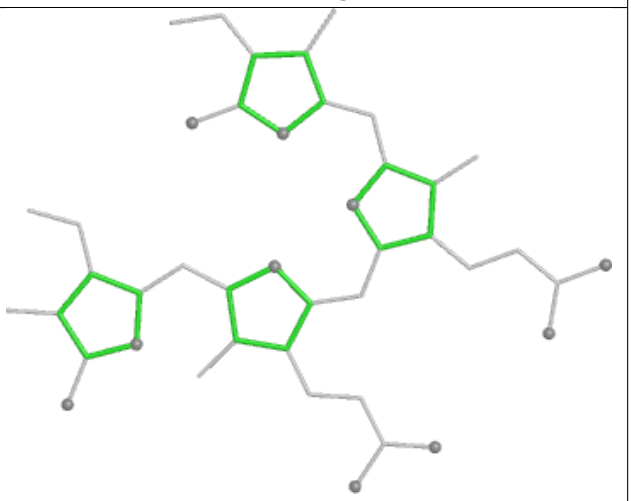
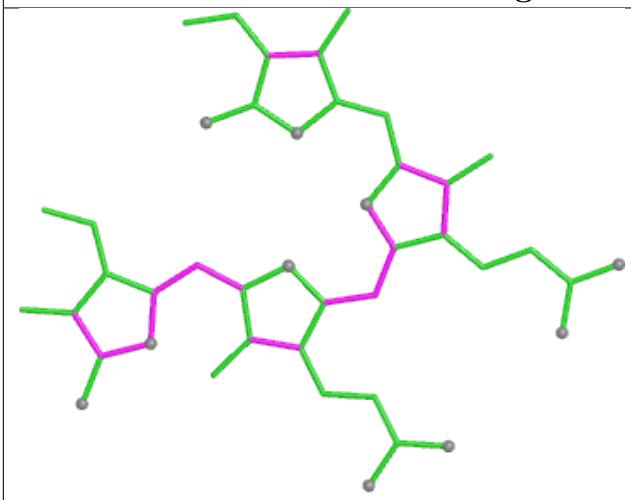


Rings

Ligand PEB U4 201



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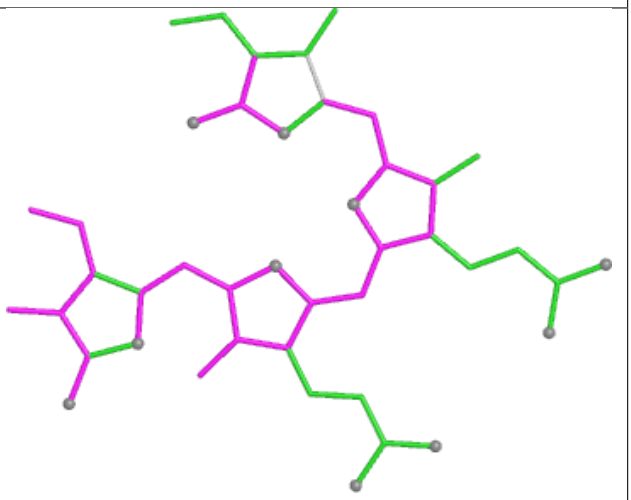

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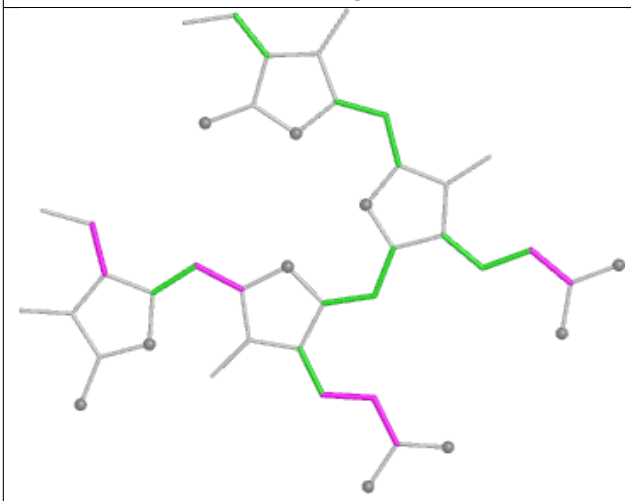

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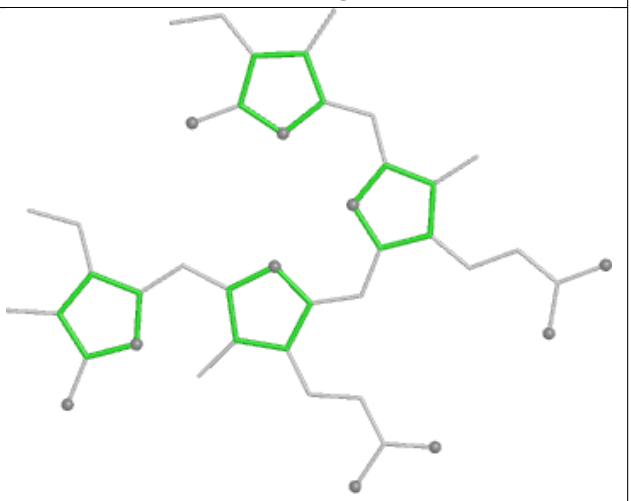
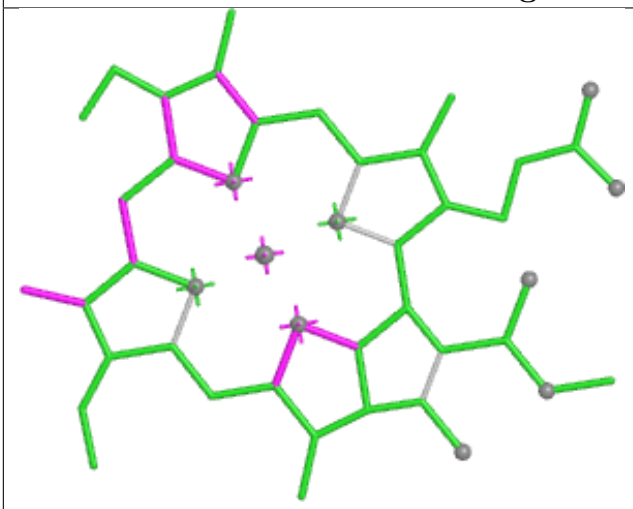


Rings

Ligand CLA 32 308



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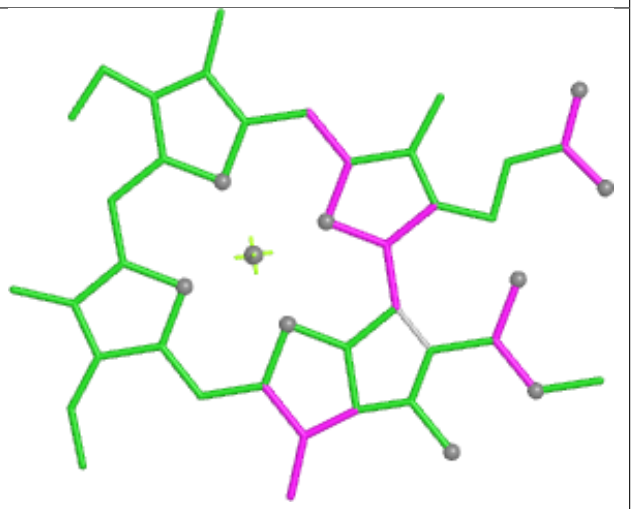

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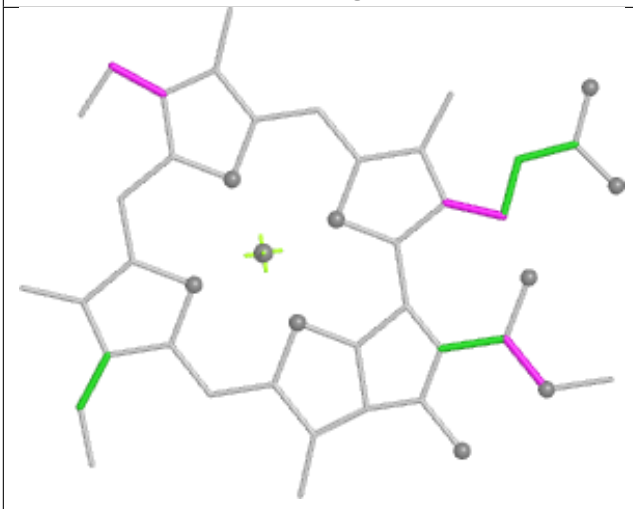
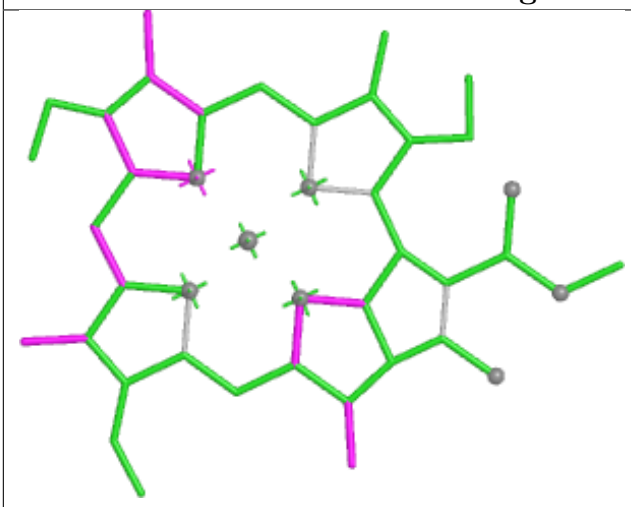


Torsions



Rings

Ligand CLA 52 604



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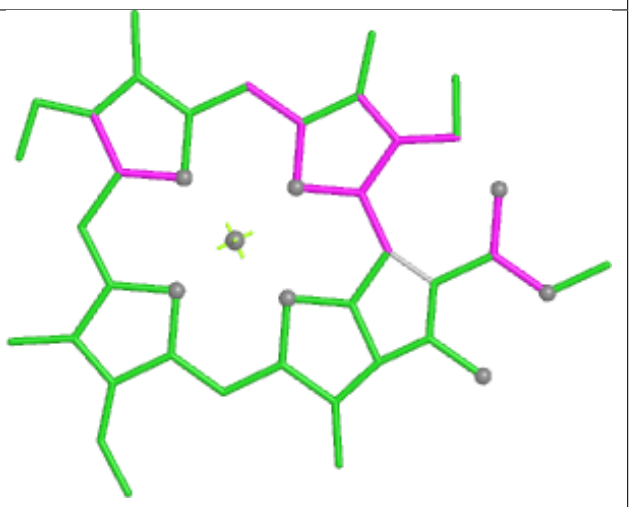
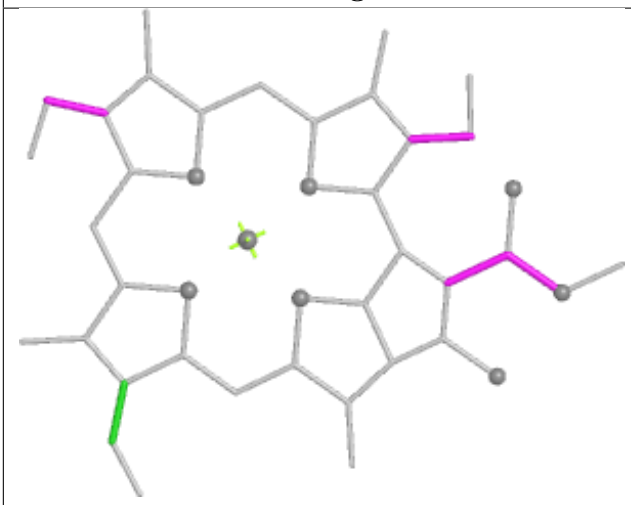


Bond angles

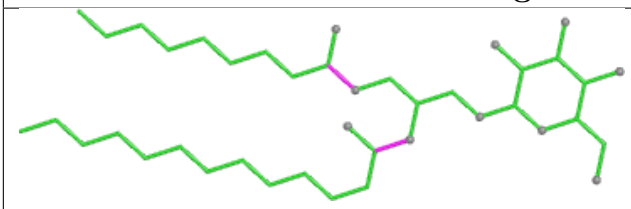


Torsions



Rings

Ligand LMG b6 619



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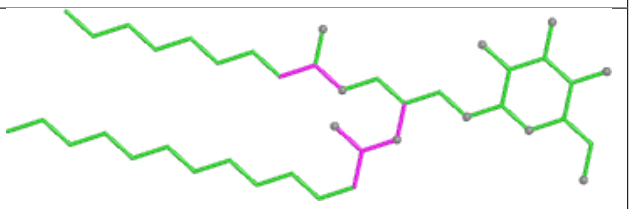

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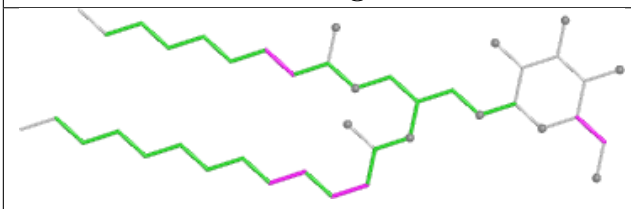

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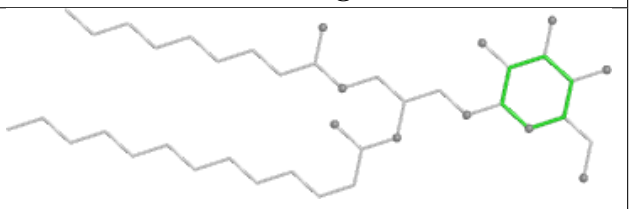
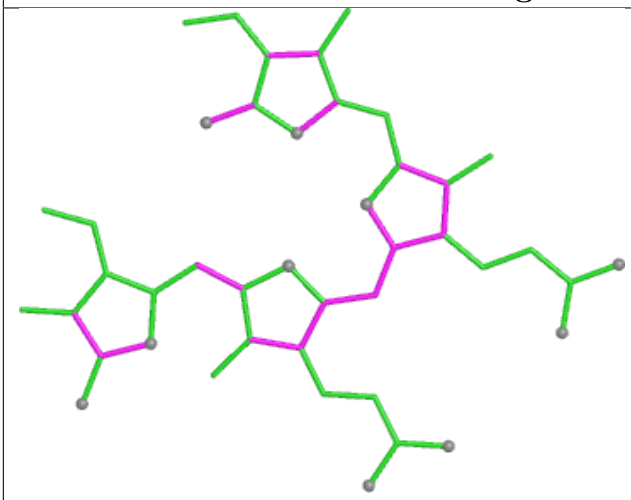


Rings

Ligand PEB vC 202



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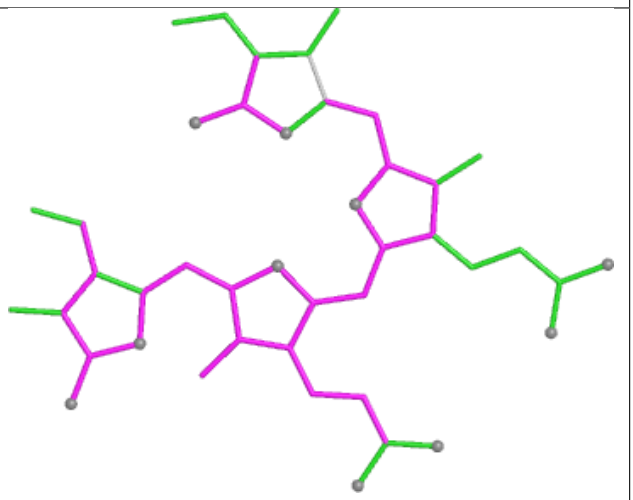

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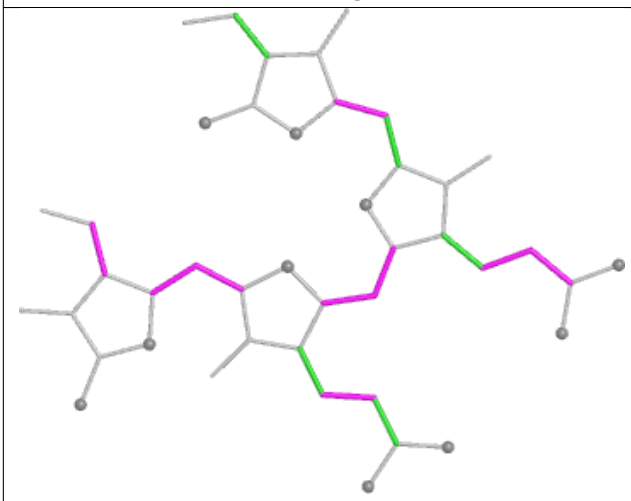

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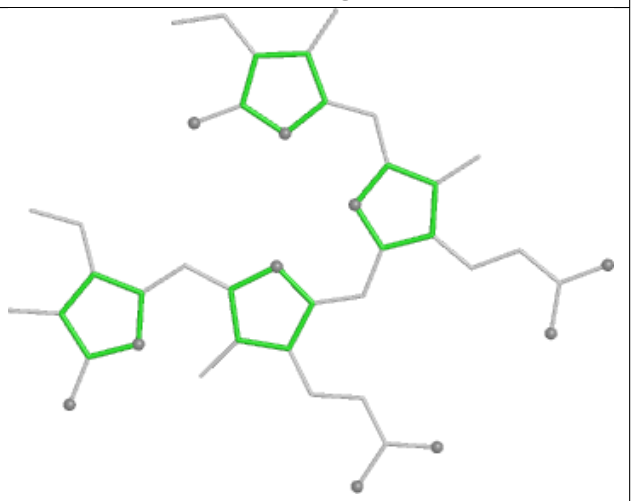
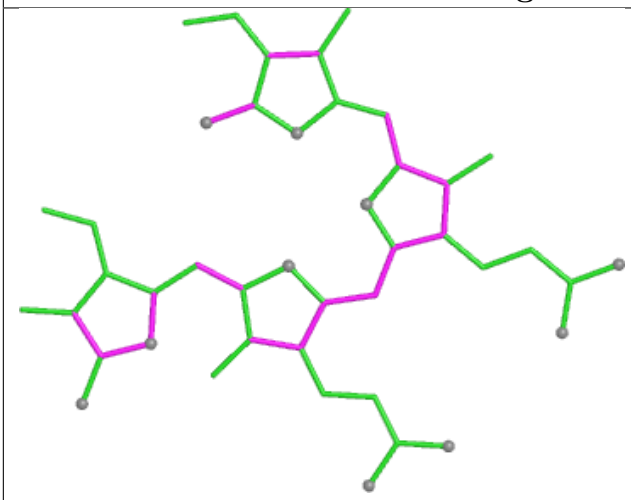


Rings

Ligand PEB cO 202



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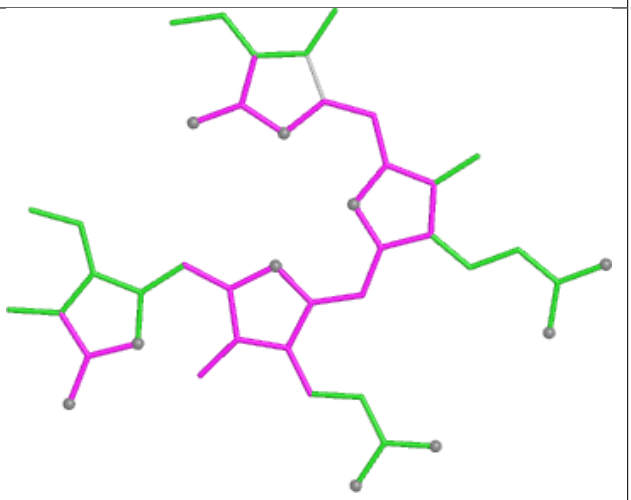
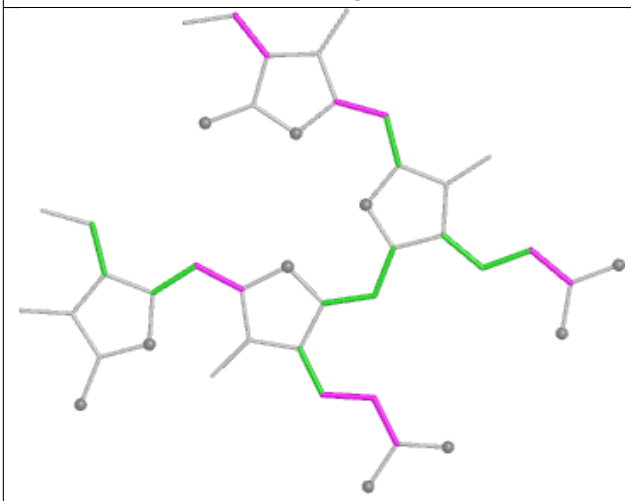


Bond angles



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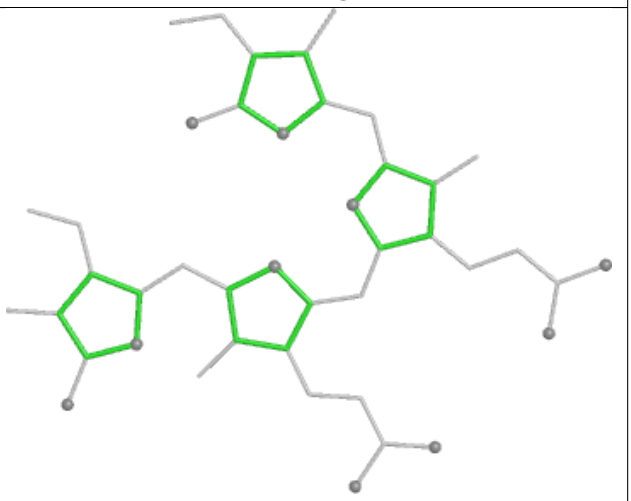
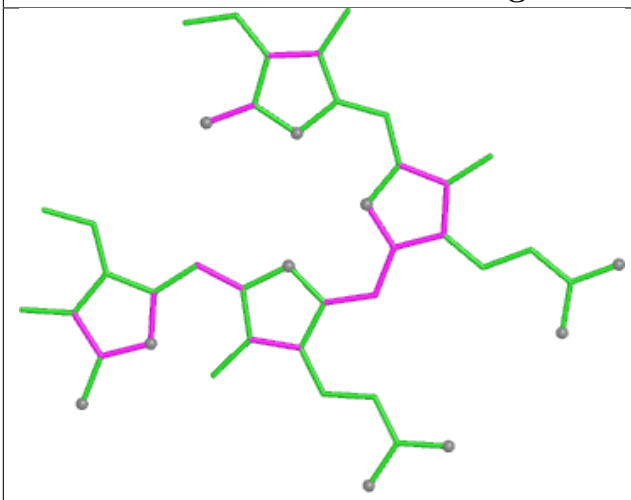


Rings

Ligand PEB PM 202



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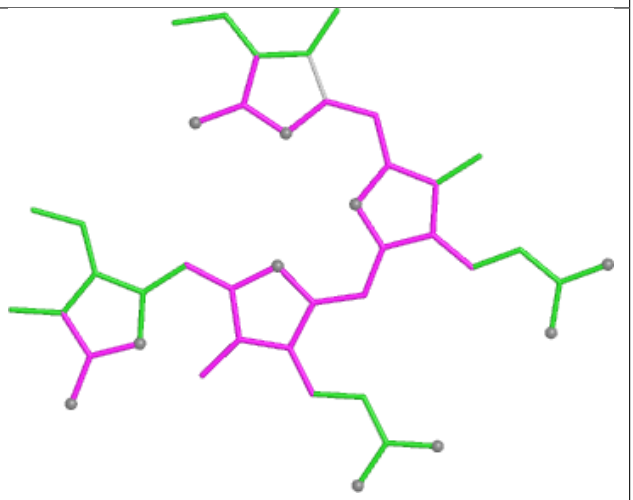
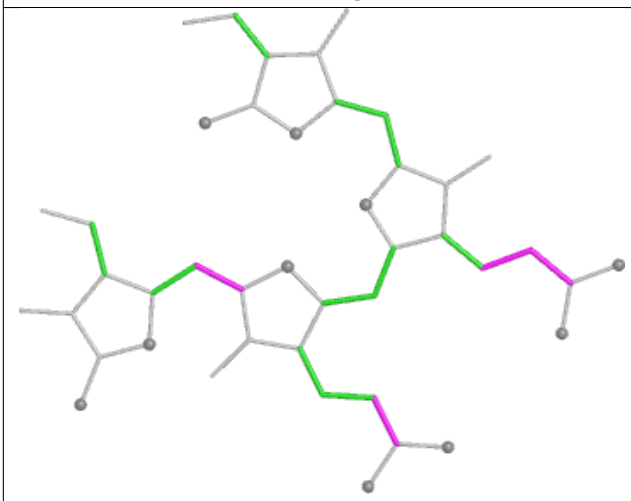


Bond angles



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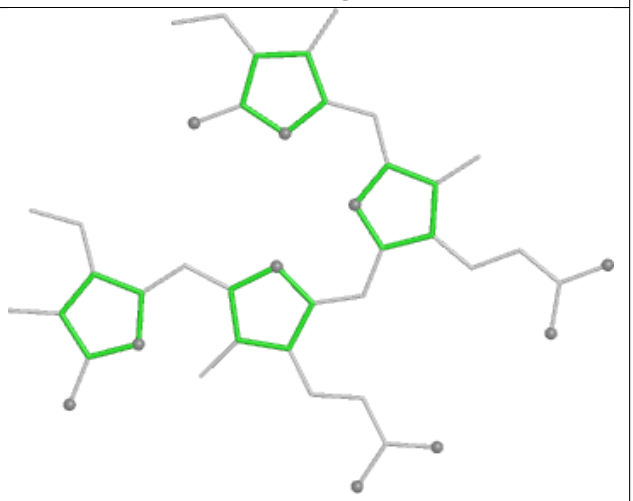
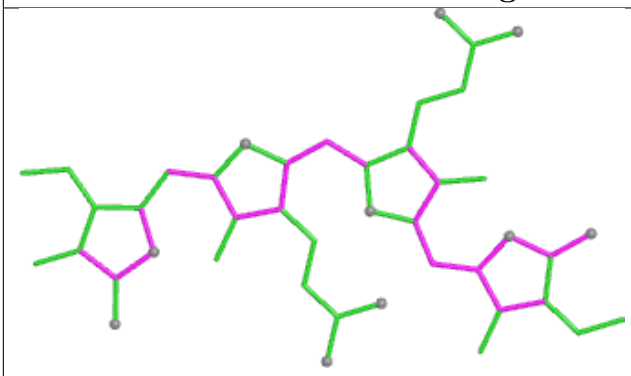


Rings

Ligand CYC CG 1001



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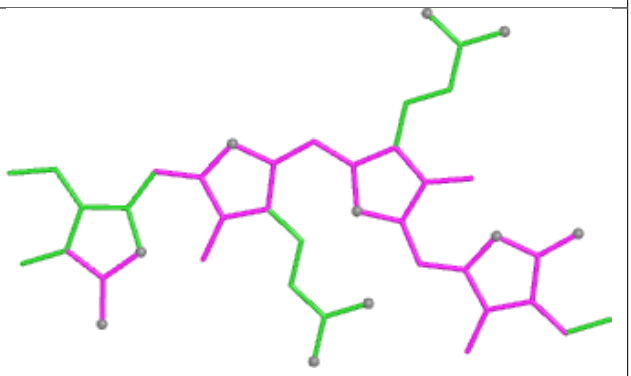

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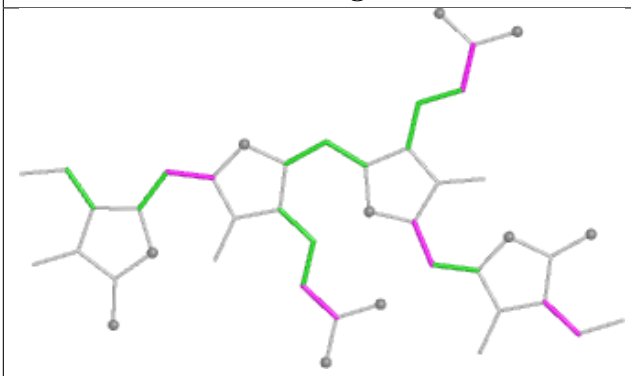

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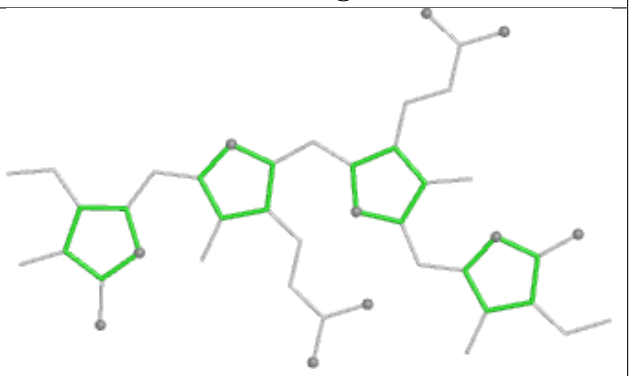
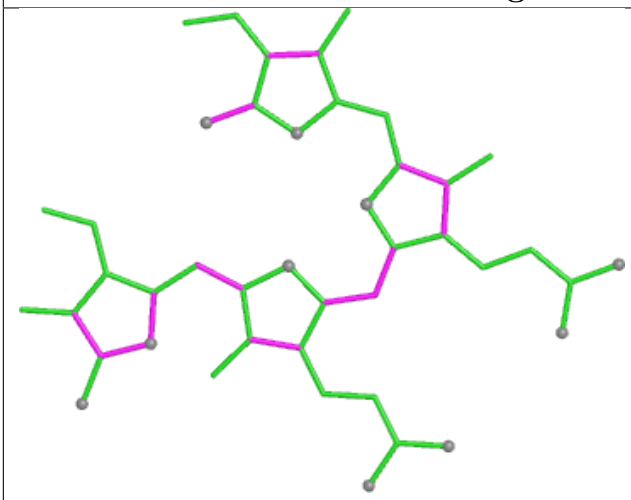


Rings

Ligand PEB WE 203



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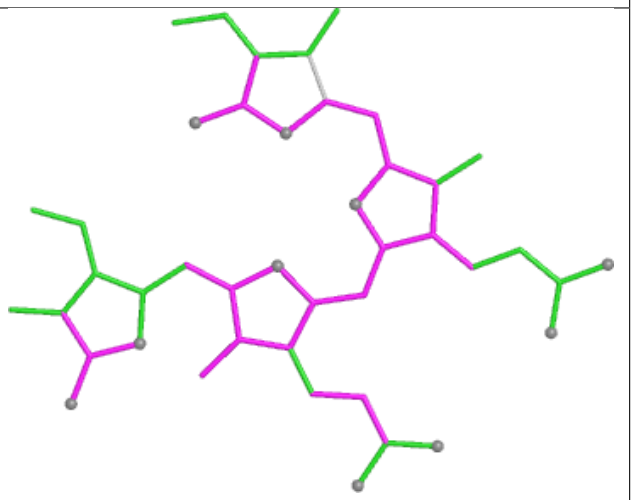

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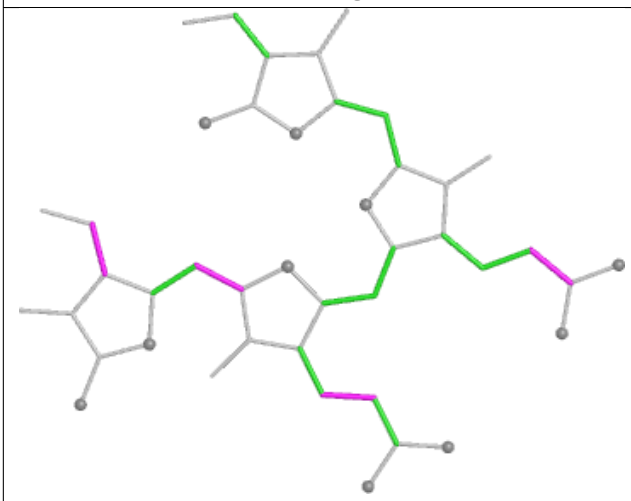

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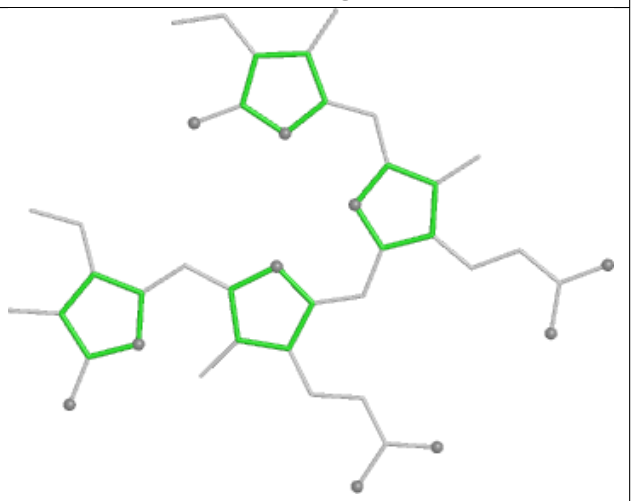
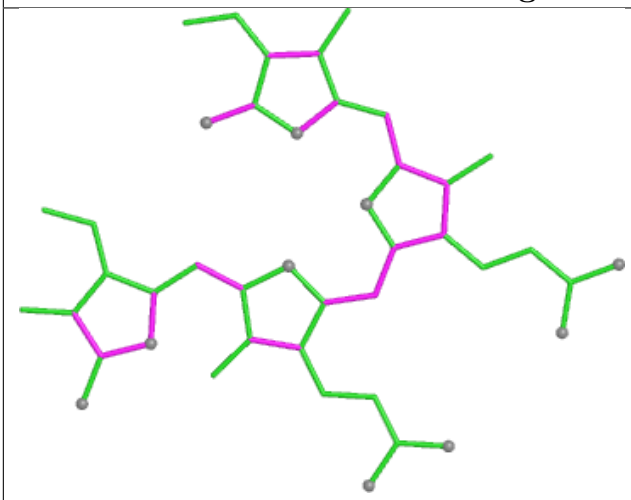


Rings

Ligand PEB b1 203



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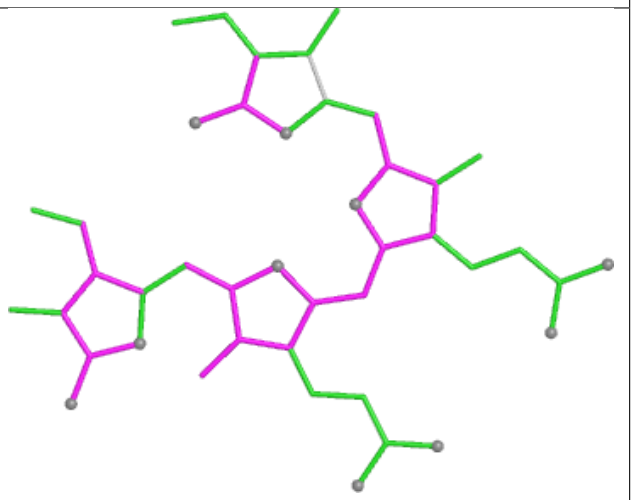

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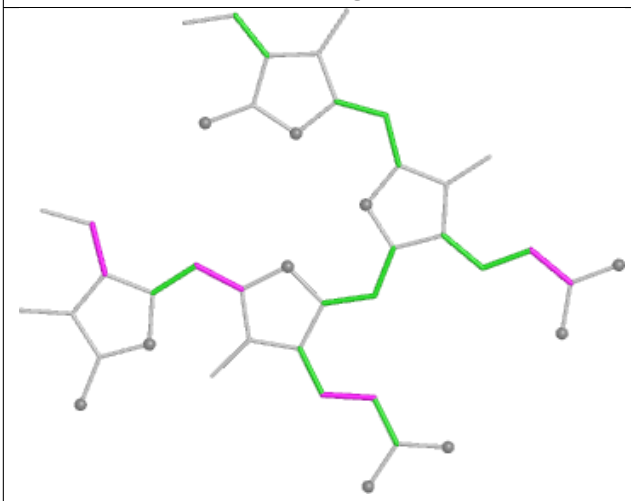

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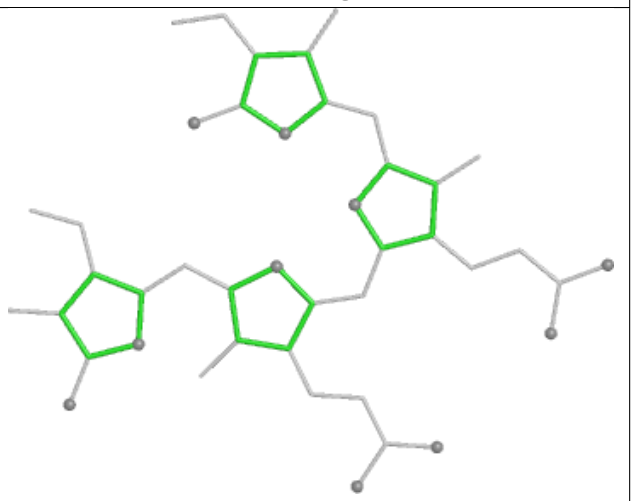
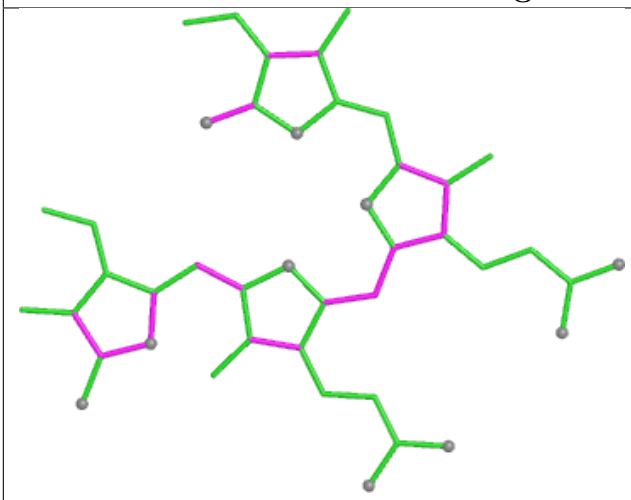


Rings

Ligand PEB GJ 203



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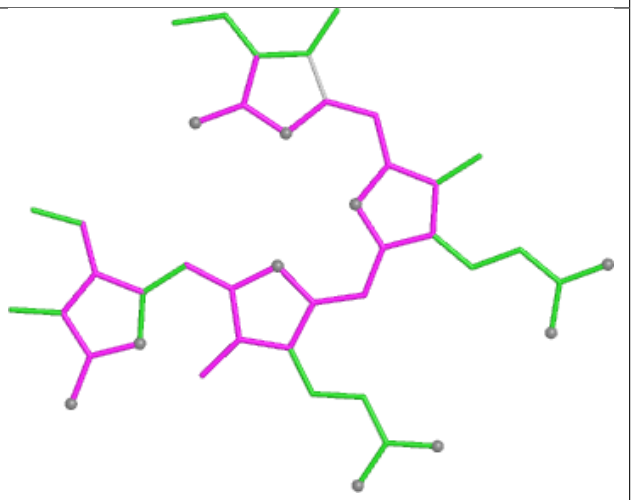

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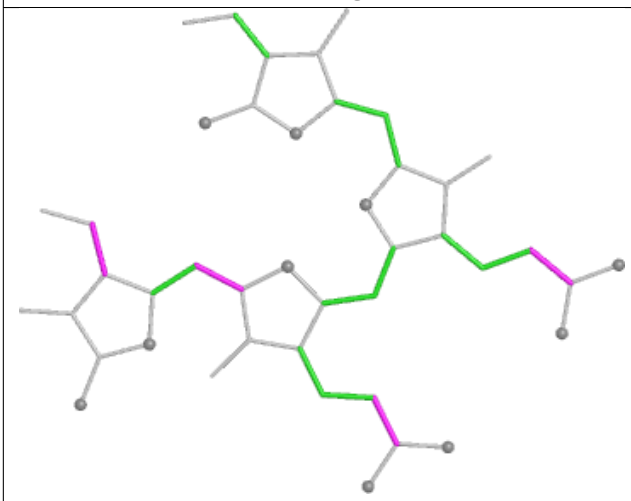

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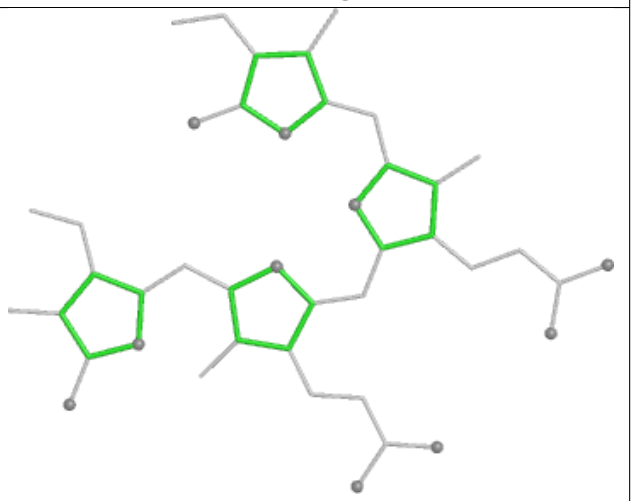
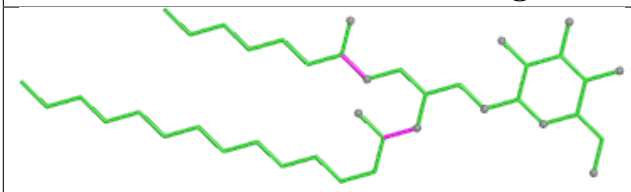


Rings

Ligand LMG B6 618



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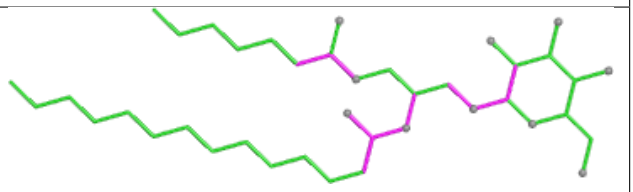

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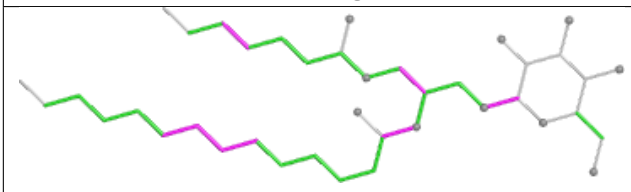

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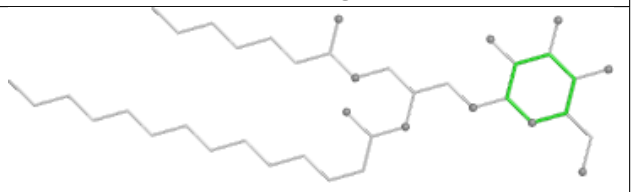
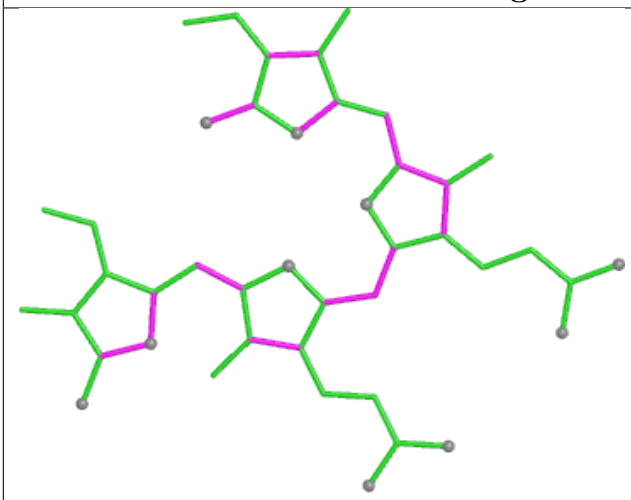


Rings

Ligand PEB W1 201



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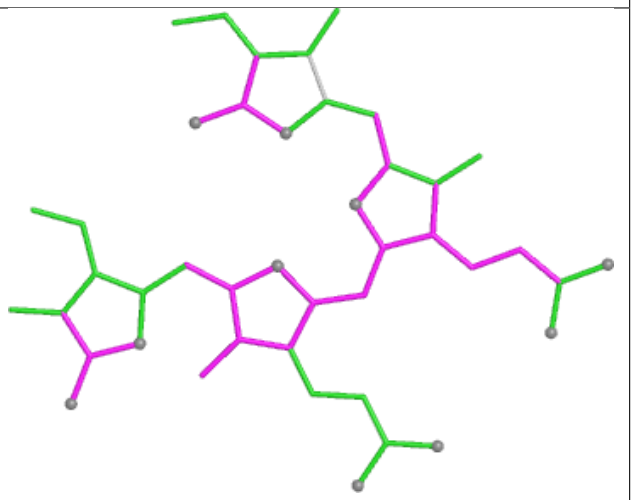

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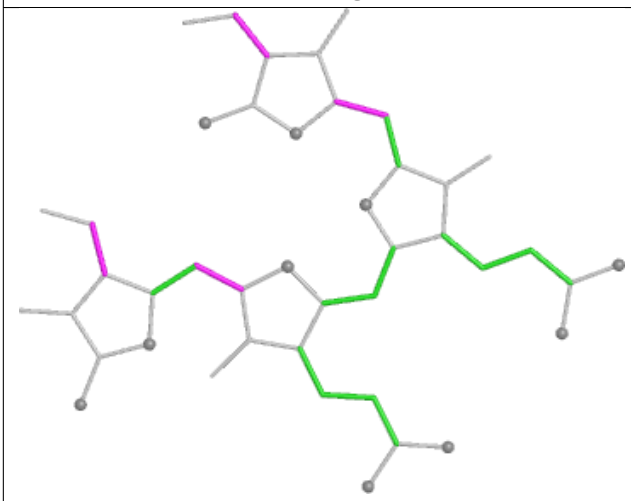

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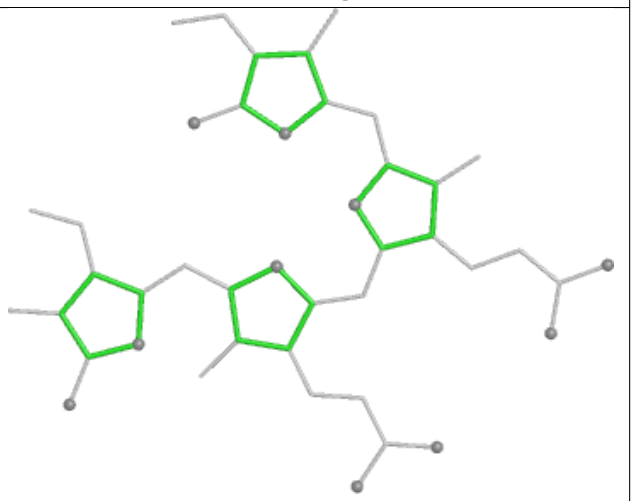
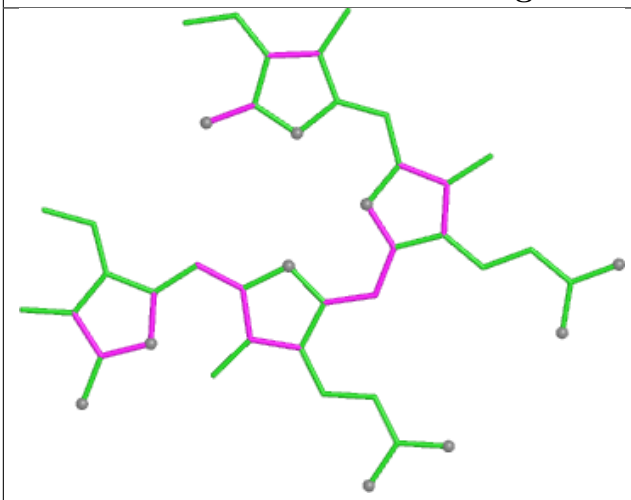


Rings

Ligand PEB Q5 203



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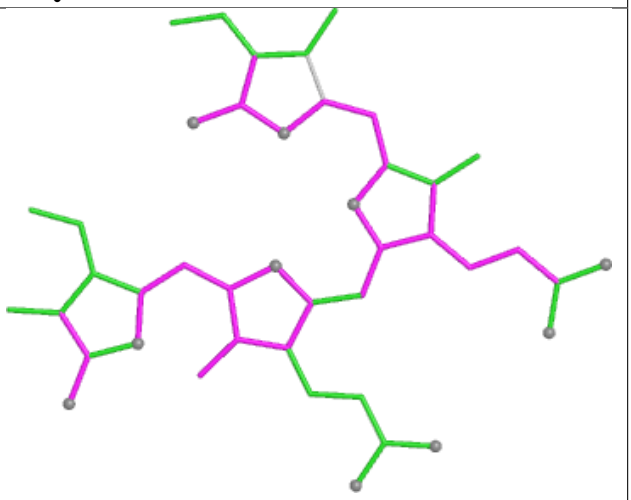

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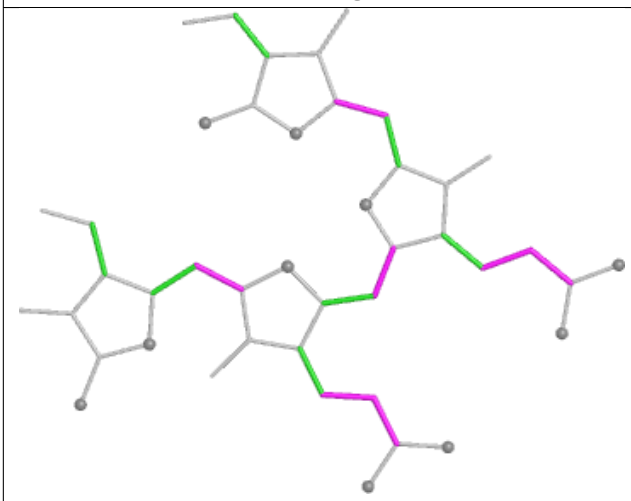

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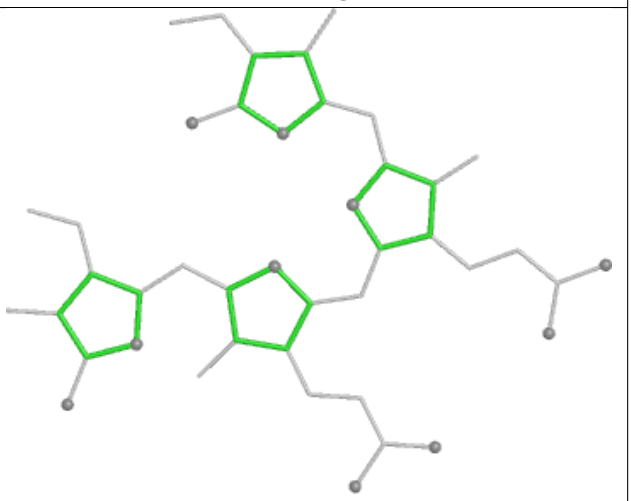

Rings

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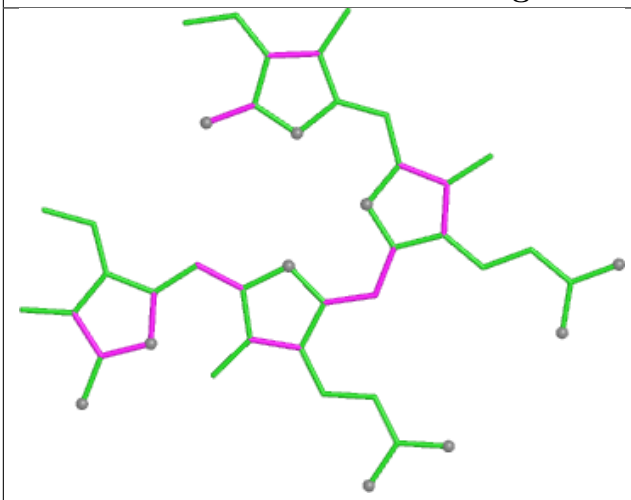

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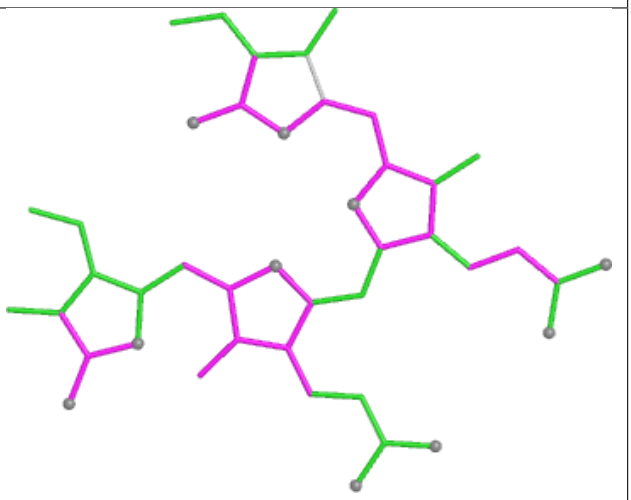

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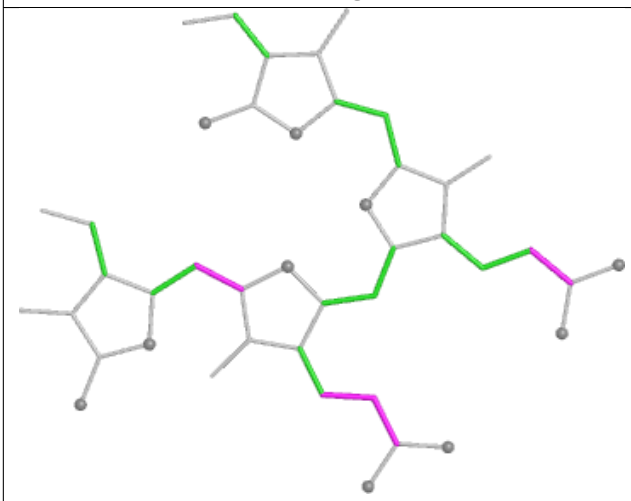

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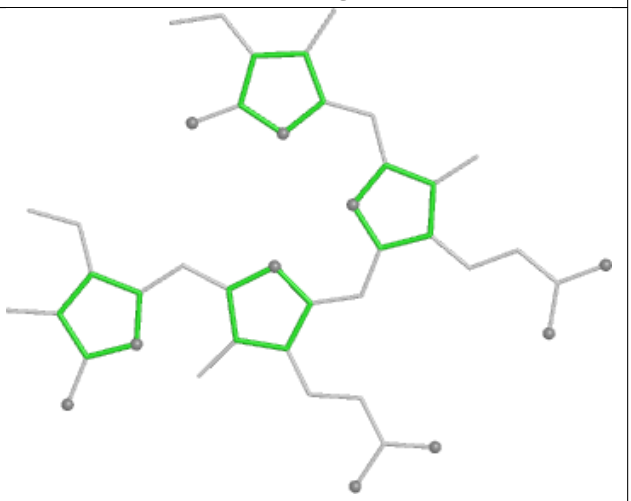
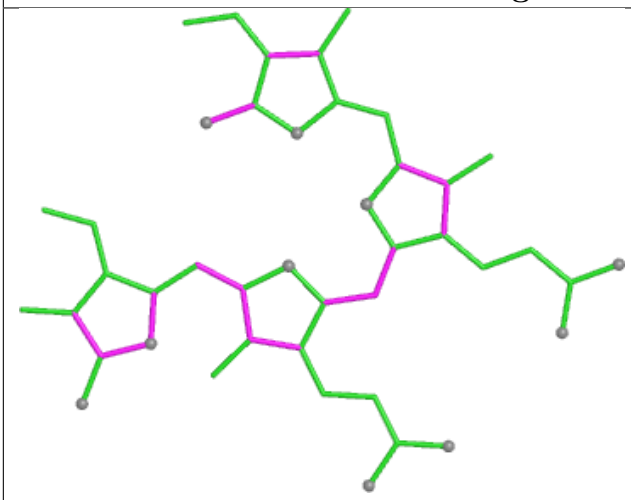


Rings

Ligand PEB PQ 202



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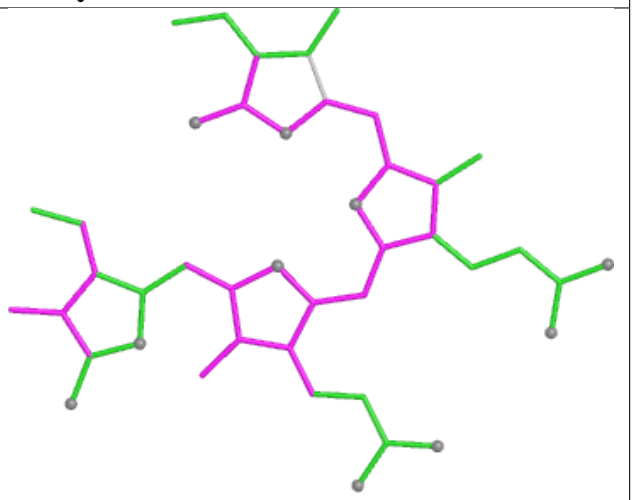

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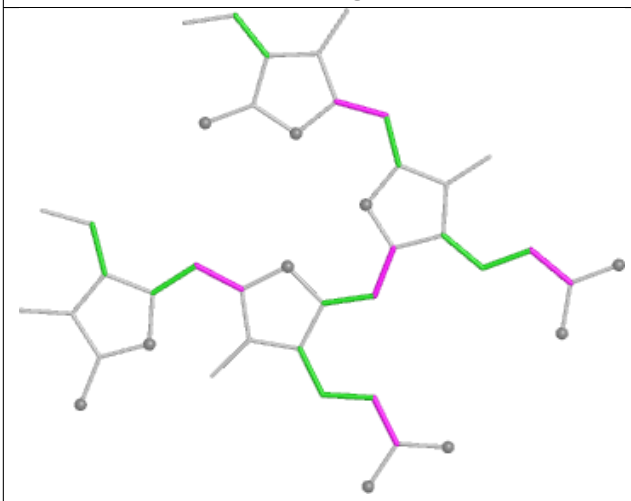

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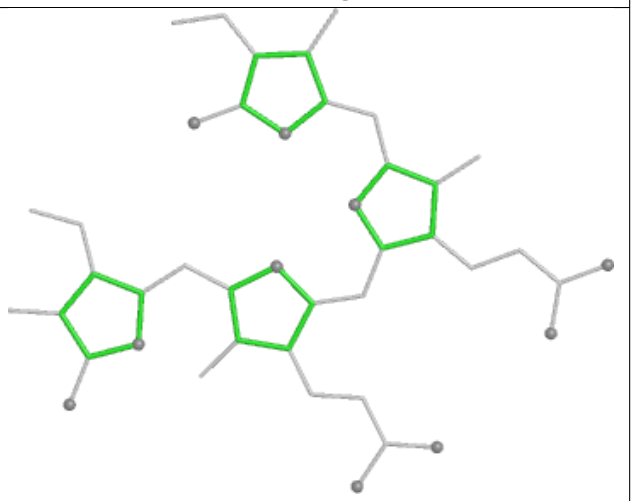
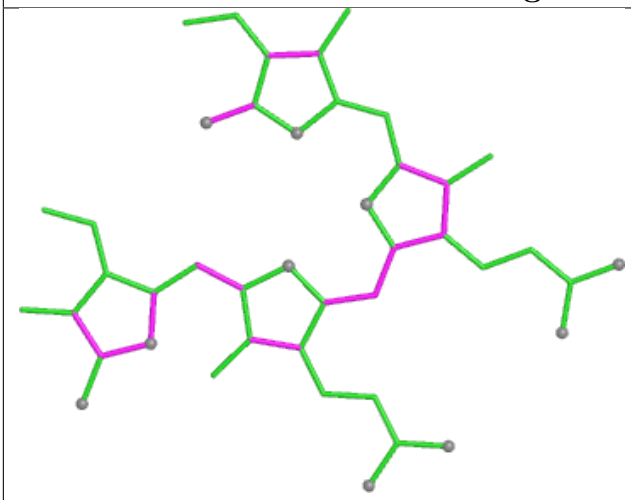


Rings

Ligand PEB l1 202



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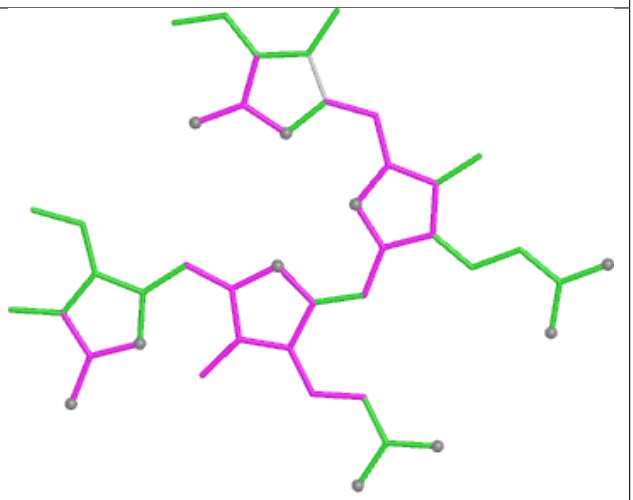

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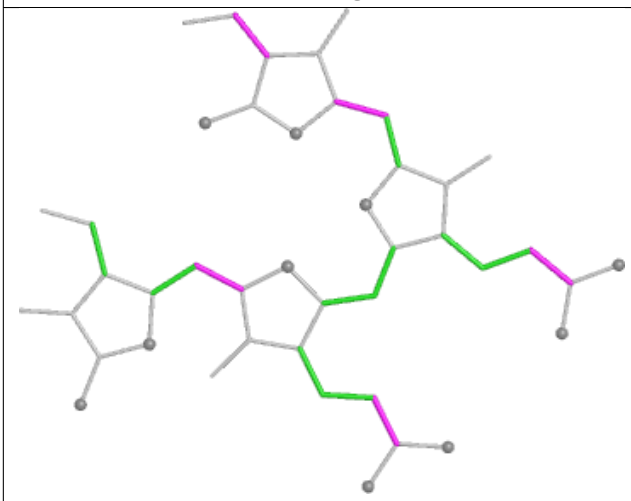

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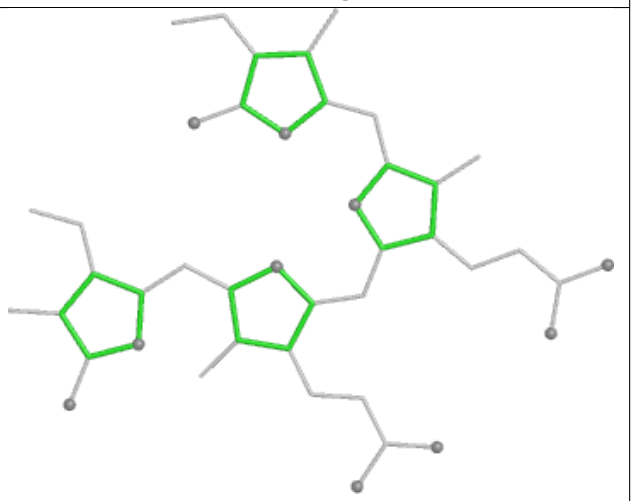
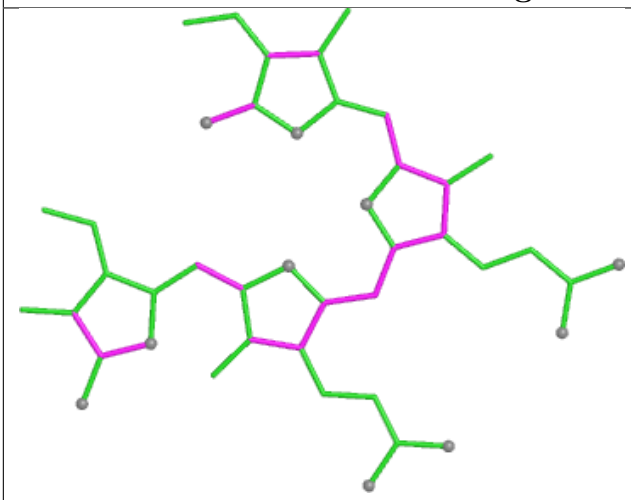


Rings

Ligand PEB H7 202



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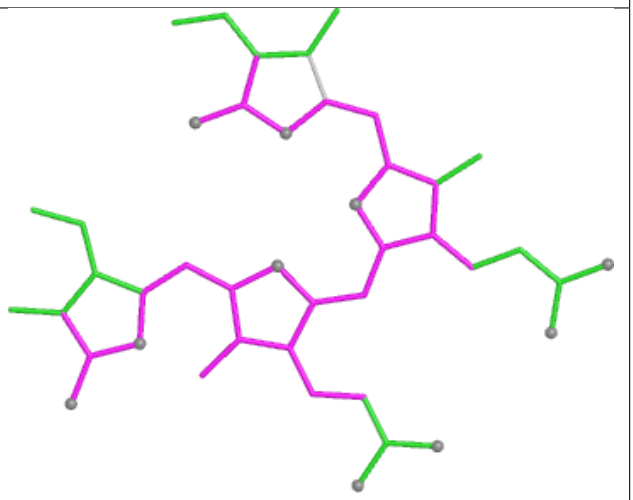

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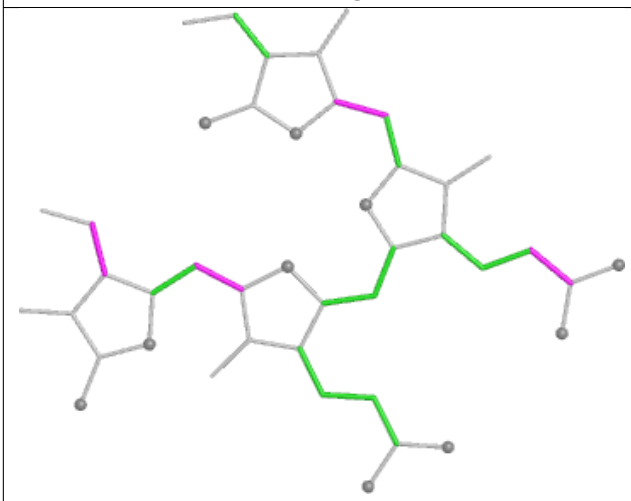

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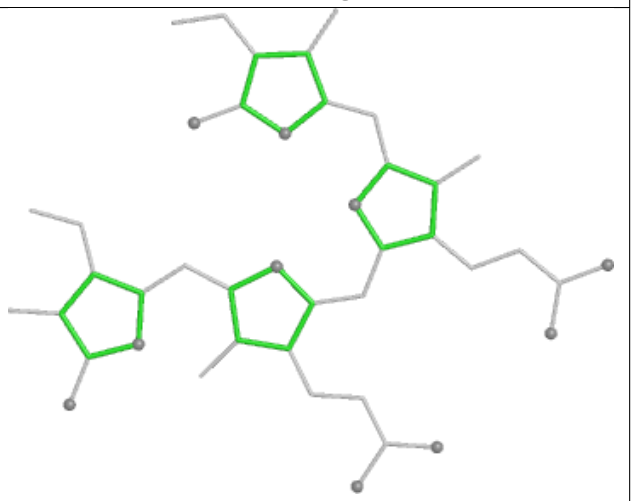
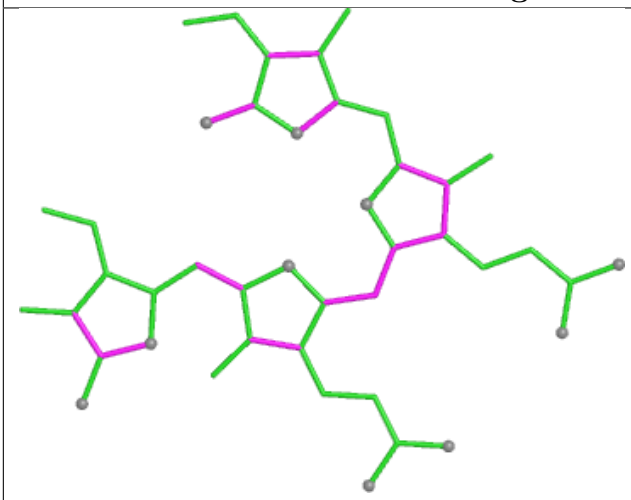


Rings

Ligand PEB OQ 201



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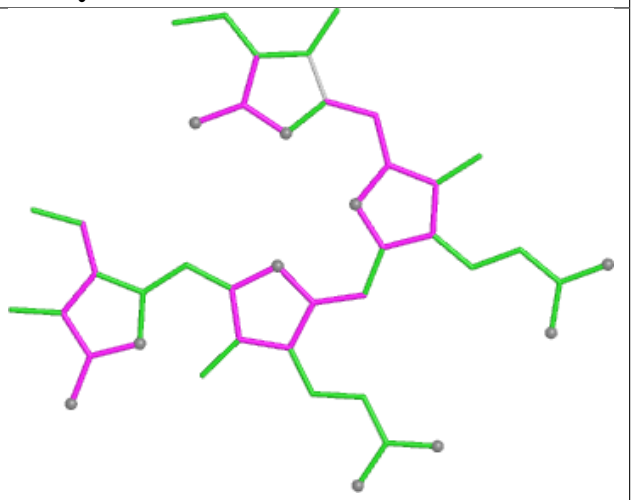
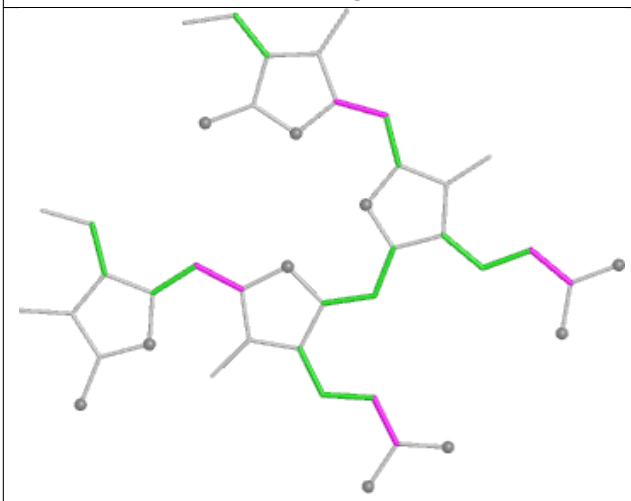


Bond angles



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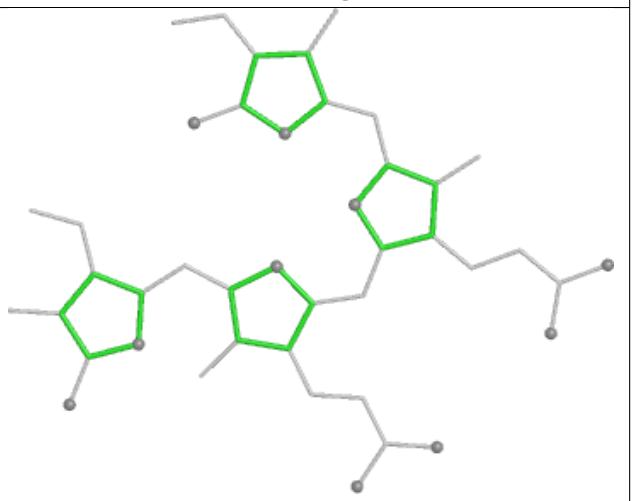
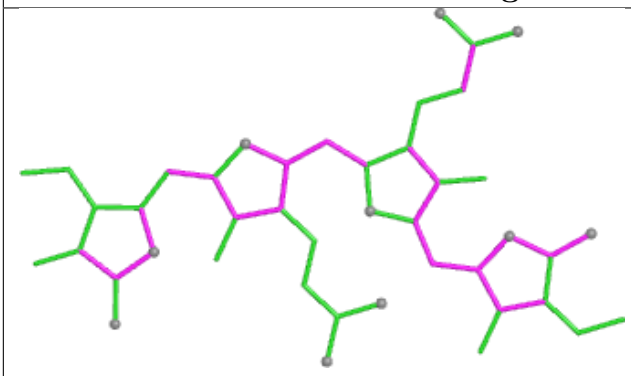


Rings

Ligand CYC LH 1002



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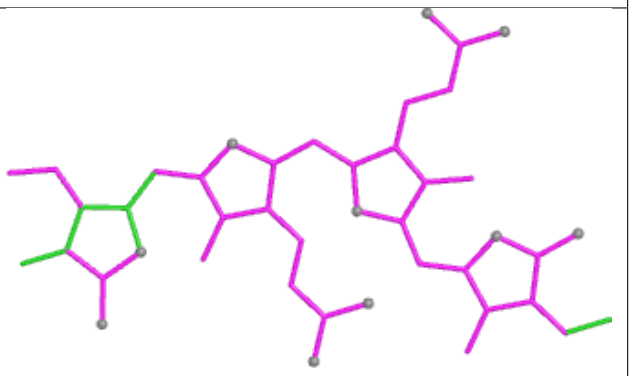
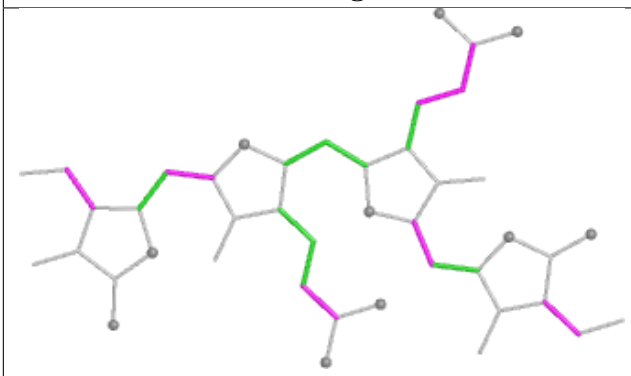


Bond angles



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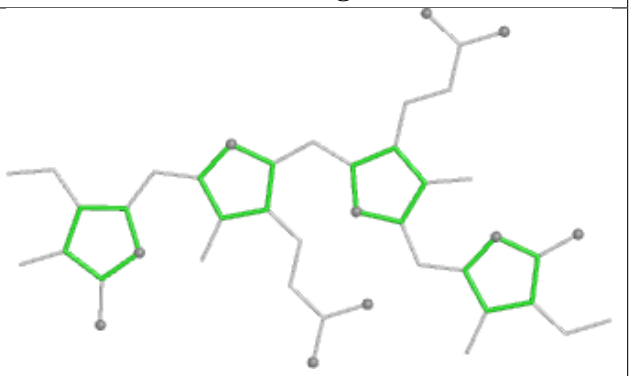
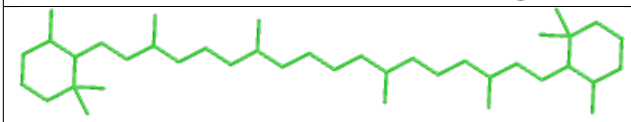
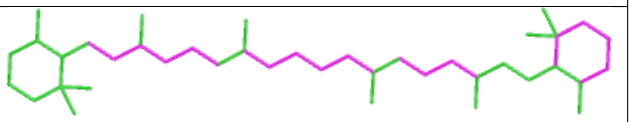


Rings

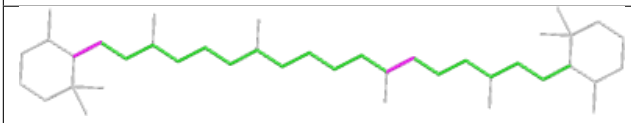
Ligand BCR BL 616



Bond lengths



Bond angles



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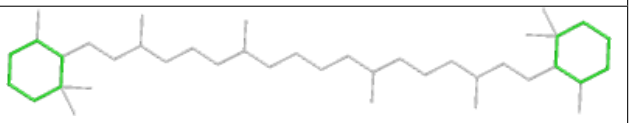
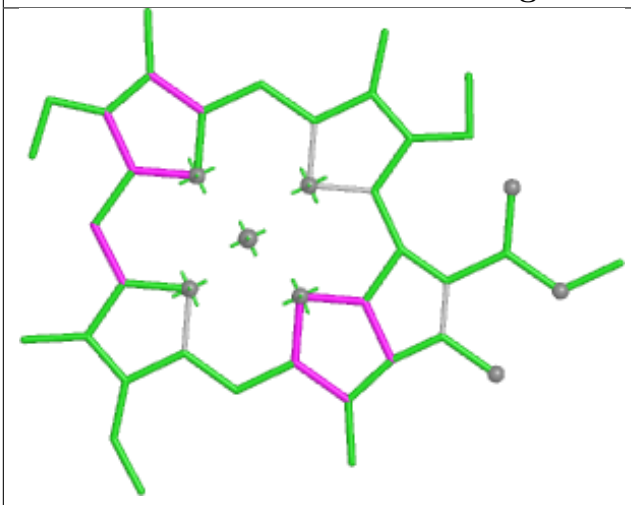
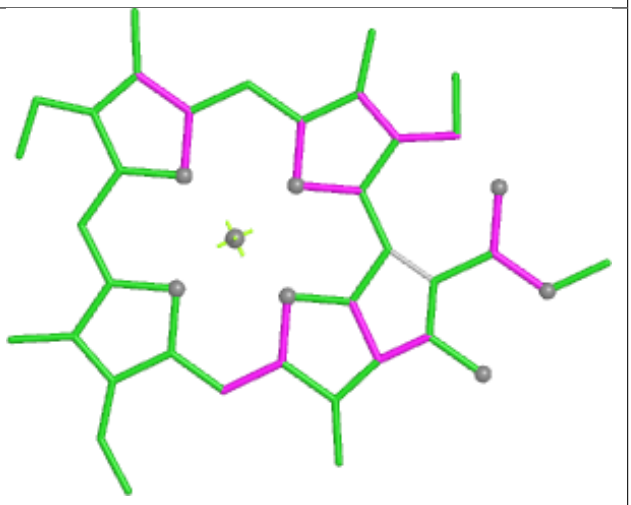


Rings

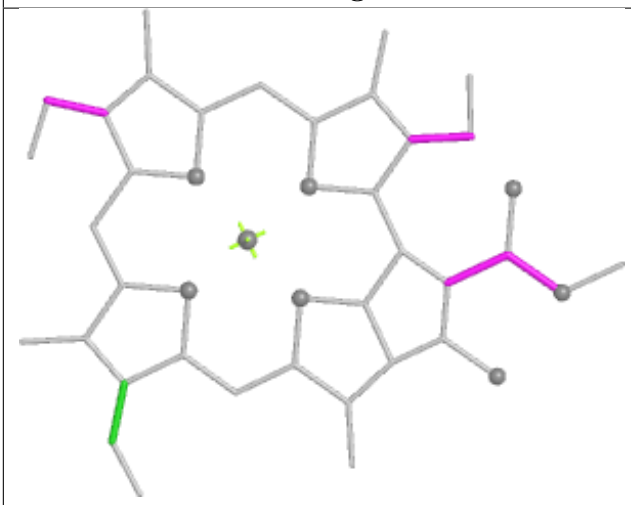
Ligand CLA 62 305



Bond lengths



Bond angles

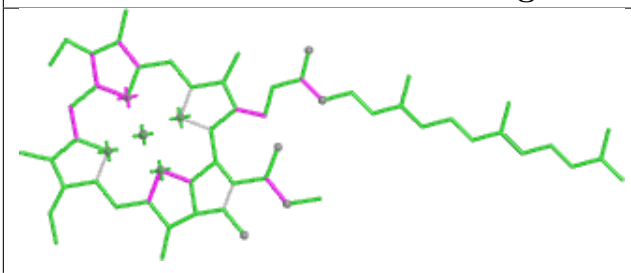


Torsions



Rings

Ligand CLA aL 606



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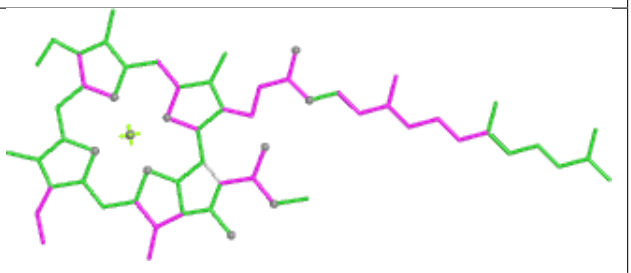

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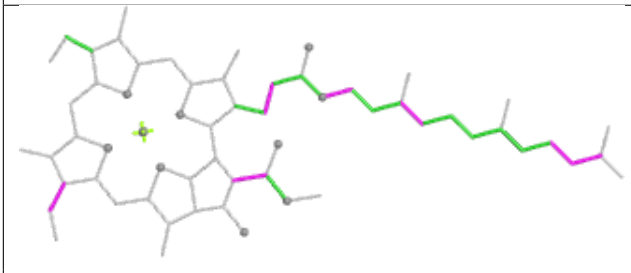

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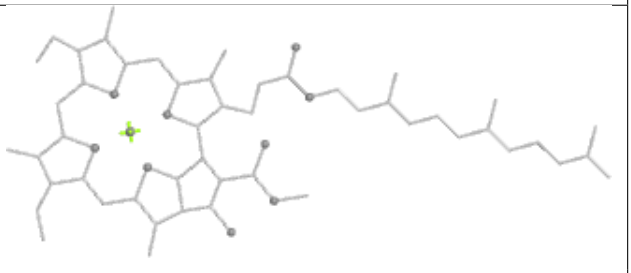
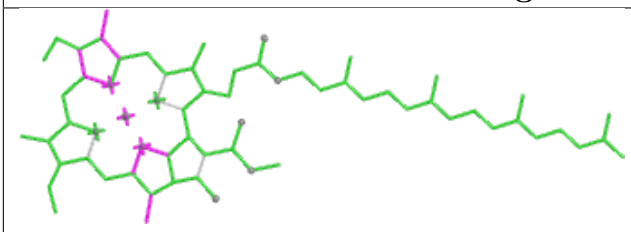


Rings

Ligand CLA B2 826



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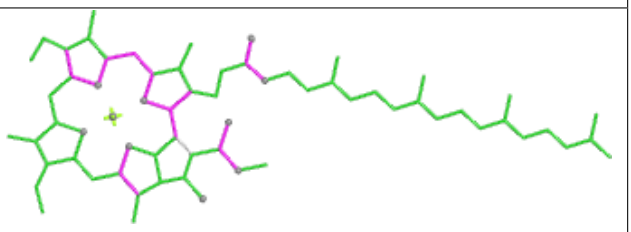

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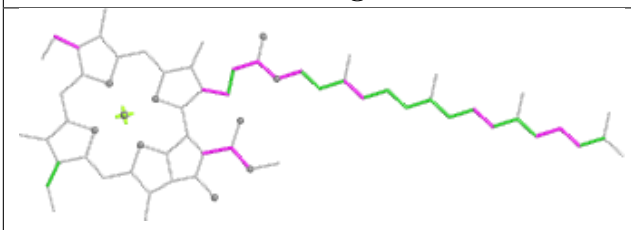

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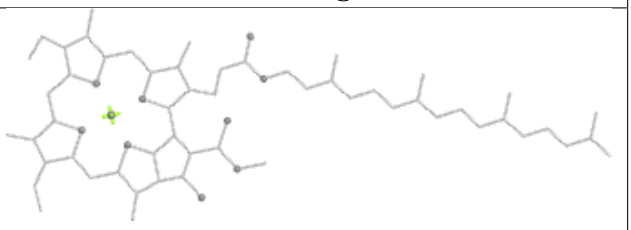
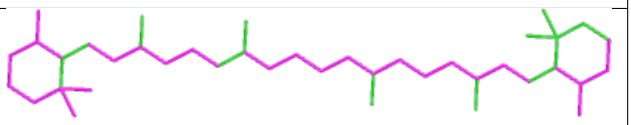


Rings

Ligand BCR J2 103



Bond lengths



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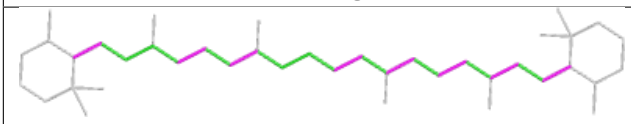

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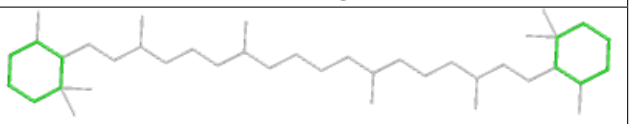
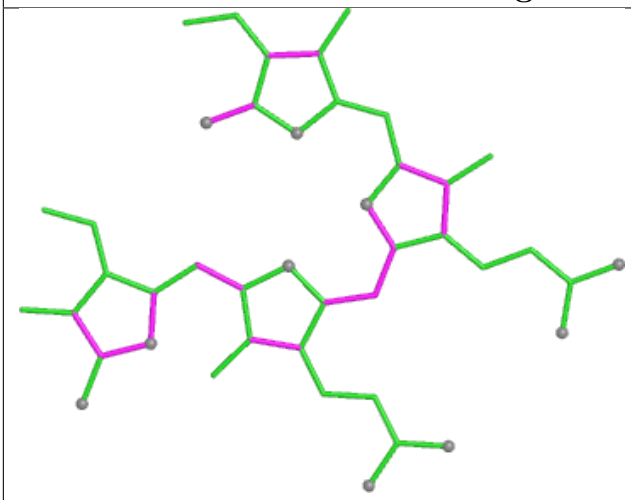


Rings

Ligand PEB O7 202



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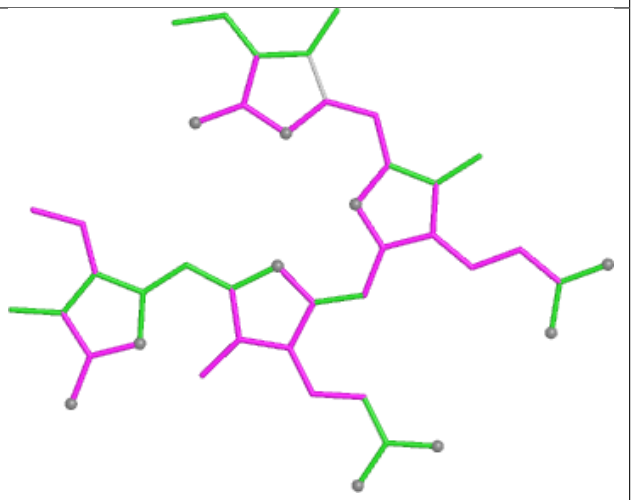

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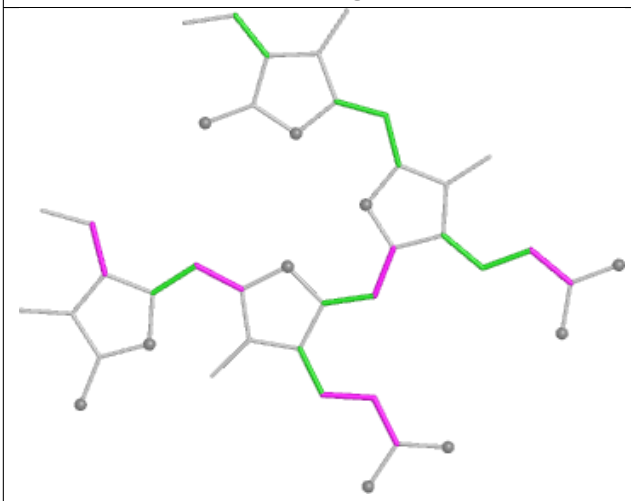

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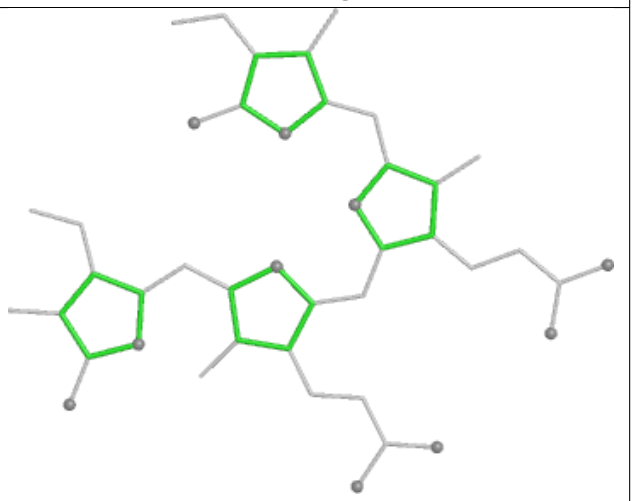
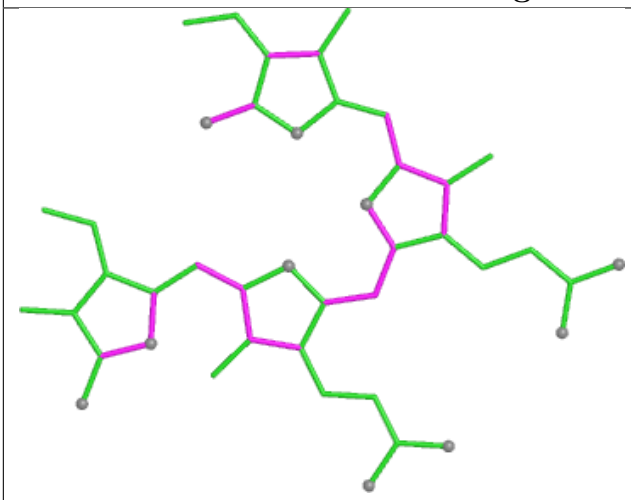


Rings

Ligand PEB wF 303



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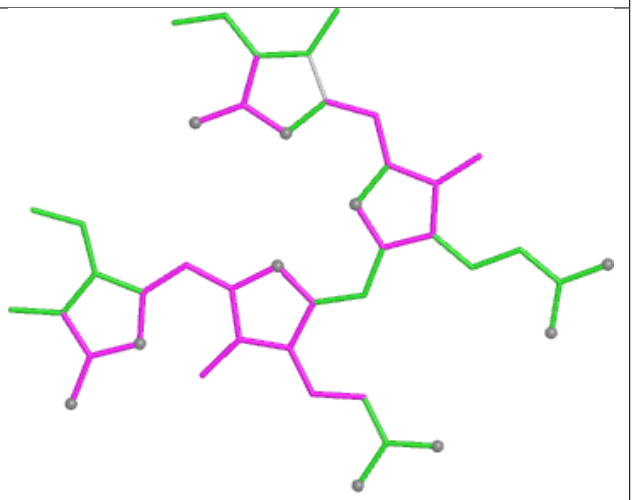

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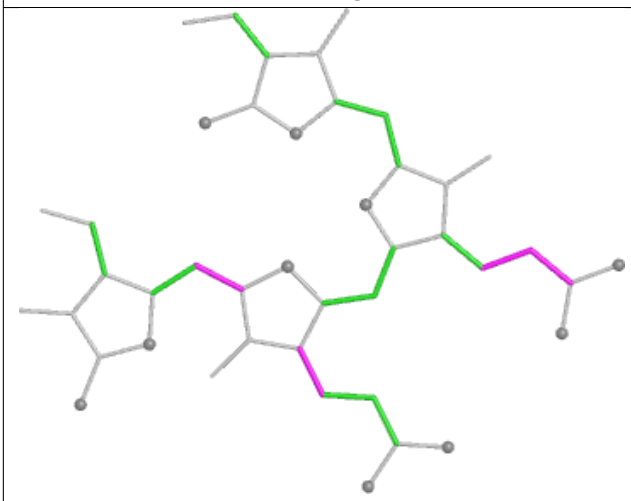

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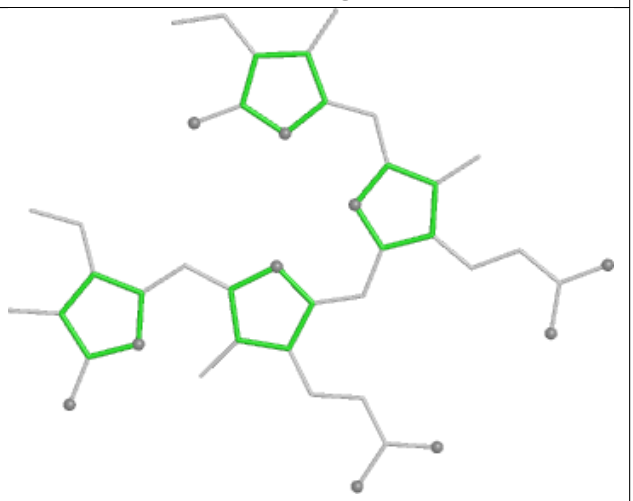
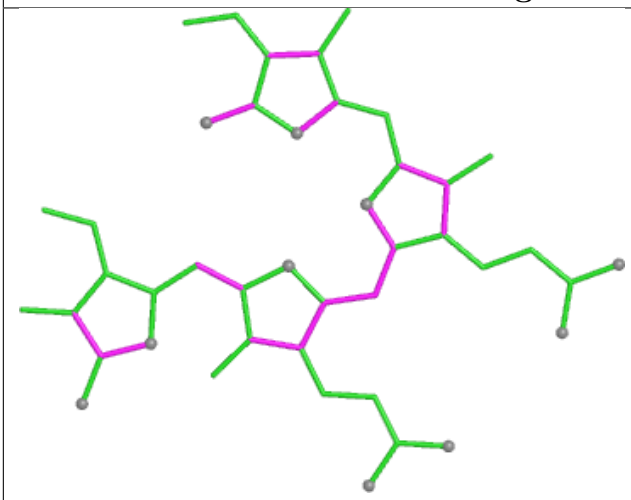


Rings

Ligand PEB D9 201



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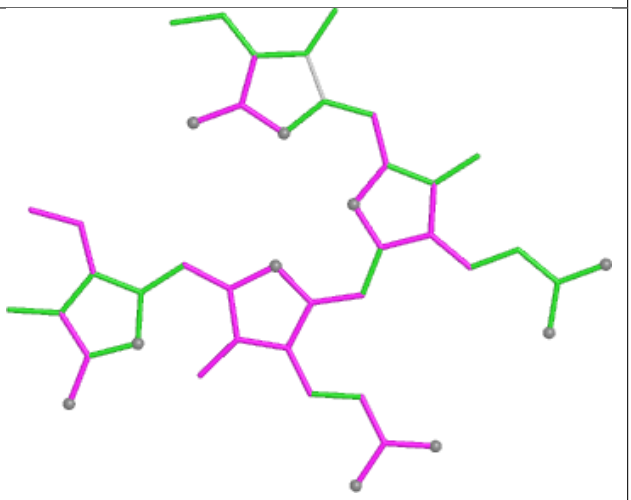

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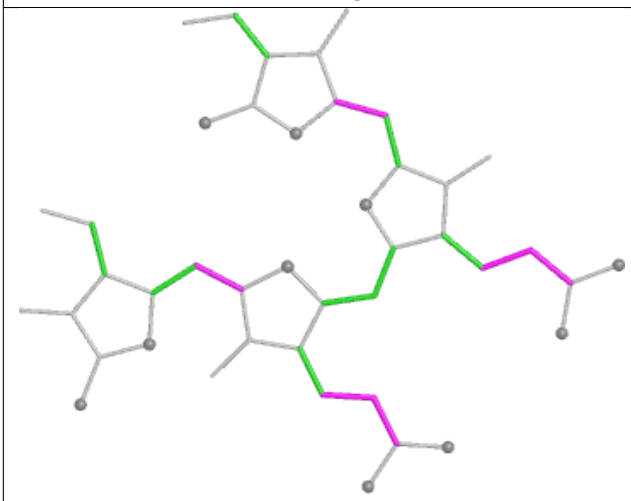

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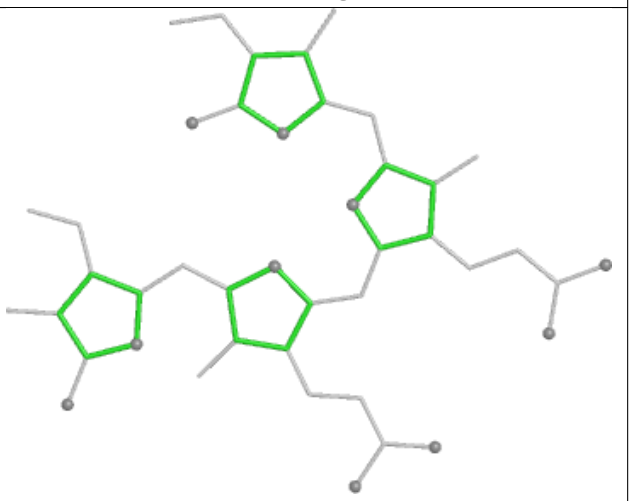

Rings

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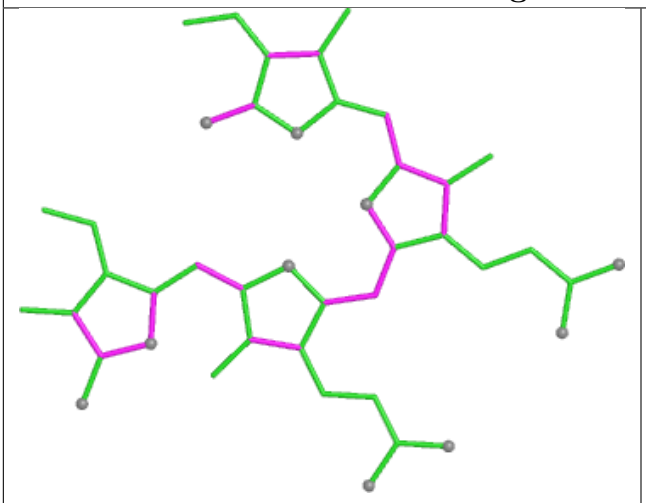

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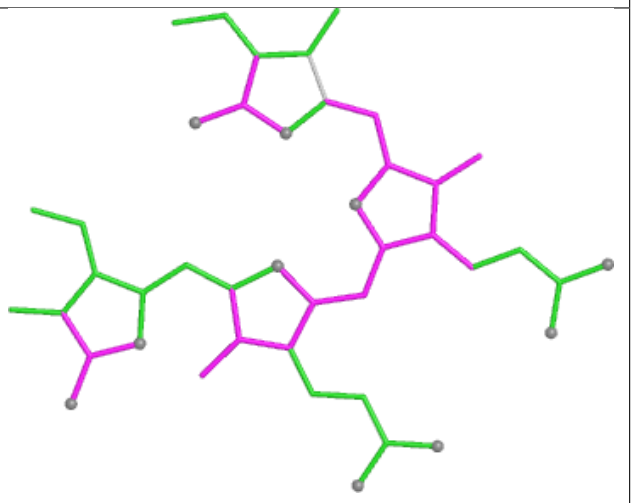
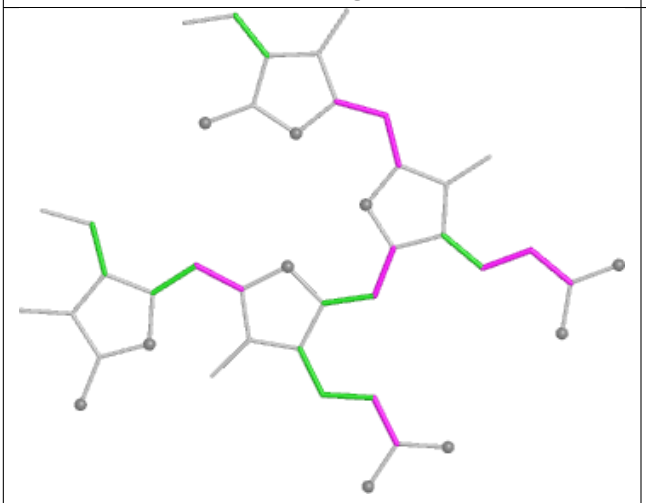


Bond angles



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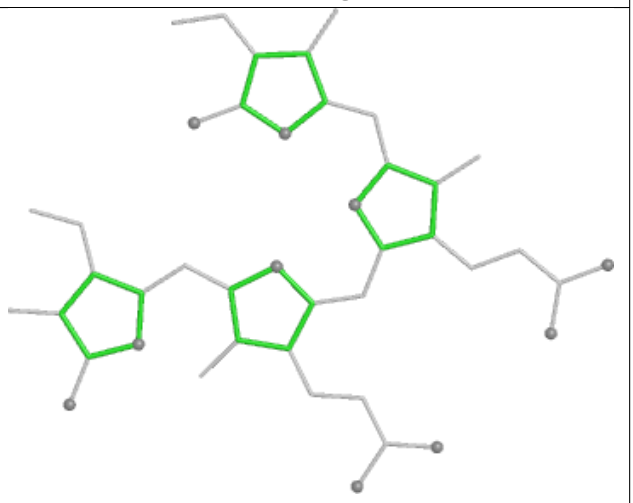
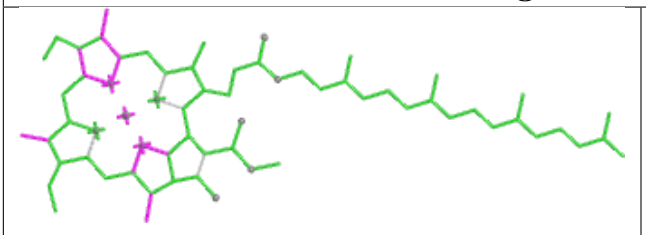


Rings

Ligand CLA bL 607



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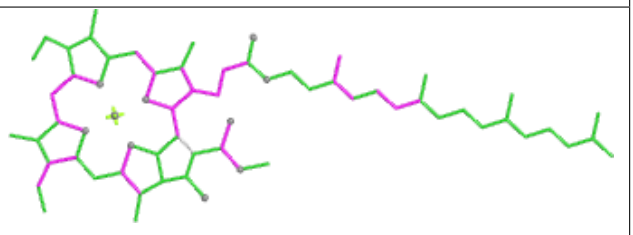

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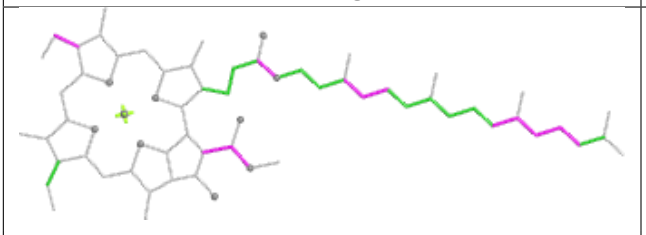

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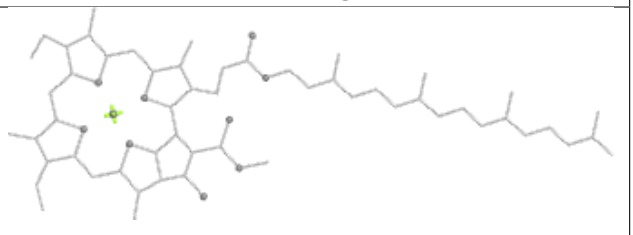
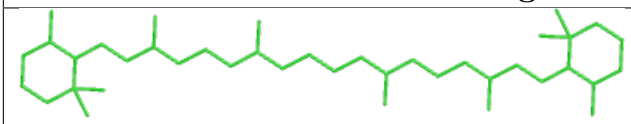


Rings

Ligand BCR c6 602



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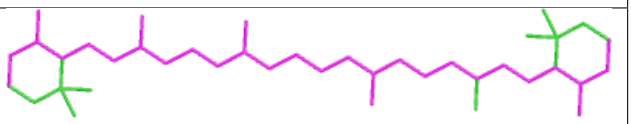

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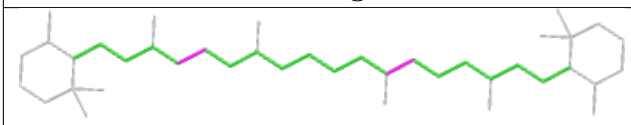

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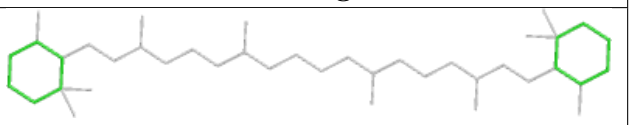
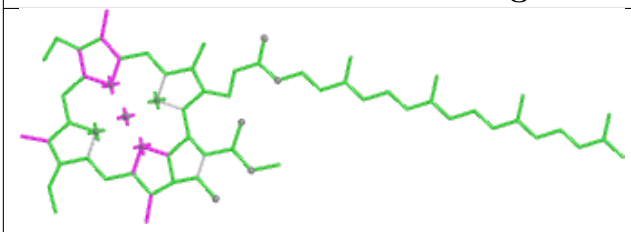


Rings

Ligand CLA BN 826



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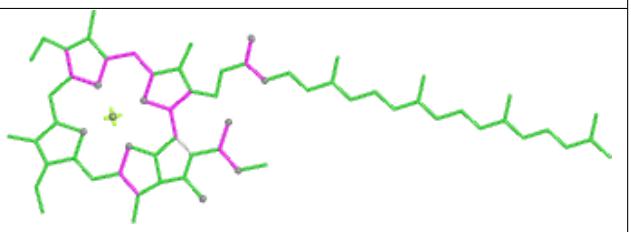

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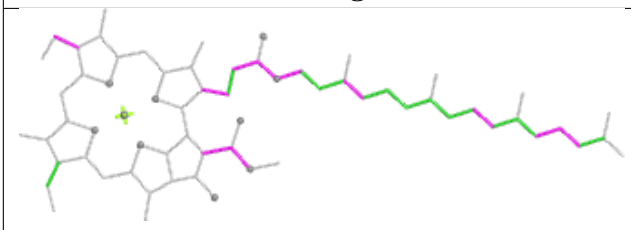

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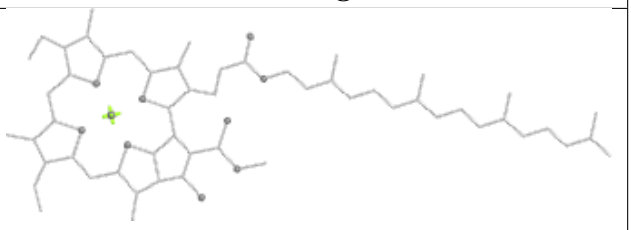
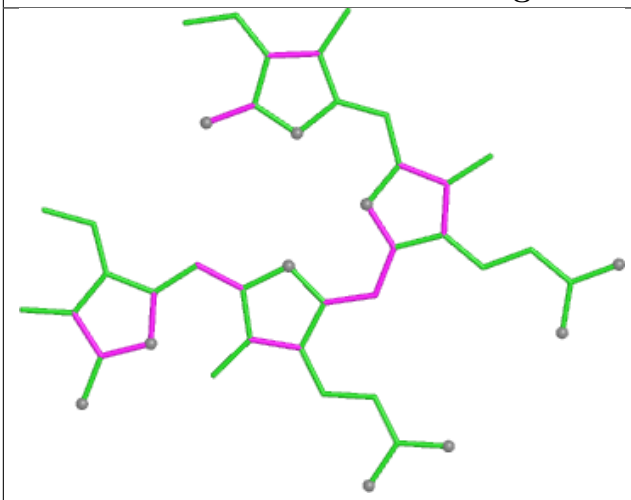


Rings

Ligand PEB TA 203



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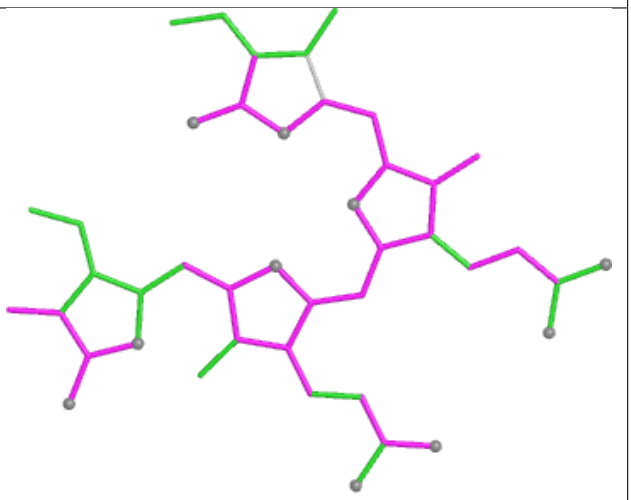
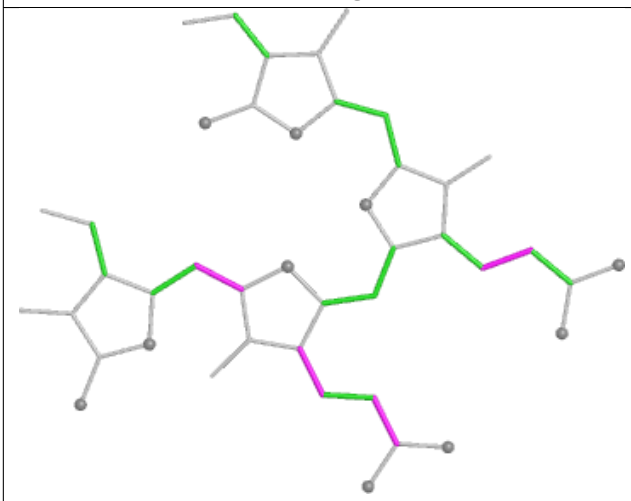


Bond angles



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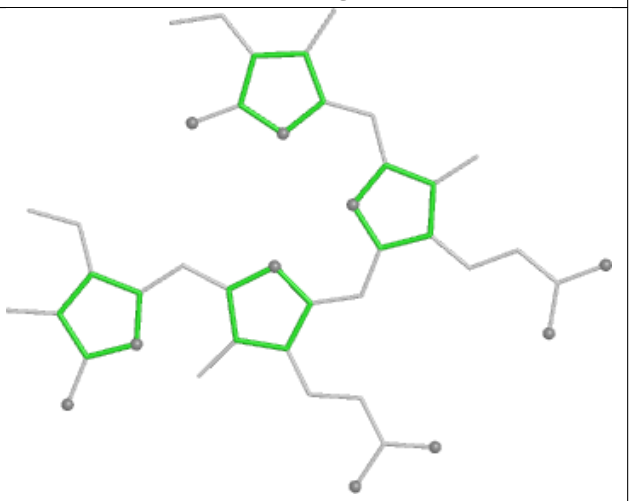
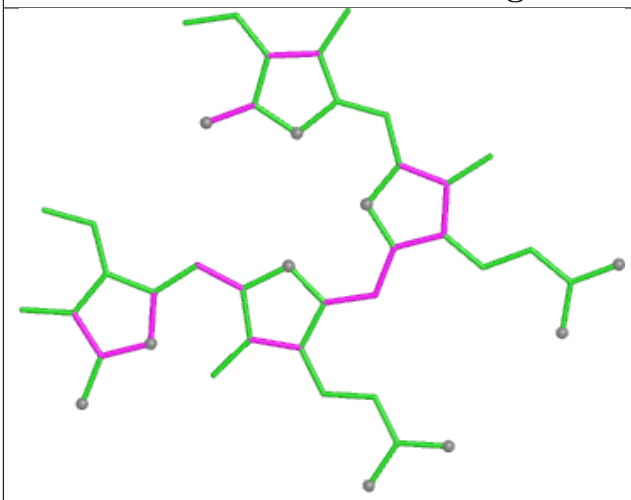


Rings

Ligand PEB KM 203



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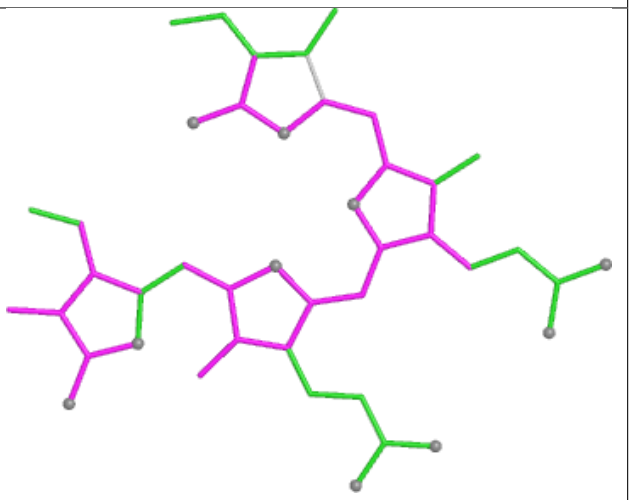
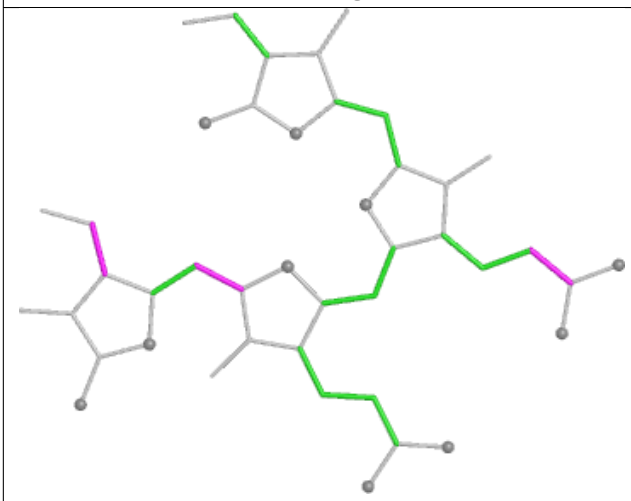


Bond angles



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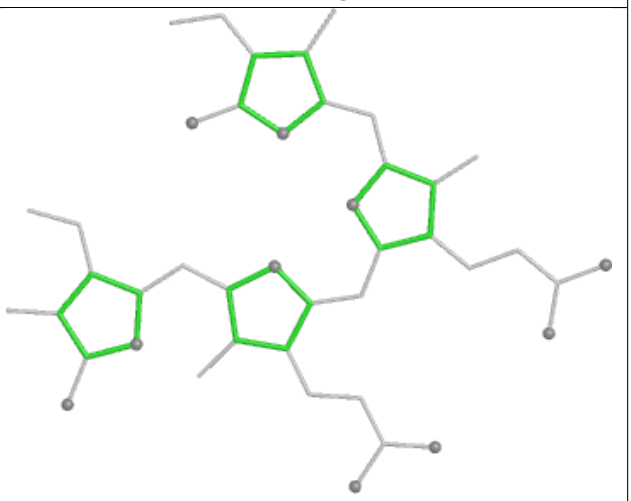
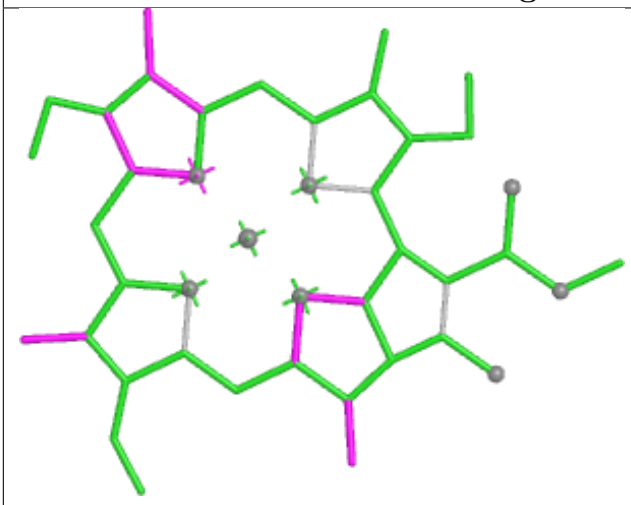


Rings

Ligand CLA 32 306



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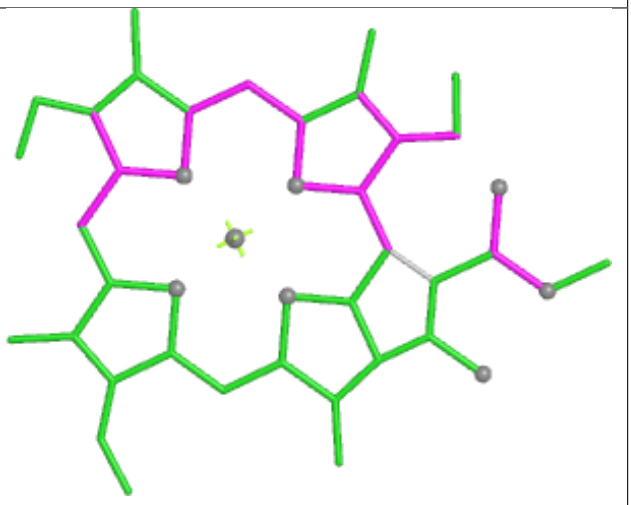
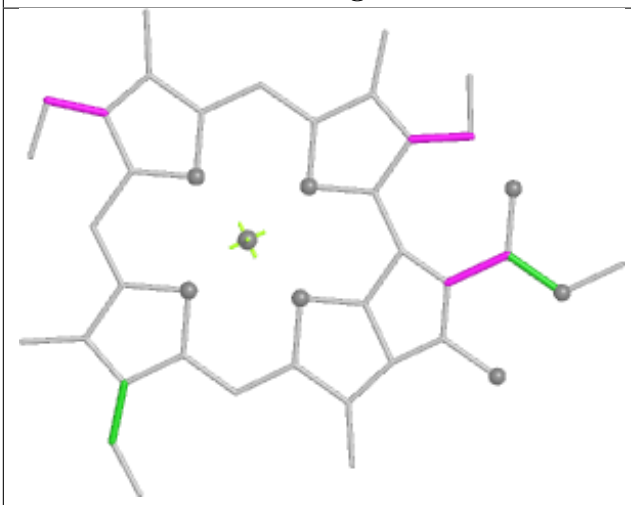


Bond angles

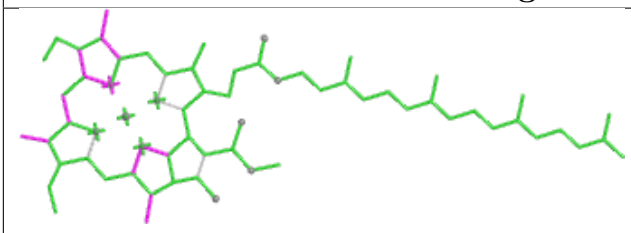


Torsions



Rings

Ligand CLA d6 403



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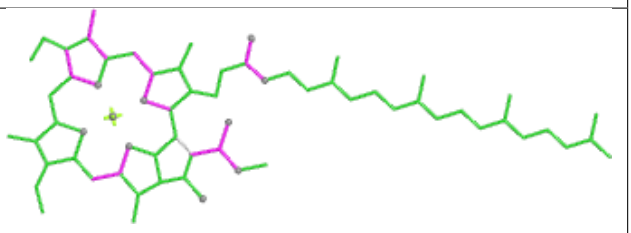
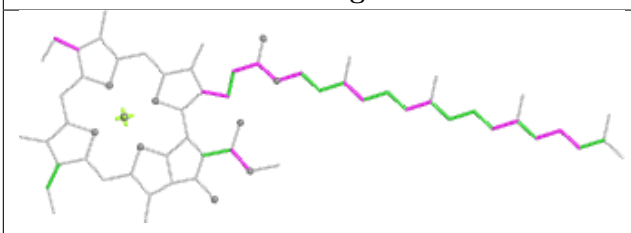


Bond angles



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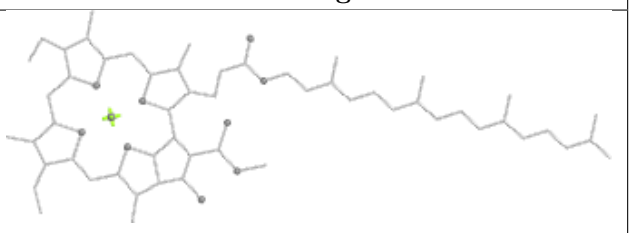
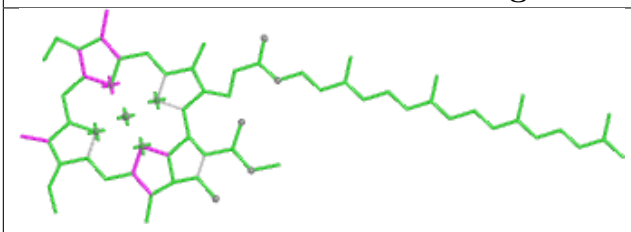


Rings

Ligand CLA AN 802



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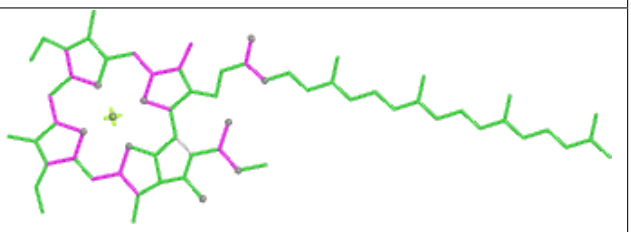
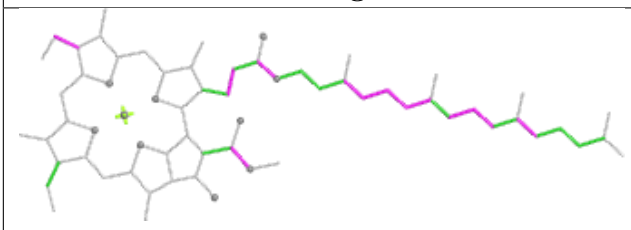
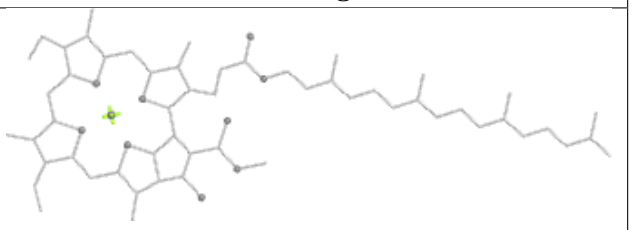


Bond angles

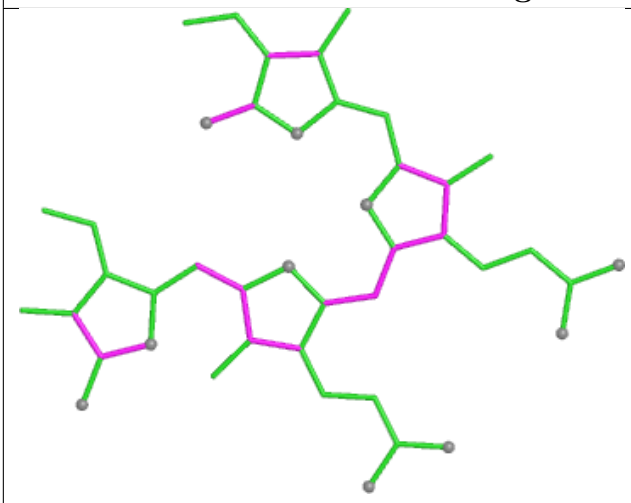


Torsions



Rings

Ligand PEB SQ 202



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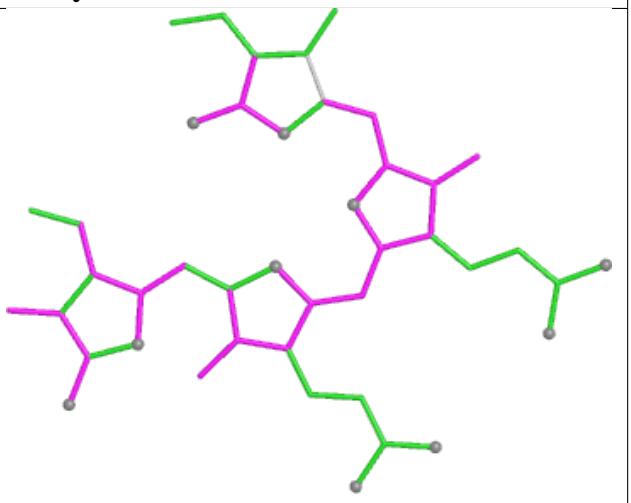

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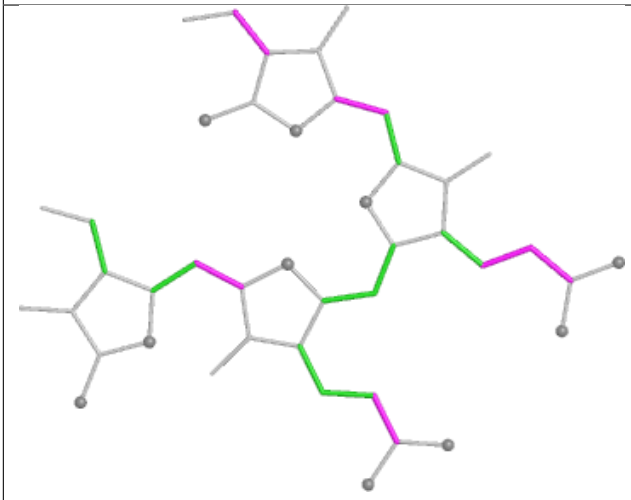

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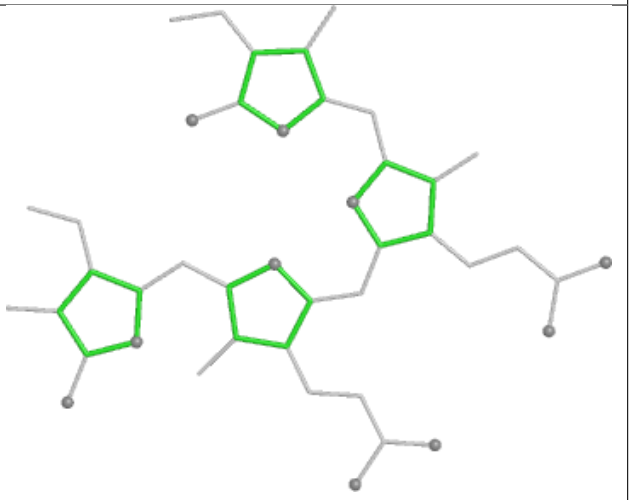
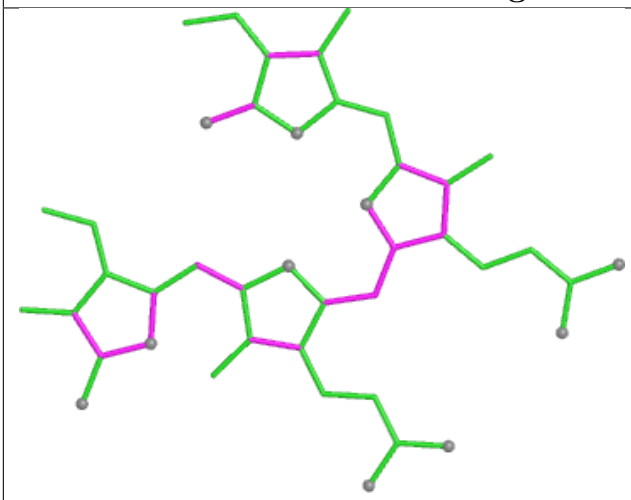


Rings

Ligand PEB TM 202



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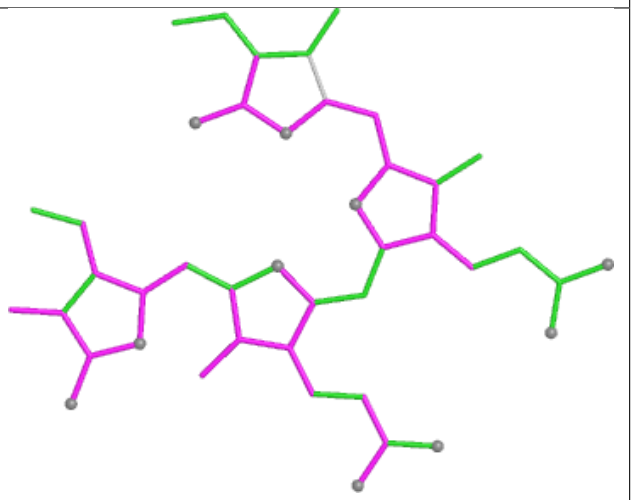

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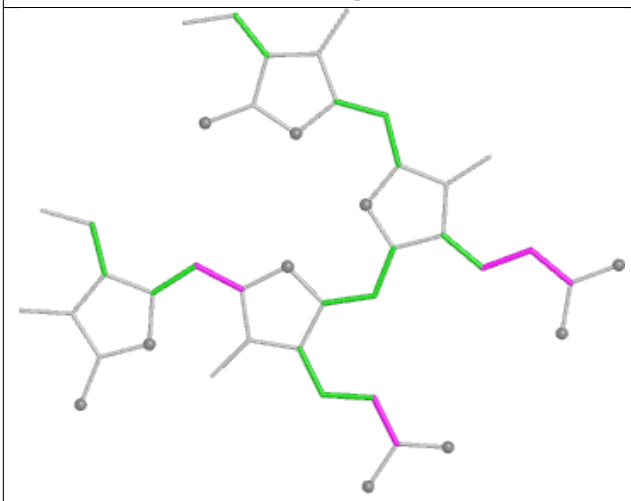

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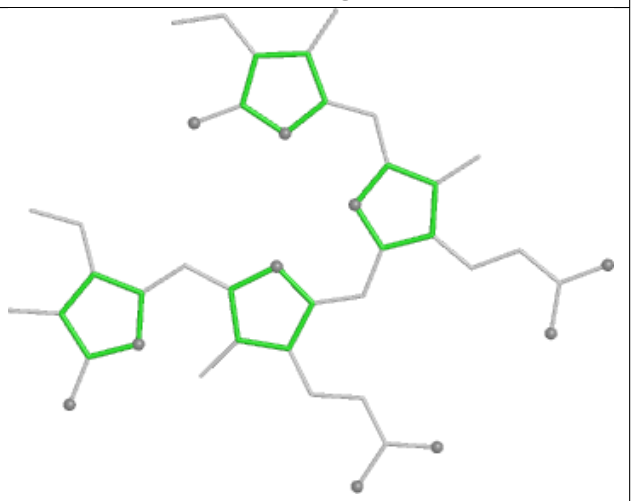
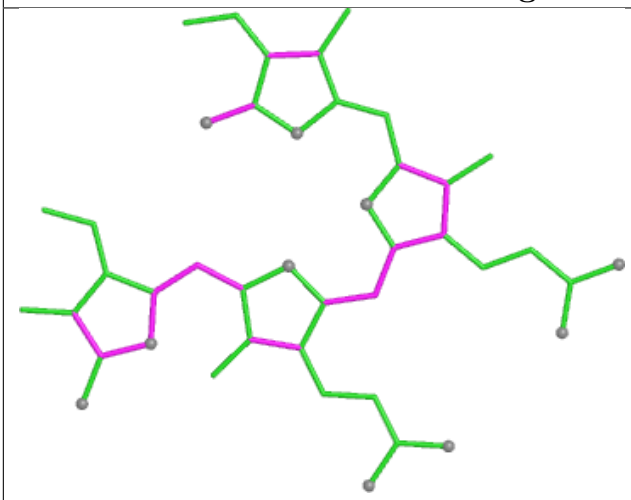


Rings

Ligand PEB jO 201



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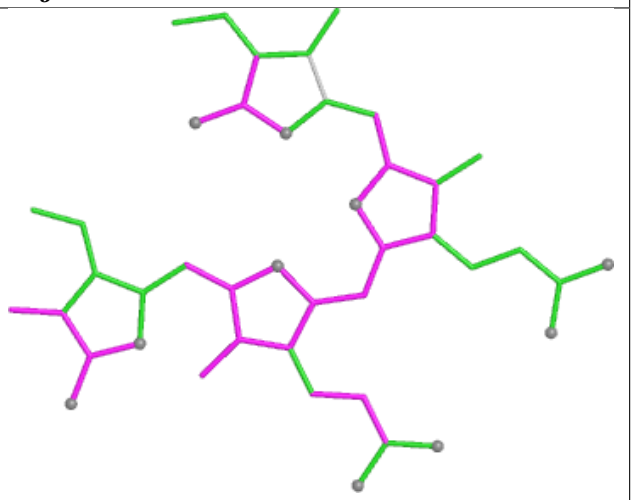

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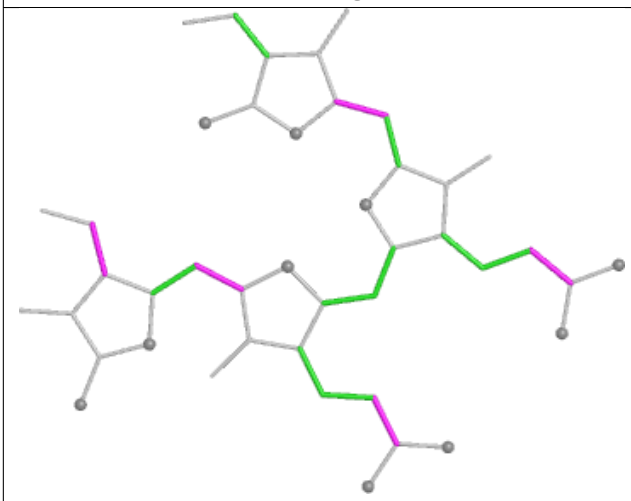

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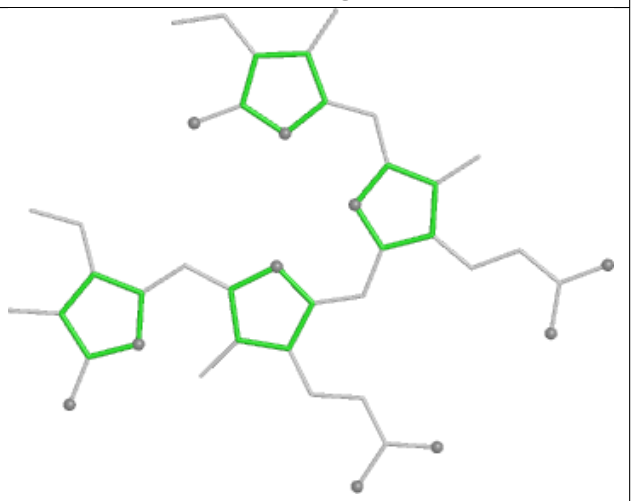
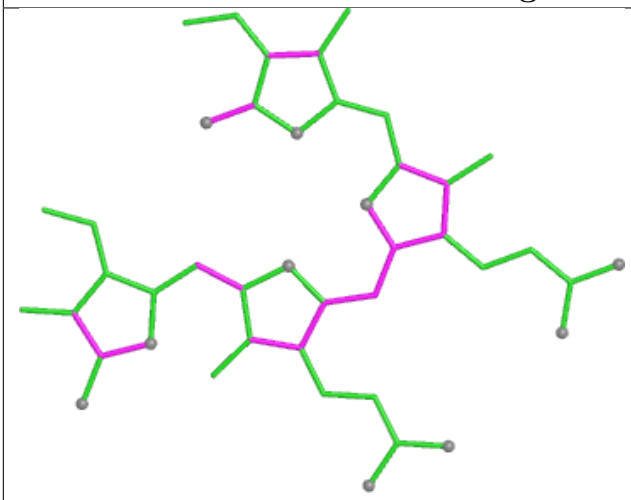


Rings

Ligand PEB x8 202



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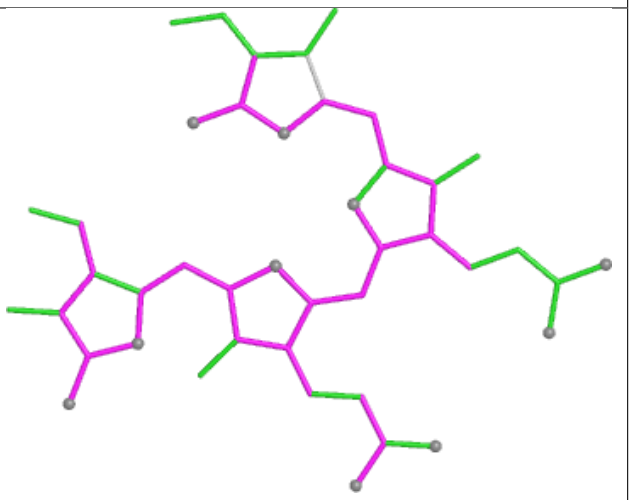

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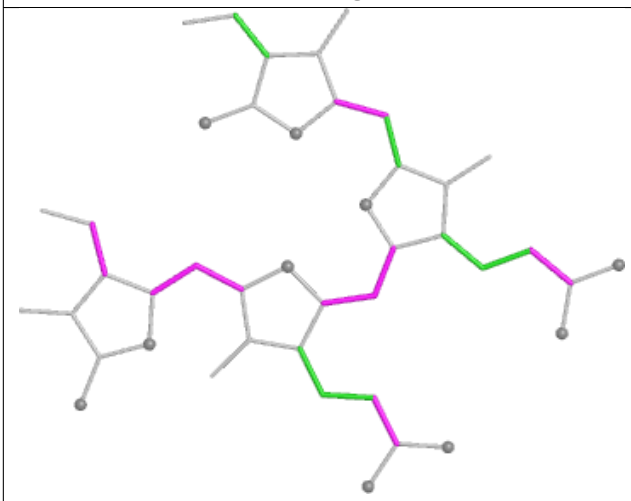

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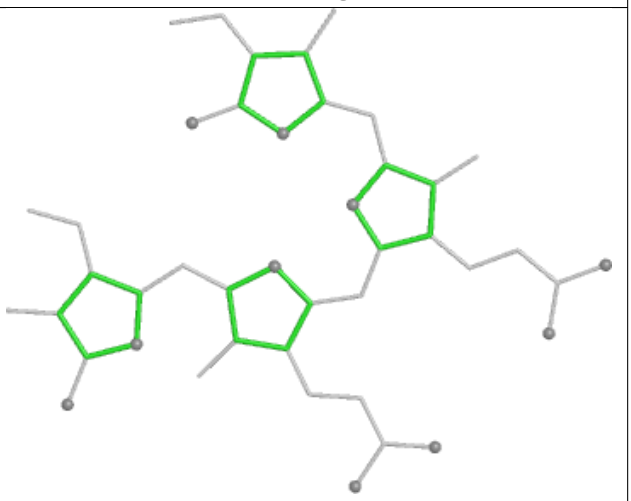
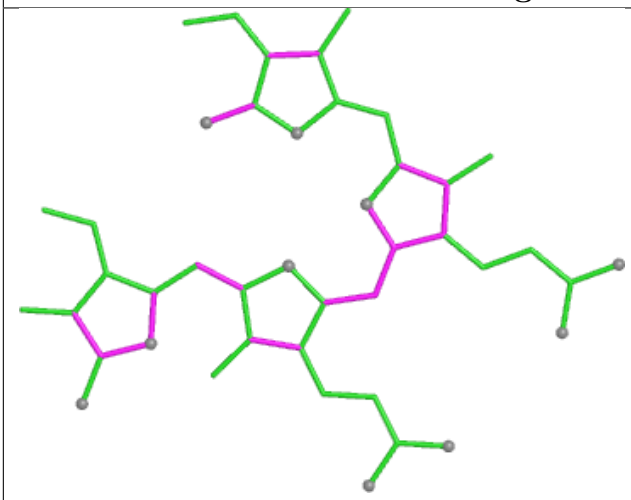


Rings

Ligand PEB DJ 201



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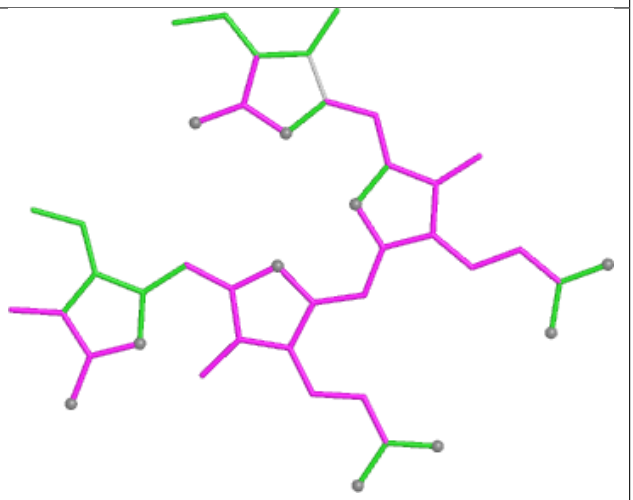

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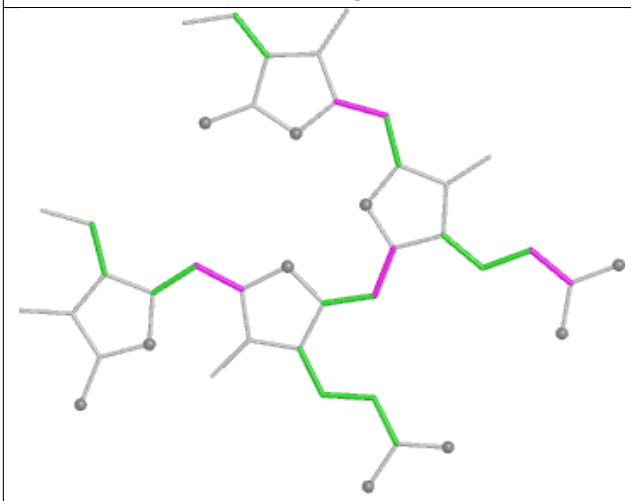

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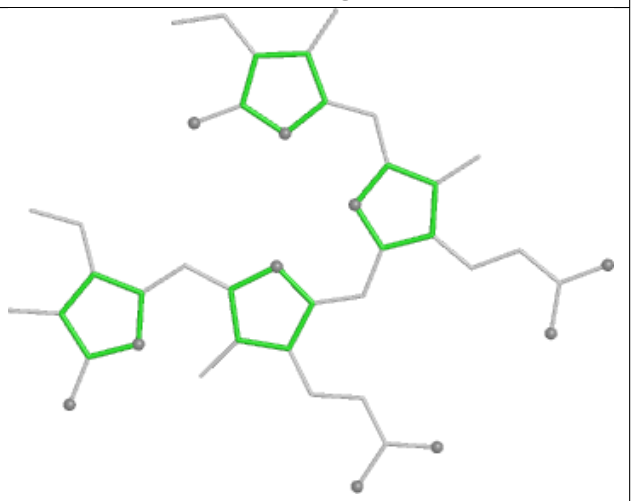
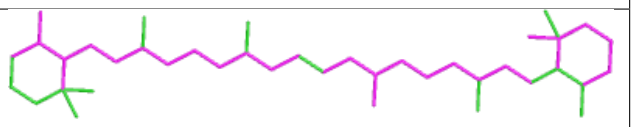


Rings

Ligand BCR BN 843



Bond lengths



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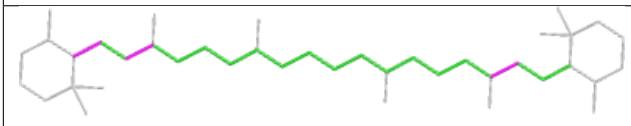

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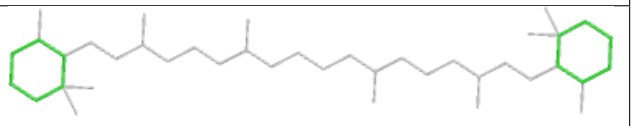
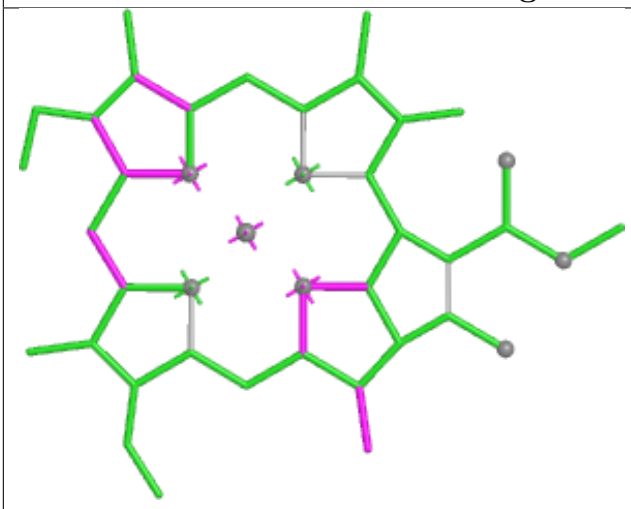


Rings

Ligand CLA 52 608



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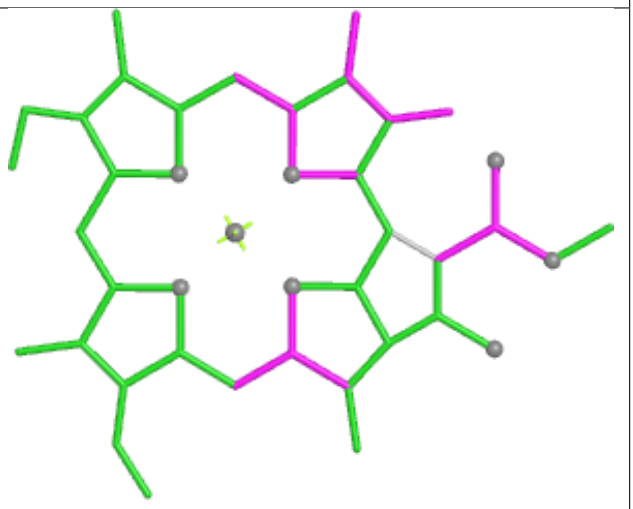

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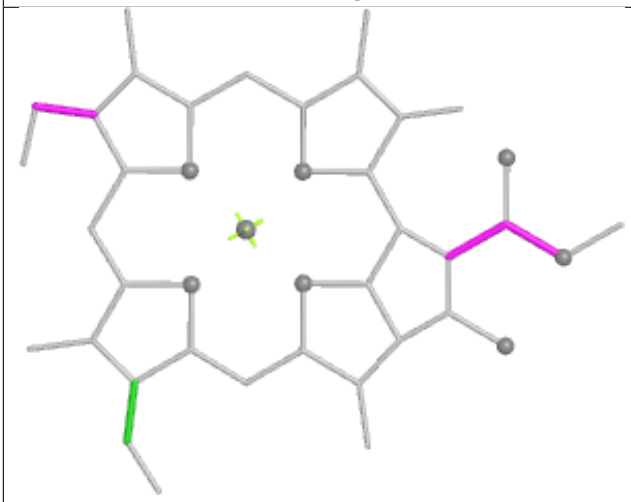

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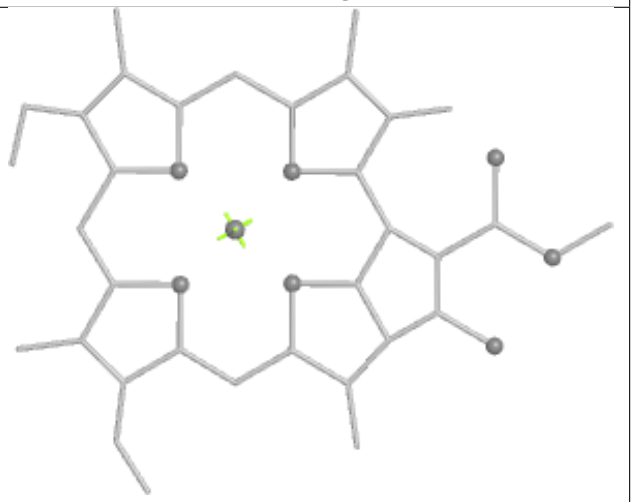
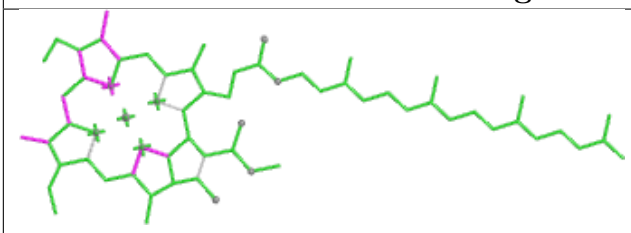


Rings

Ligand CLA 5N 602



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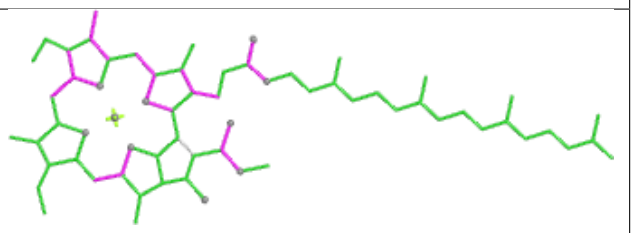

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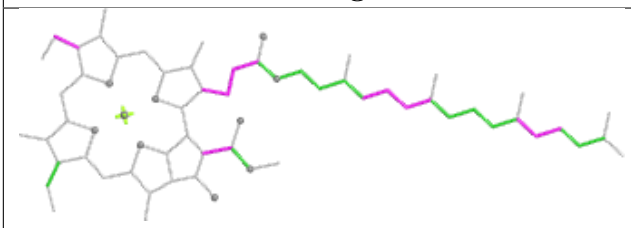

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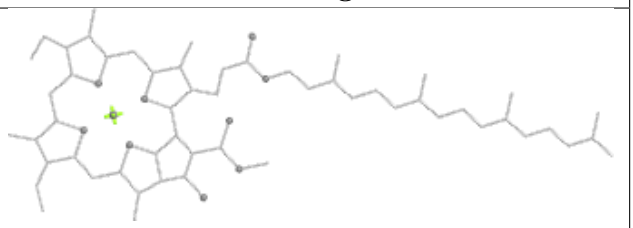
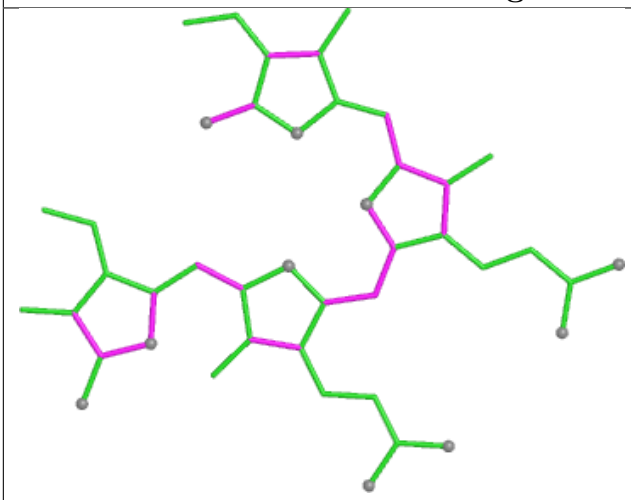


Rings

Ligand PEB HM 201



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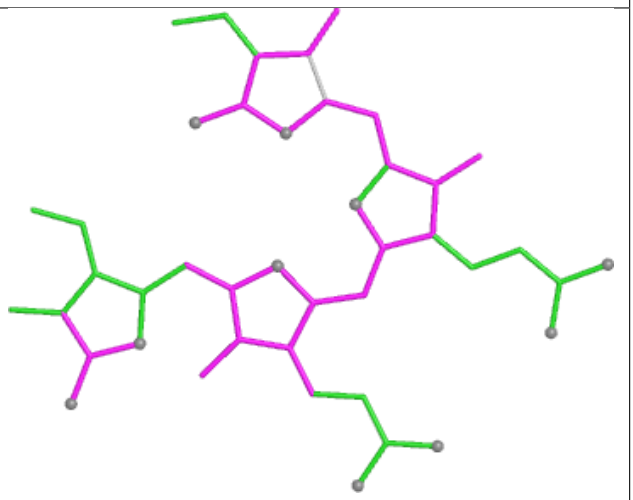

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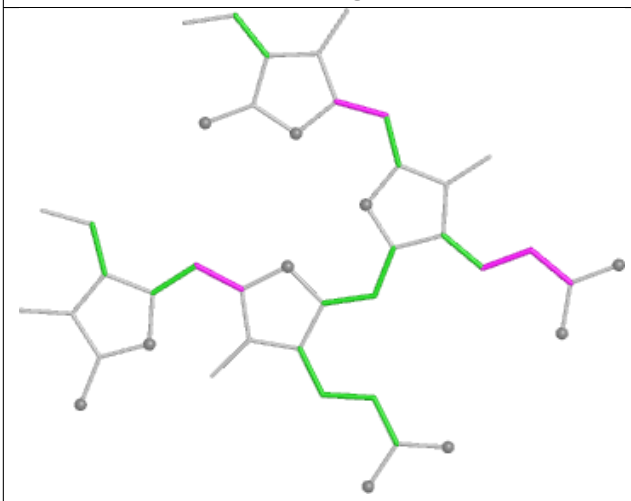

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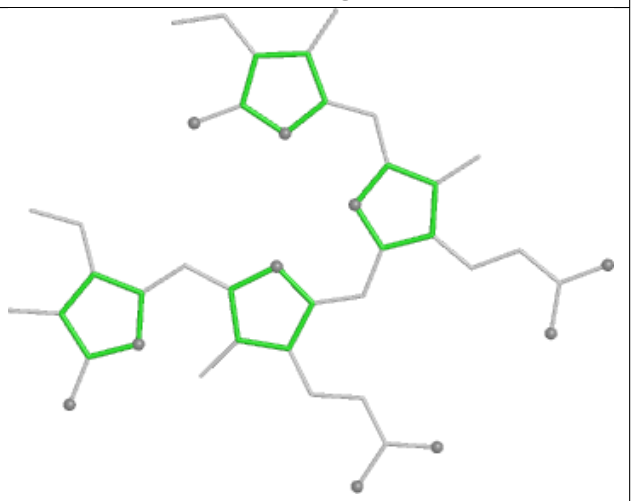
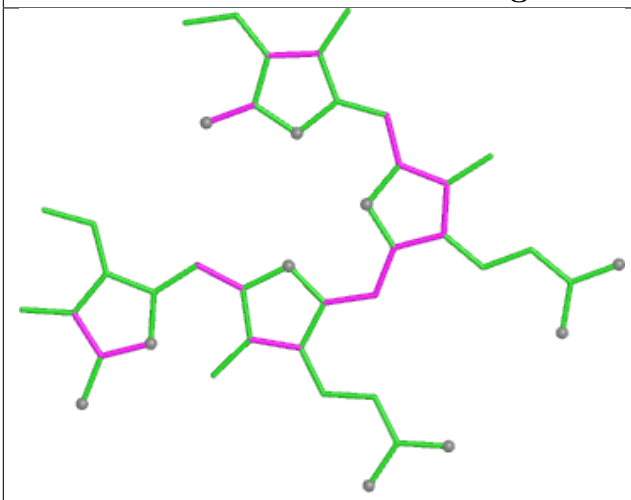


Rings

Ligand PEB UQ 202



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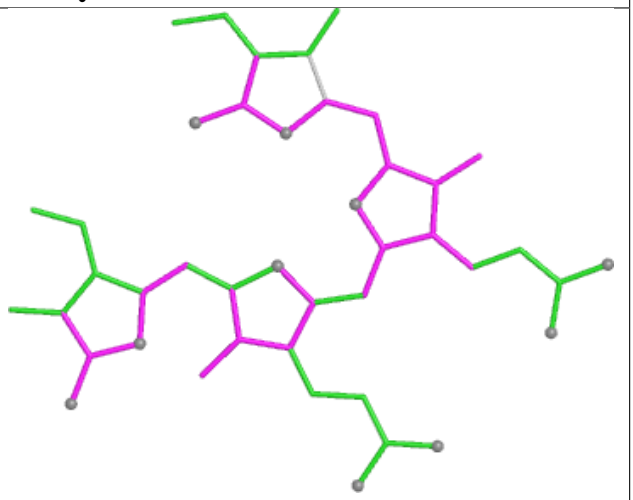

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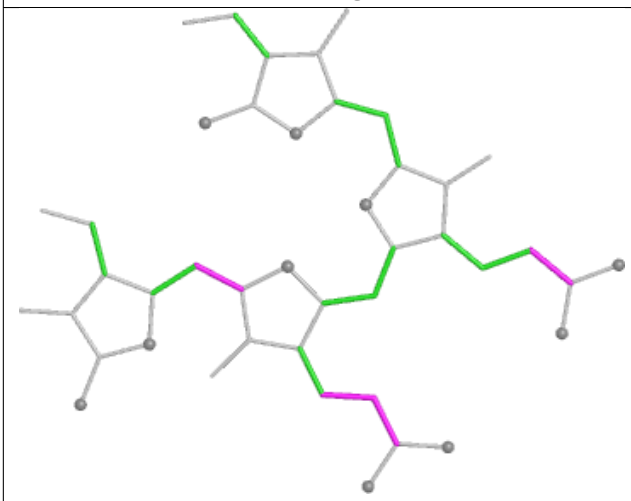

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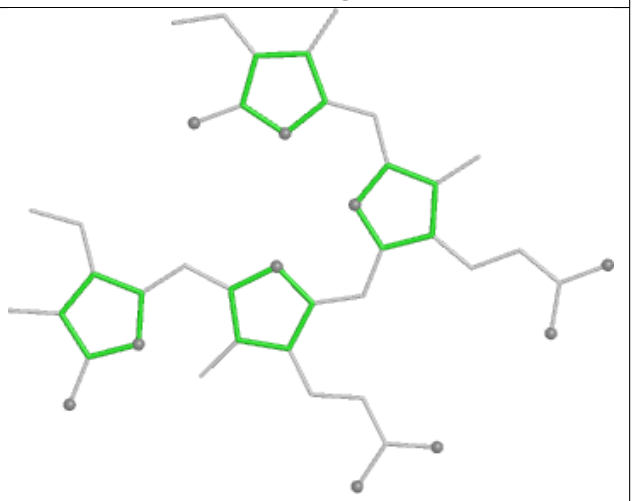
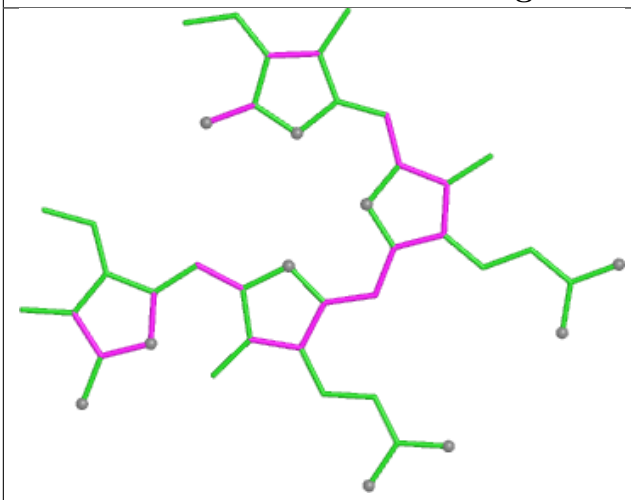


Rings

Ligand PEB A7 201



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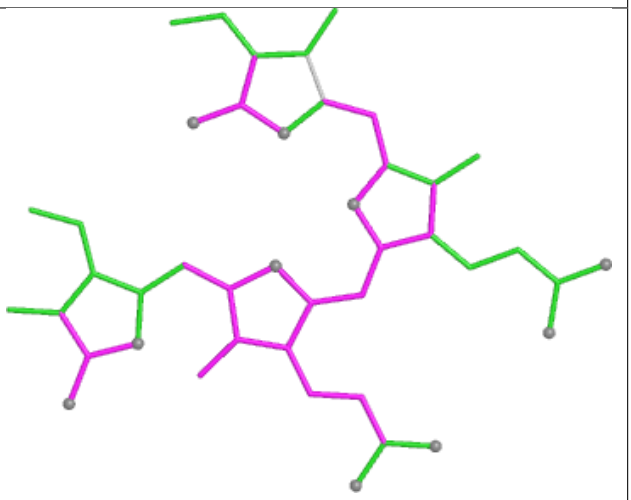
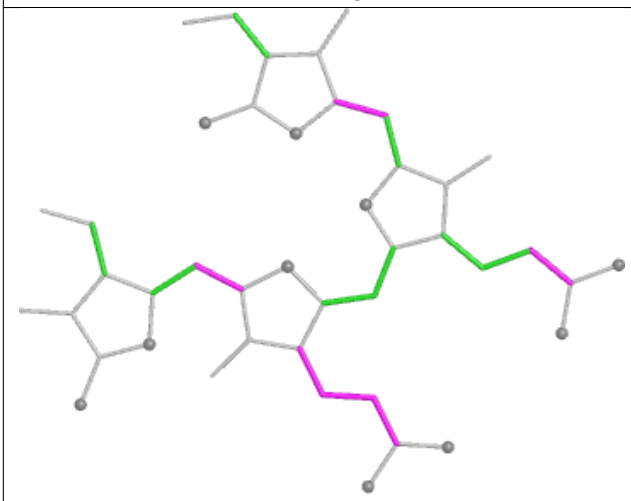


Bond angles



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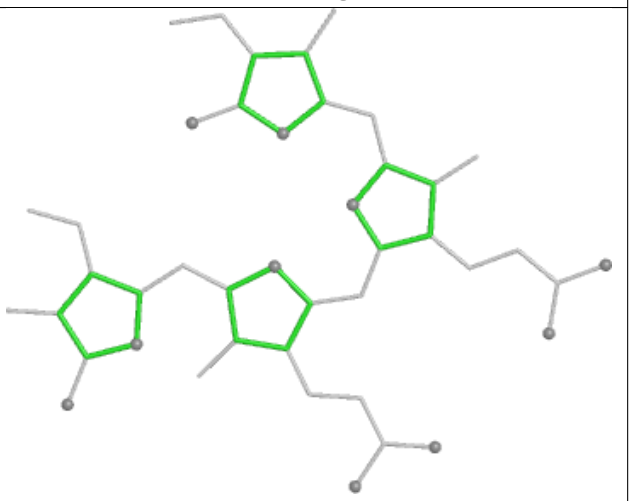
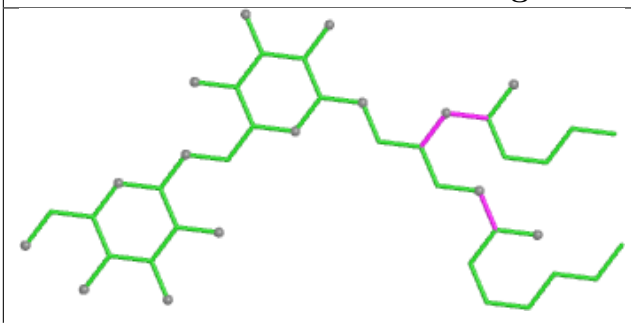


Rings

Ligand DGD C6 504



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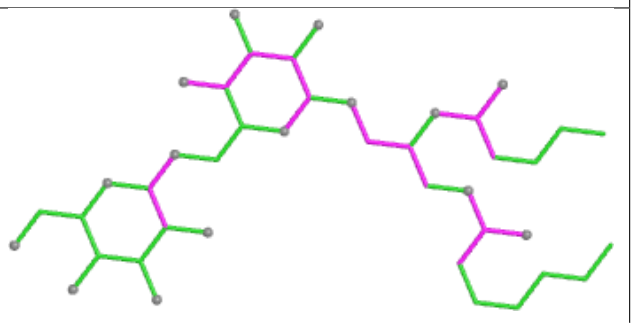
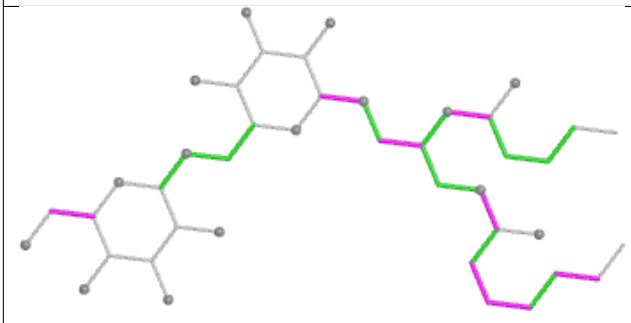


Bond angles



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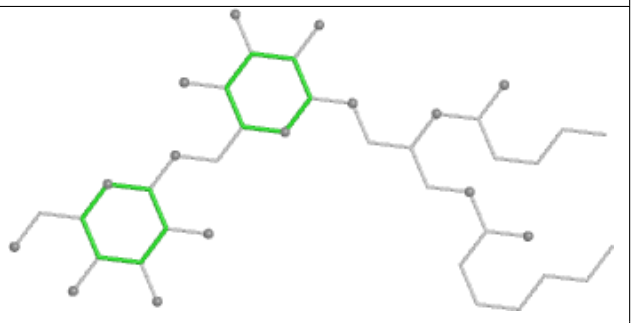
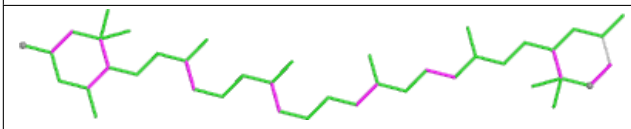


Rings

Ligand ZEX 82 310



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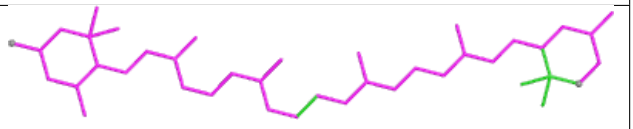
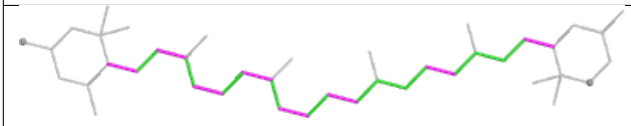


Bond angles



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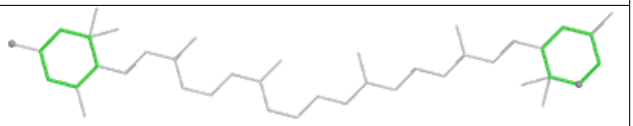
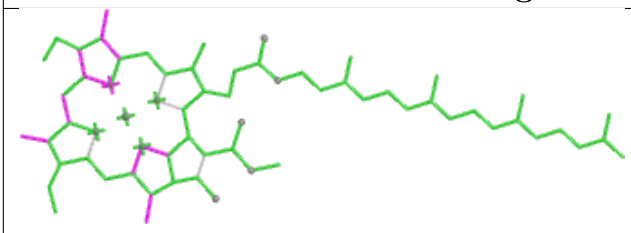


Rings

Ligand CLA B6 609



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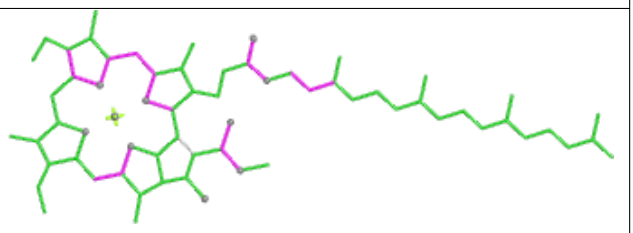
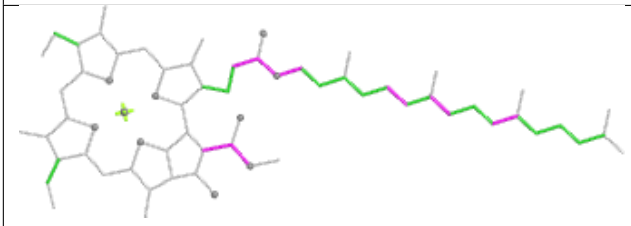


Bond angles



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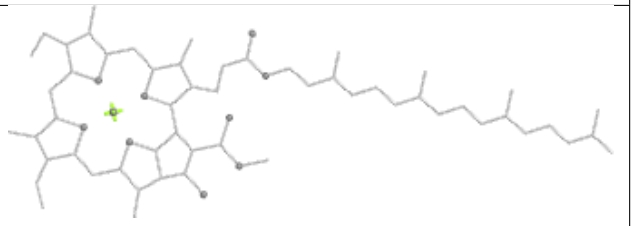
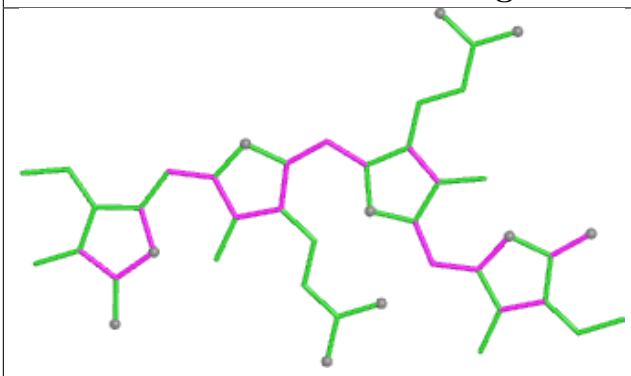
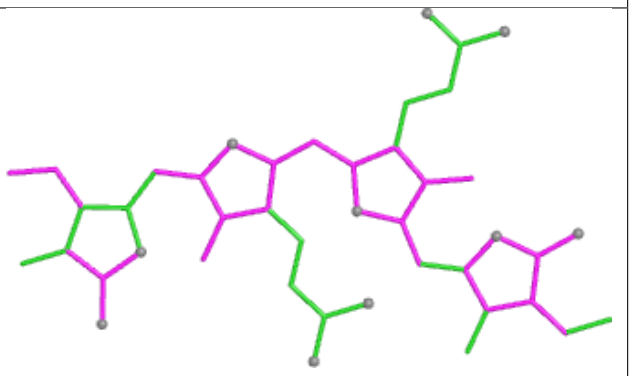


Rings

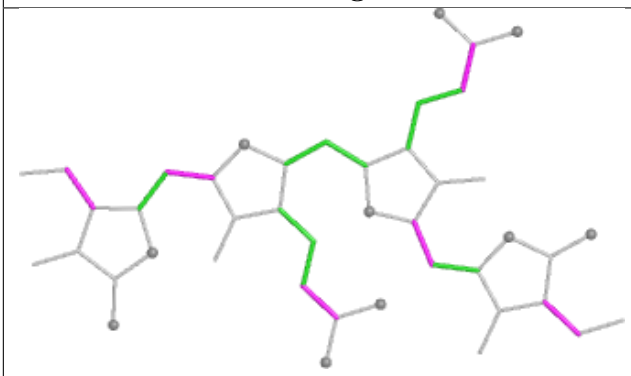
Ligand CYC MO 1001



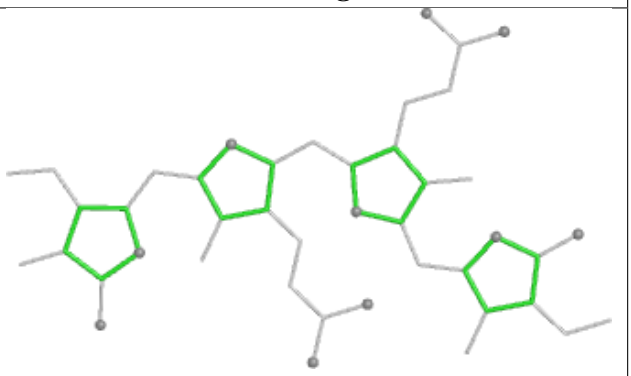
Bond lengths



Bond angles

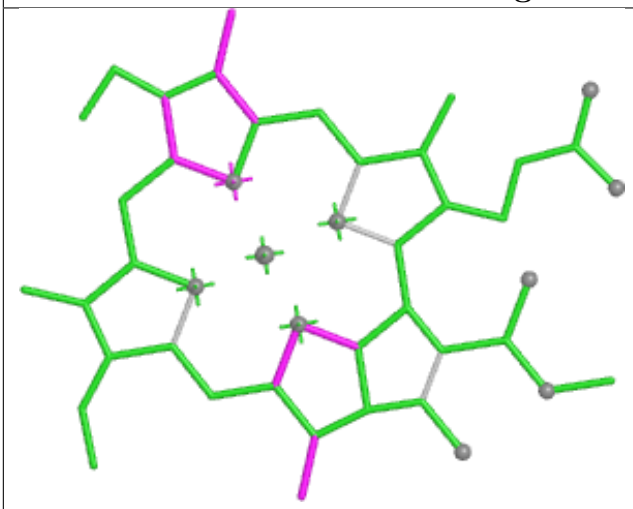


Torsions



Rings

Ligand CLA 2N 304



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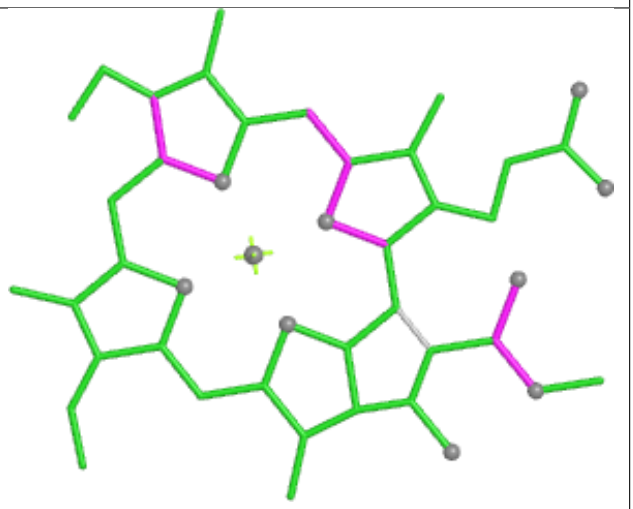

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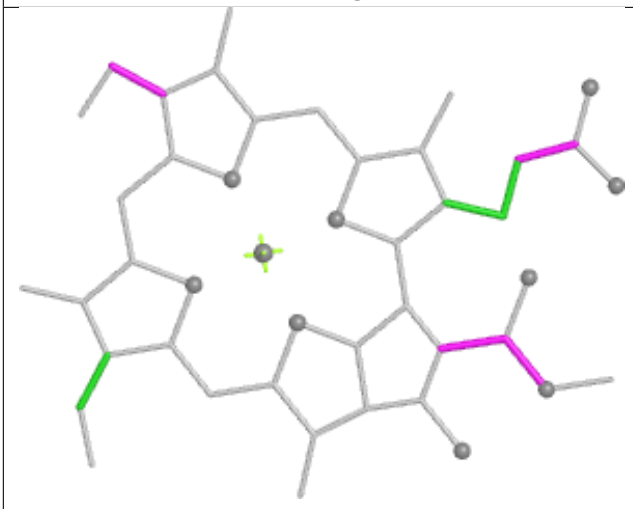
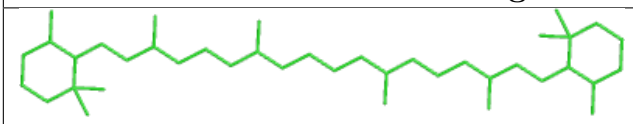


Torsions



Rings

Ligand BCR BN 803



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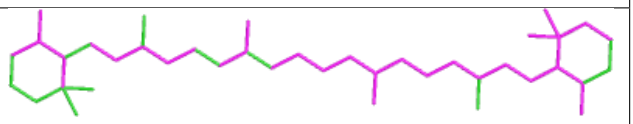

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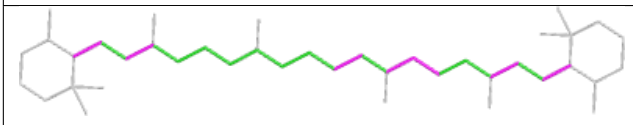

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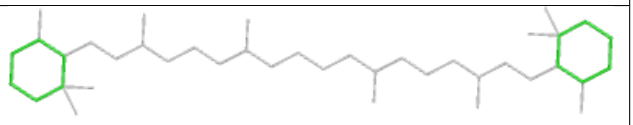
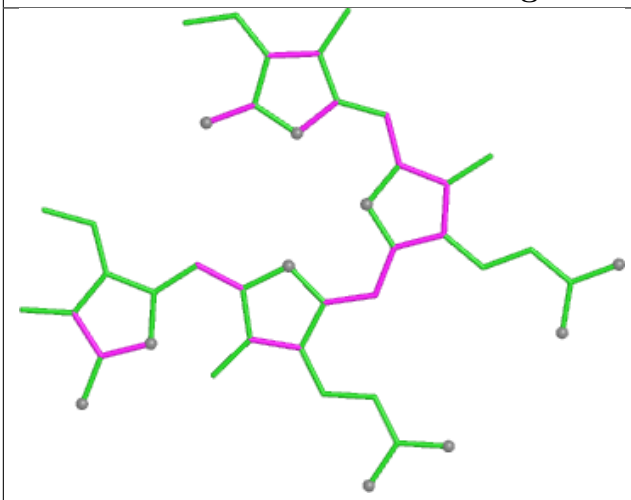


Rings

Ligand PEB e1 202



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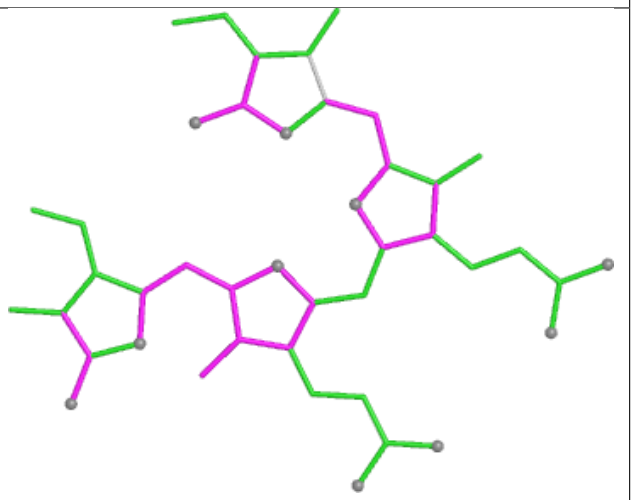

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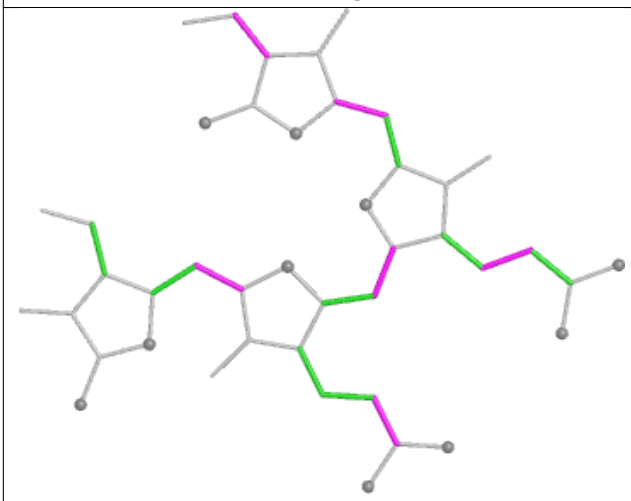

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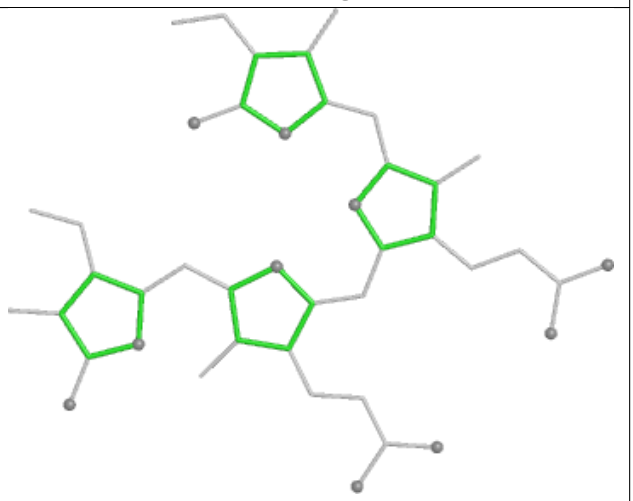
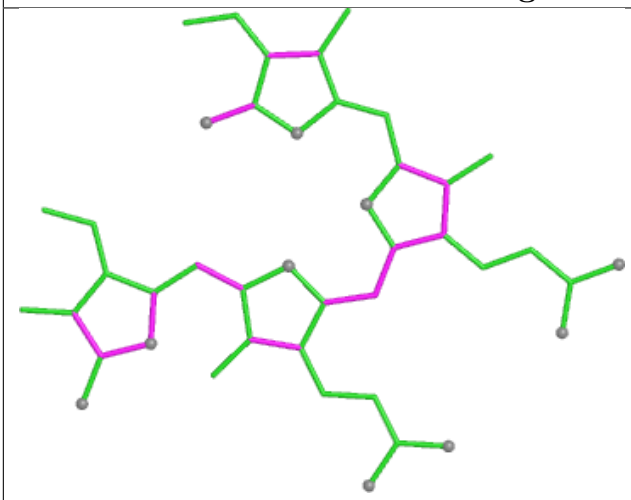


Rings

Ligand PEB SJ 201



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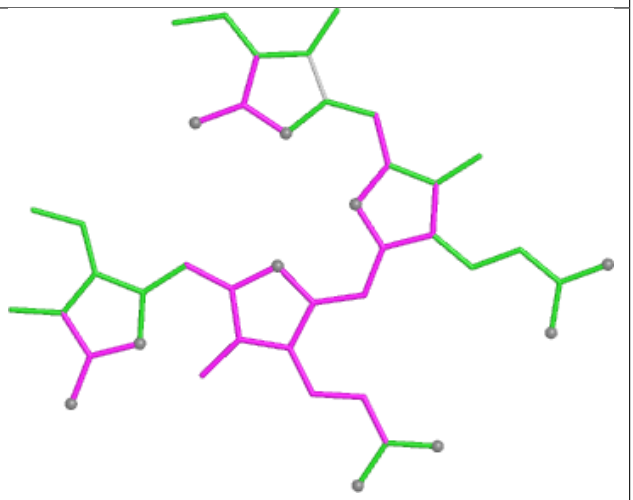
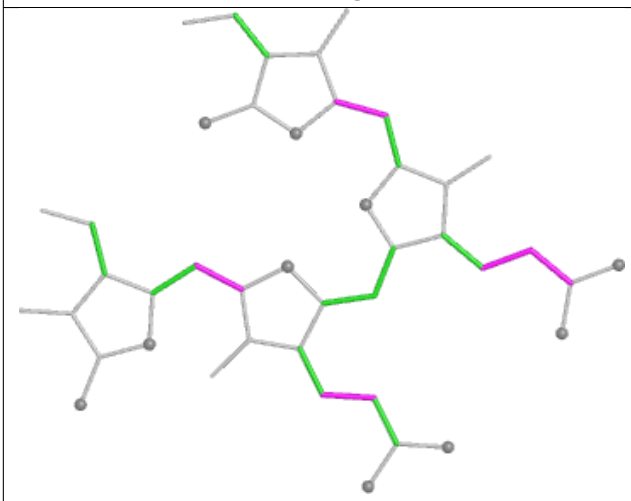


Bond angles



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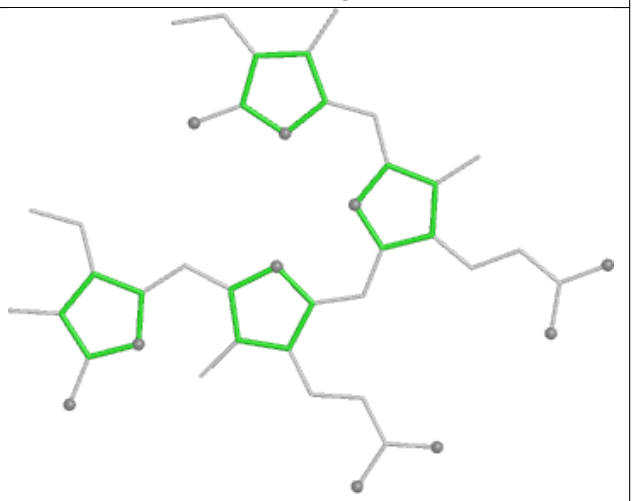
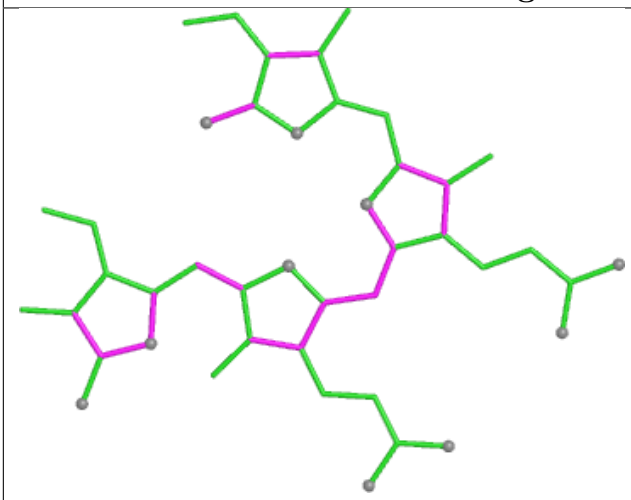


Rings

Ligand PEB Z5 305



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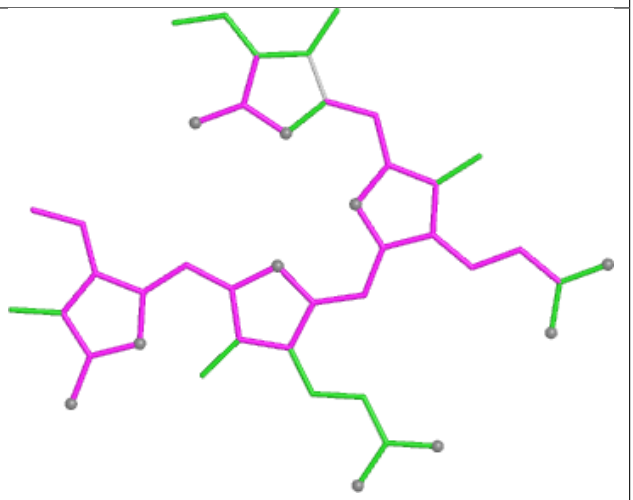

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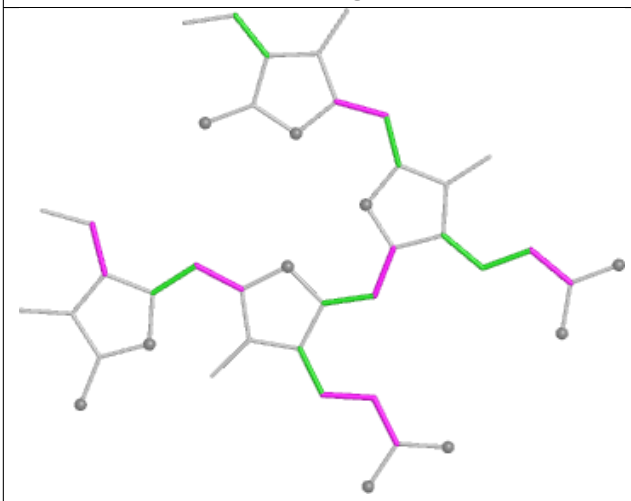

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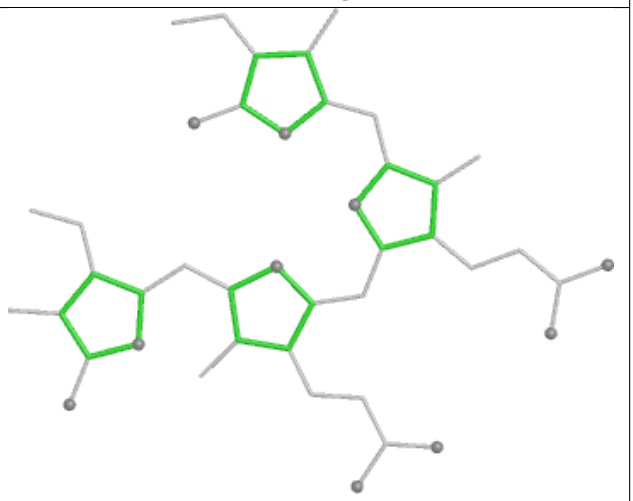
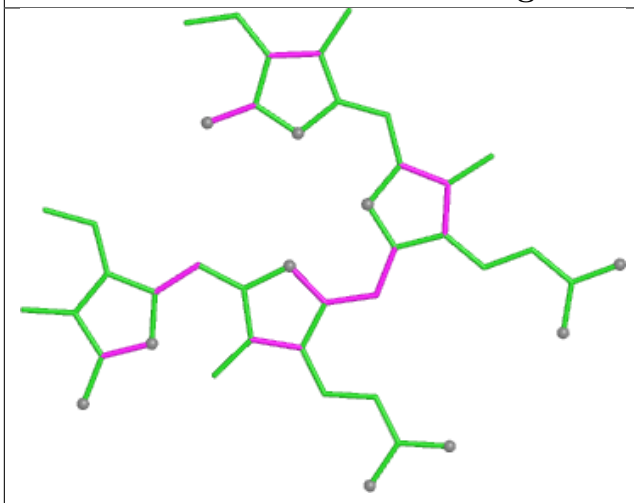


Rings

Ligand PEB T7 202



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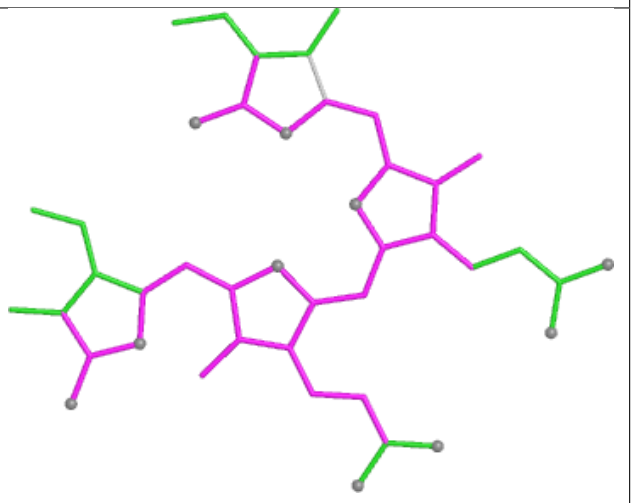

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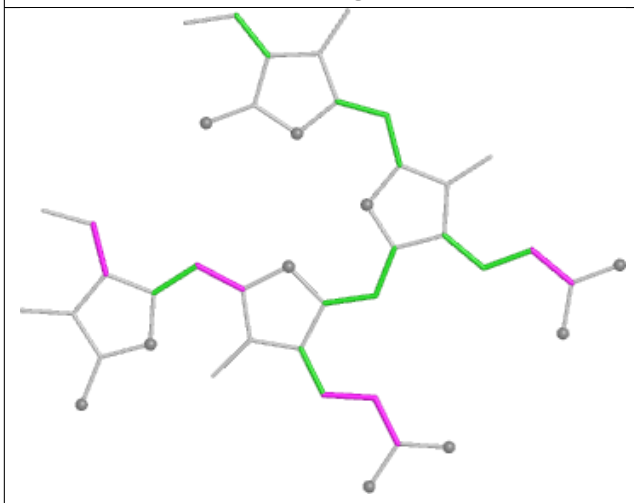

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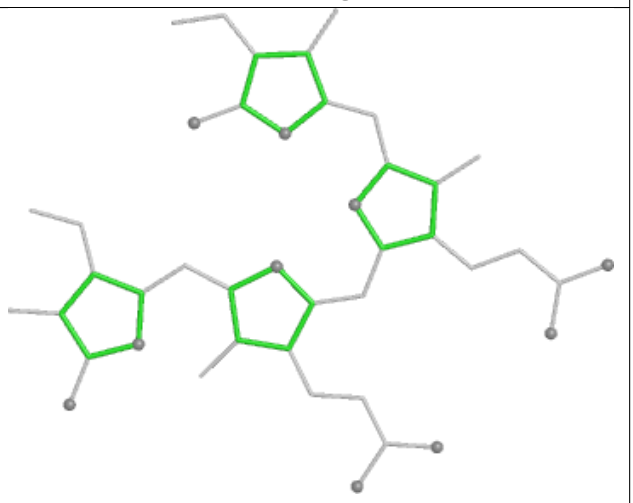
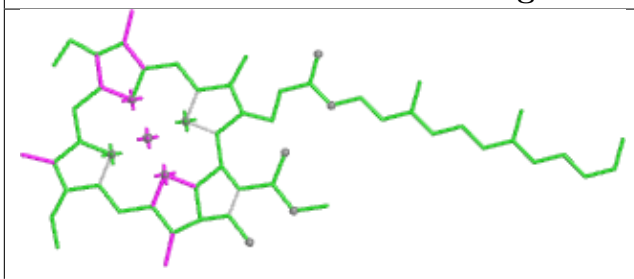


Rings

Ligand CLA bL 619



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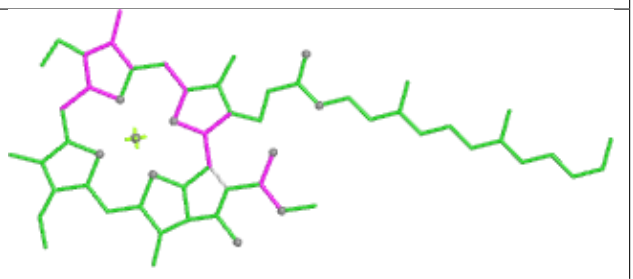

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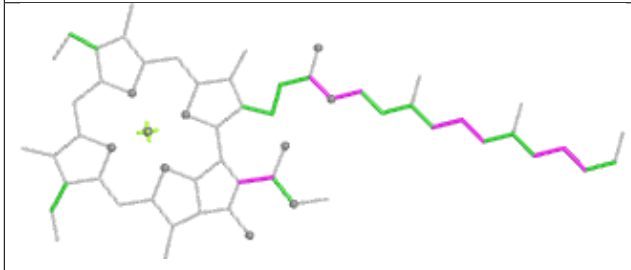

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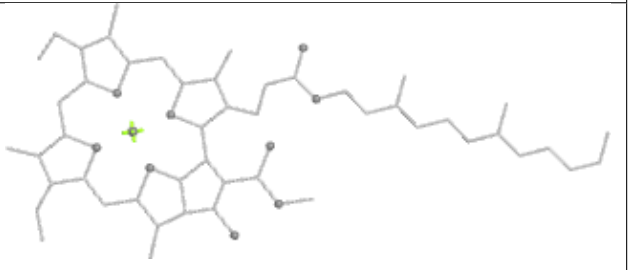
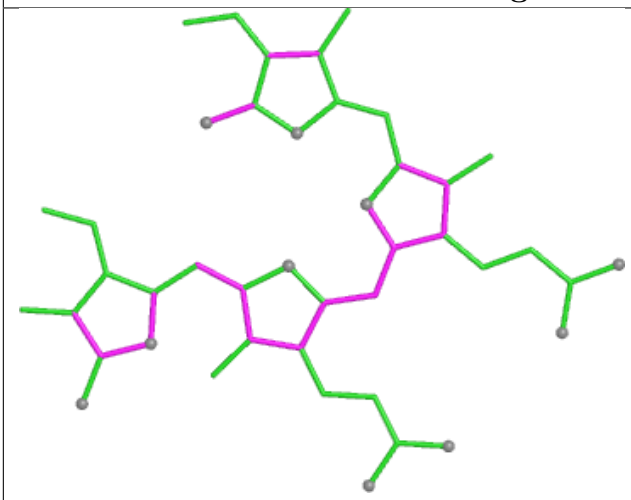


Rings

Ligand PEB UD 201



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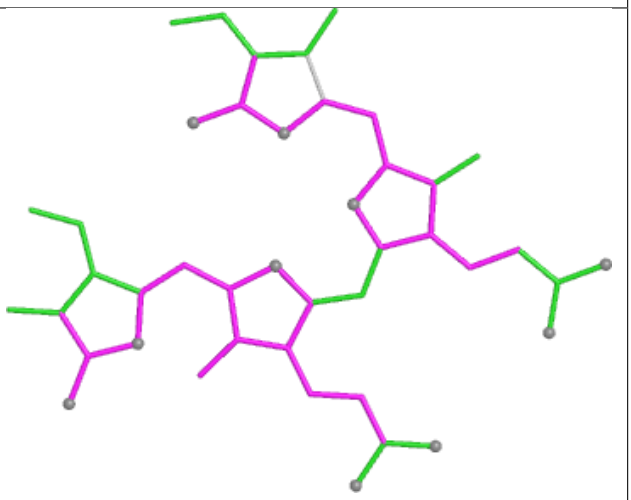

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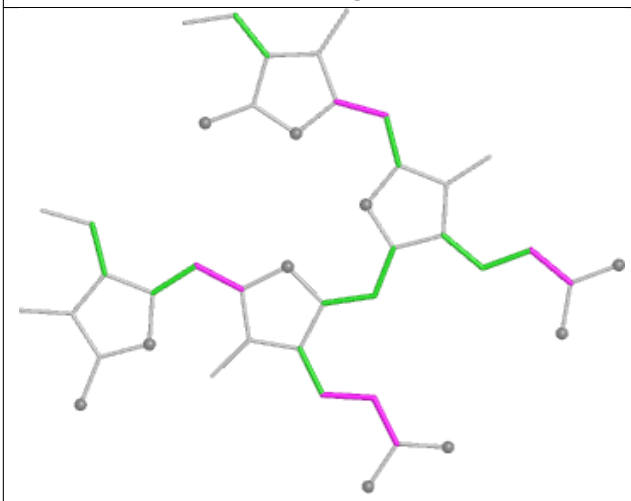

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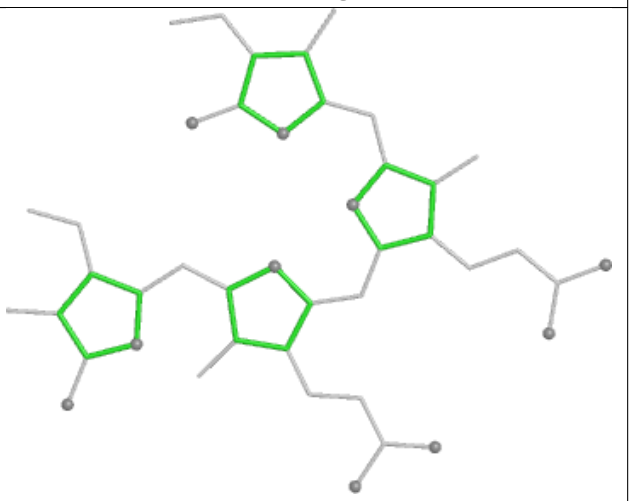
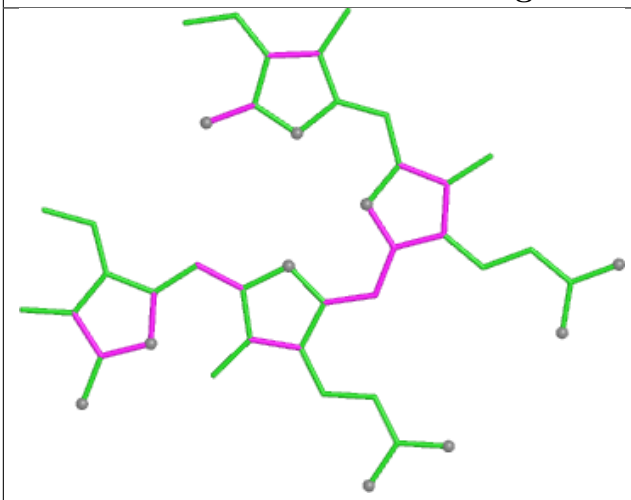


Rings

Ligand PEB A4 304



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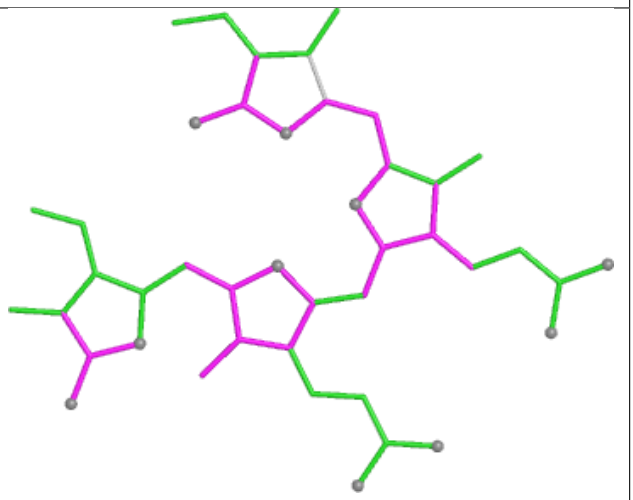

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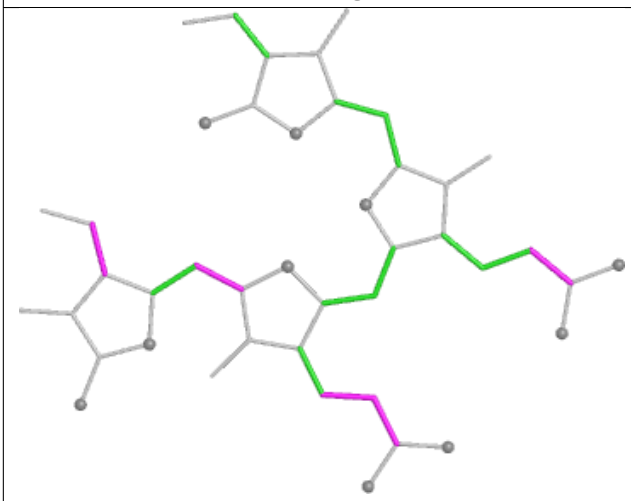

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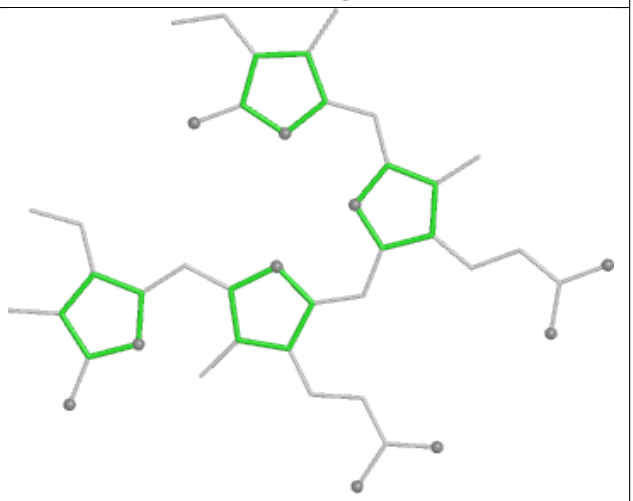
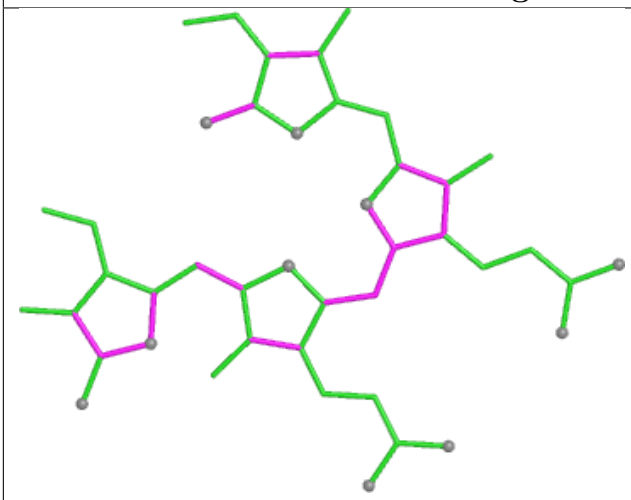


Rings

Ligand PEB DP 202



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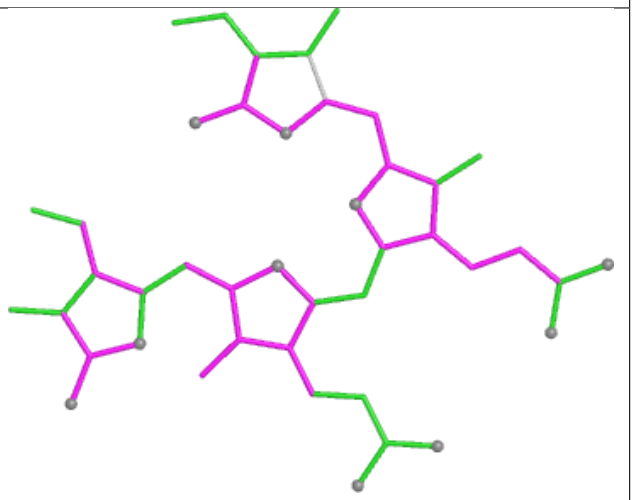

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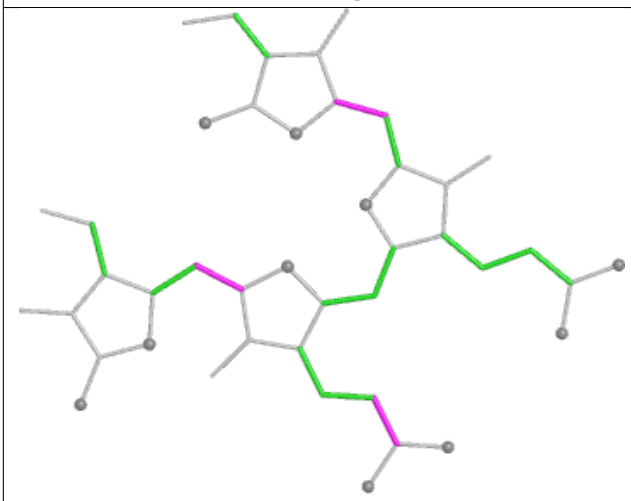

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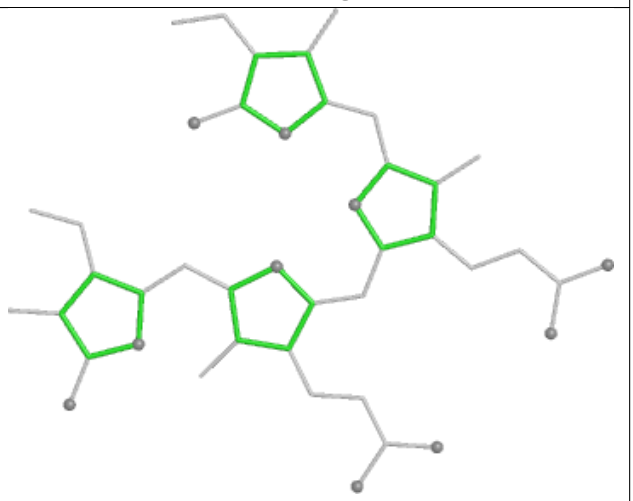
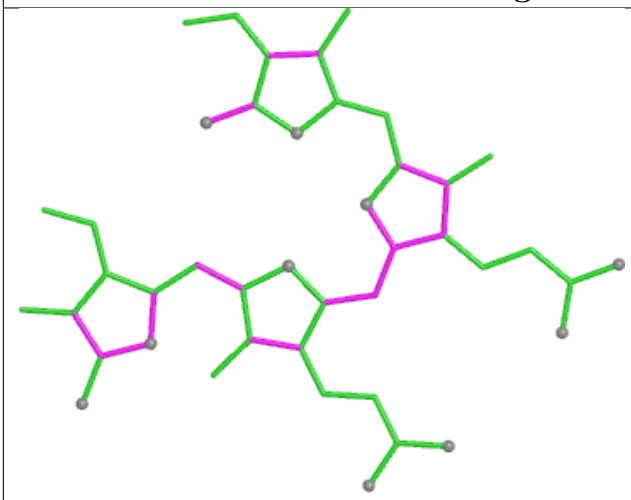


Rings

Ligand PEB bG 201



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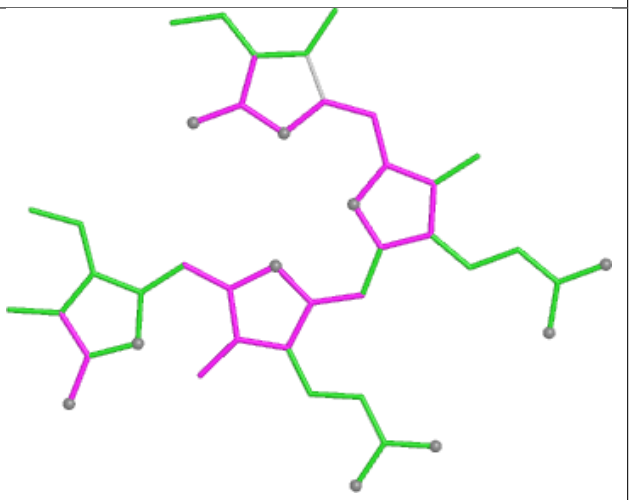

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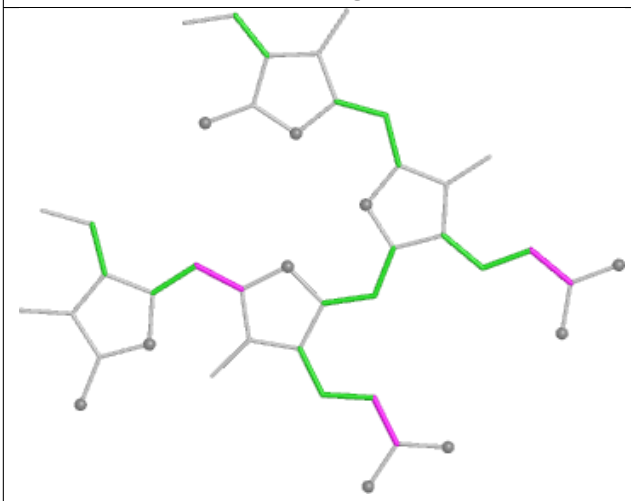

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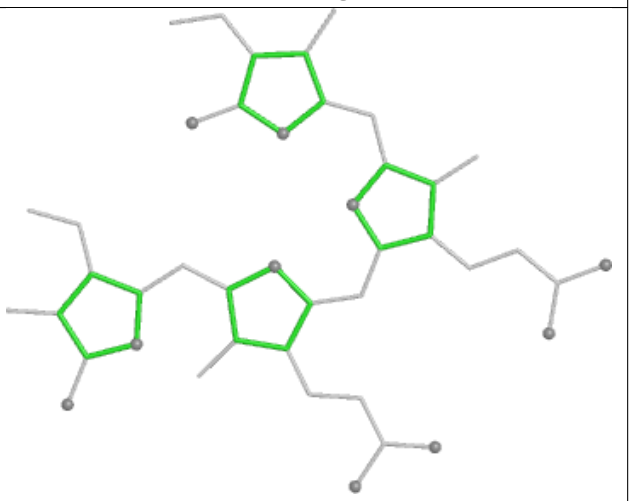
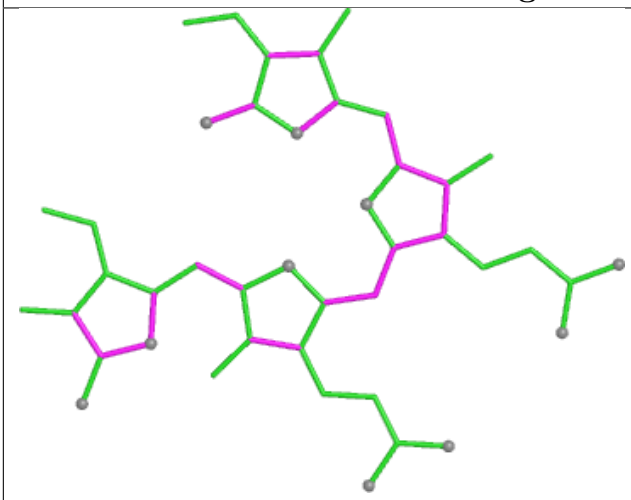


Rings

Ligand PEB lH 201



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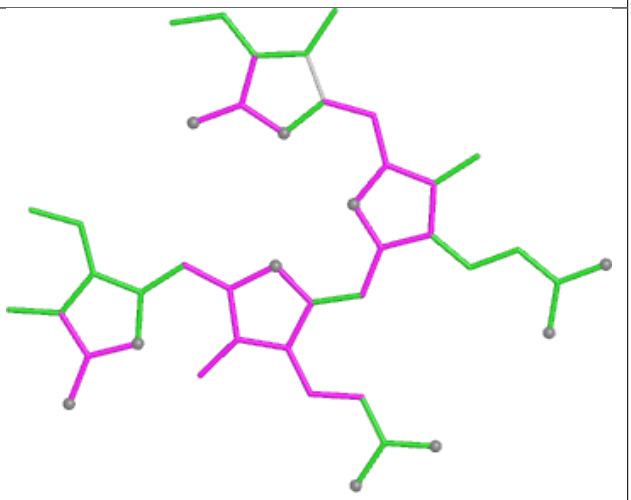
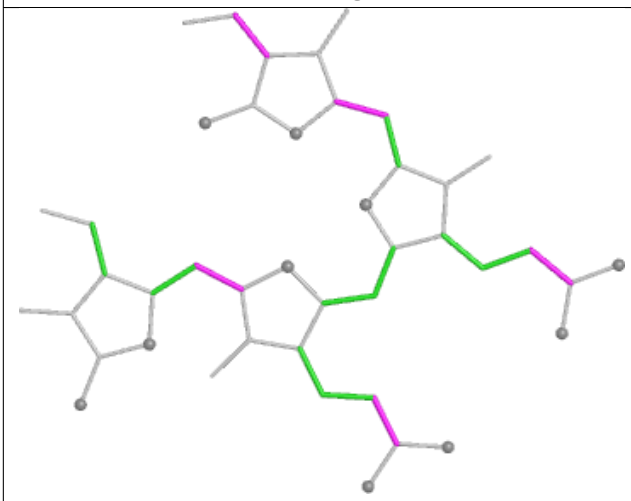


Bond angles



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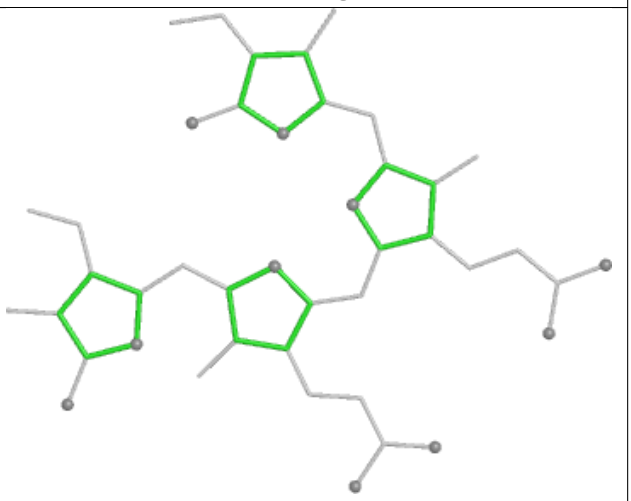
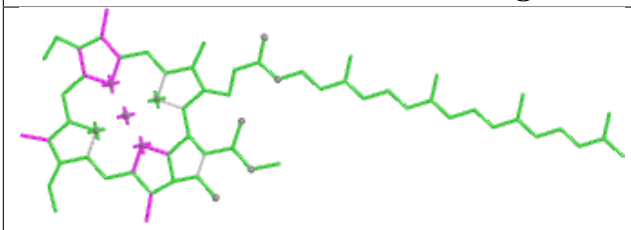


Rings

Ligand CLA A2 823



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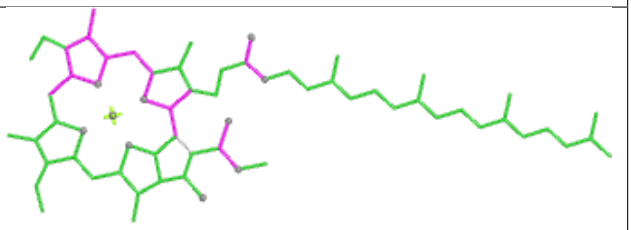
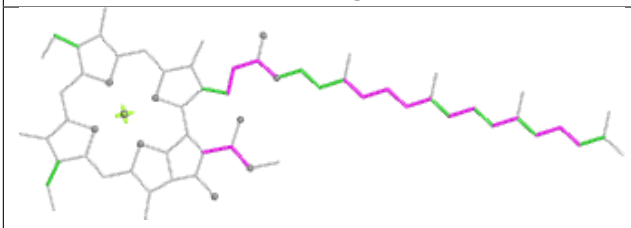


Bond angles



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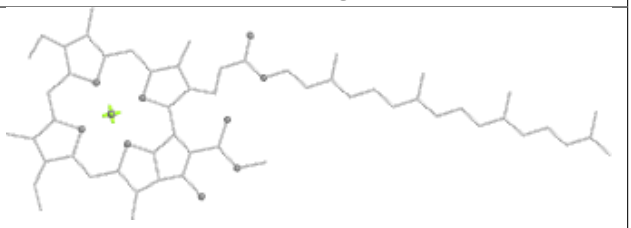
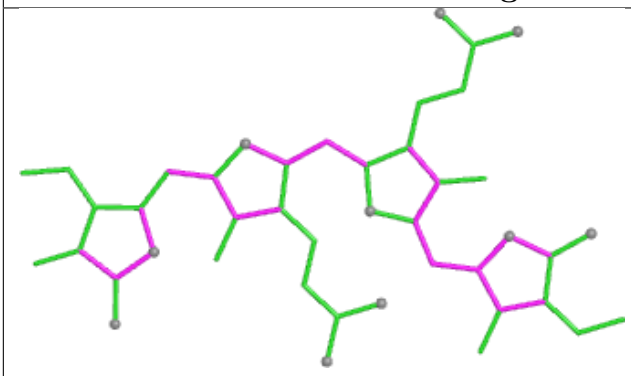


Rings

Ligand CYC EH 1001



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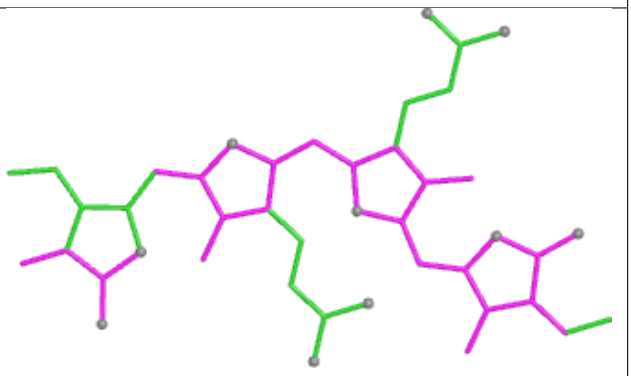
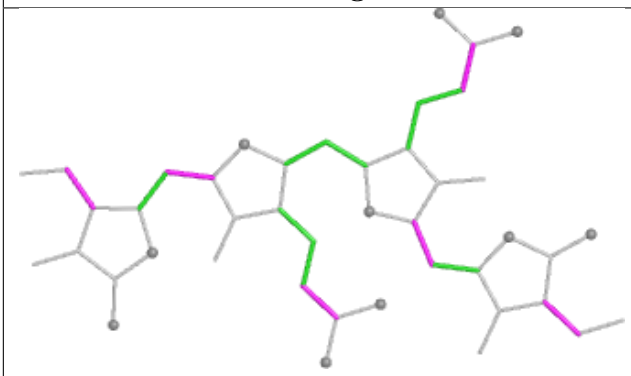


Bond angles



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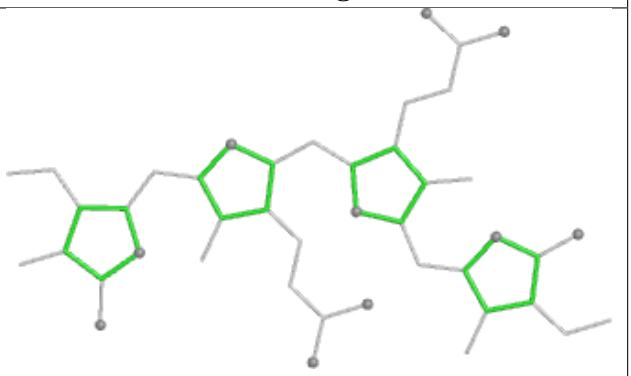
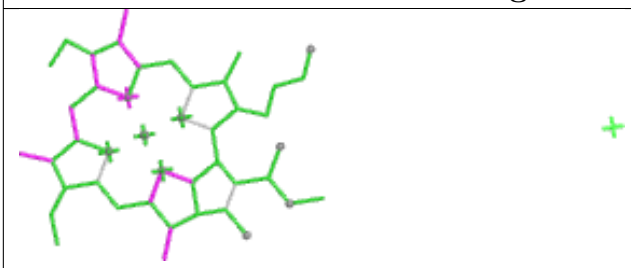


Rings

Ligand CLA AN 801



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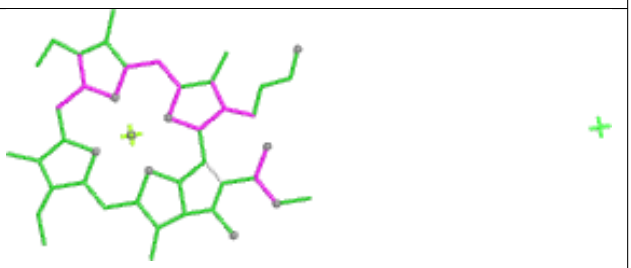

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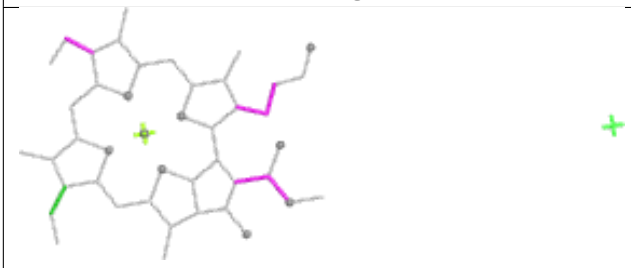

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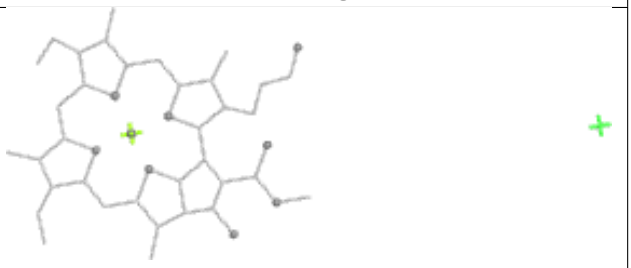
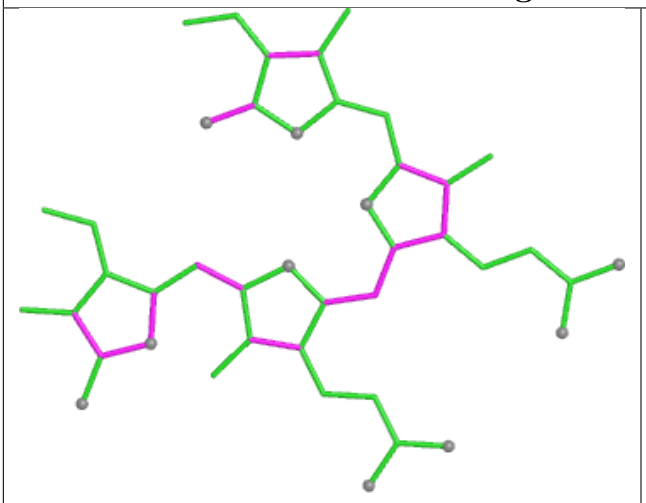


Rings

Ligand PEB QJ 203



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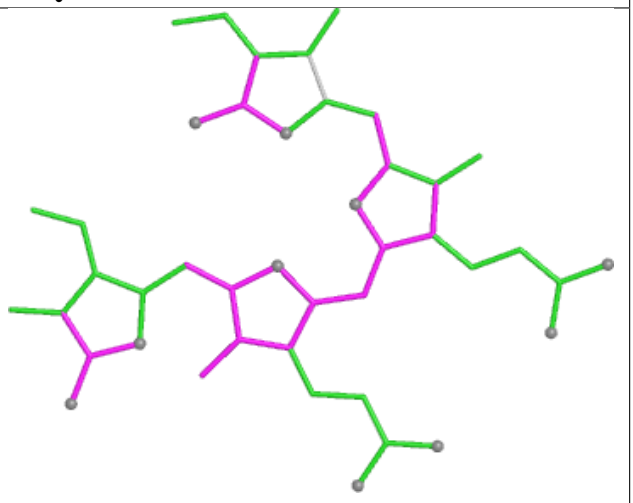

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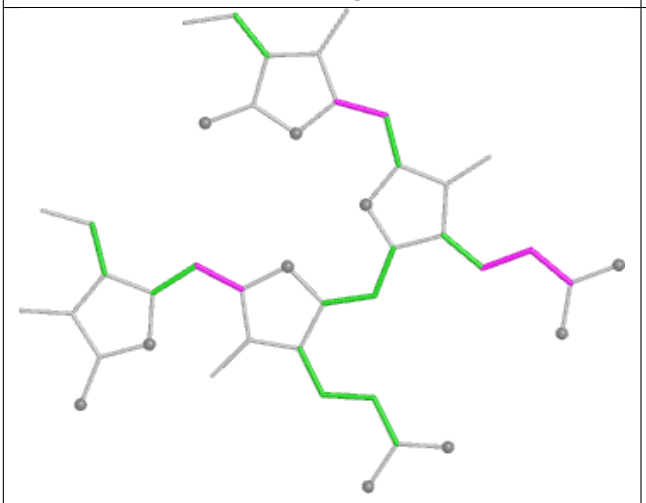

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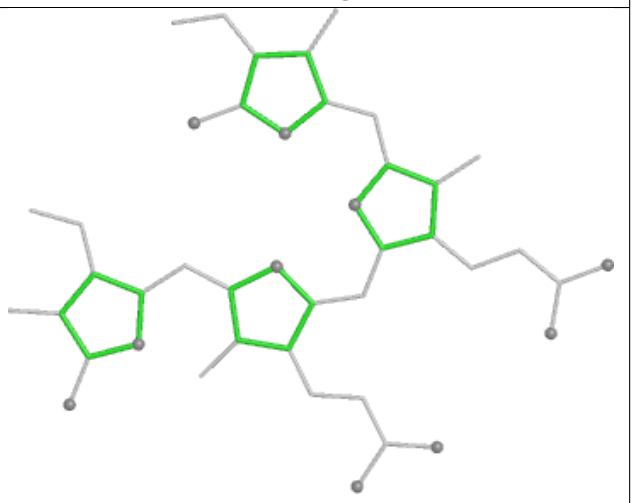
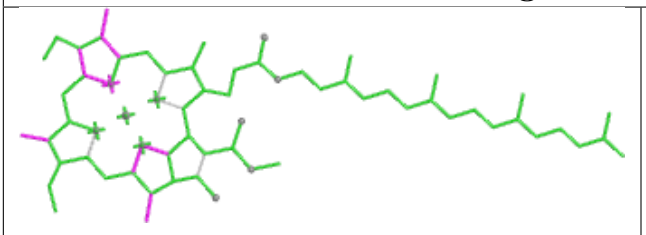


Rings

Ligand CLA b6 606



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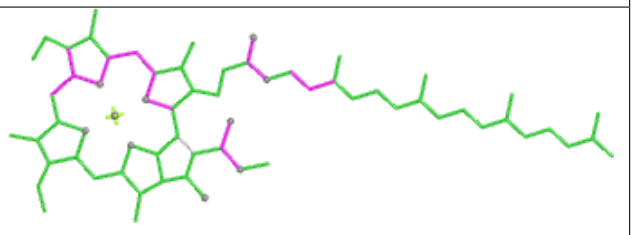

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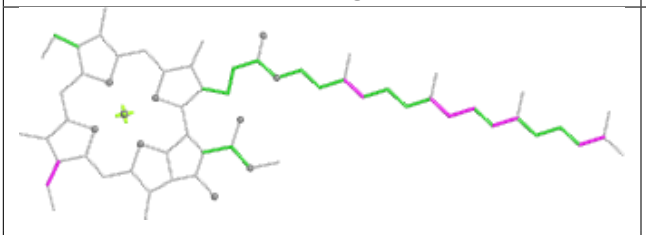

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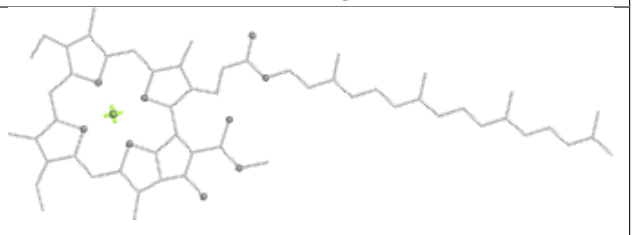
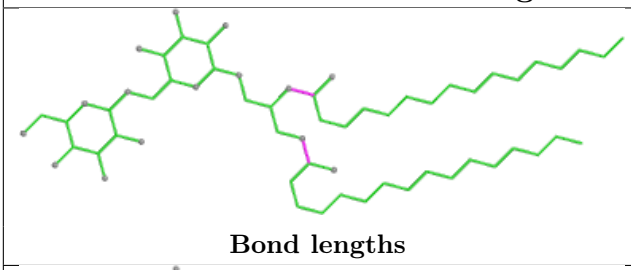


Rings

Ligand DGD c6 618



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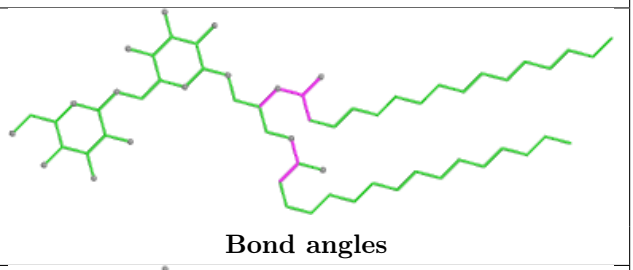

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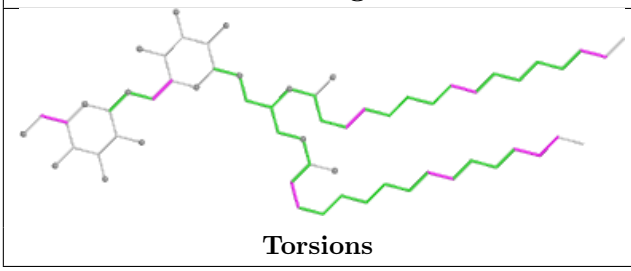

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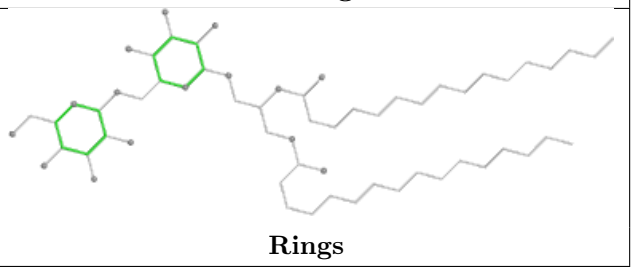
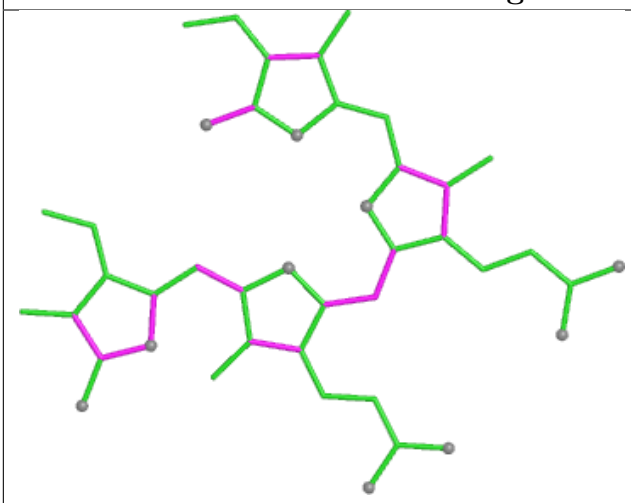


Rings

Ligand PEB MK 201



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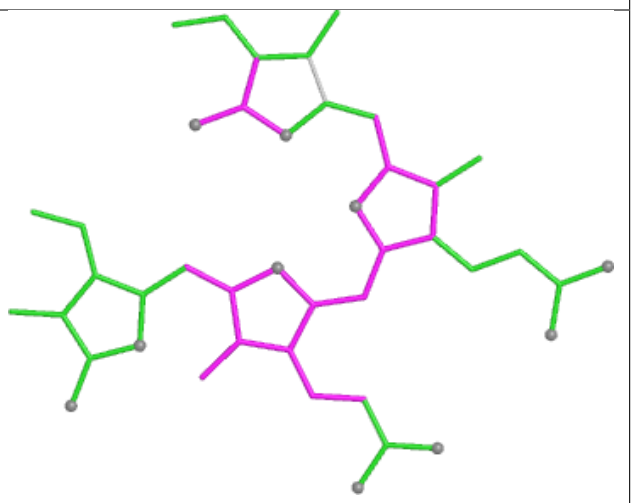

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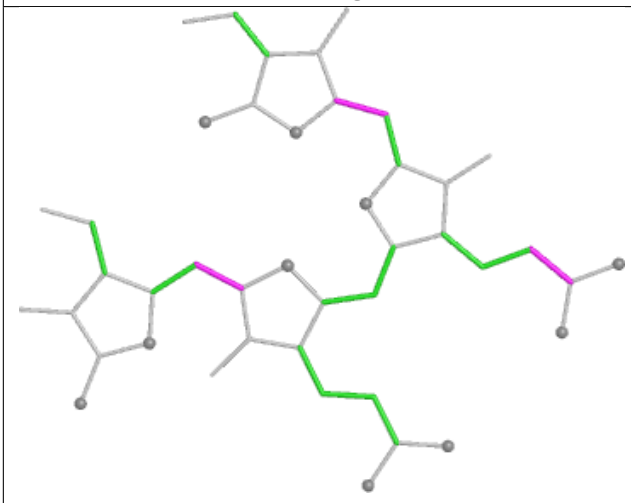

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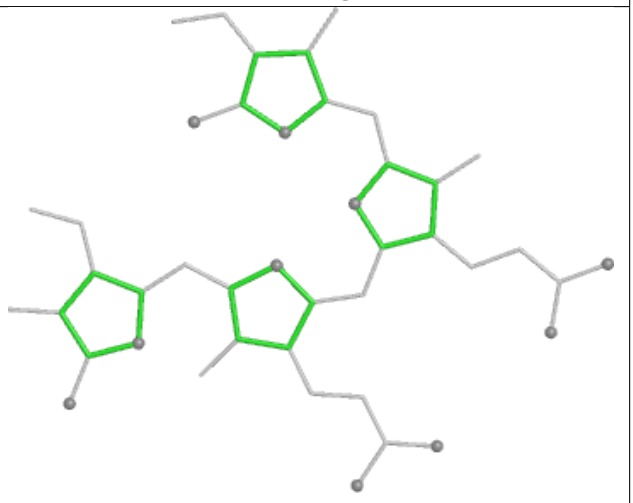
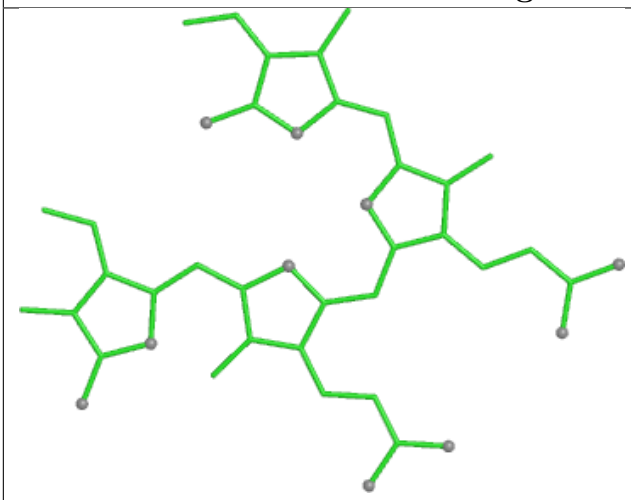


Rings

Ligand PEB bE 202



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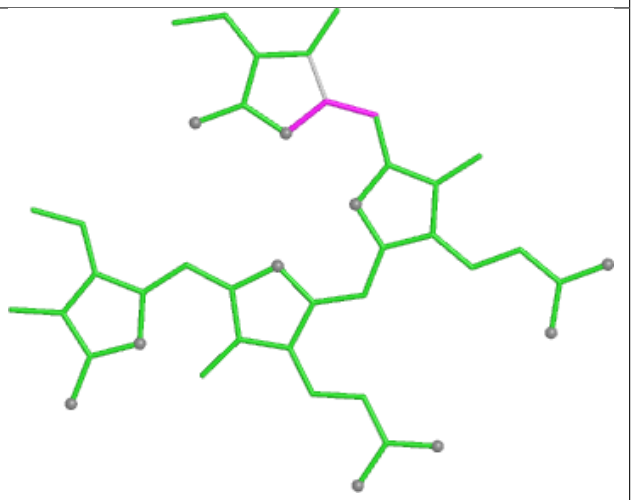

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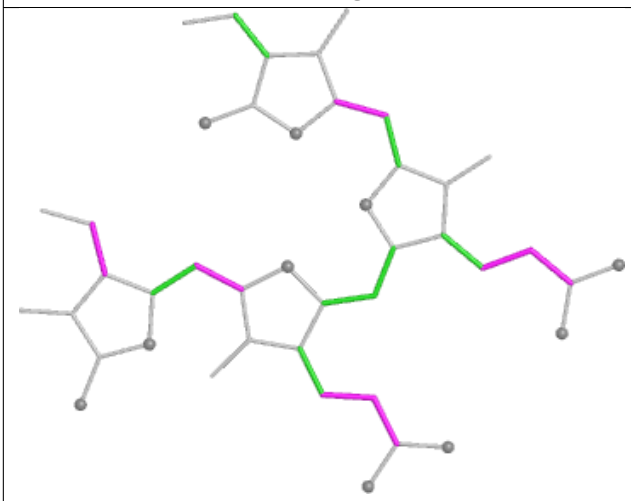

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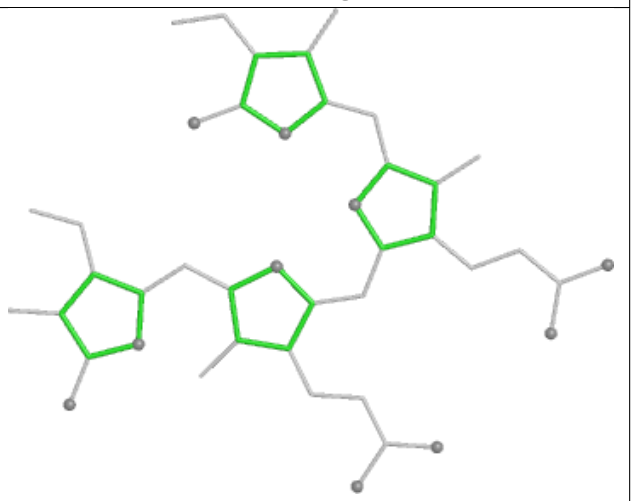

Rings

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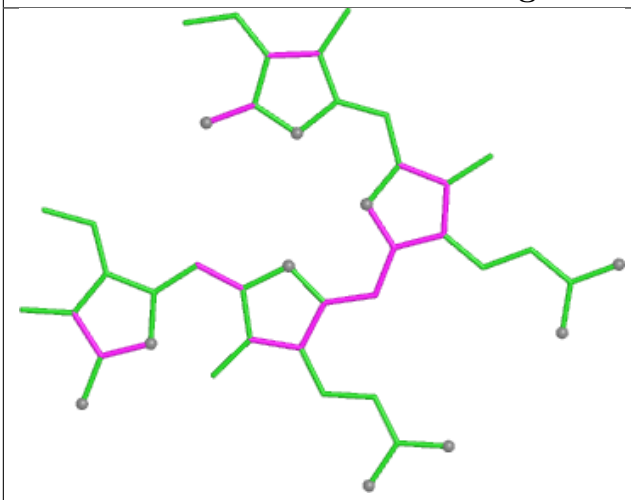

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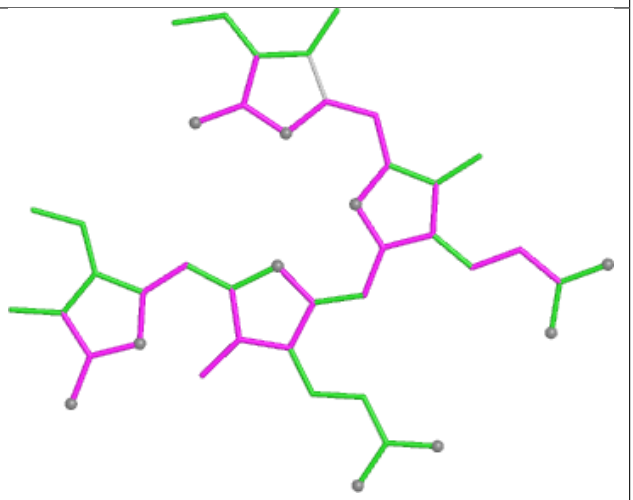

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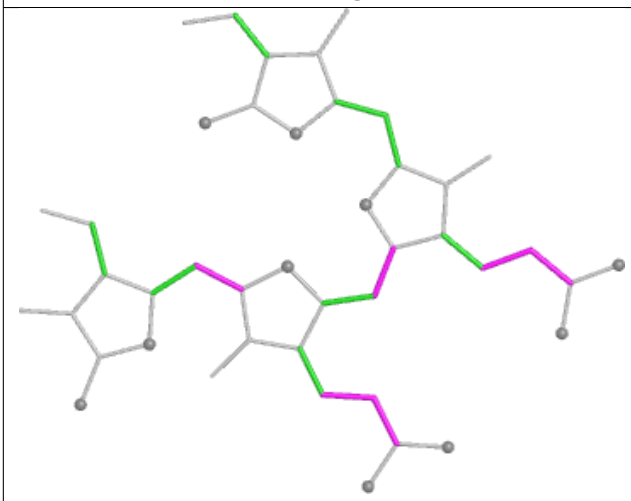

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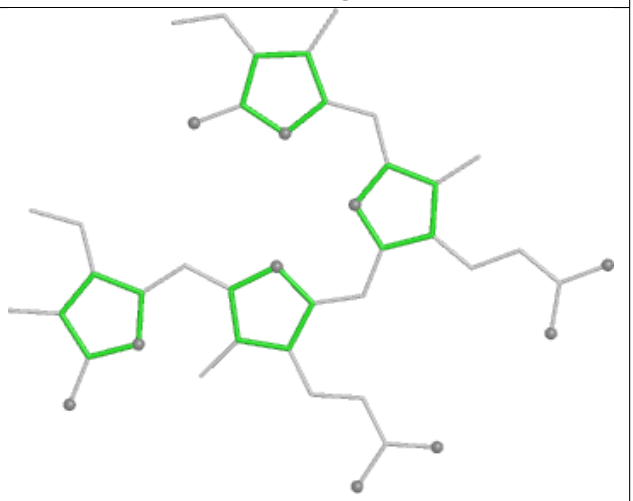
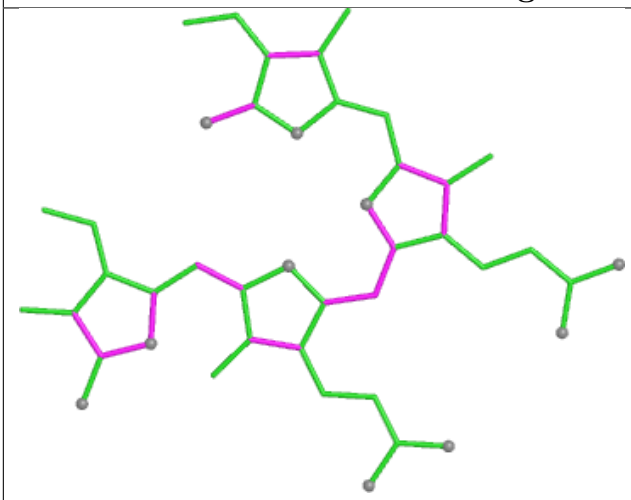


Rings

Ligand PEB LJ 201



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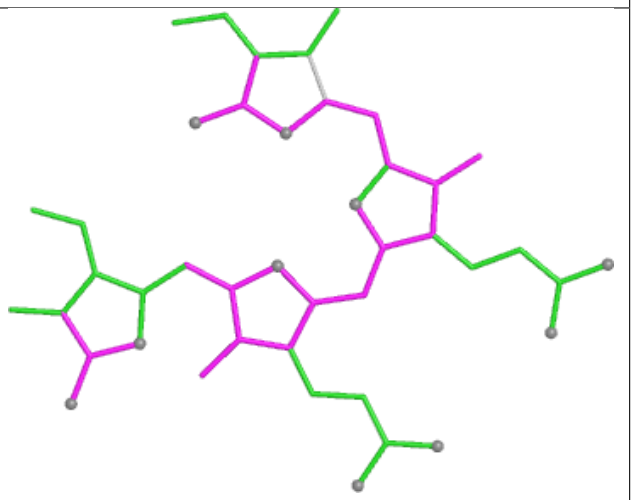

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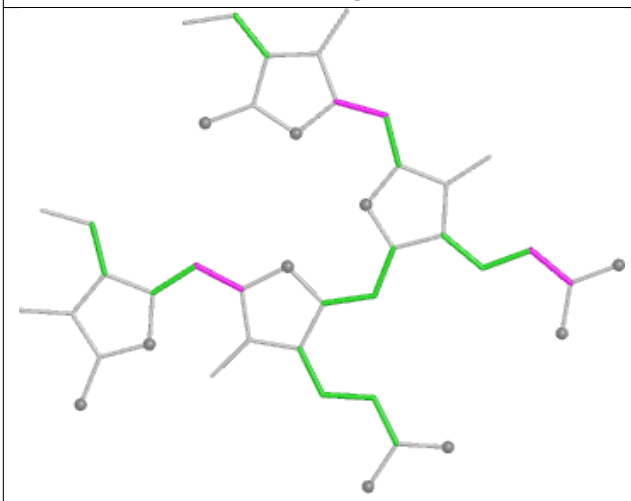

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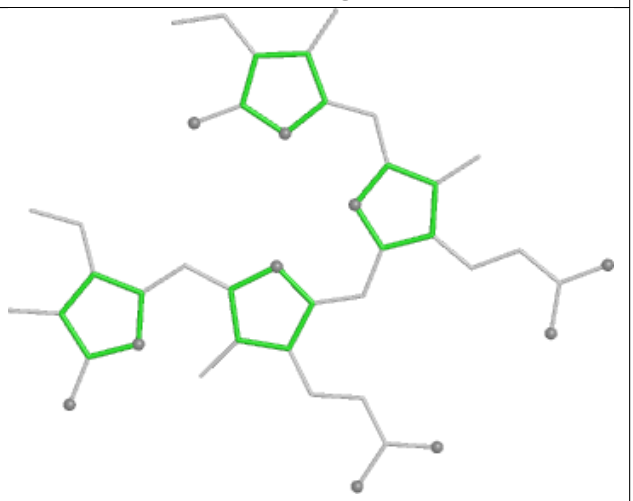
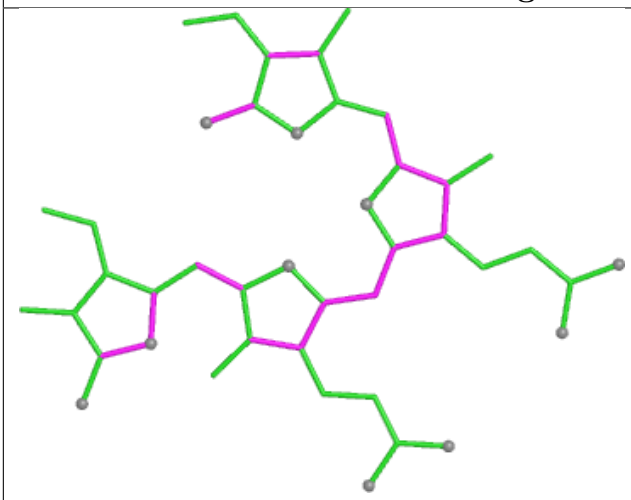


Rings

Ligand PEB aF 201



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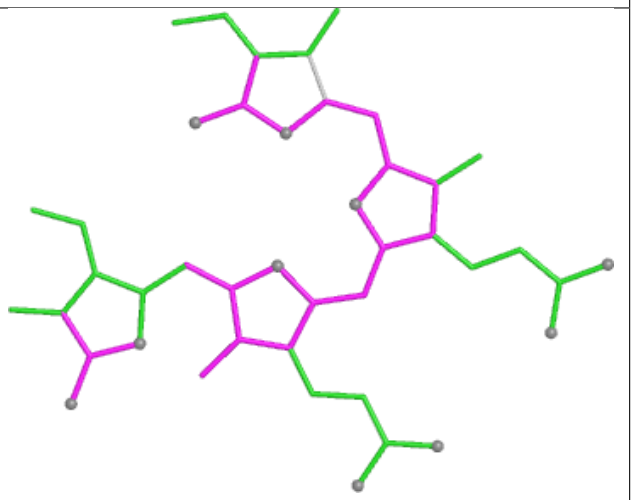

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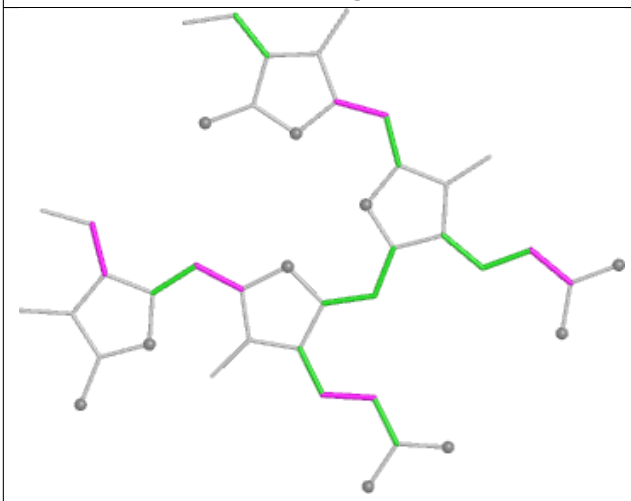

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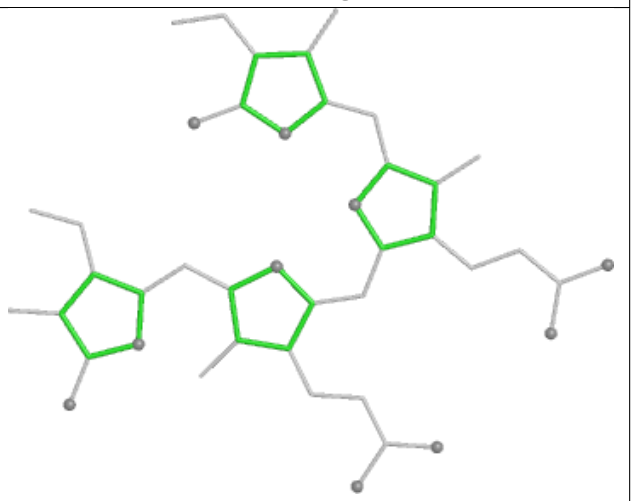
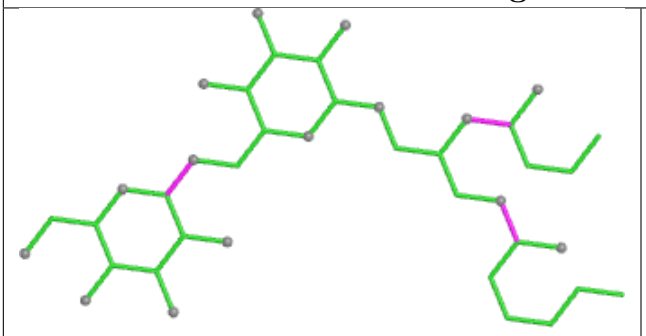


Rings

Ligand DGD BL 613



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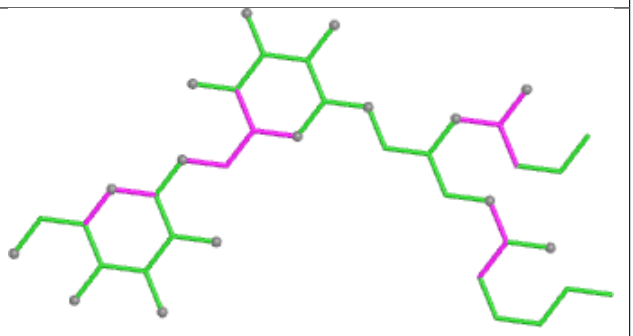

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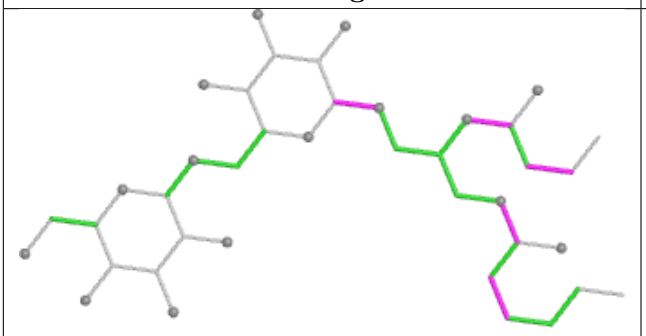

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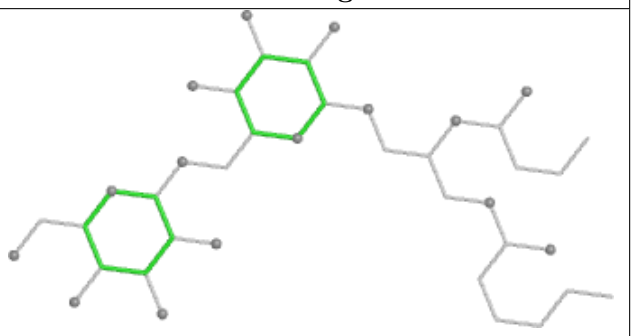
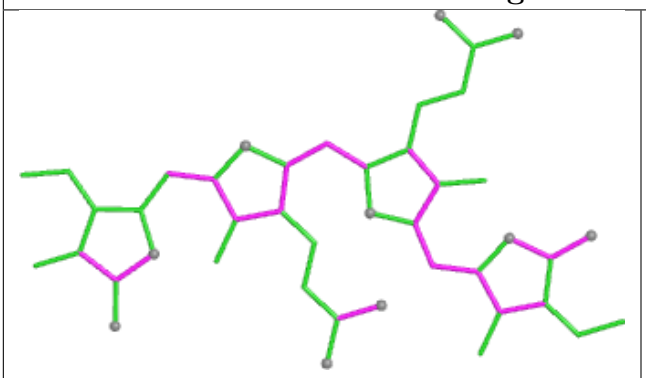


Rings

Ligand CYC d3 1001



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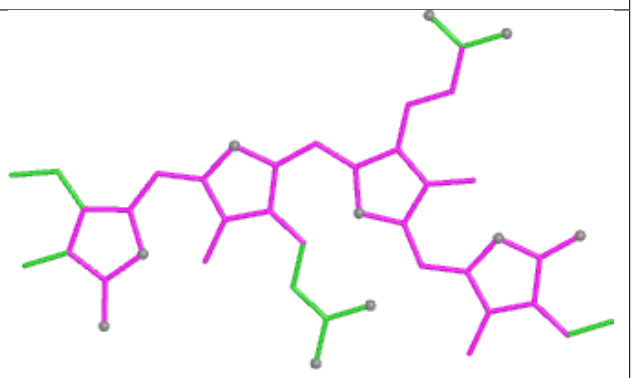

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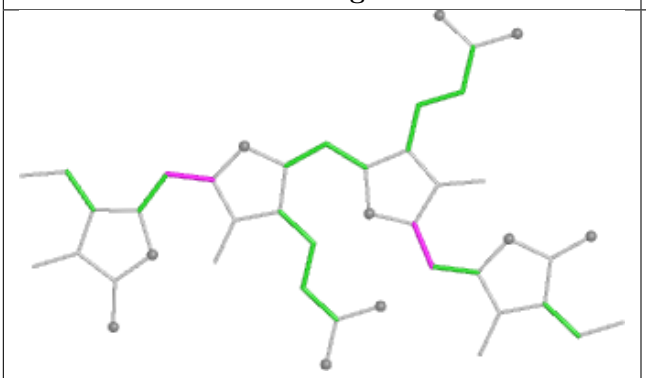

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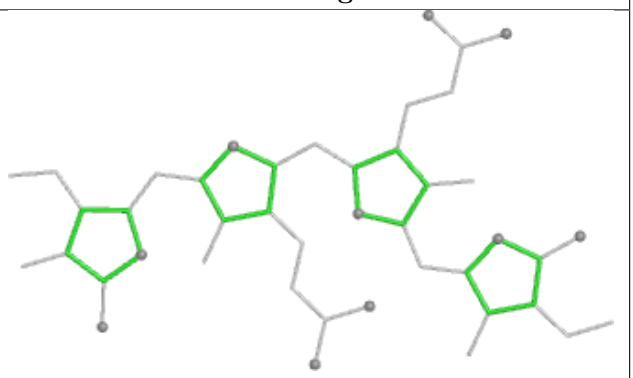
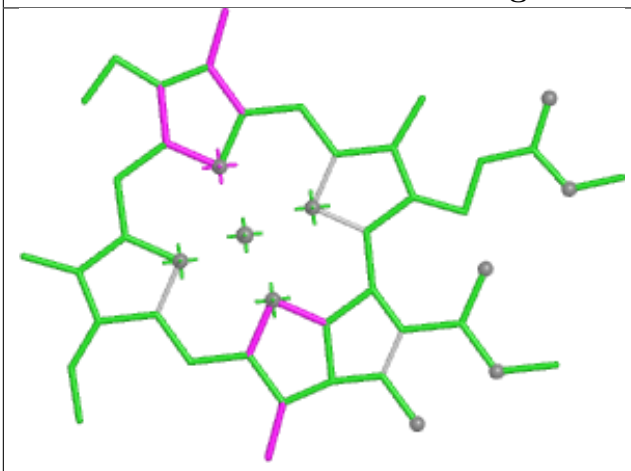


Rings

Ligand CLA RN 203



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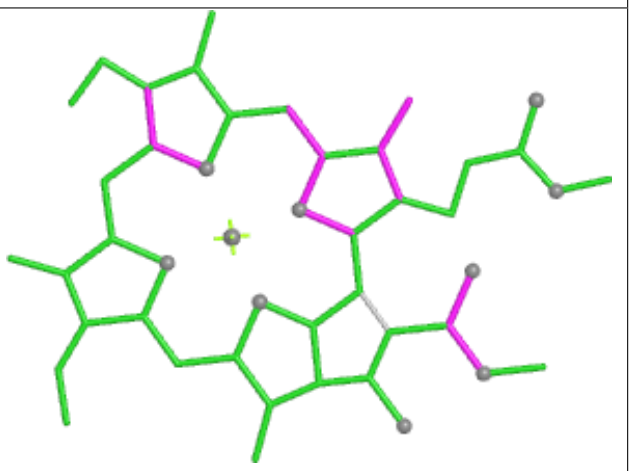

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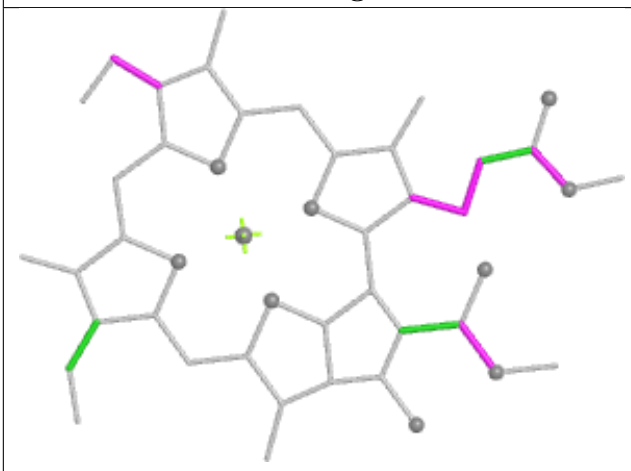

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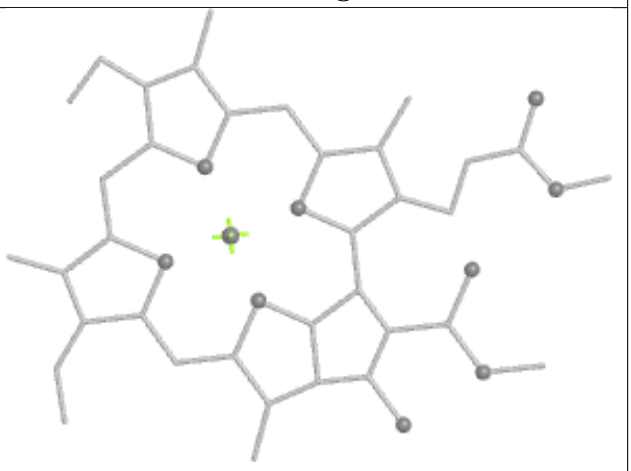
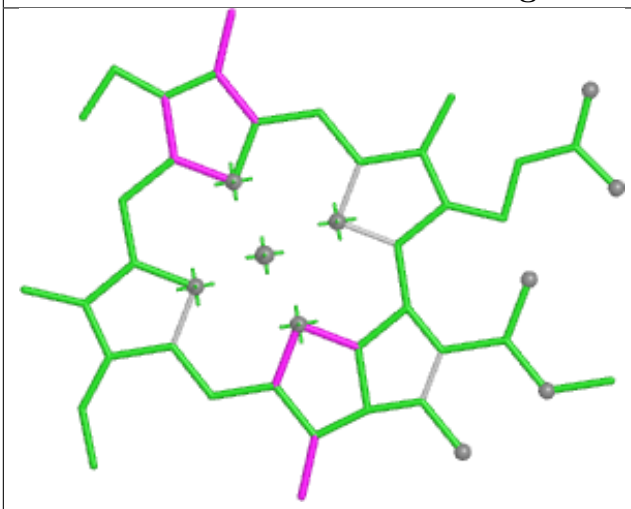


Rings

Ligand CLA 52 606



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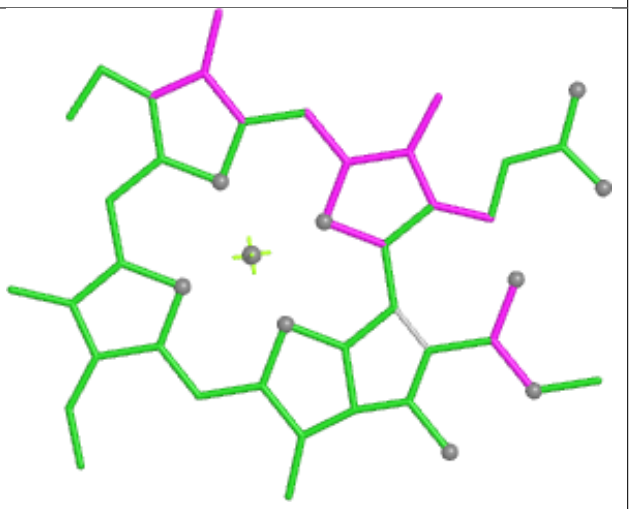

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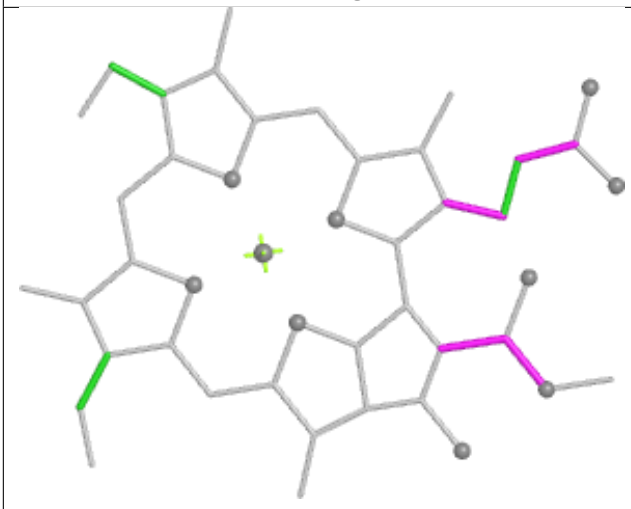
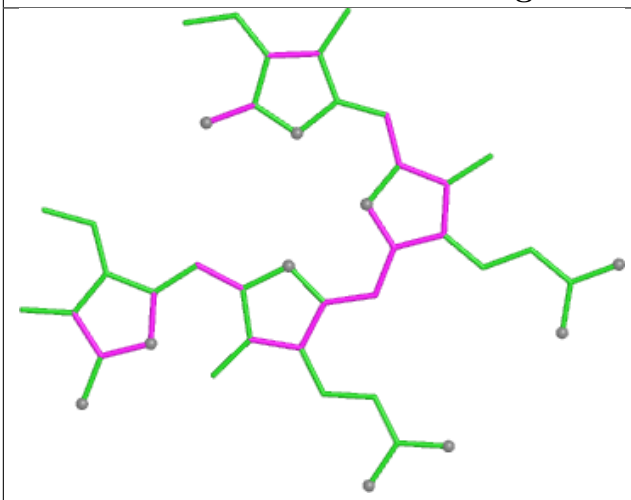


Torsions



Rings

Ligand PEB ZF 202



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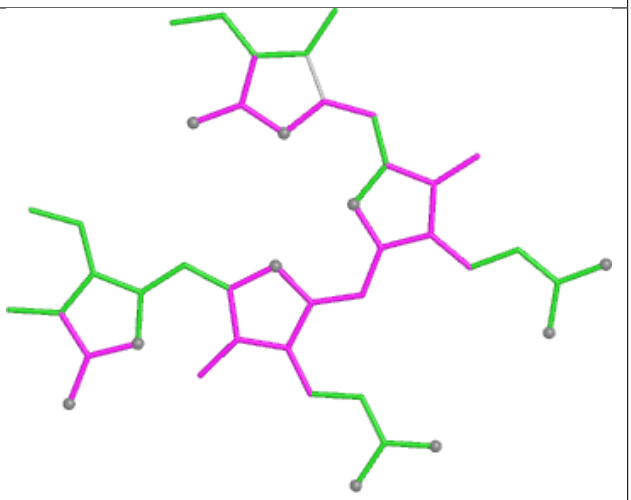

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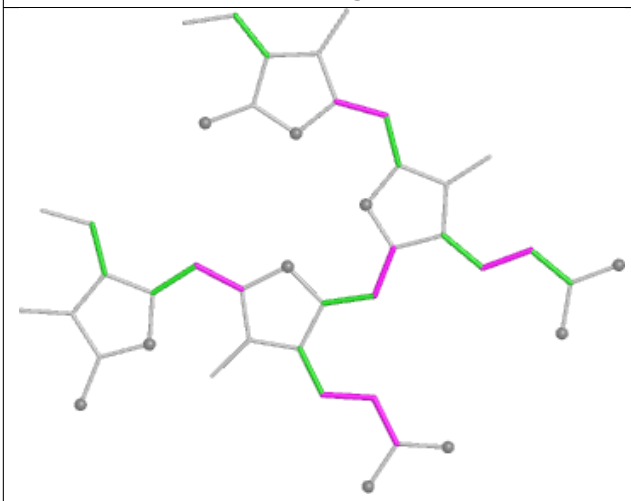

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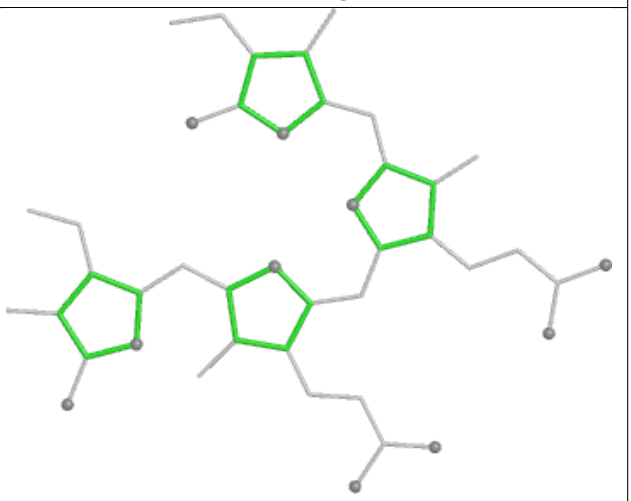
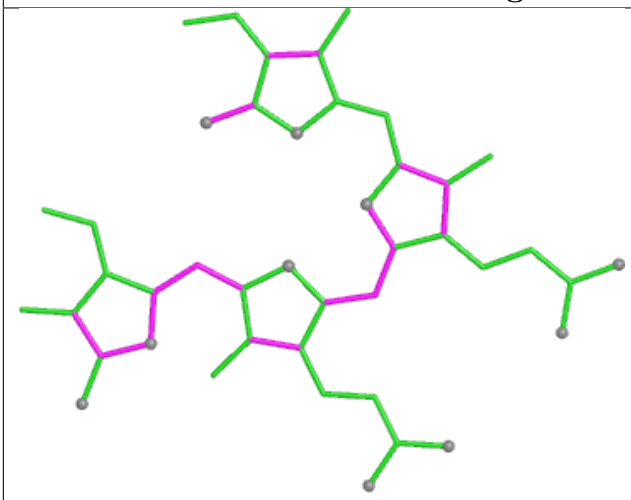


Rings

Ligand PEB WO 201



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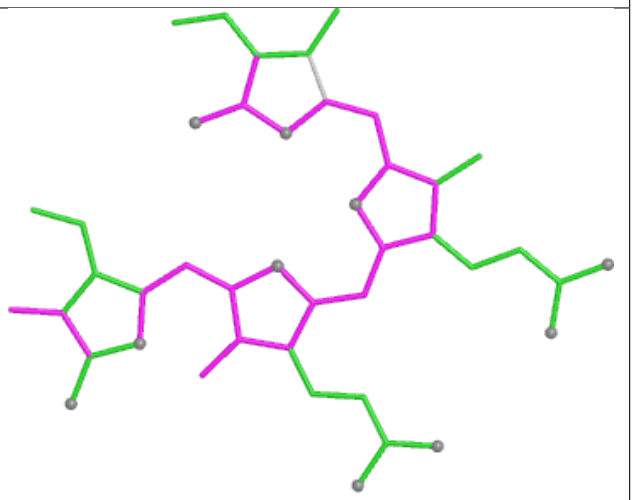
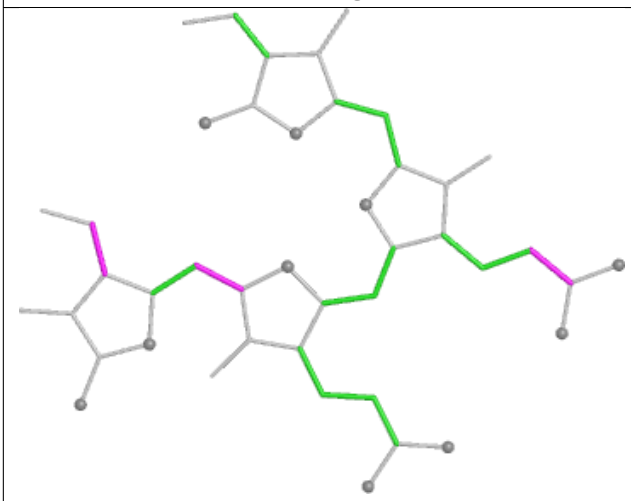


Bond angles



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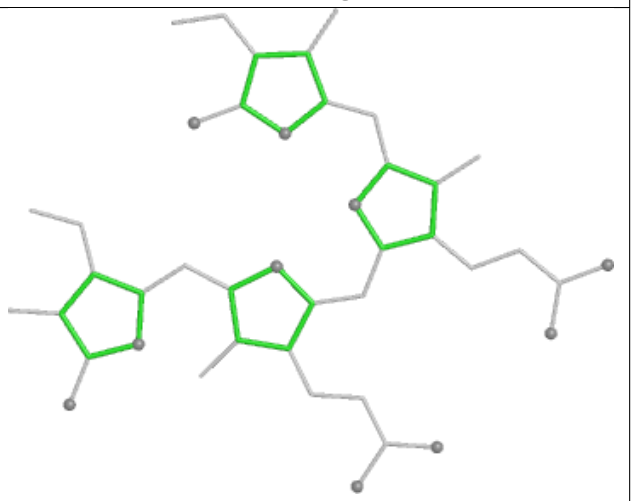
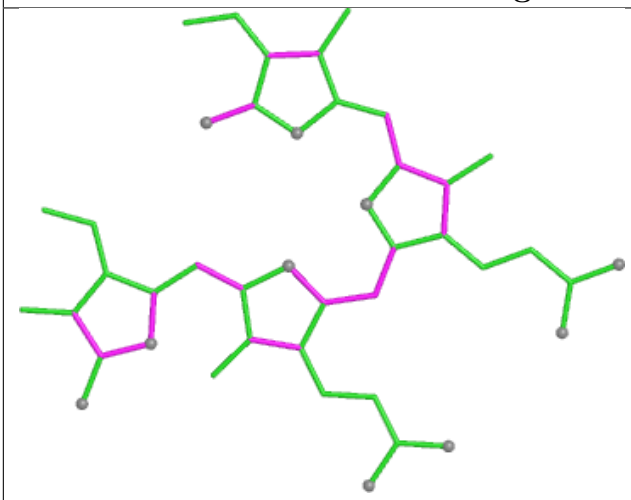


Rings

Ligand PEB SH 201



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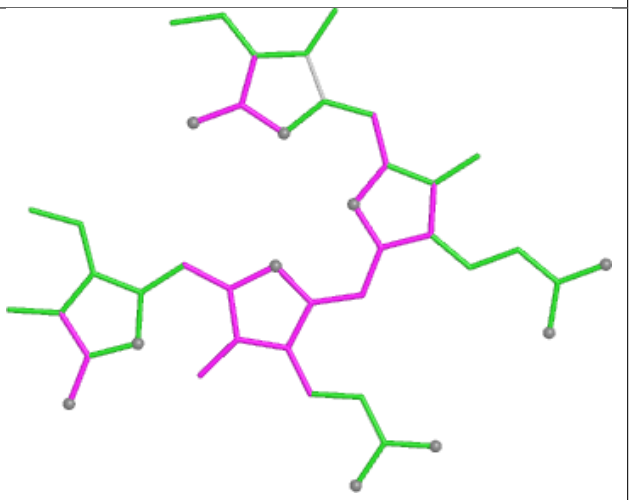

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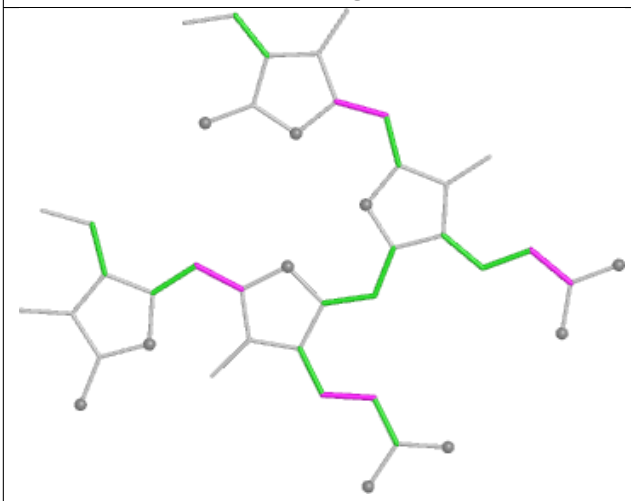

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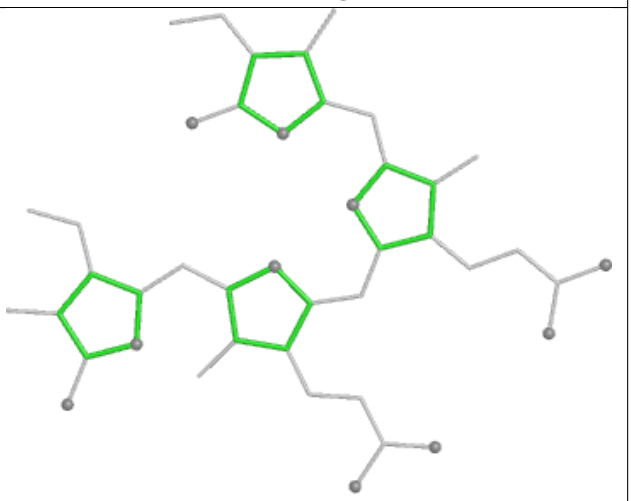
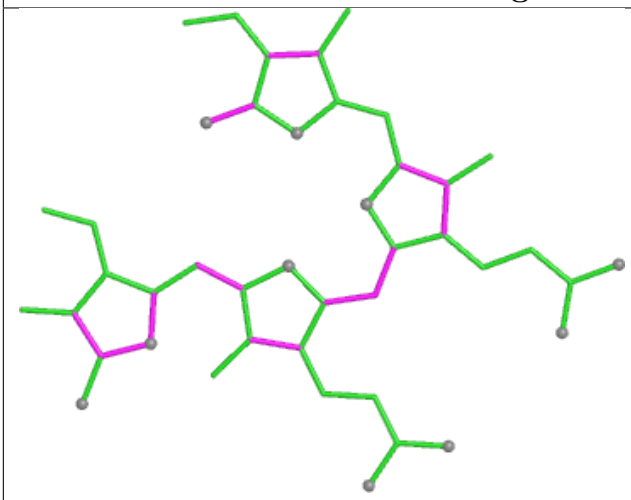


Rings

Ligand PEB MJ 201



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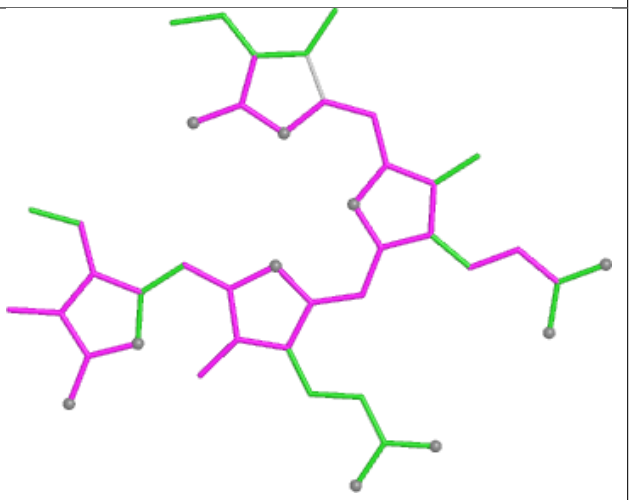

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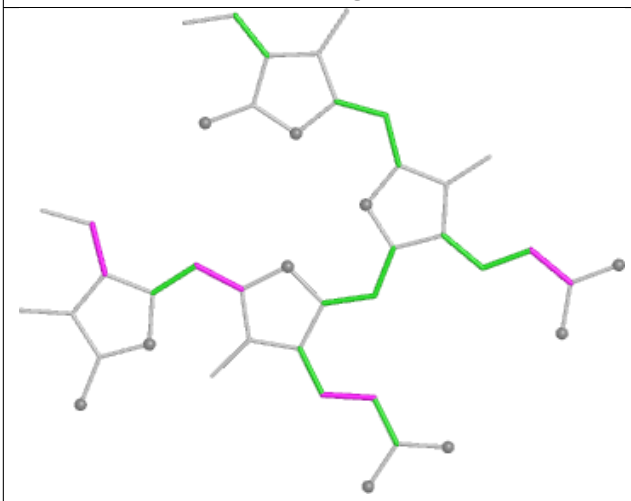

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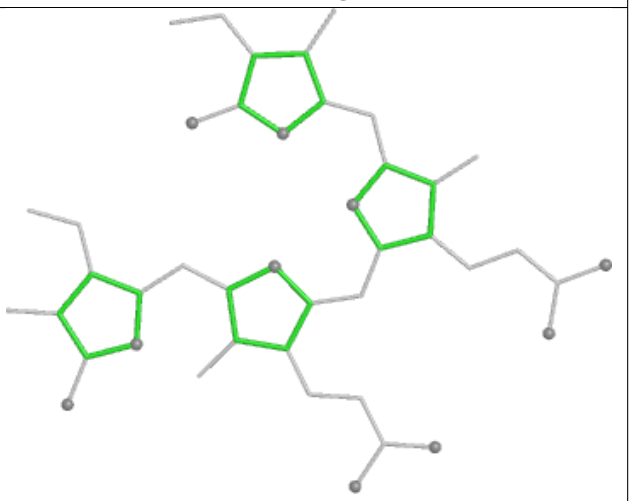
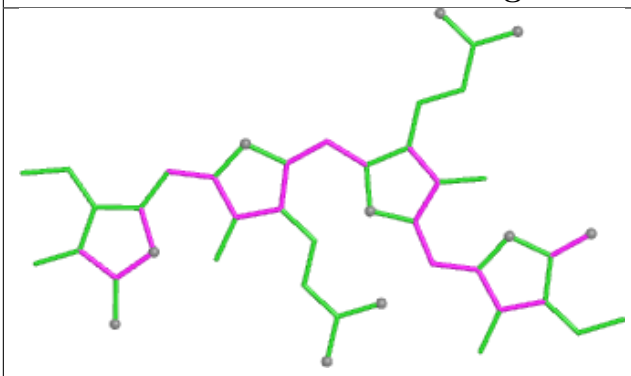


Rings

Ligand CYC C1 1001



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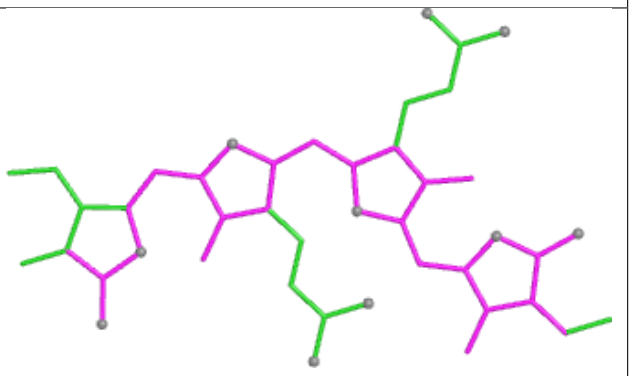

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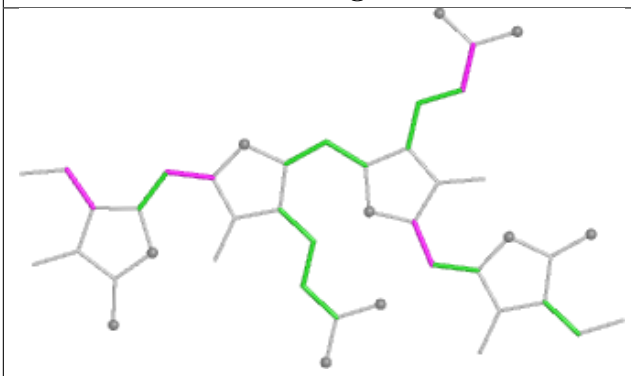

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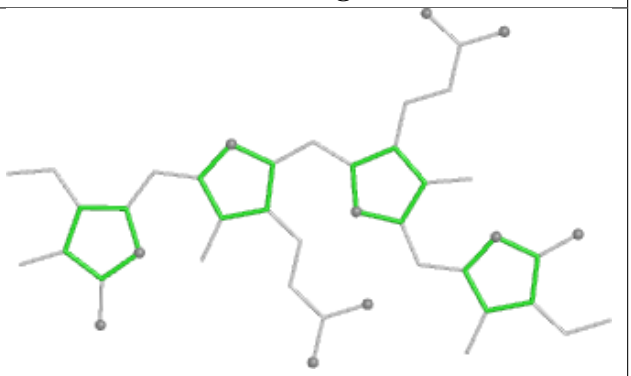
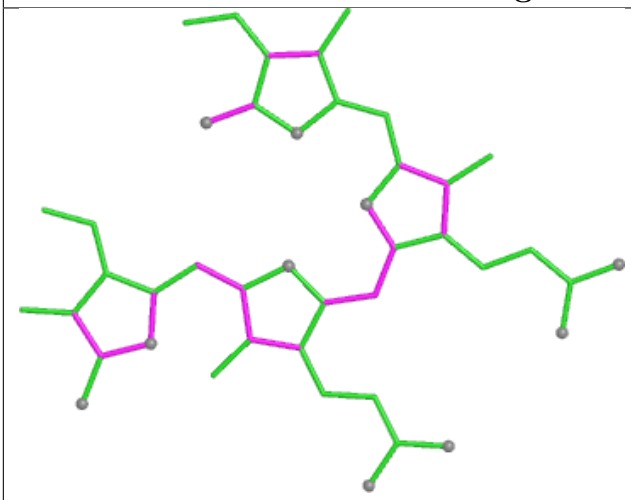


Rings

Ligand PEB N5 201



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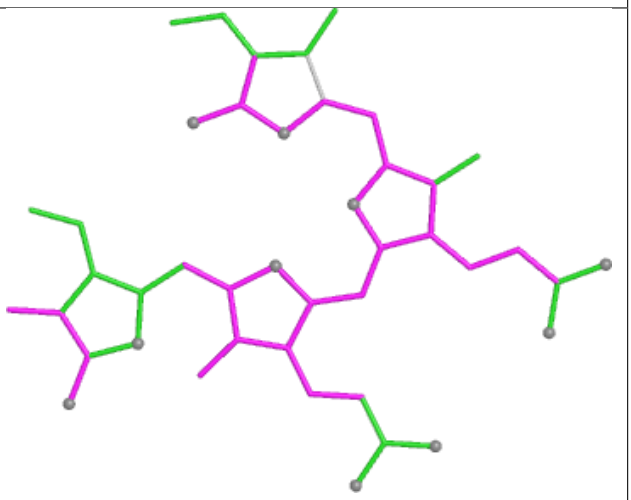

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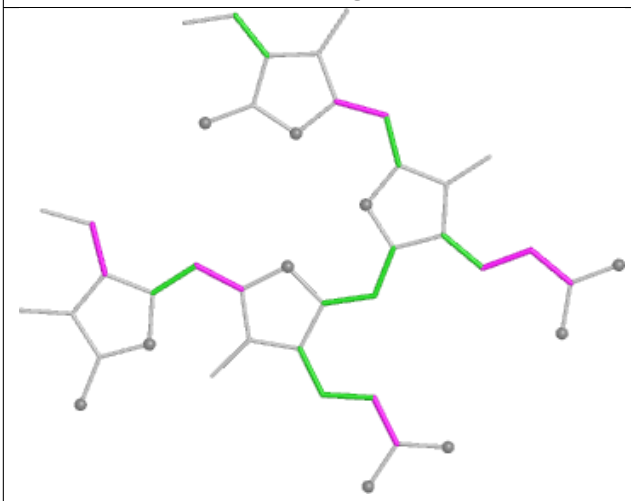

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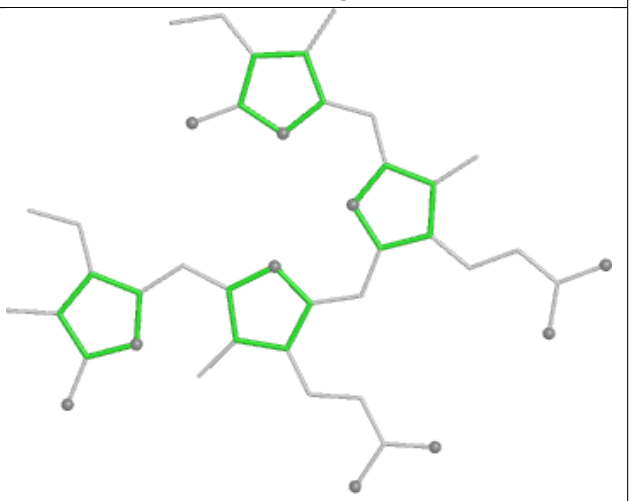

Rings

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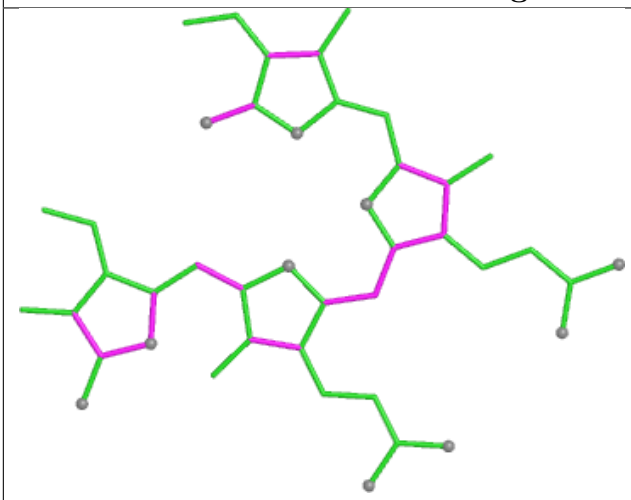

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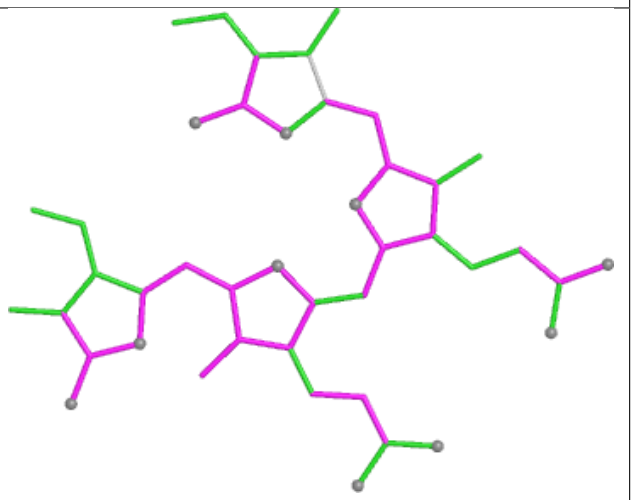

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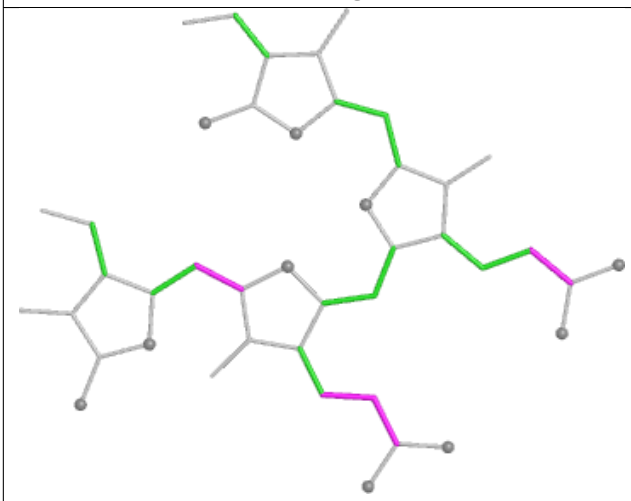

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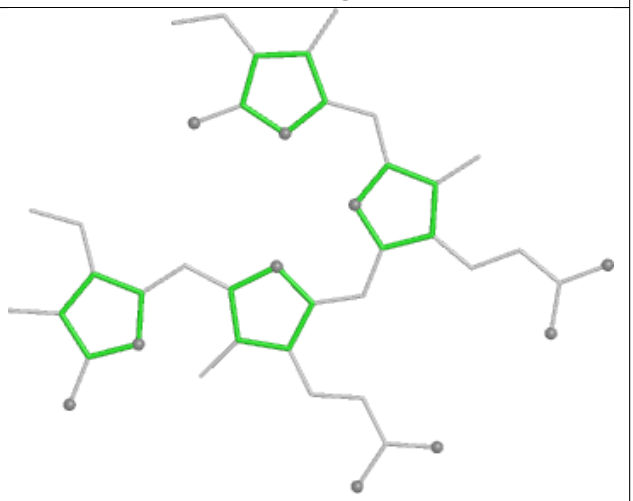

Rings

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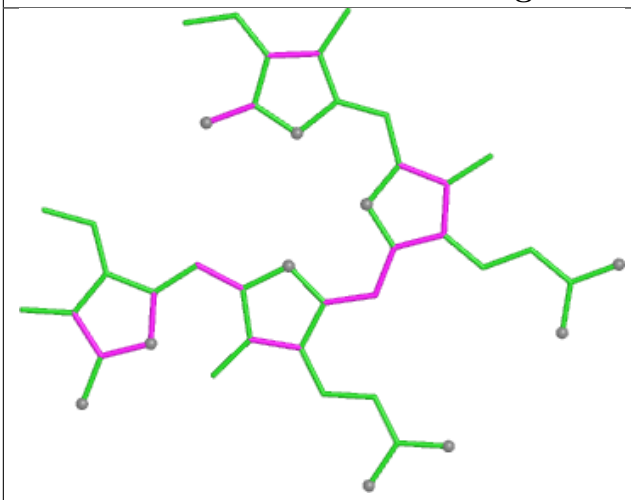

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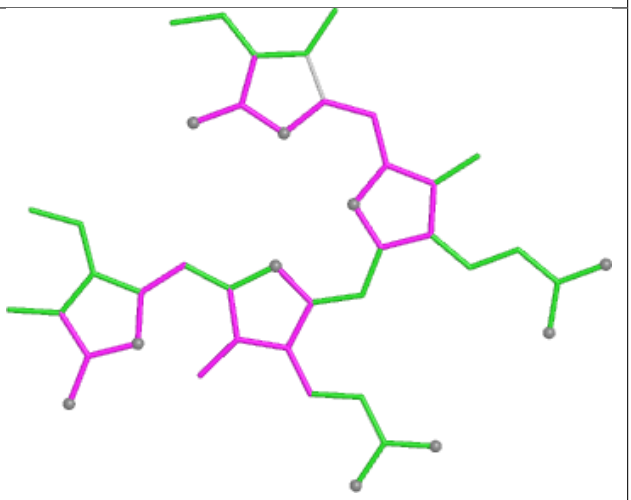

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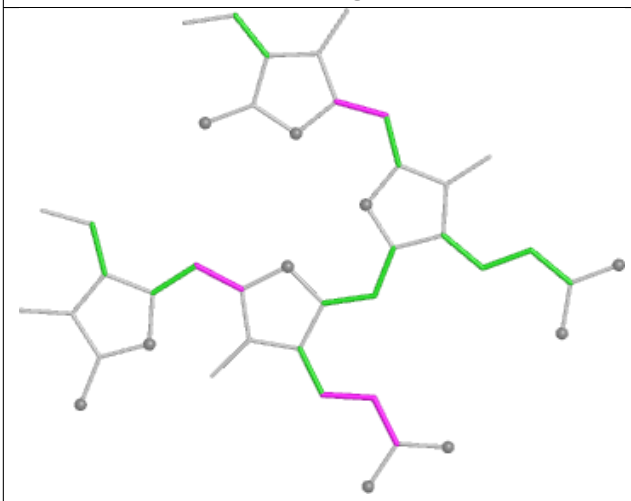

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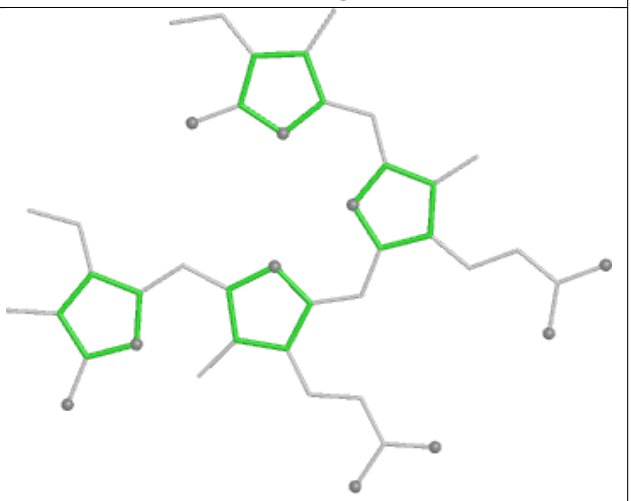

Rings

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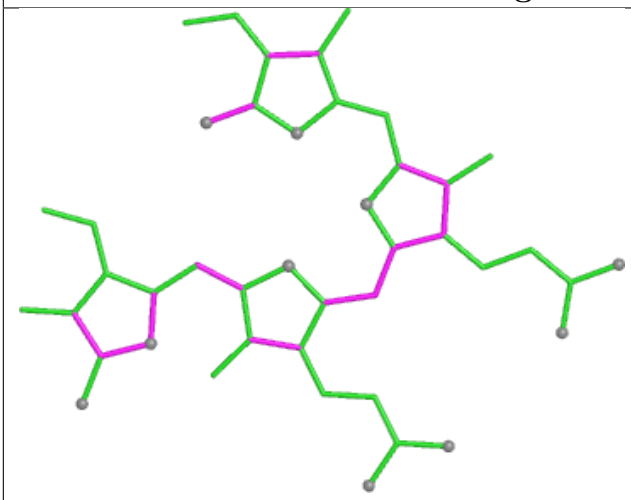

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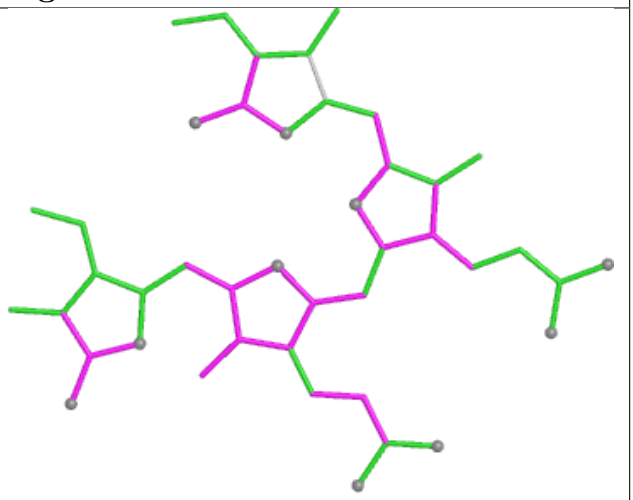

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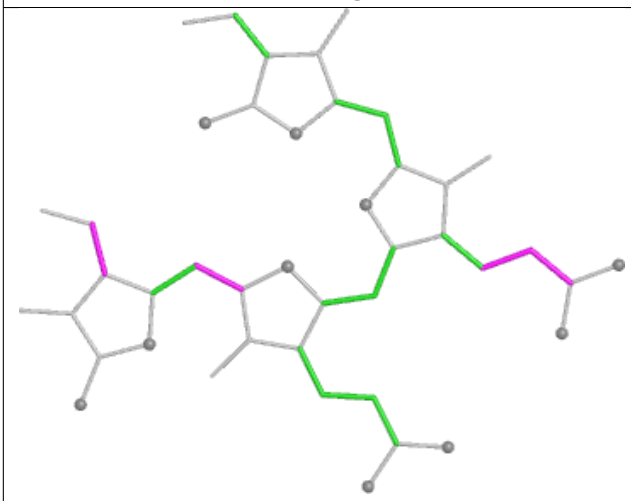

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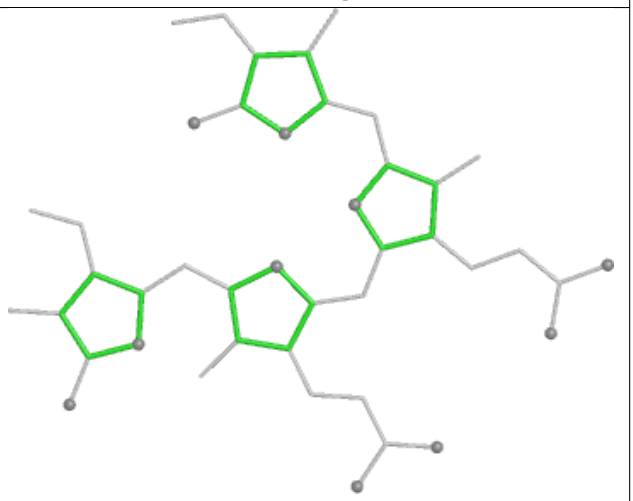

Rings

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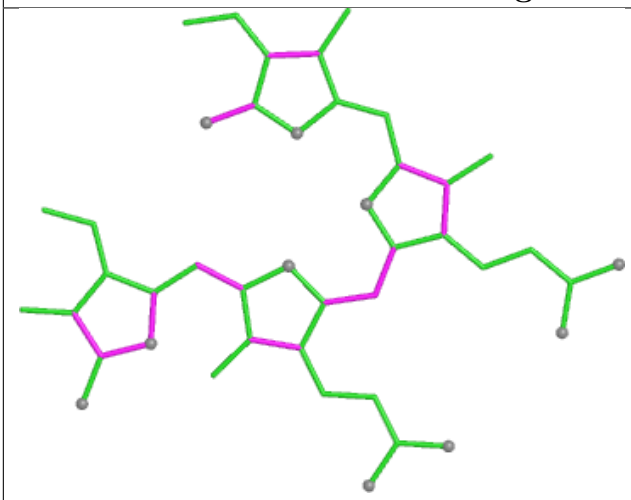

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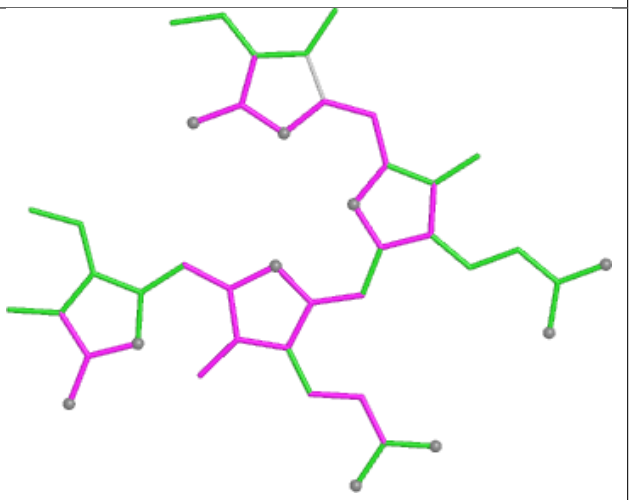

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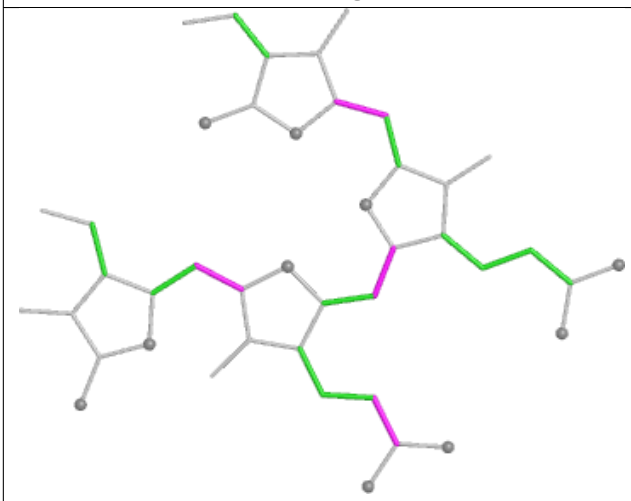

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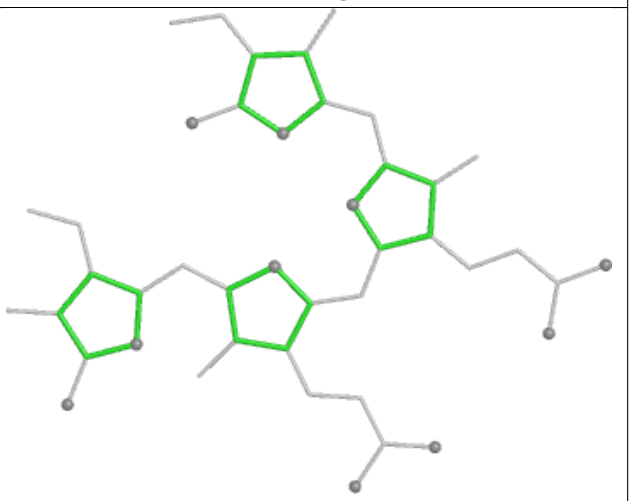
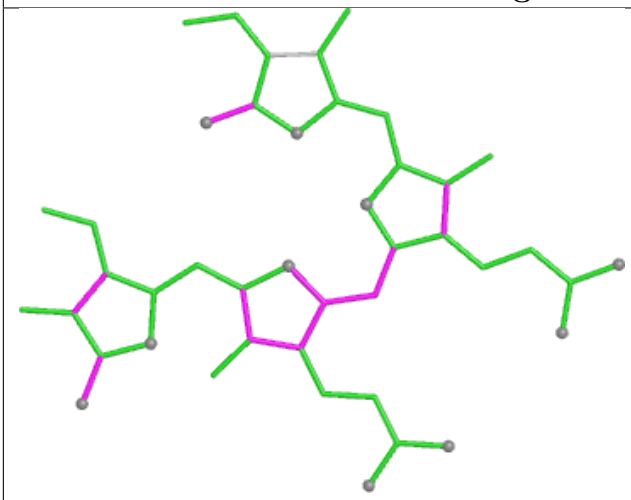


Rings

Ligand PUB A1 303



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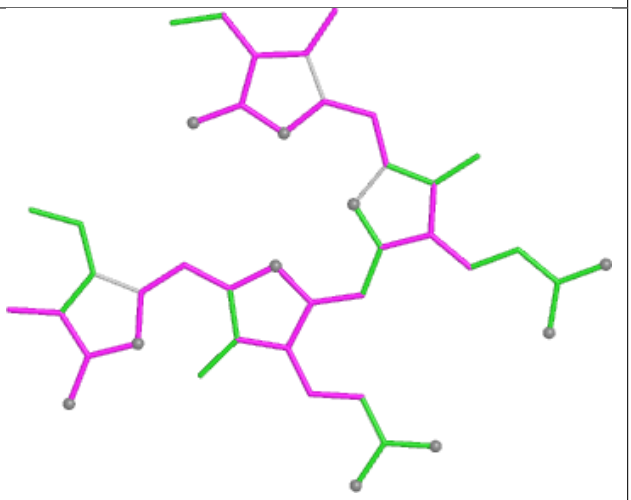

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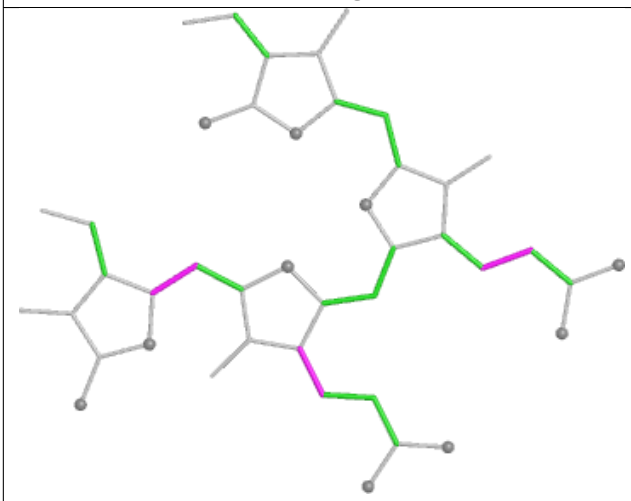

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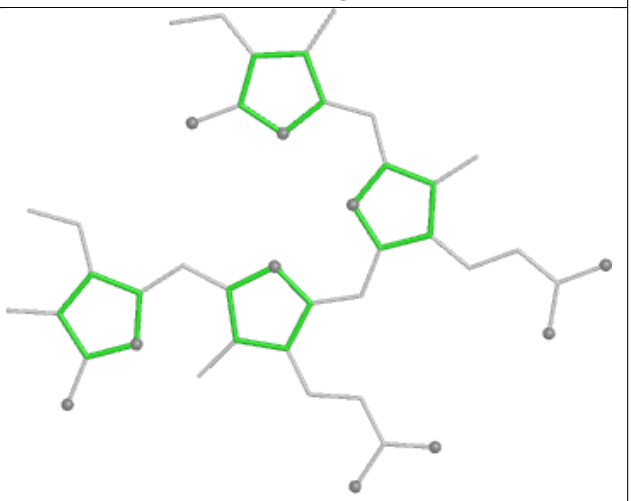
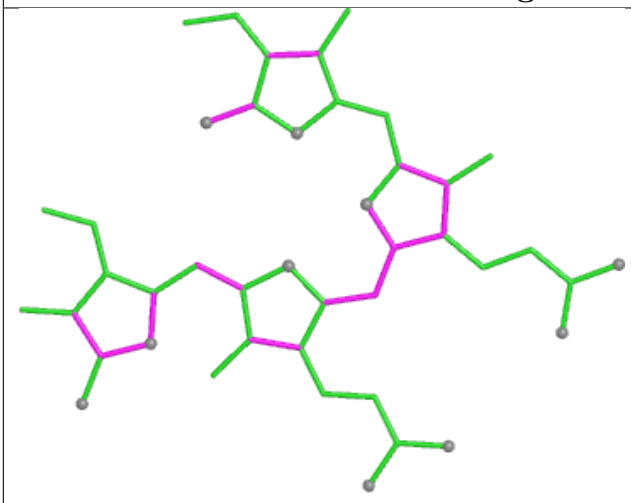


Rings

Ligand PEB GI 203



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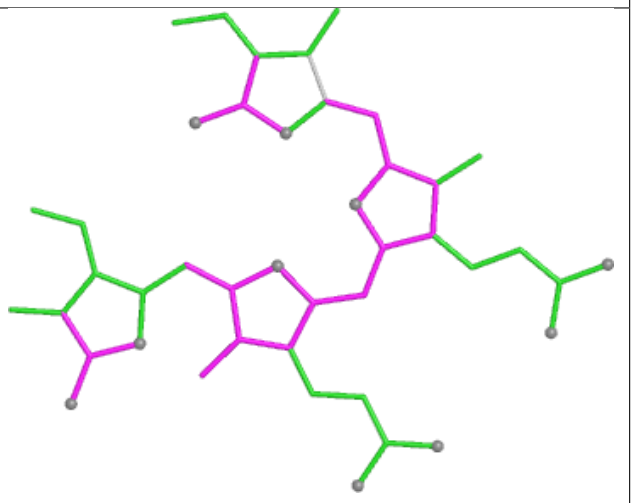

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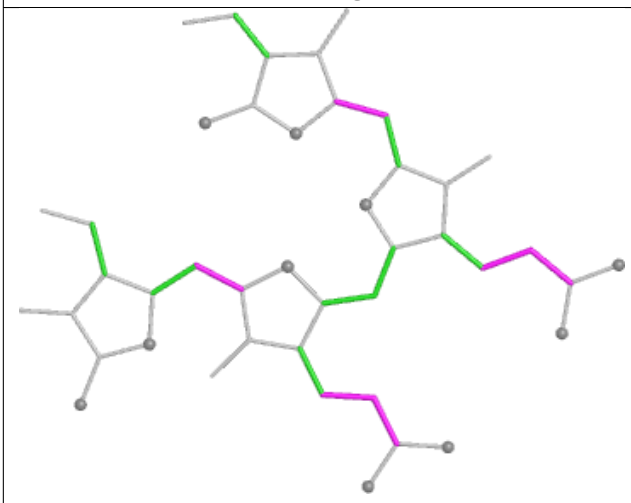

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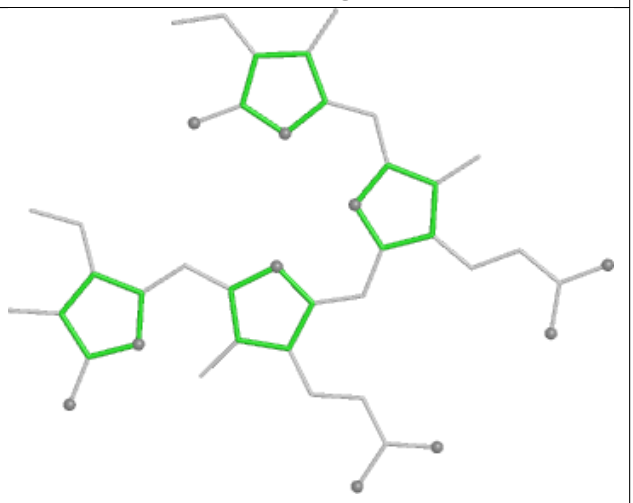
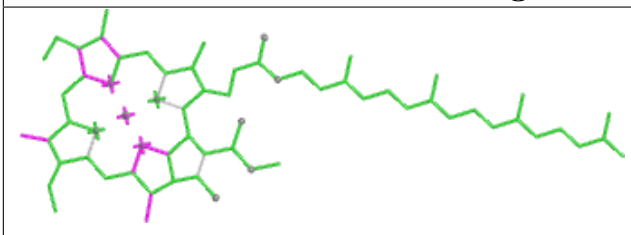


Rings

Ligand CLA AN 829



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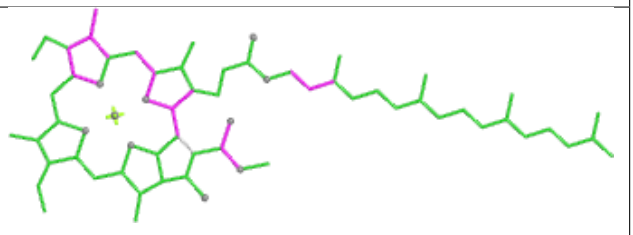

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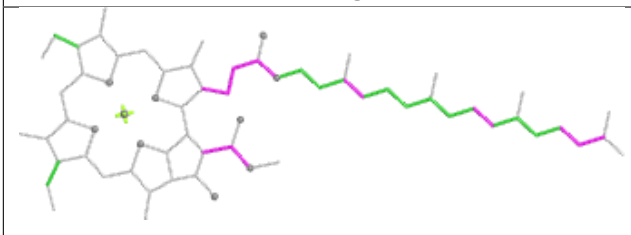

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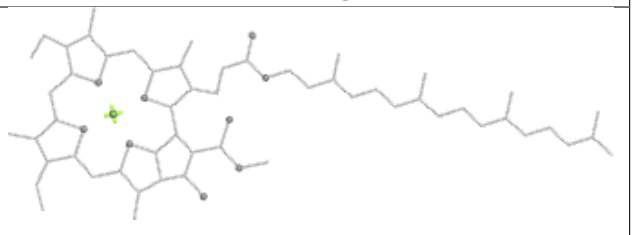
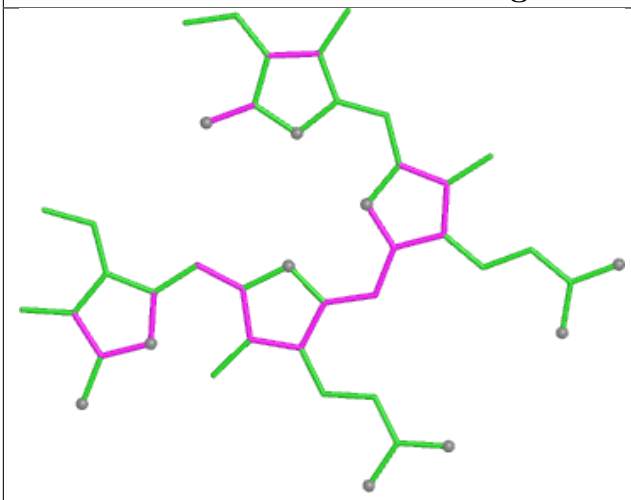


Rings

Ligand PEB UQ 201



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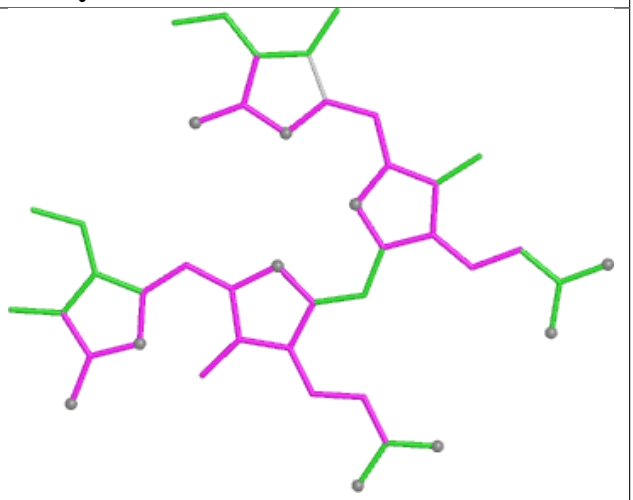

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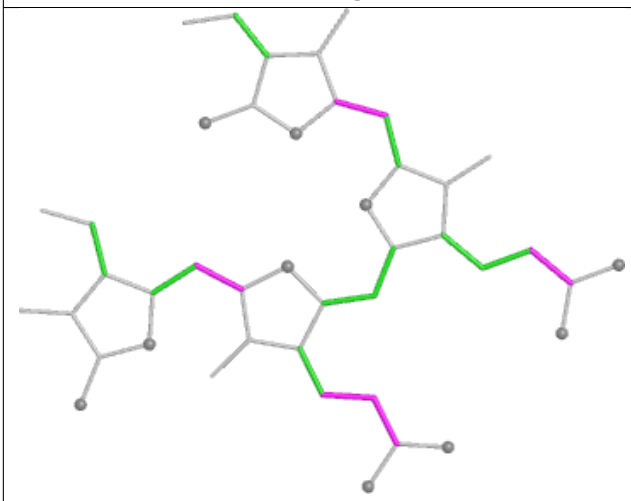

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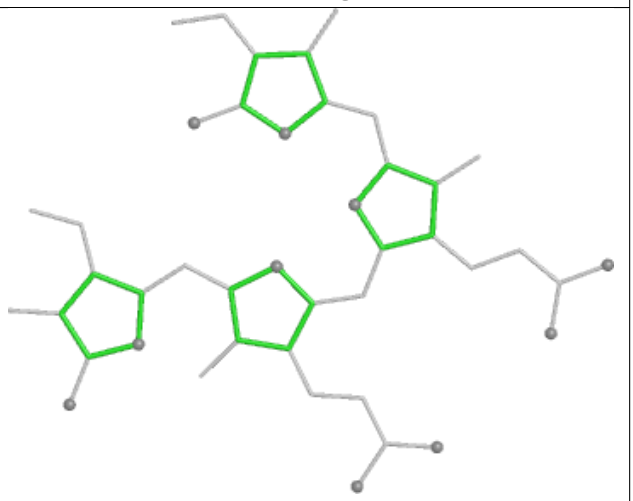
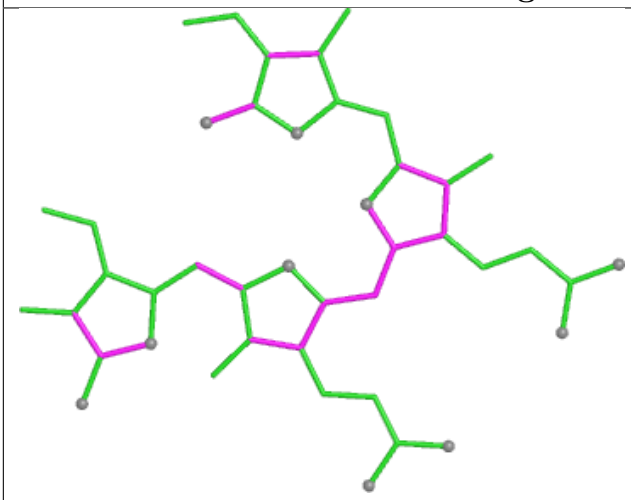


Rings

Ligand PEB tC 202



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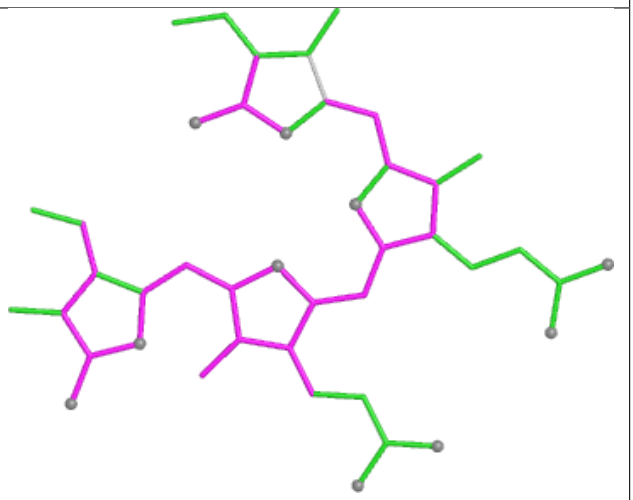

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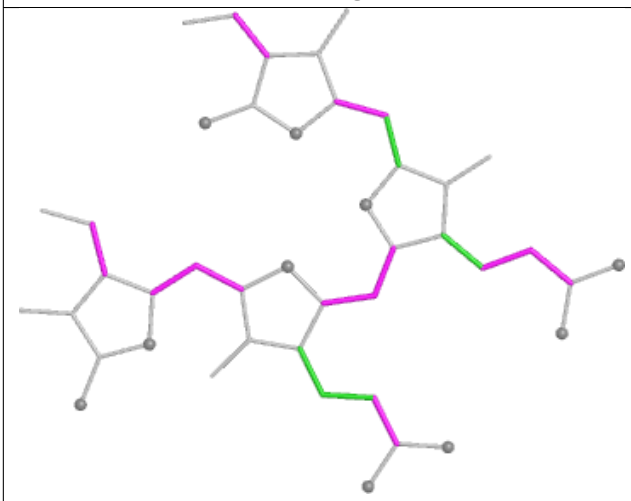

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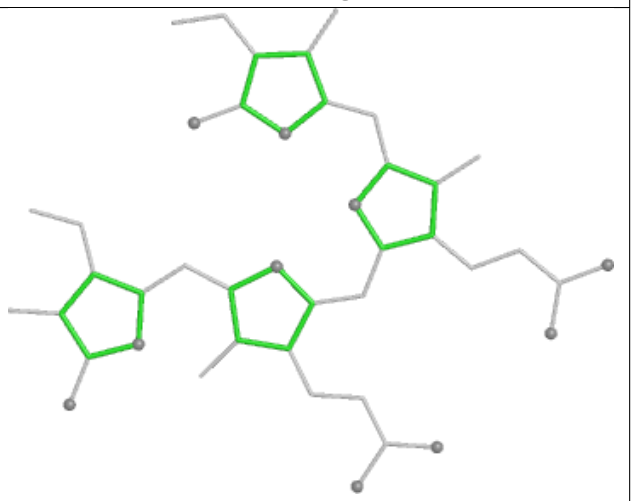
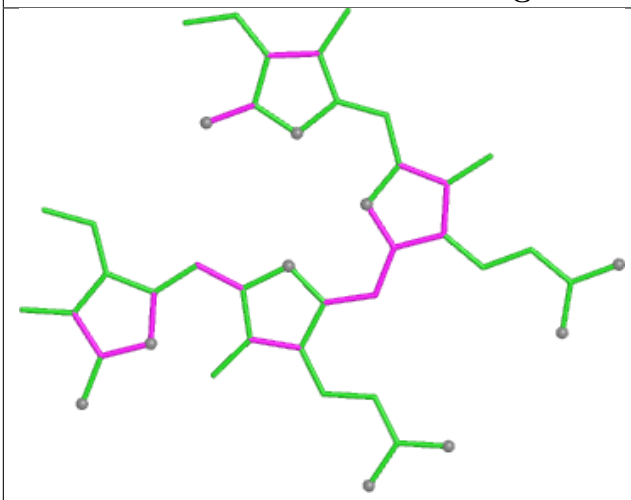


Rings

Ligand PEB bK 201



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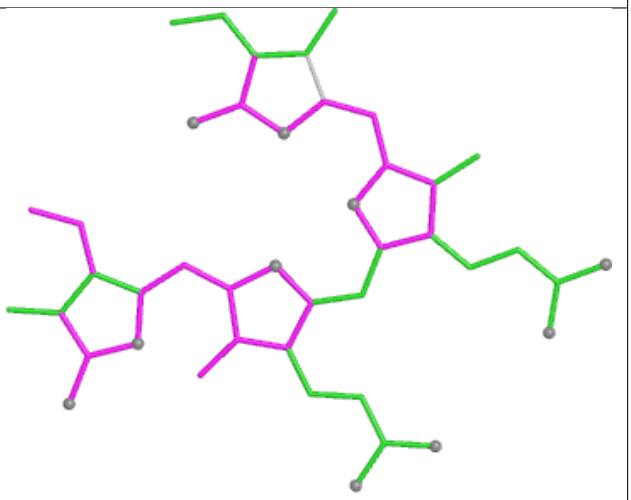
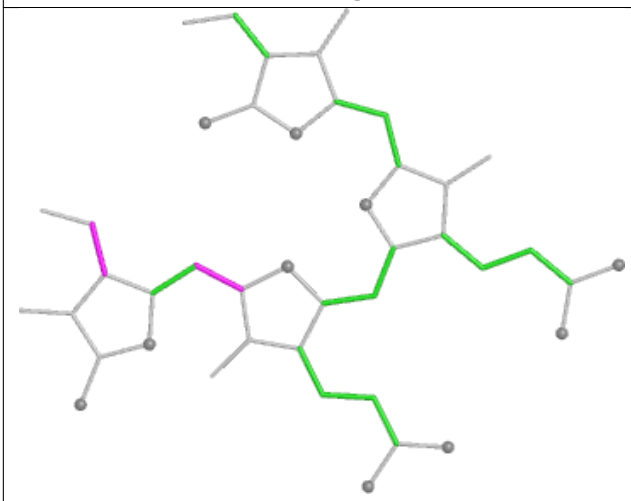


Bond angles



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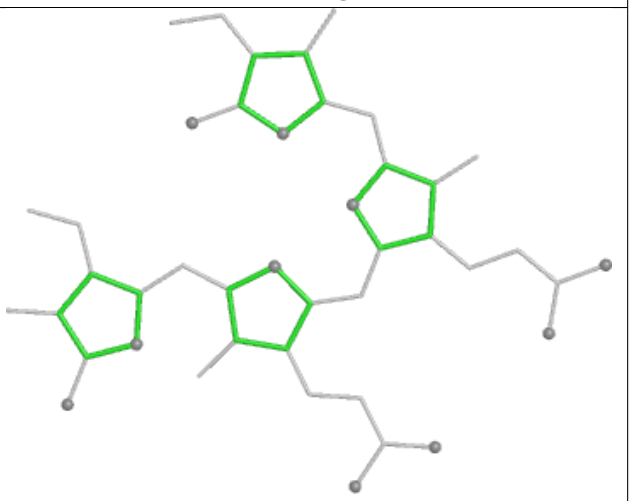
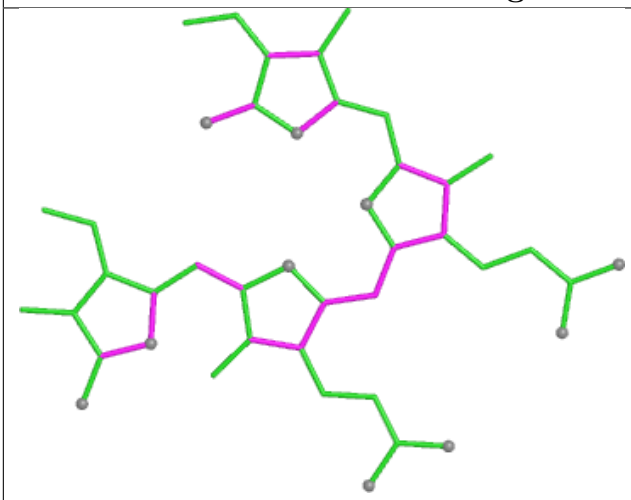


Rings

Ligand PEB AM 301



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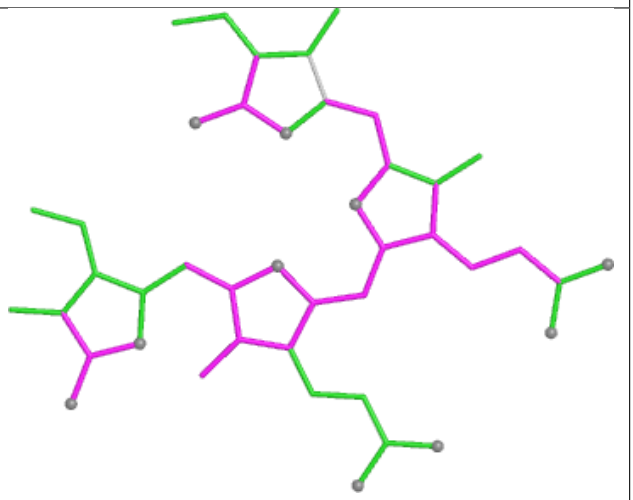
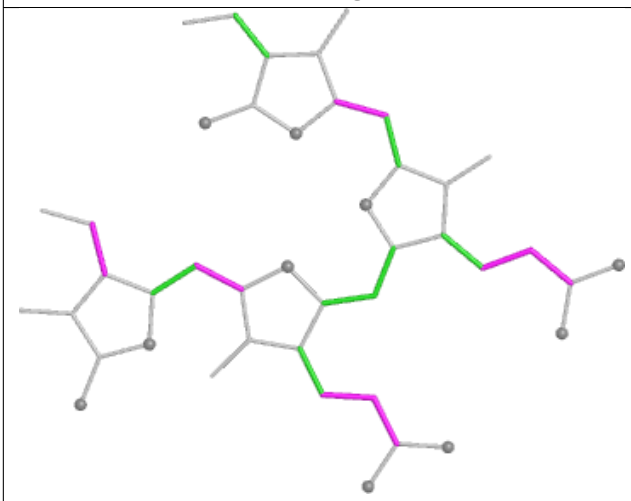
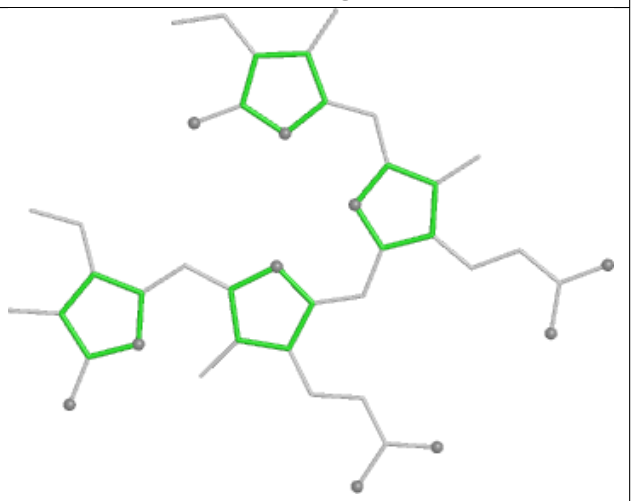


Bond angles

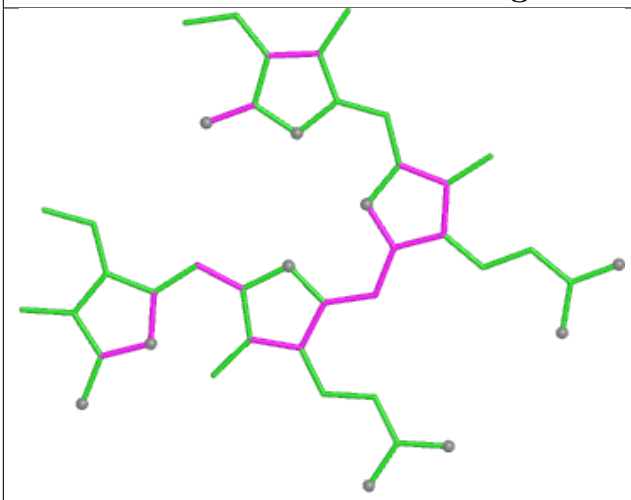


Torsions



Rings

Ligand PEB YQ 202



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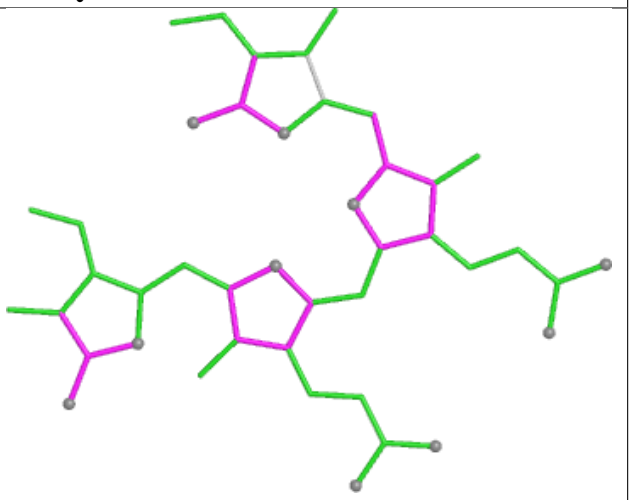
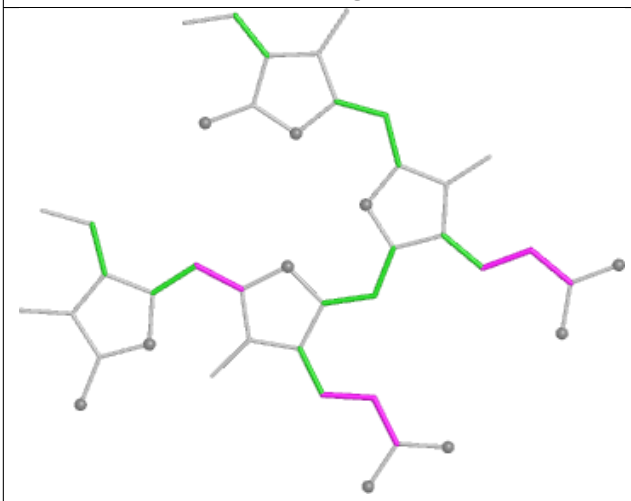


Bond angles



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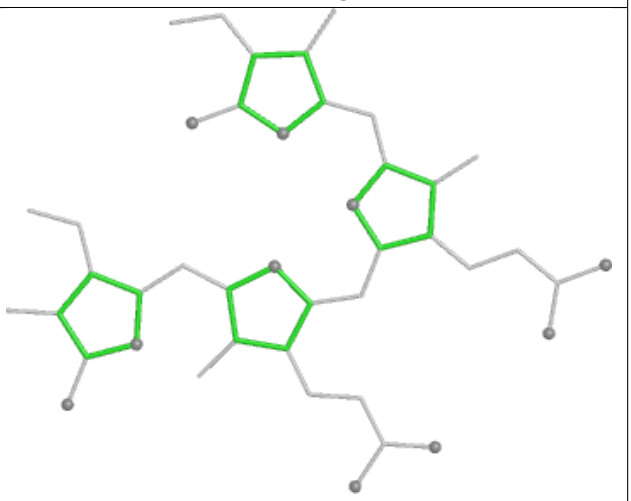
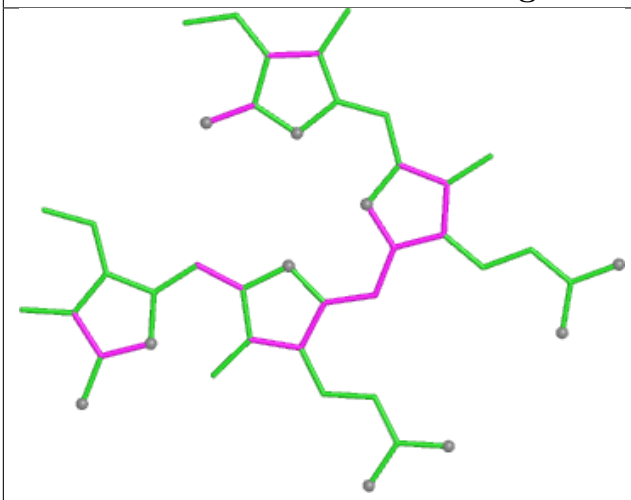


Rings

Ligand PEB p8 202



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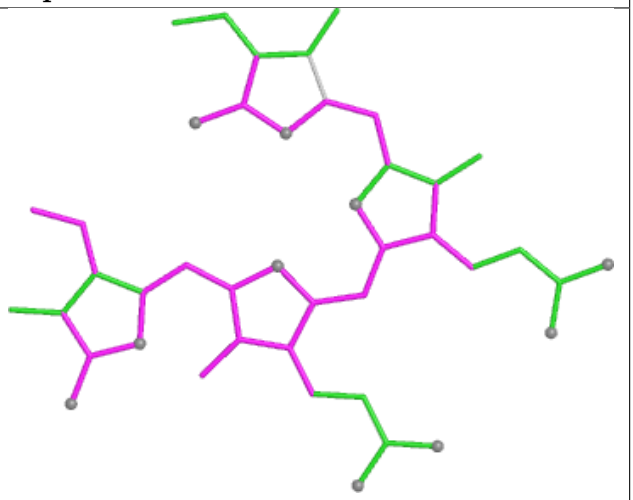

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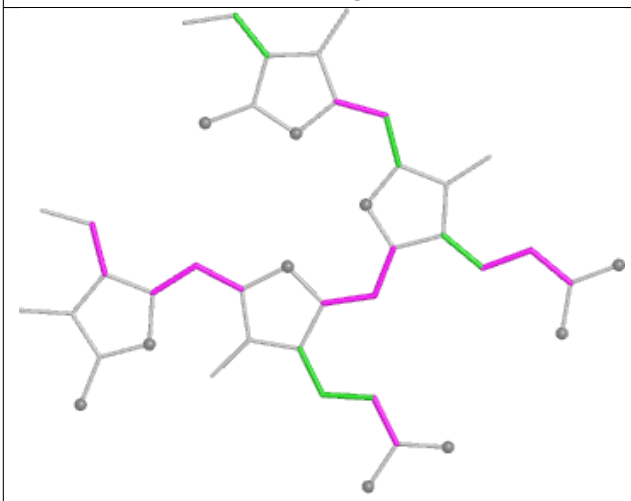

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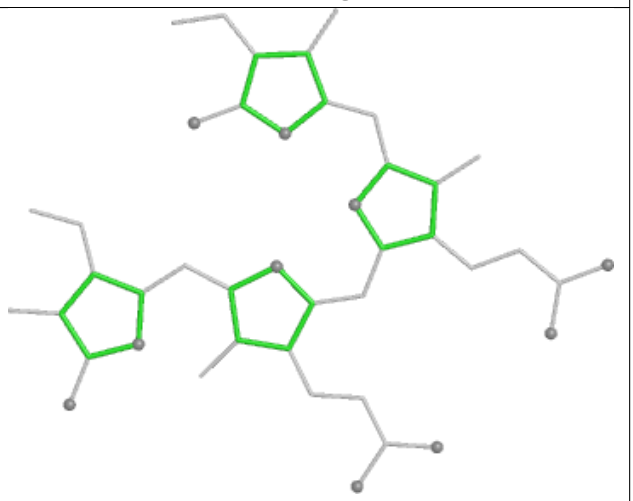
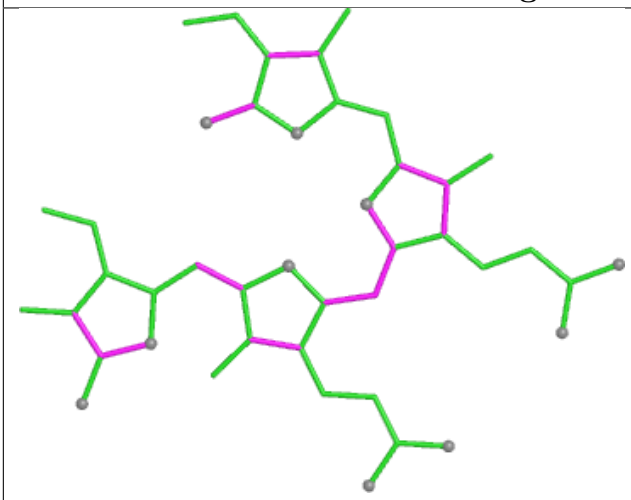


Rings

Ligand PEB FI 202



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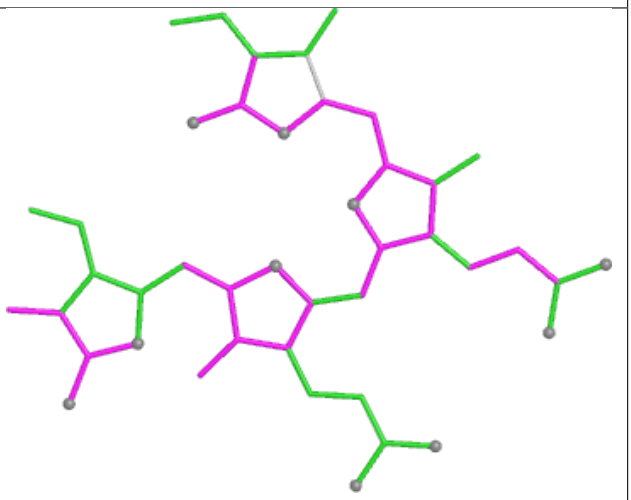

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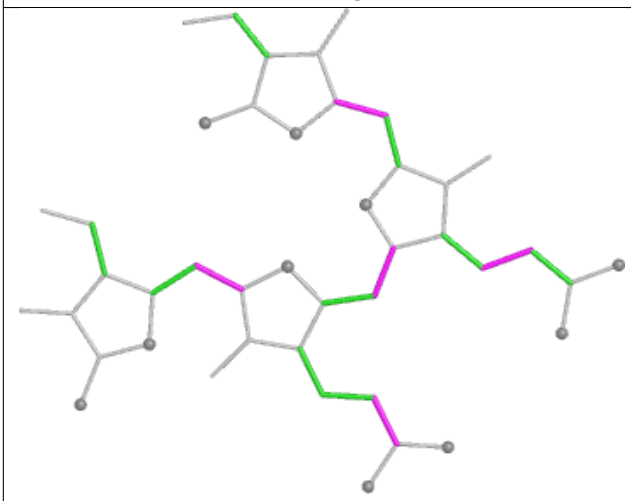

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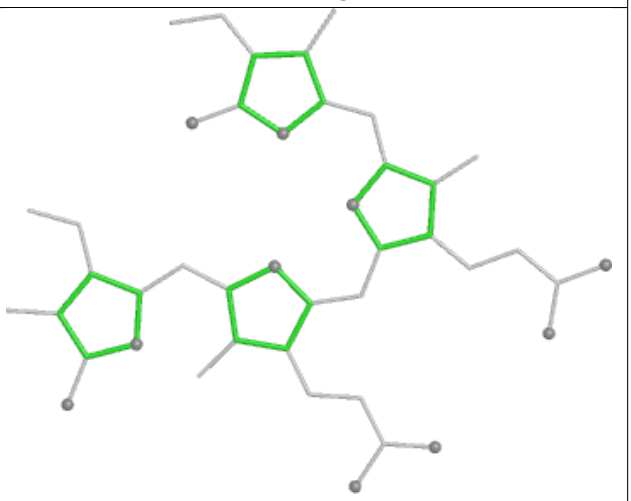
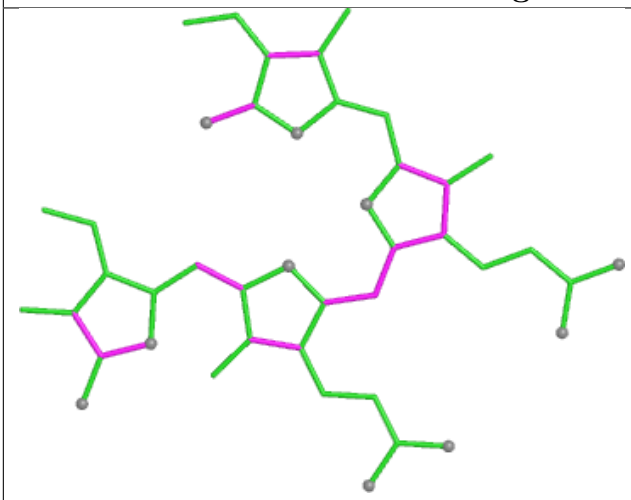


Rings

Ligand PEB NF 201



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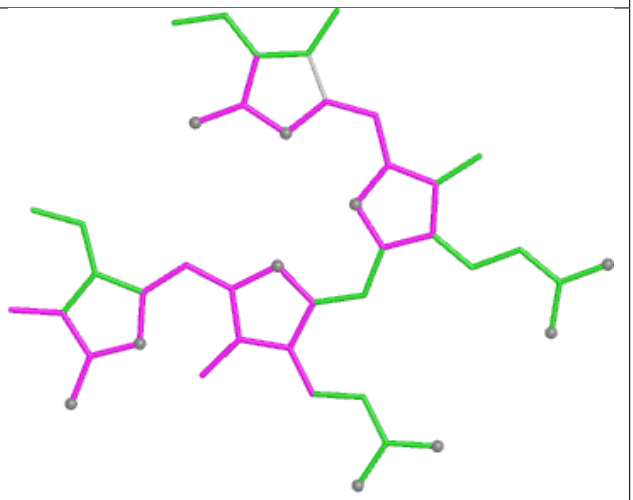

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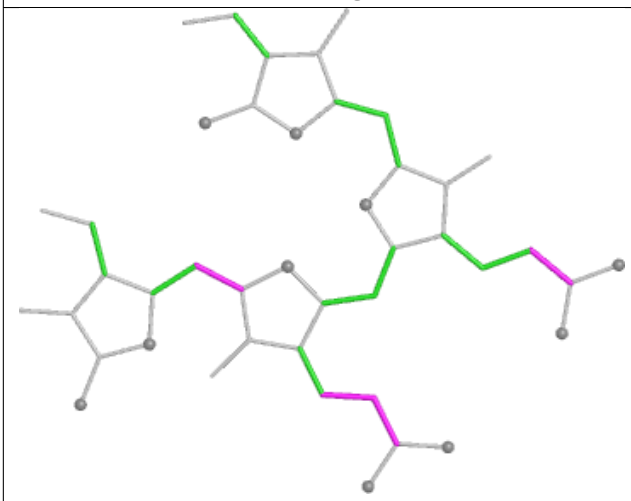

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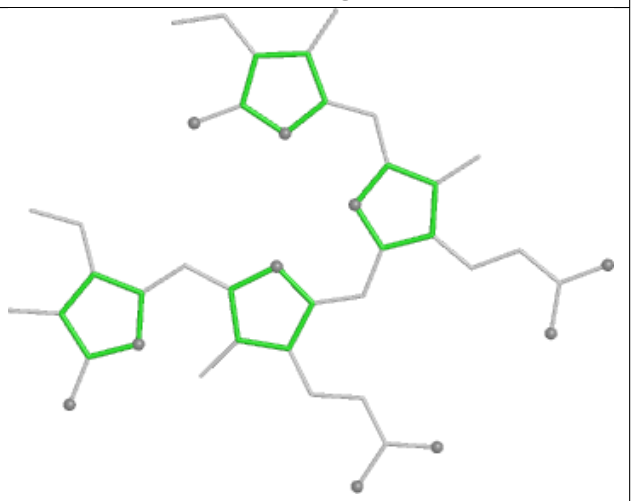
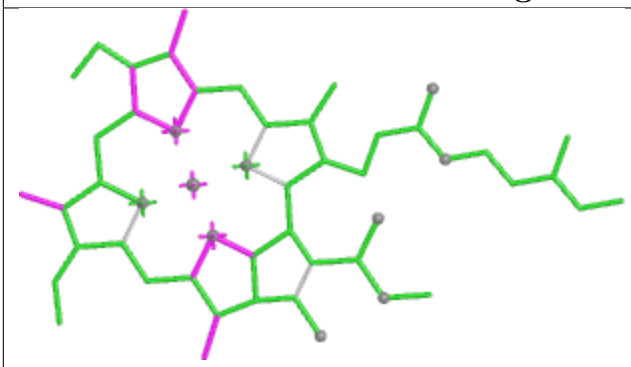


Rings

Ligand CLA A2 837



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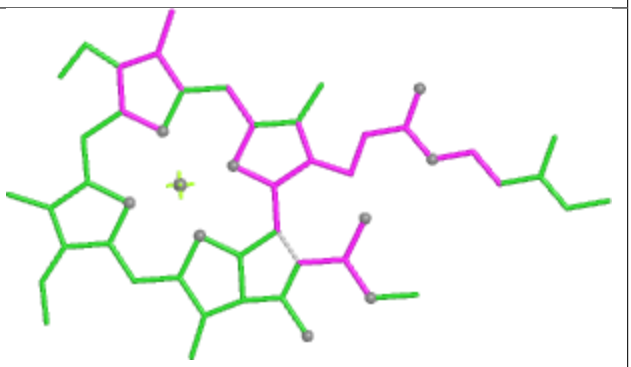

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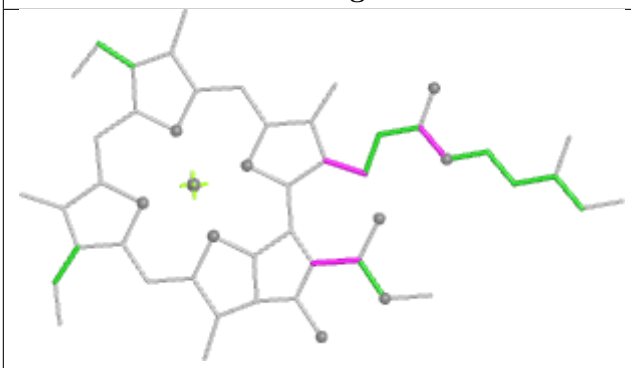

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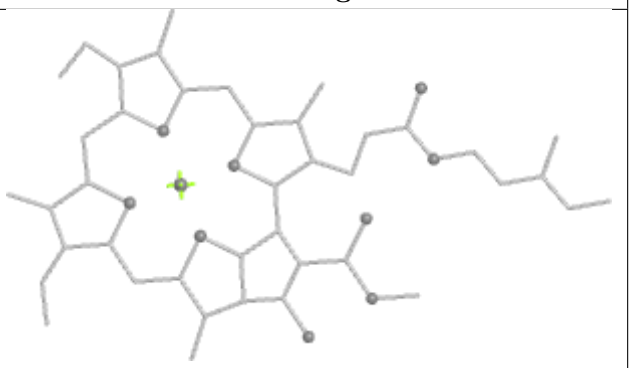
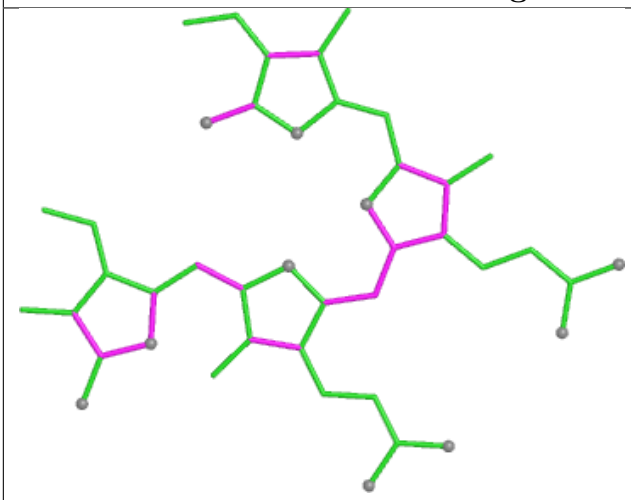


Rings

Ligand PEB UG 202



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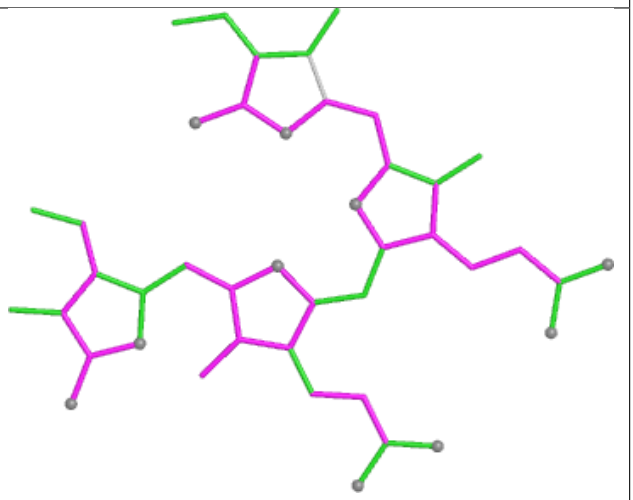

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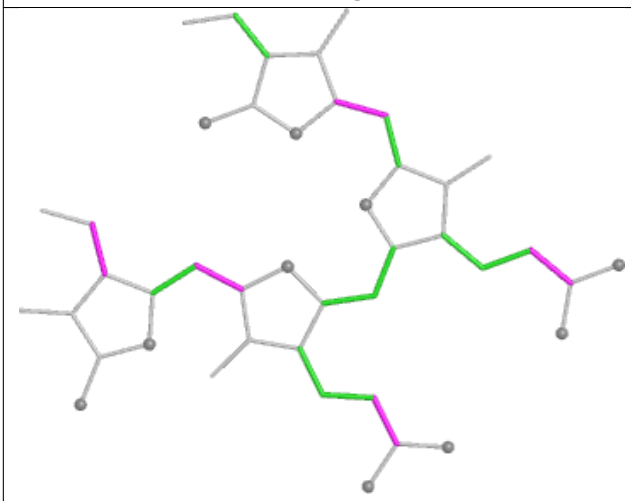

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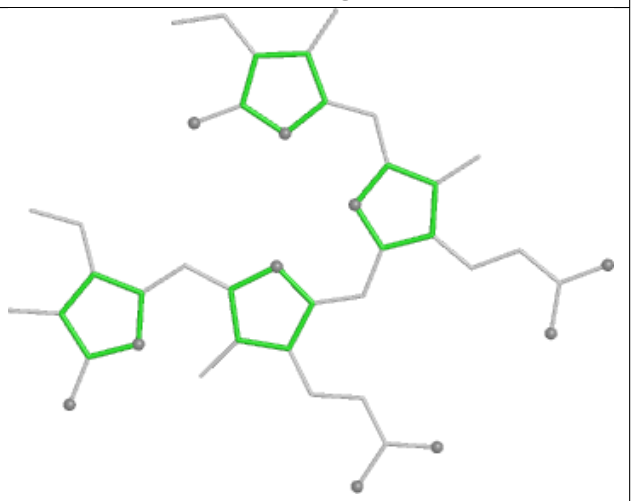
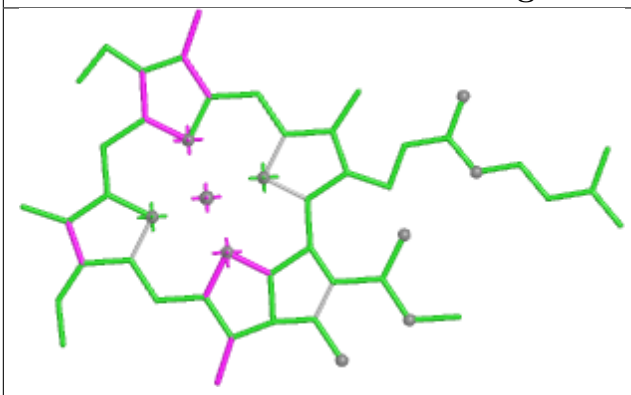


Rings

Ligand CLA L2 204



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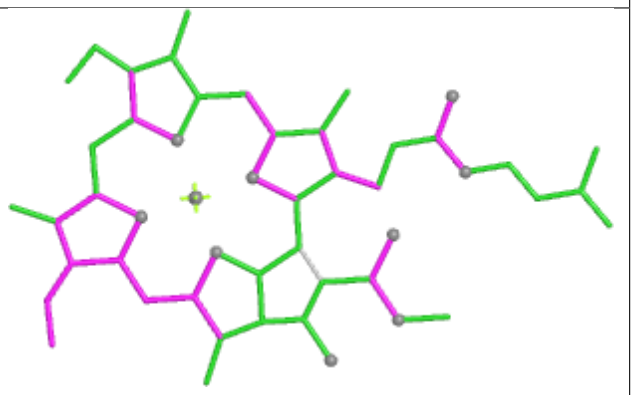

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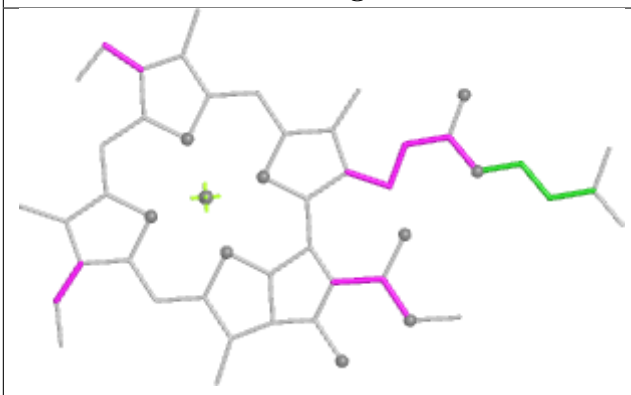

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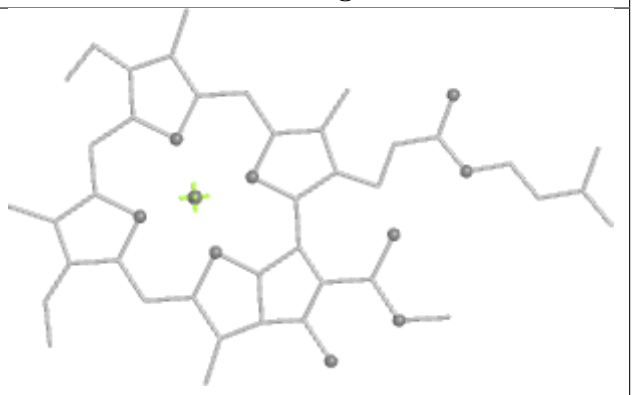
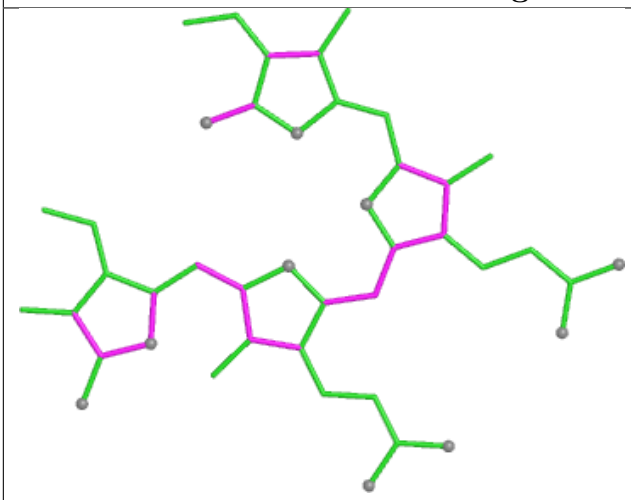


Rings

Ligand PEB BA 201



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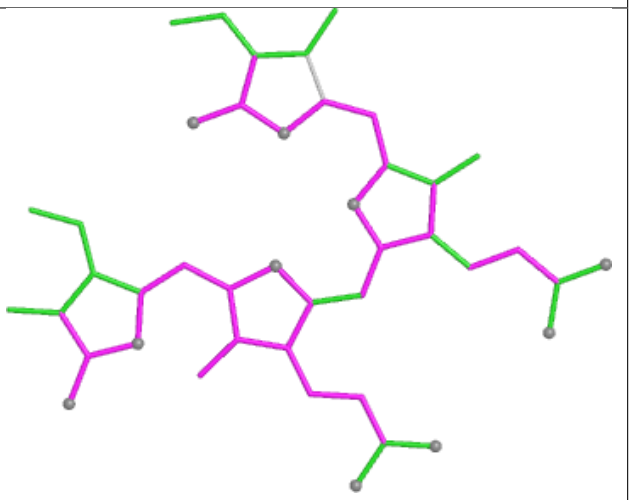

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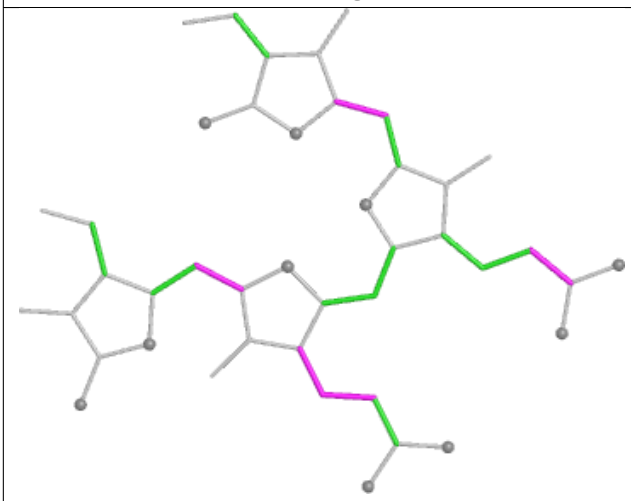

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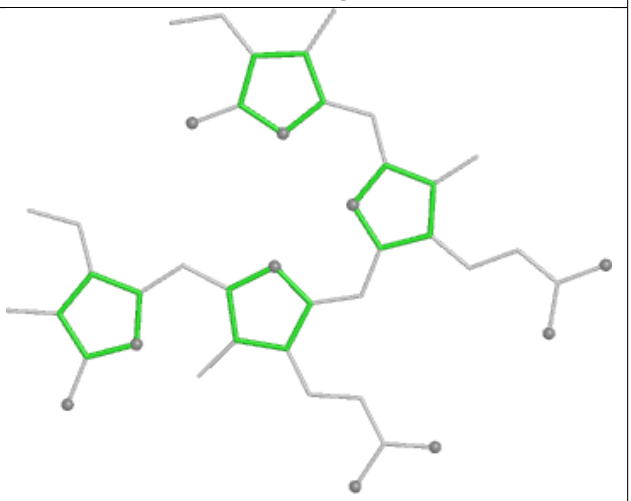
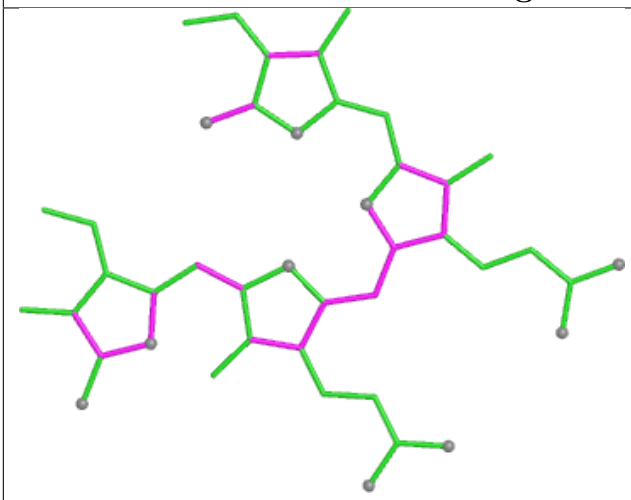


Rings

Ligand PEB Y9 201



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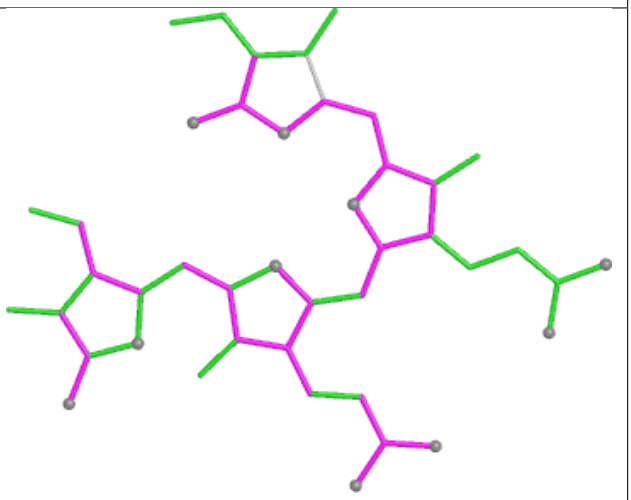

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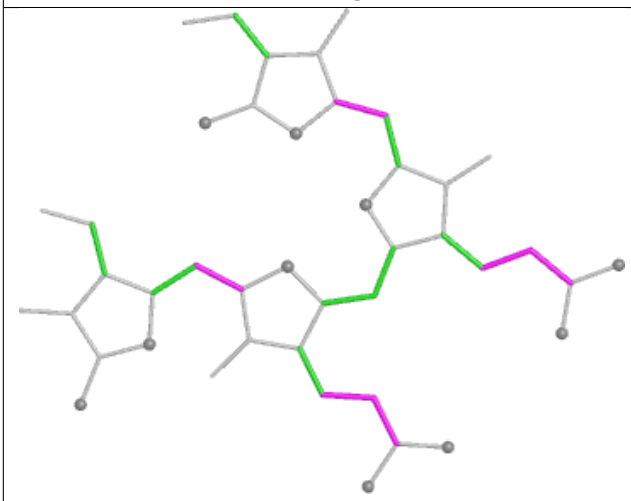

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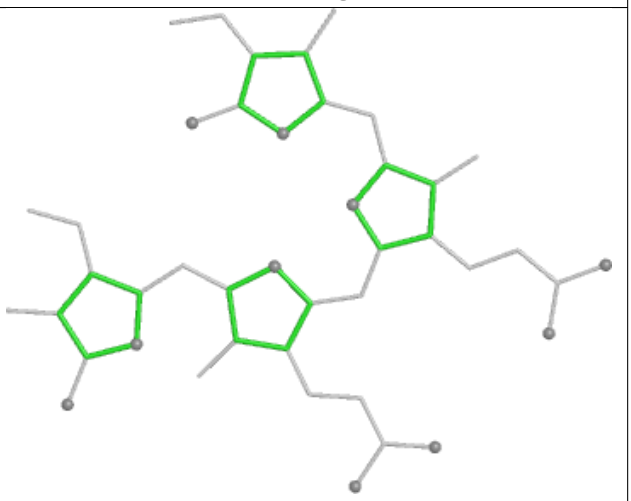
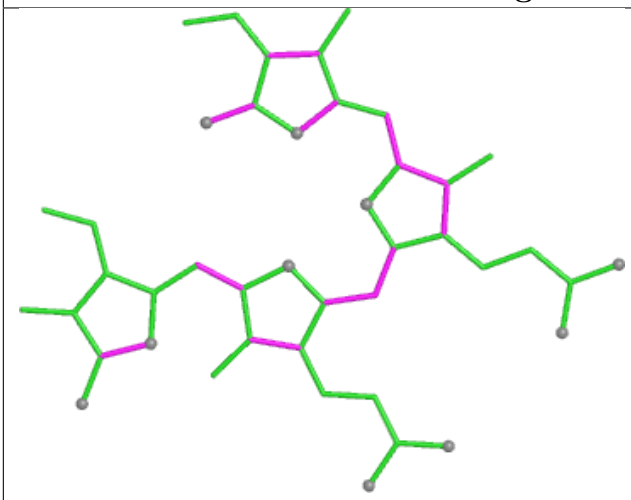


Rings

Ligand PEB JQ 202



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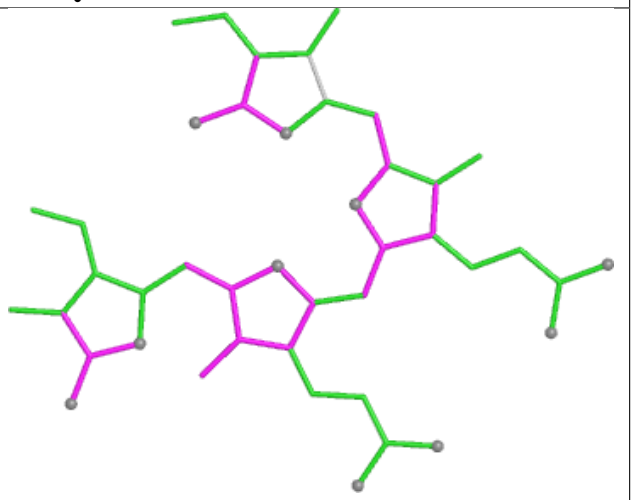

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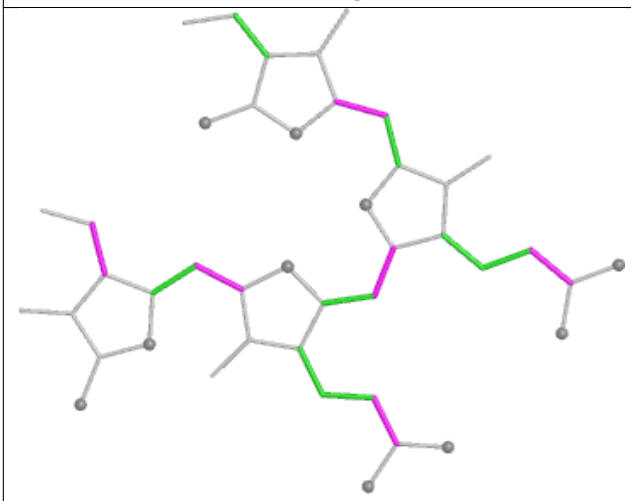

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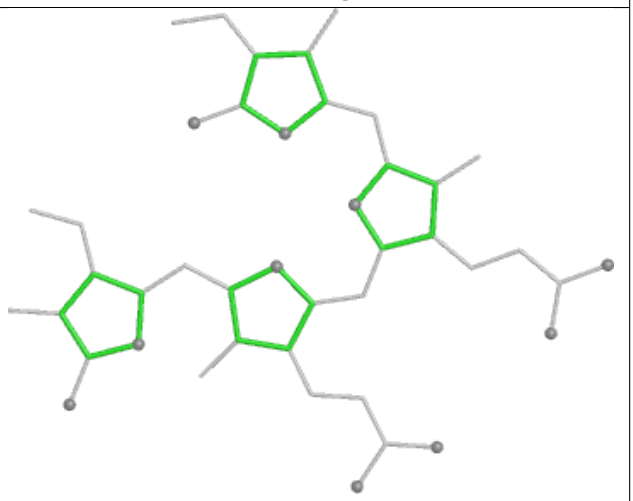
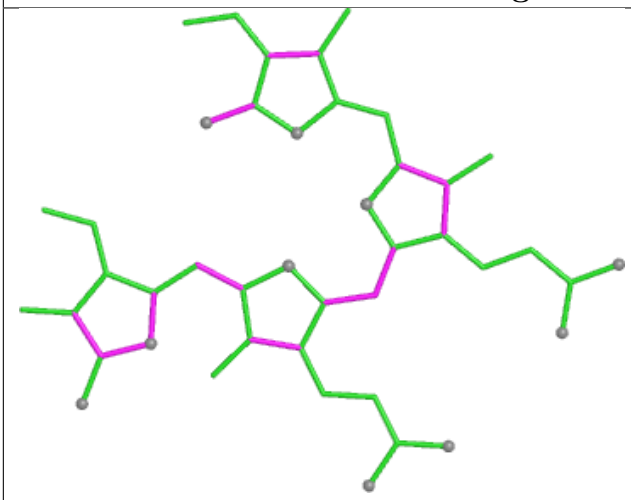


Rings

Ligand PEB OP 202



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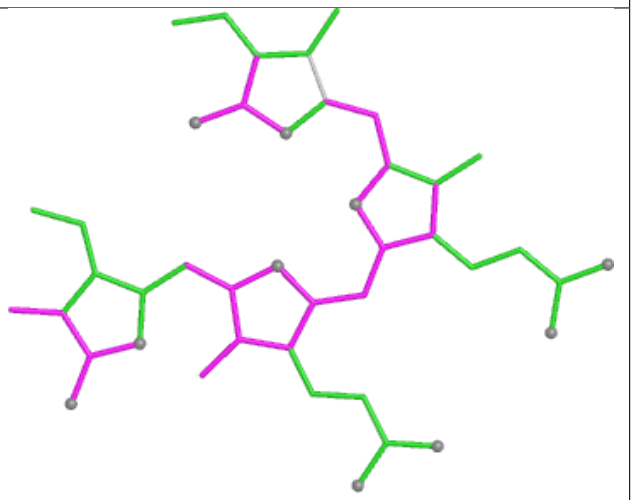

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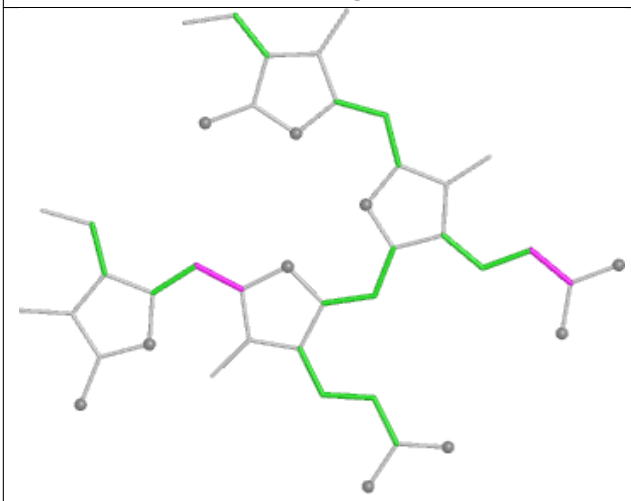

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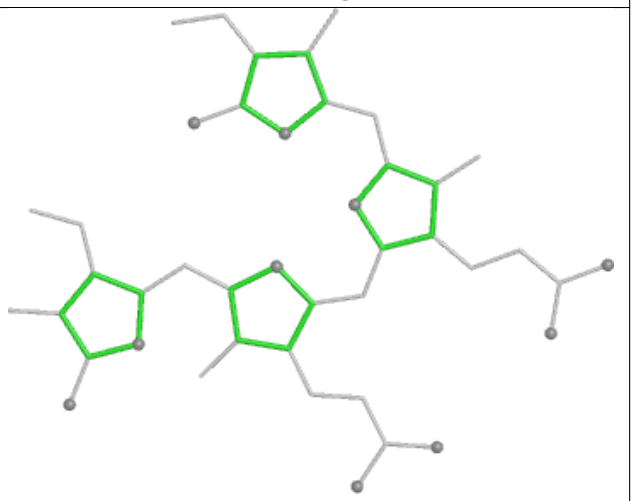
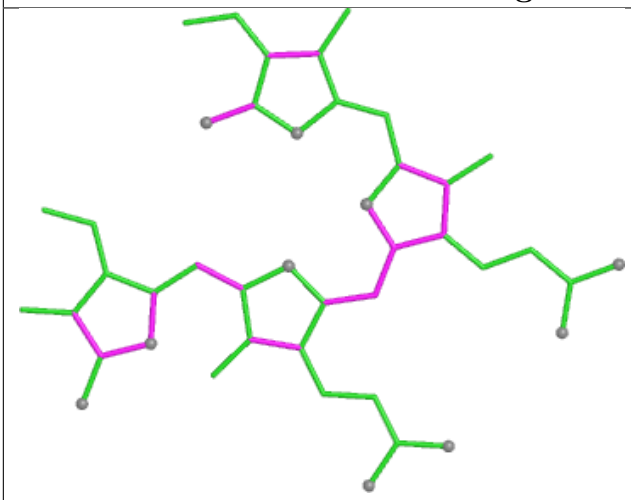


Rings

Ligand PEB R5 202



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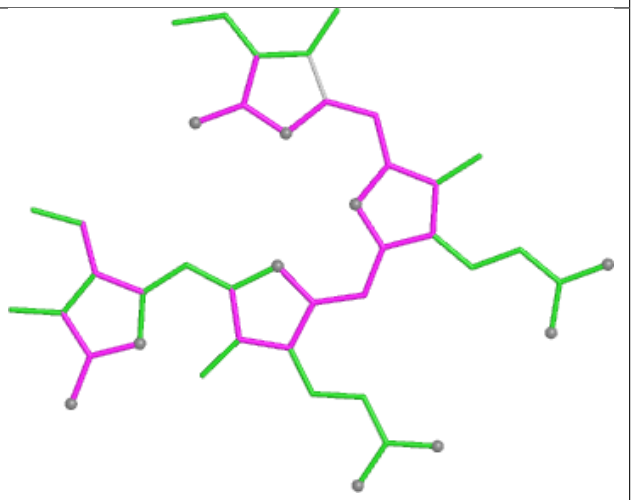

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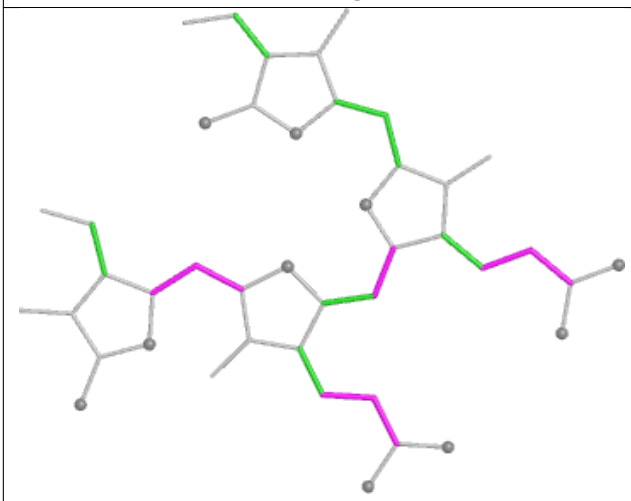

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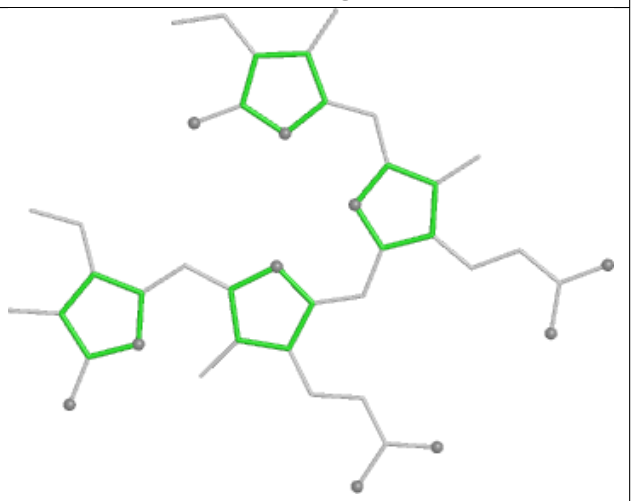
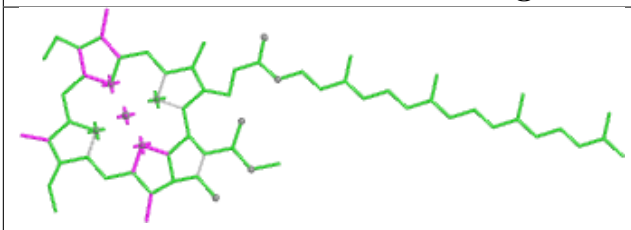


Rings

Ligand CLA B2 807



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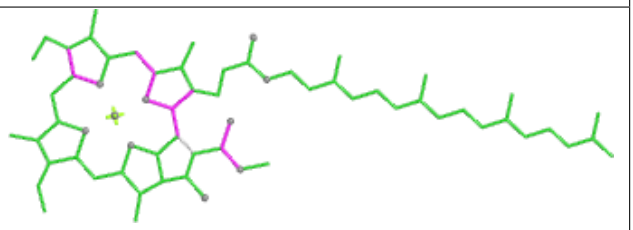

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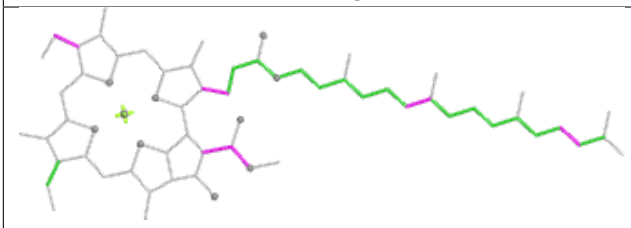

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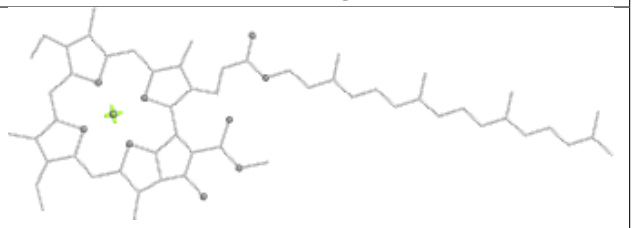
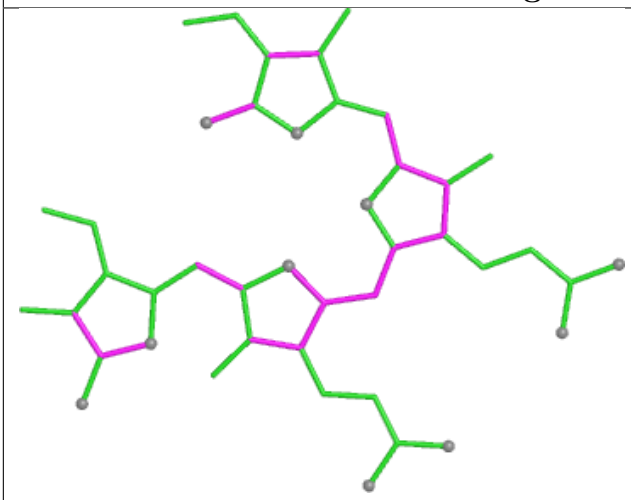


Rings

Ligand PEB l1 203



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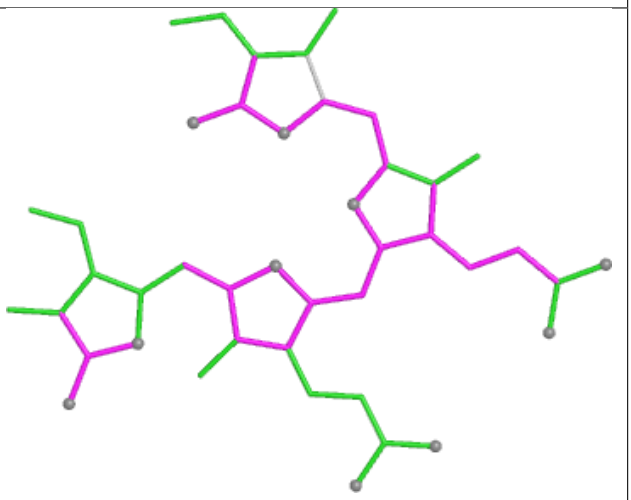
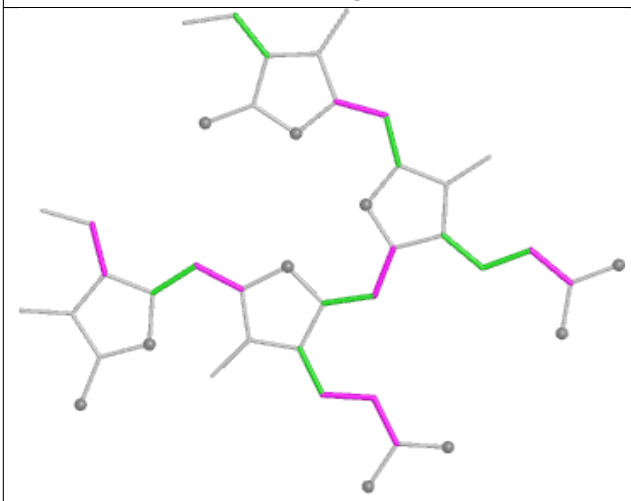


Bond angles



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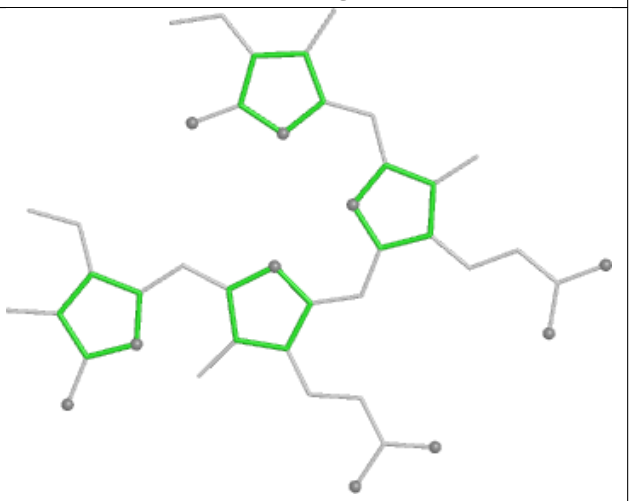
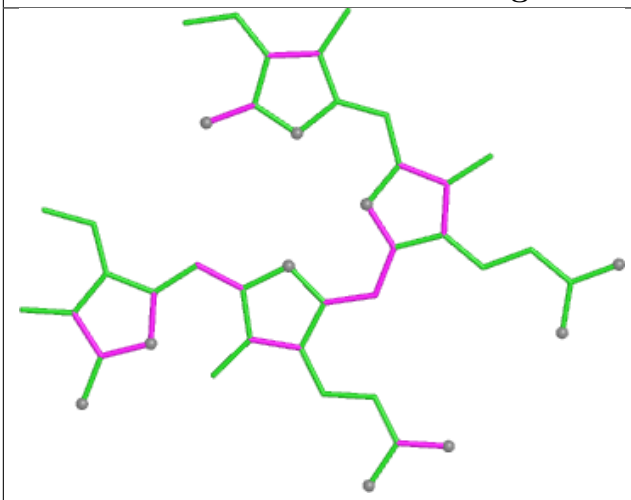
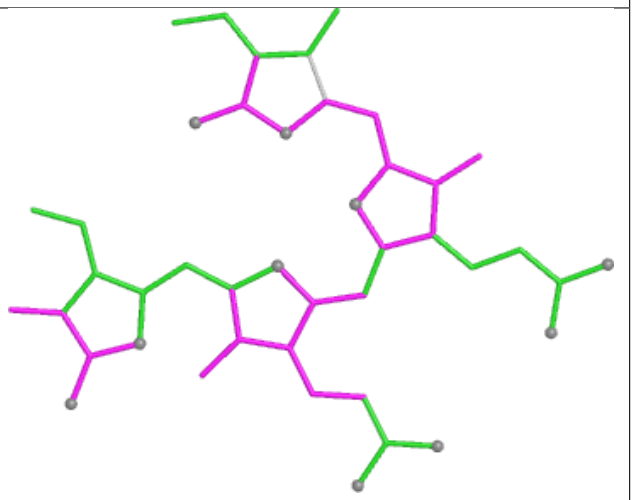


Rings

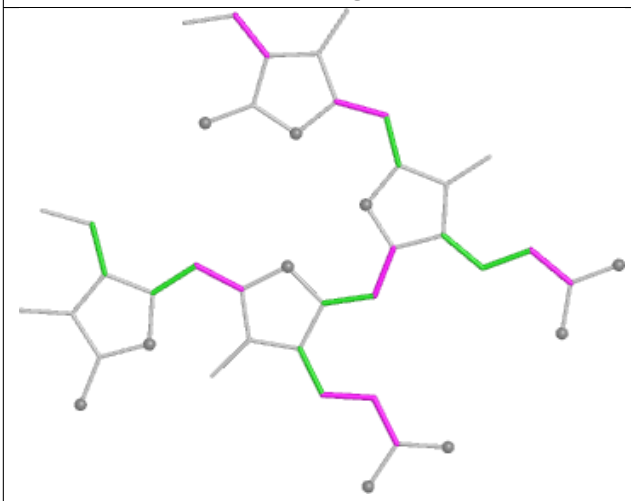
Ligand PEB NB 203



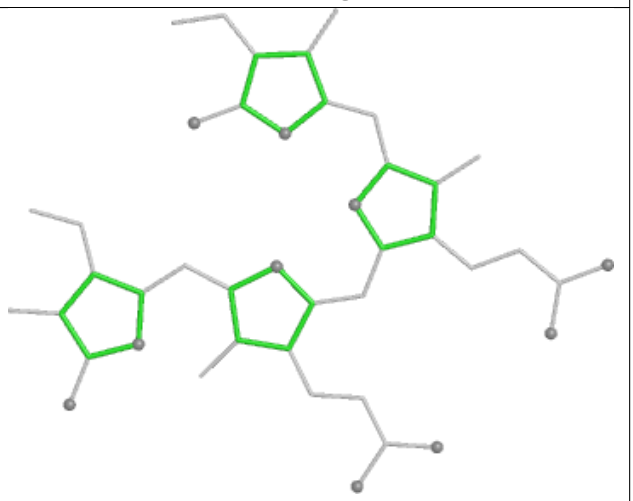
Bond lengths



Bond angles

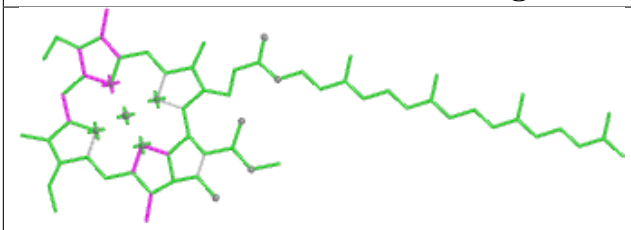


Torsions



Rings

Ligand CLA BN 830



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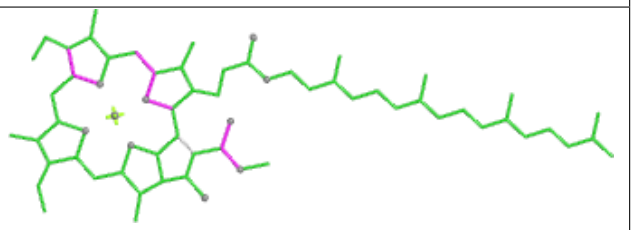

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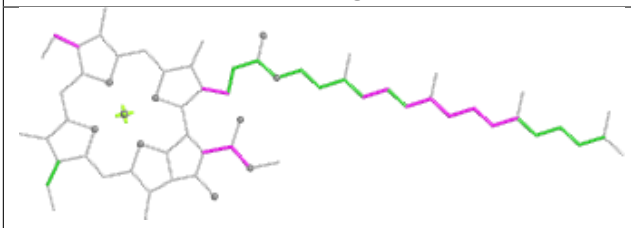

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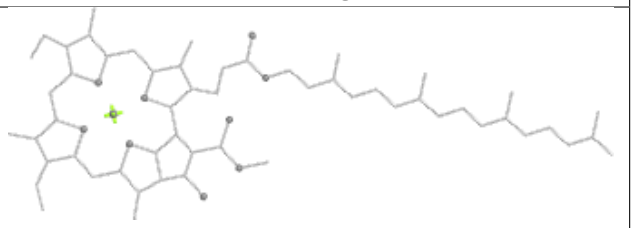
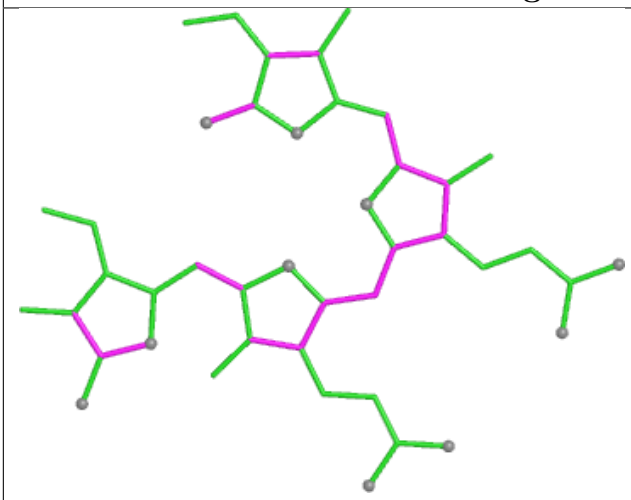


Rings

Ligand PEB f1 203



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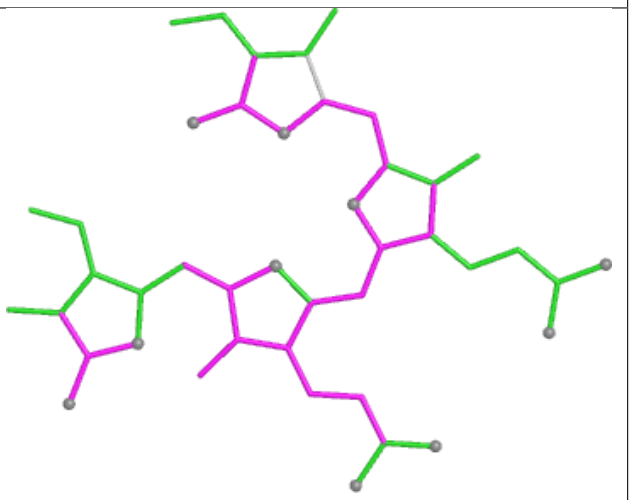

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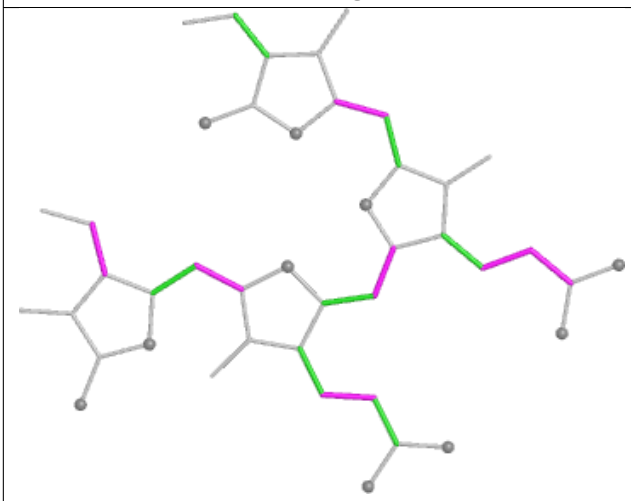

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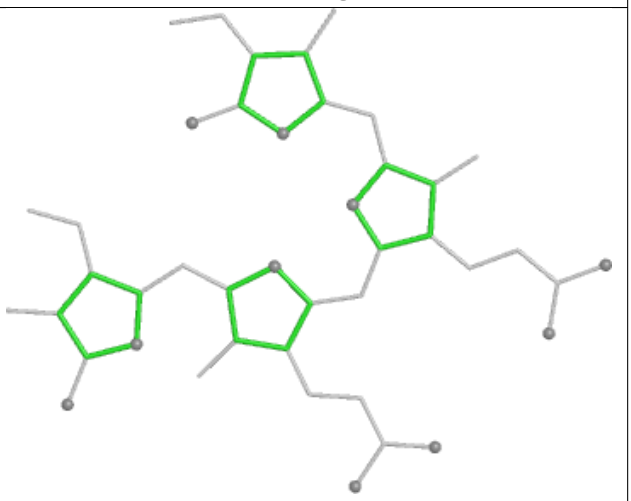
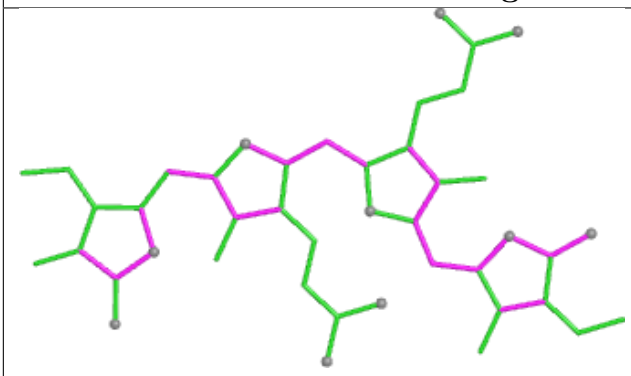


Rings

Ligand CYC LG 1001



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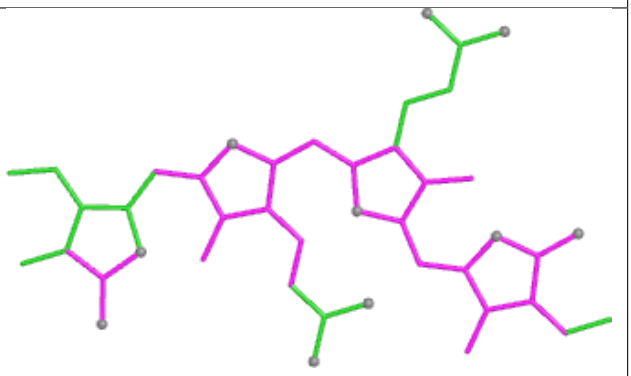
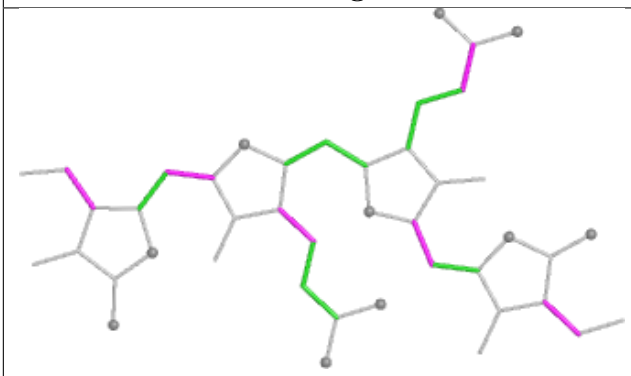


Bond angles



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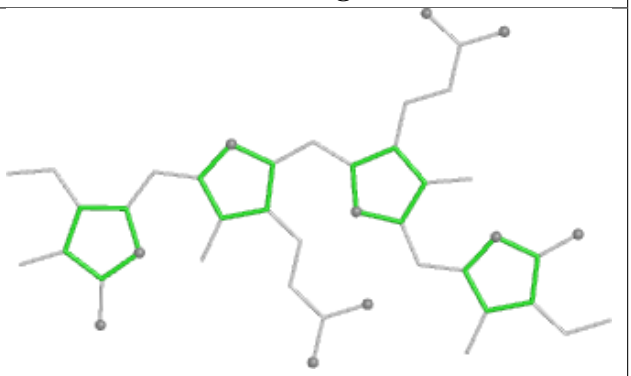
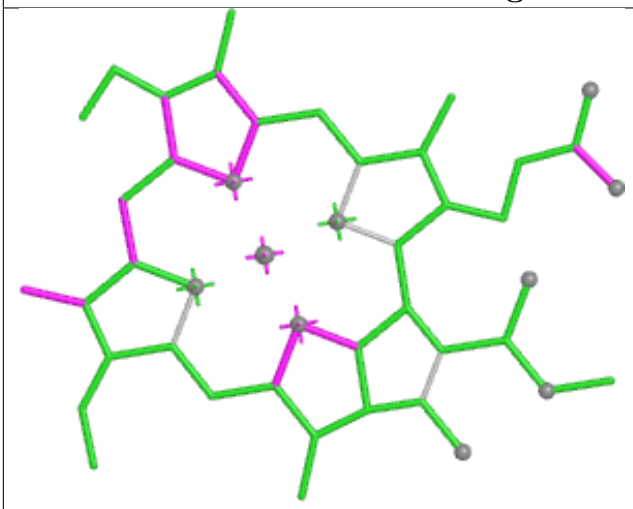


Rings

Ligand CLA MN 101



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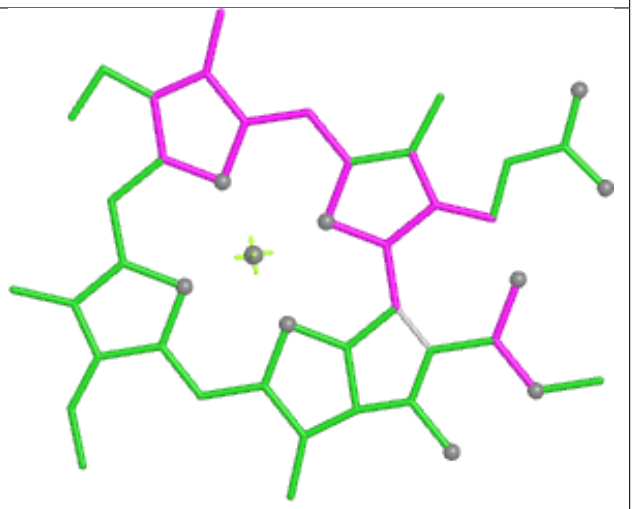
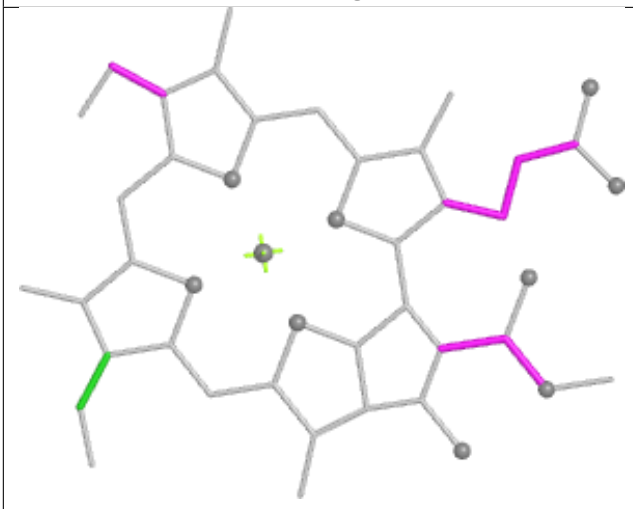


Bond angles

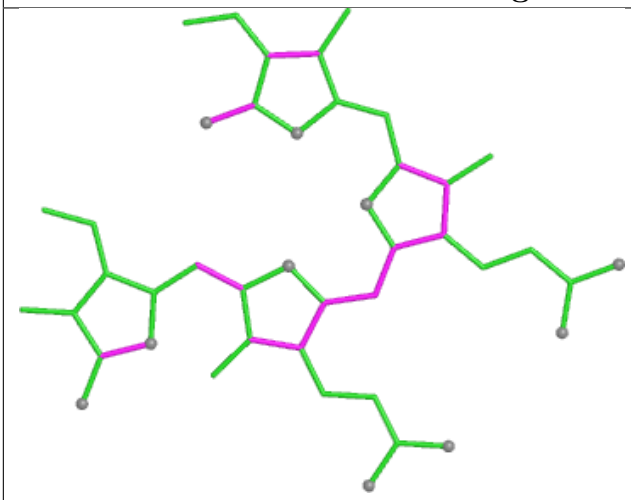


Torsions



Rings

Ligand PEB TO 203



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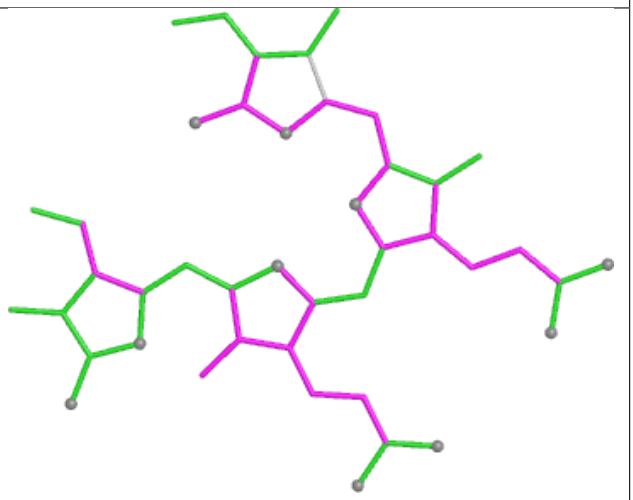

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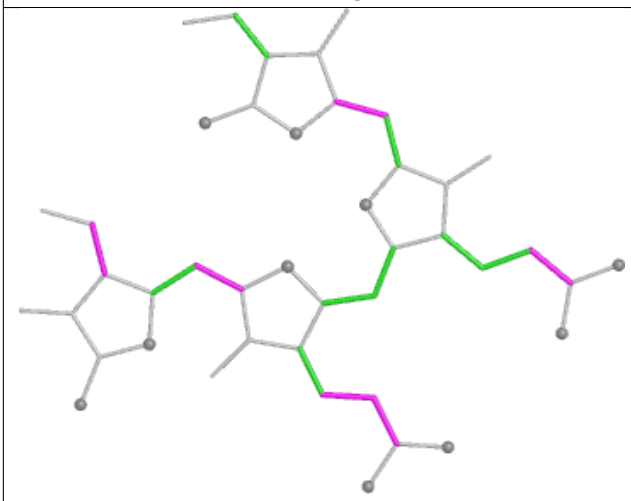

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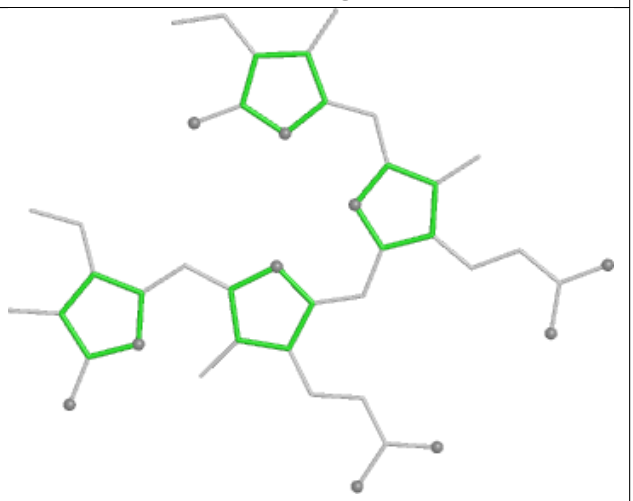
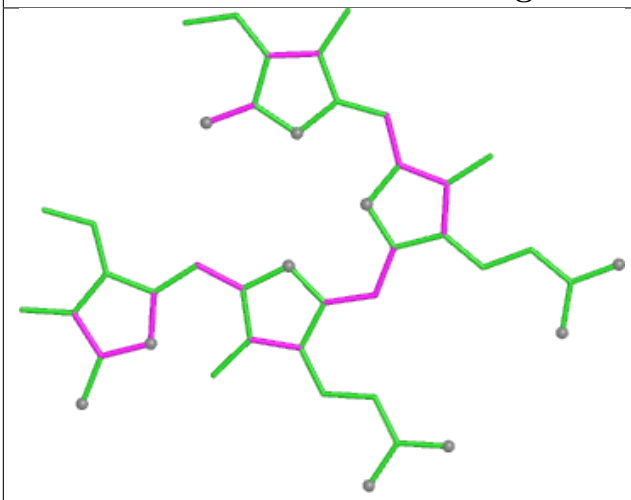


Rings

Ligand PEB V4 202



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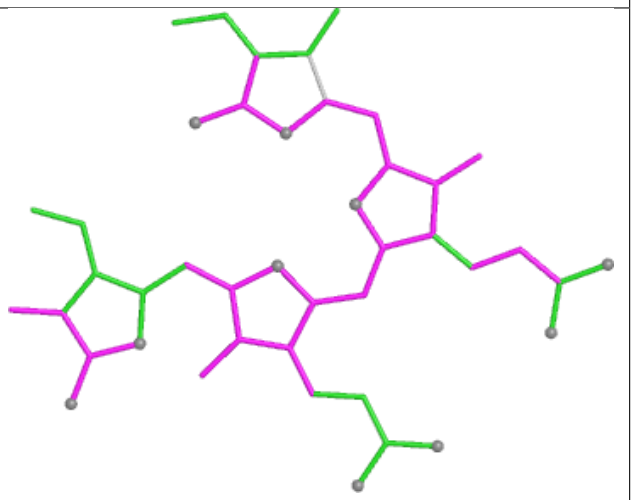
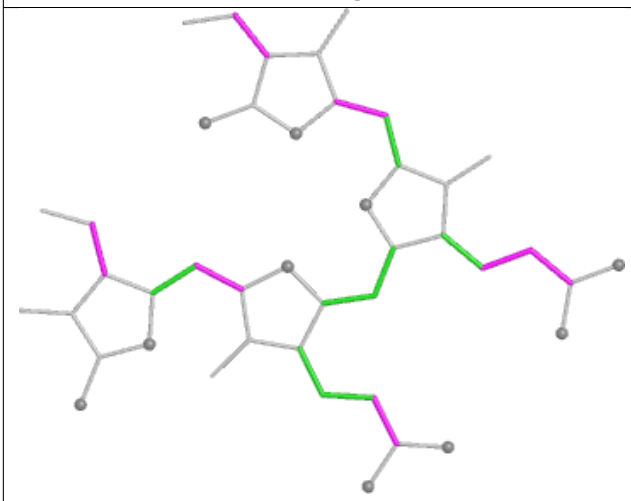


Bond angles



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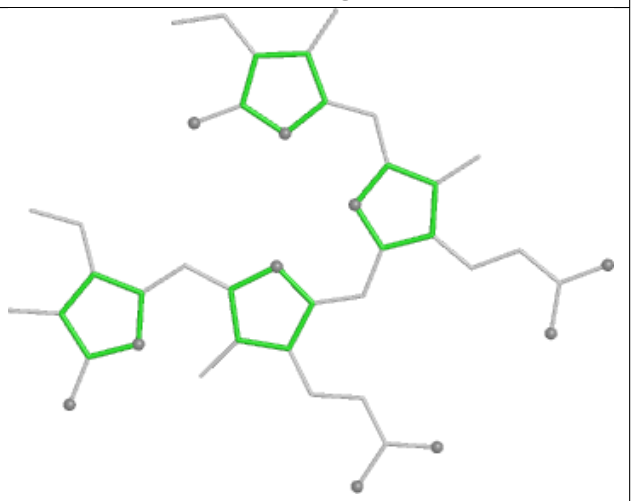
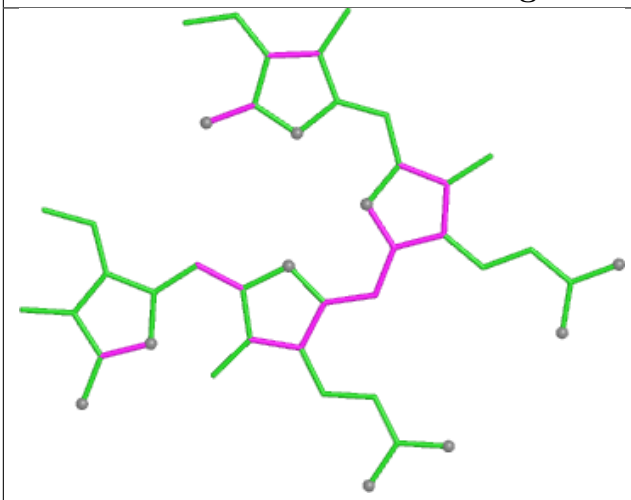


Rings

Ligand PEB x8 201



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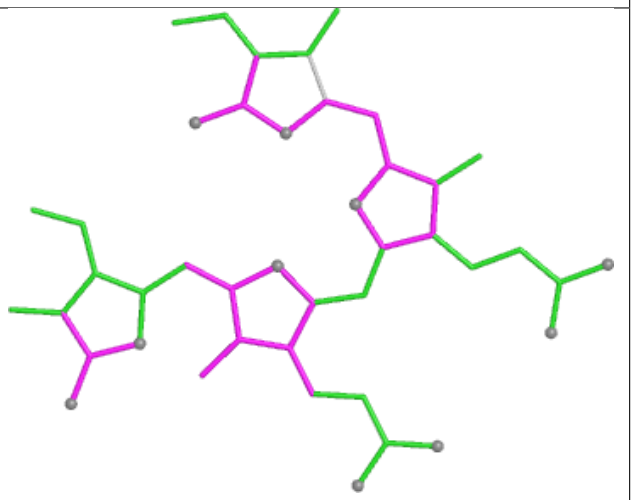
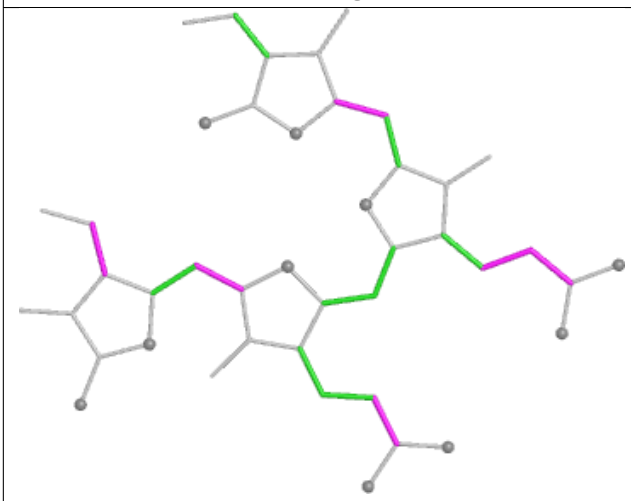


Bond angles



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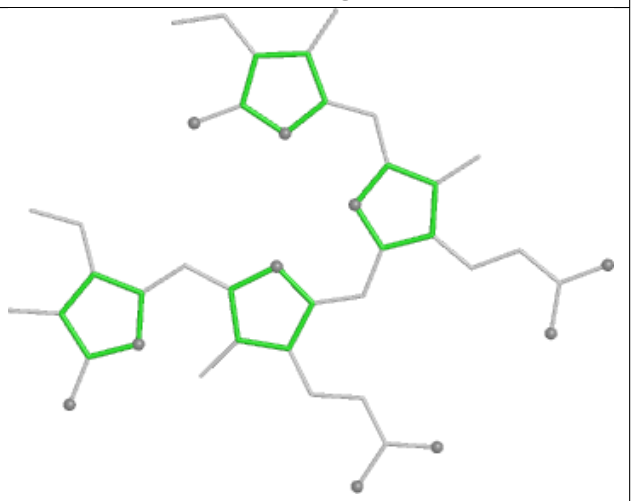
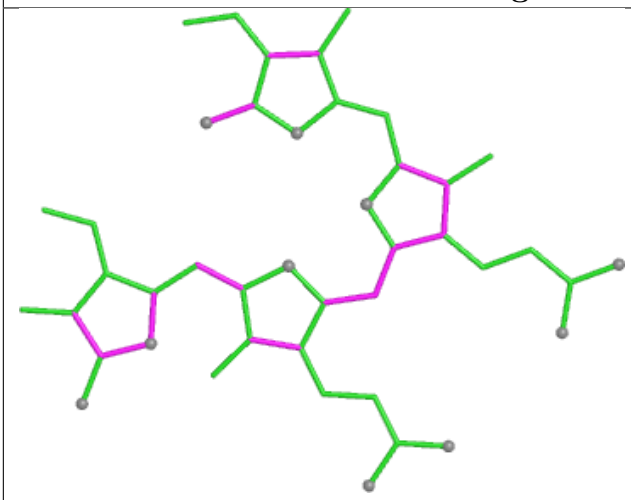


Rings

Ligand PEB NP 202



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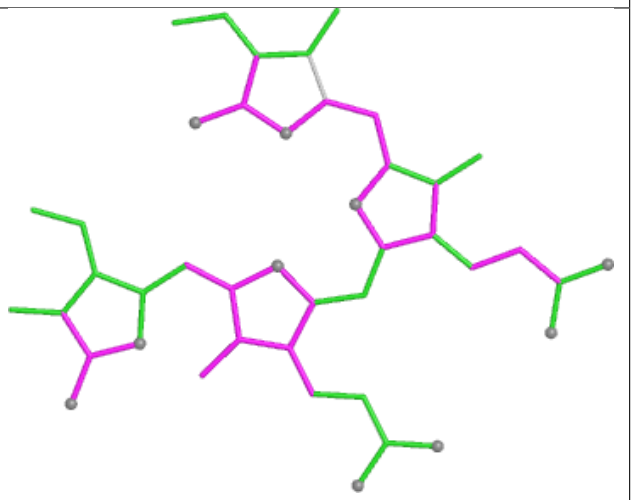
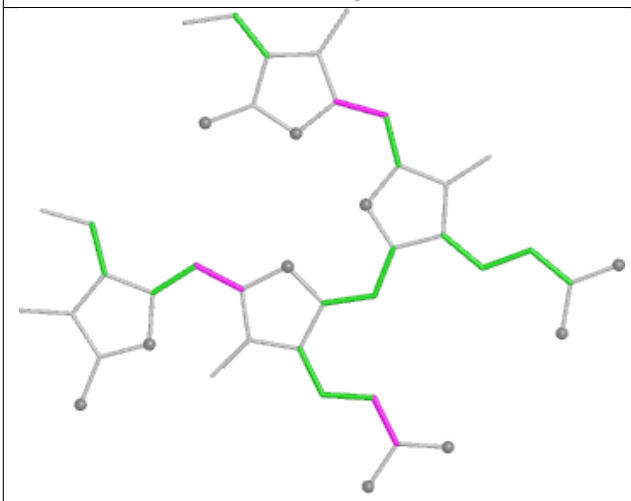


Bond angles



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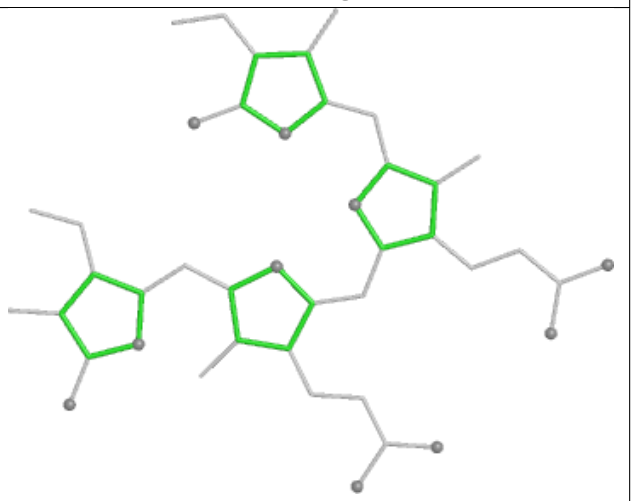
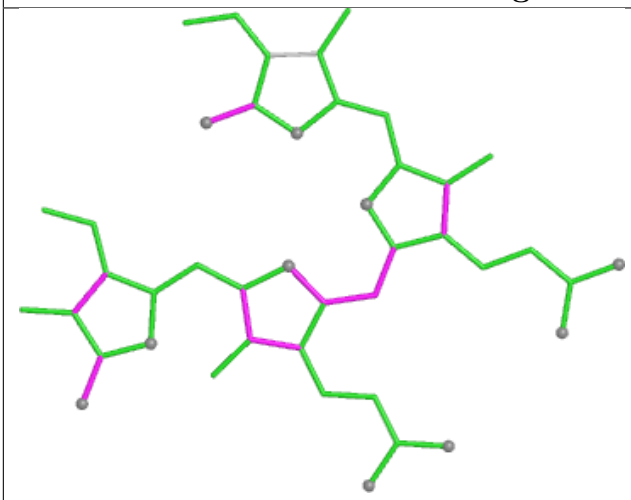


Rings

Ligand PUB yK 303



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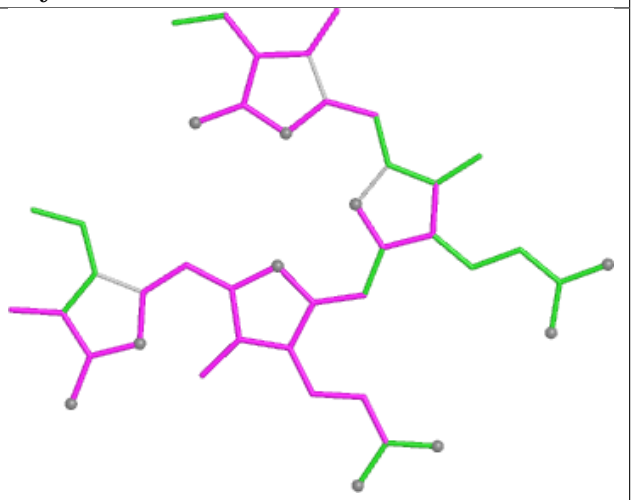
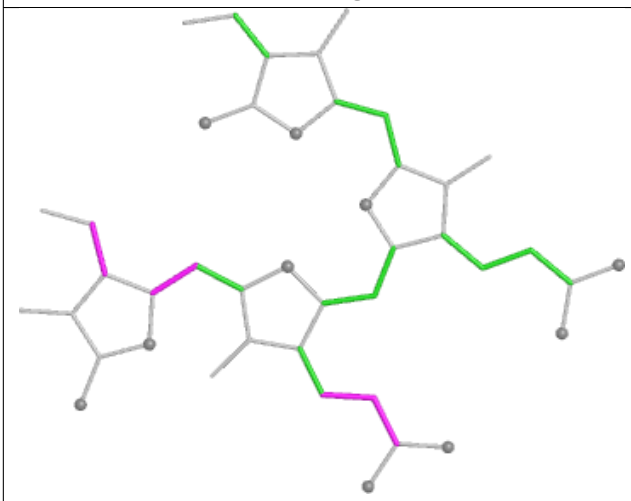


Bond angles



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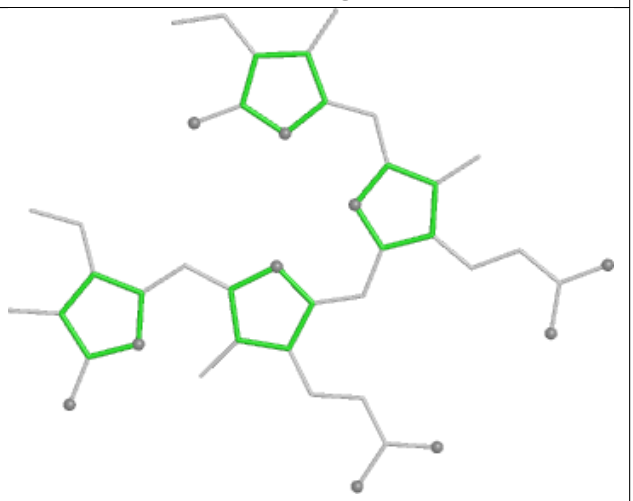
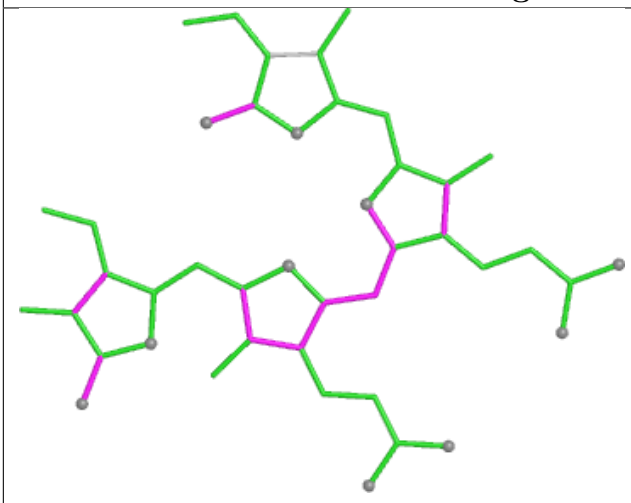


Rings

Ligand PUB xK 301



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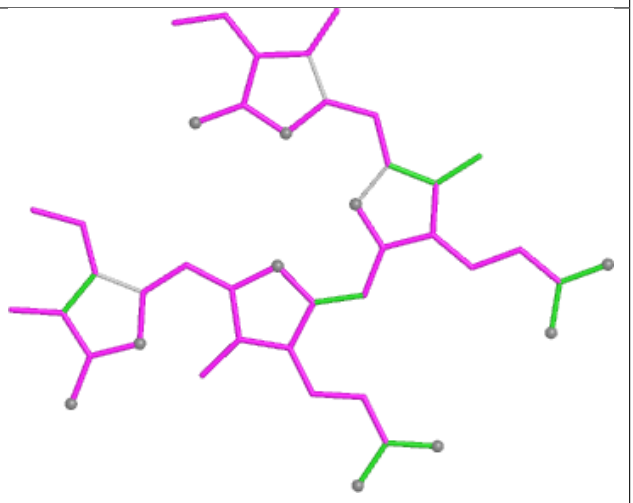
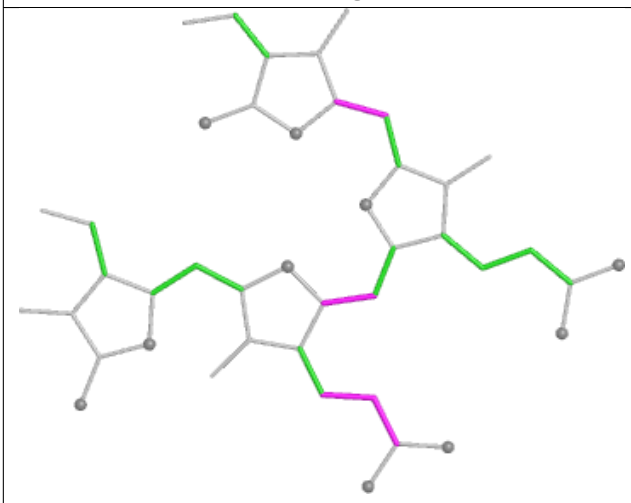


Bond angles



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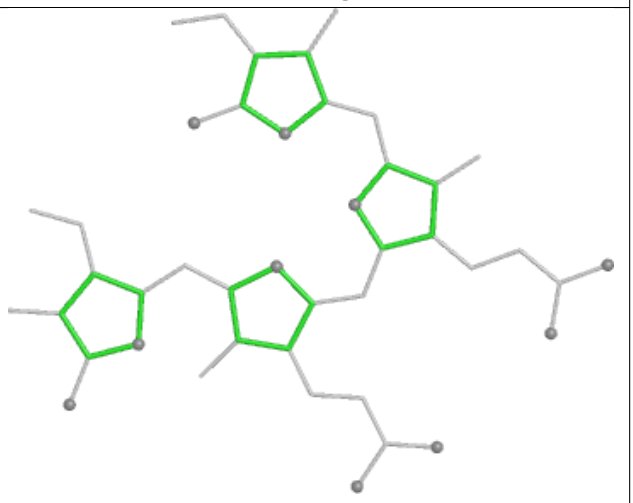
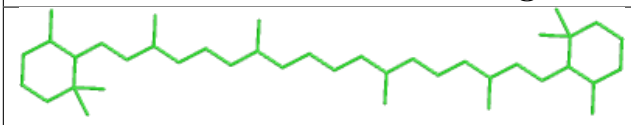


Rings

Ligand BCR c6 617



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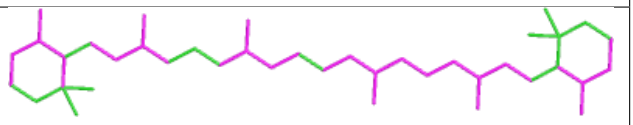

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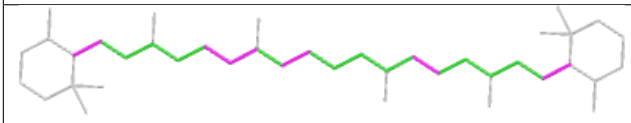

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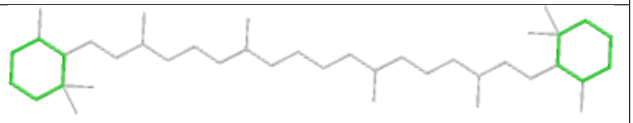
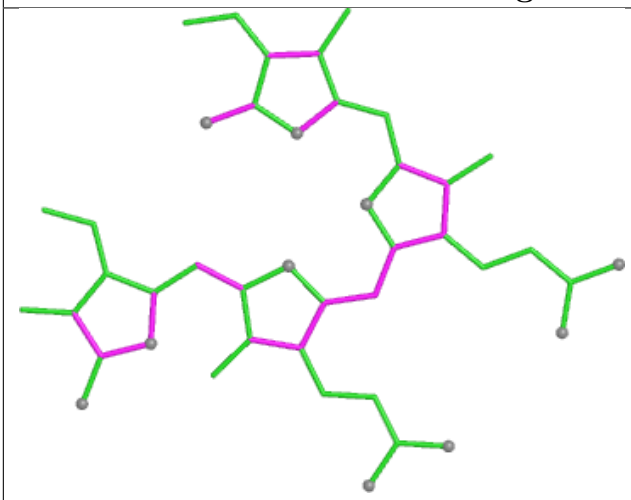


Rings

Ligand PEB dE 204



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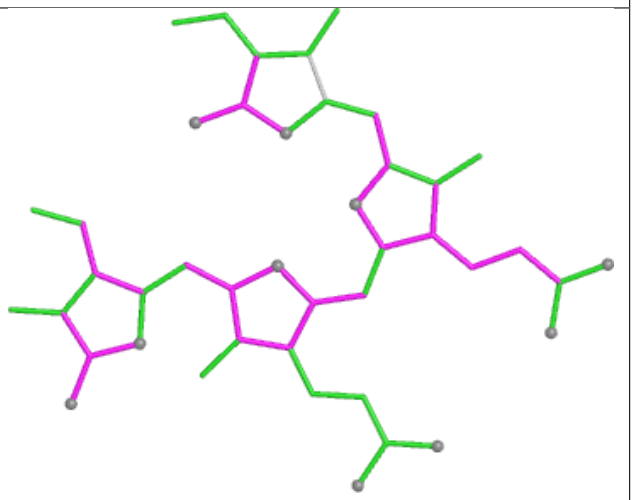
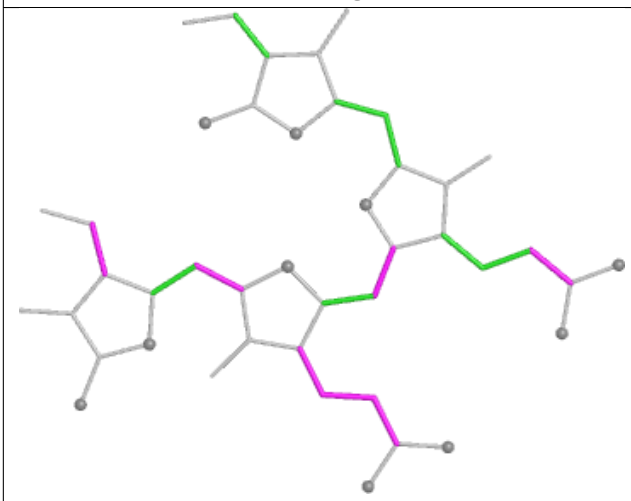


Bond angles



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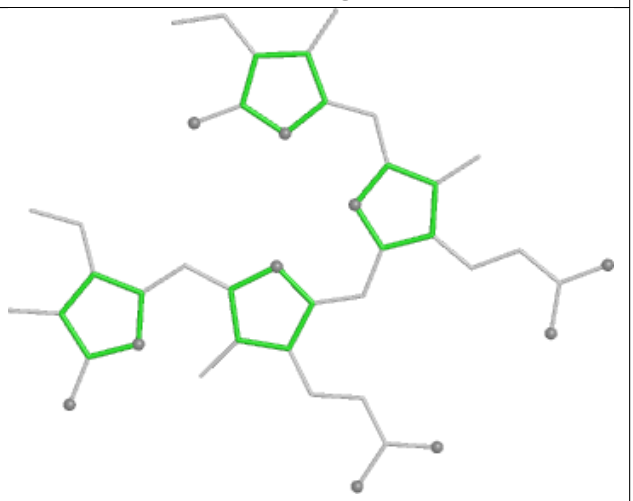
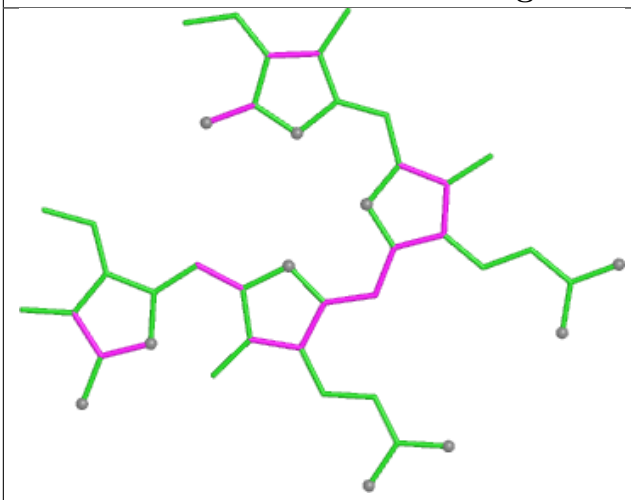


Rings

Ligand PEB rK 201



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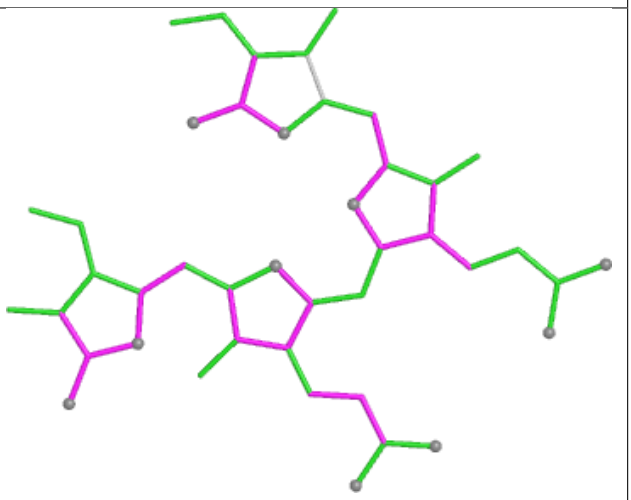
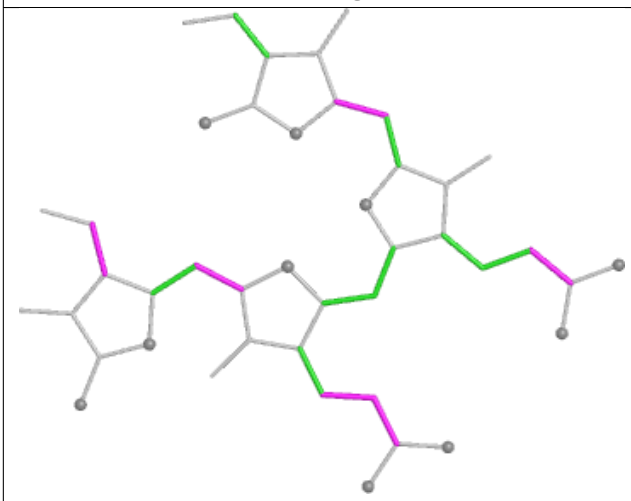


Bond angles



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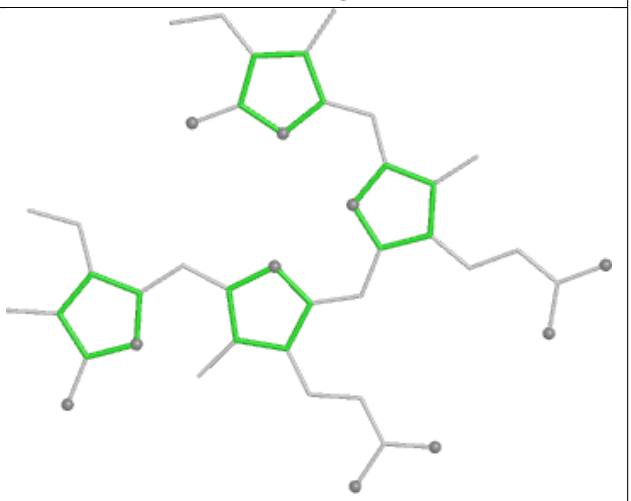
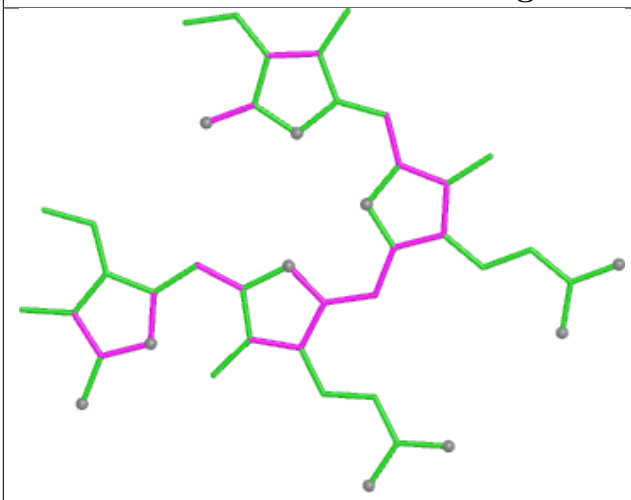


Rings

Ligand PEB sK 203



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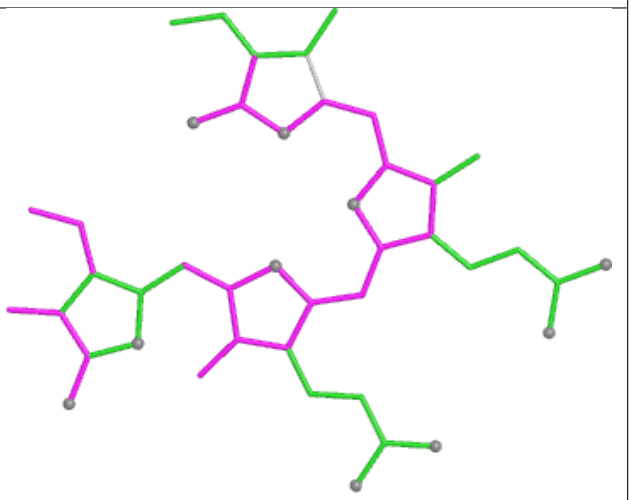
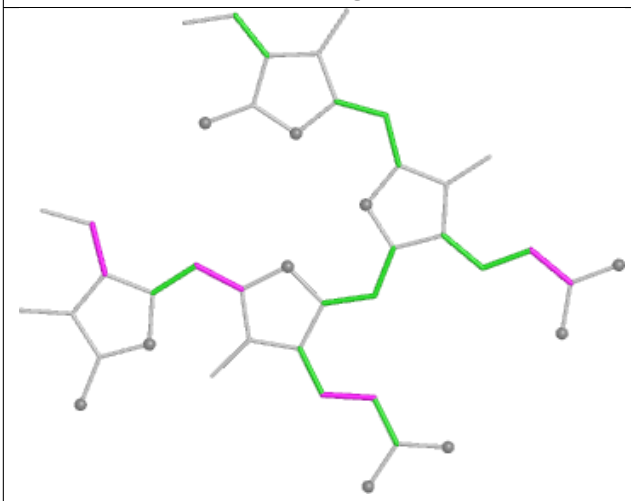


Bond angles



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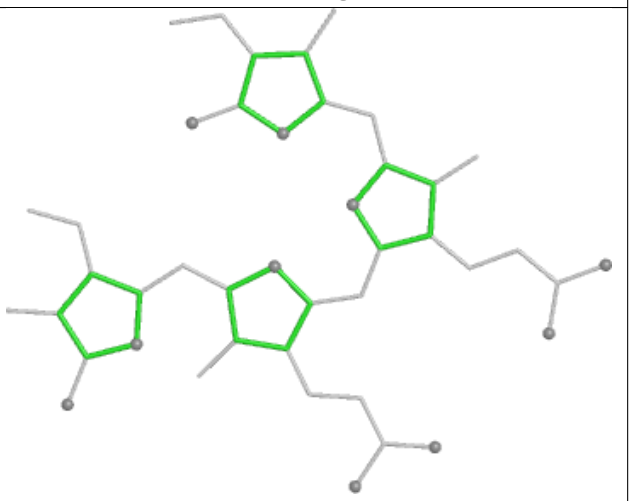
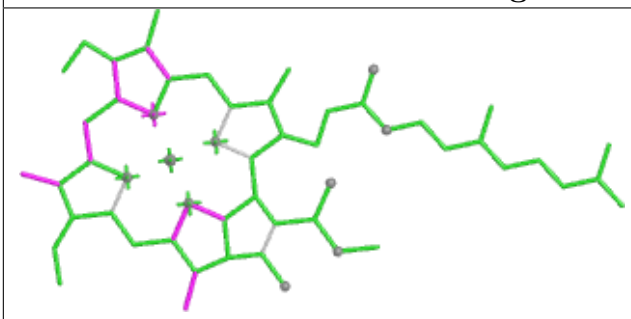


Rings

Ligand CLA AN 806



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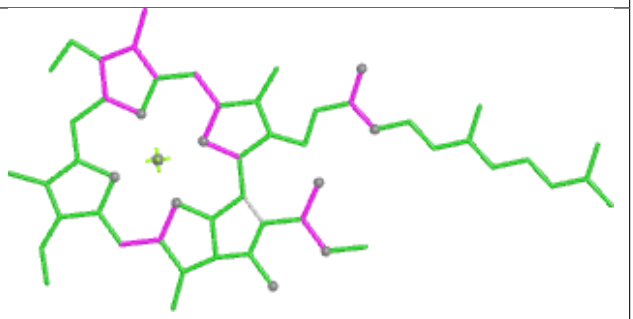
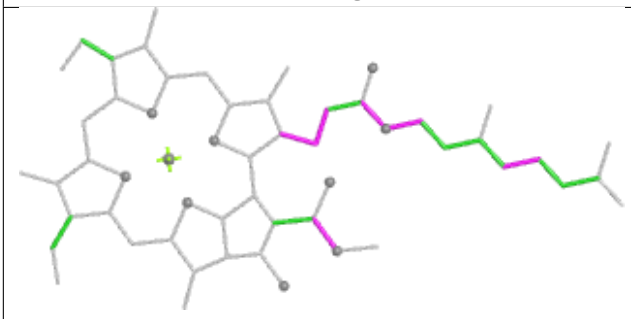
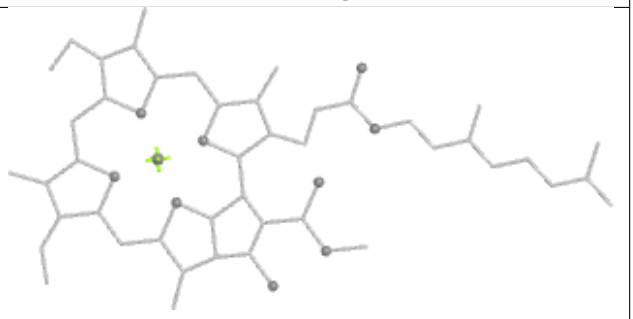


Bond angles

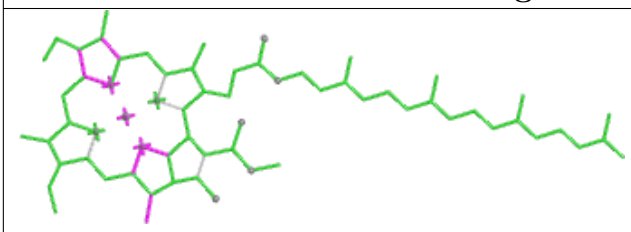


Torsions



Rings

Ligand CLA A2 850



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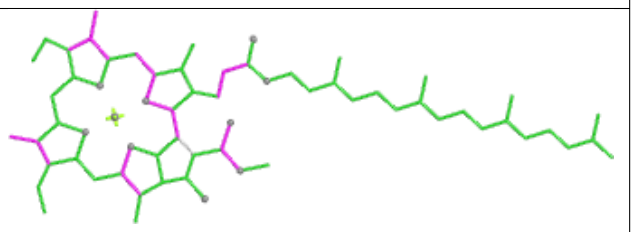

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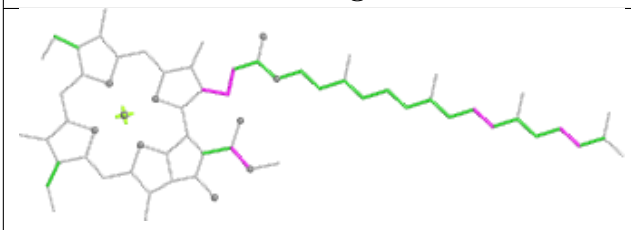

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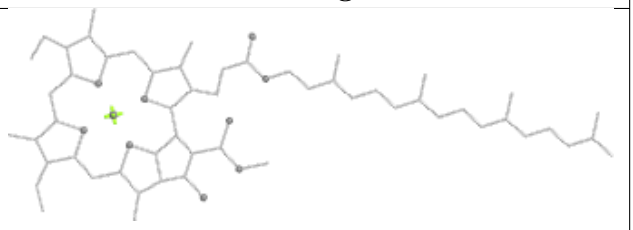
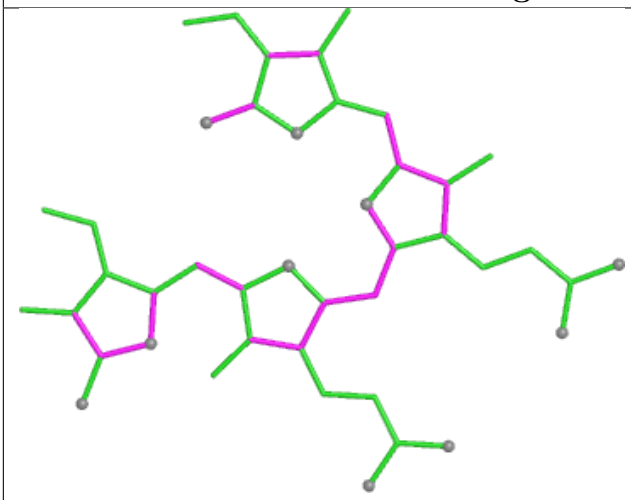


Rings

Ligand PEB RF 202



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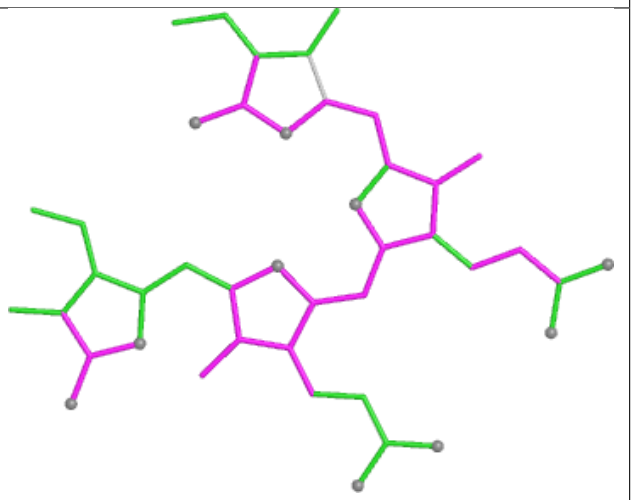

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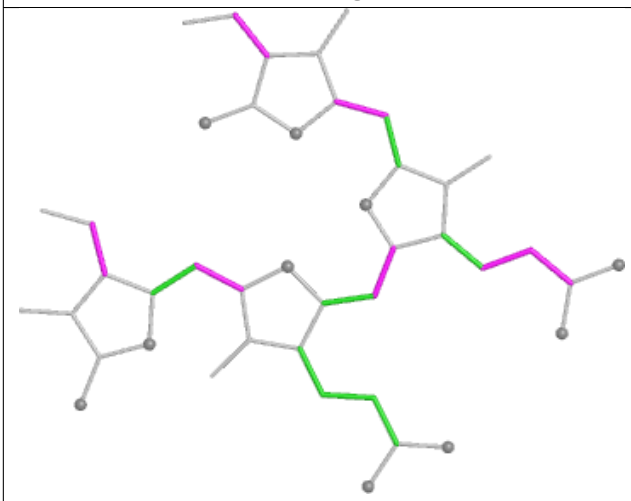

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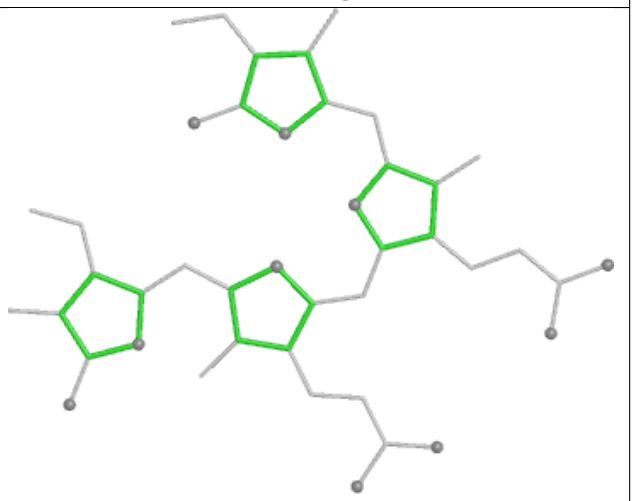
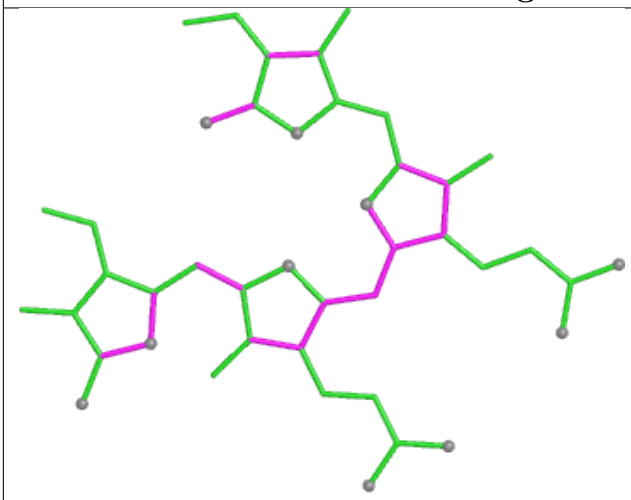


Rings

Ligand PEB KI 203



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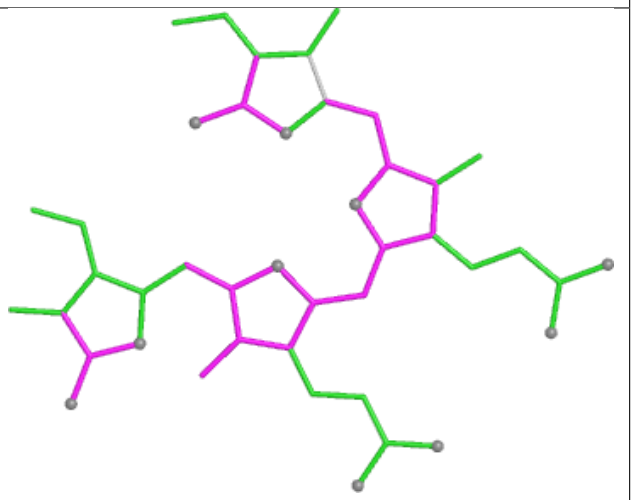

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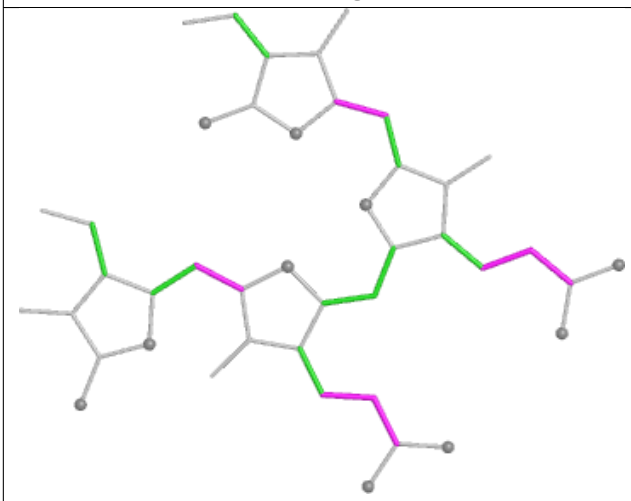

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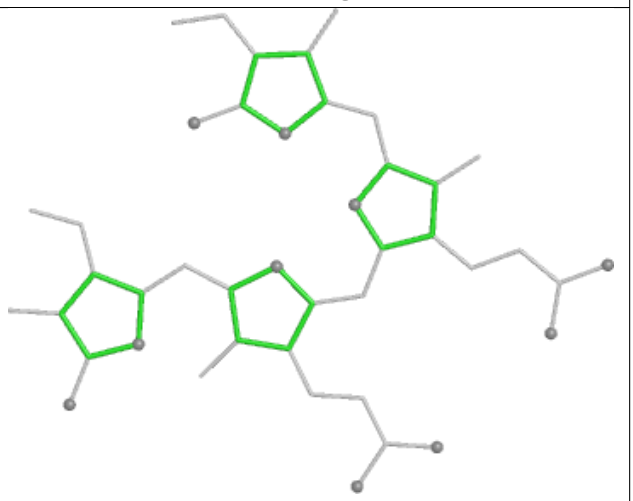
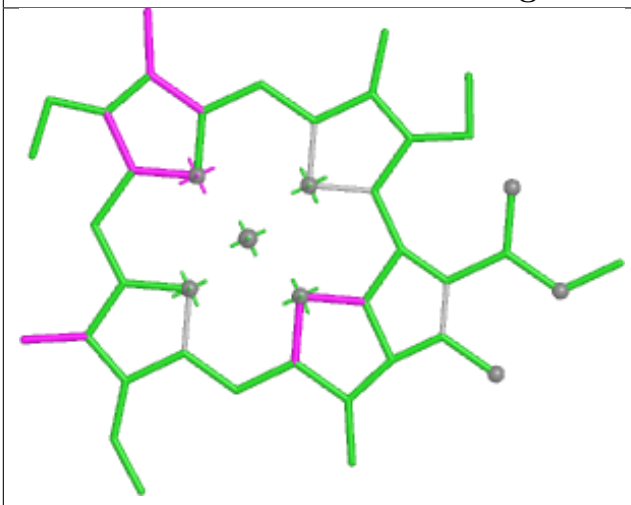


Rings

Ligand CLA 62 311



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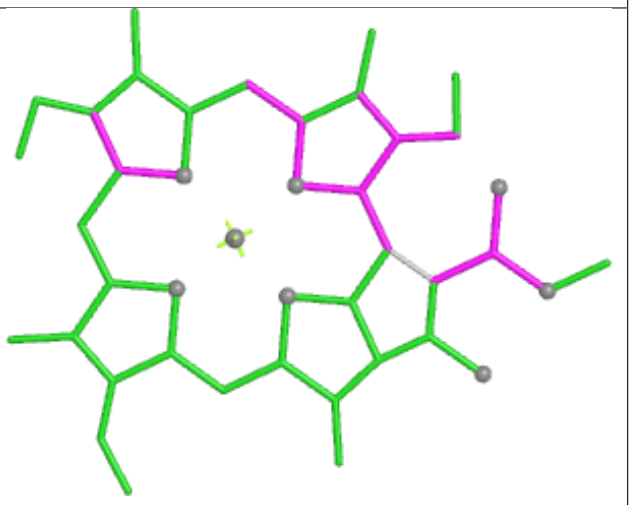

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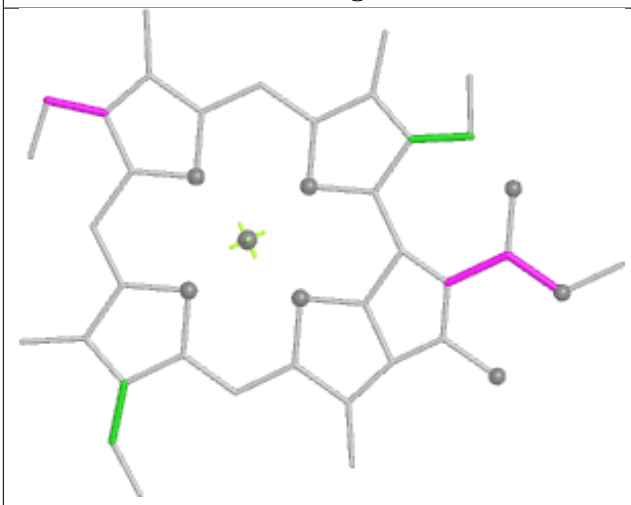
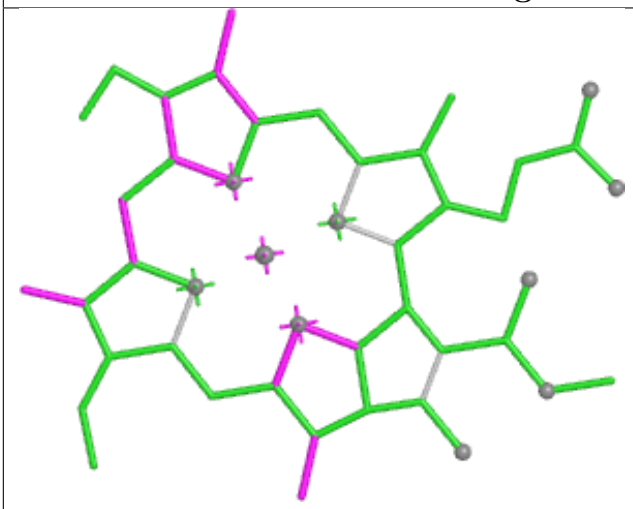


Torsions



Rings

Ligand CLA 8N 302



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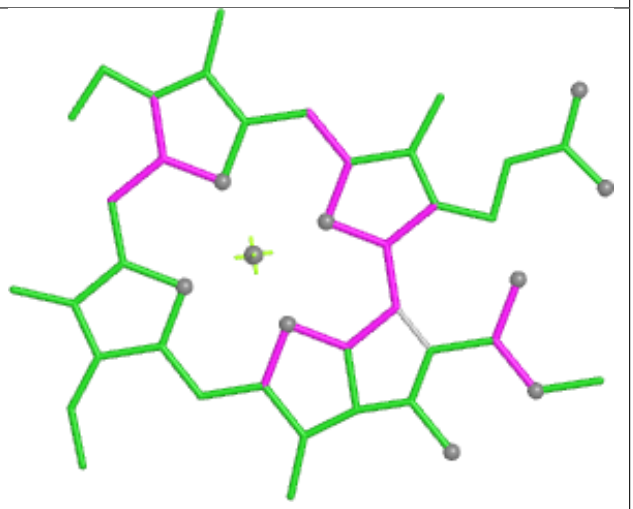

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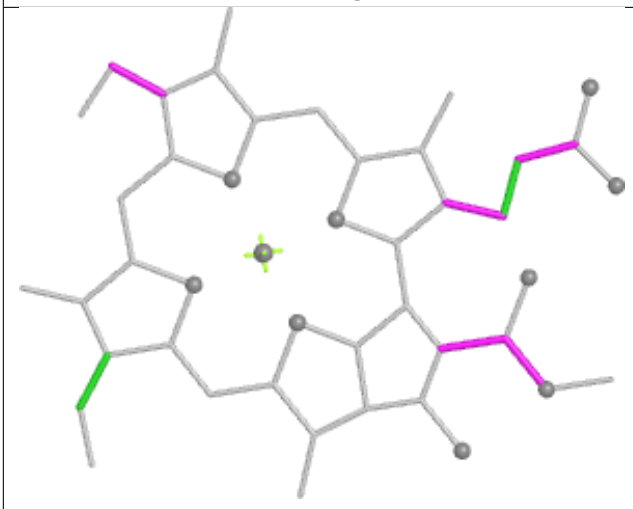
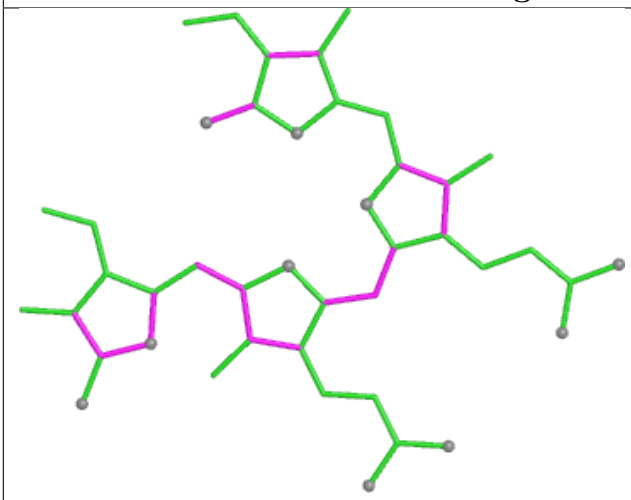


Torsions



Rings

Ligand PEB FQ 201



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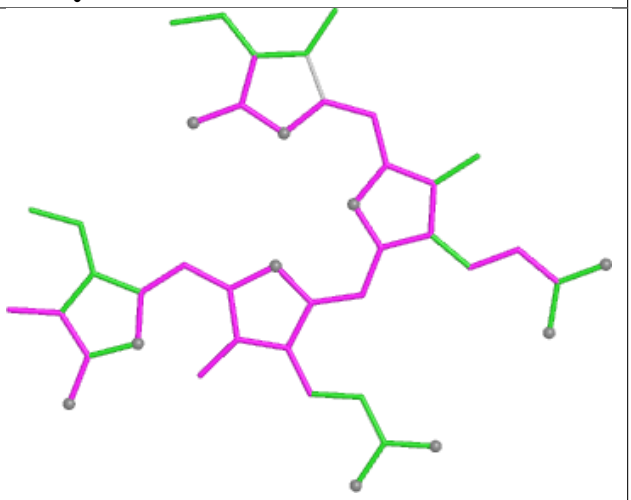

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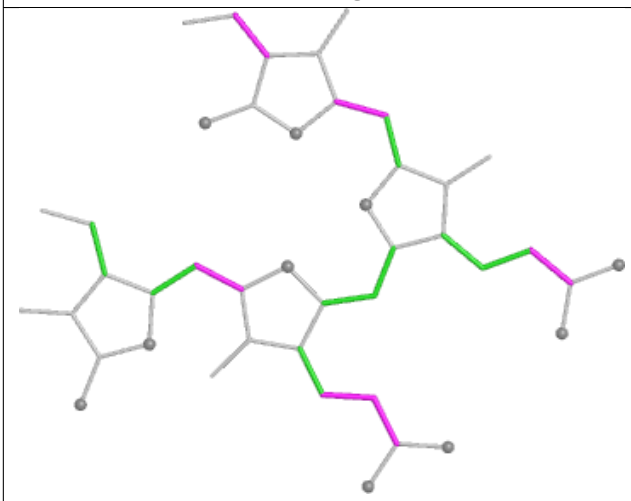

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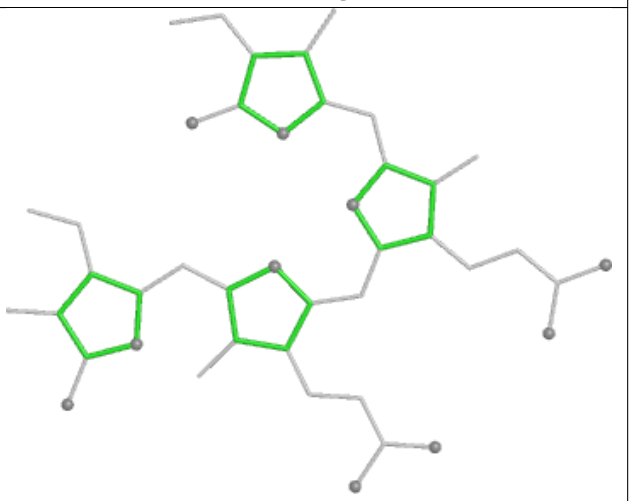
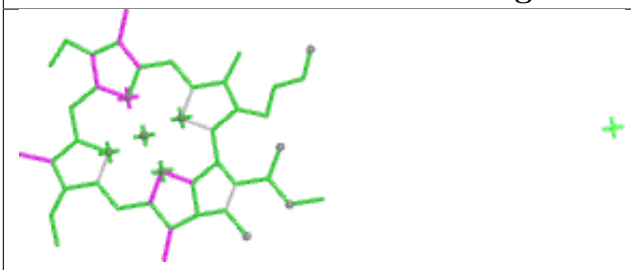


Rings

Ligand CLA A2 802



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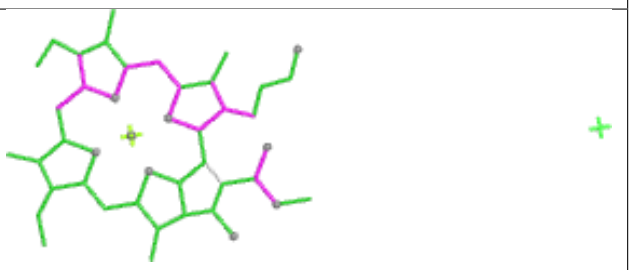

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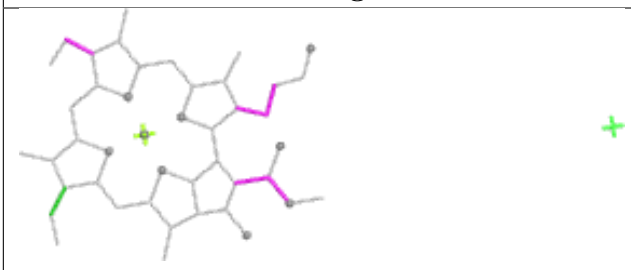

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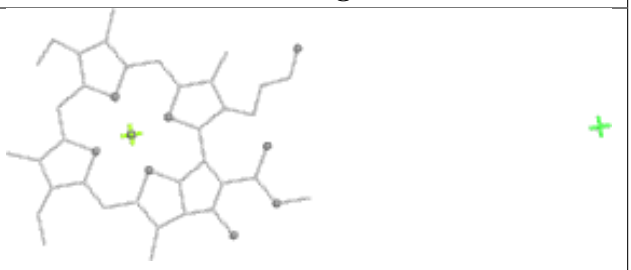
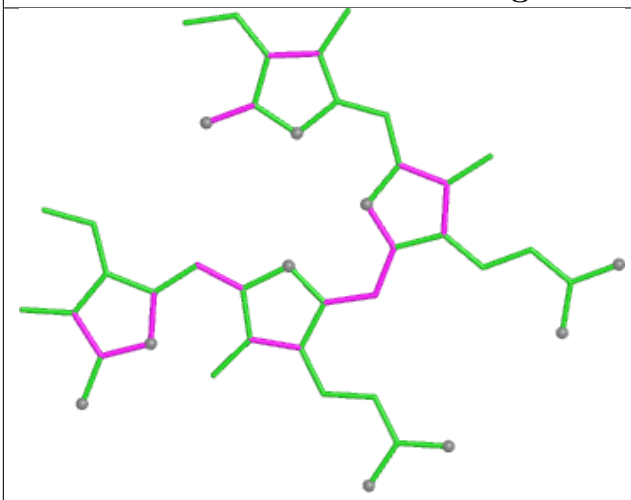


Rings

Ligand PEB VO 201



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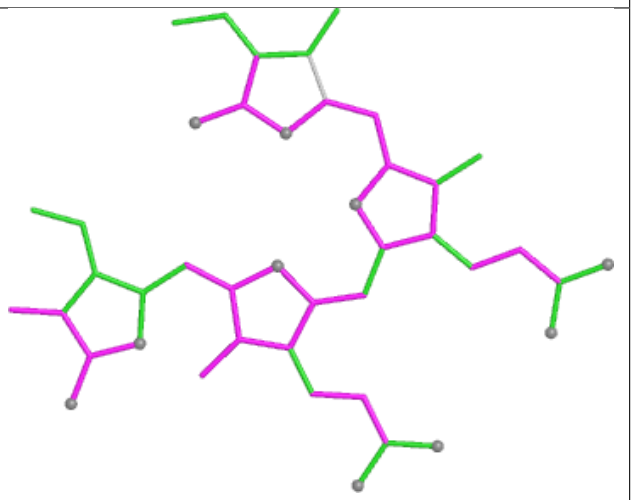

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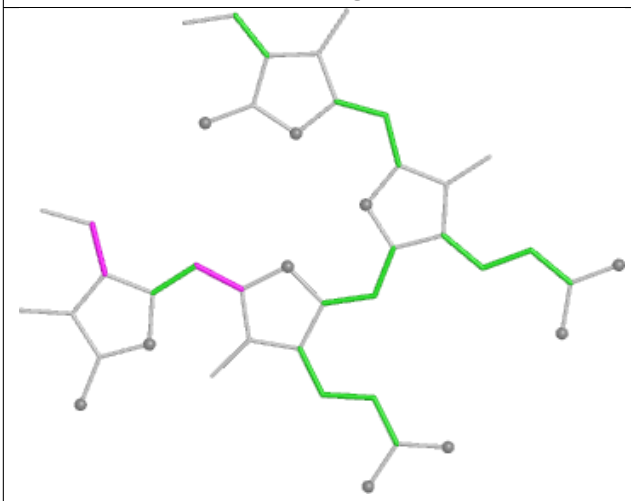

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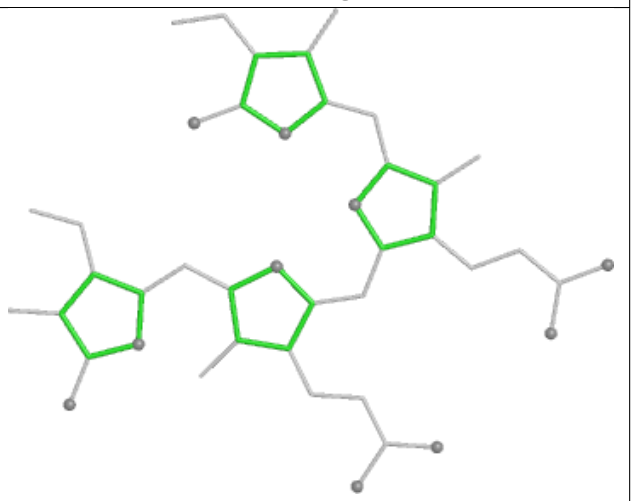
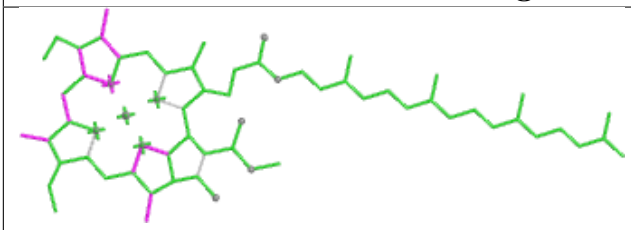


Rings

Ligand CLA B6 610



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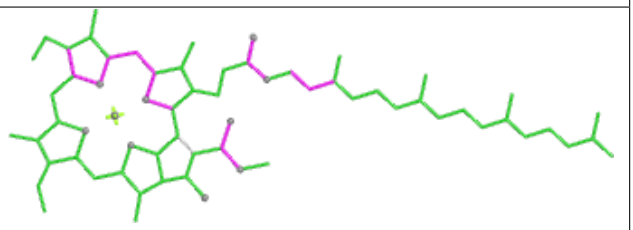
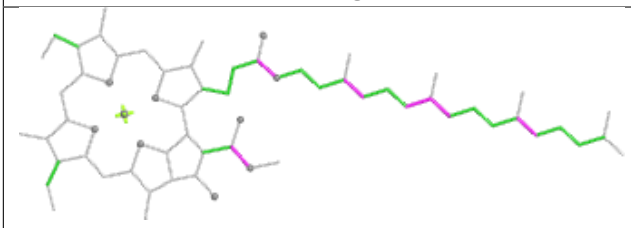


Bond angles



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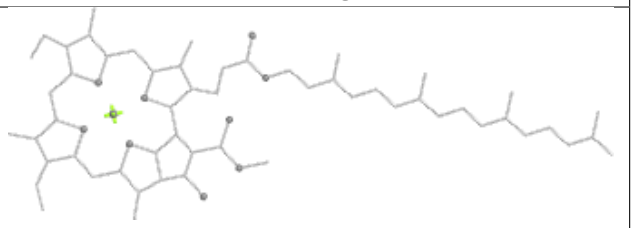
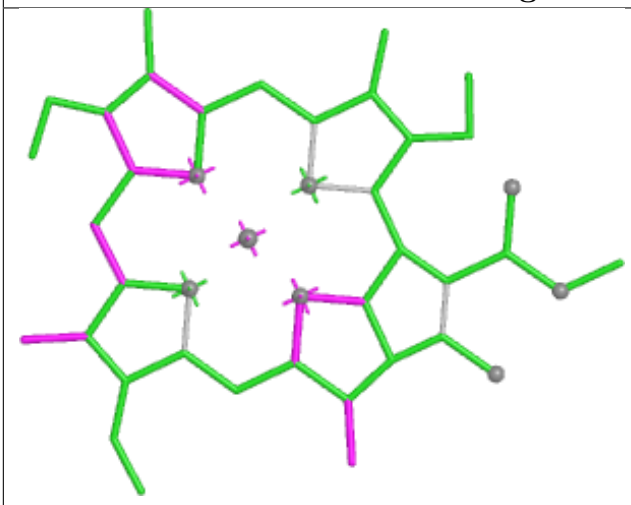


Rings

Ligand CLA 82 307



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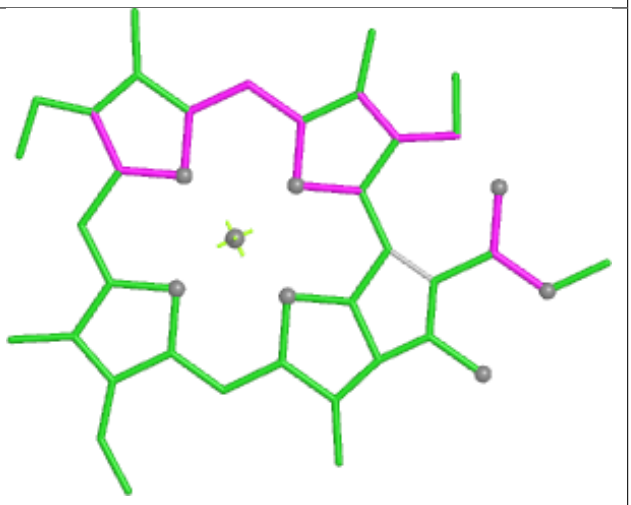

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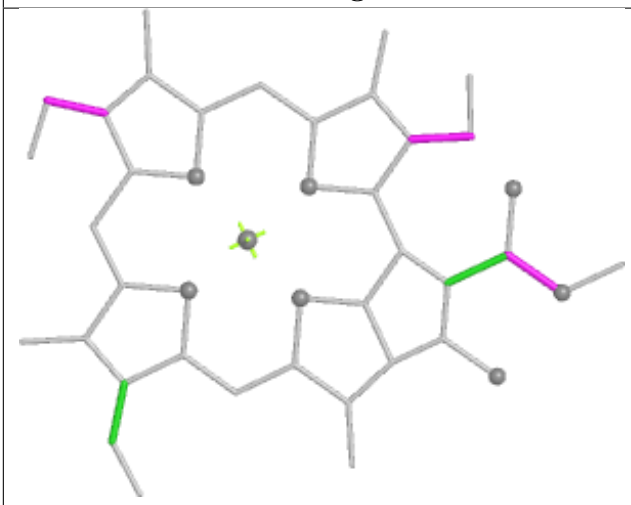
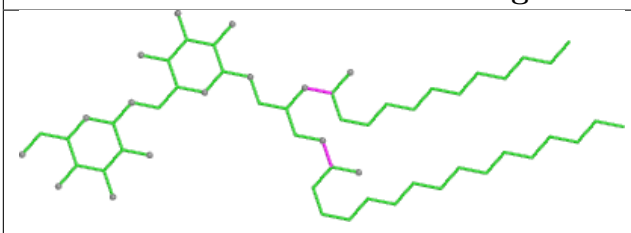


Torsions



Rings

Ligand DGD B6 620



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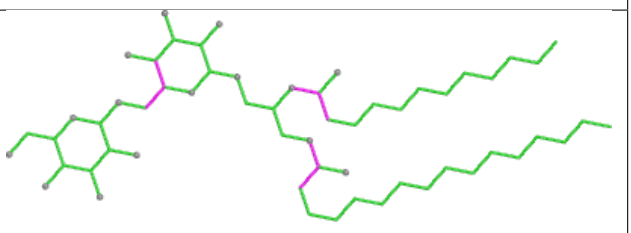

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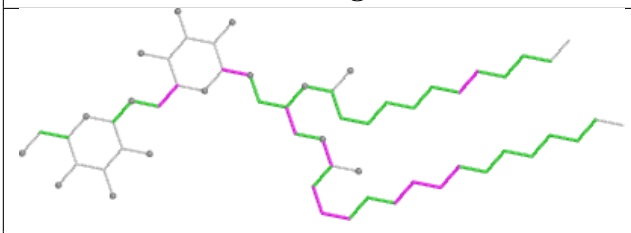

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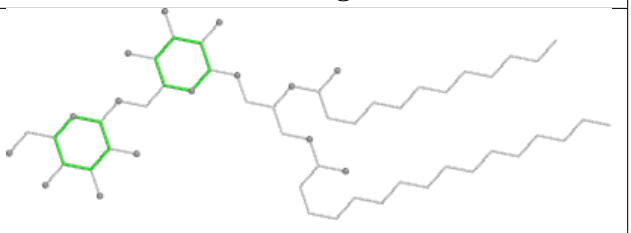
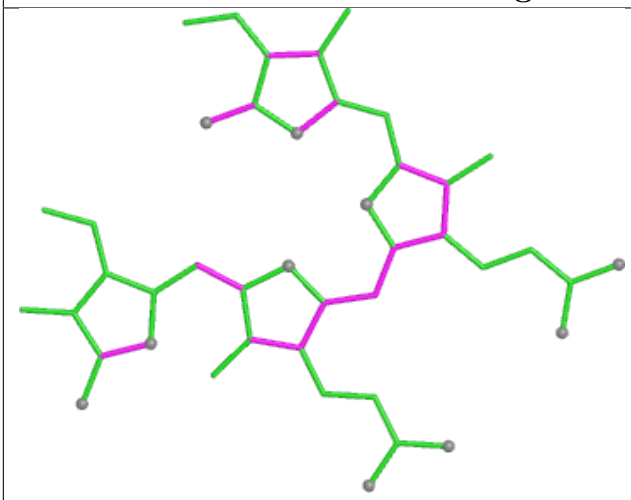


Rings

Ligand PEB JD 203



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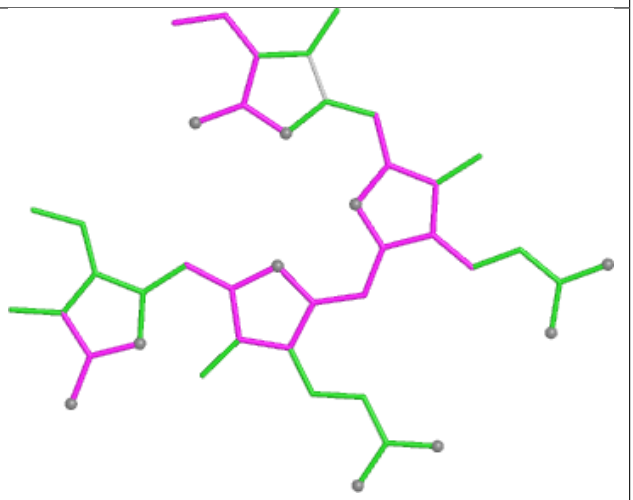

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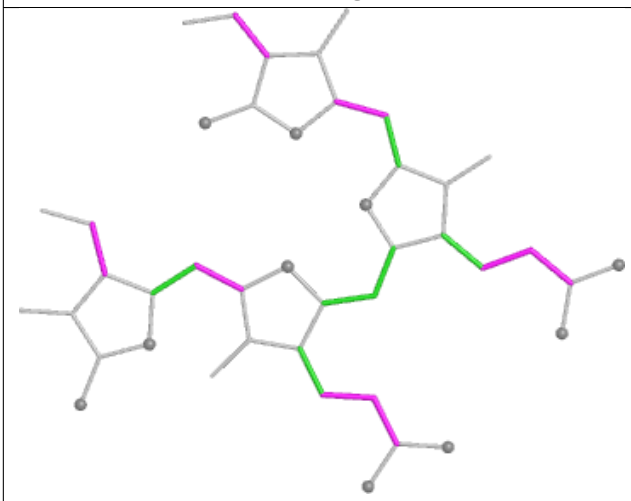

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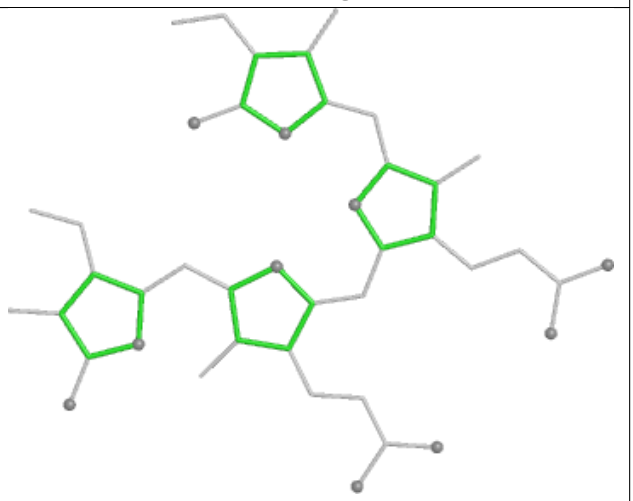
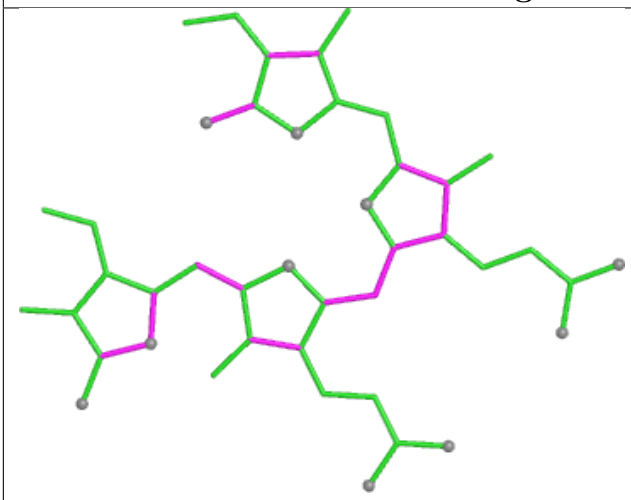


Rings

Ligand PEB U1 203



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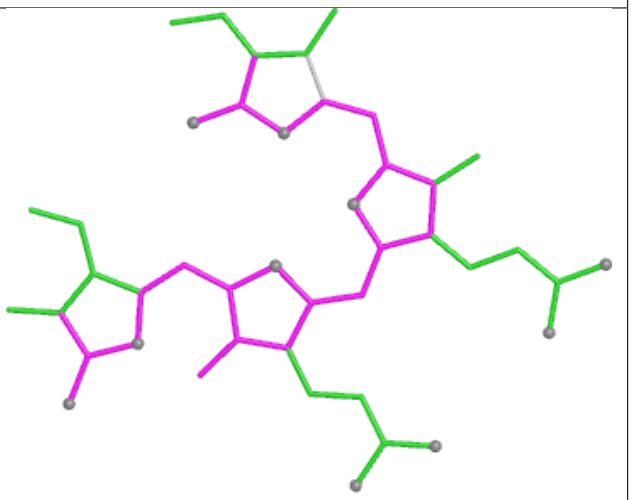
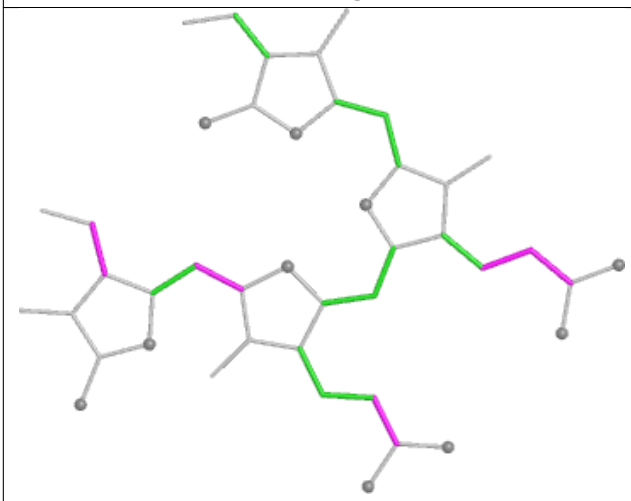


Bond angles



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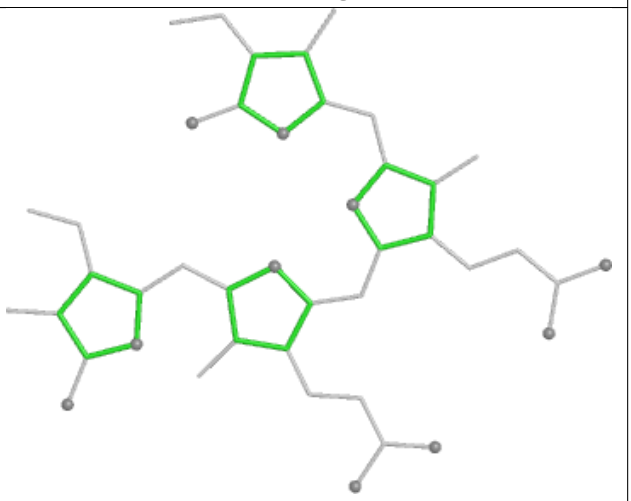
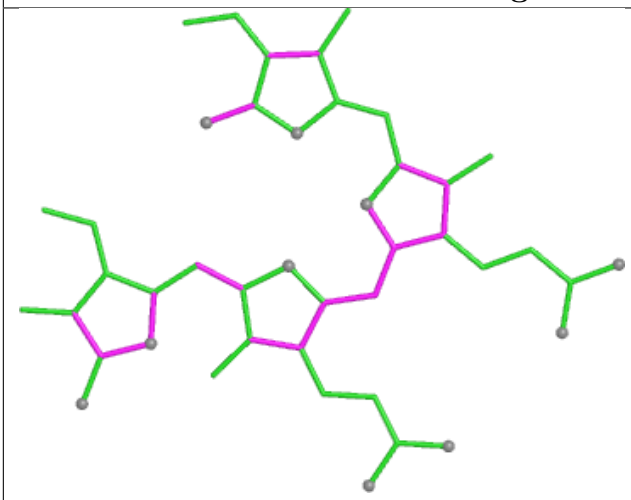


Rings

Ligand PEB XA 203



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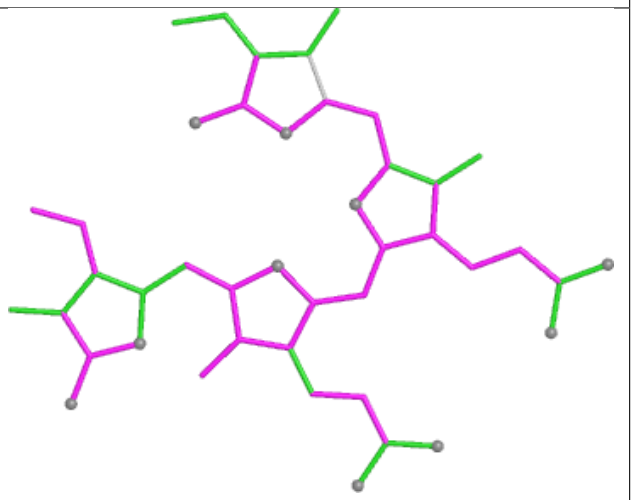
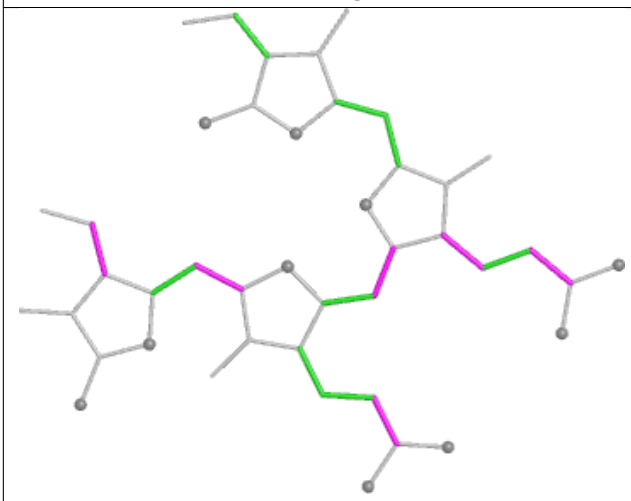


Bond angles



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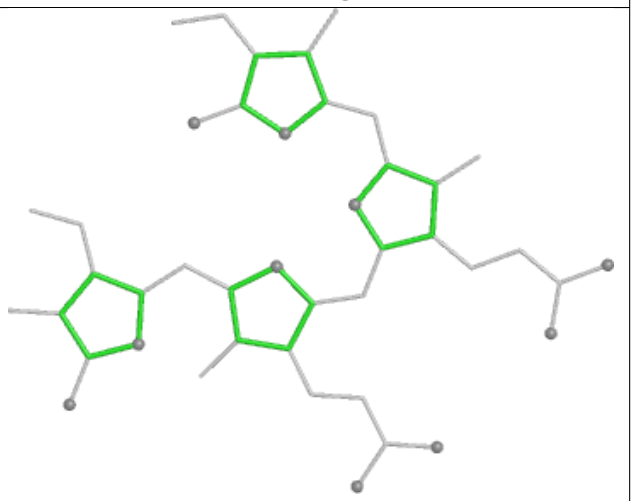
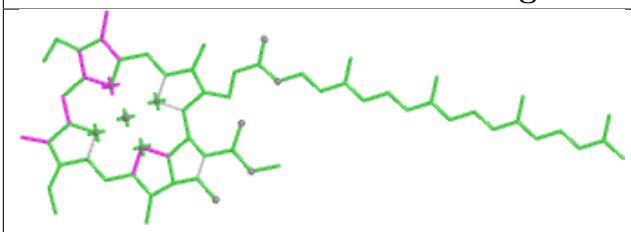
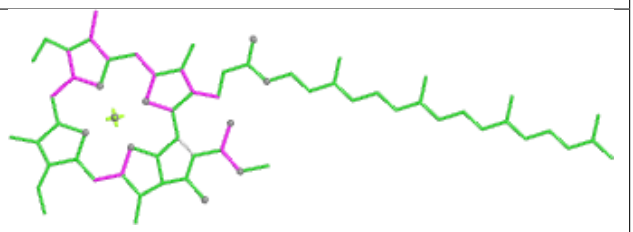


Rings

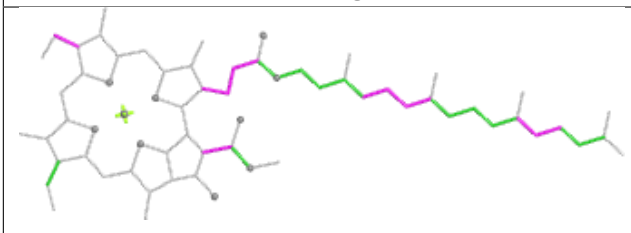
Ligand CLA 52 602



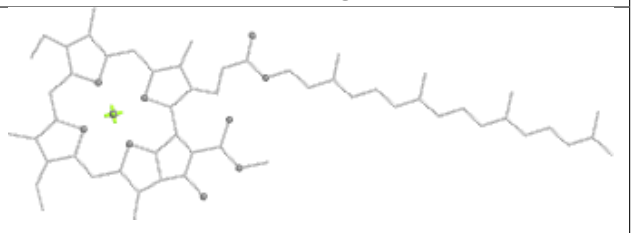
Bond lengths



Bond angles

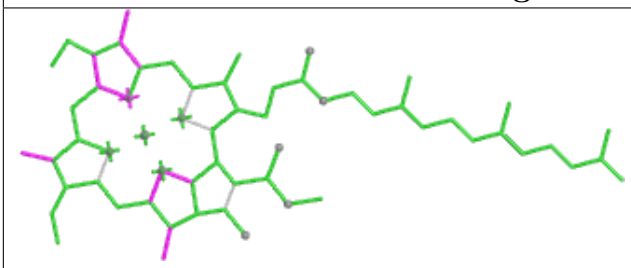


Torsions



Rings

Ligand CLA AL 404



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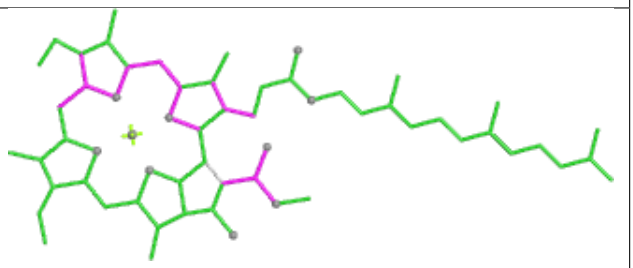
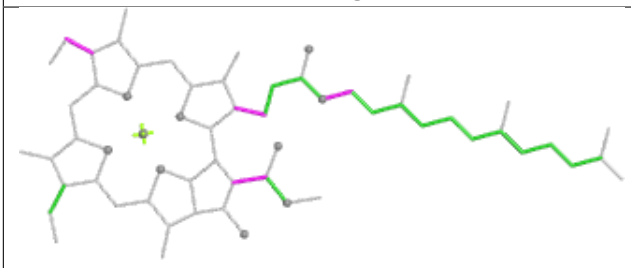


Bond angles



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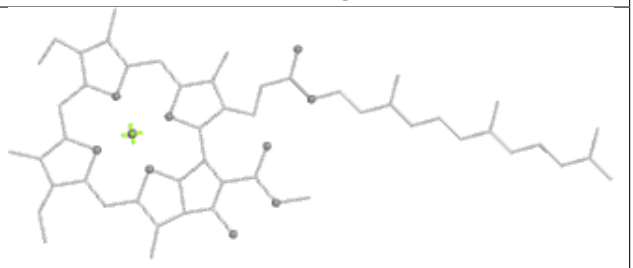
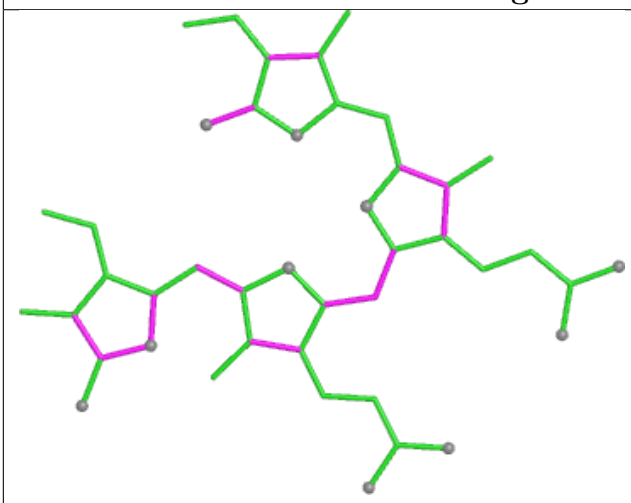


Rings

Ligand PEB VB 202



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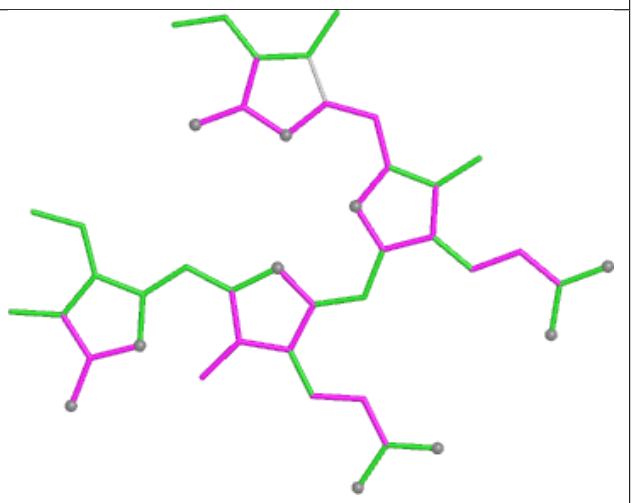

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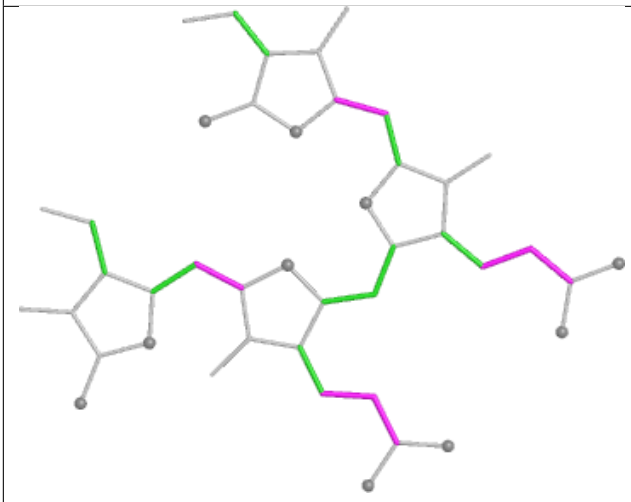

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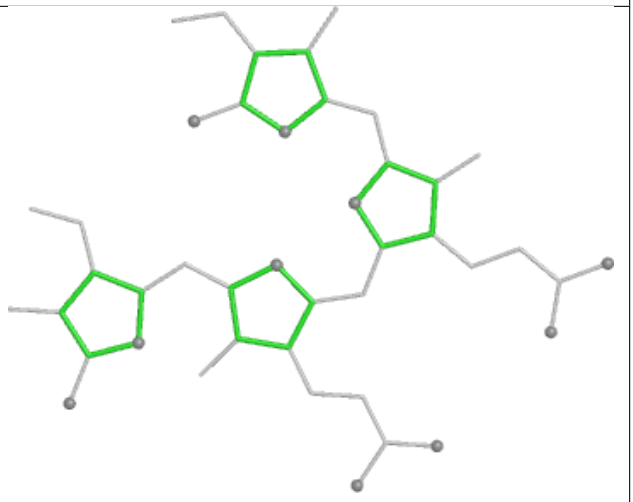
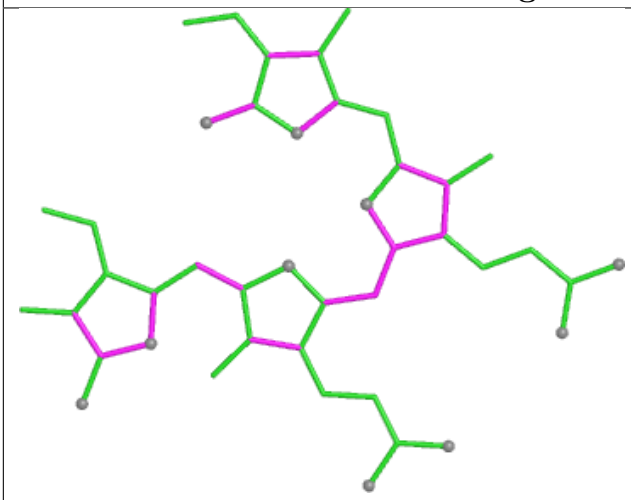


Rings

Ligand PEB S4 202



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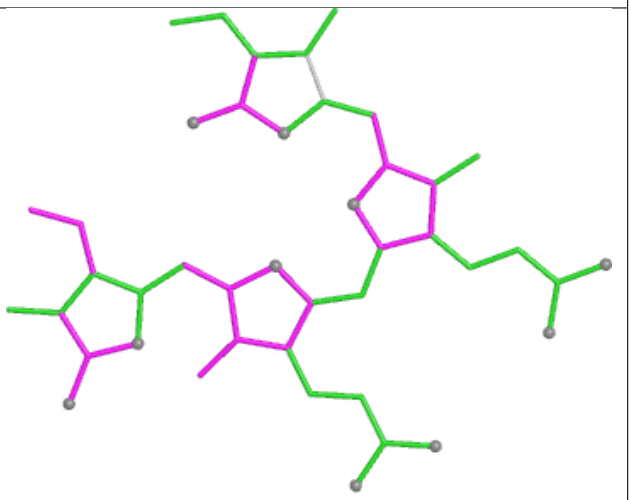
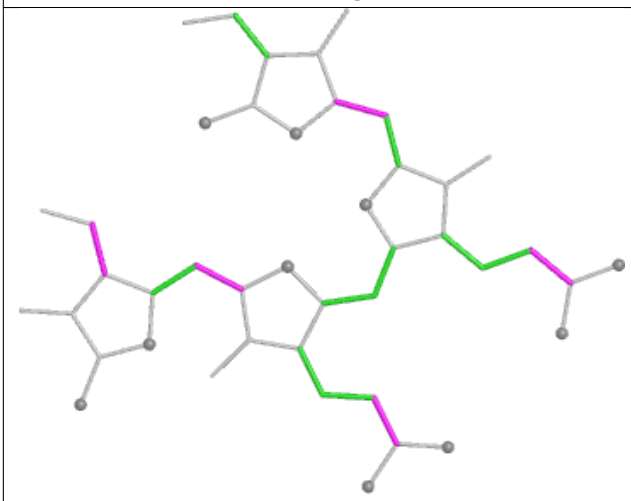


Bond angles



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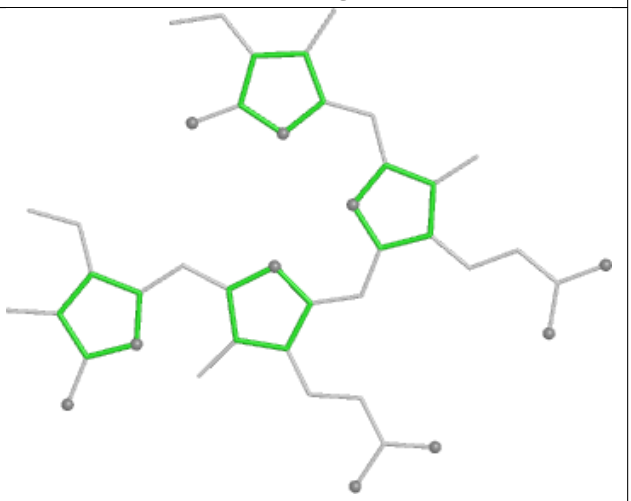
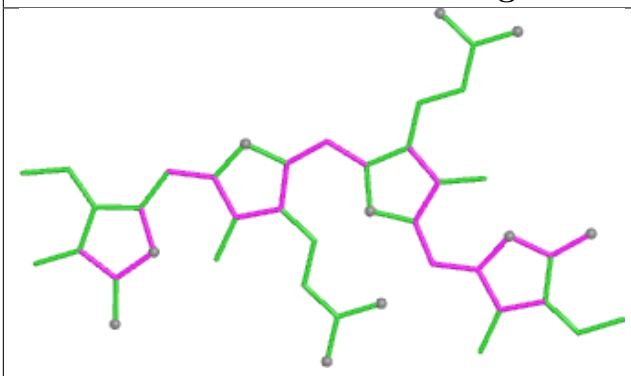


Rings

Ligand CYC HH 1001



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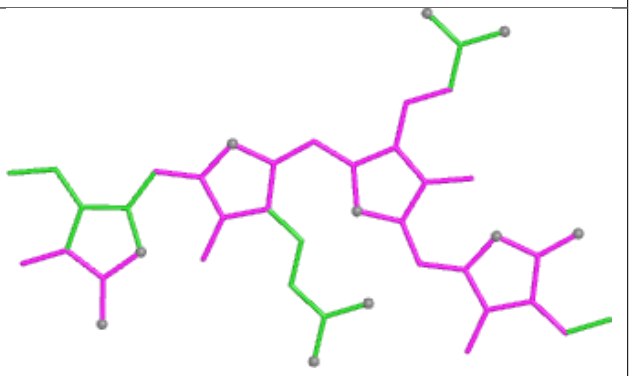
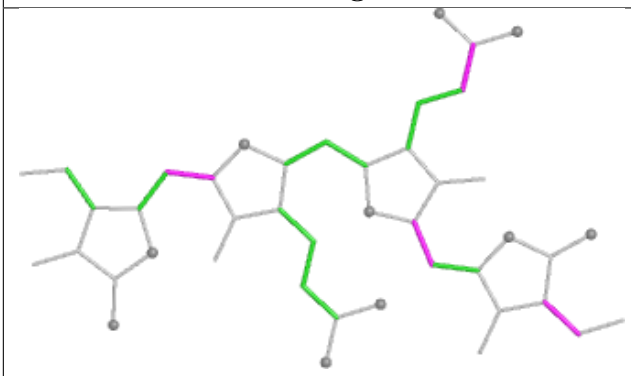


Bond angles



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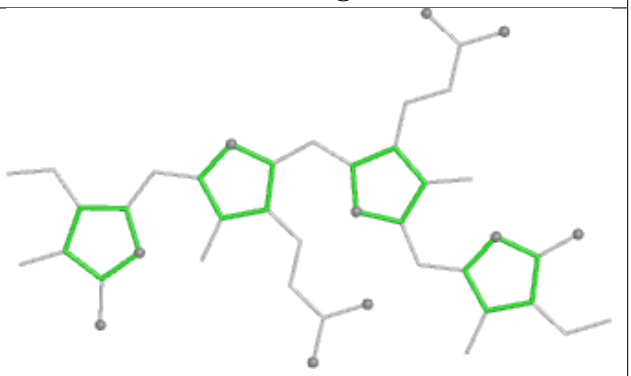
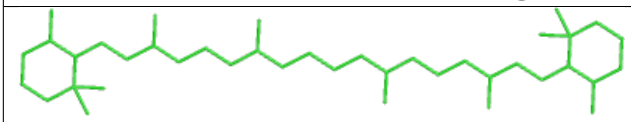


Rings

Ligand BCR A2 804



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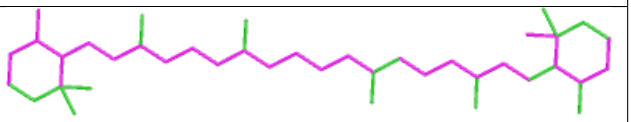

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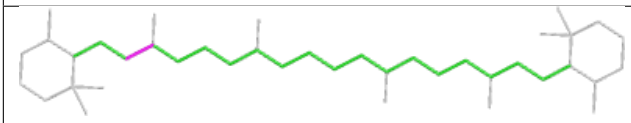

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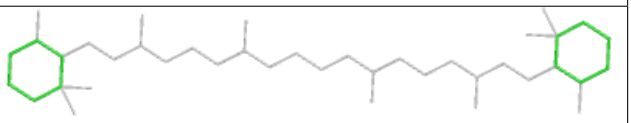
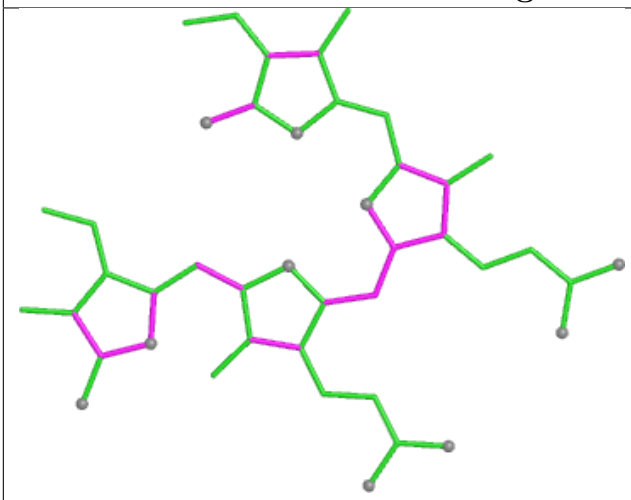


Rings

Ligand PEB P5 202



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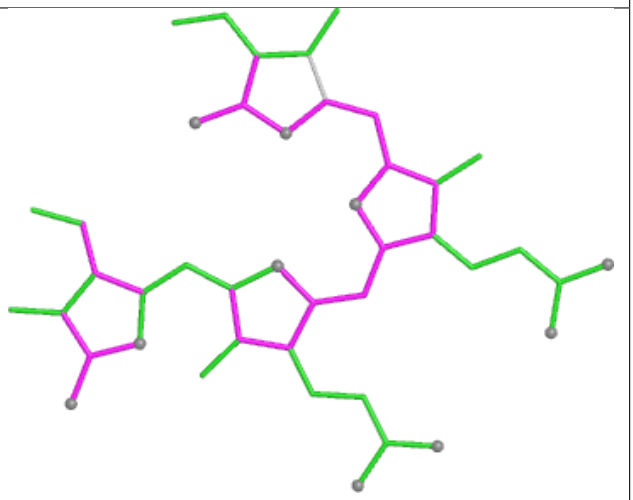
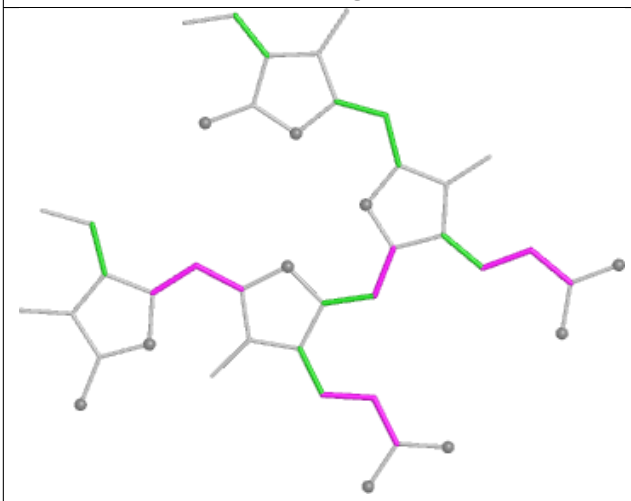


Bond angles



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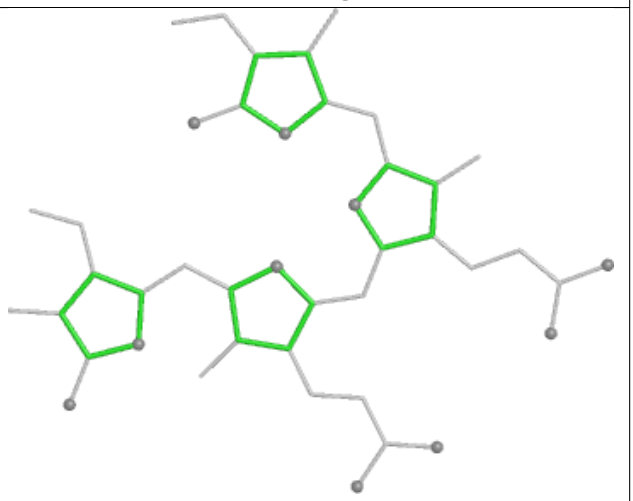
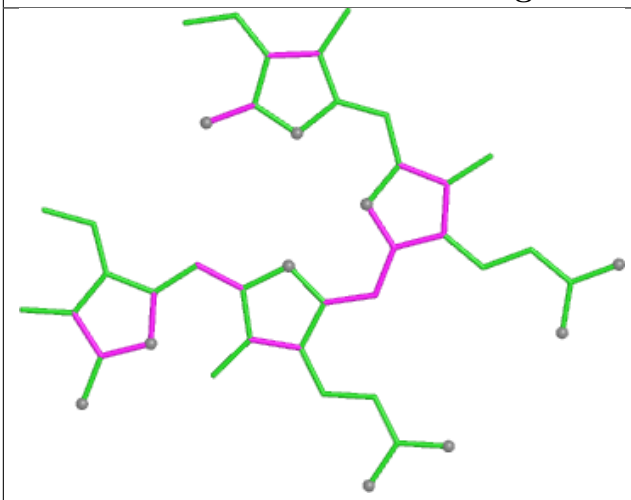


Rings

Ligand PEB D7 203



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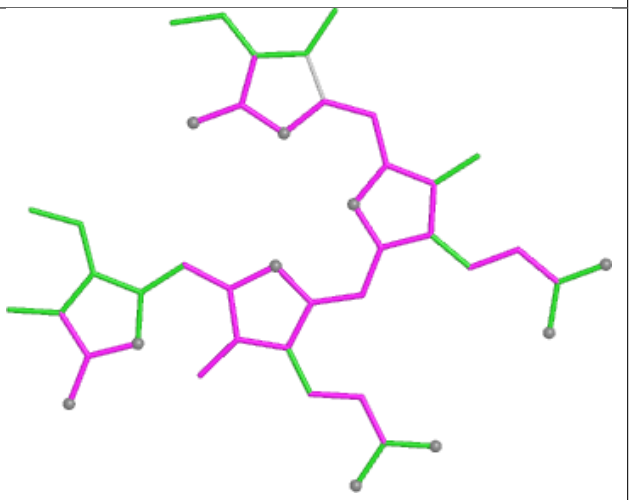
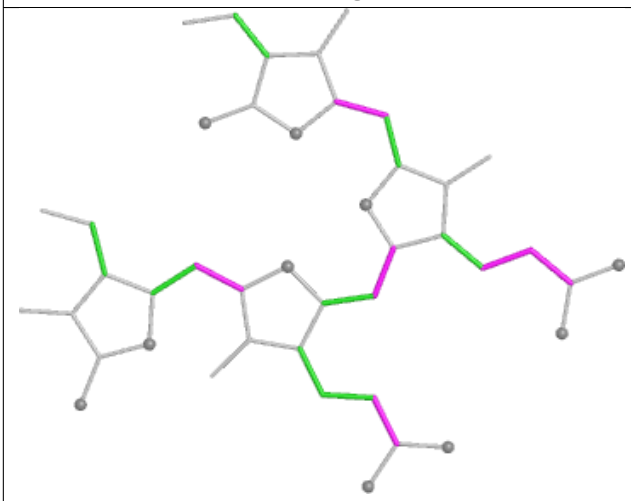


Bond angles



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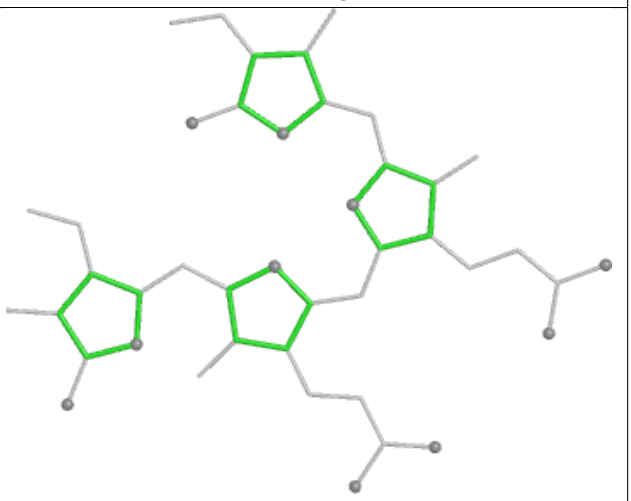
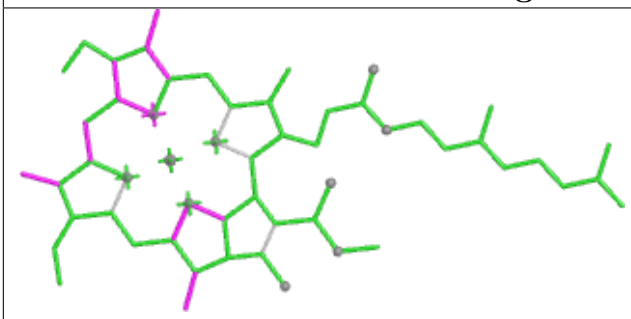


Rings

Ligand CLA B2 821



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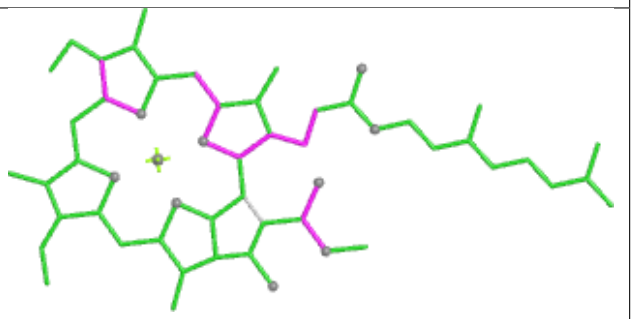
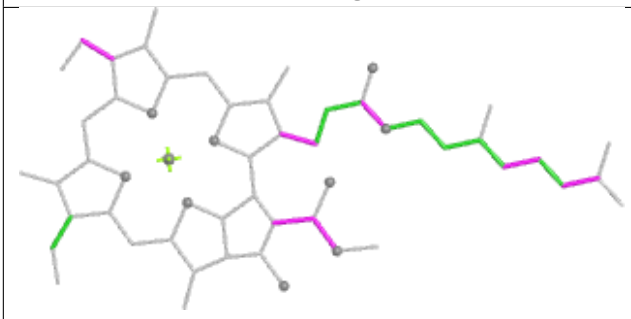


Bond angles



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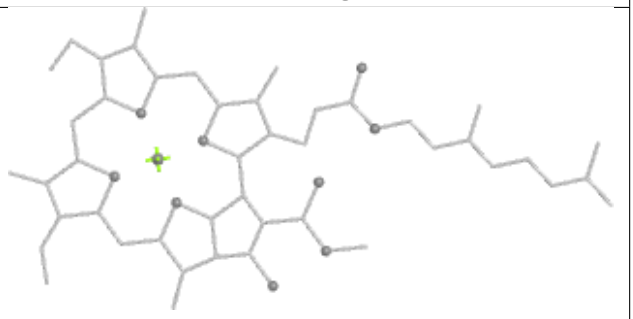
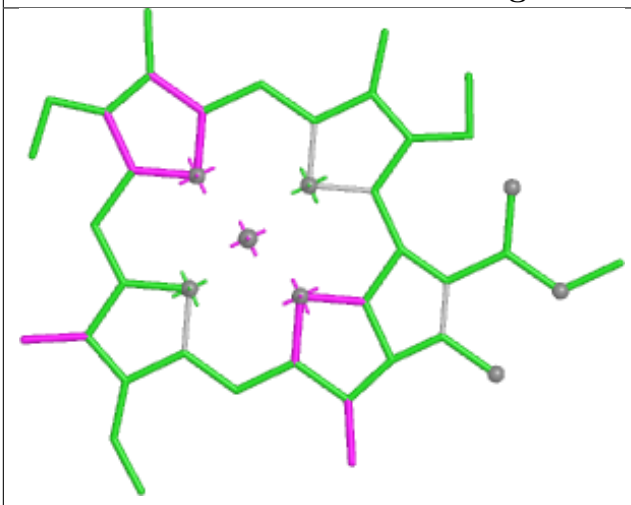


Rings

Ligand CLA KN 103



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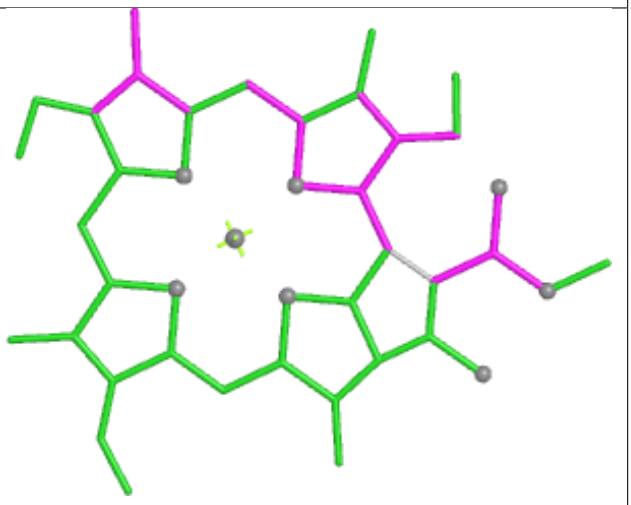
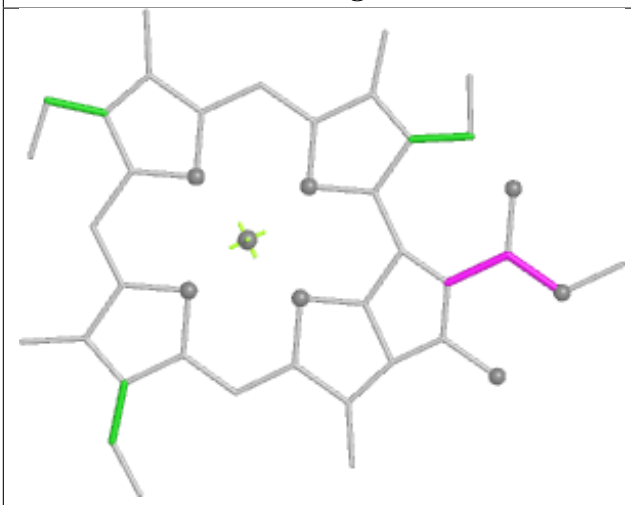


Bond angles

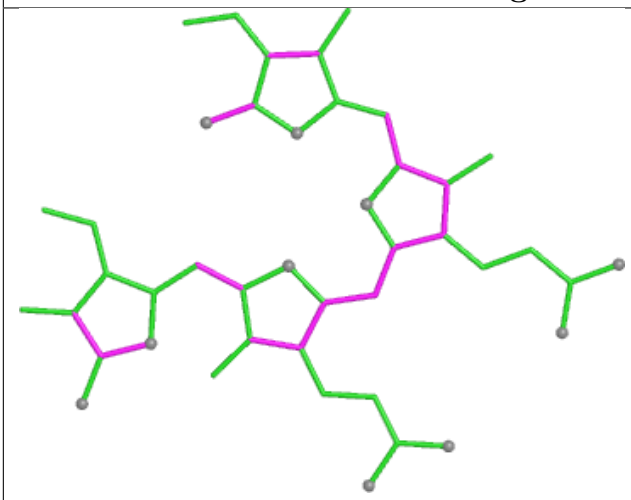


Torsions



Rings

Ligand PEB ND 202



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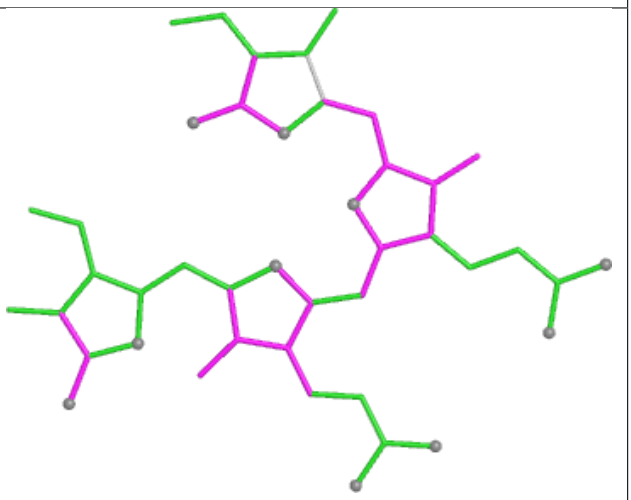
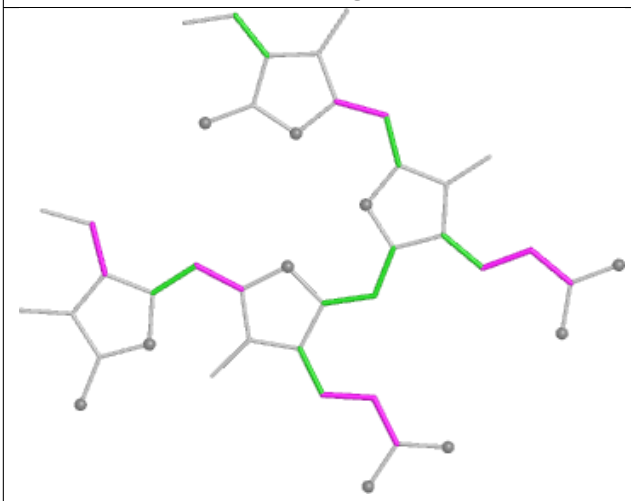


Bond angles



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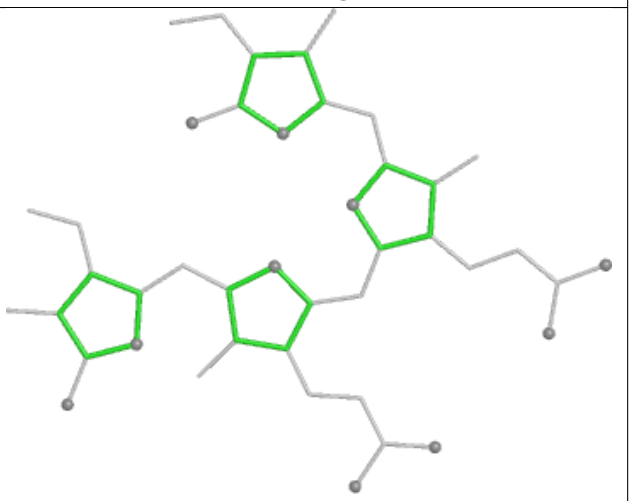
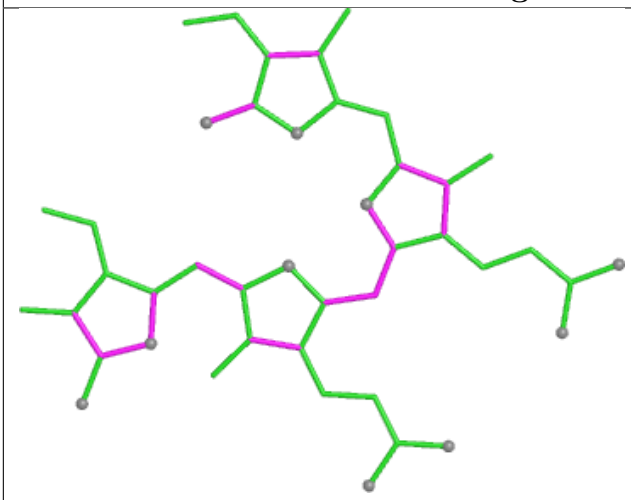


Rings

Ligand PEB GB 203



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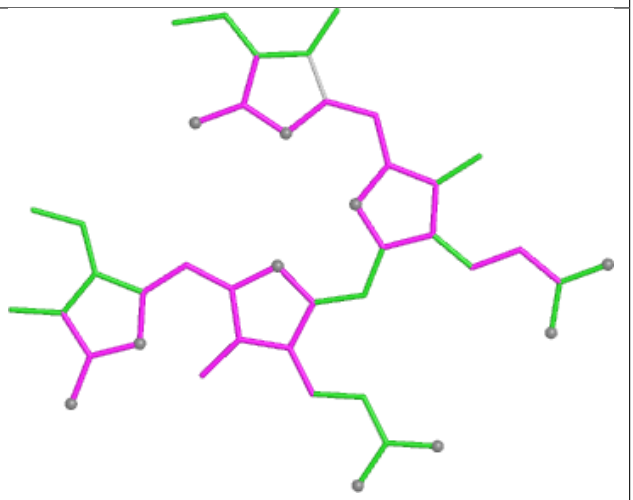
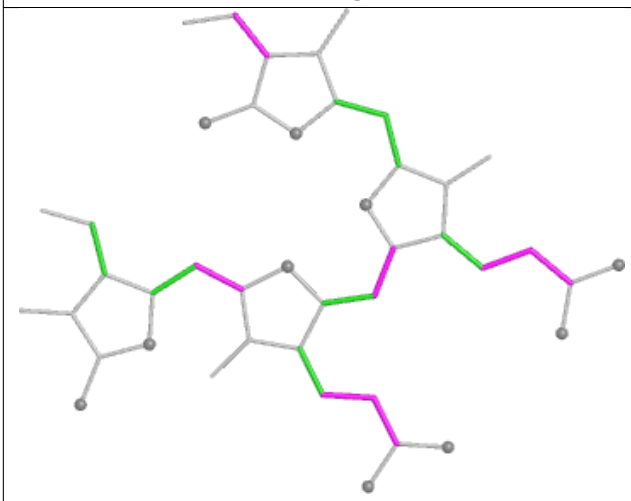


Bond angles



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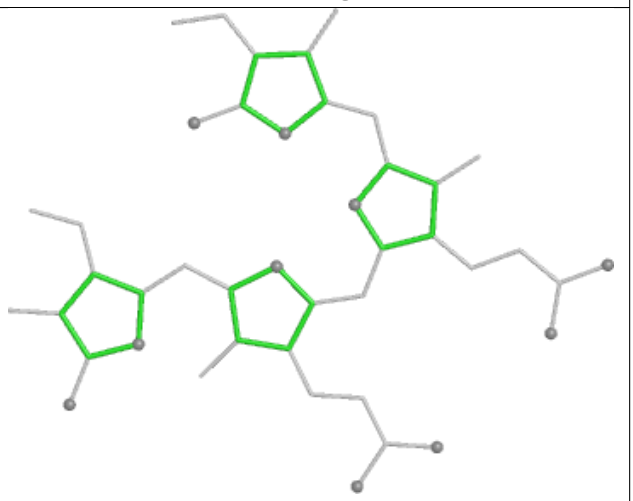
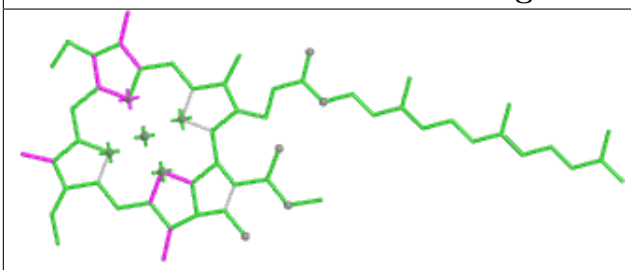


Rings

Ligand CLA B2 817



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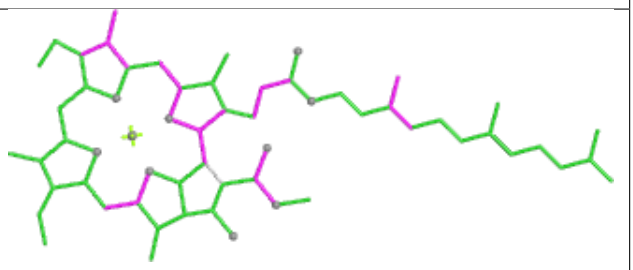
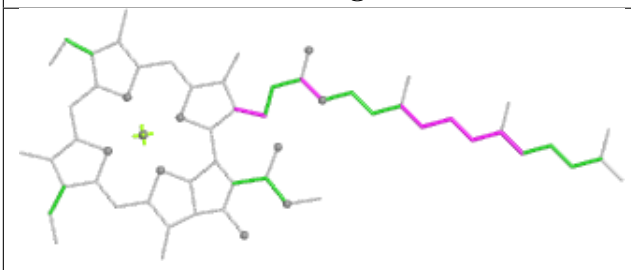


Bond angles



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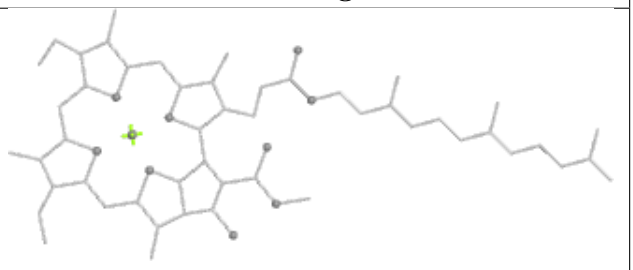
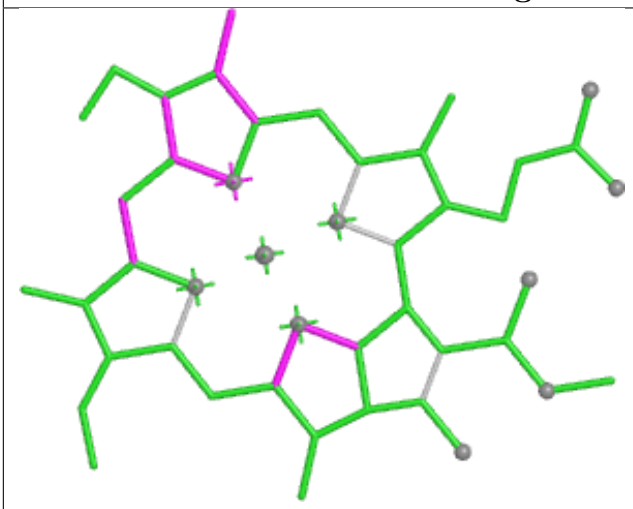


Rings

Ligand CLA 2N 306



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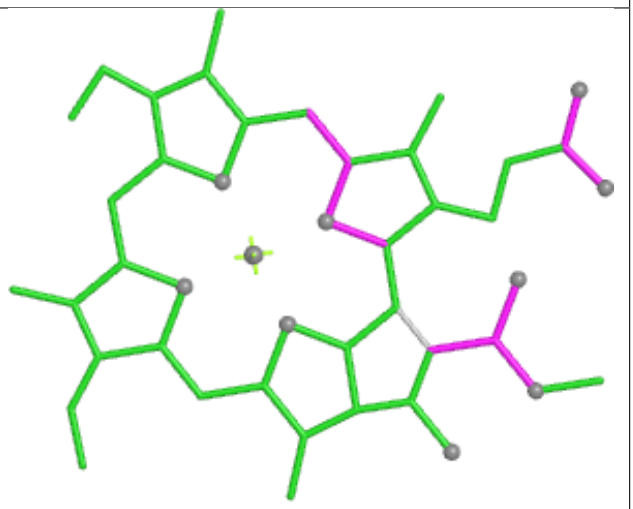
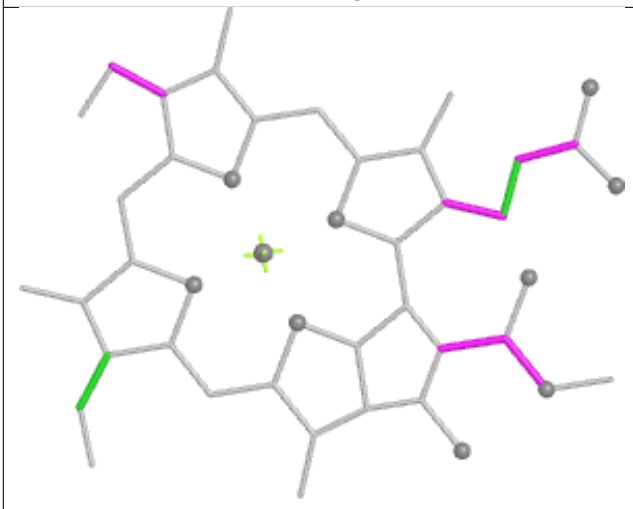


Bond angles

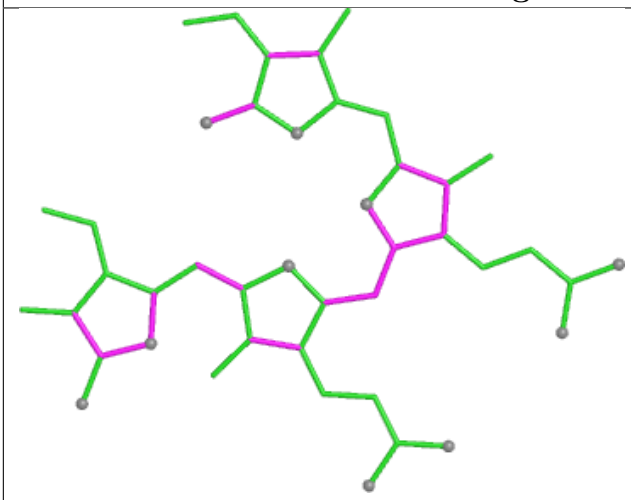


Torsions



Rings

Ligand PEB OE 201



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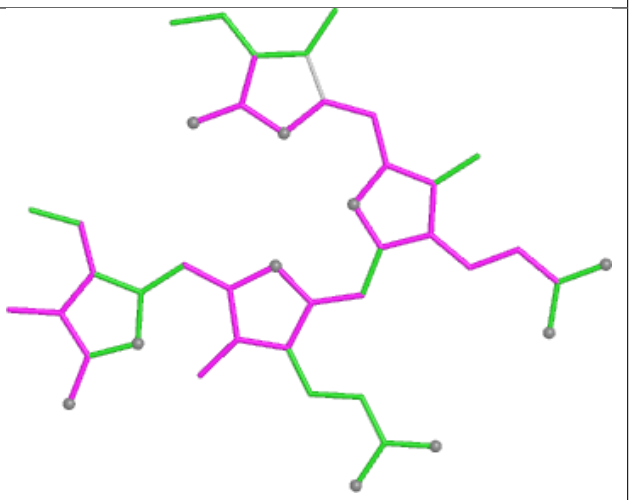
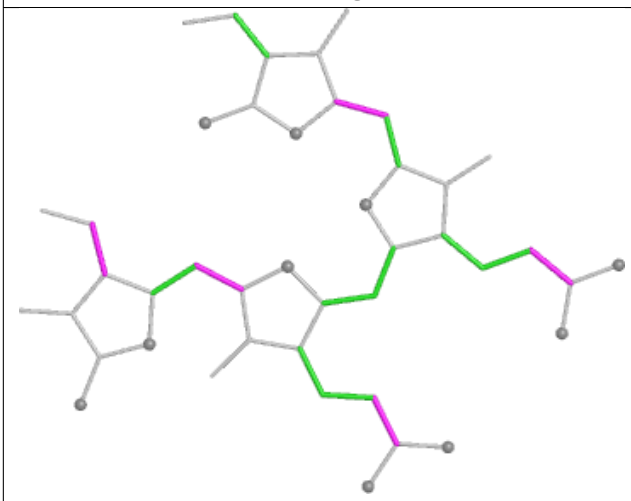


Bond angles



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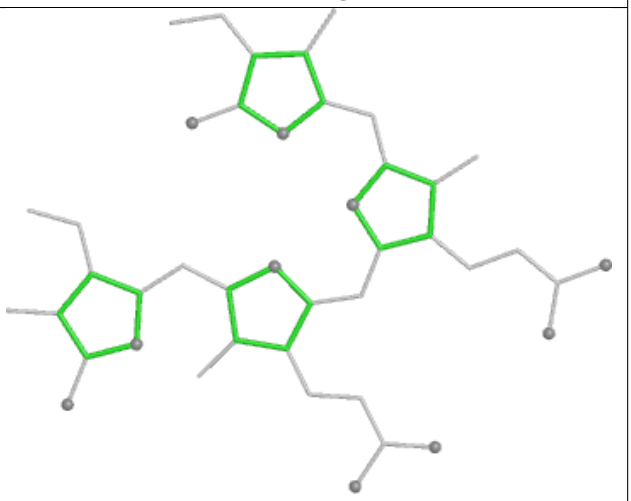
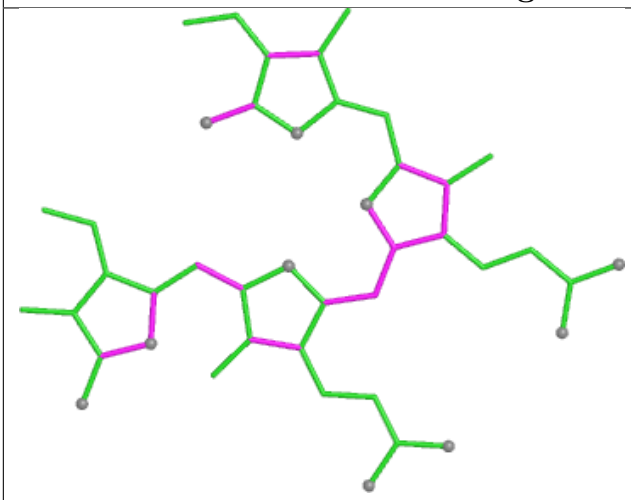


Rings

Ligand PEB VI 201



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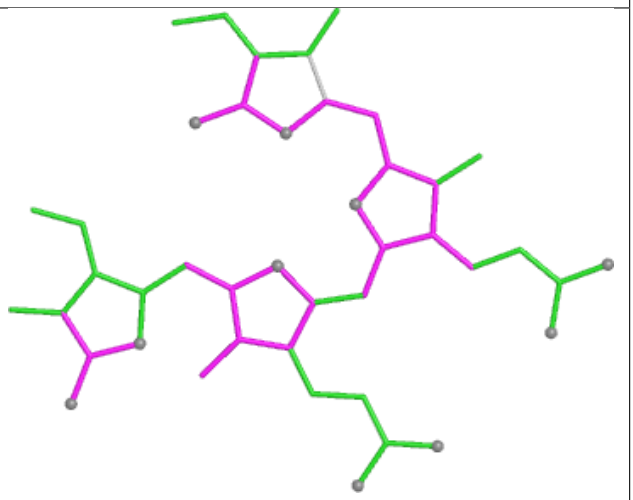
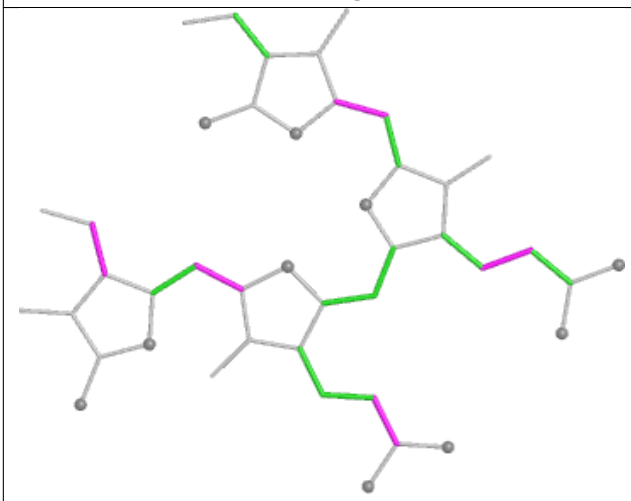


Bond angles



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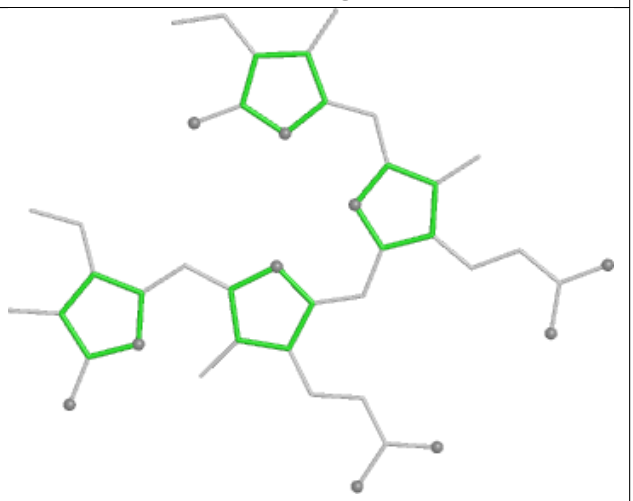
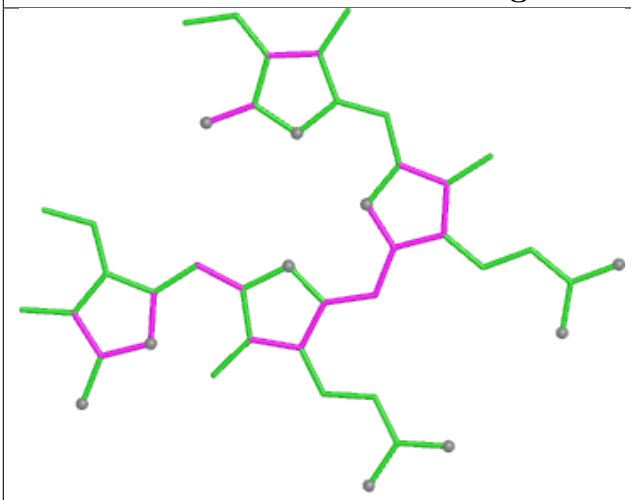


Rings

Ligand PEB GD 201



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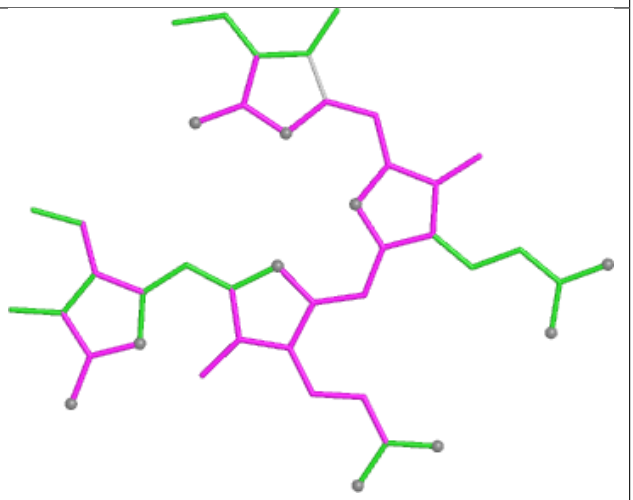

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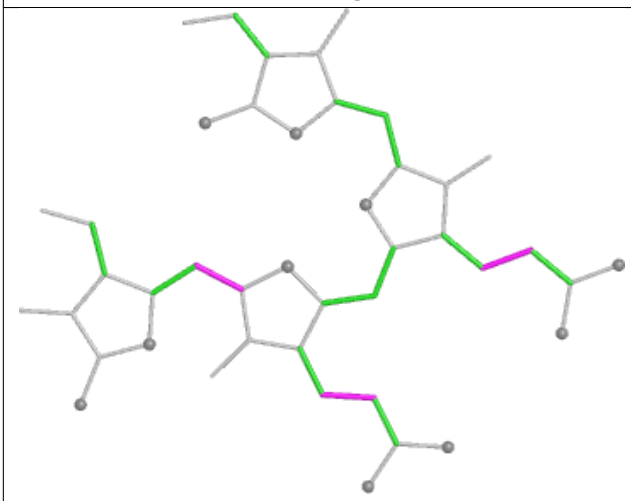

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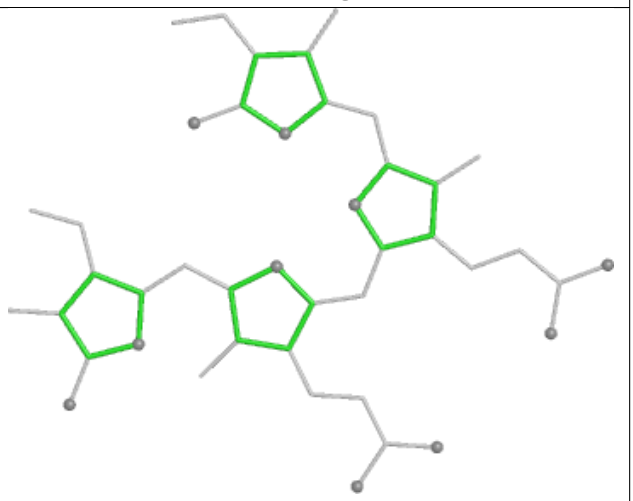

Rings

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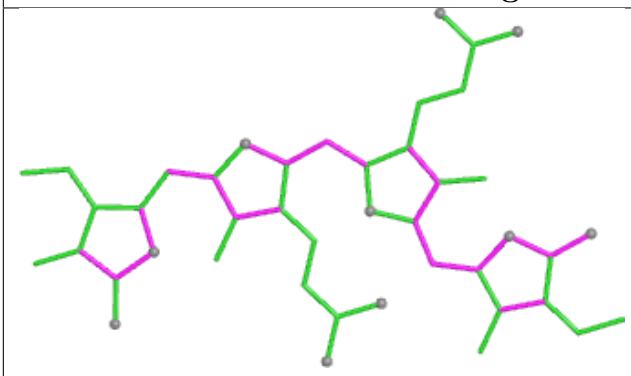

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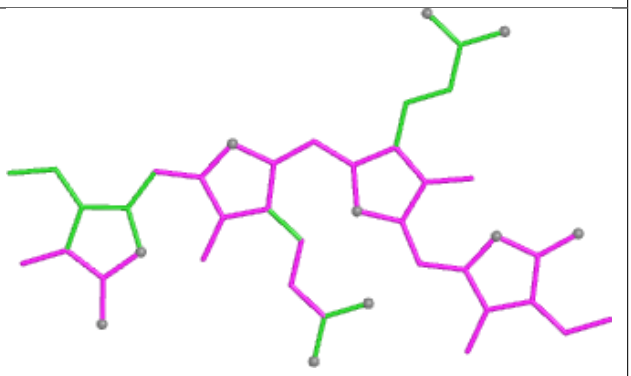

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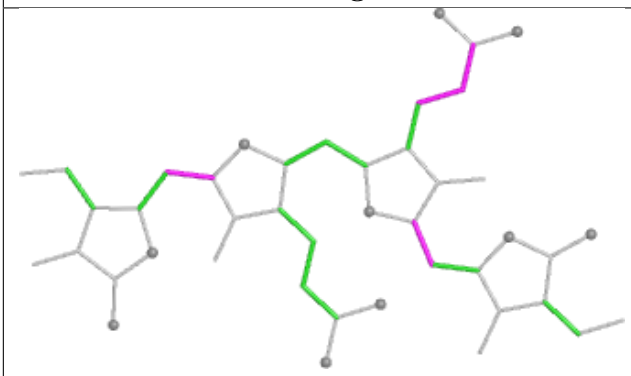

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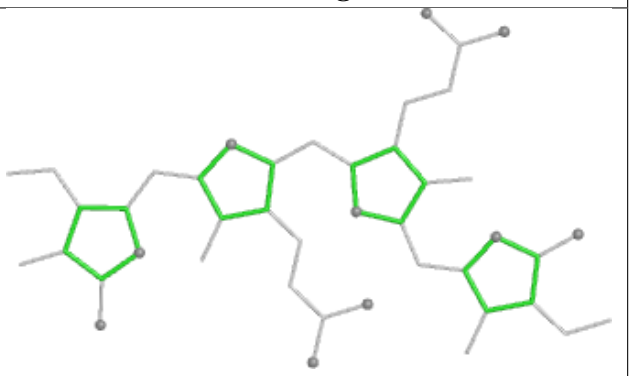
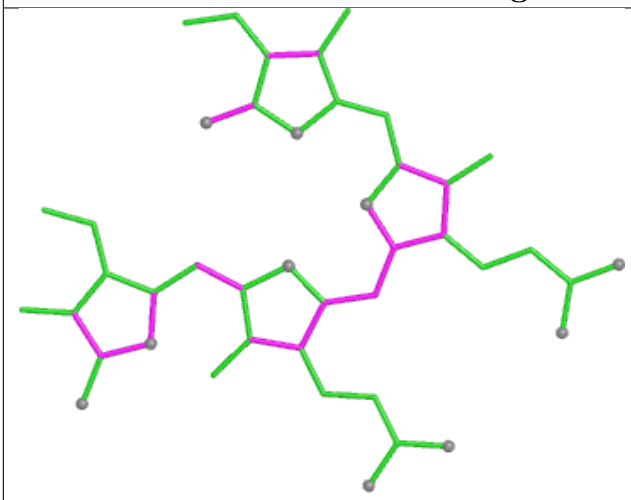


Rings

Ligand PEB RH 201



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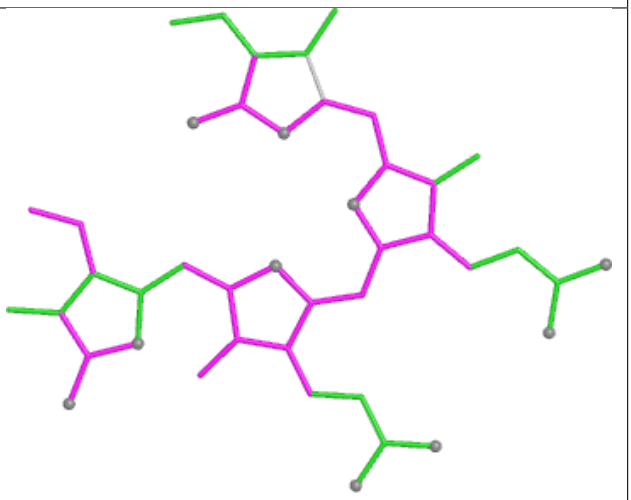

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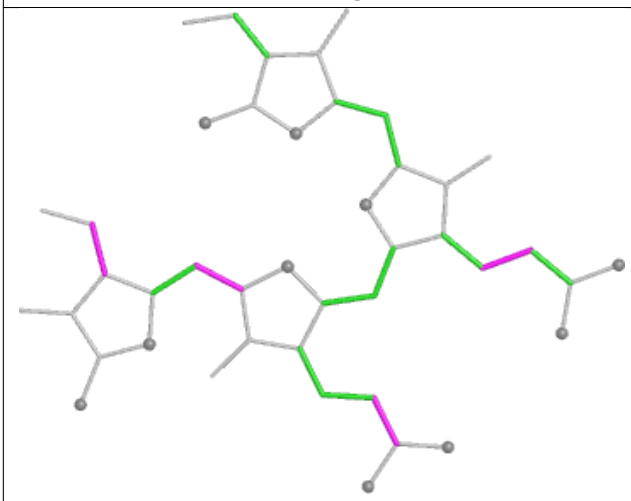

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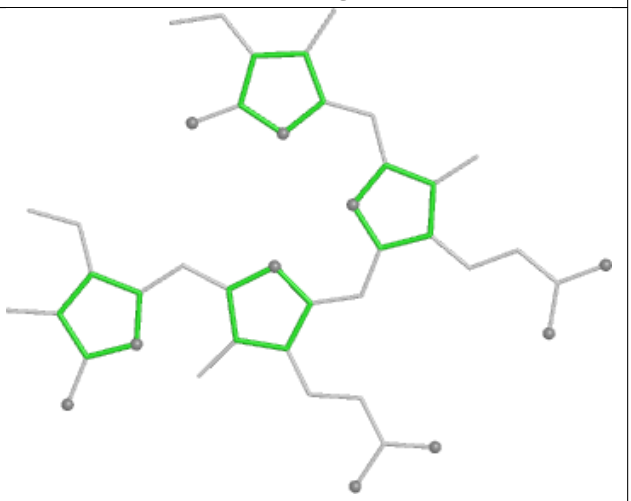
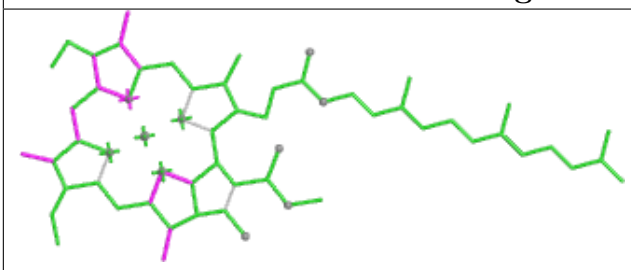


Rings

Ligand CLA A6 403



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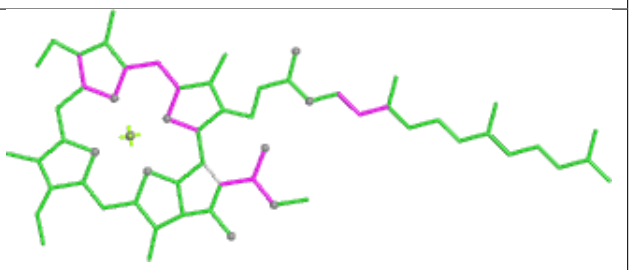

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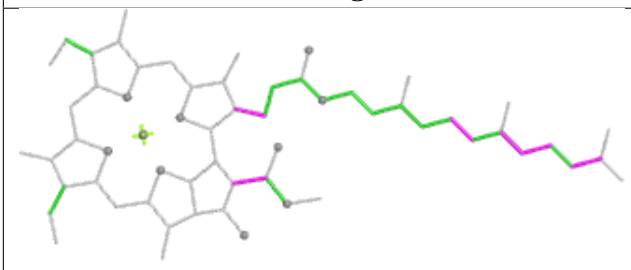

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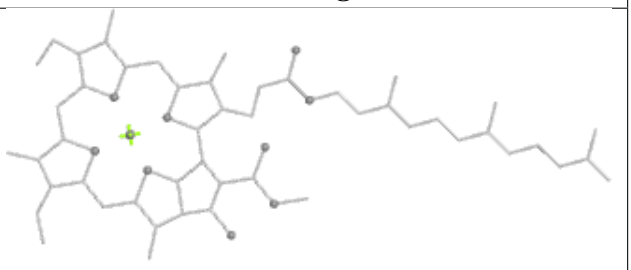
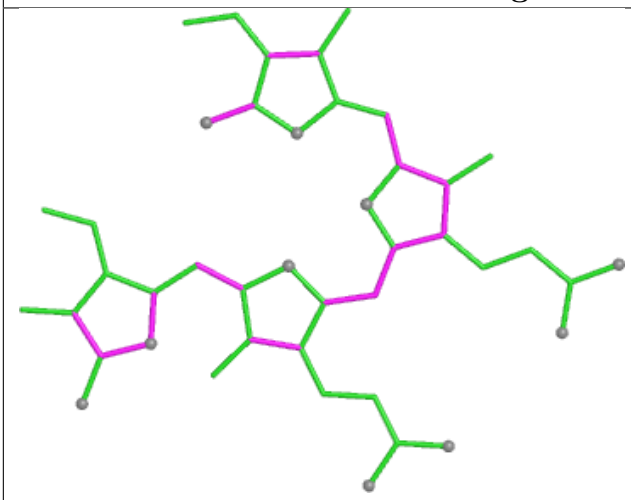


Rings

Ligand PEB mE 202



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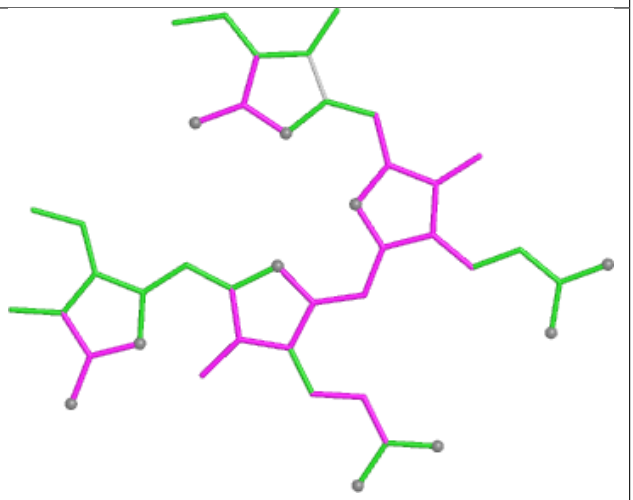

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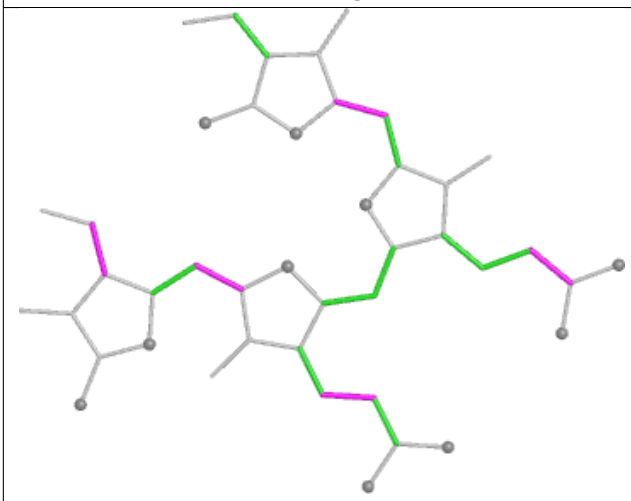

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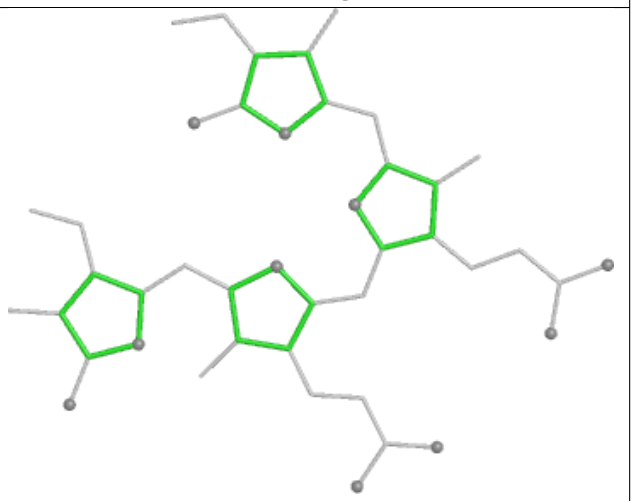
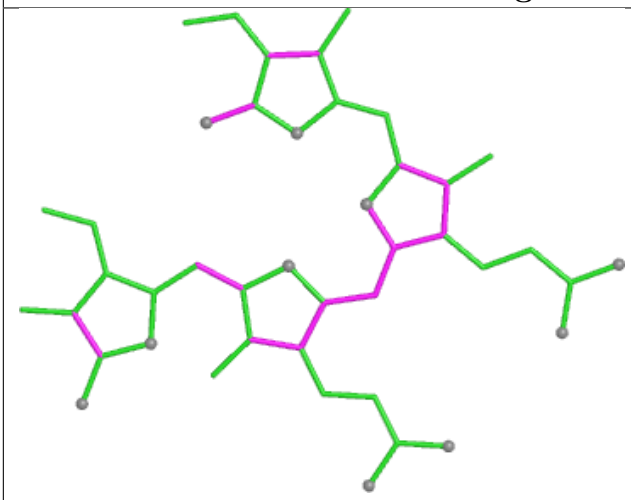


Rings

Ligand PEB FF 201



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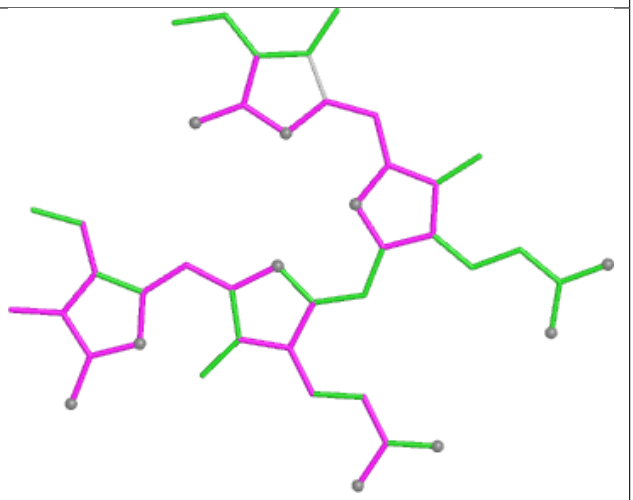

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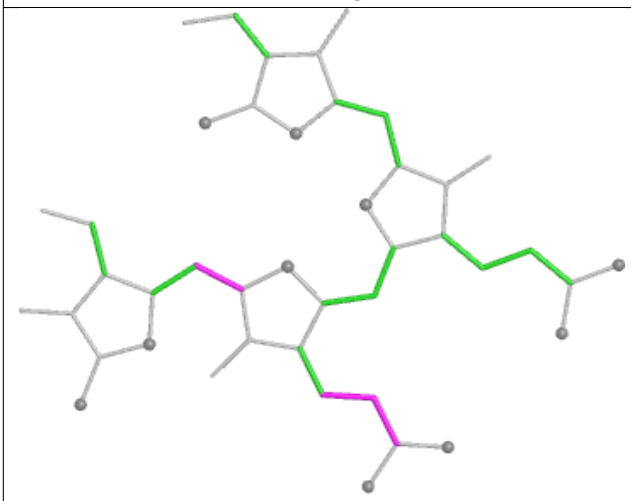

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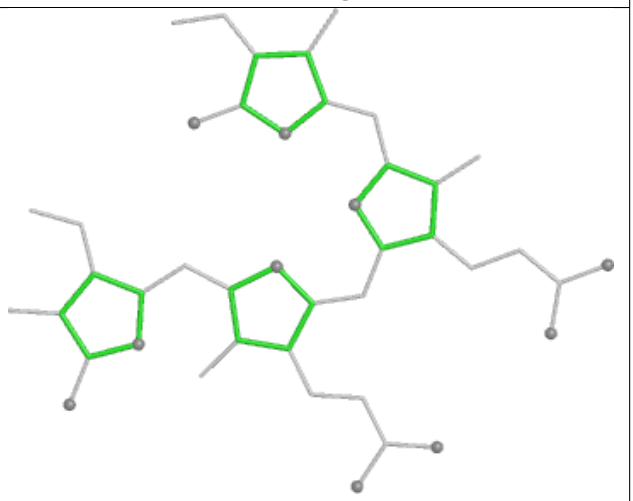
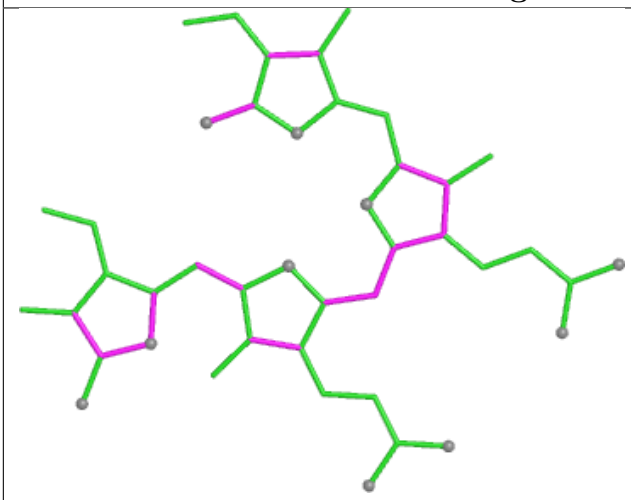


Rings

Ligand PEB KG 201



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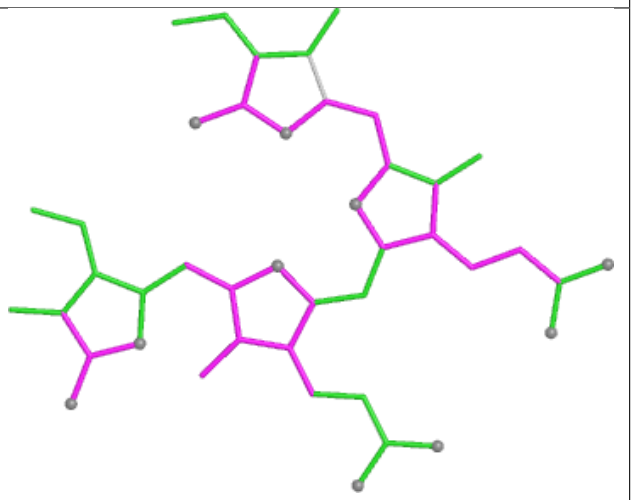

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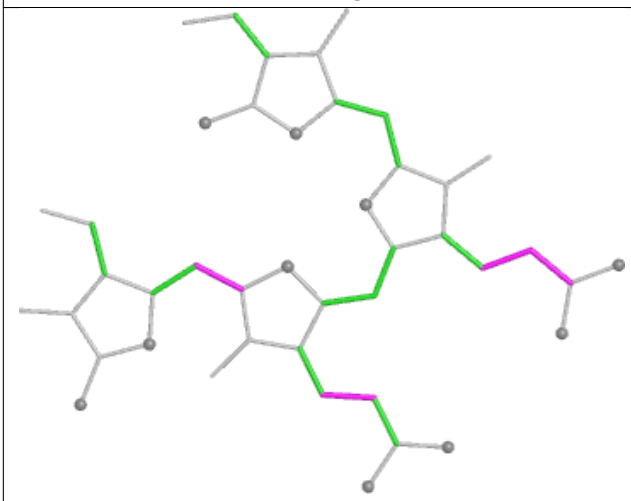

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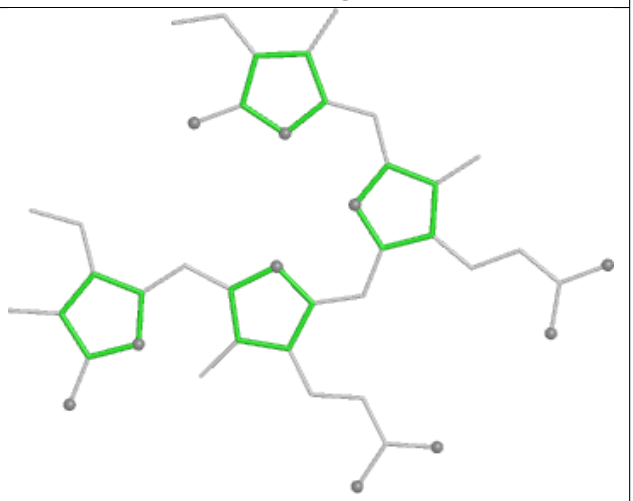
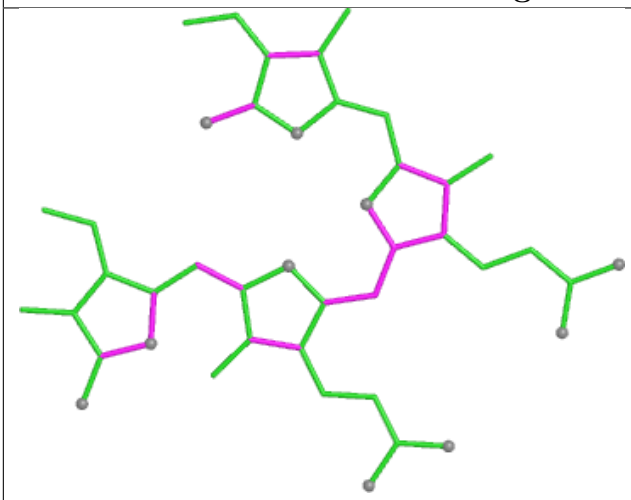


Rings

Ligand PEB dG 201



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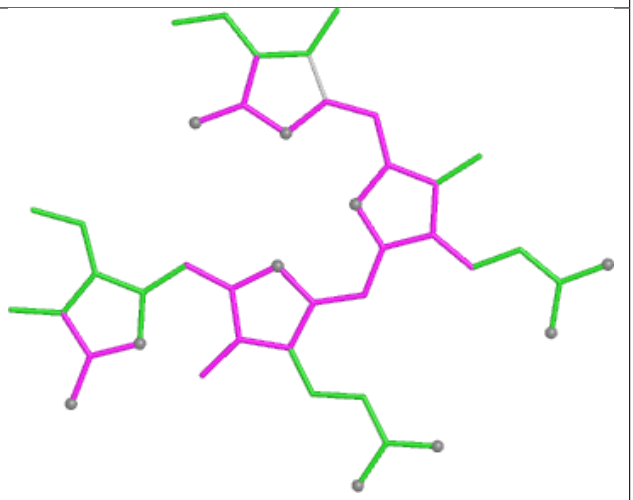

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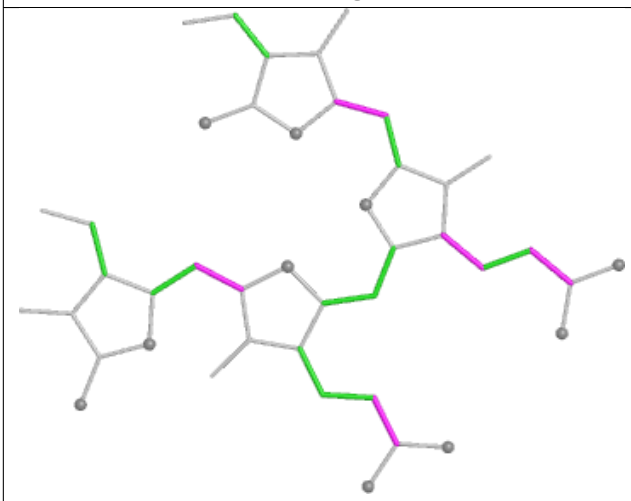

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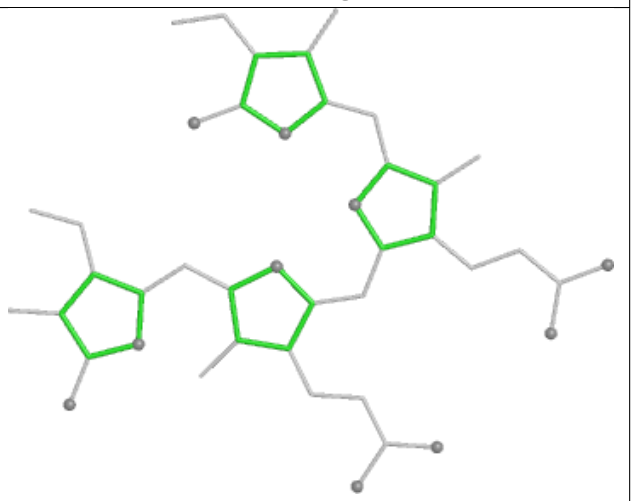
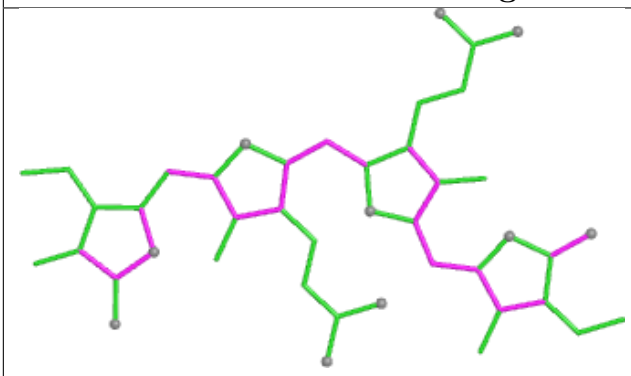


Rings

Ligand CYC CH 1001



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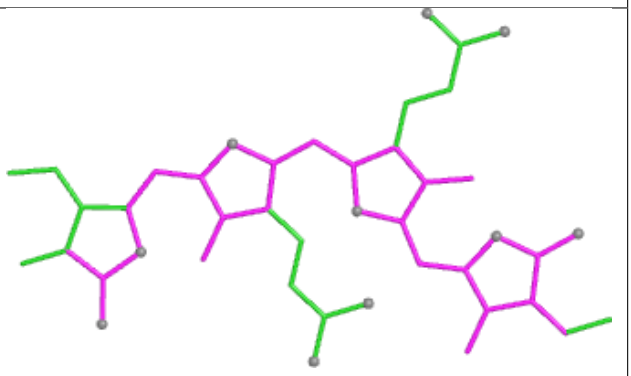
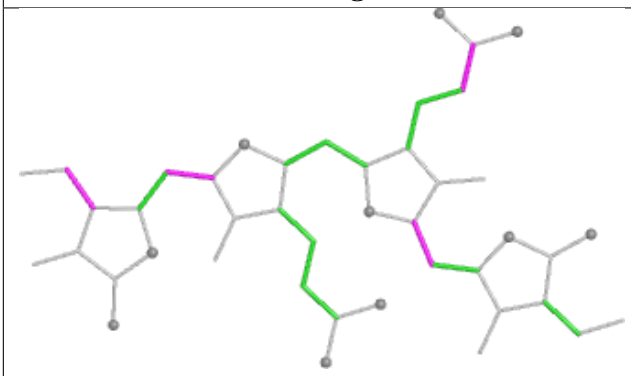


Bond angles



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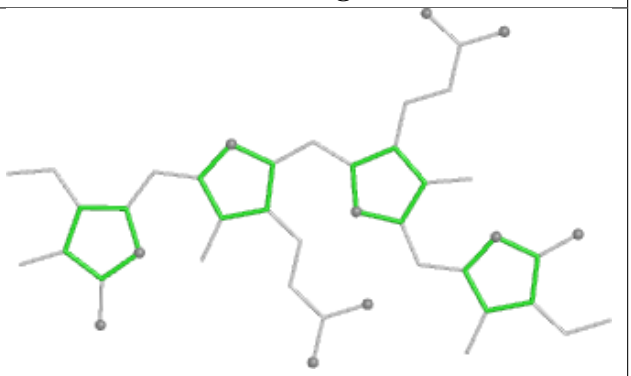
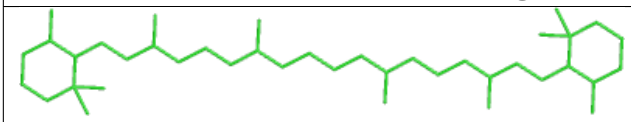


Rings

Ligand BCR B2 840



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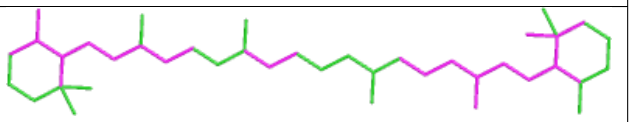

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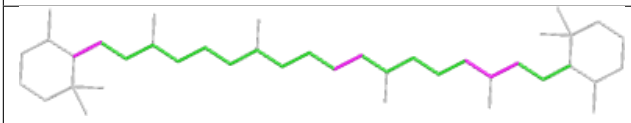

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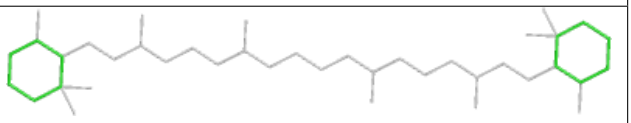
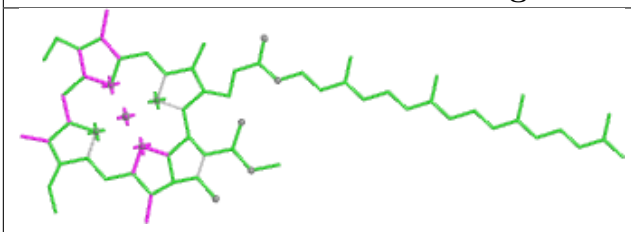


Rings

Ligand CLA AN 808



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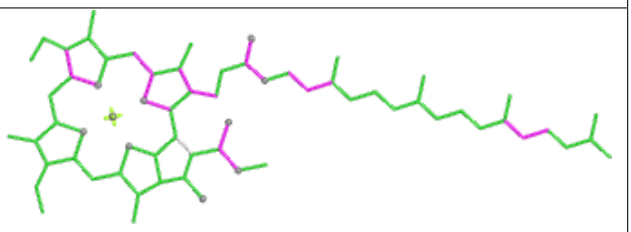

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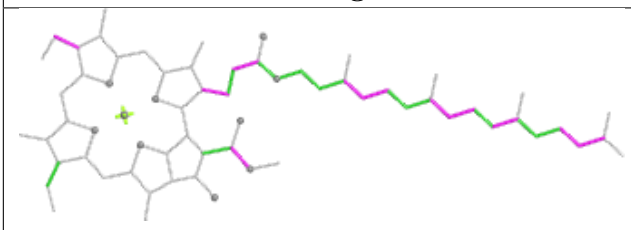

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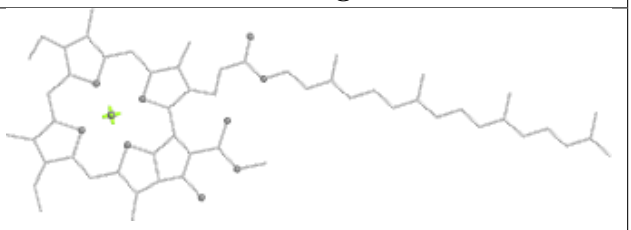
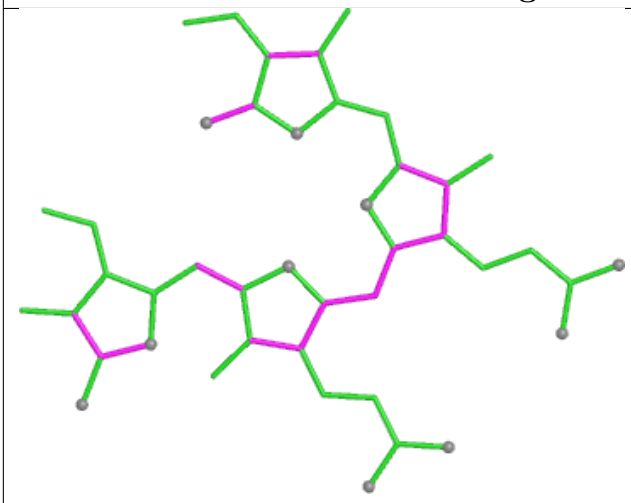


Rings

Ligand PEB rF 201



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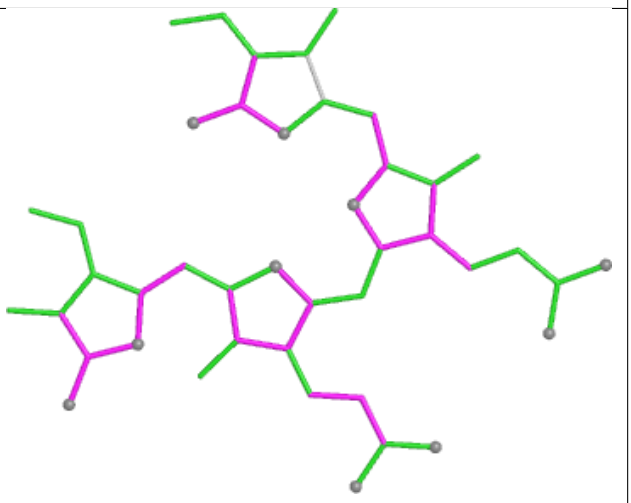
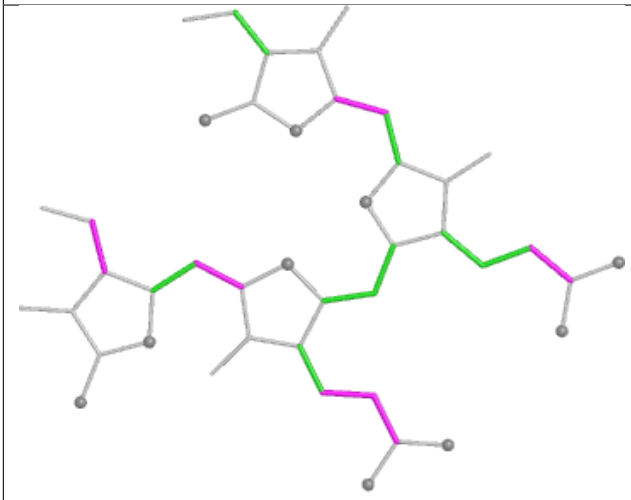


Bond angles



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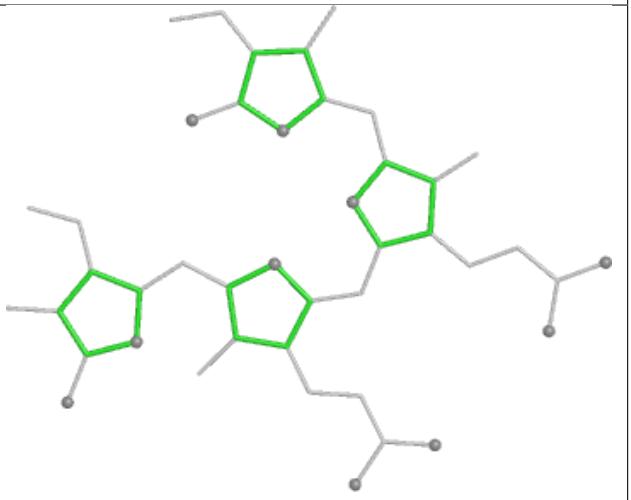
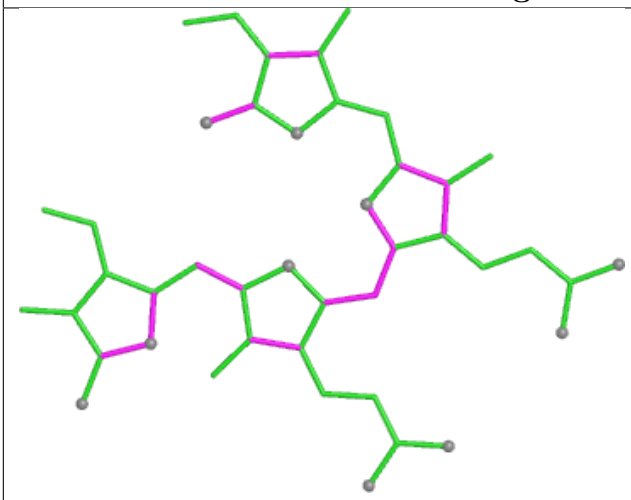


Rings

Ligand PEB OF 202



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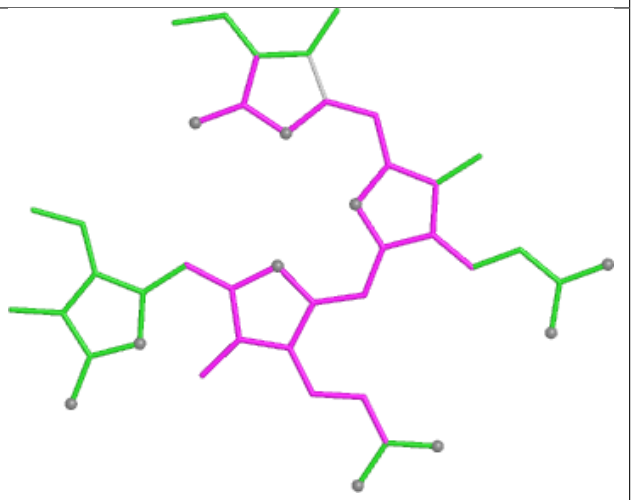

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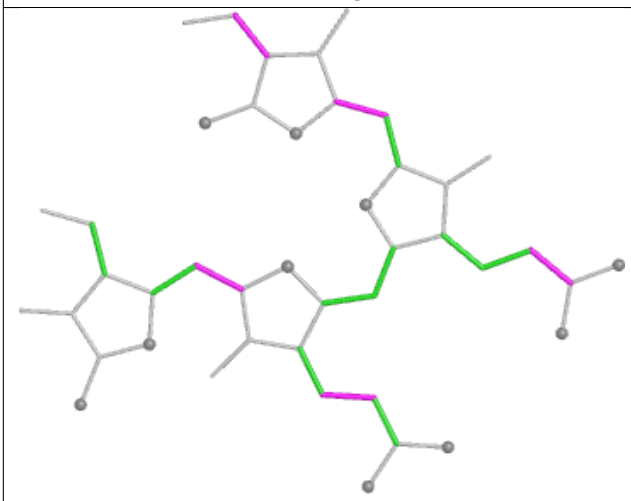

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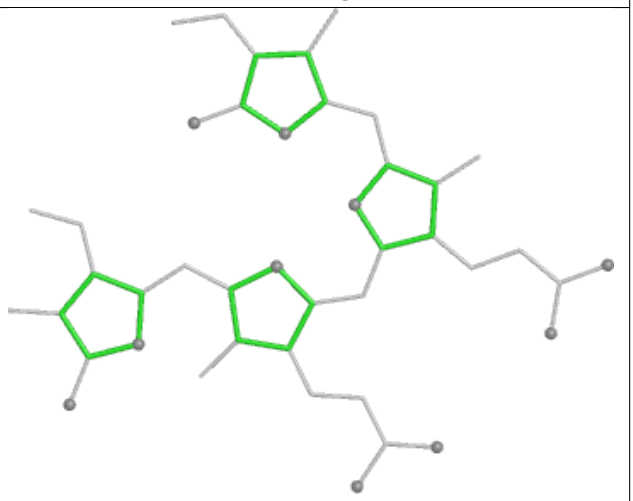
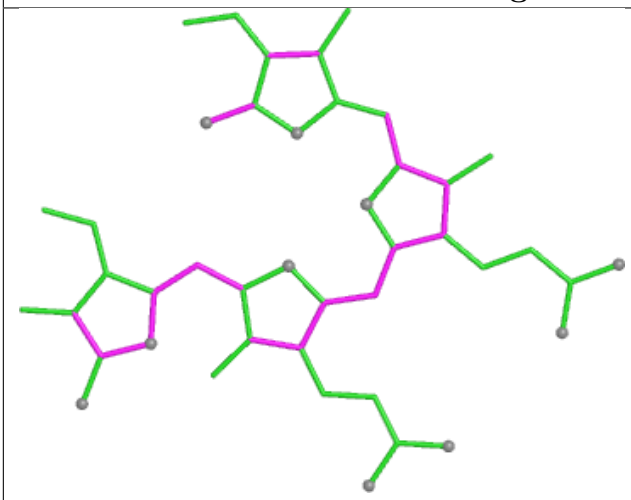


Rings

Ligand PEB UH 202



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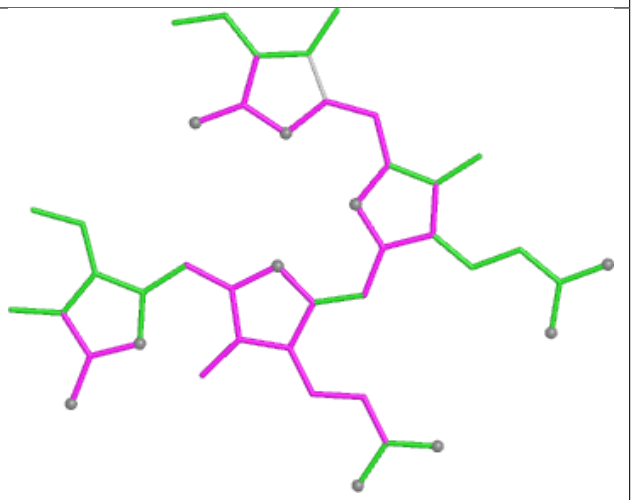
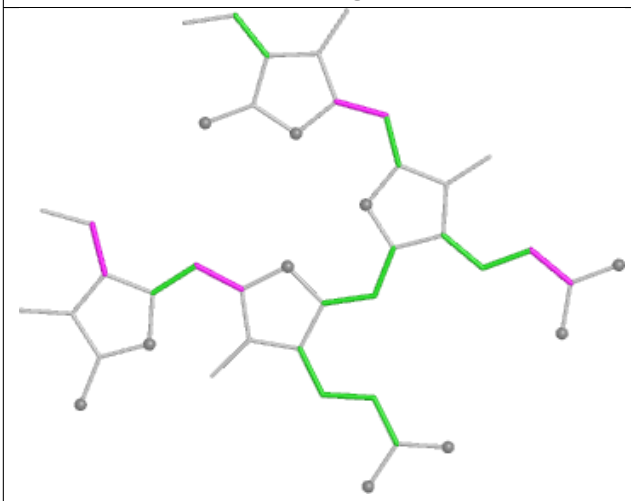


Bond angles



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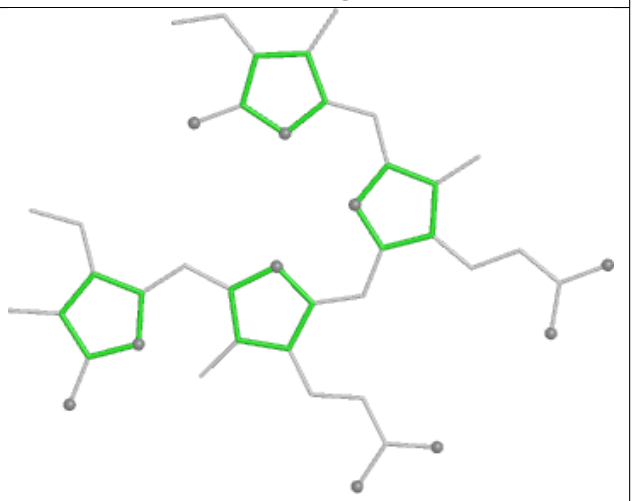
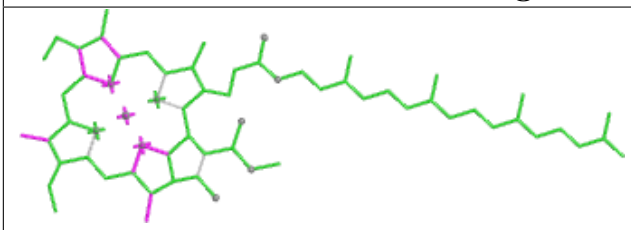


Rings

Ligand CLA A2 829



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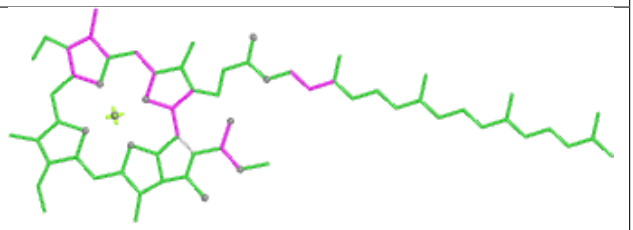

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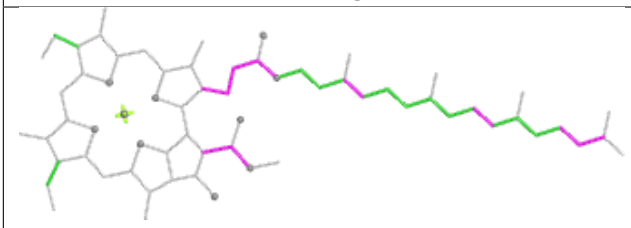
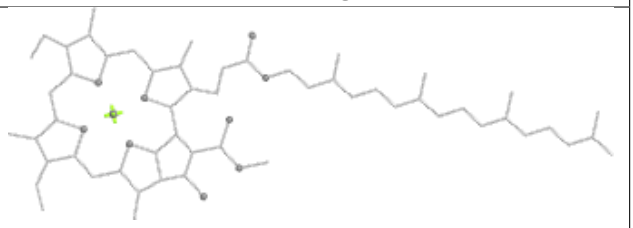
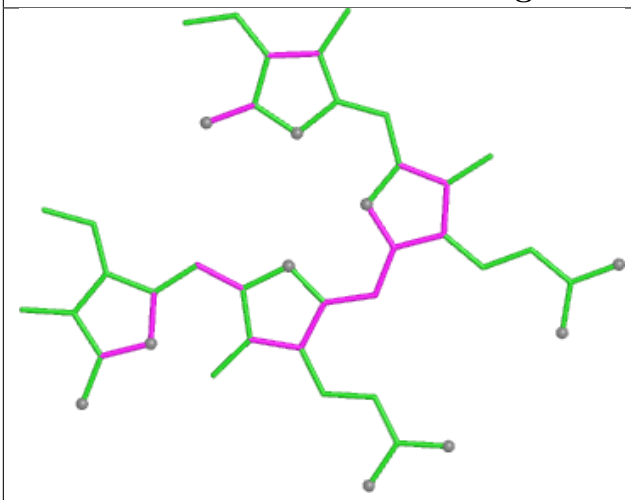


Torsions



Rings

Ligand PEB OJ 202



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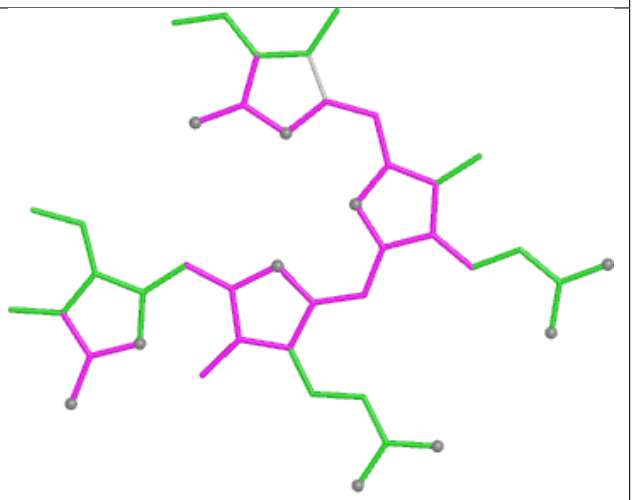

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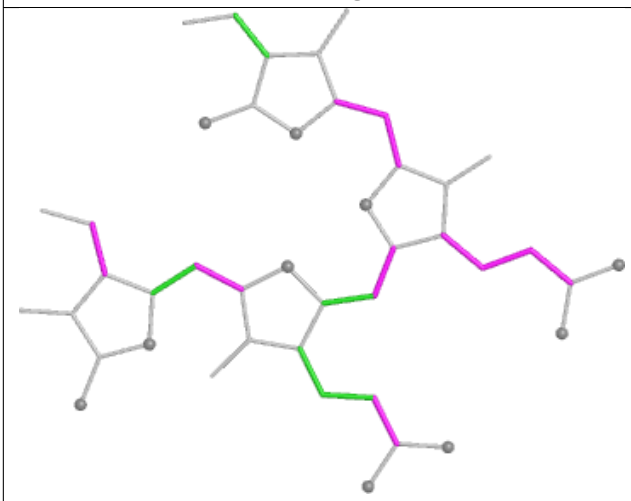

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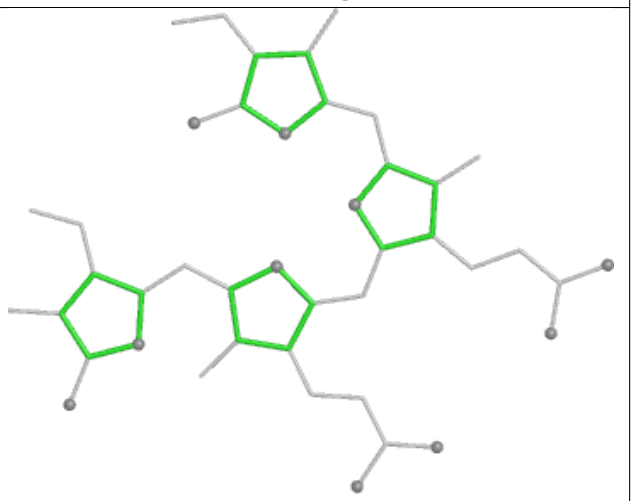
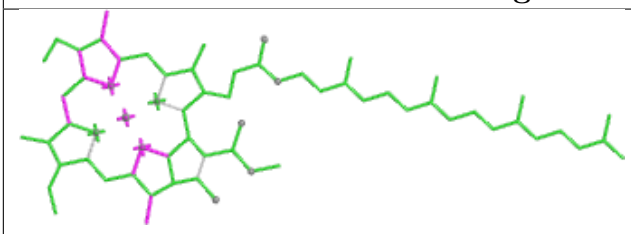


Rings

Ligand CLA CL 507



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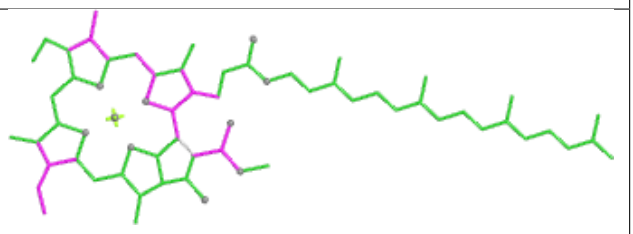

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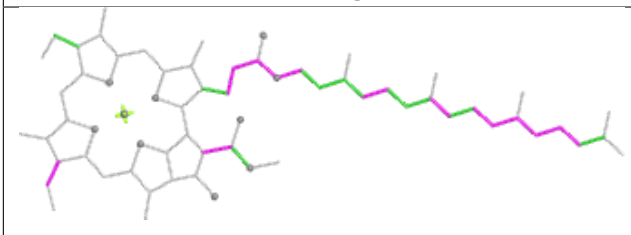

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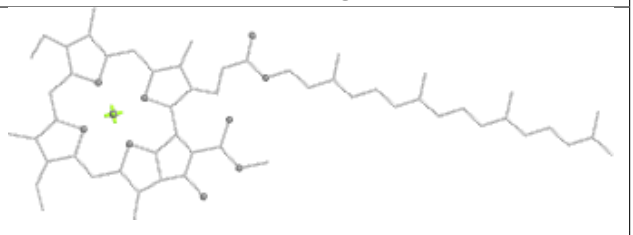
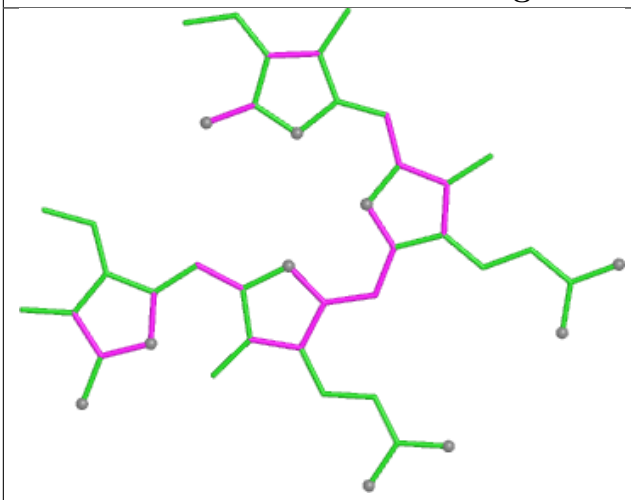


Rings

Ligand PEB FQ 203



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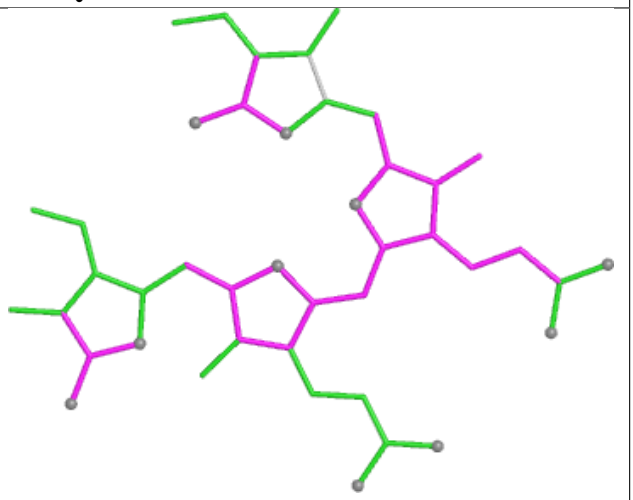

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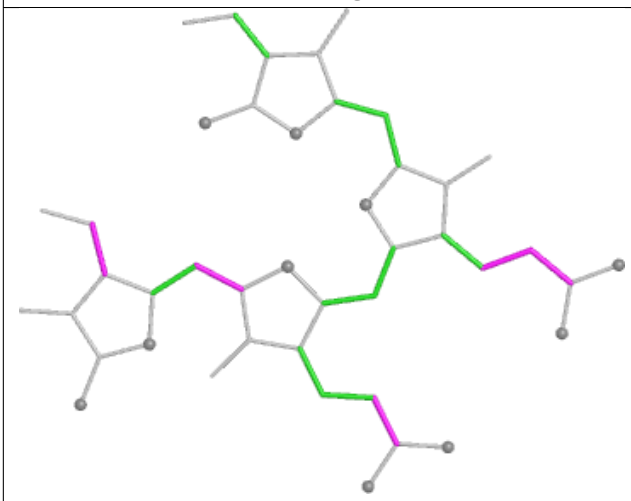

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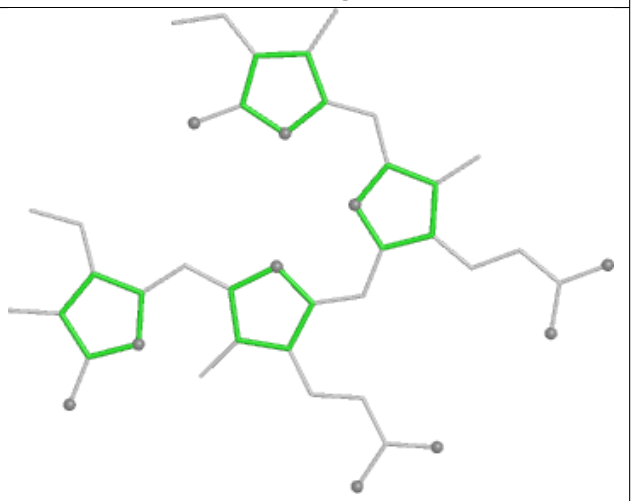
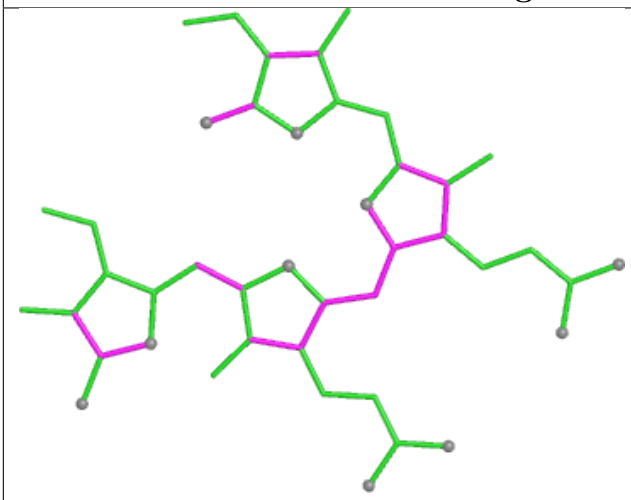


Rings

Ligand PEB U9 201



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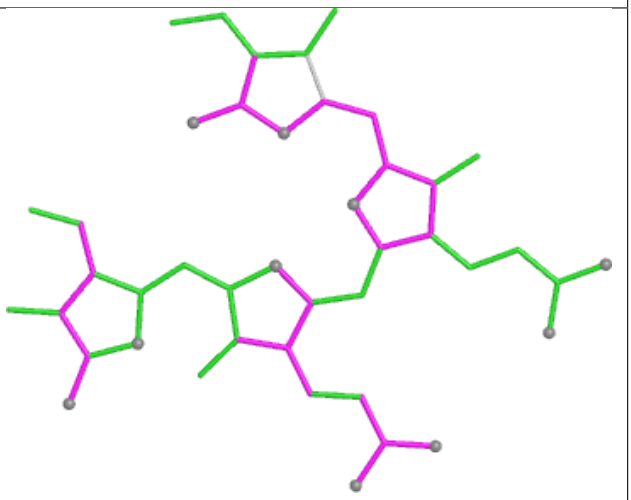

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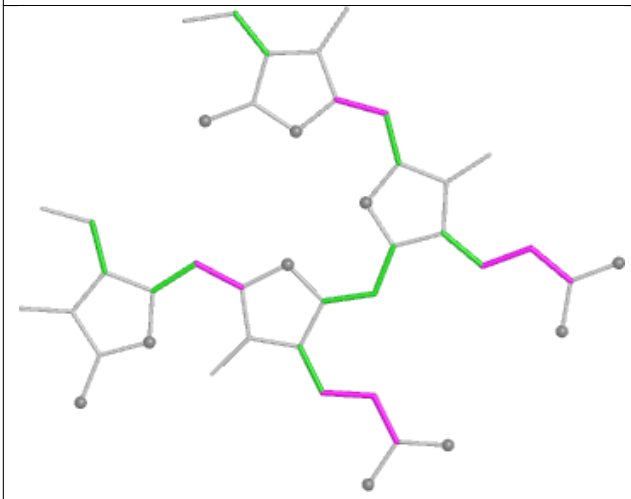

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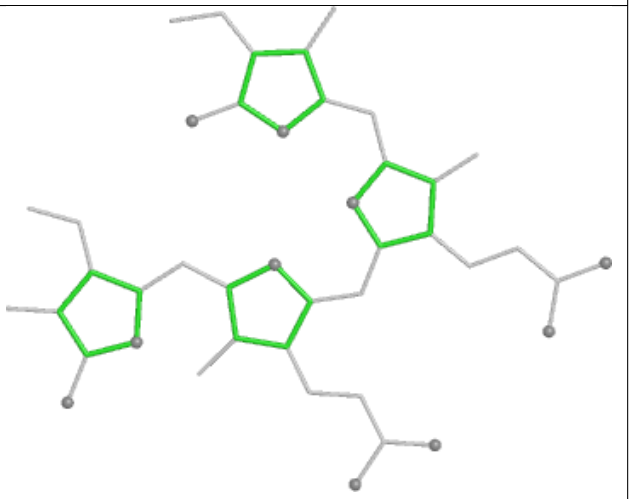
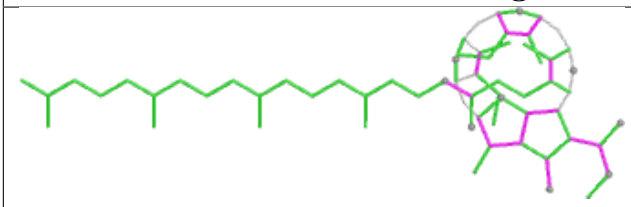


Rings

Ligand PHO DL 405



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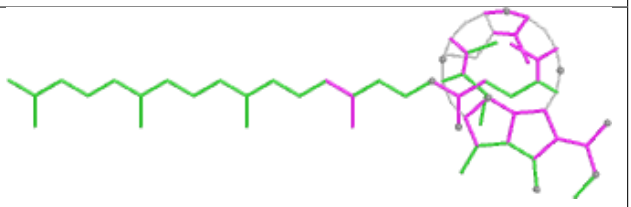

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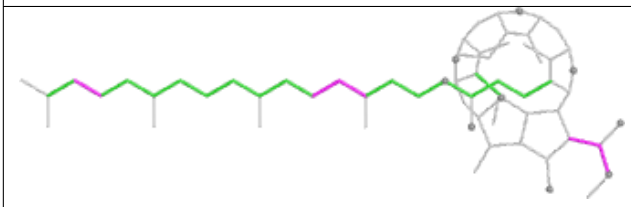

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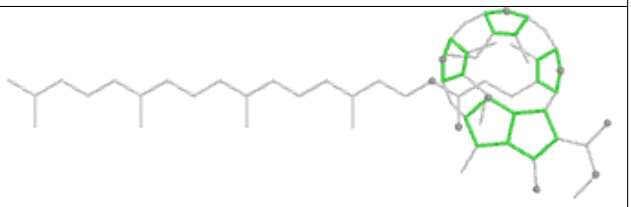
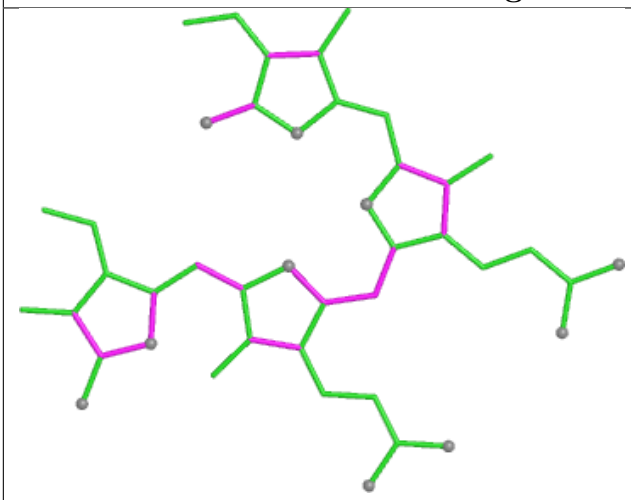


Rings

Ligand PEB WK 201



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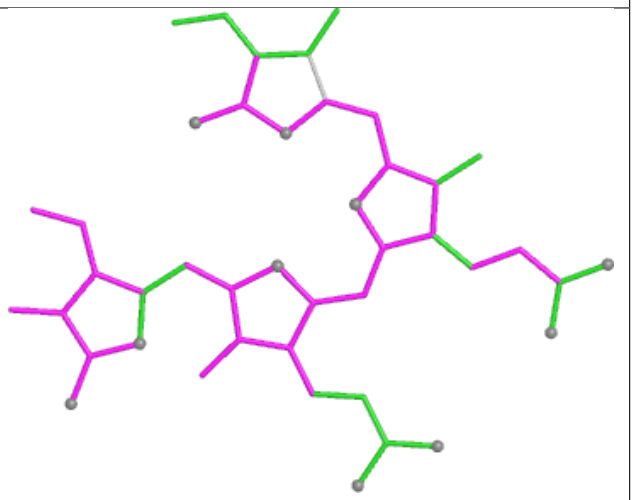

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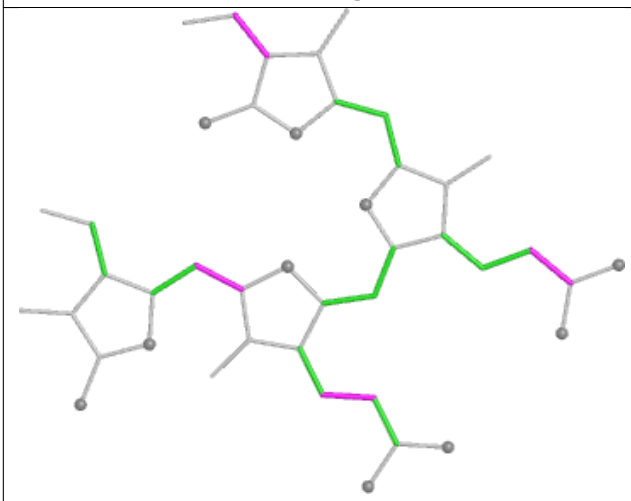

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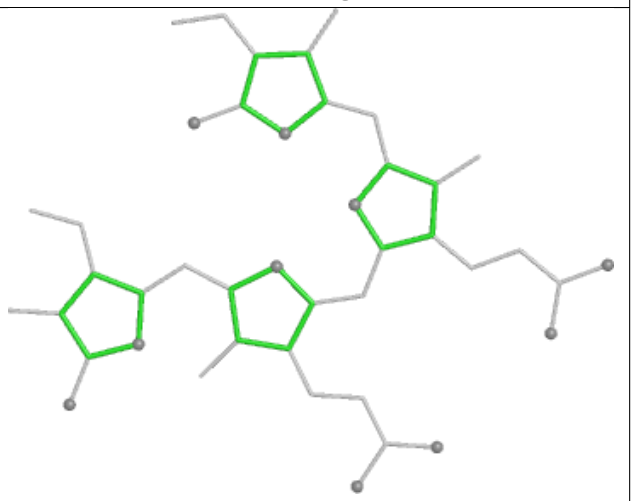
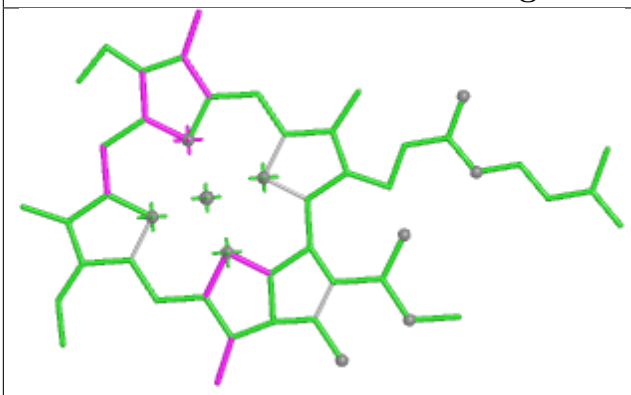


Rings

Ligand CLA 12 607



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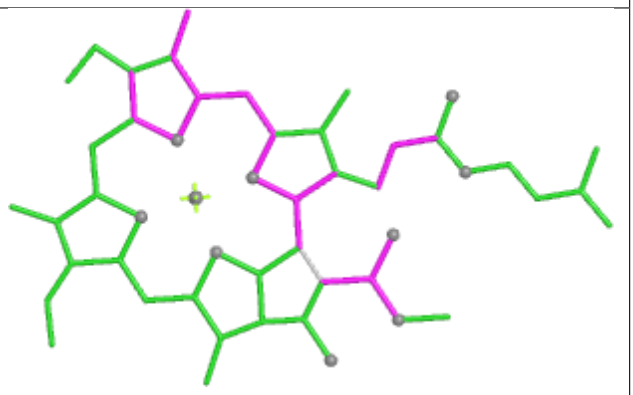

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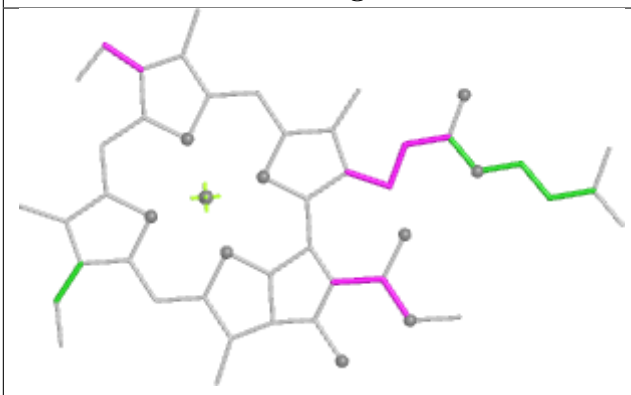

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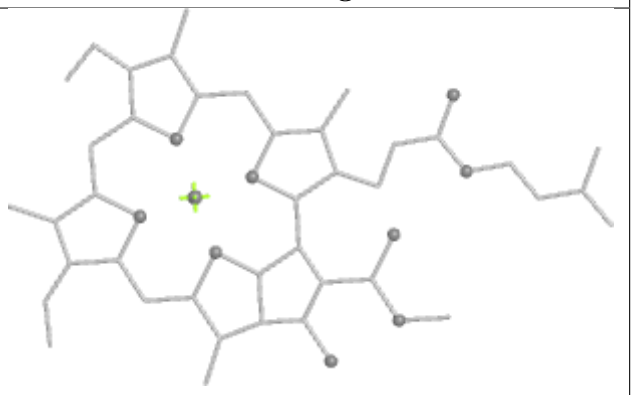
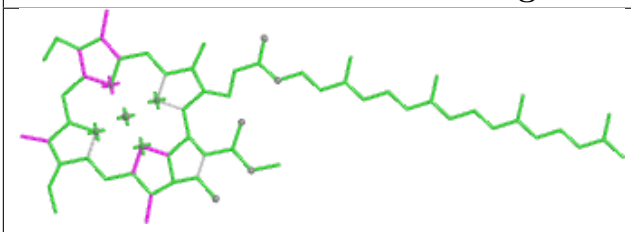


Rings

Ligand CLA cL 514



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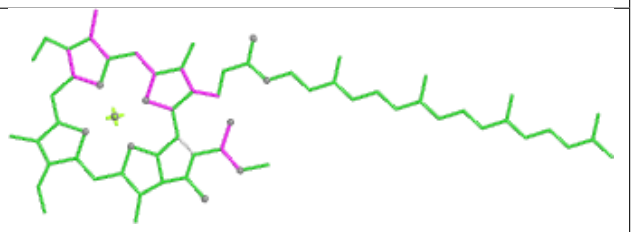

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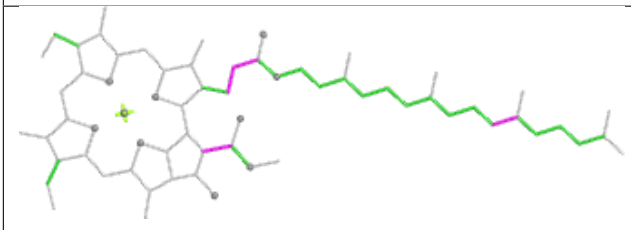

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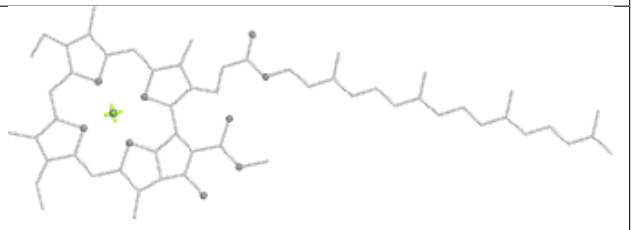
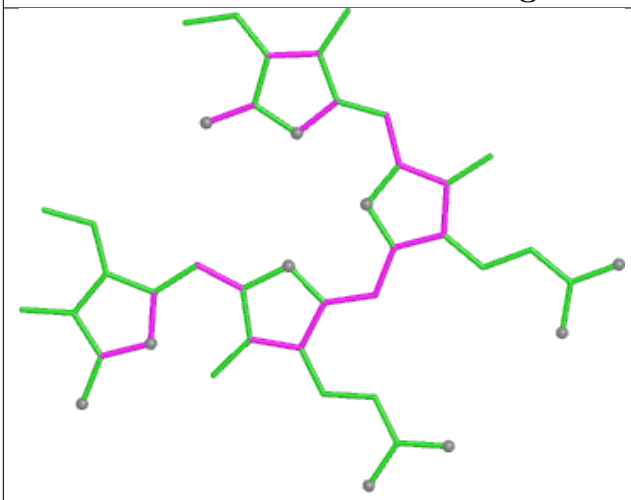


Rings

Ligand PEB tF 202



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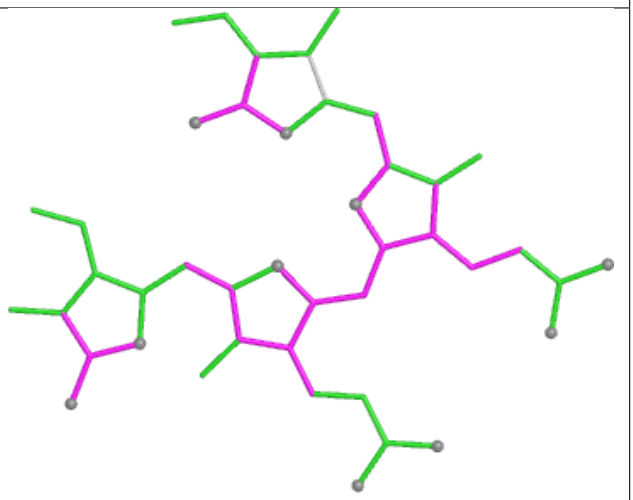

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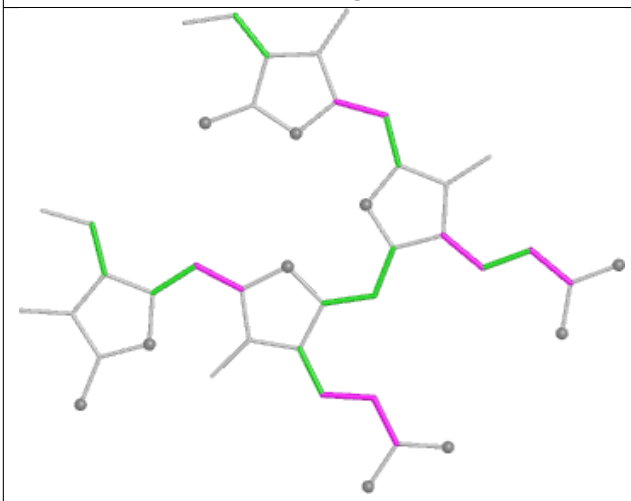

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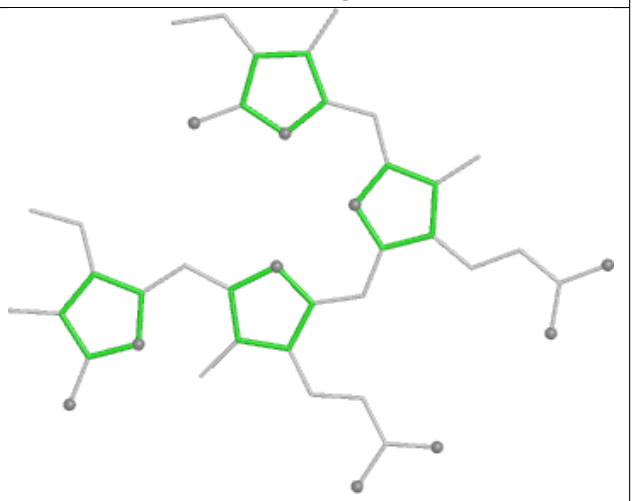
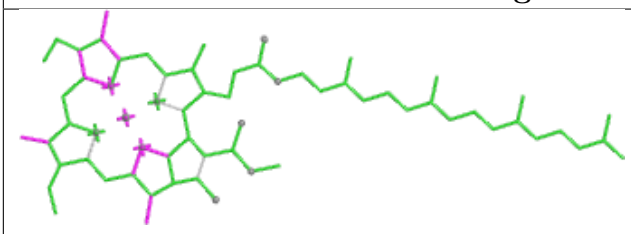


Rings

Ligand CLA BL 602



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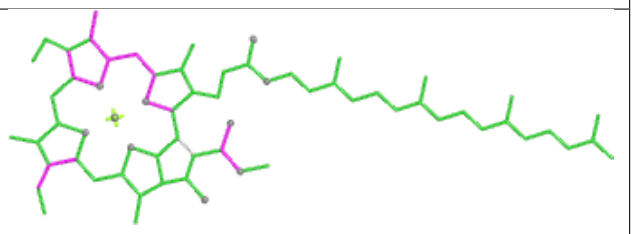

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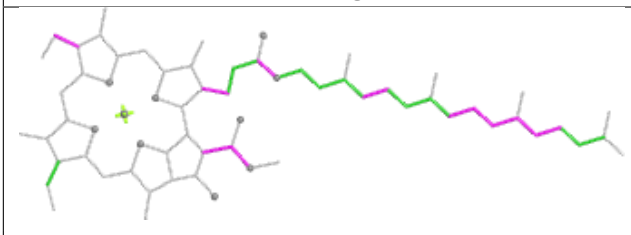

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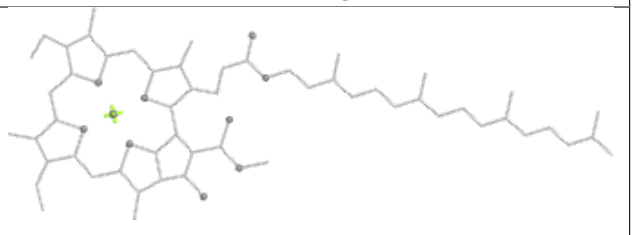
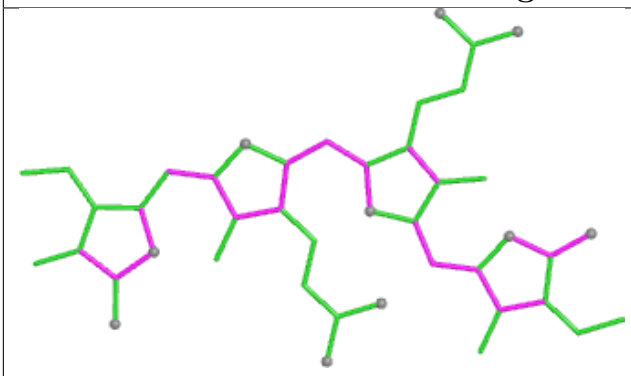


Rings

Ligand CYC 63 901



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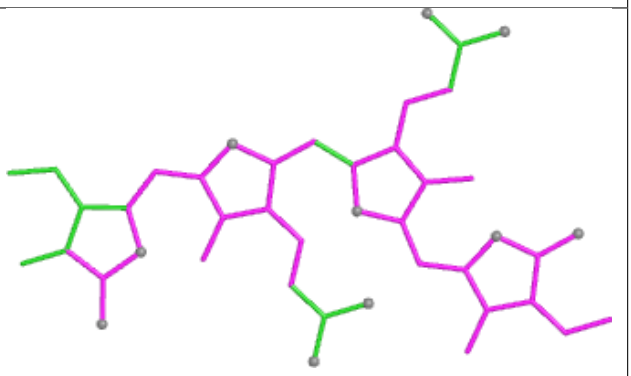

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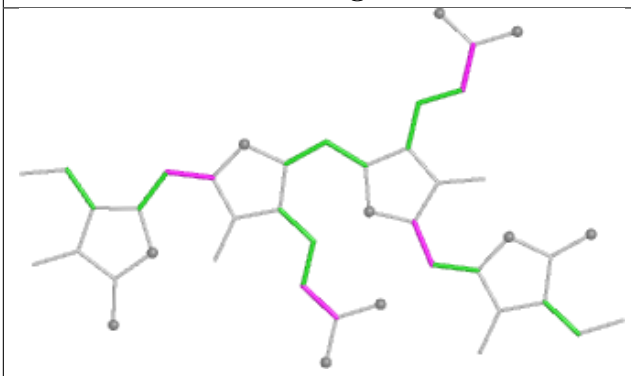

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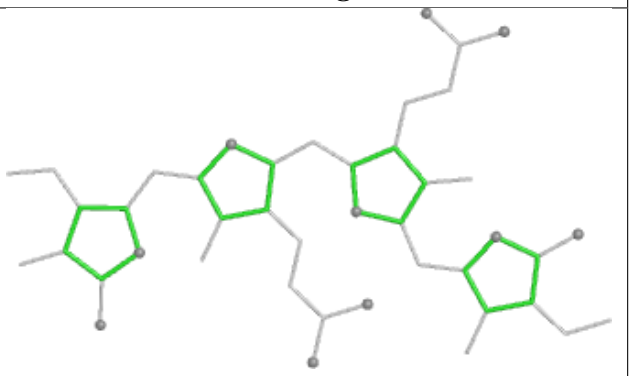
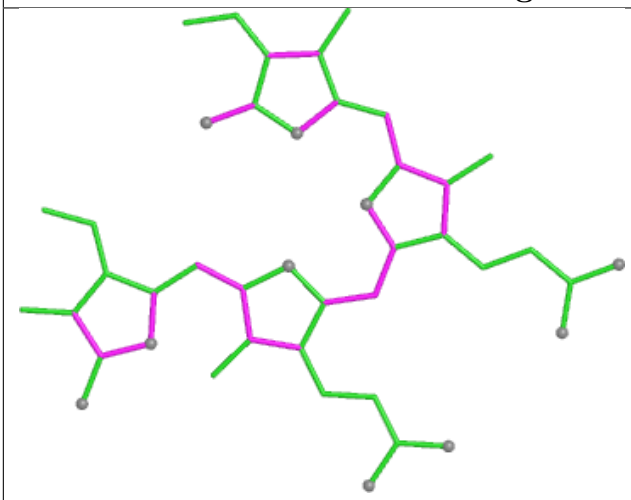


Rings

Ligand PEB iM 201



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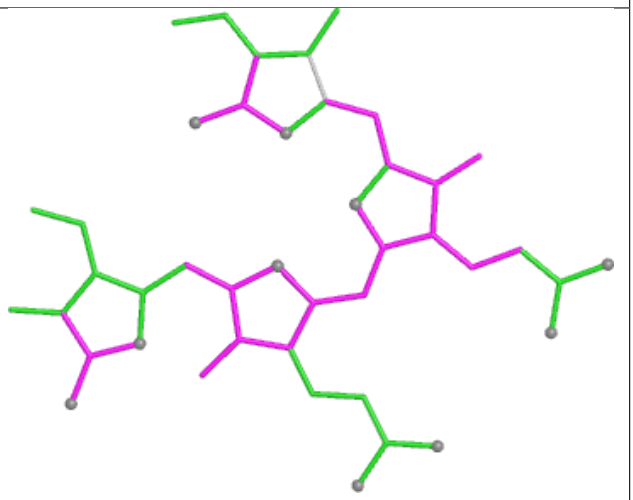
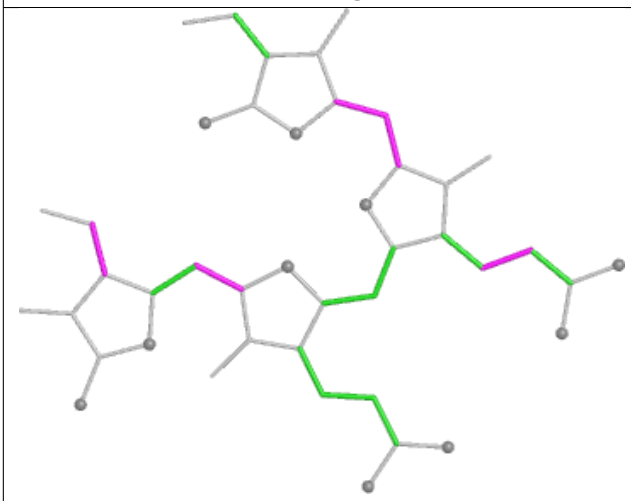


Bond angles



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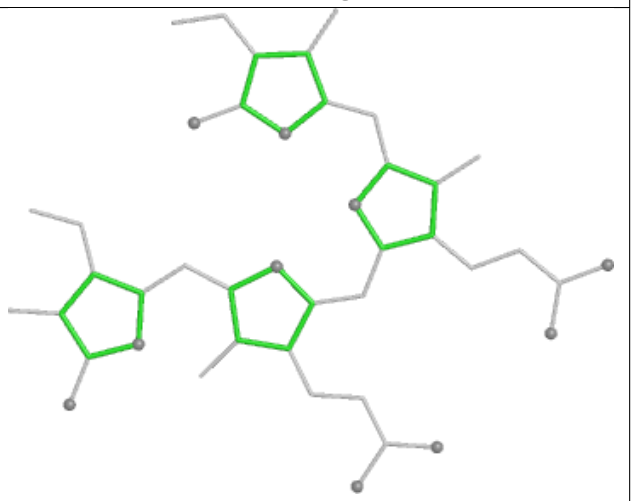
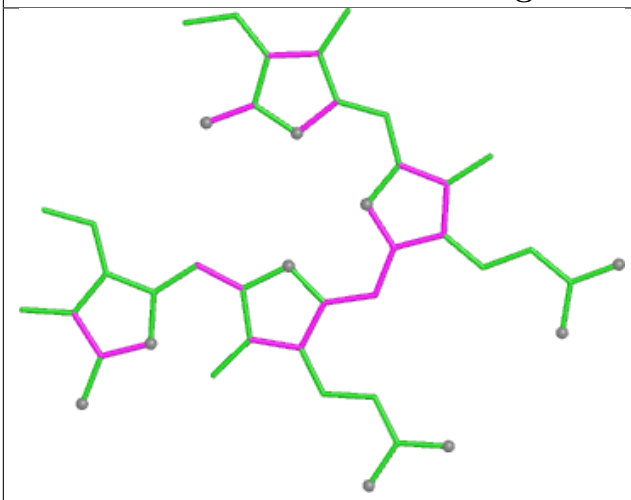


Rings

Ligand PEB X9 202



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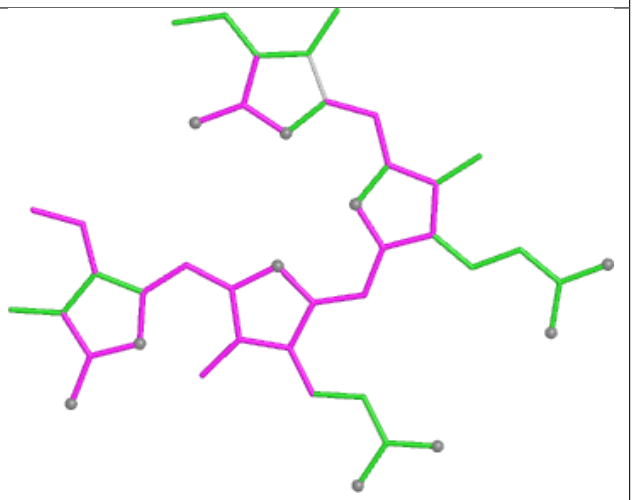
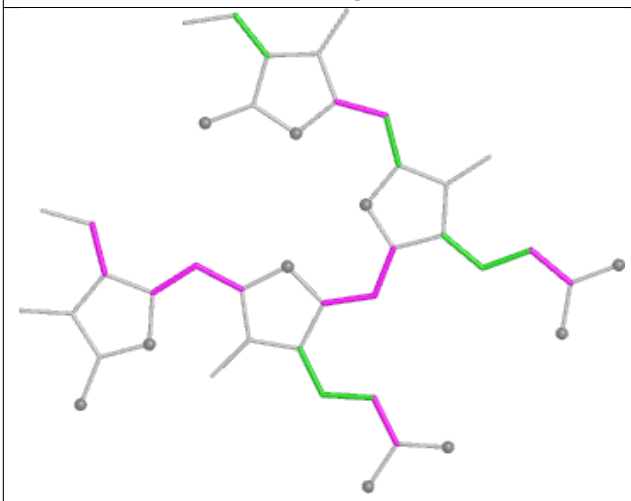


Bond angles



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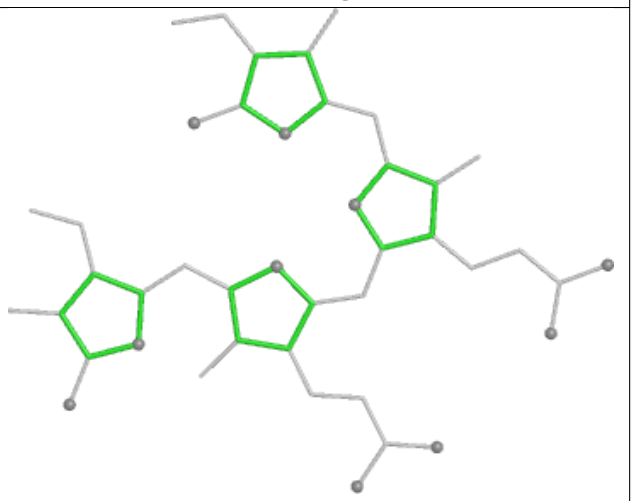
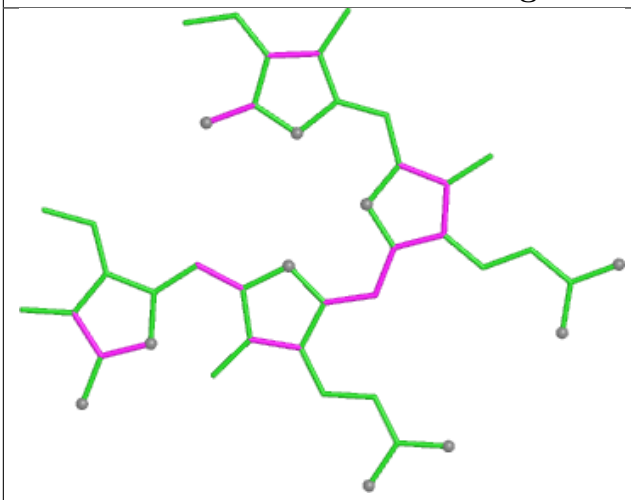


Rings

Ligand PEB g4 202



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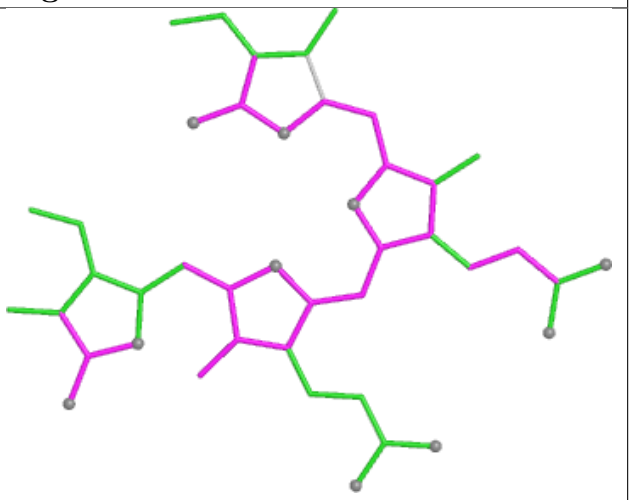
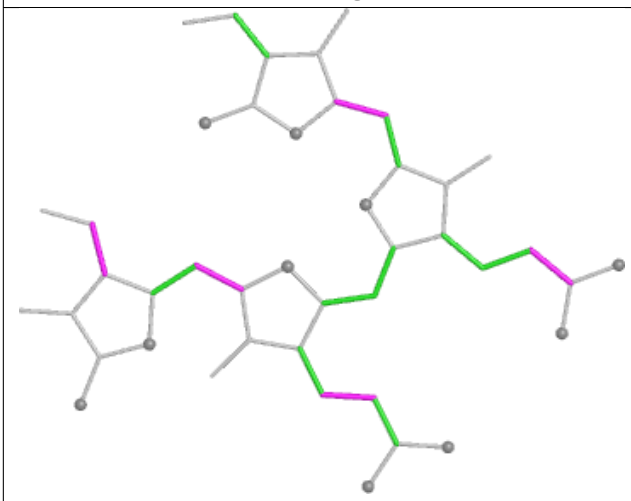
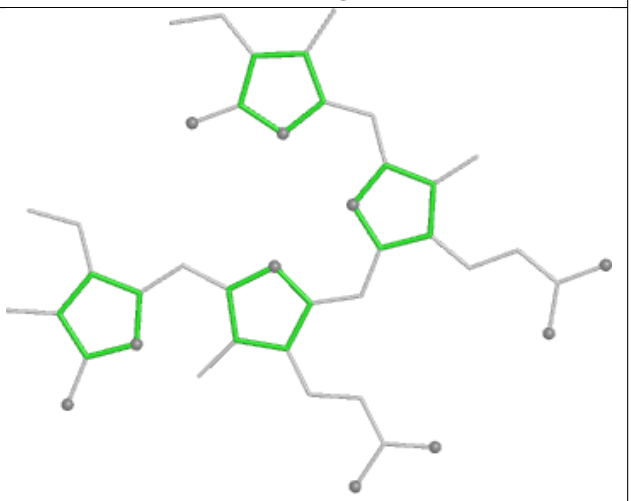


Bond angles

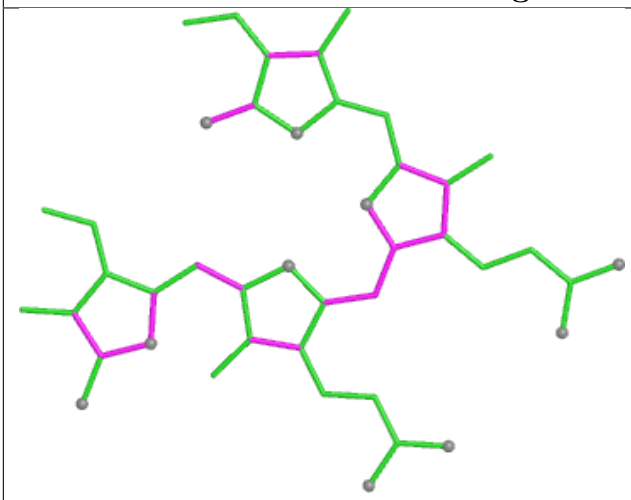


Torsions



Rings

Ligand PEB UE 202



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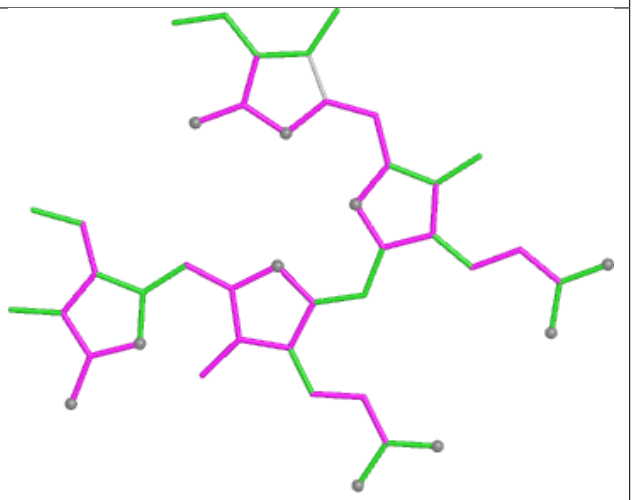

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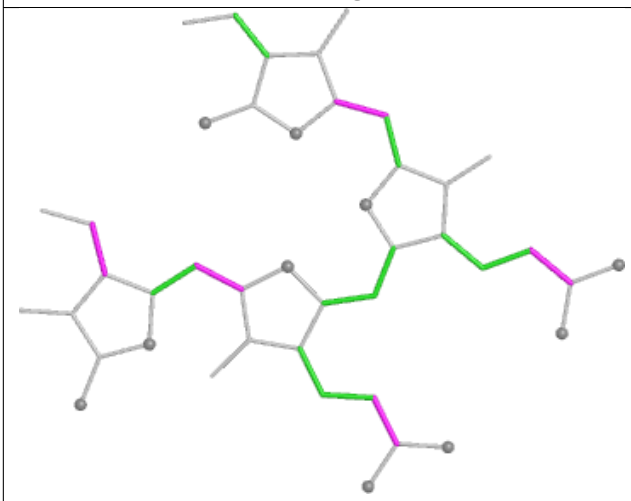

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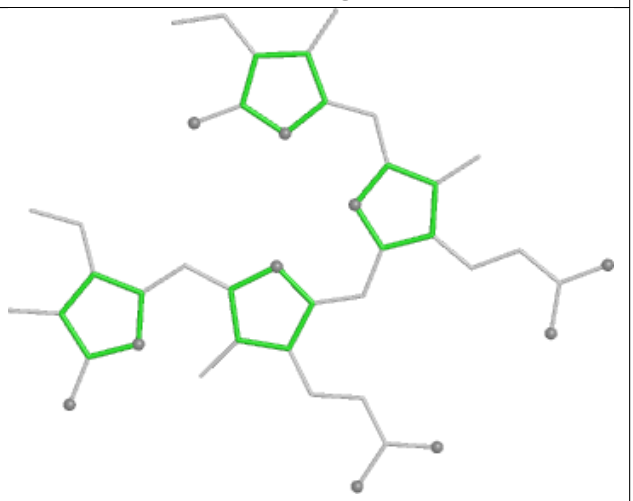
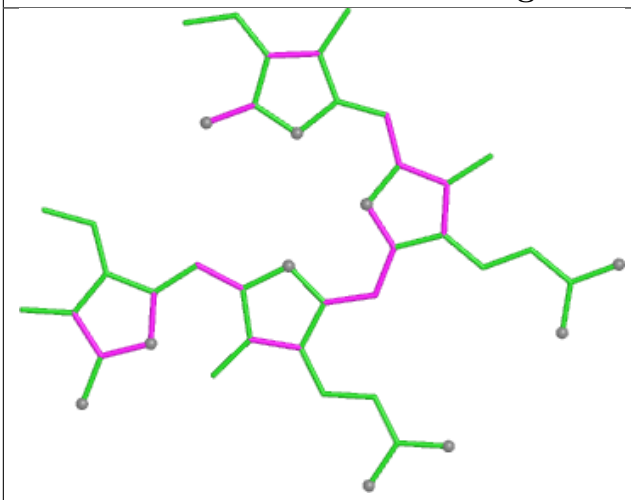


Rings

Ligand PEB ZJ 201



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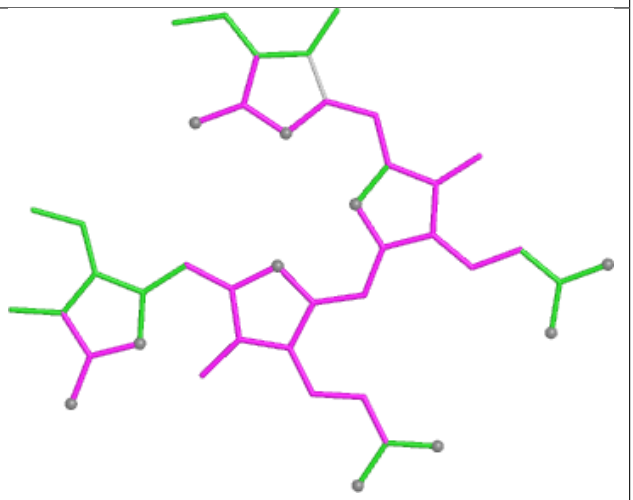

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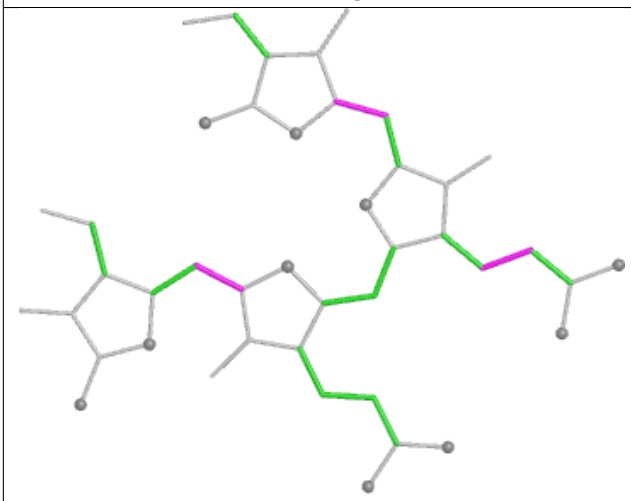

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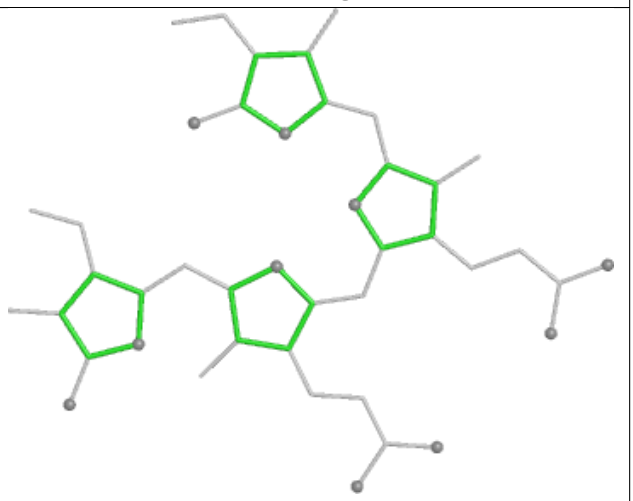

Rings

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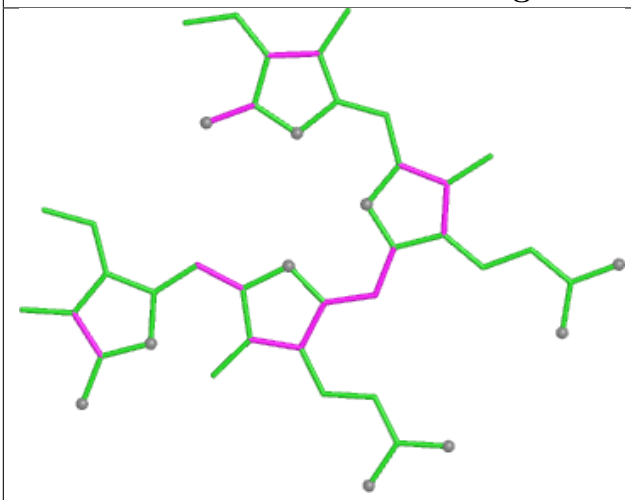

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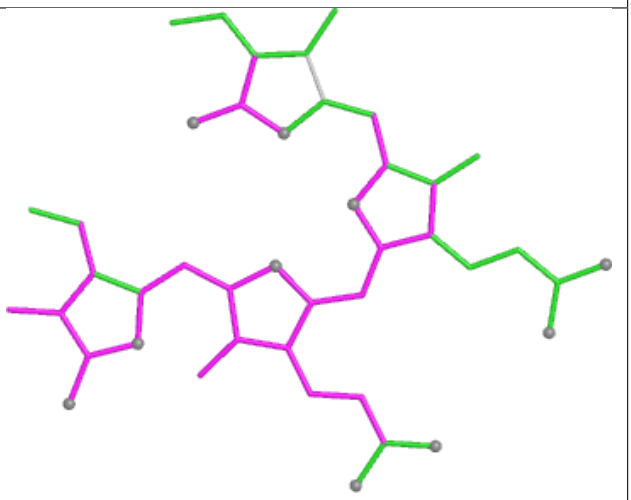

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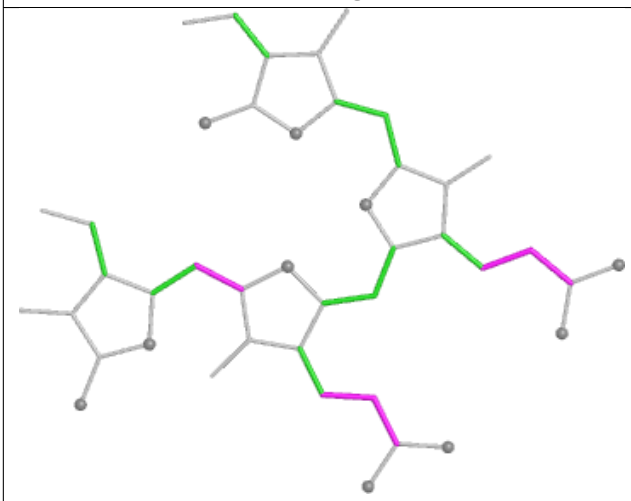

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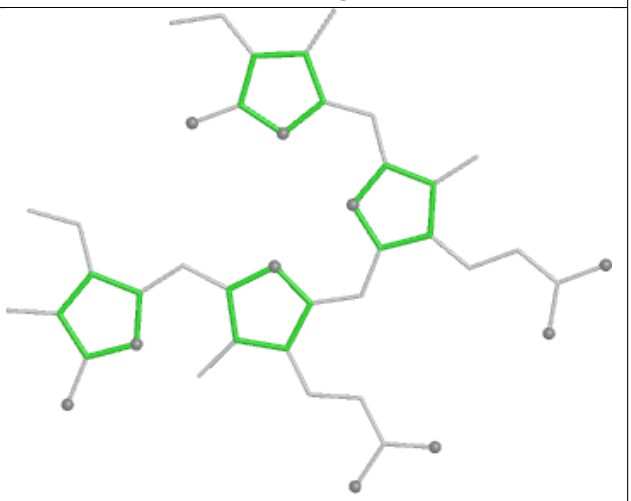

Rings

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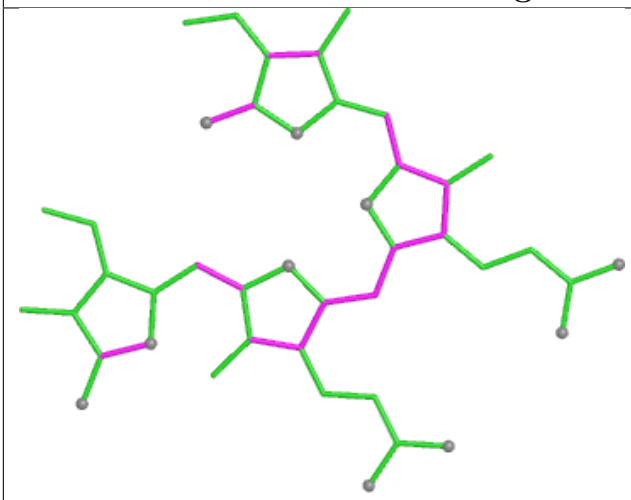

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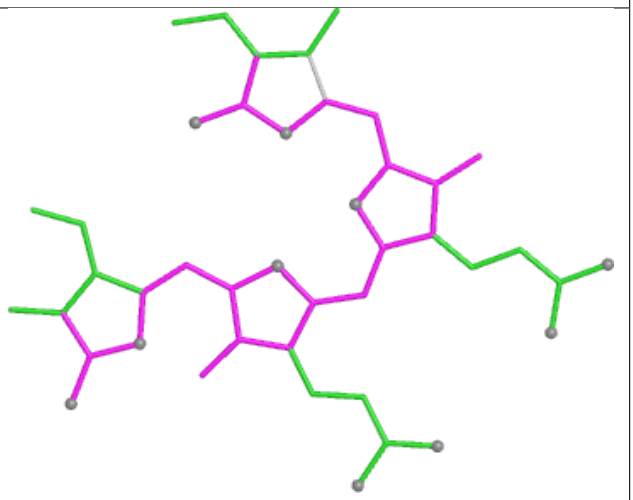

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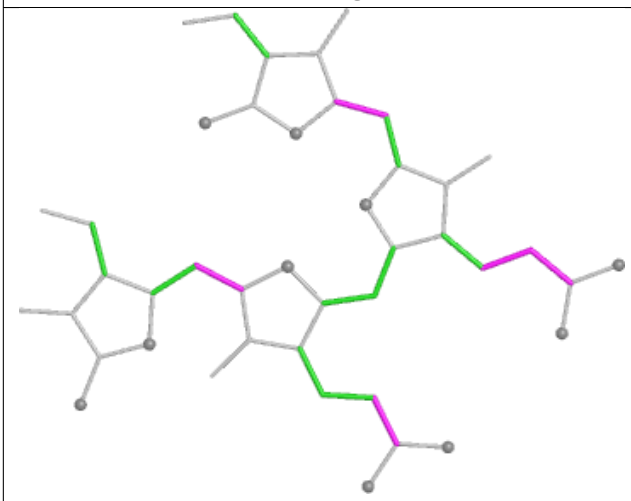

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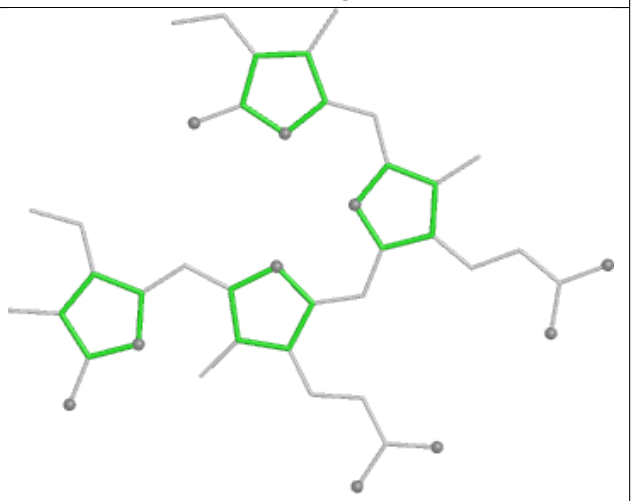

Rings

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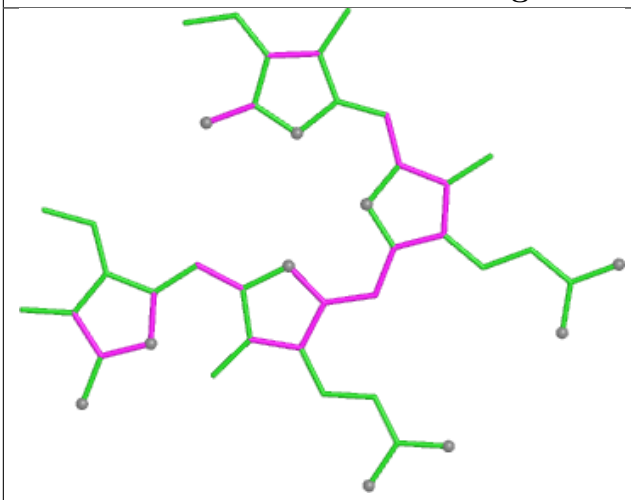

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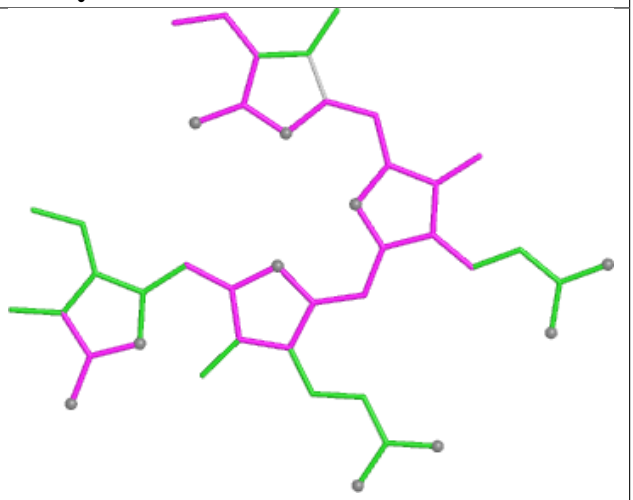

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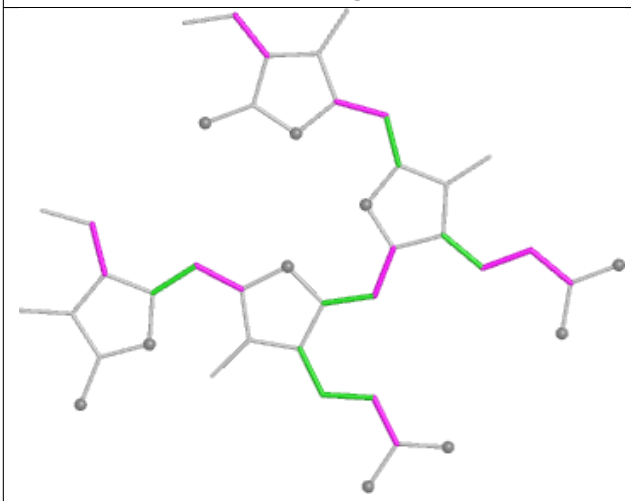

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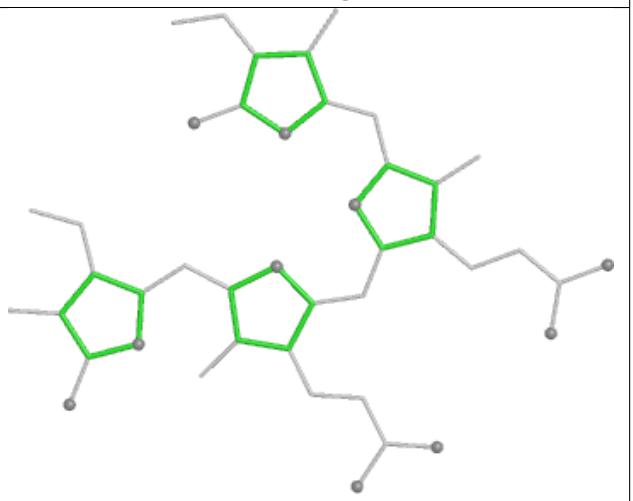
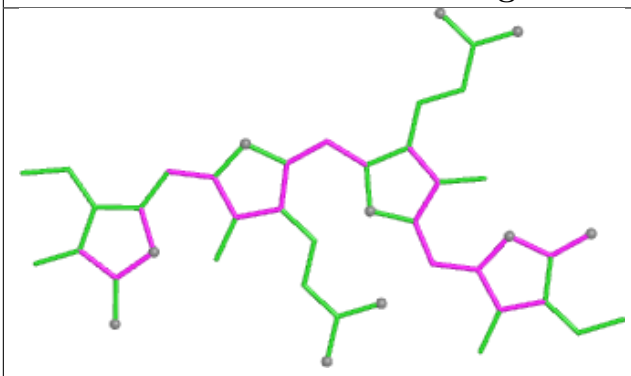


Rings

Ligand CYC NH 1001



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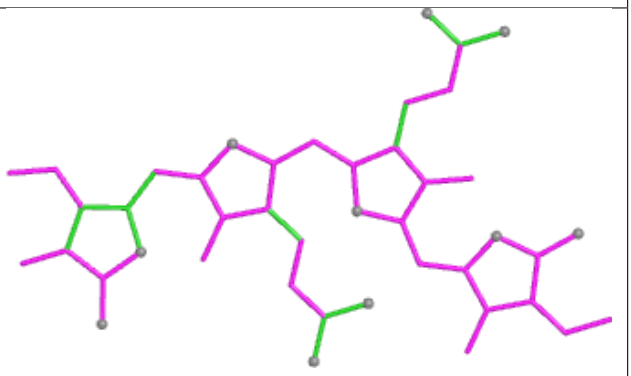

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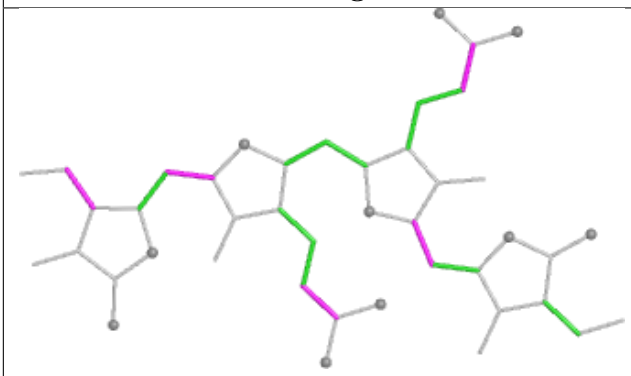

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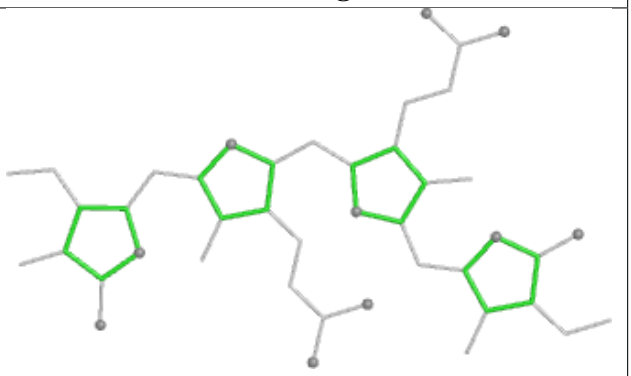
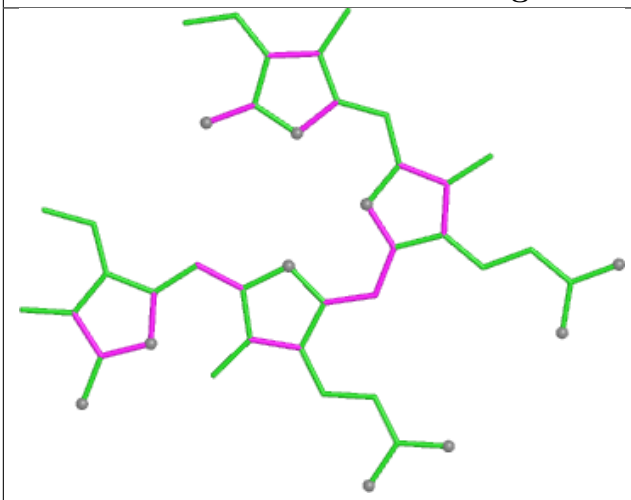


Rings

Ligand PEB UB 302



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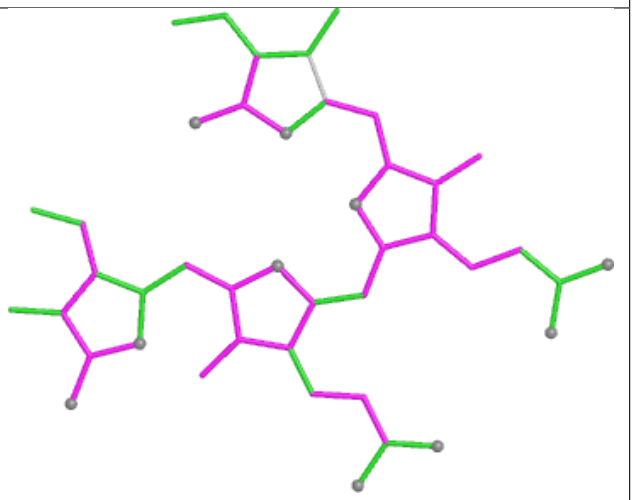

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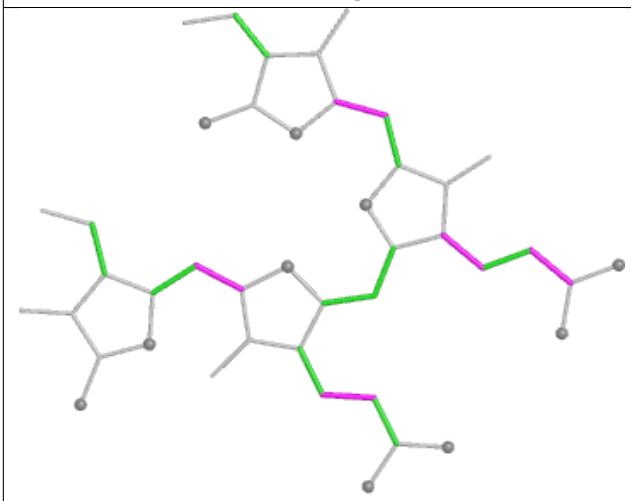

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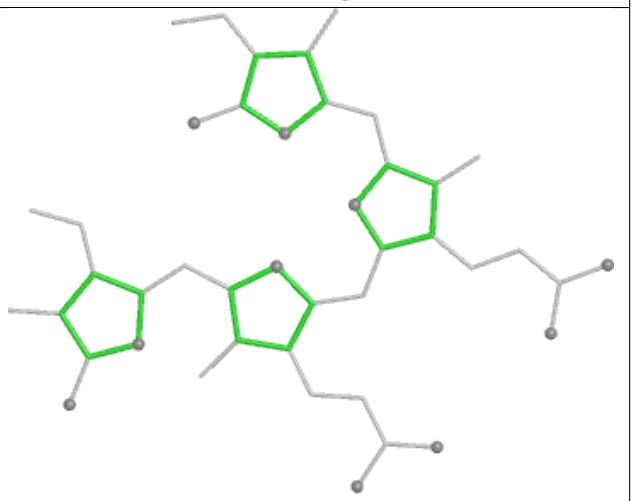
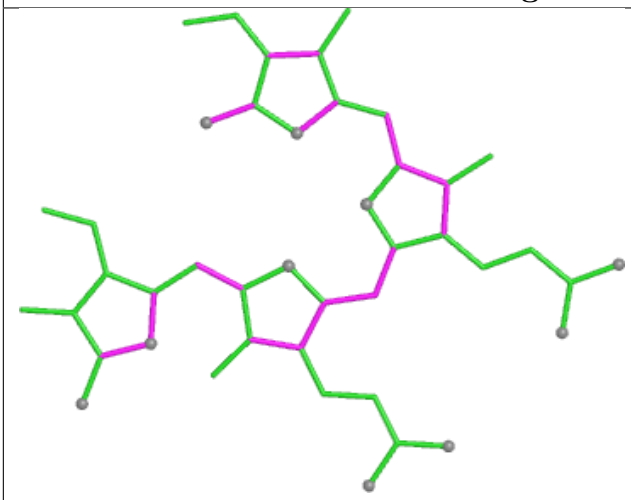


Rings

Ligand PEB lF 202



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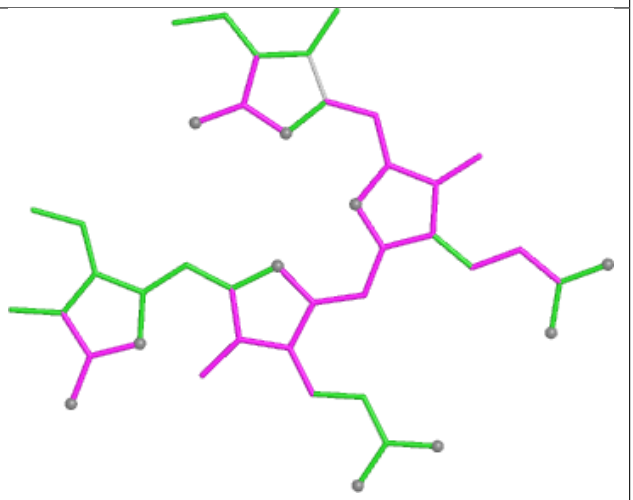

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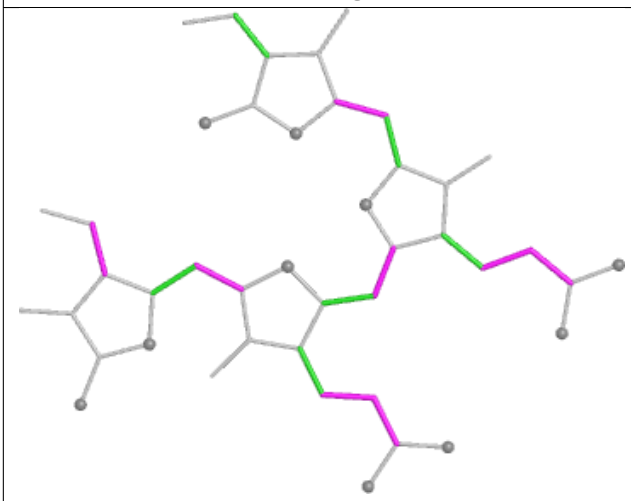

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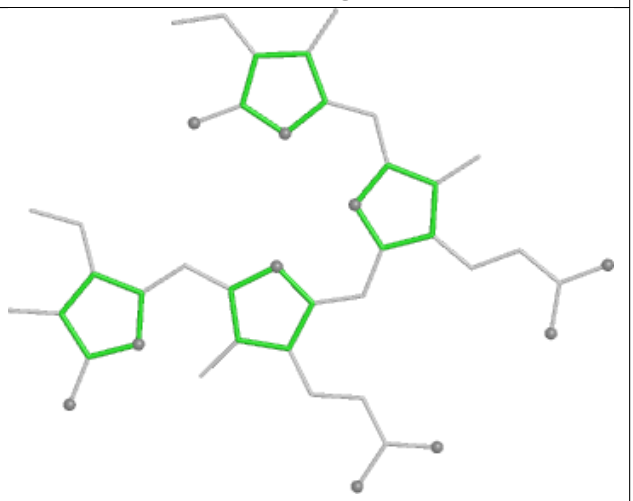
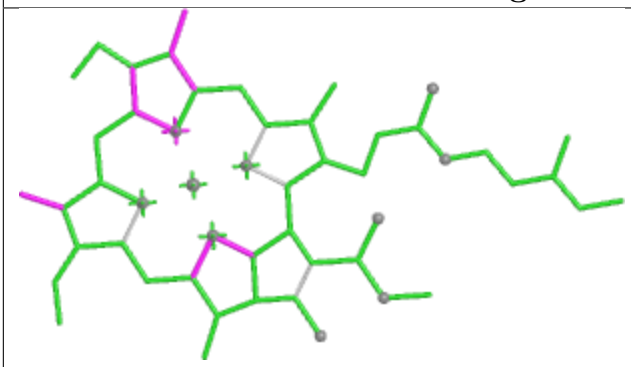


Rings

Ligand CLA AN 824



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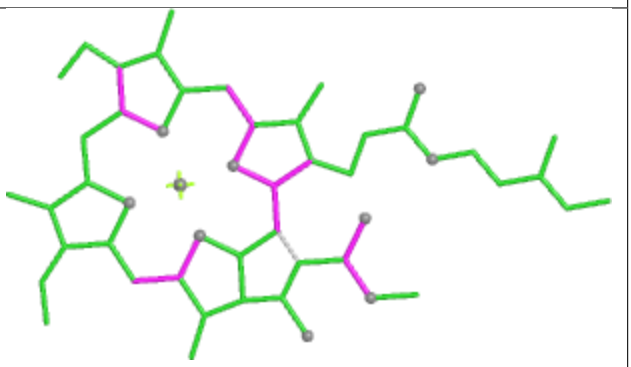

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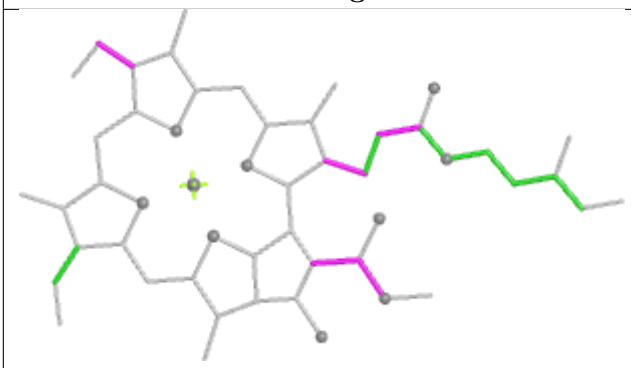

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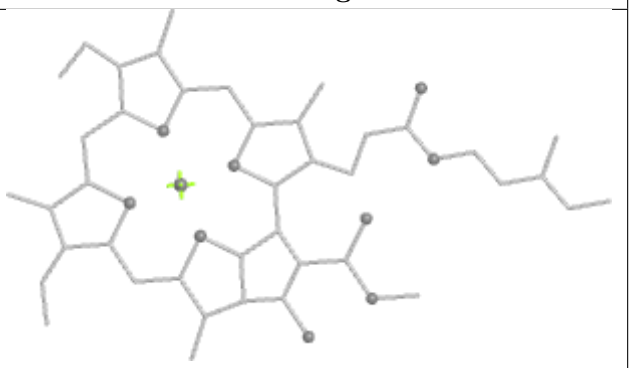
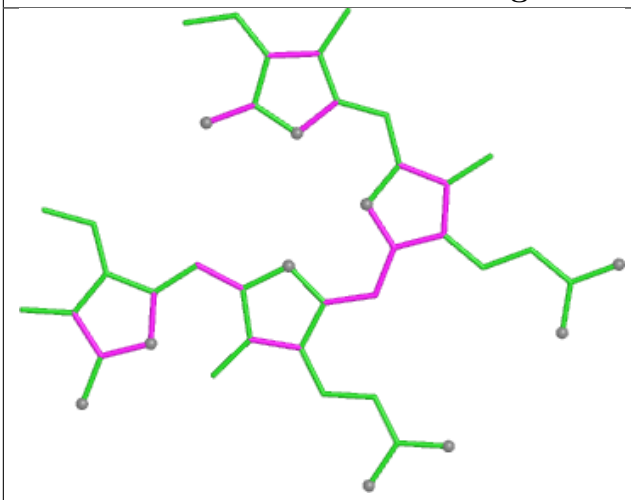


Rings

Ligand PEB OO 202



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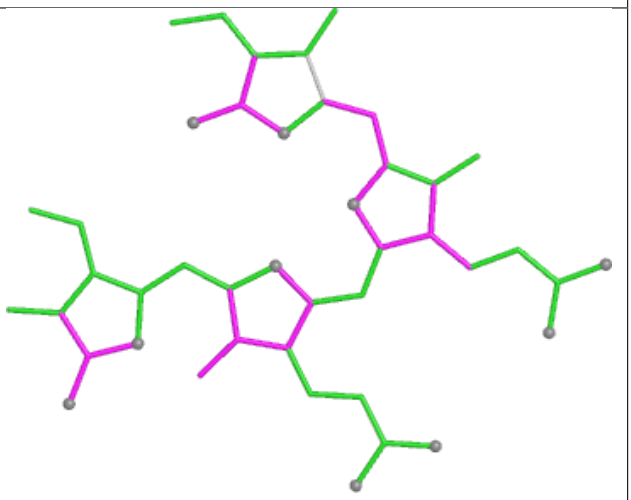

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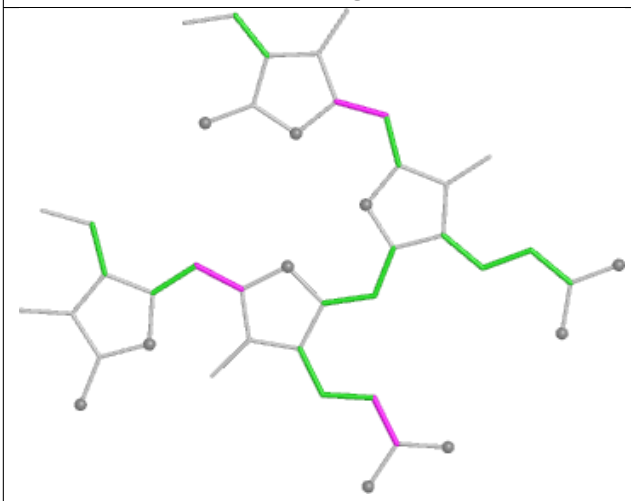

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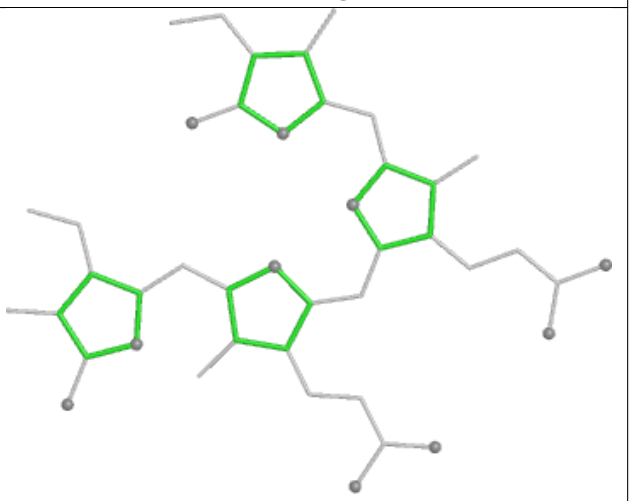
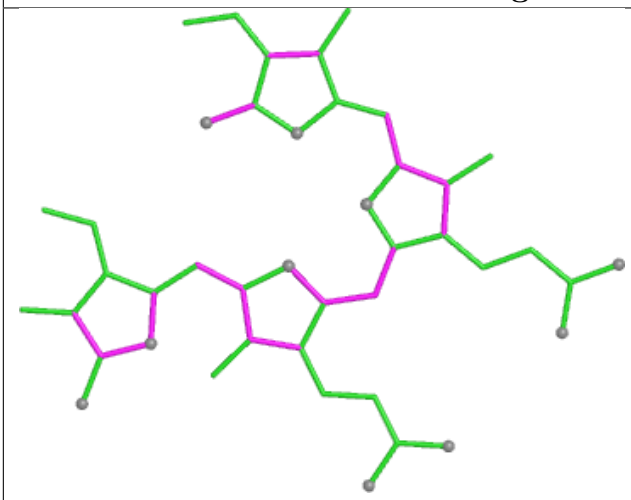


Rings

Ligand PEB CA 201



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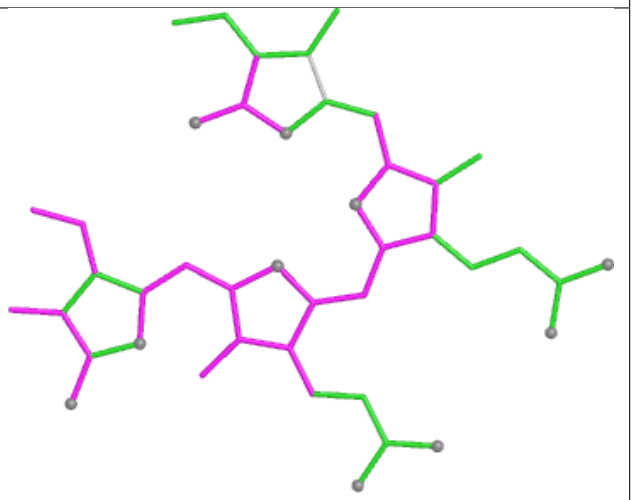

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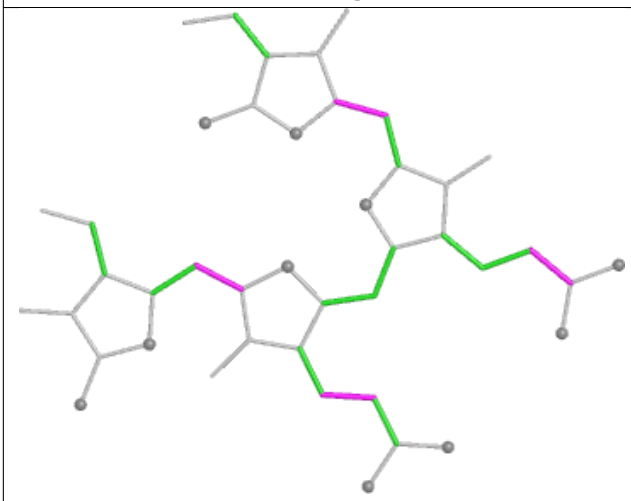

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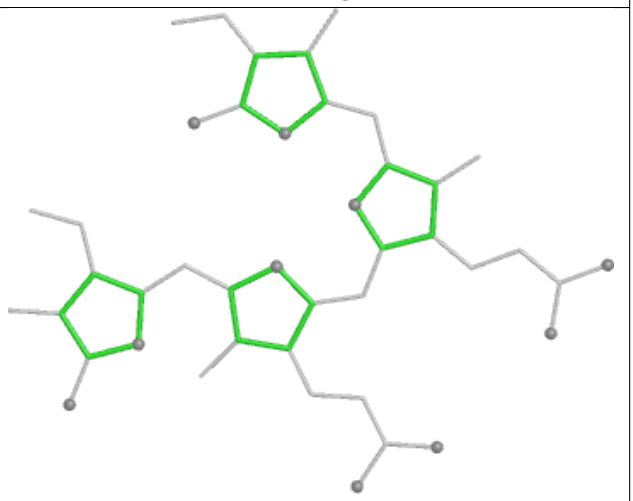

Rings

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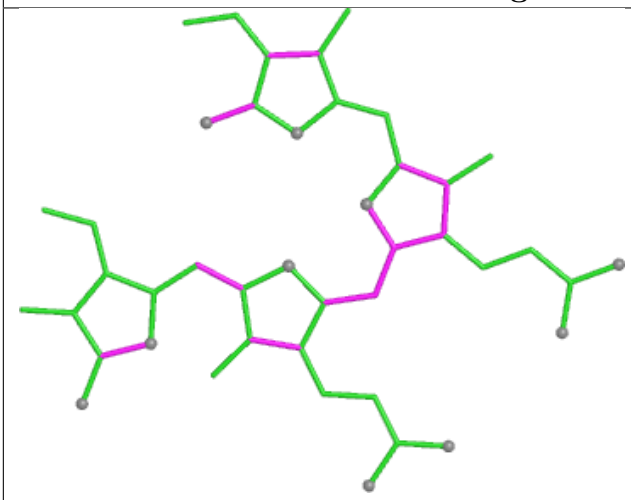

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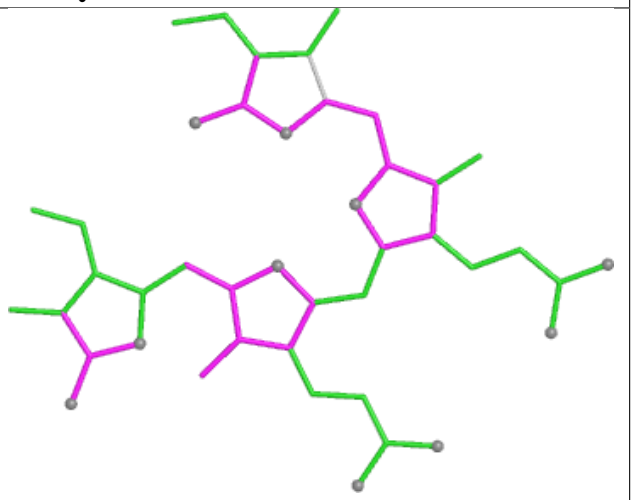

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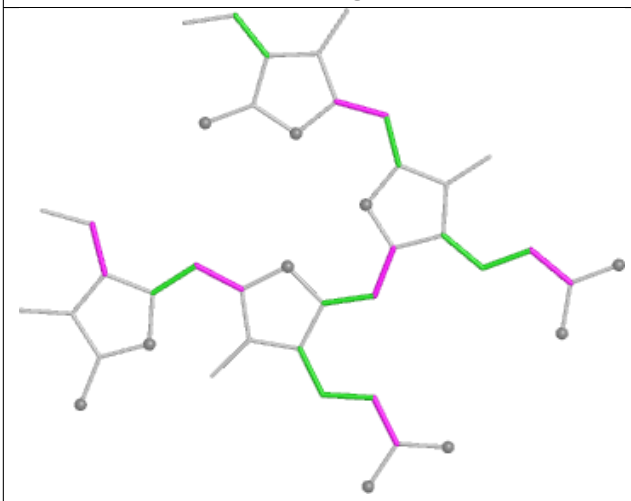

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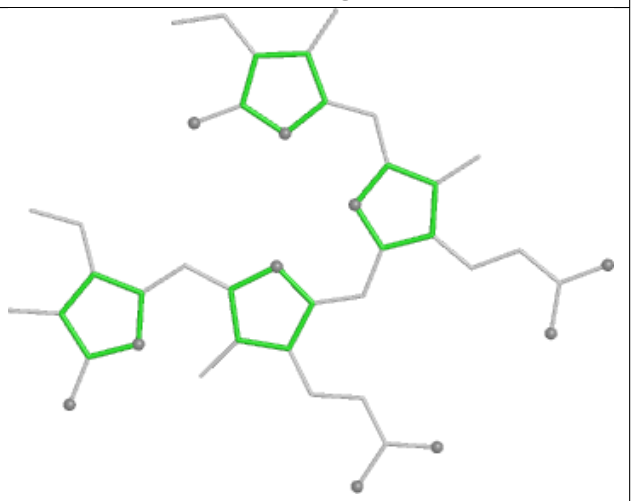

Rings

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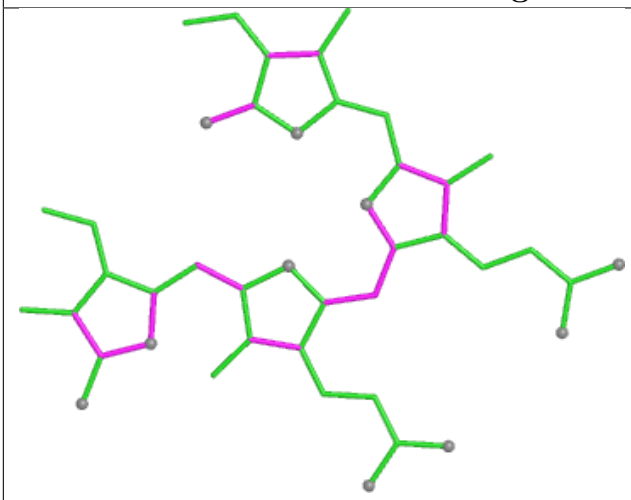

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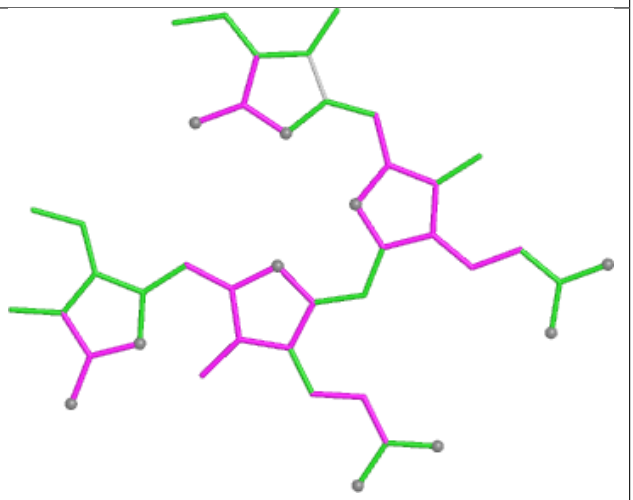

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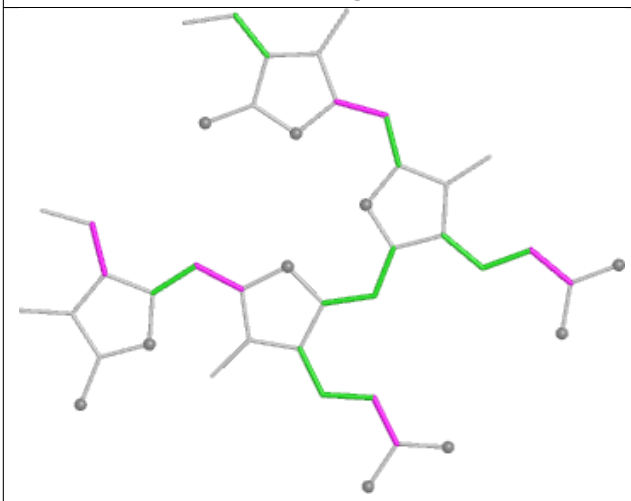

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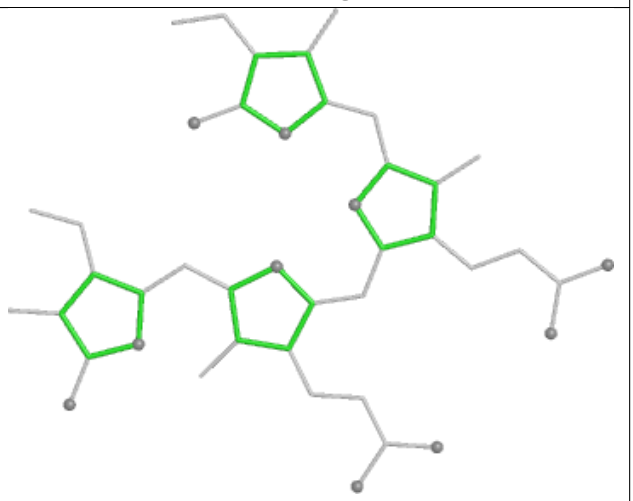

Rings

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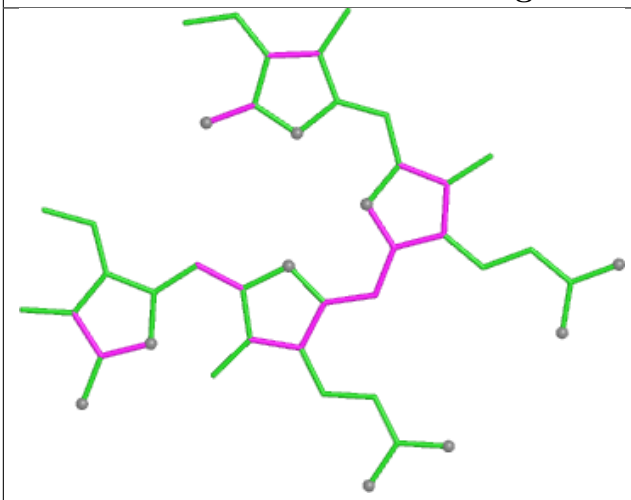

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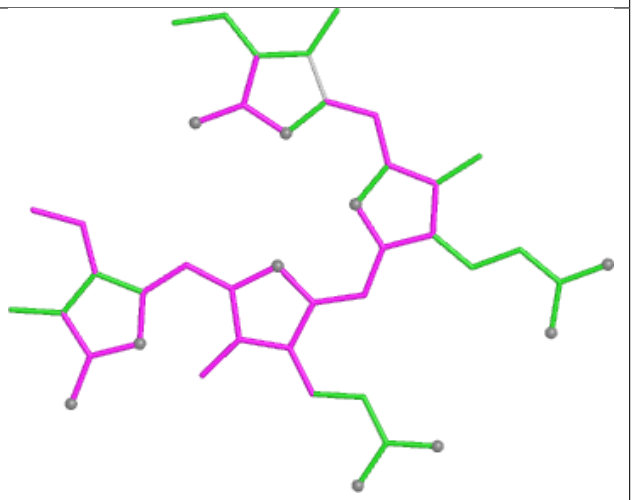

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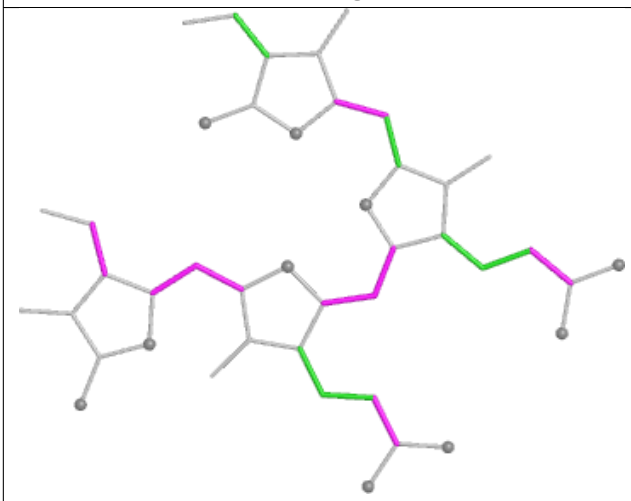

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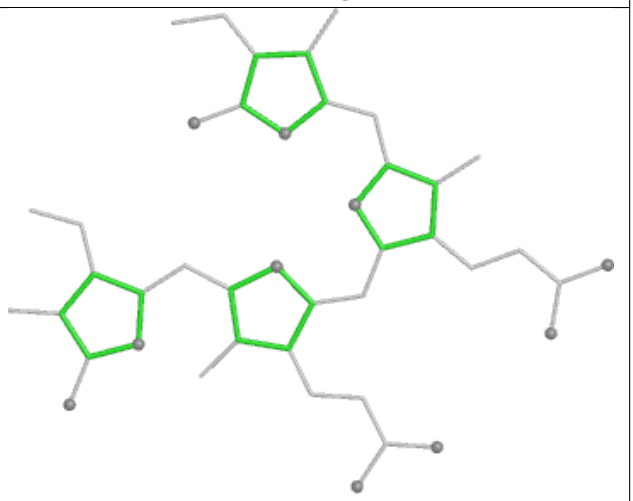

Rings

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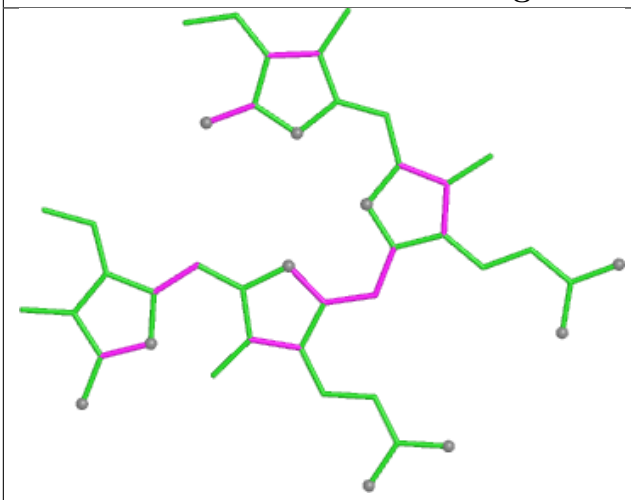
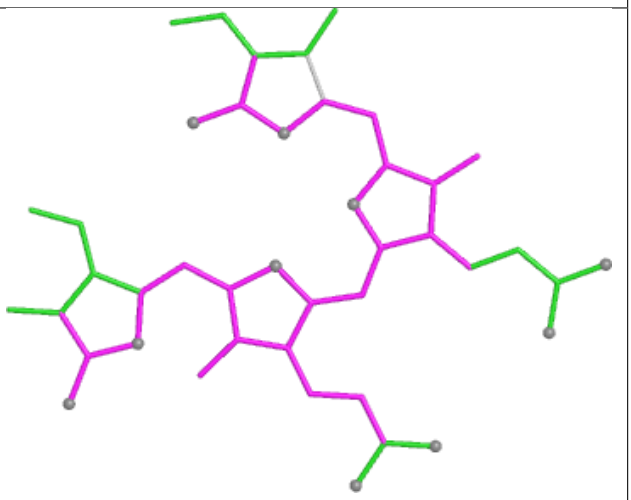
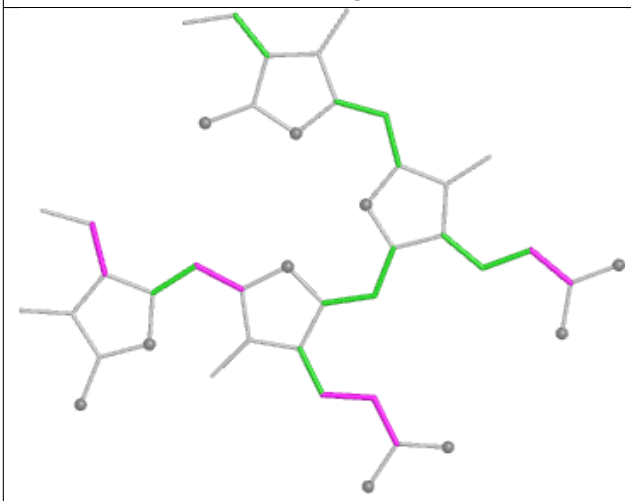


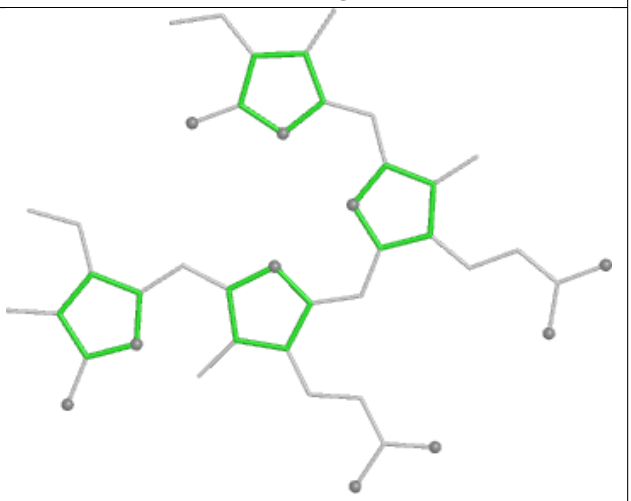
Bond lengths



Bond angles

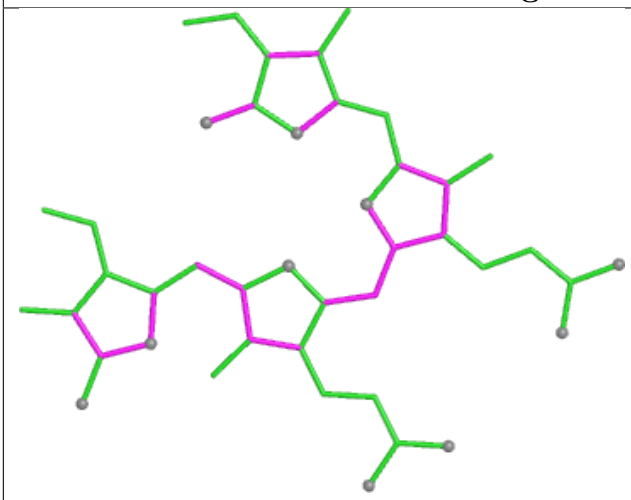


Torsions



Rings

Ligand PEB s8 201



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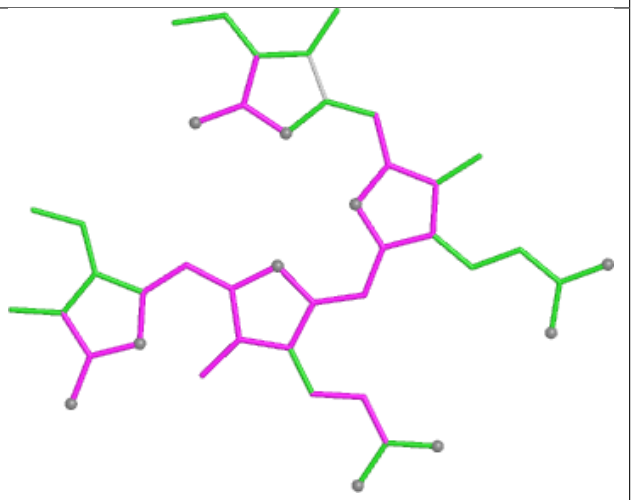

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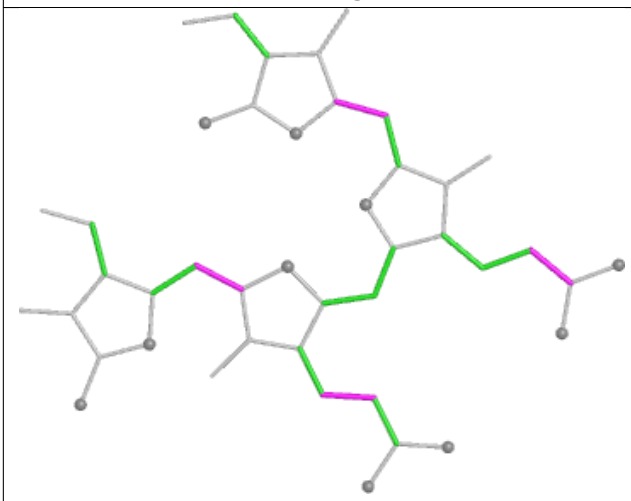

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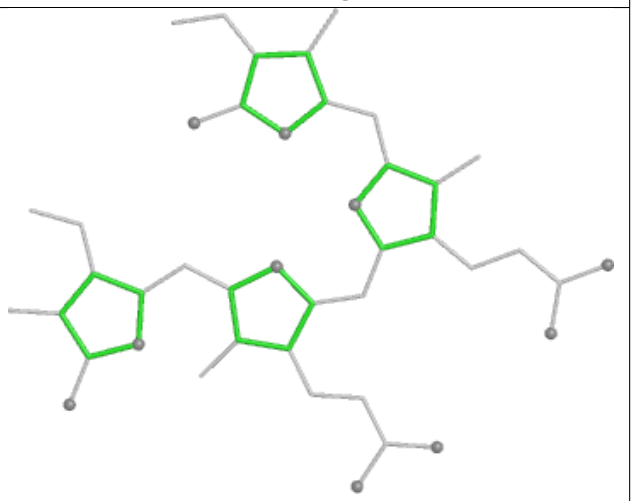
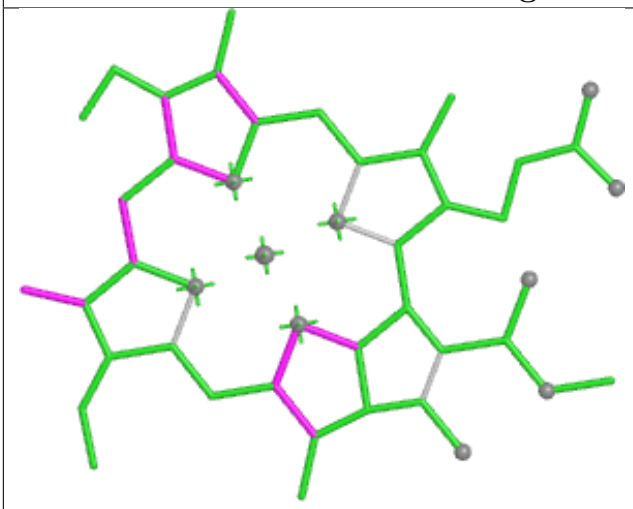


Rings

Ligand CLA 62 313



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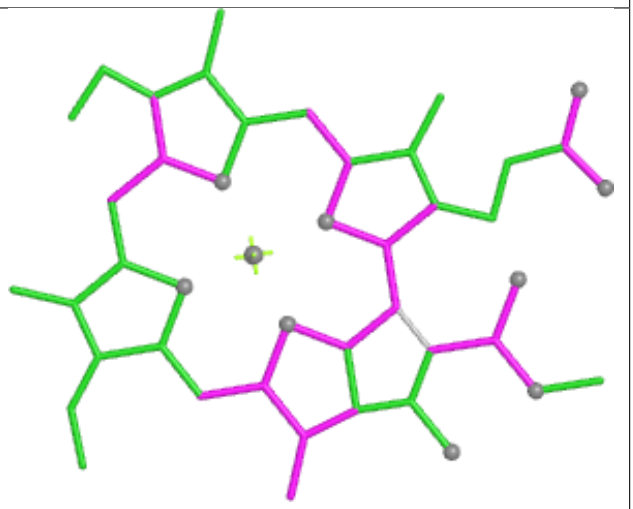

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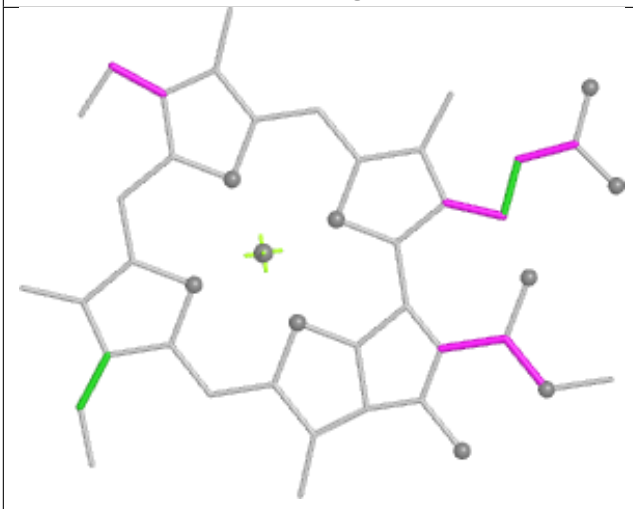
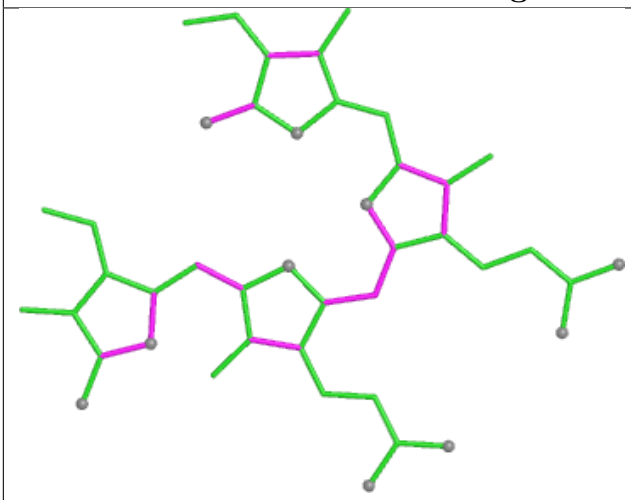


Torsions



Rings

Ligand PEB UK 202



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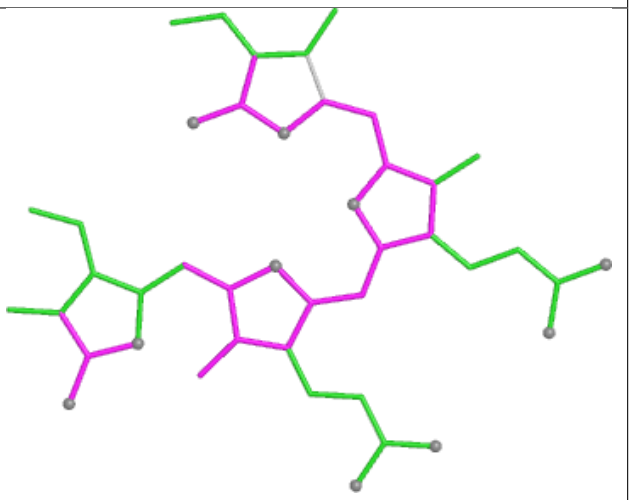

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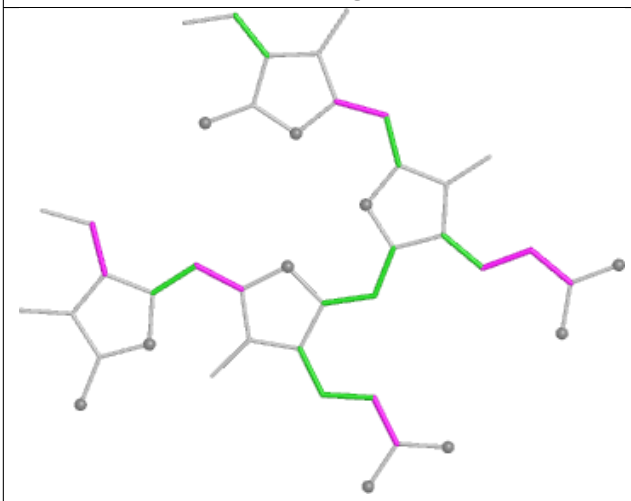

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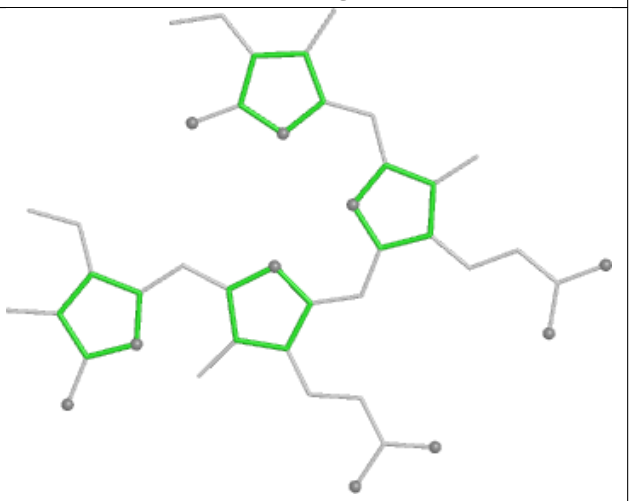
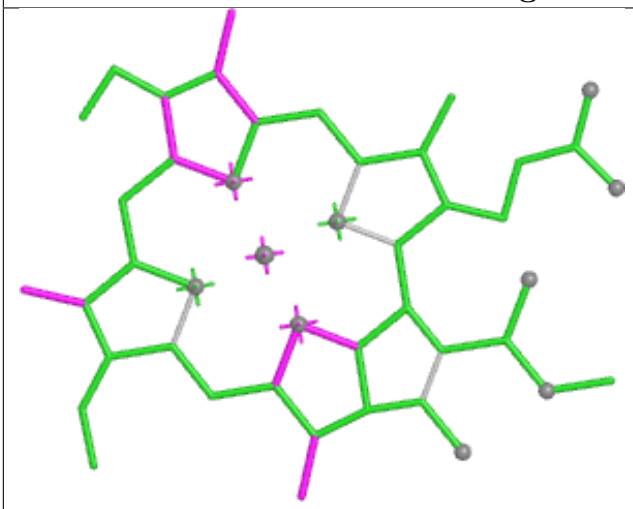


Rings

Ligand CLA 32 312



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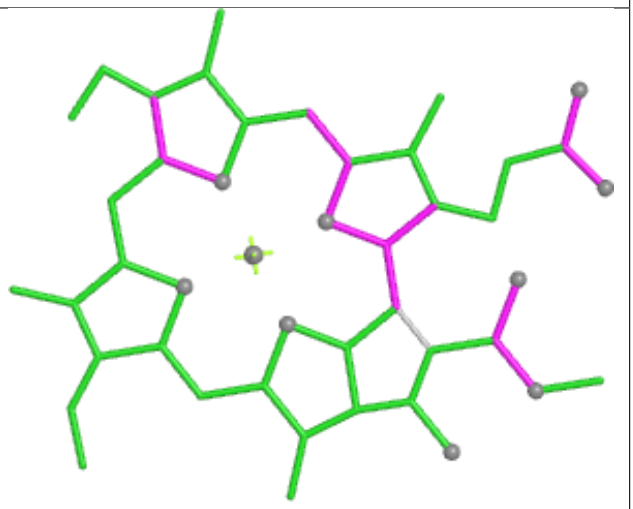

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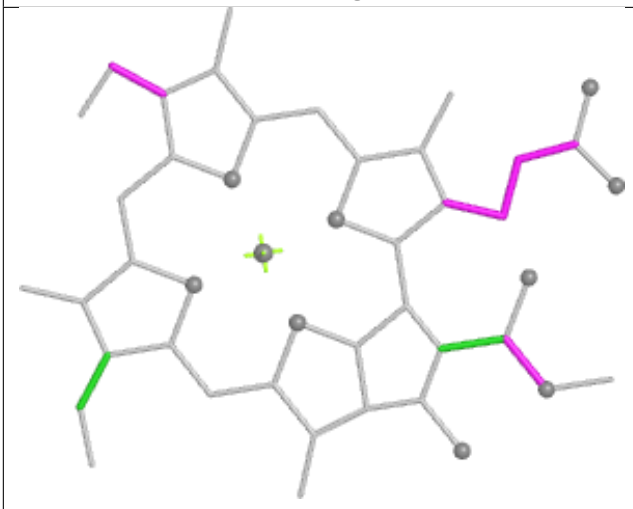
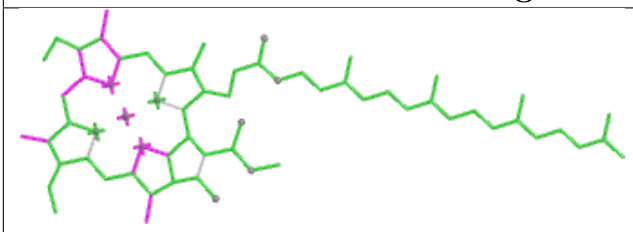


Torsions



Rings

Ligand CLA B2 810



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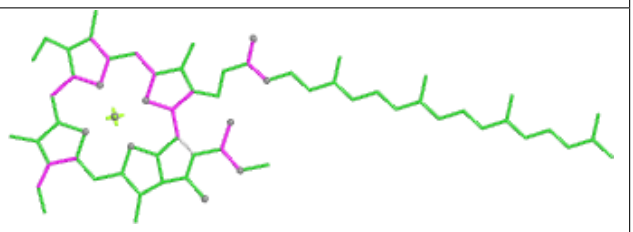

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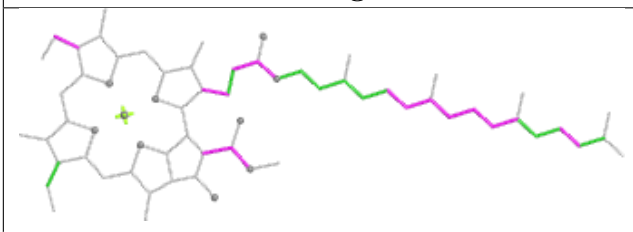

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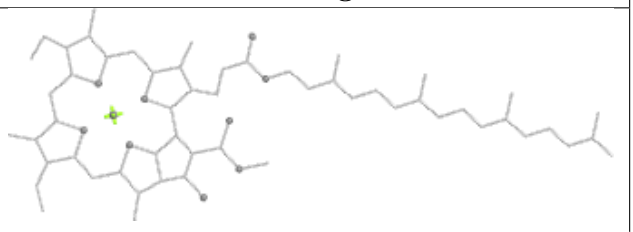
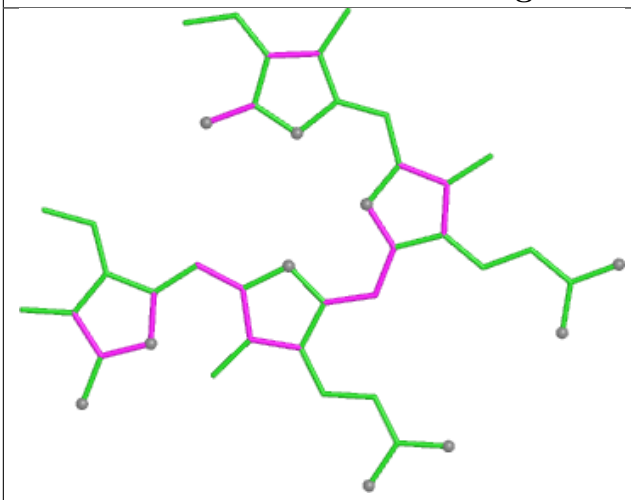


Rings

Ligand PEB A5 201



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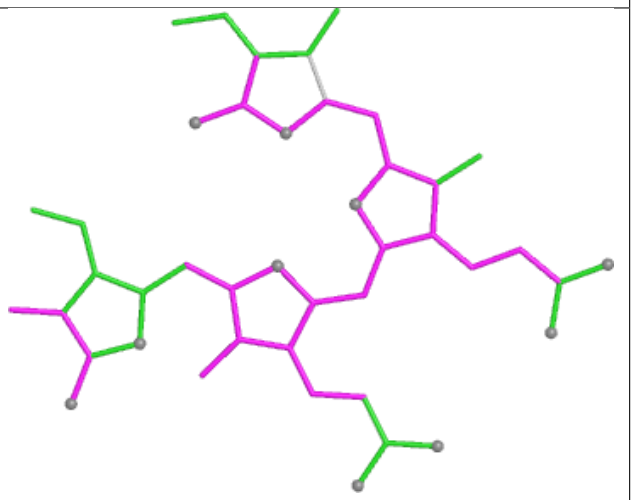

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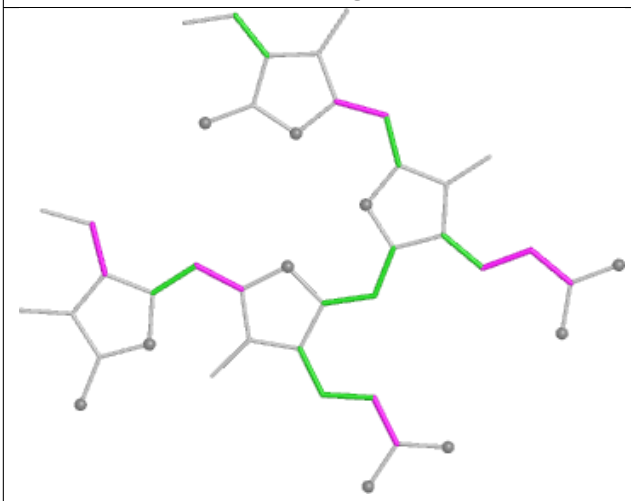

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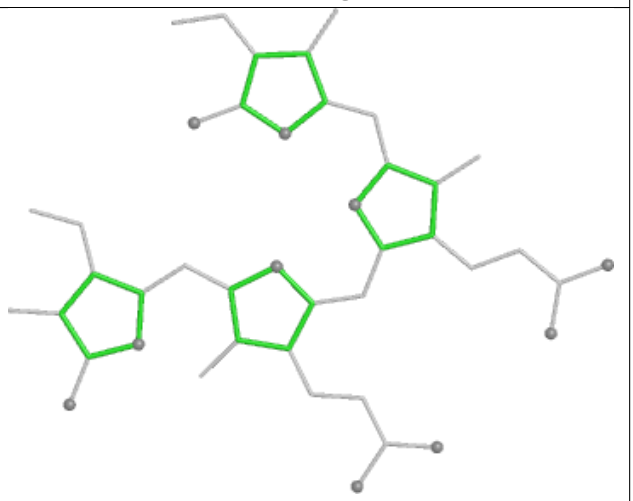

Rings

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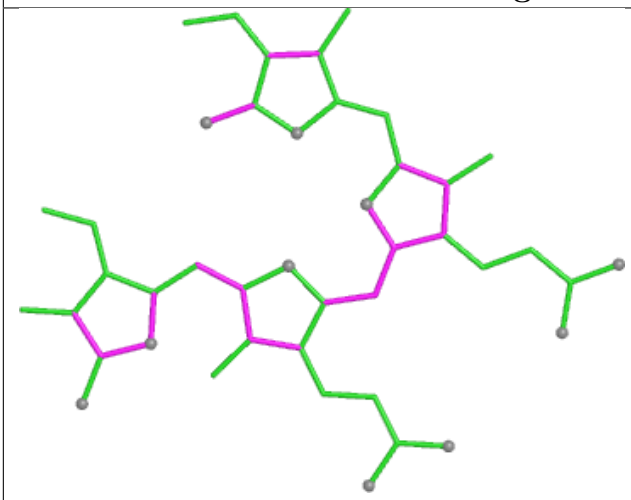

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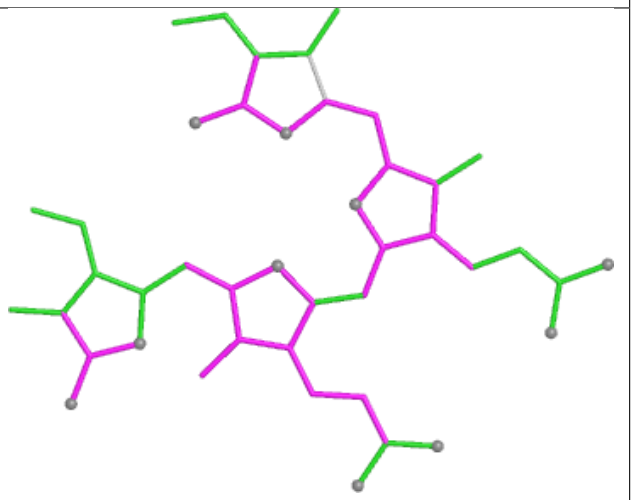

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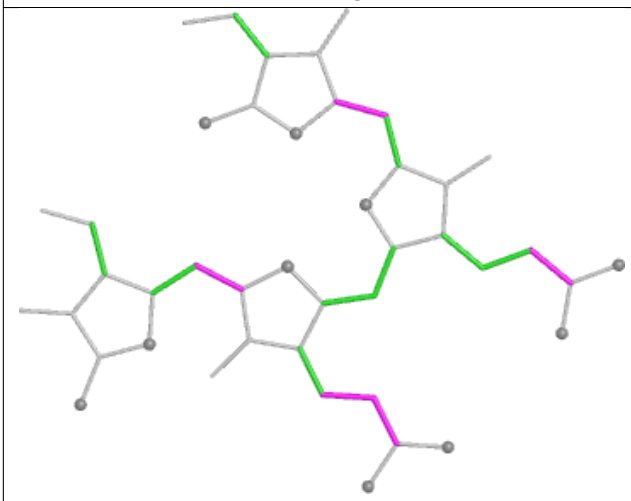

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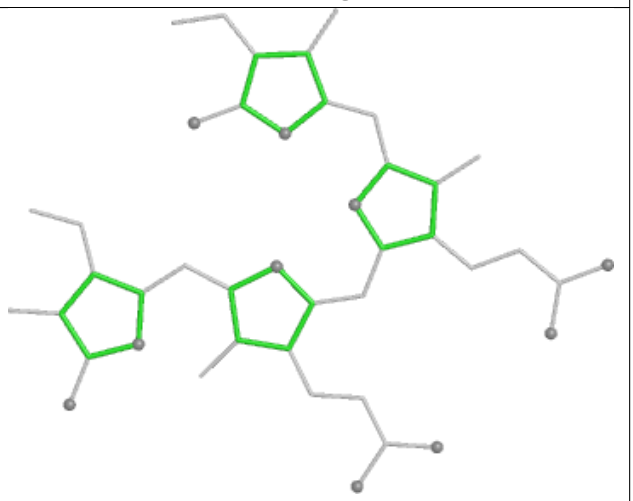
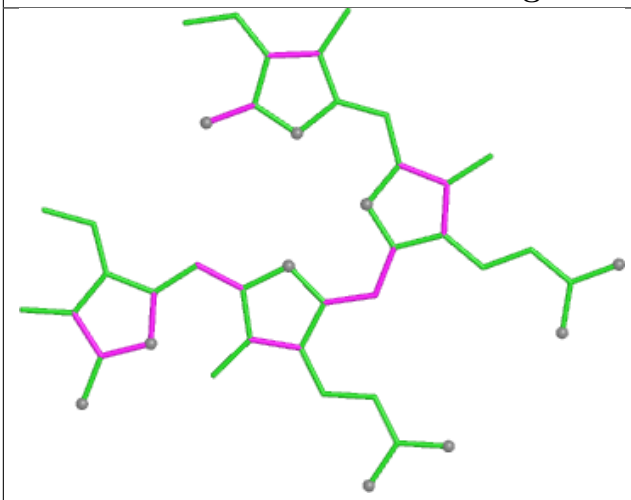


Rings

Ligand PEB jJ 201



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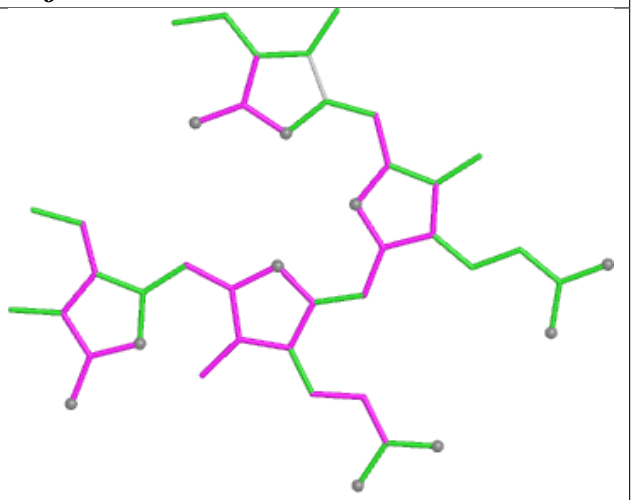

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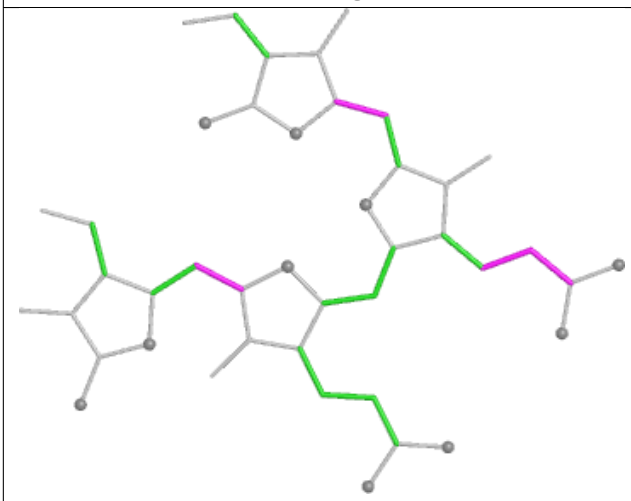

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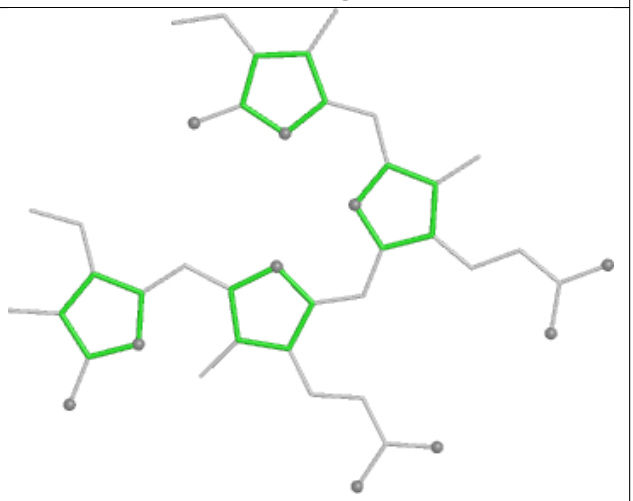
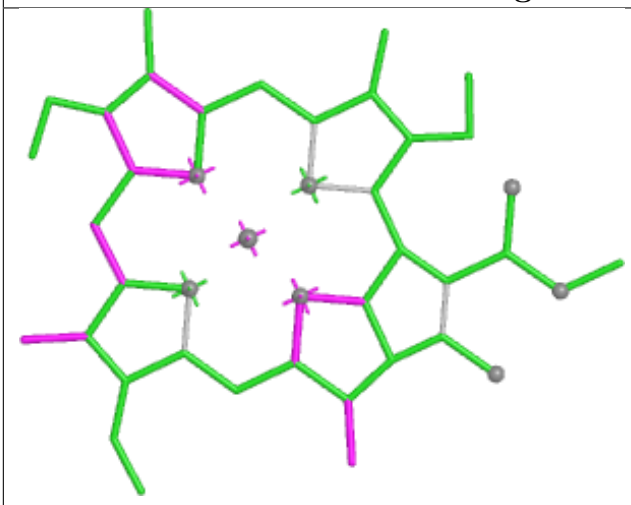


Rings

Ligand CLA 2N 305



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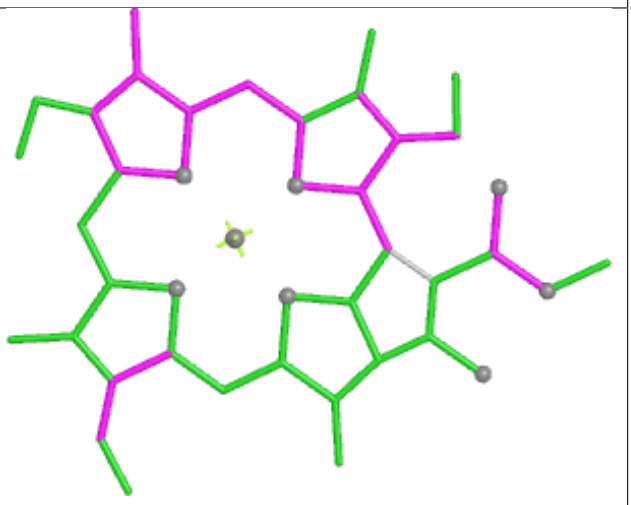

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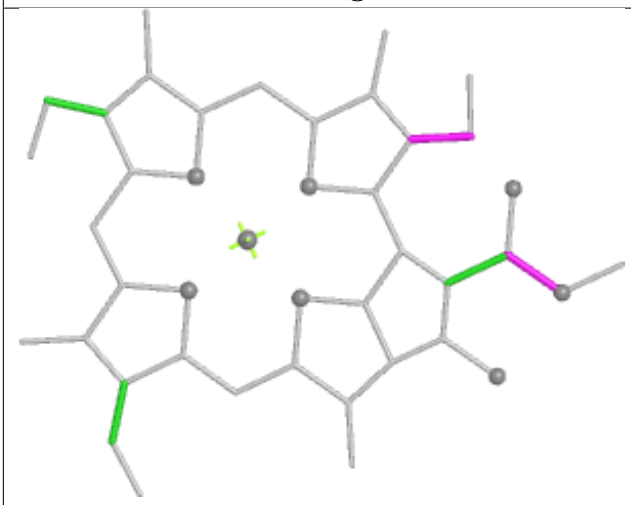
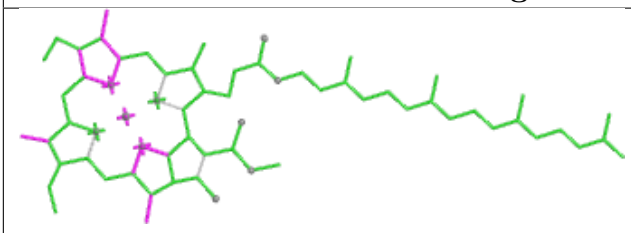


Torsions



Rings

Ligand CLA BN 809



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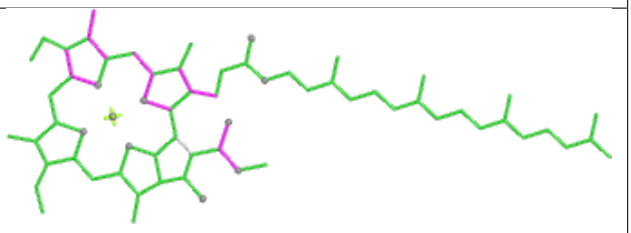

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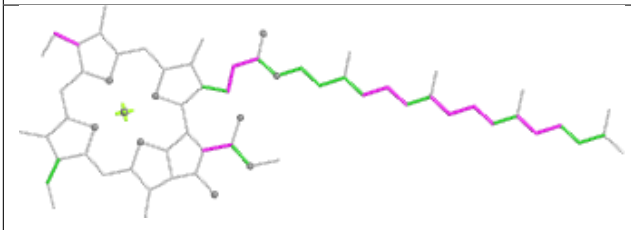

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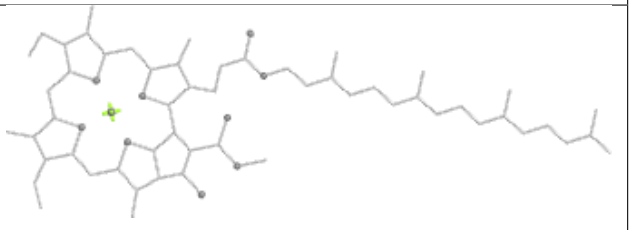
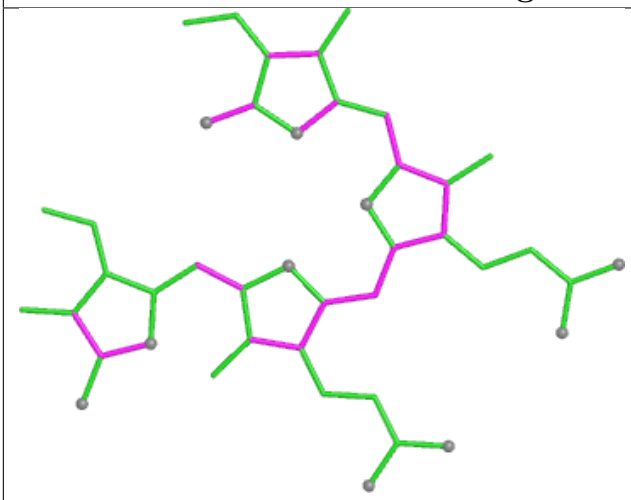


Rings

Ligand PEB tK 203



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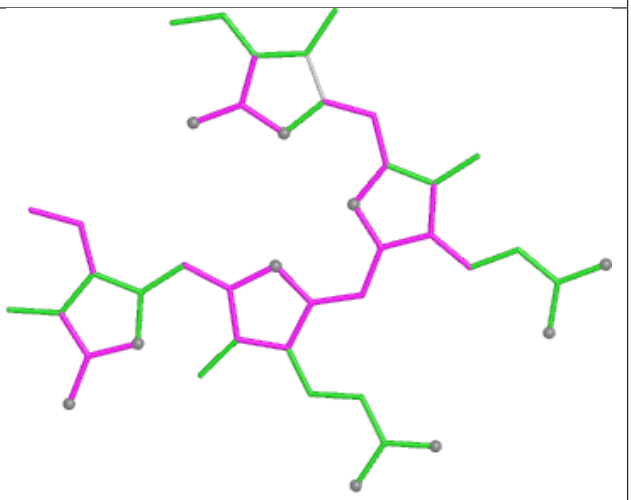

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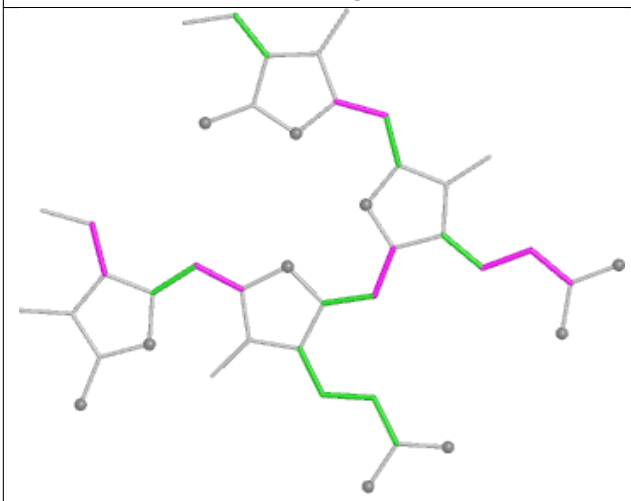

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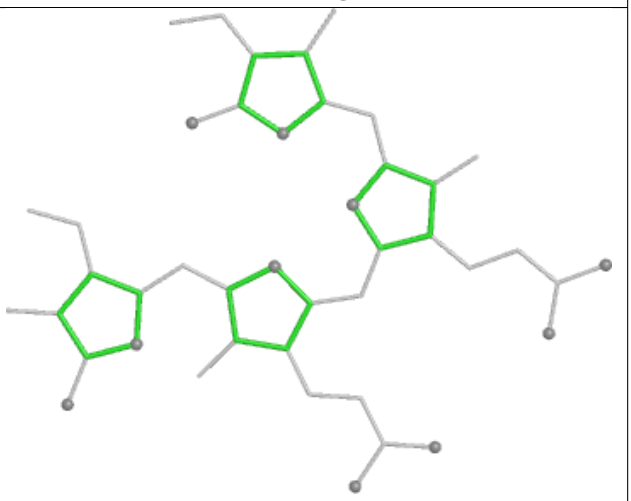
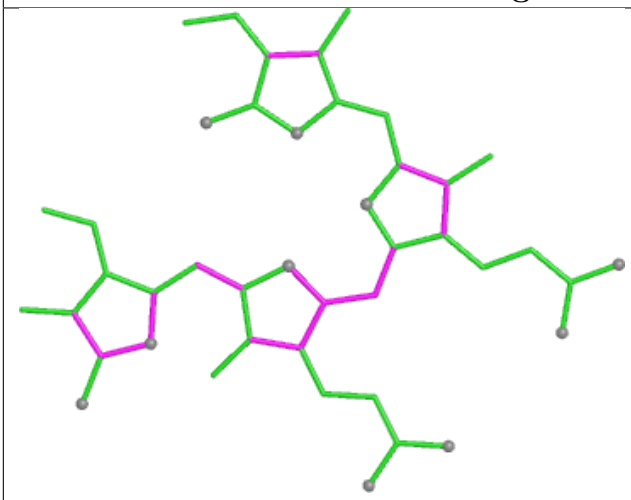


Rings

Ligand PEB GF 201



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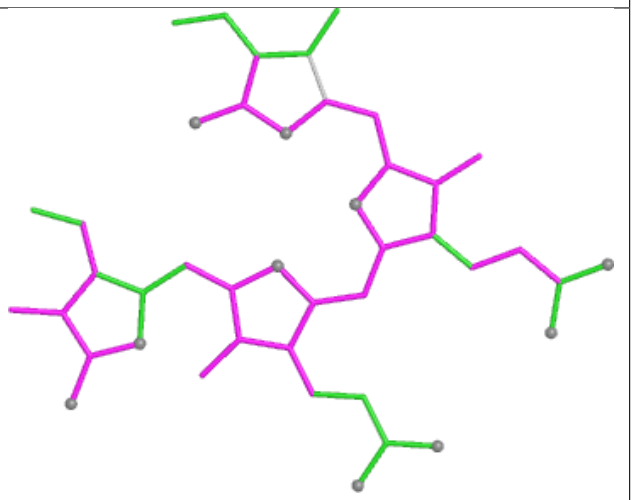
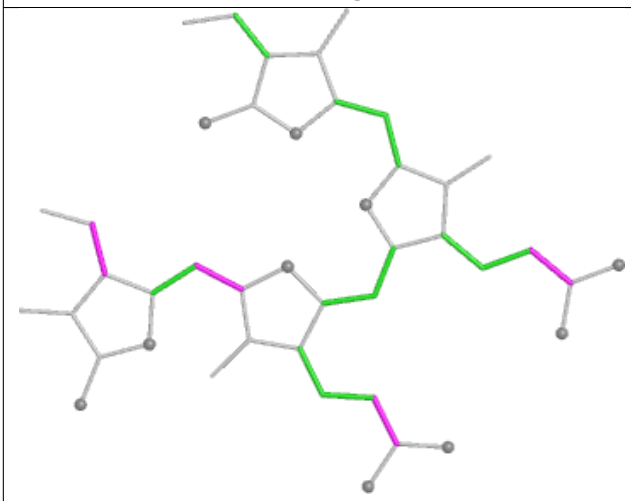


Bond angles



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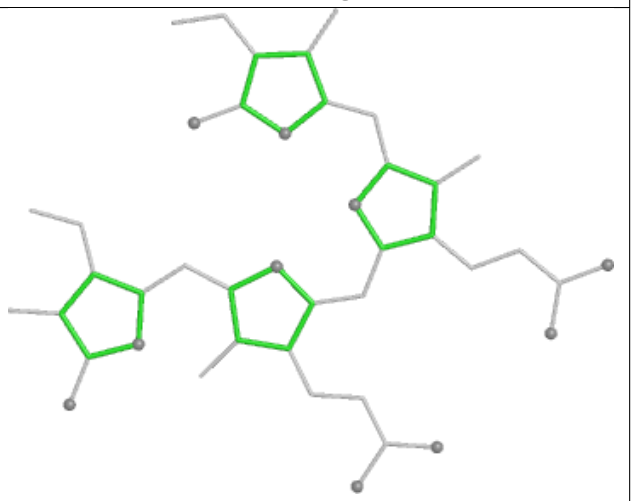
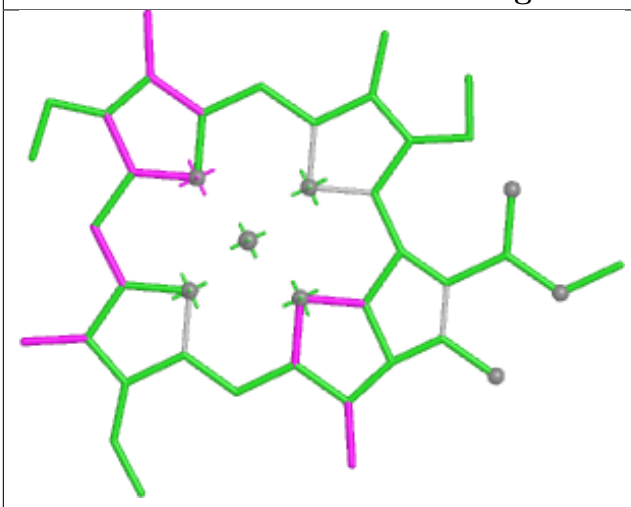


Rings

Ligand CLA 3N 311



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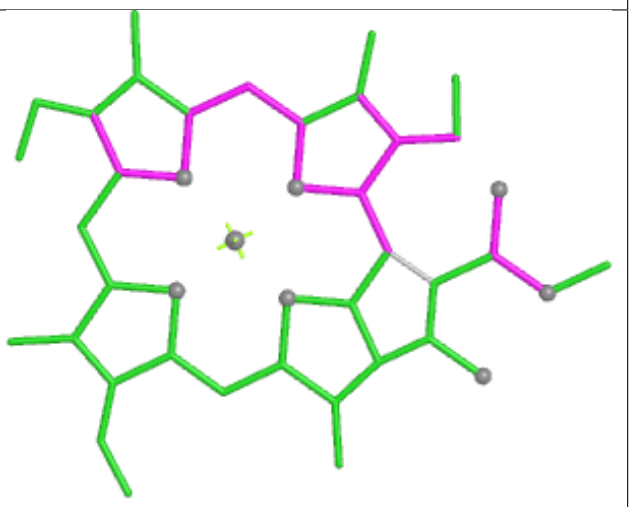
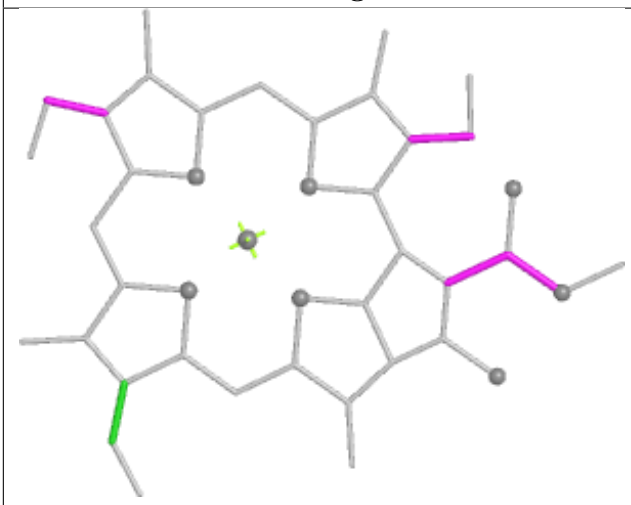


Bond angles

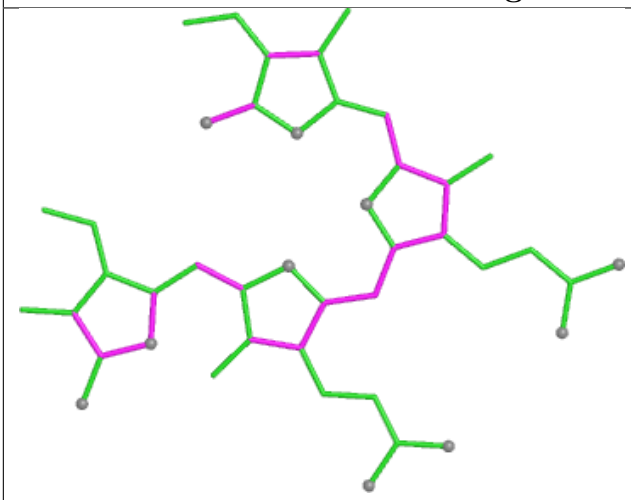


Torsions



Rings

Ligand PEB WH 203



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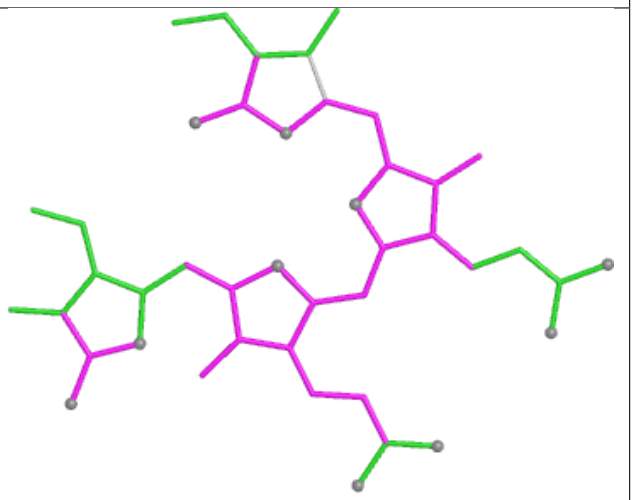
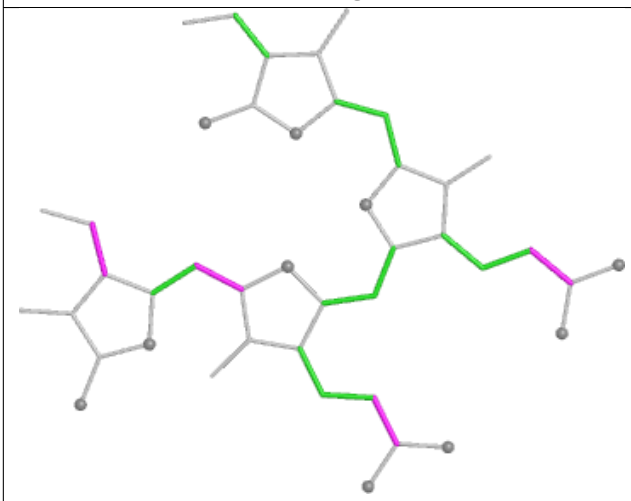


Bond angles



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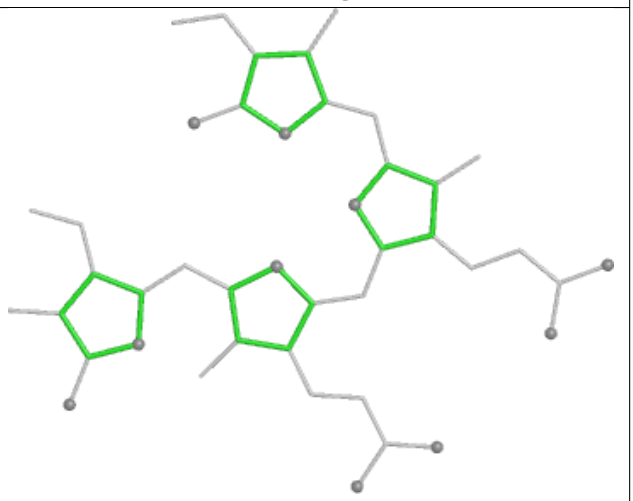
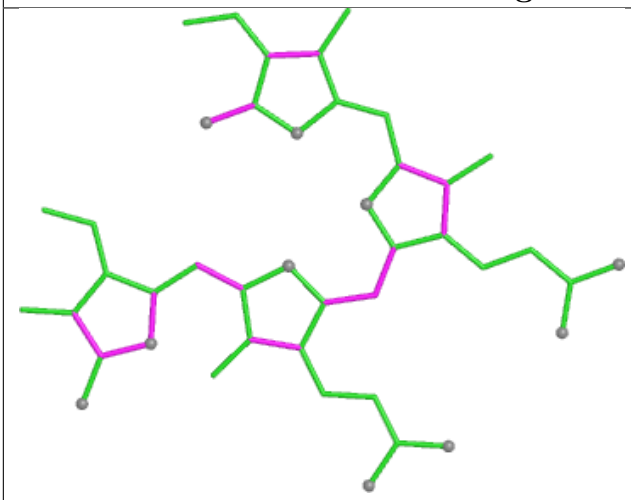


Rings

Ligand PEB CJ 203



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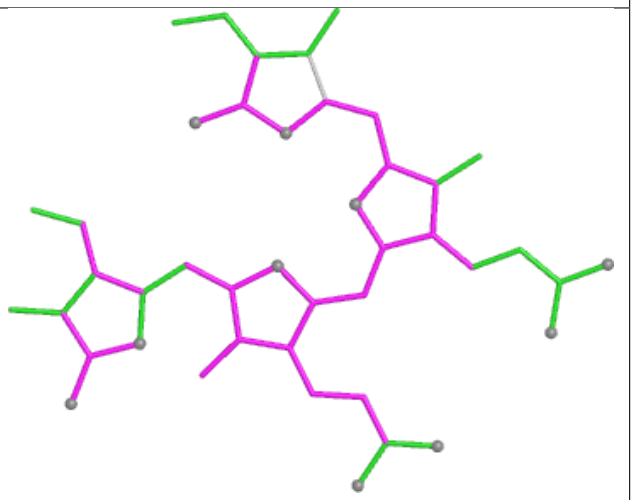
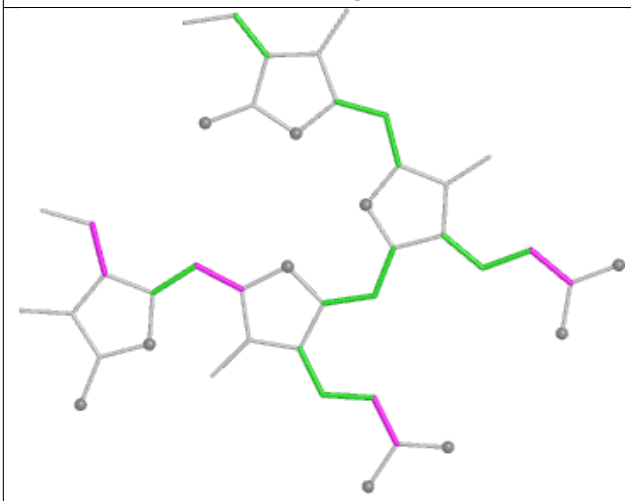
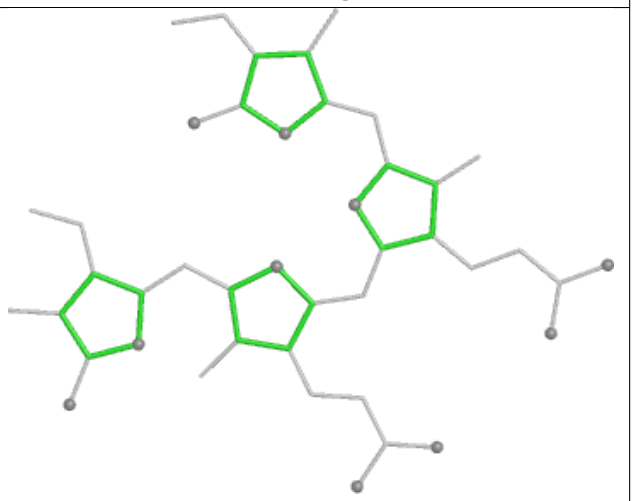


Bond angles

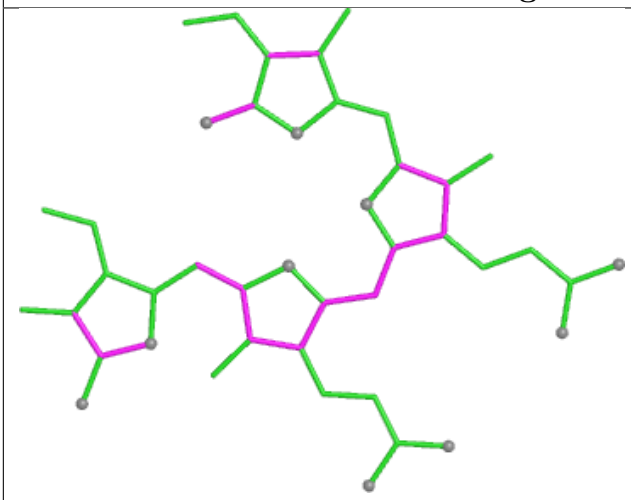


Torsions



Rings

Ligand PEB k1 202



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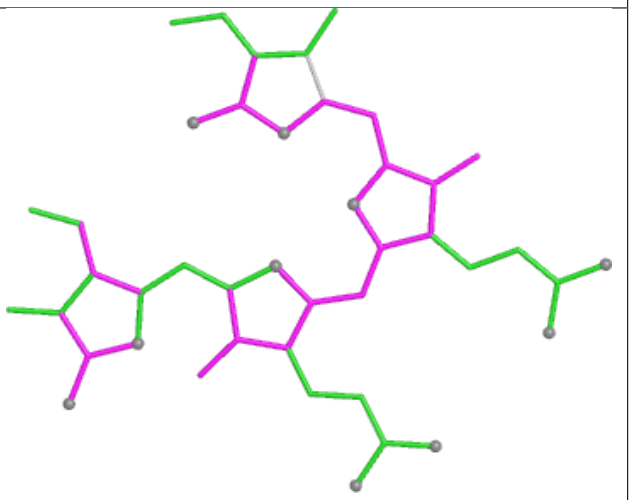

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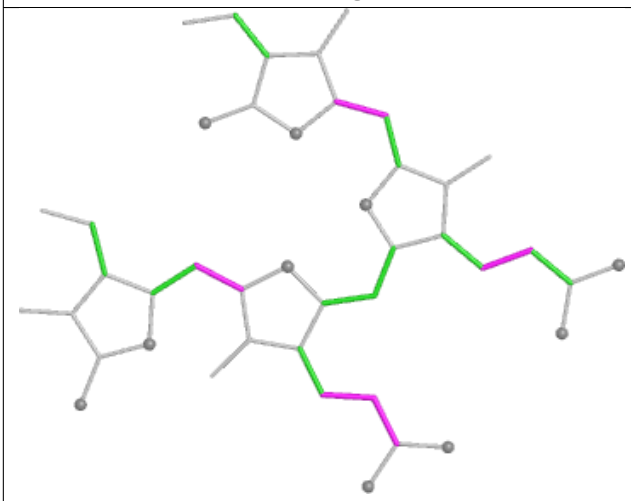

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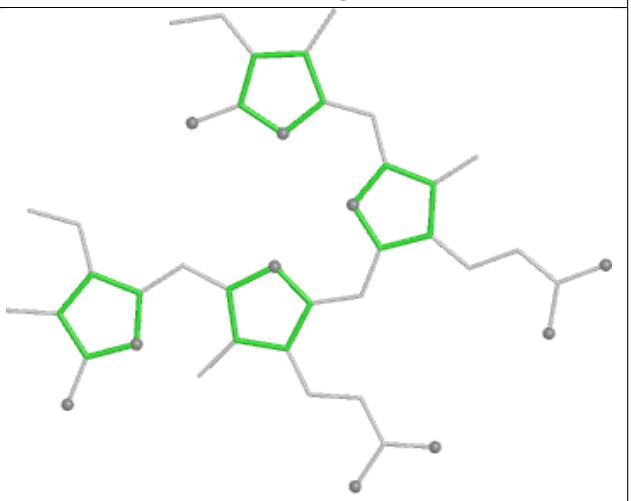
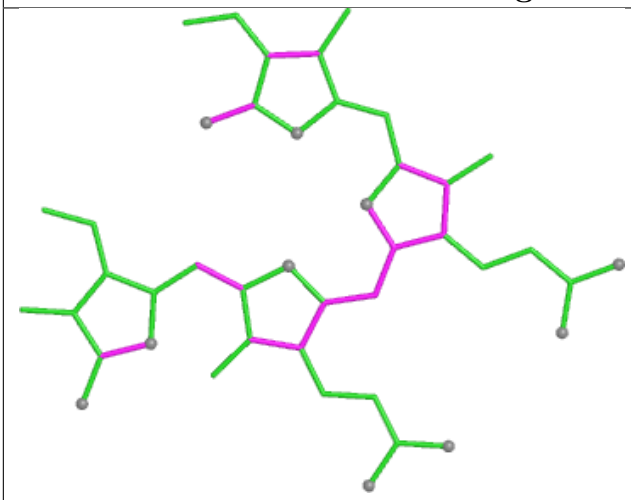


Rings

Ligand PEB qC 203



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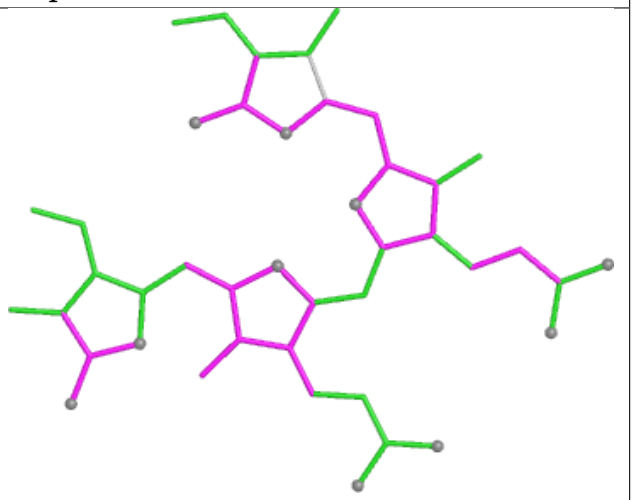

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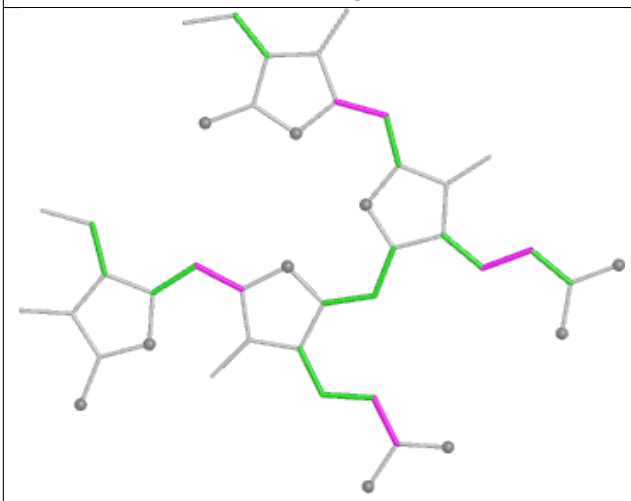

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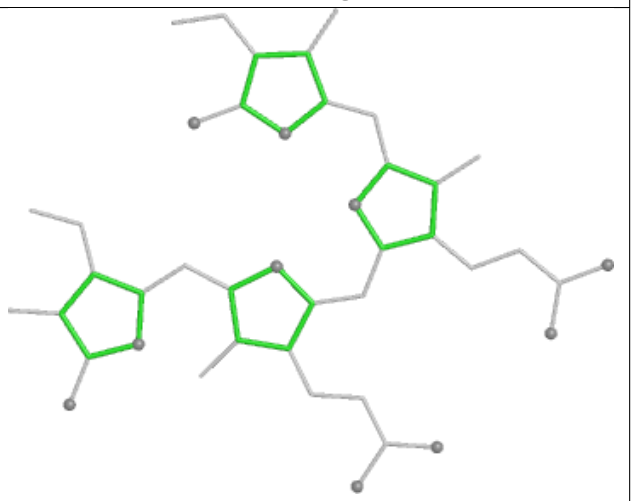
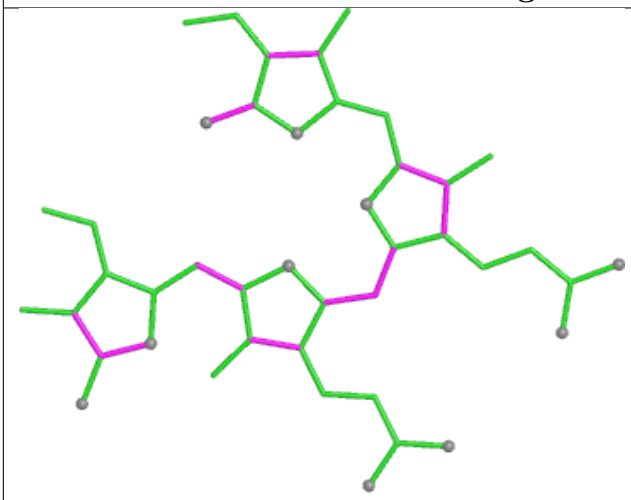


Rings

Ligand PEB eE 202



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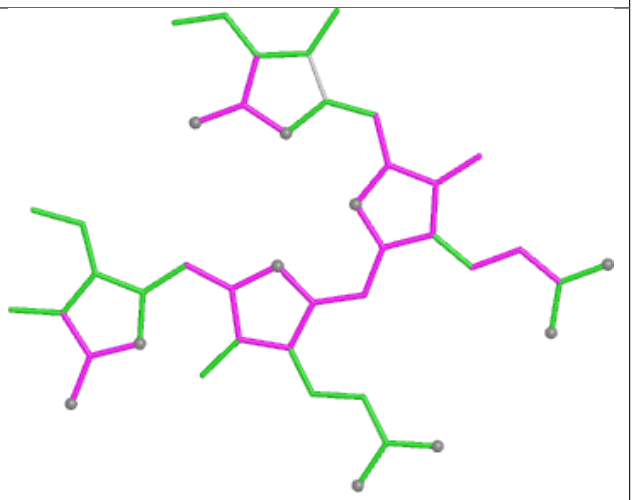
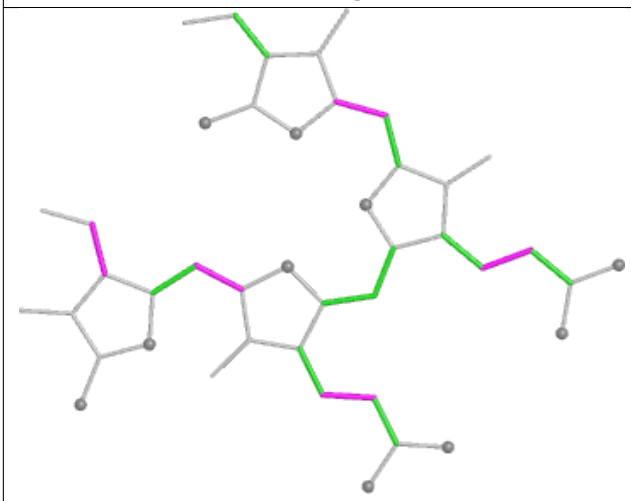


Bond angles



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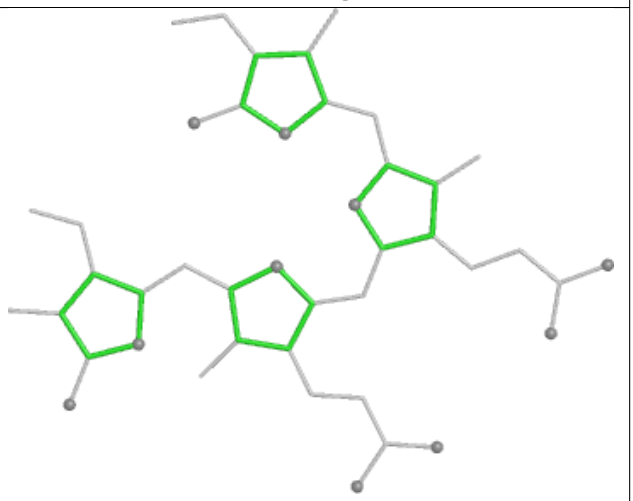
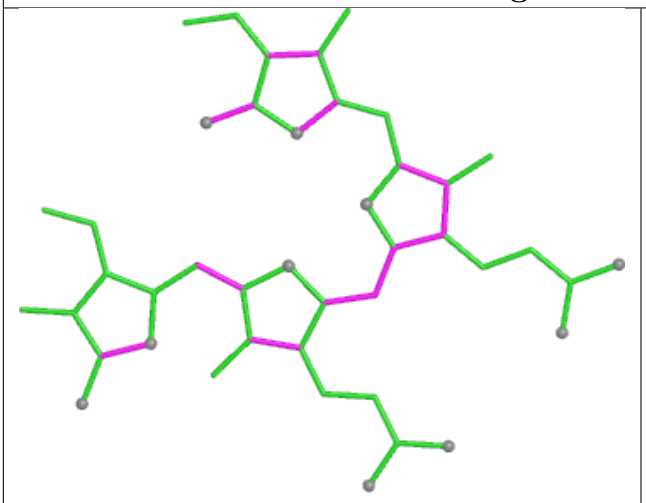


Rings

Ligand PEB QK 202



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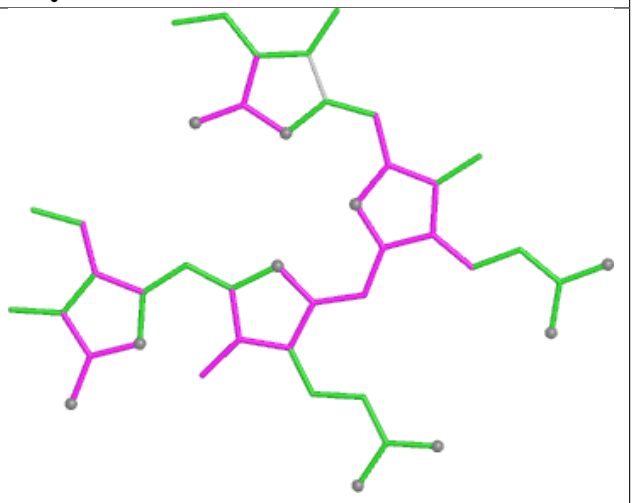

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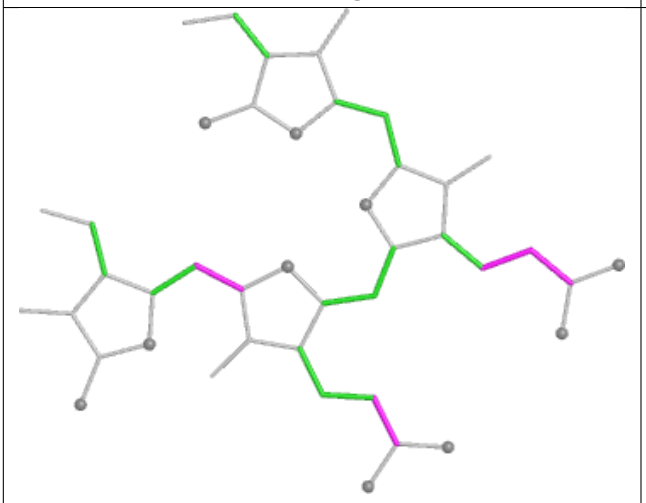

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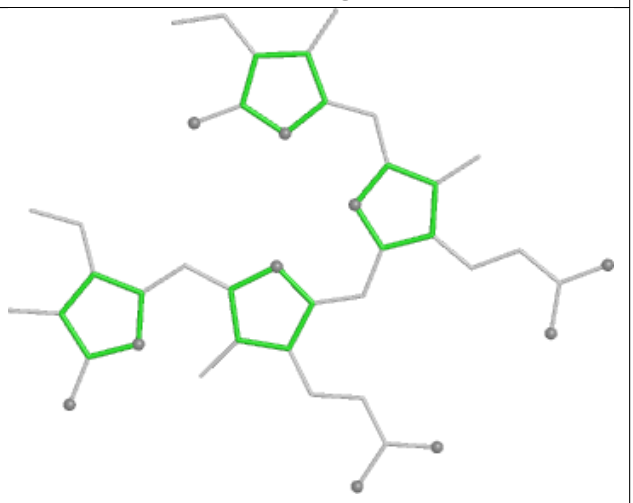
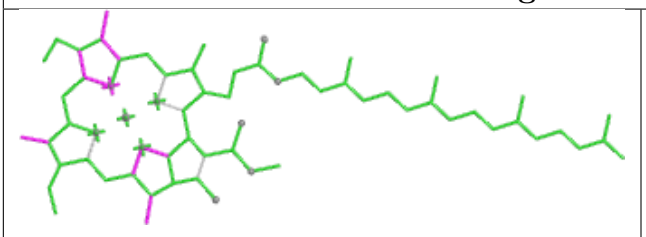


Rings

Ligand CLA b6 609



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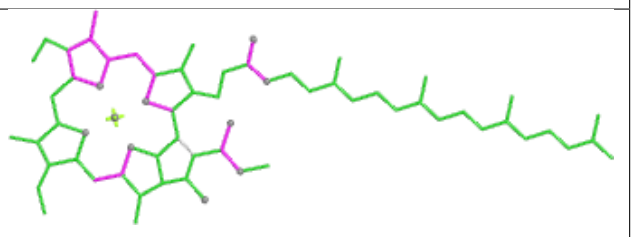

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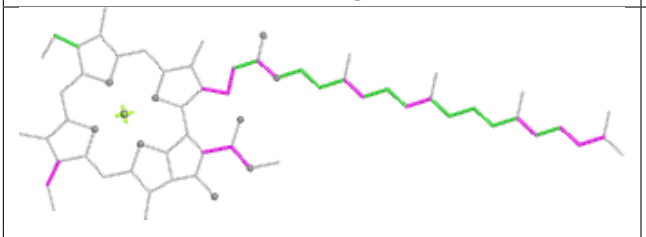

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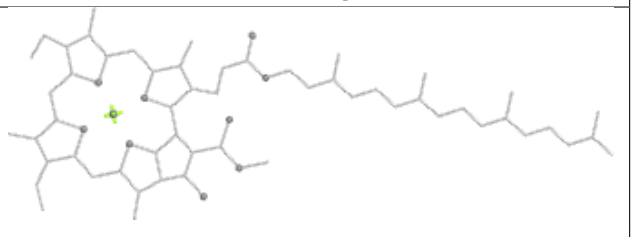

Rings

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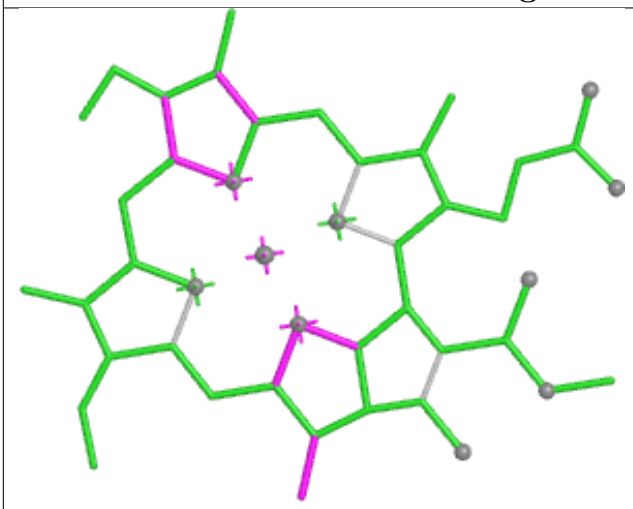

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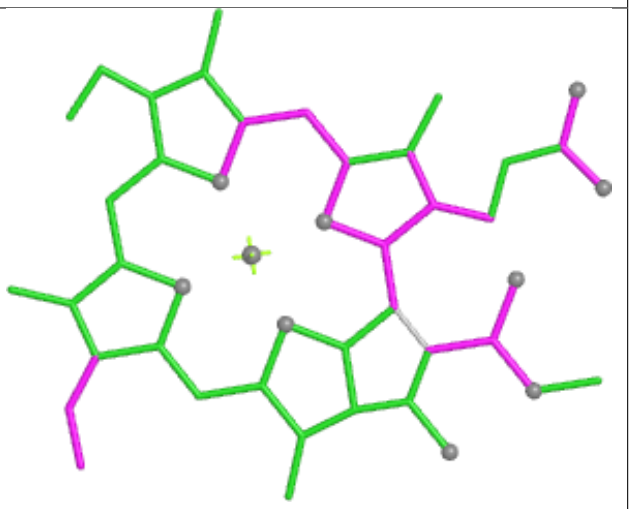

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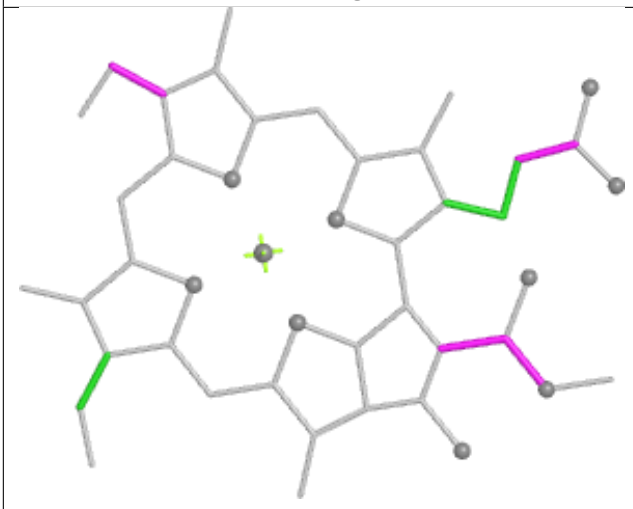
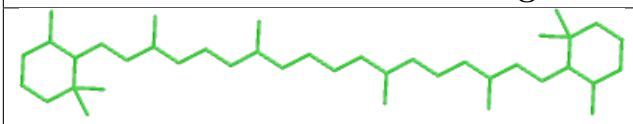


Torsions



Rings

Ligand BCR c6 603



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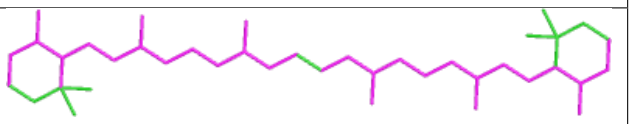

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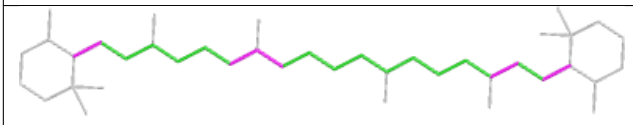

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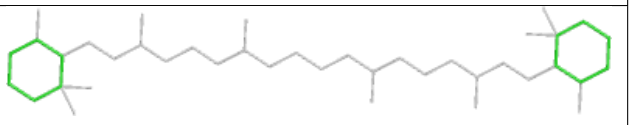
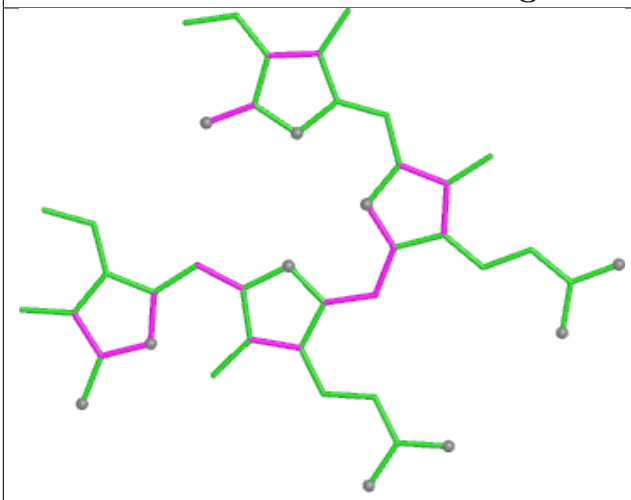


Rings

Ligand PEB lO 201



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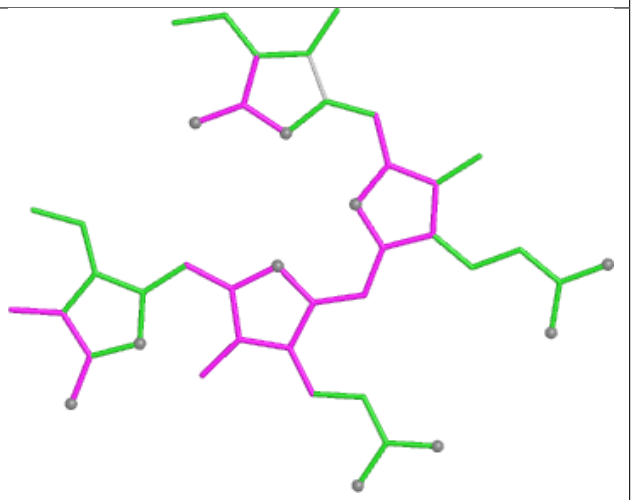

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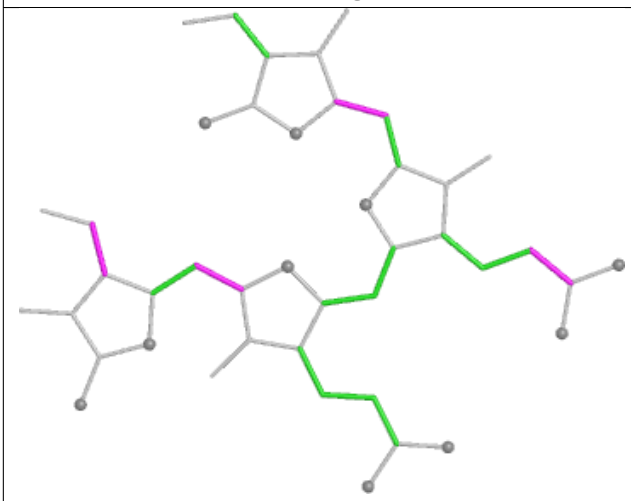

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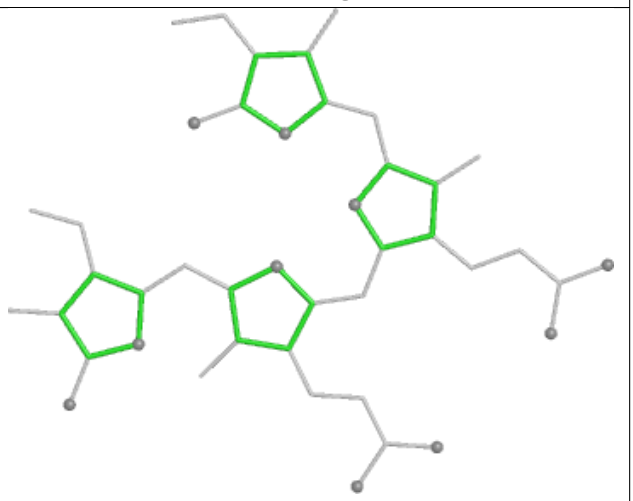
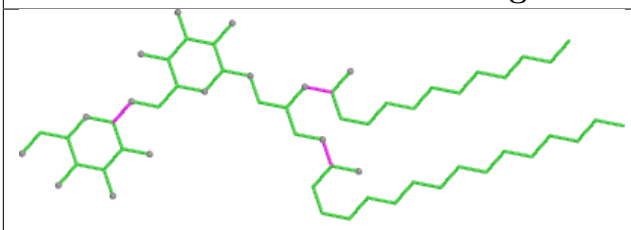


Rings

Ligand DGD BL 614



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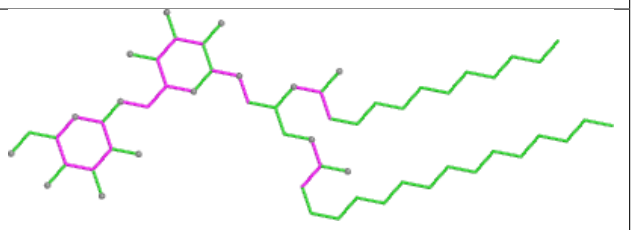

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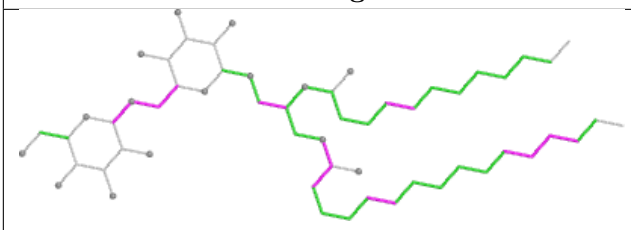

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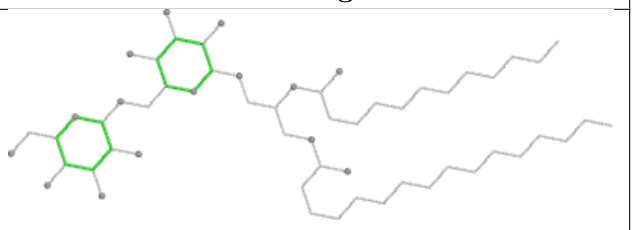
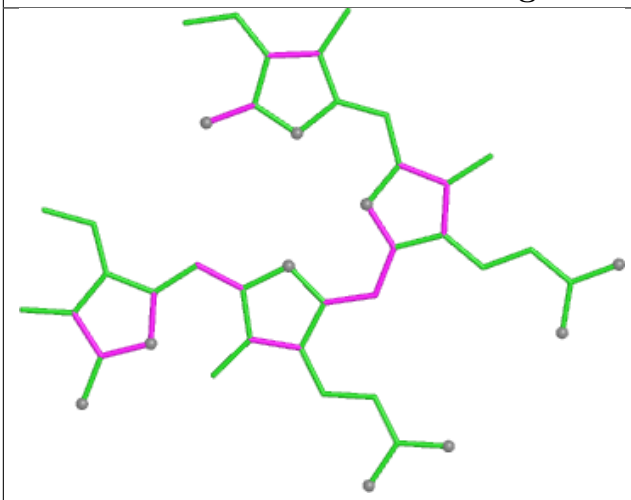


Rings

Ligand PEB IP 201



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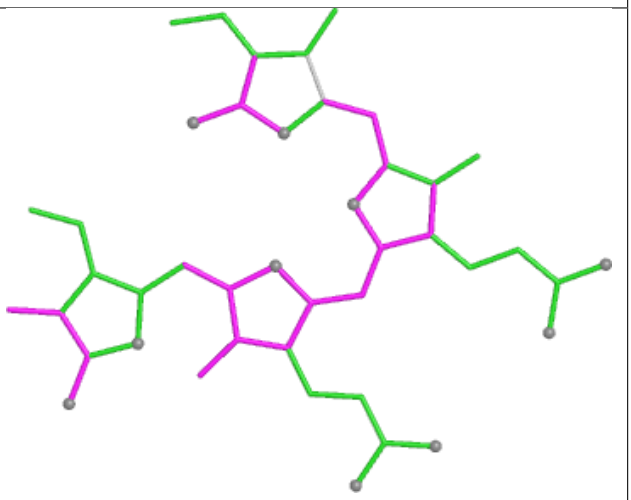

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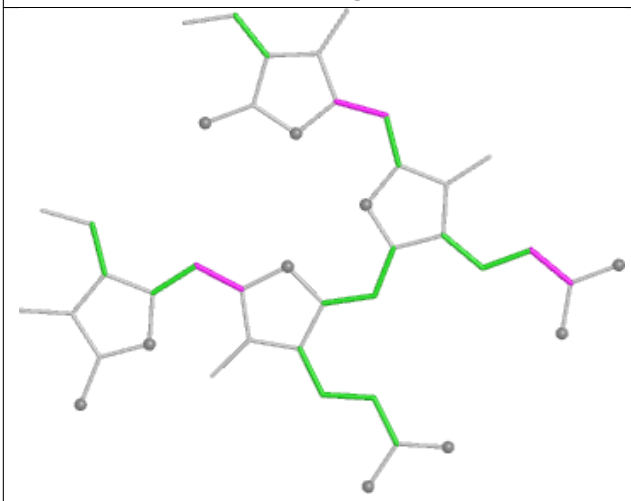

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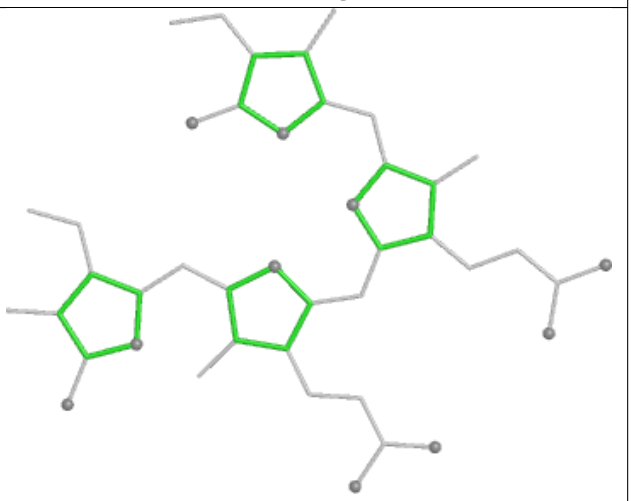
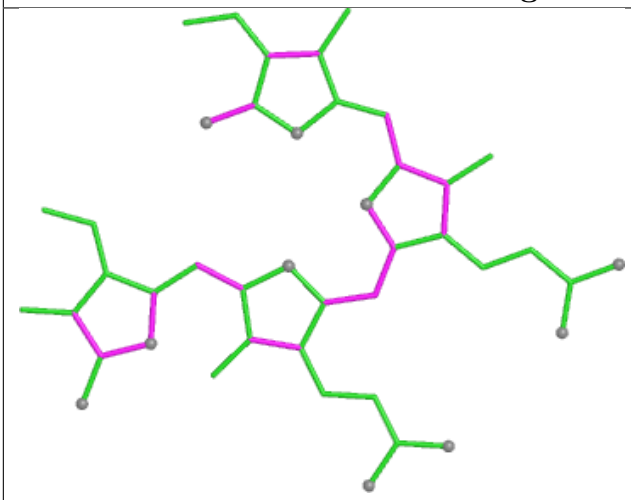


Rings

Ligand PEB cJ 201



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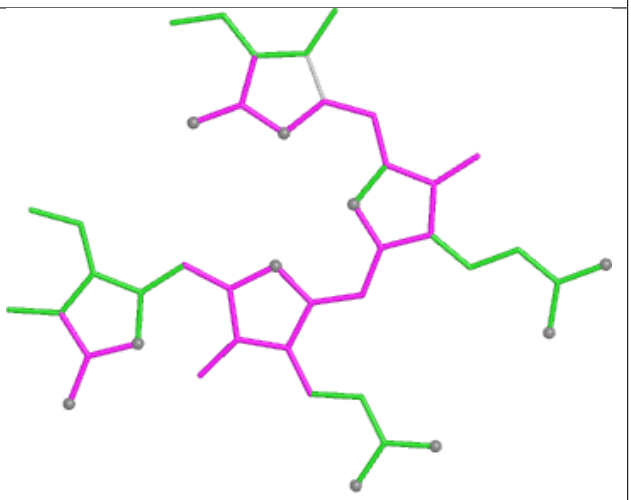

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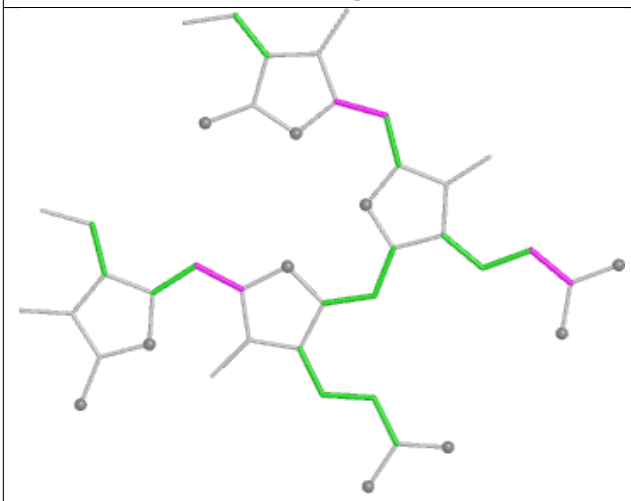

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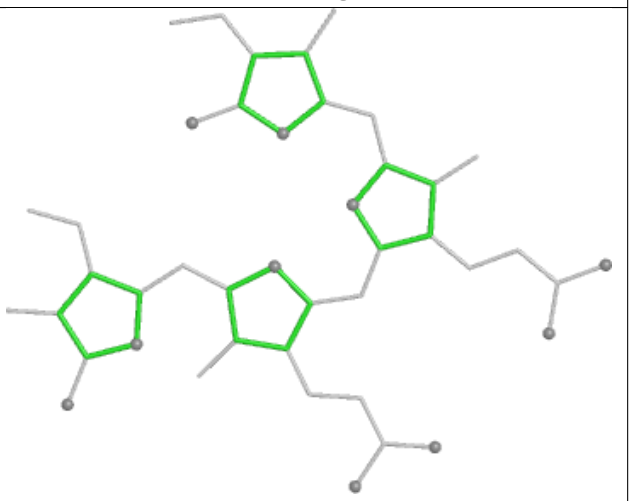
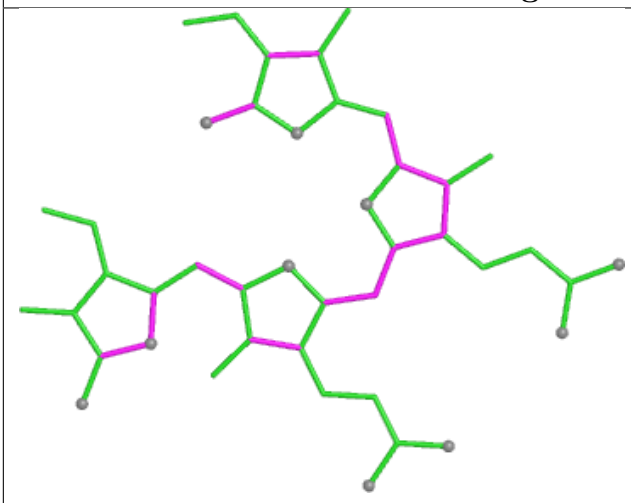


Rings

Ligand PEB iF 201



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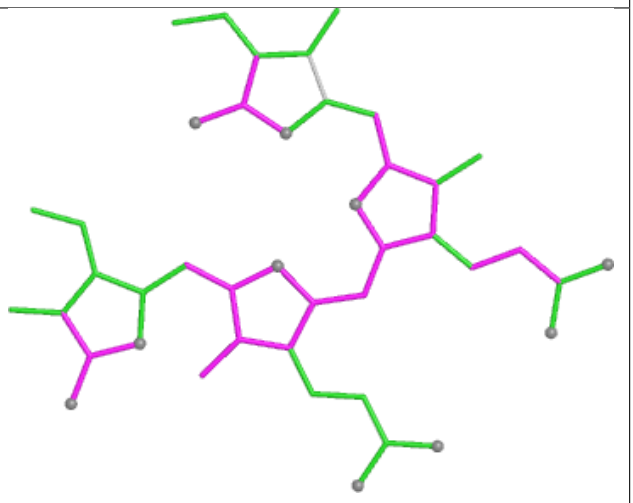
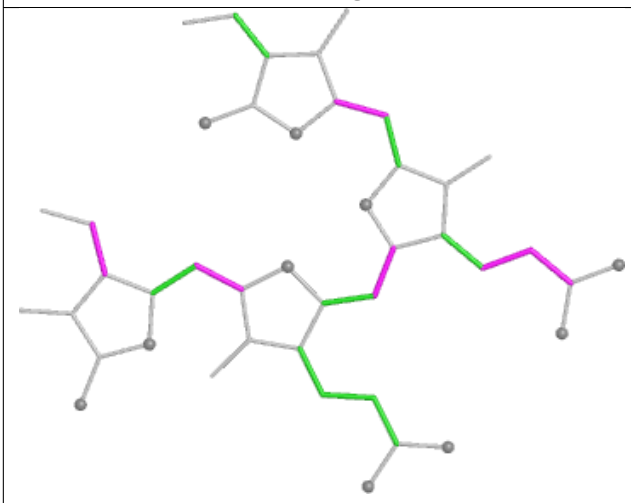


Bond angles



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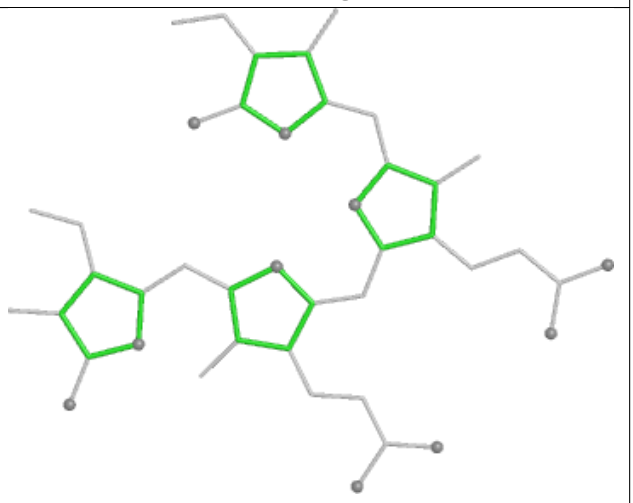
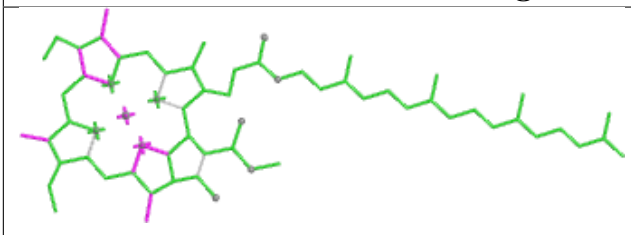


Rings

Ligand CLA A2 828



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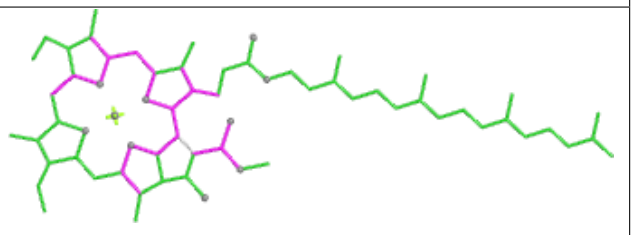
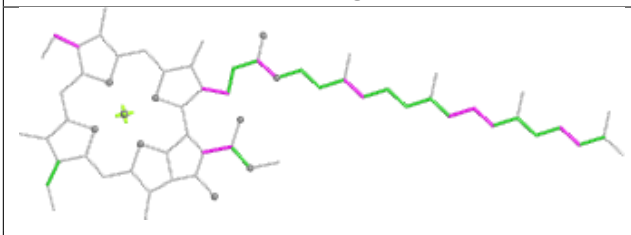


Bond angles



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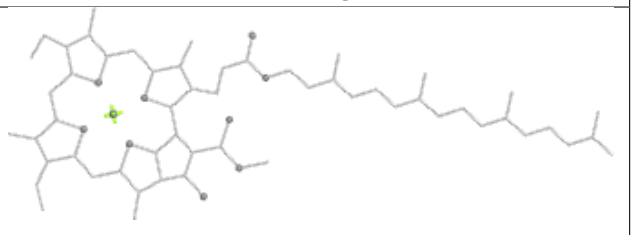
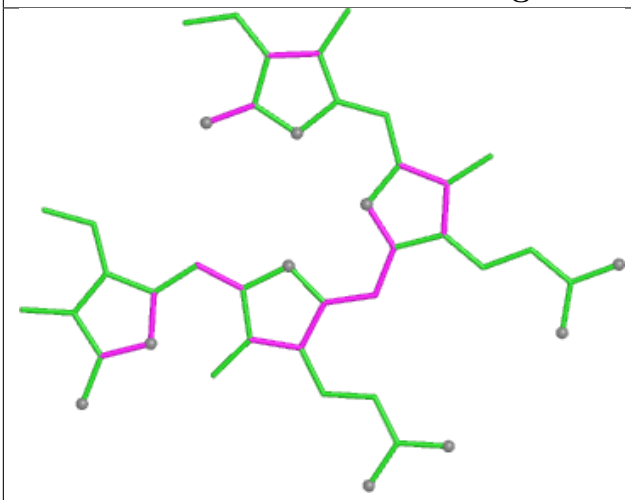


Rings

Ligand PEB KF 203



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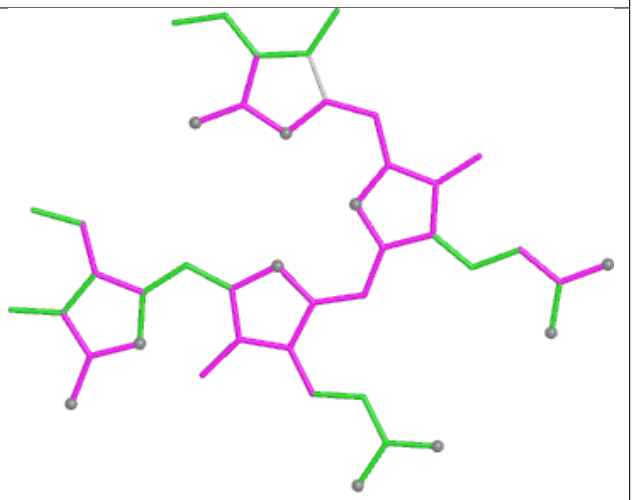
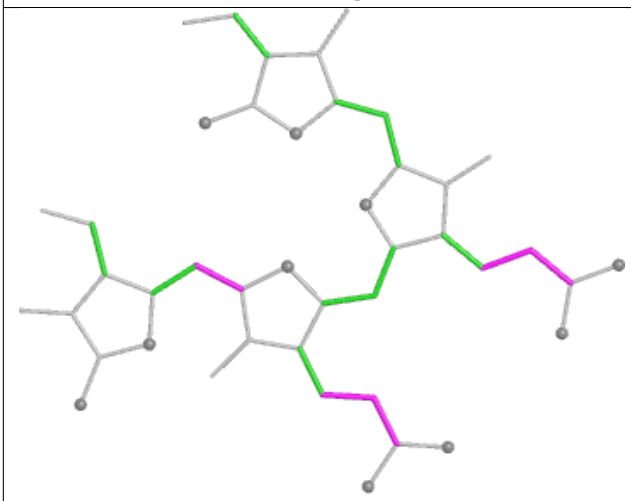


Bond angles



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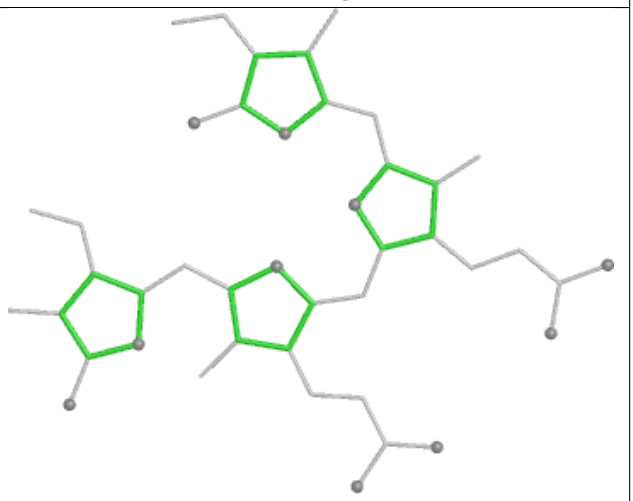
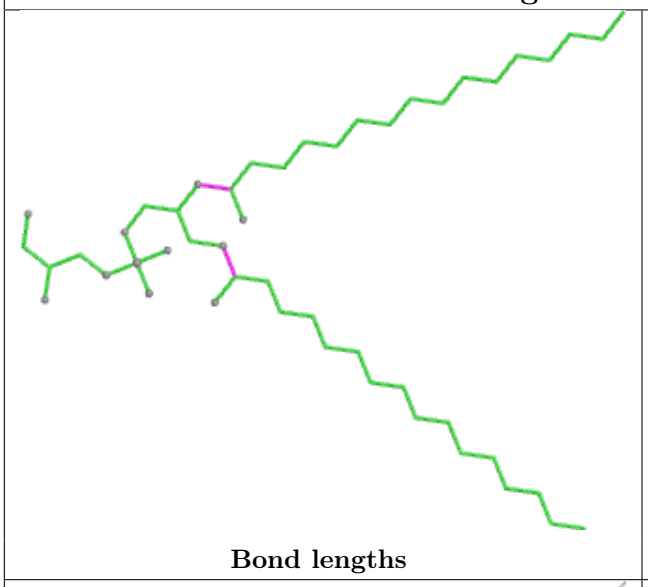
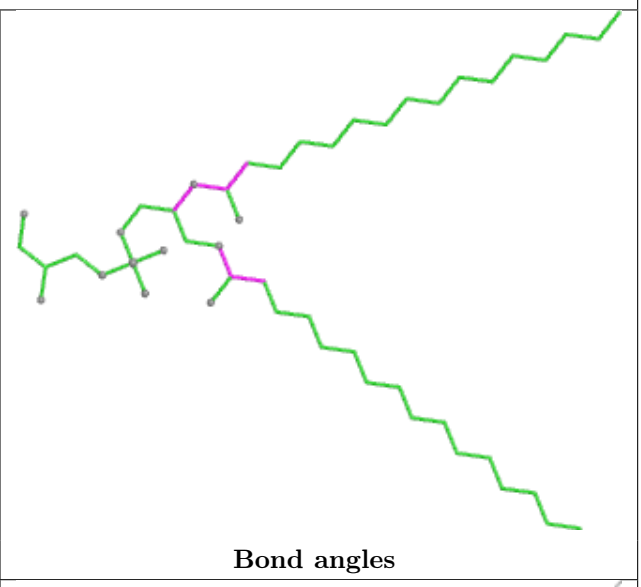


Rings

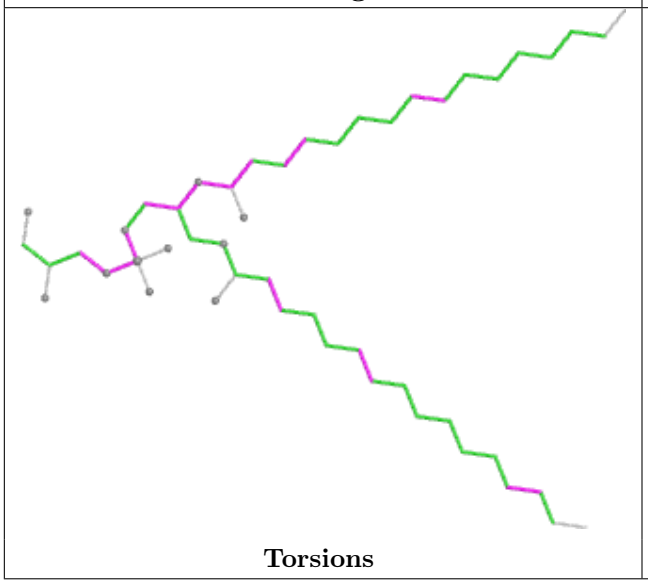
Ligand LHG iL 101



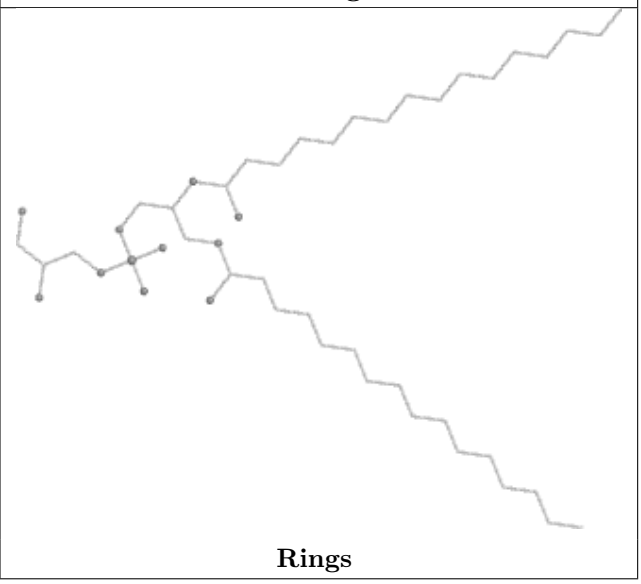
Bond lengths



Bond angles

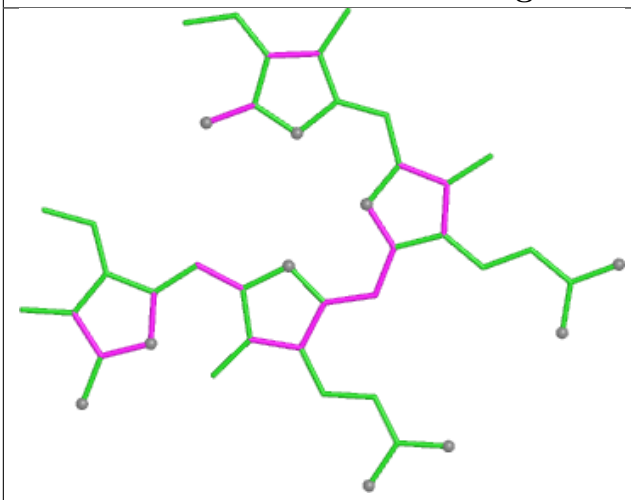


Torsions

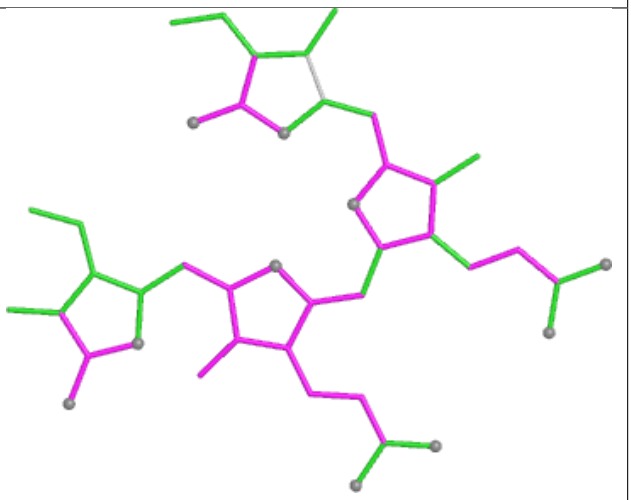


Rings

Ligand PEB cG 201



Bond lengths



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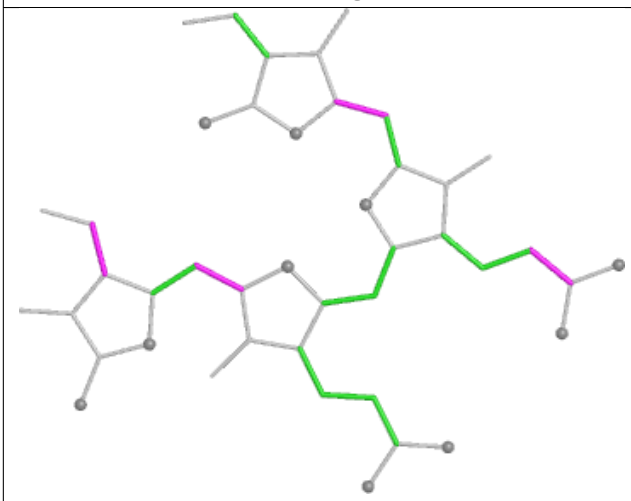

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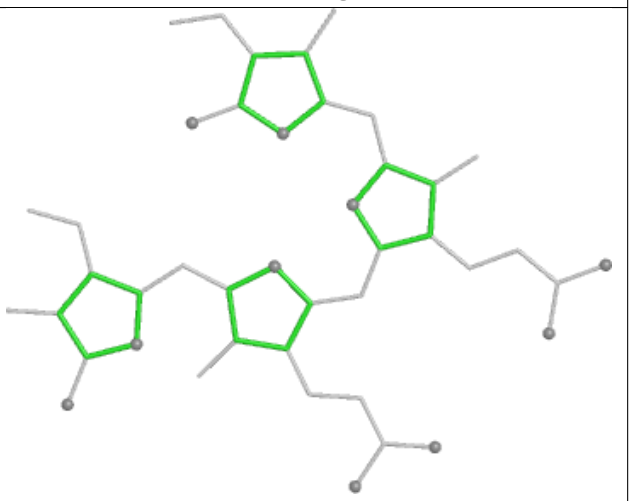
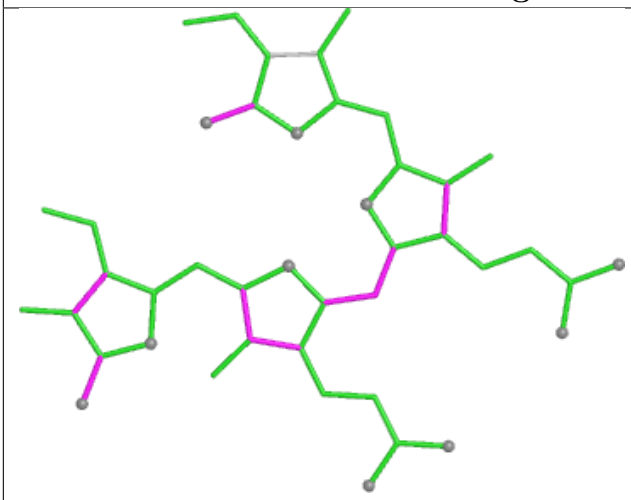


Rings

Ligand PUB yK 302



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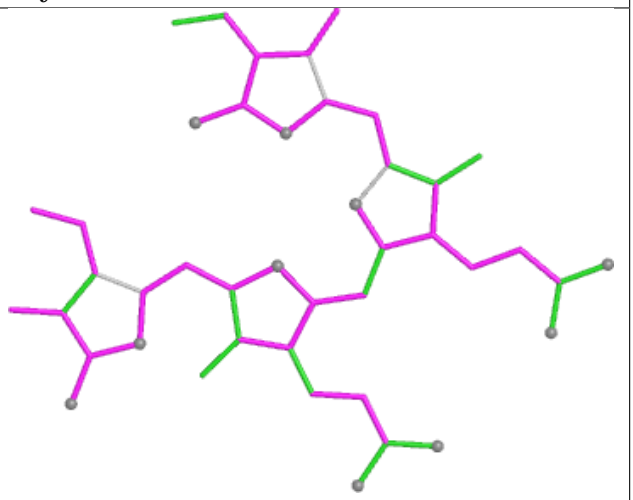

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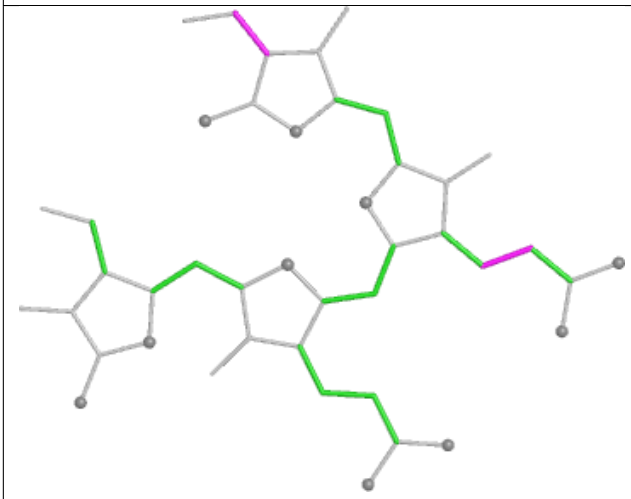

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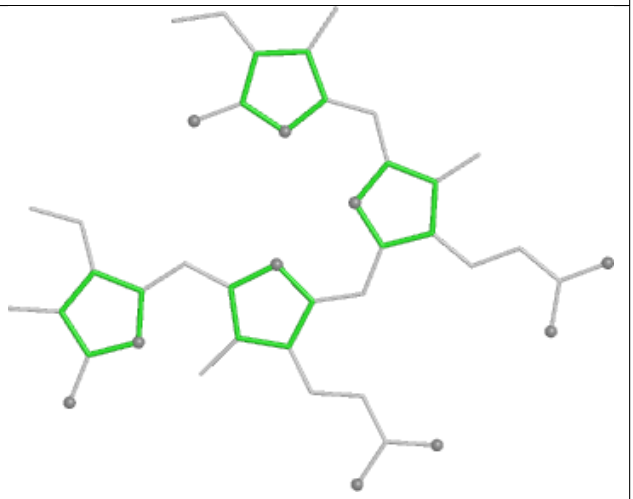
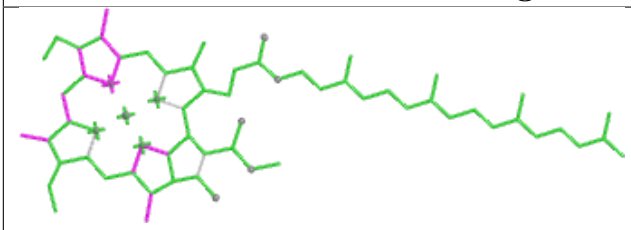


Rings

Ligand CLA bL 613



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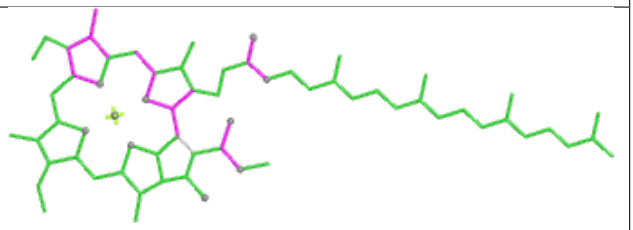

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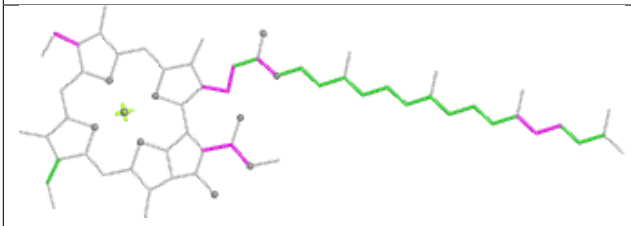

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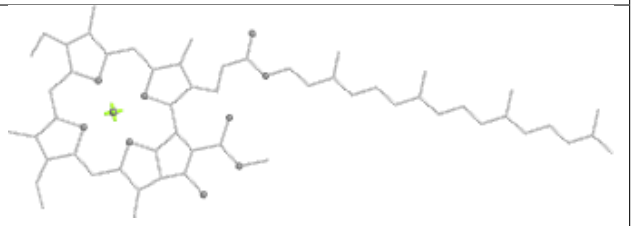
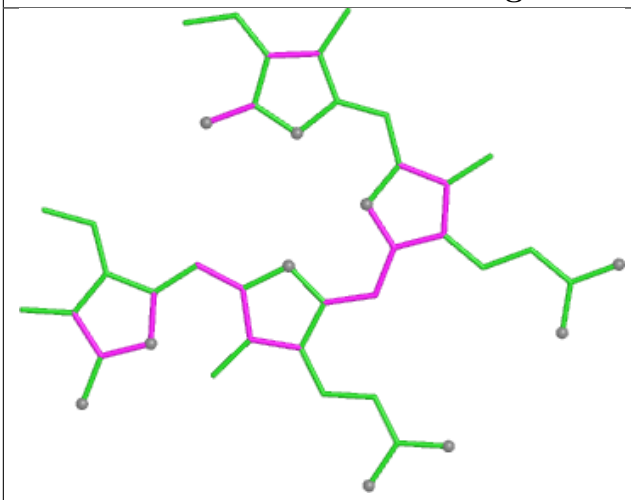


Rings

Ligand PEB WD 201



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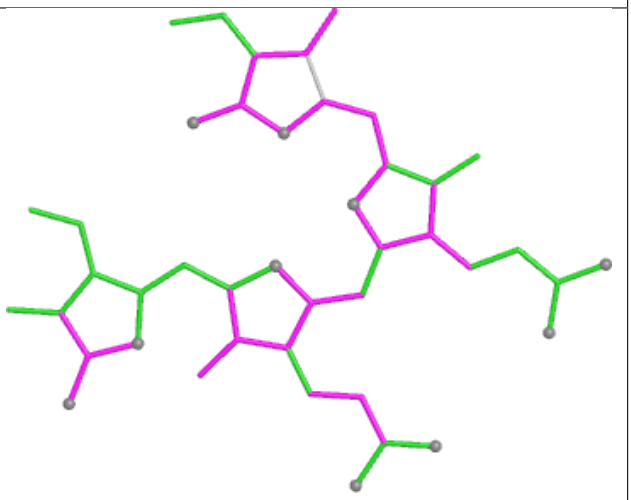
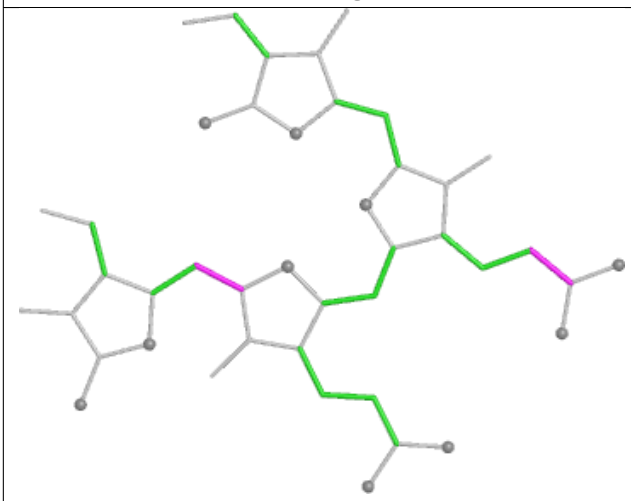


Bond angles



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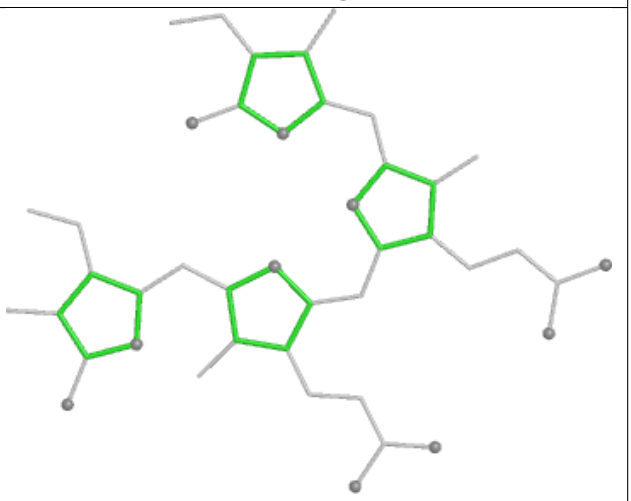
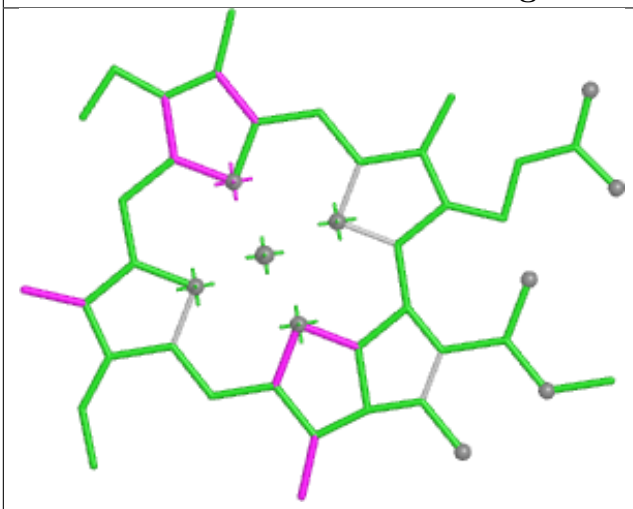


Rings

Ligand CLA 32 305



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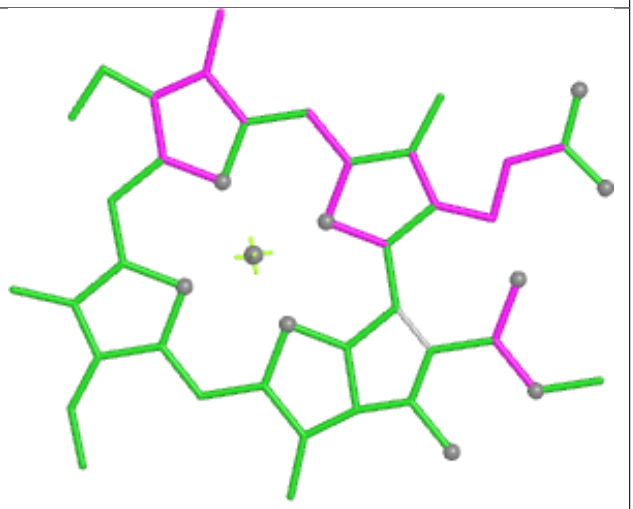

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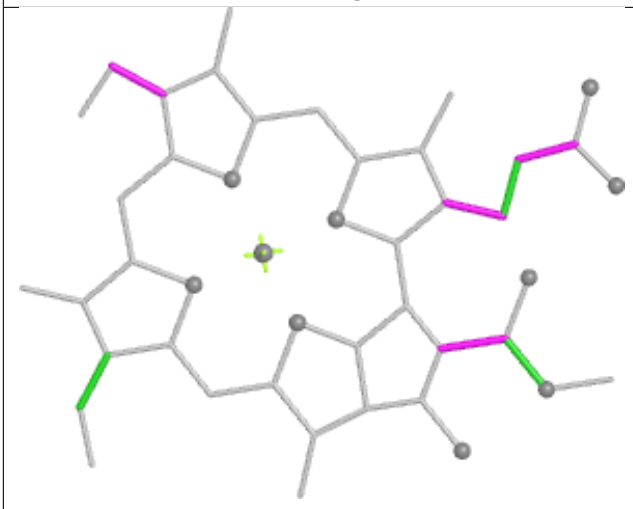
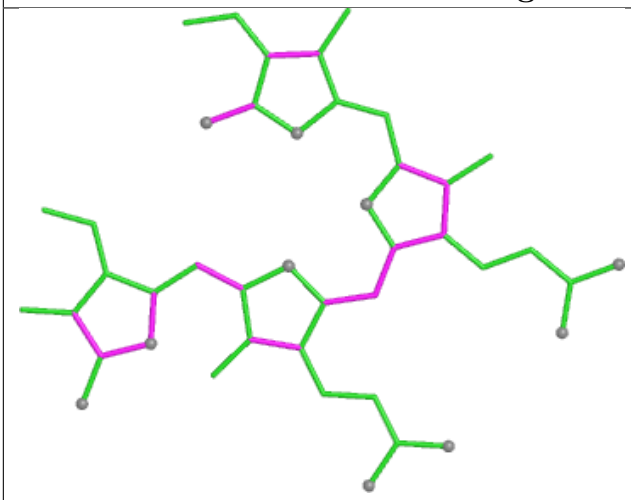


Torsions



Rings

Ligand PEB F5 202



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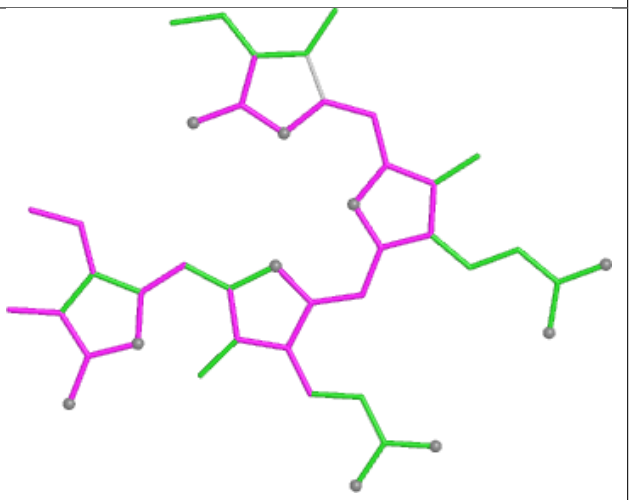

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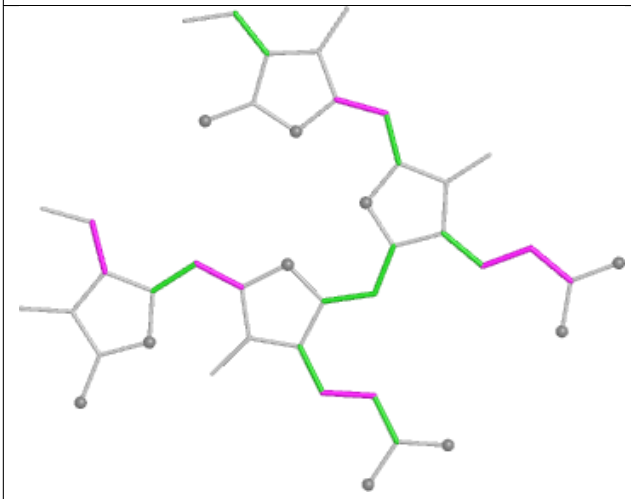

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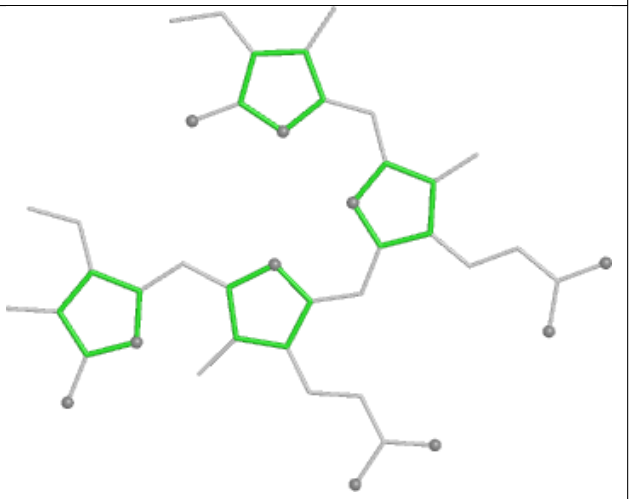
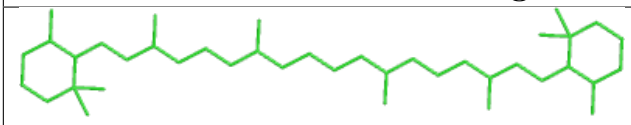


Rings

Ligand BCR LN 201



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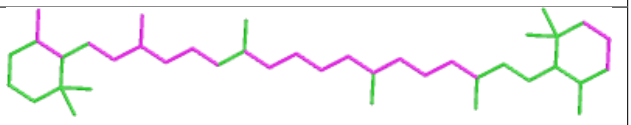
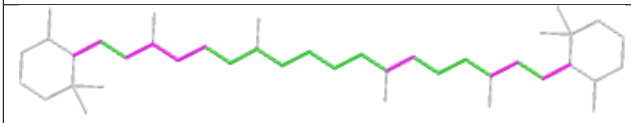


Bond angles



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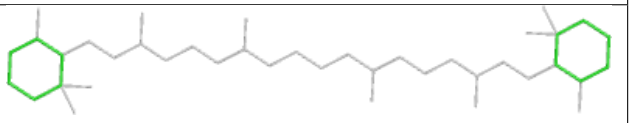
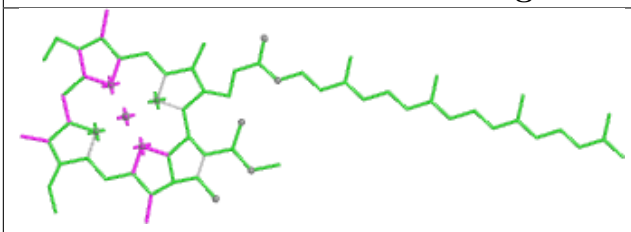


Rings

Ligand CLA B2 834



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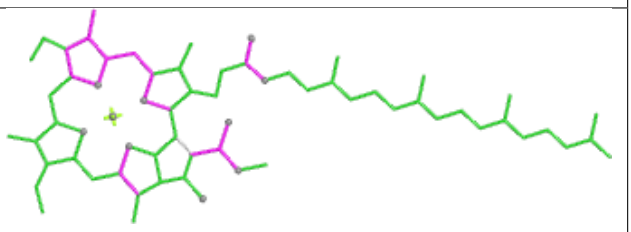
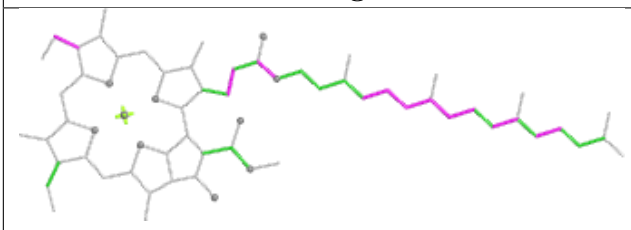


Bond angles



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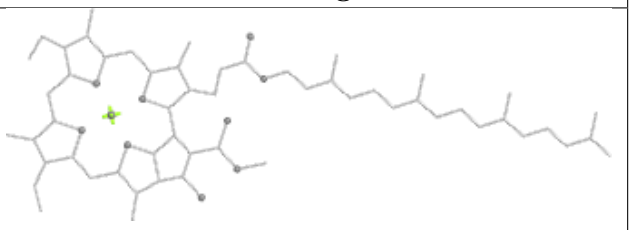
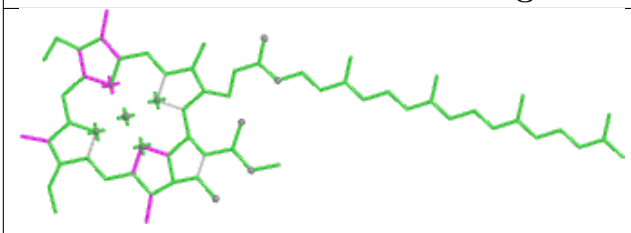


Rings

Ligand CLA bL 605



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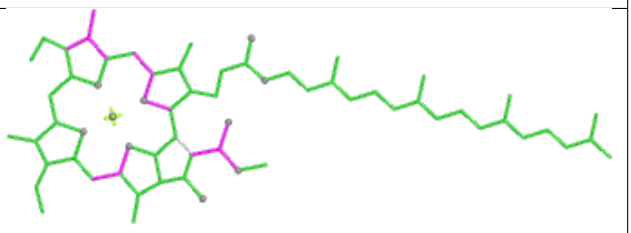
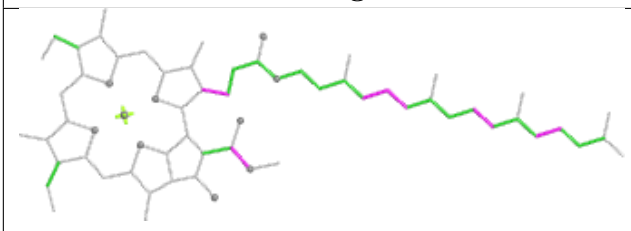


Bond angles



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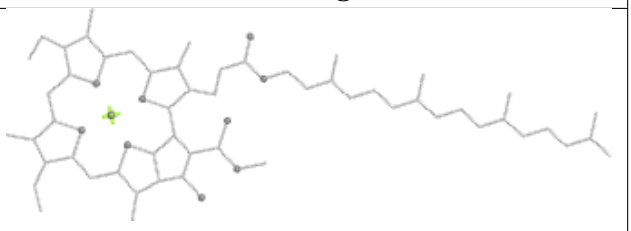
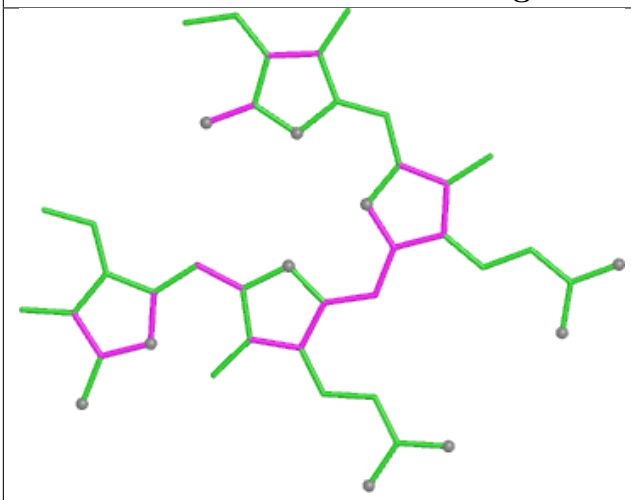


Rings

Ligand PEB TP 201



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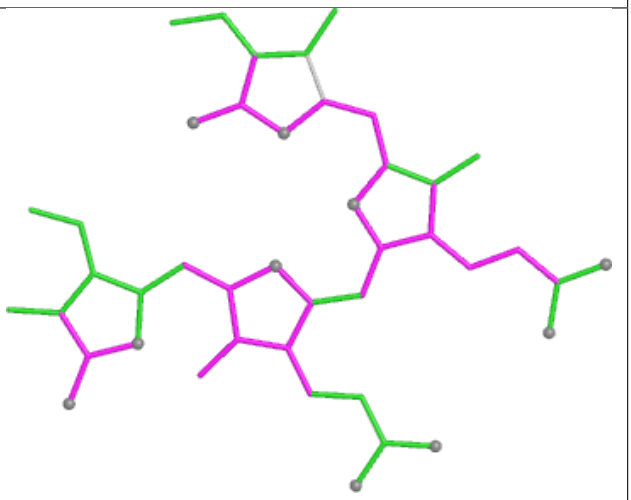

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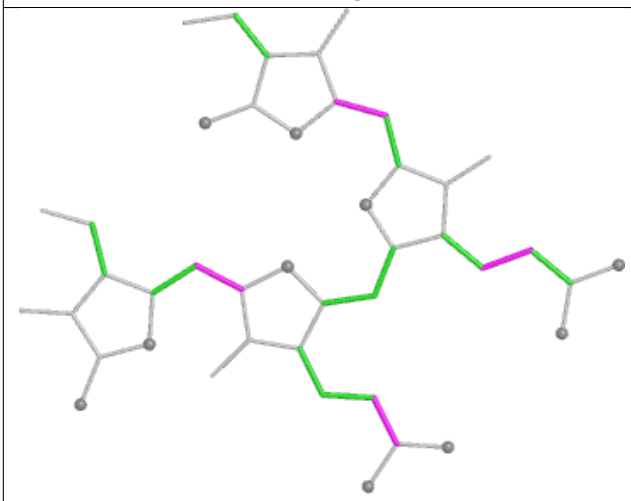

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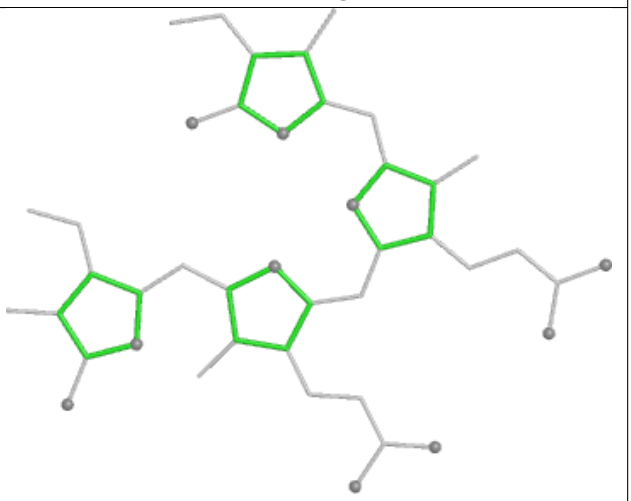
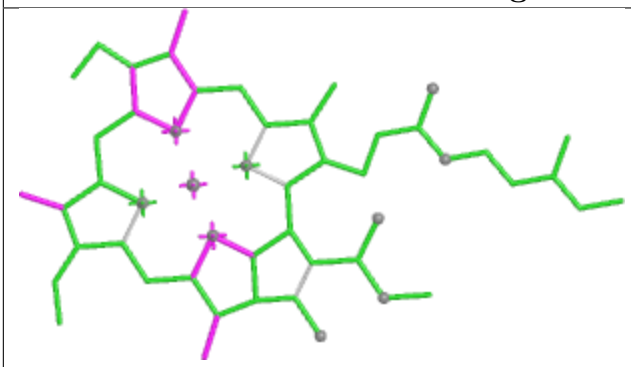


Rings

Ligand CLA AN 837



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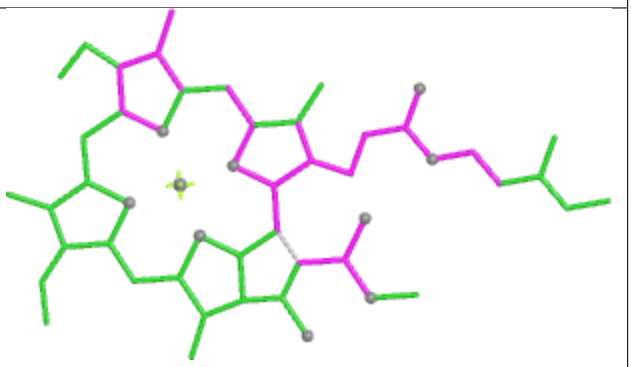

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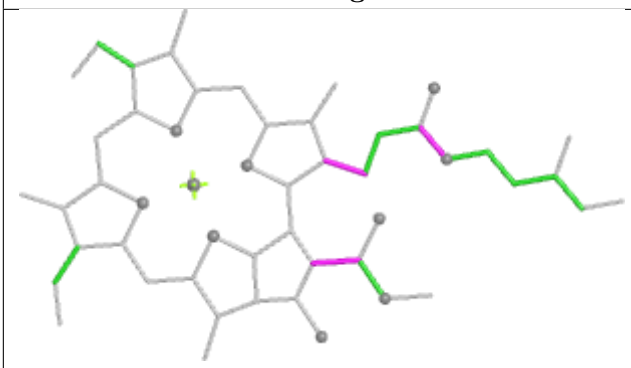

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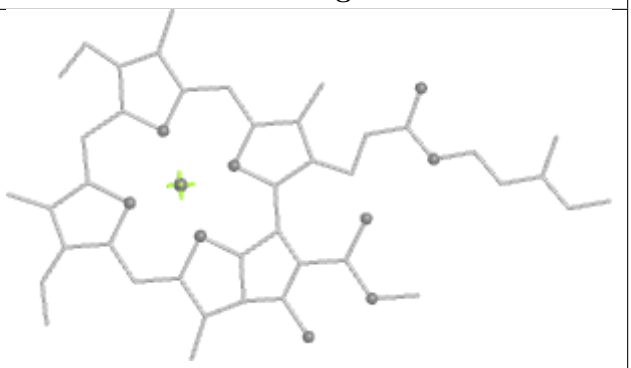
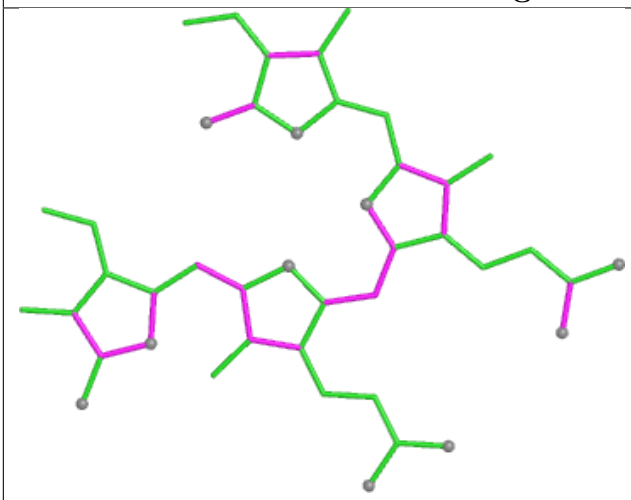


Rings

Ligand PEB SK 202



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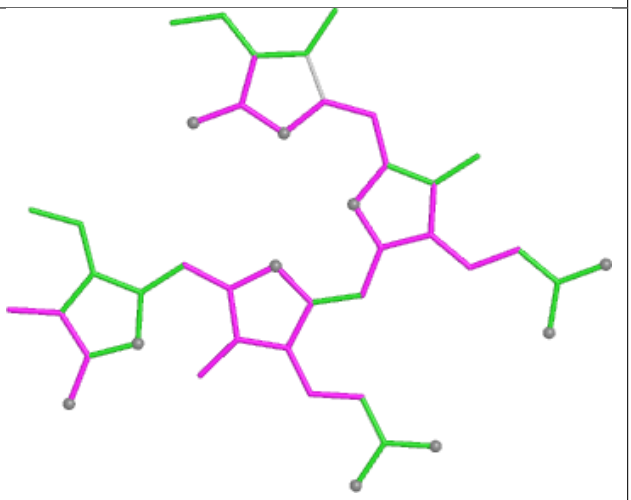
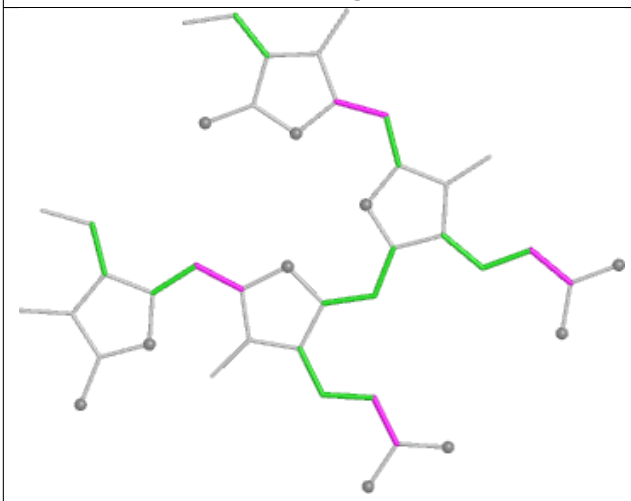


Bond angles



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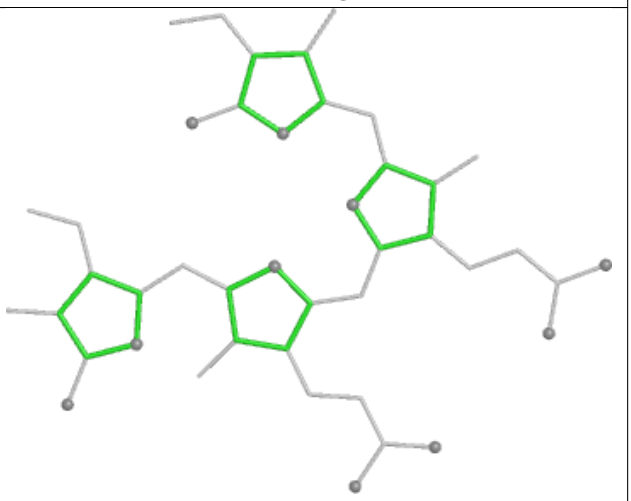
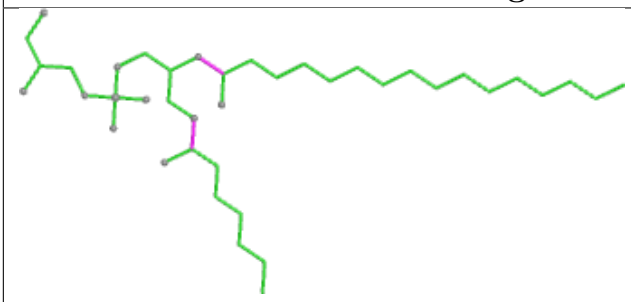
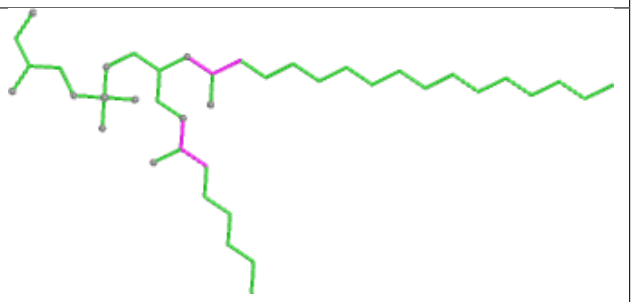


Rings

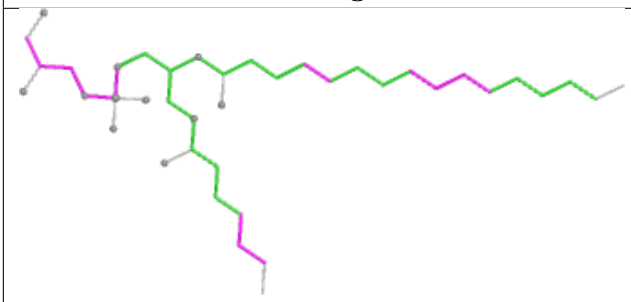
Ligand LHG AN 844



Bond lengths



Bond angles



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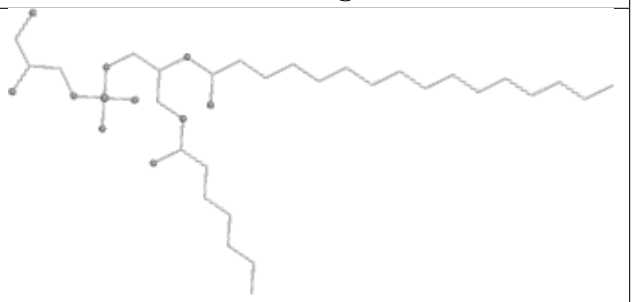
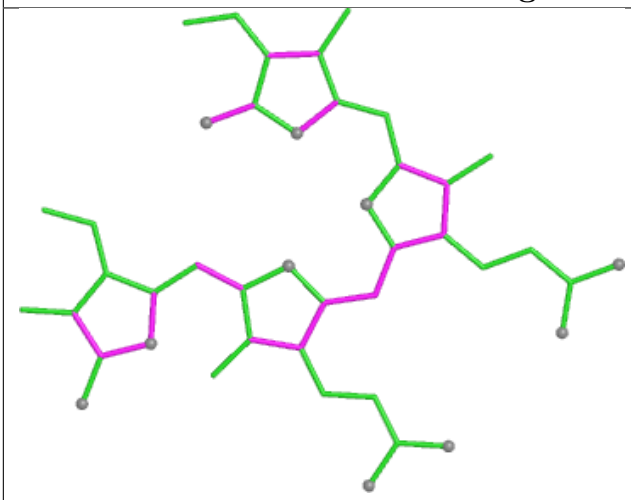
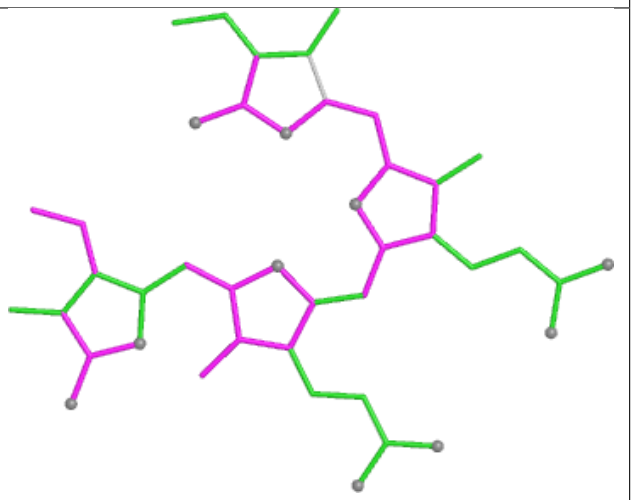


Rings

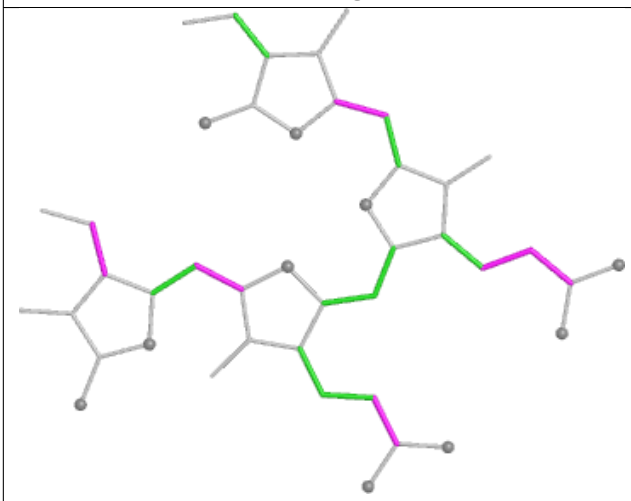
Ligand PEB fO 202



Bond lengths



Bond angles



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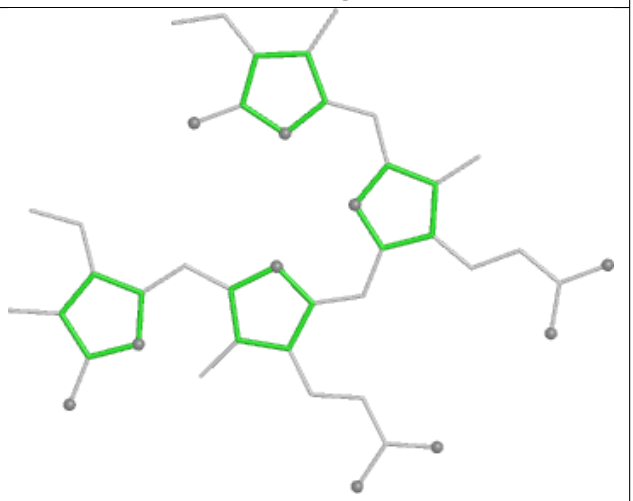
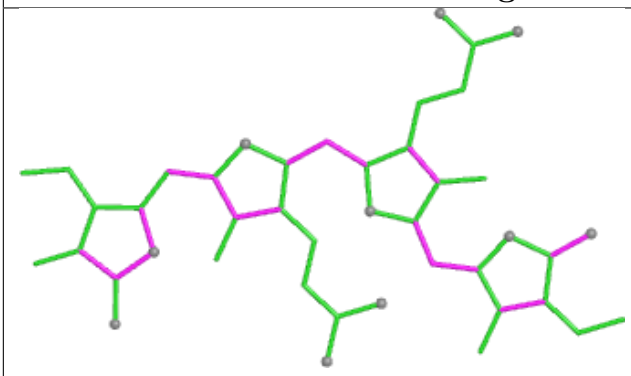
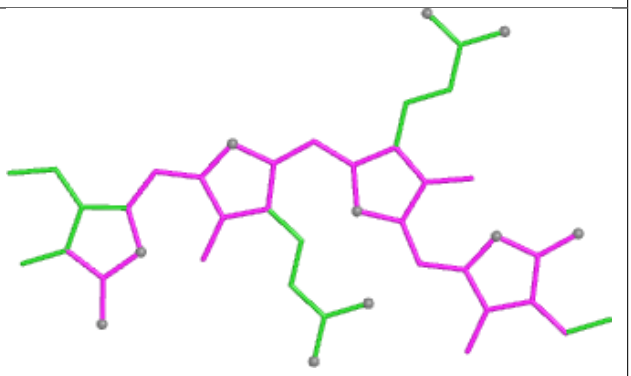


Rings

Ligand CYC KH 1001



Bond lengths



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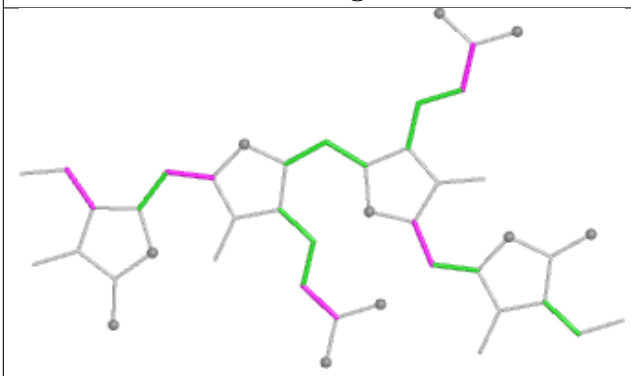

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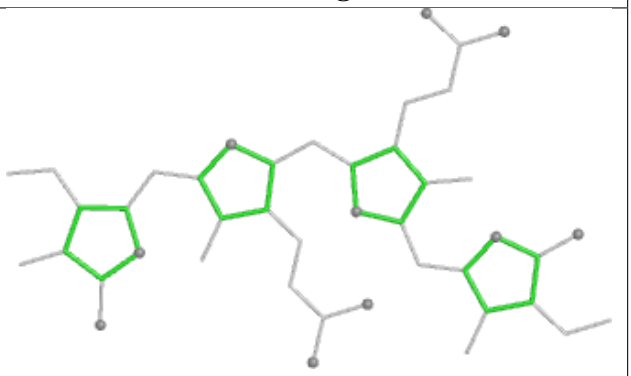
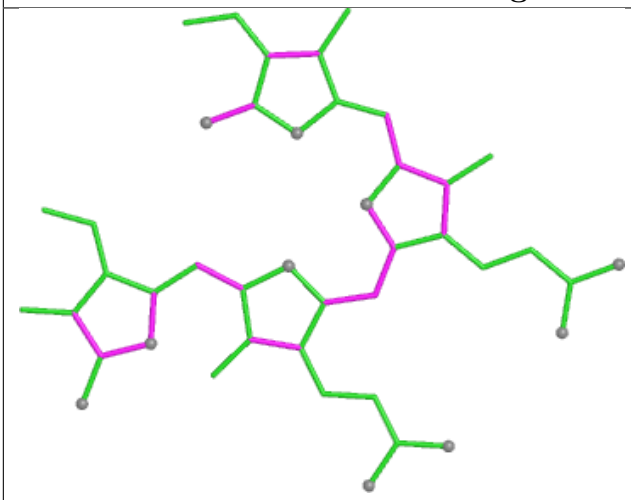


Rings

Ligand PEB LM 201



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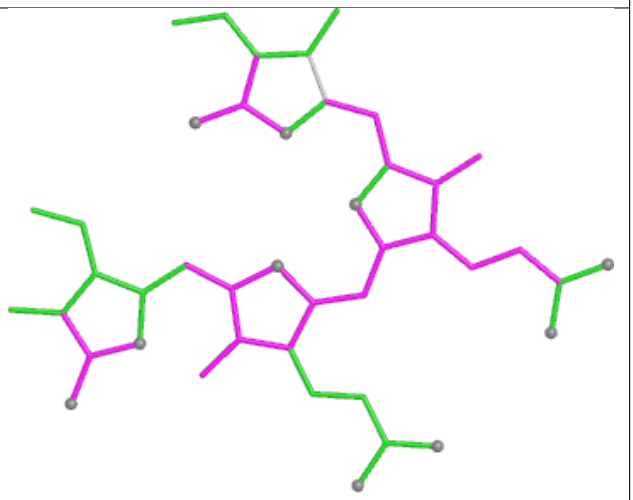

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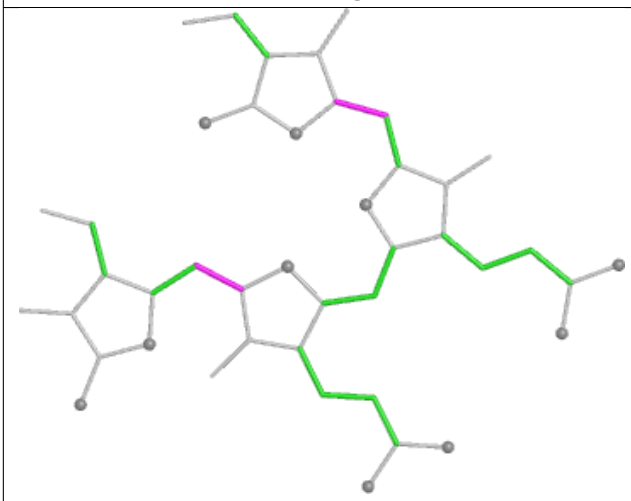

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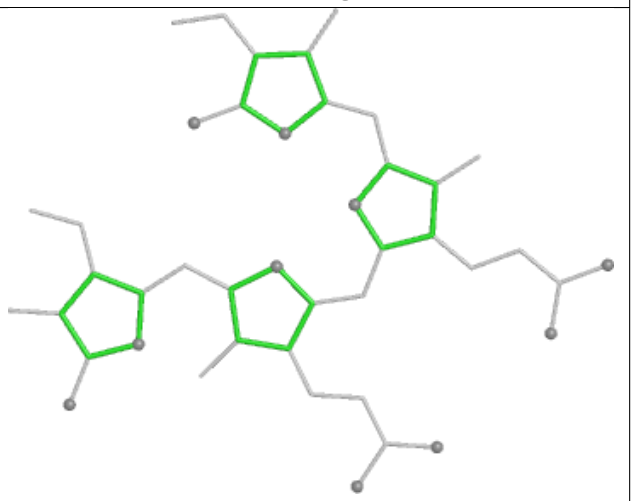
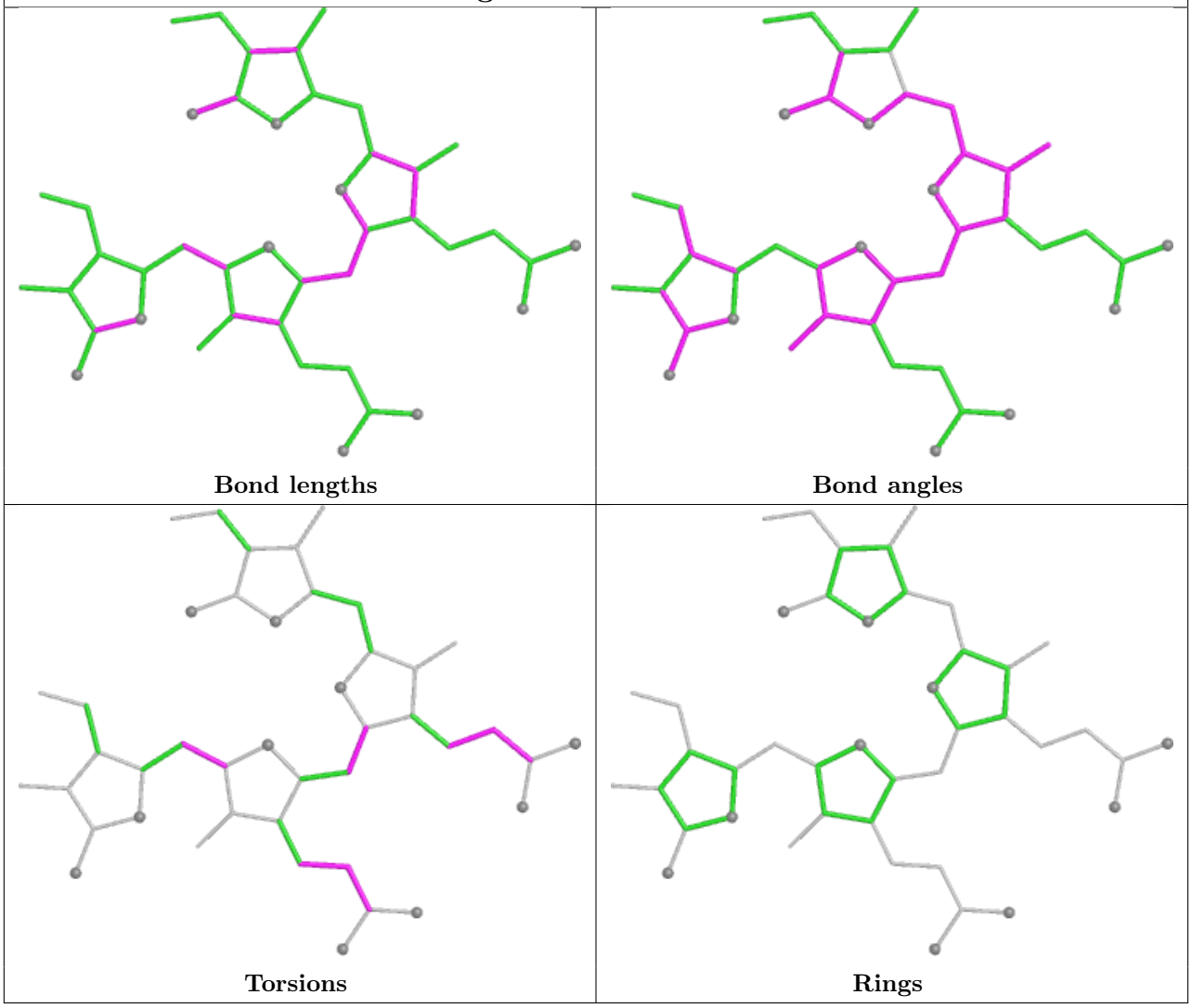
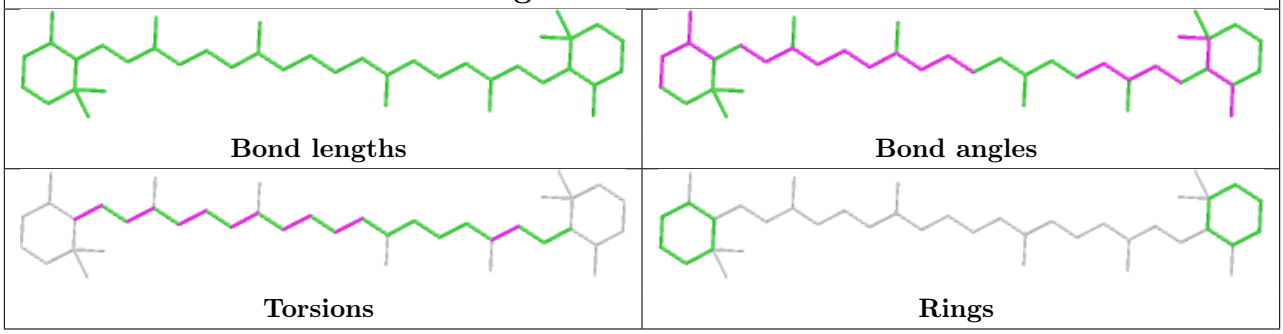


Rings

Ligand PEB OF 203



Ligand BCR A2 845



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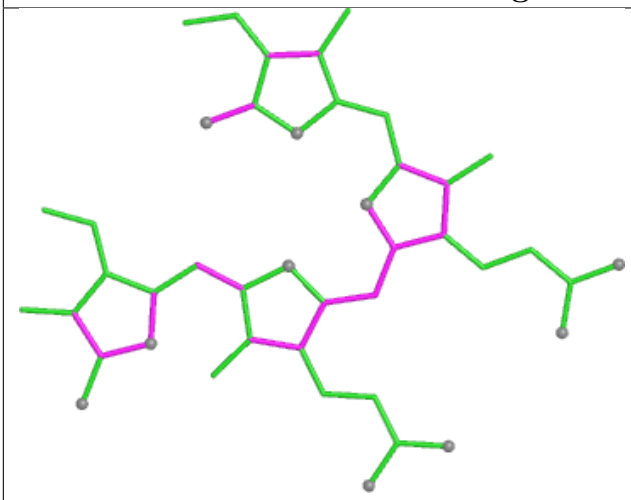

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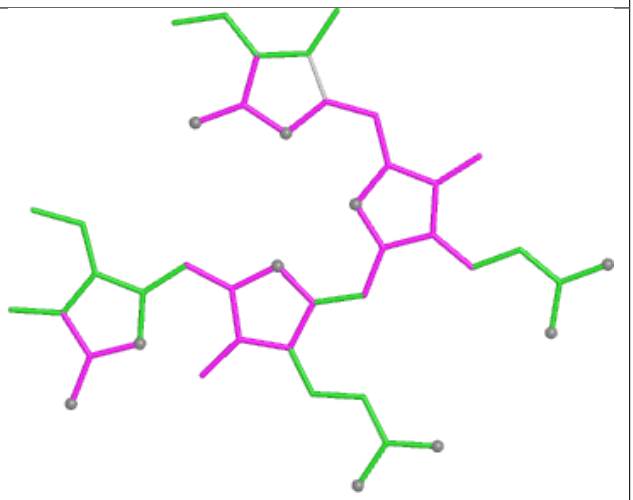

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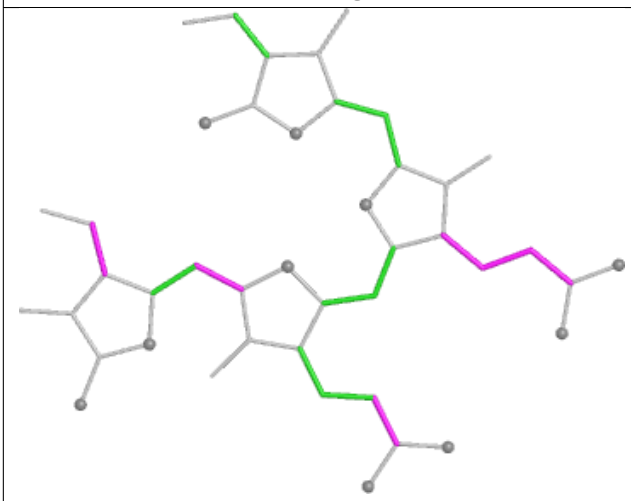

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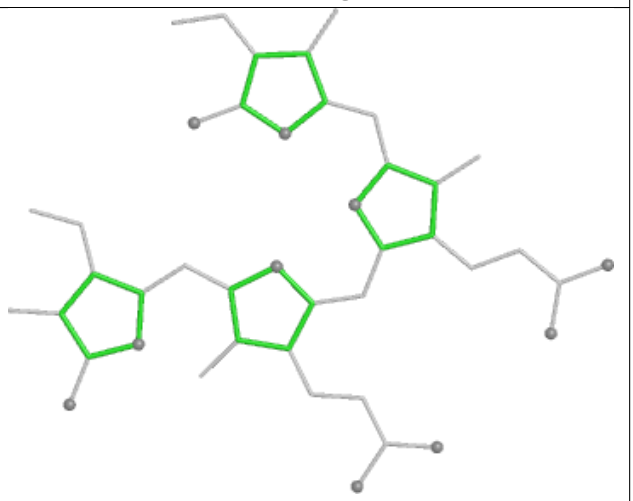

Rings

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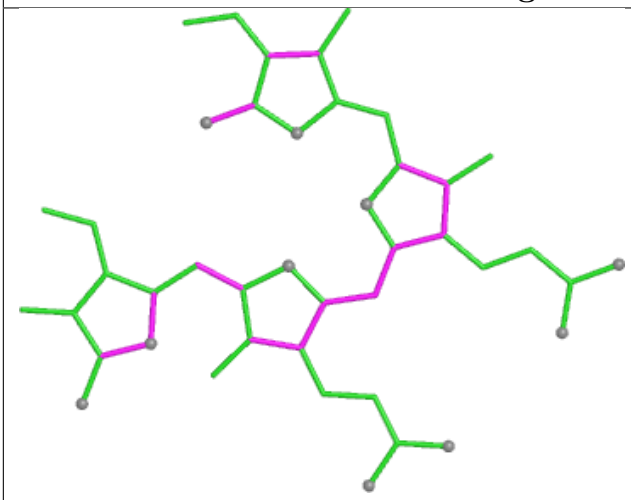

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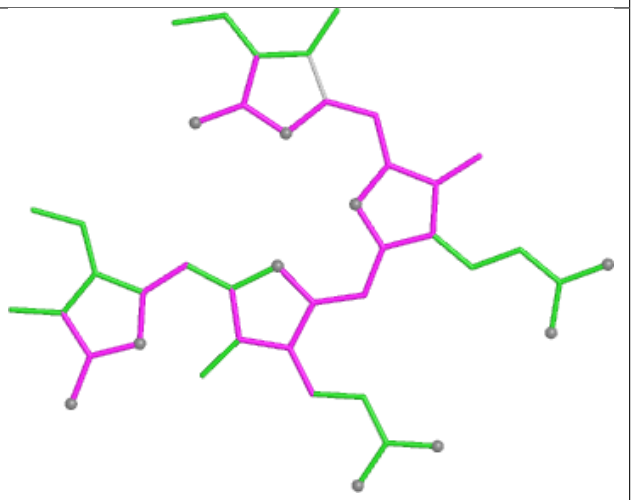

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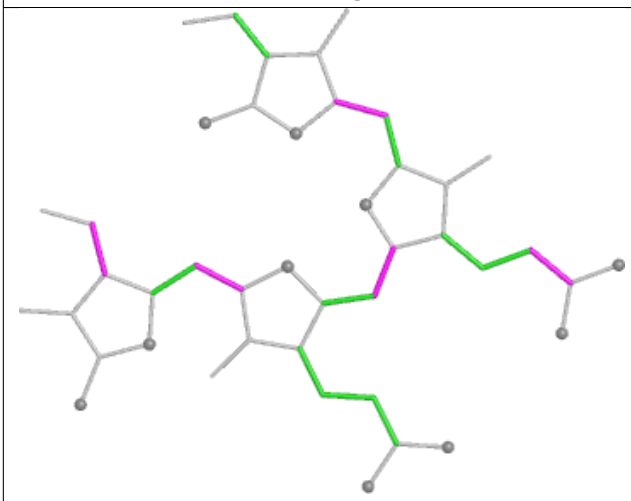

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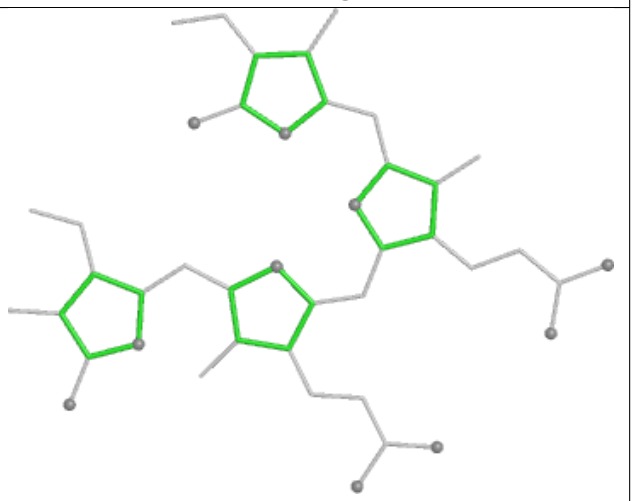
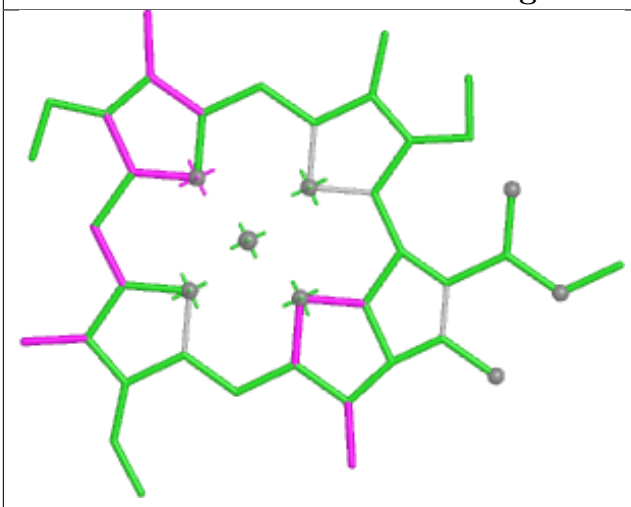


Rings

Ligand CLA 32 311



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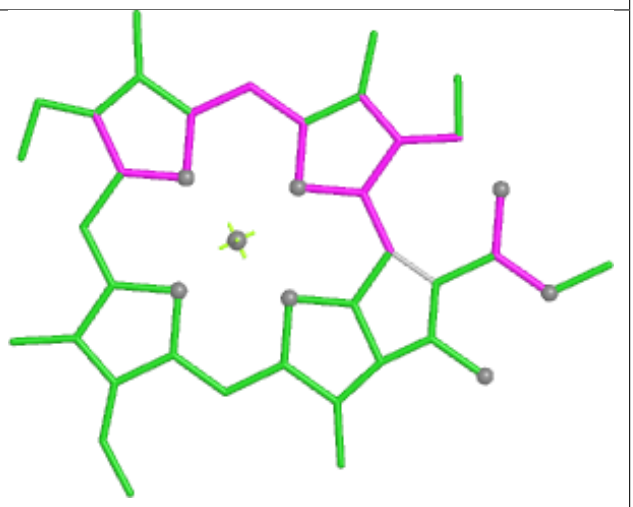

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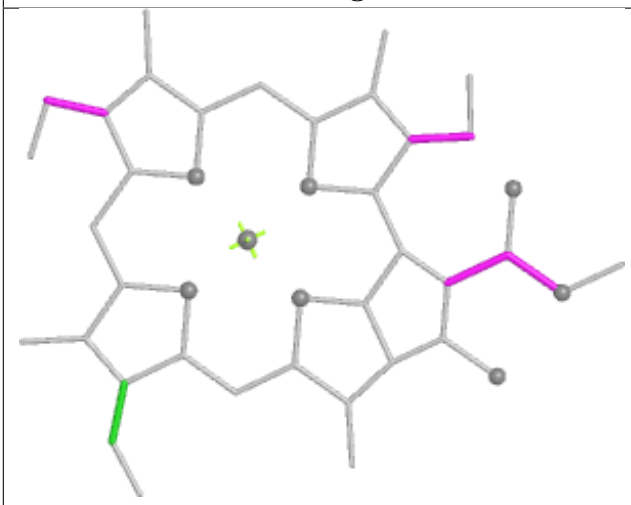
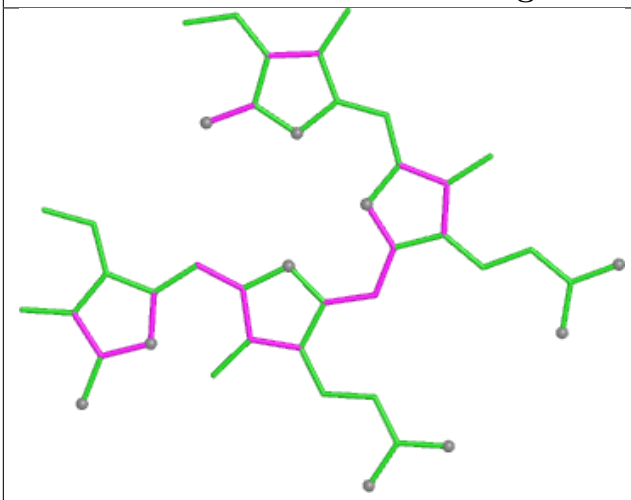


Torsions



Rings

Ligand PEB E5 201



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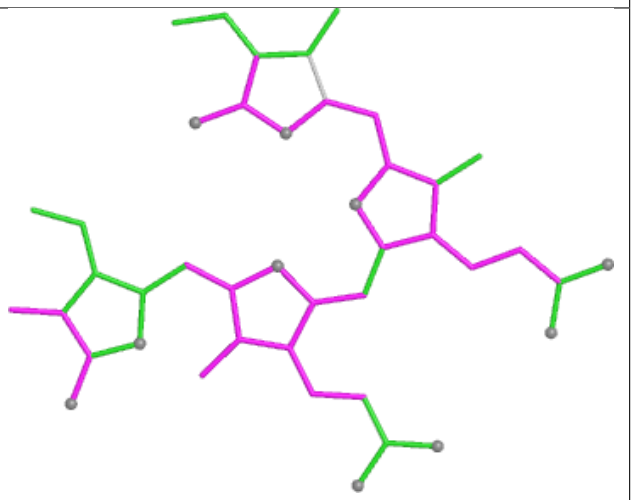

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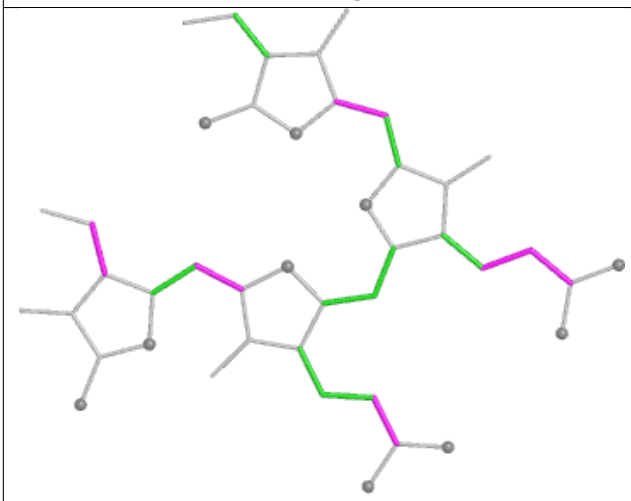

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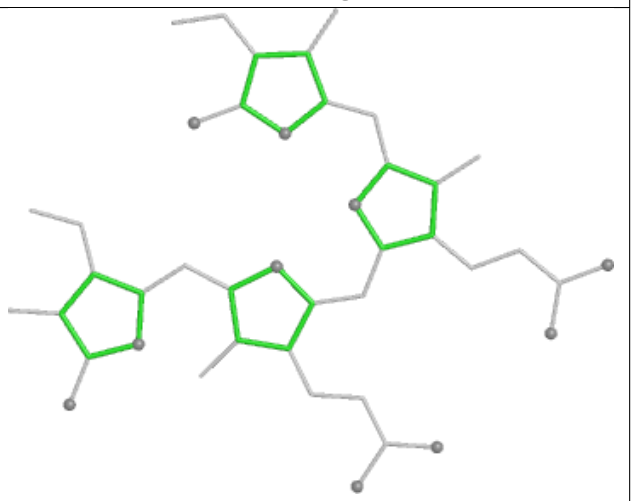
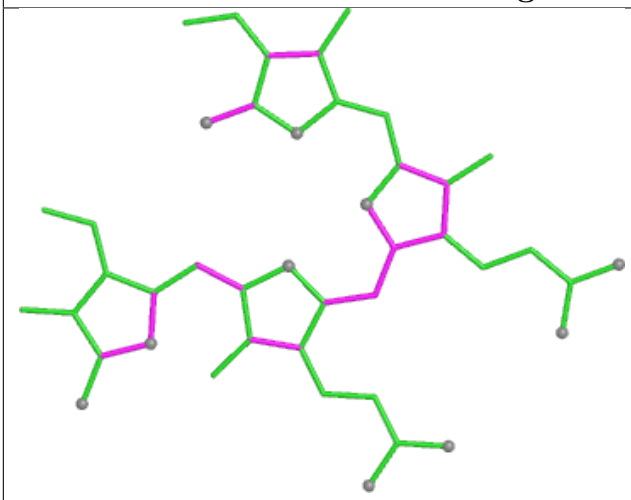


Rings

Ligand PEB AI 201



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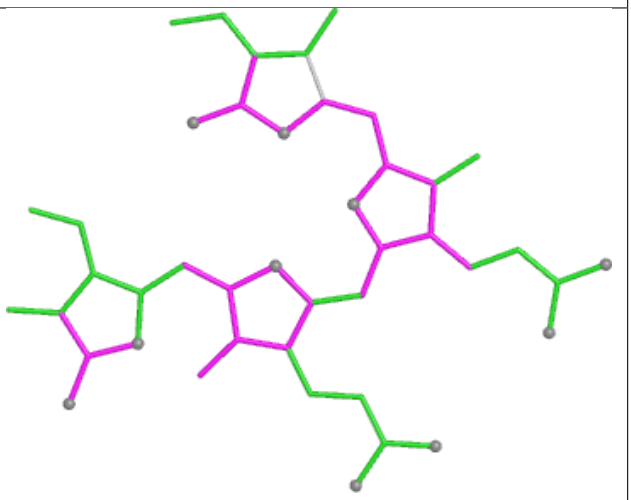

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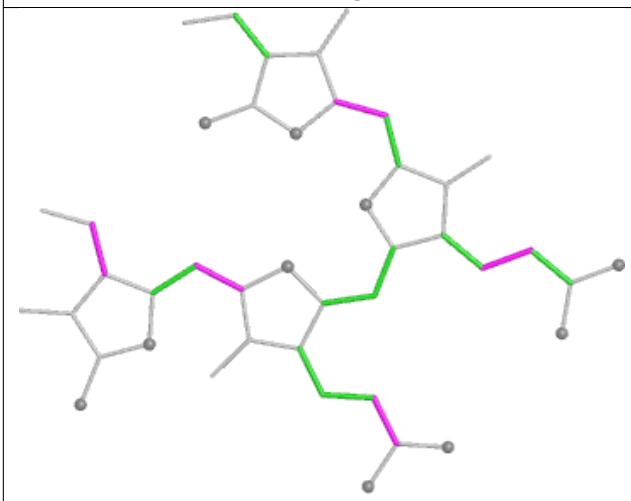

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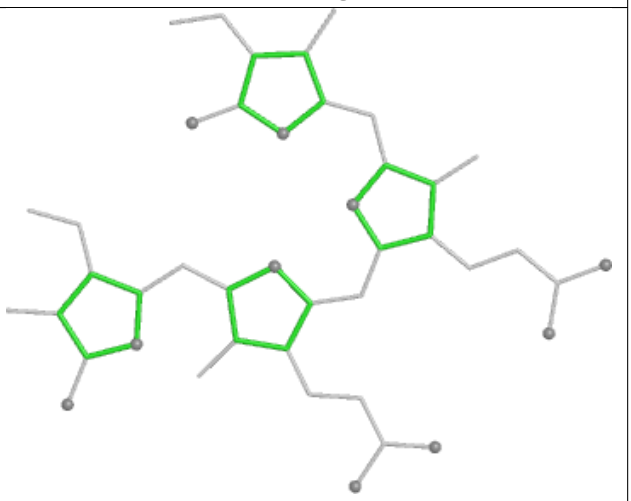
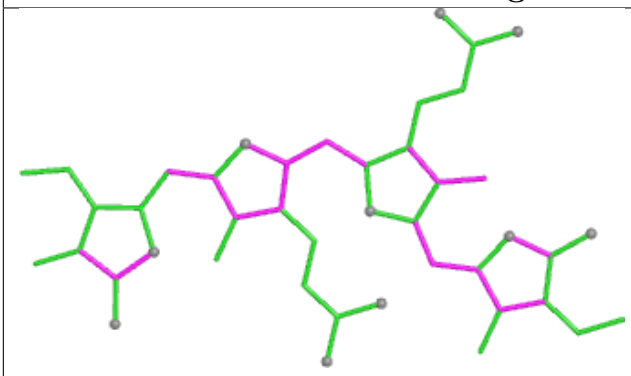


Rings

Ligand CYC x3 1001



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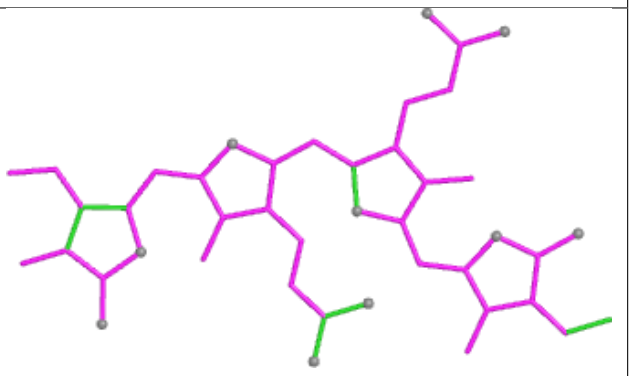

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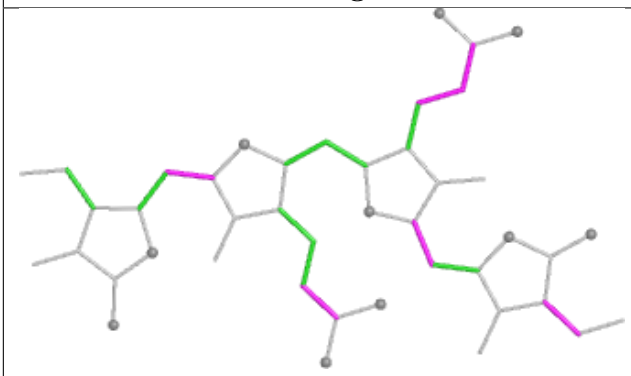

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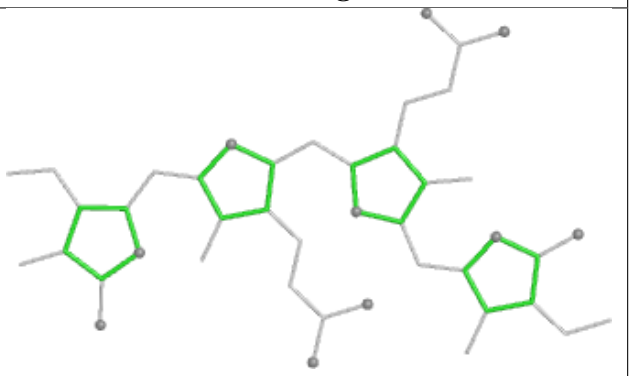
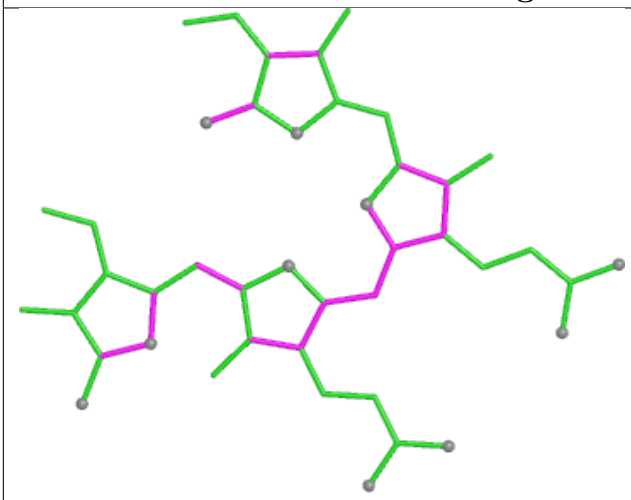


Rings

Ligand PEB zC 201



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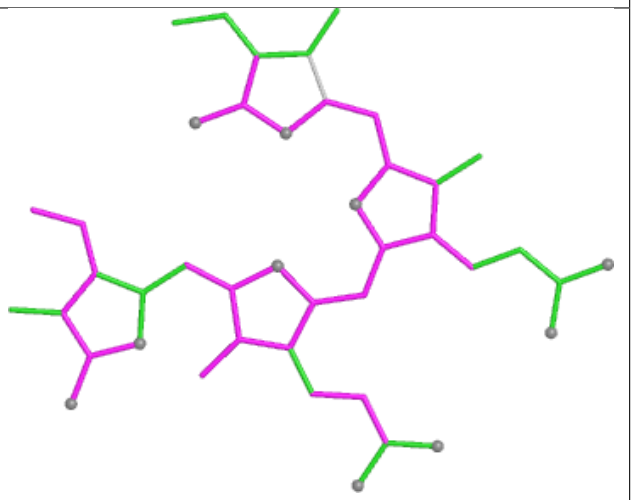

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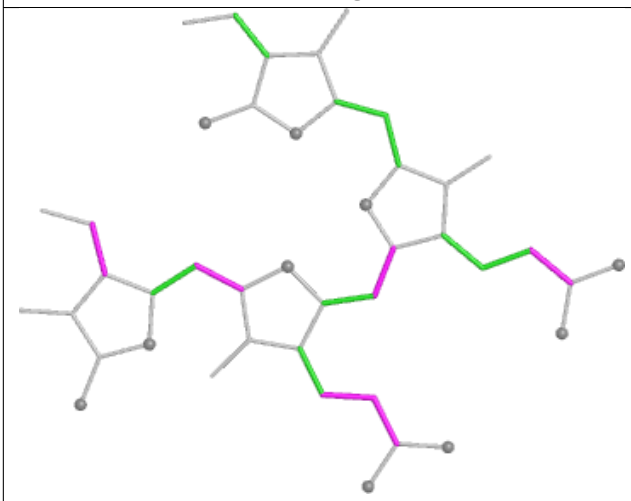

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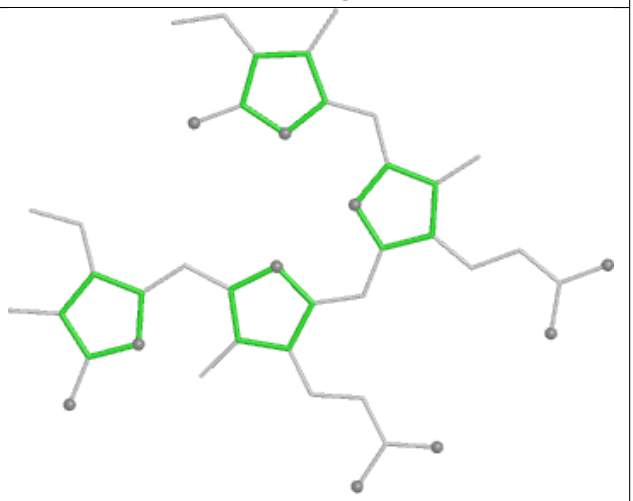
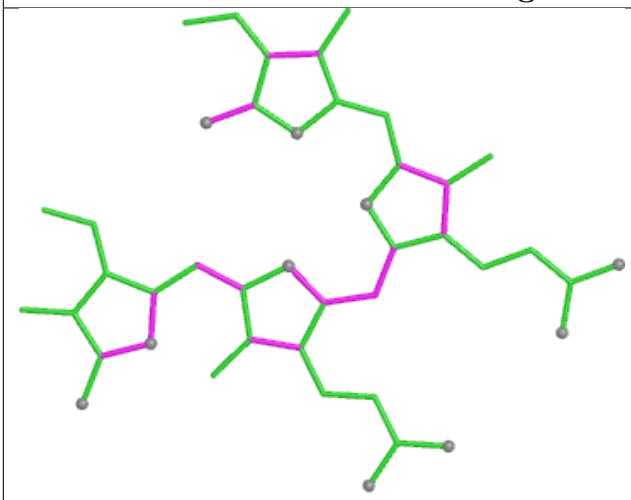


Rings

Ligand PEB RI 203



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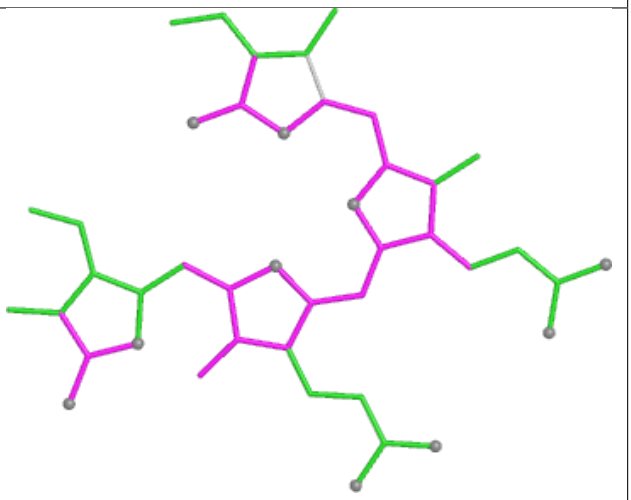

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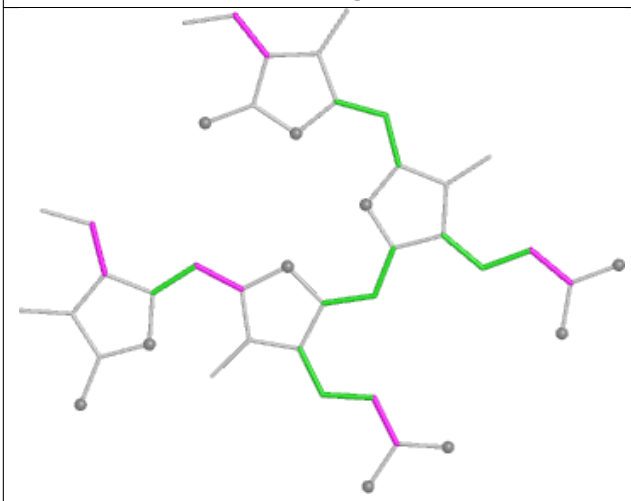

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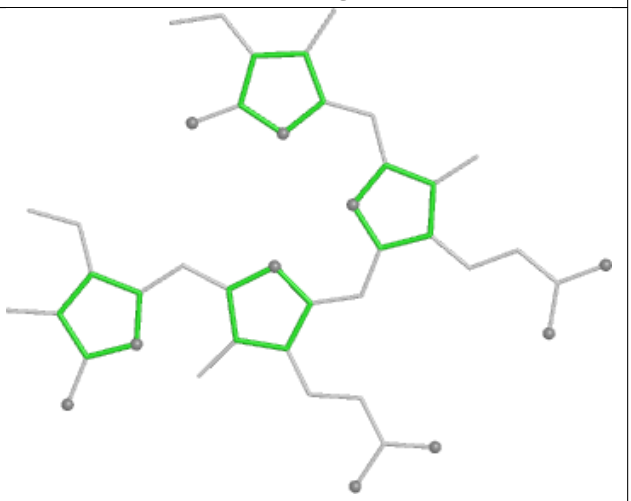

Rings

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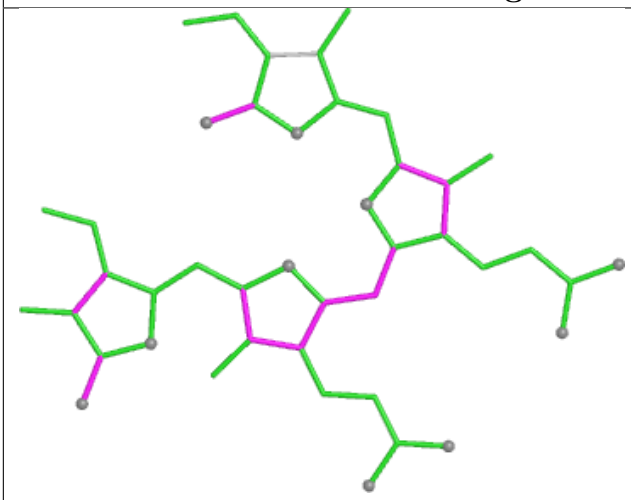

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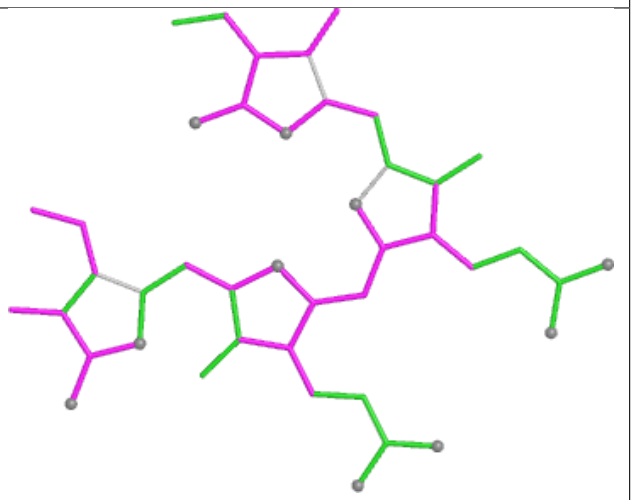

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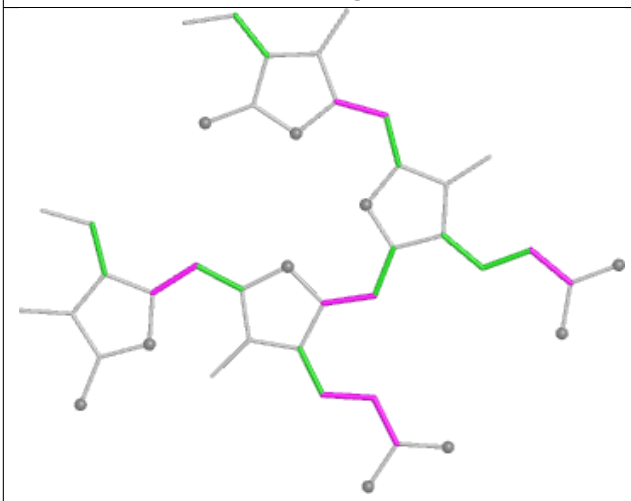

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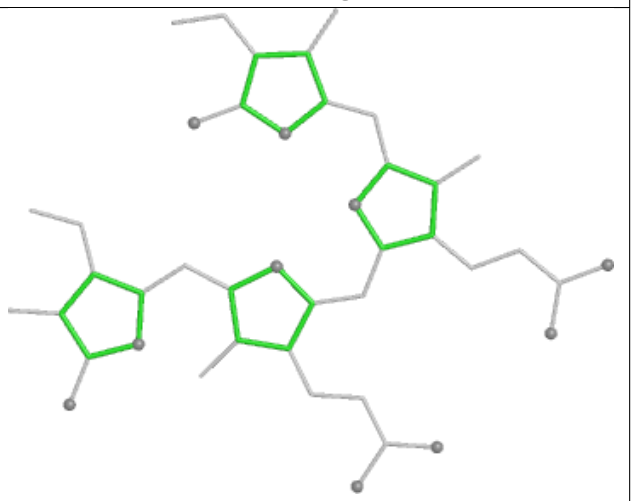
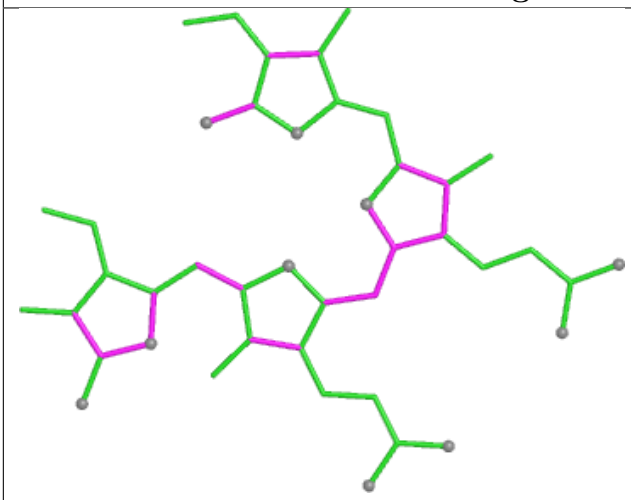


Rings

Ligand PEB YP 503



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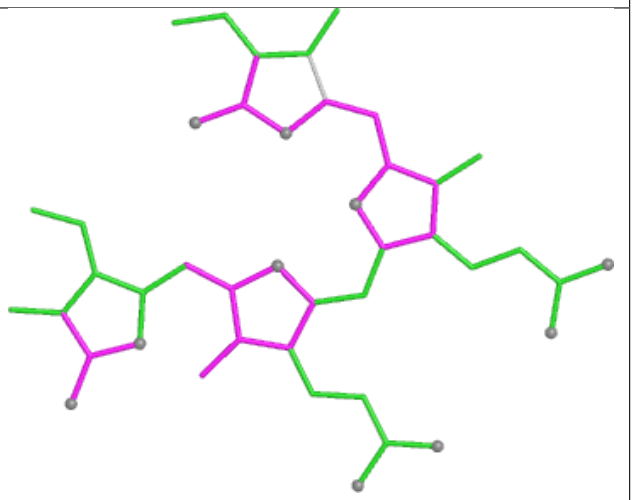

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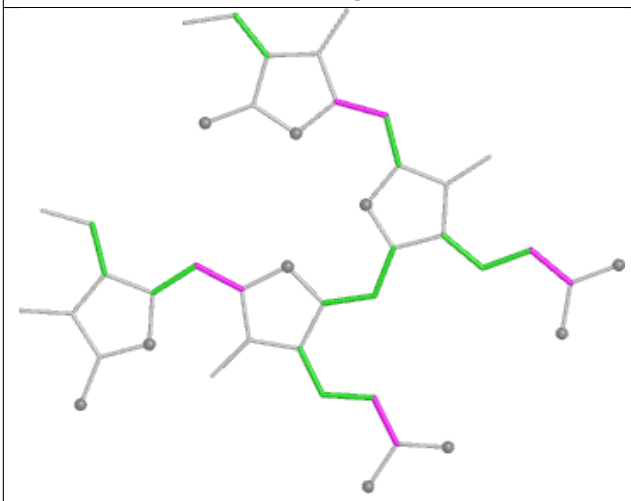

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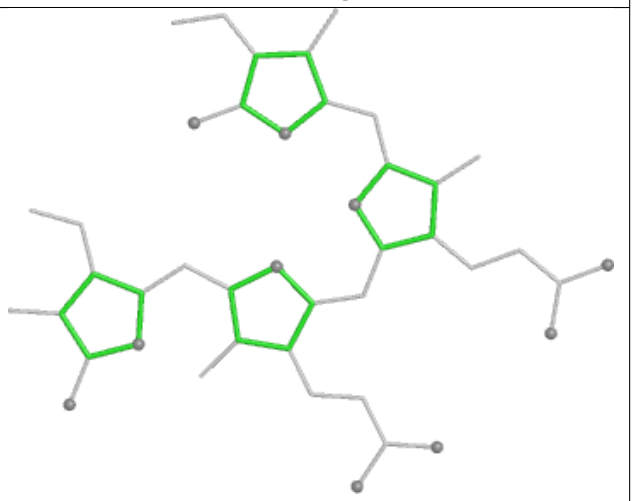
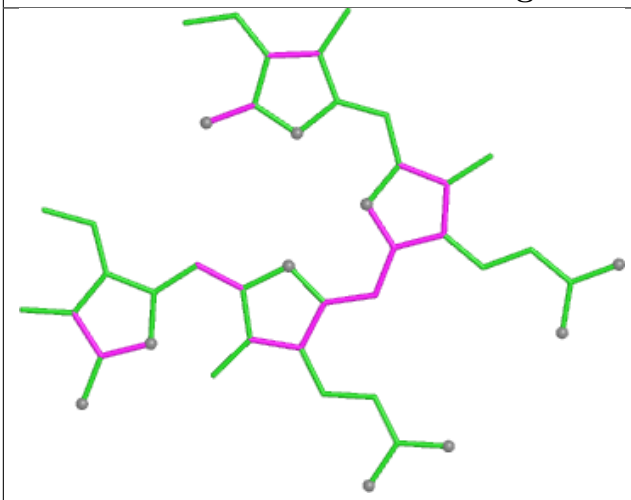


Rings

Ligand PEB T9 202



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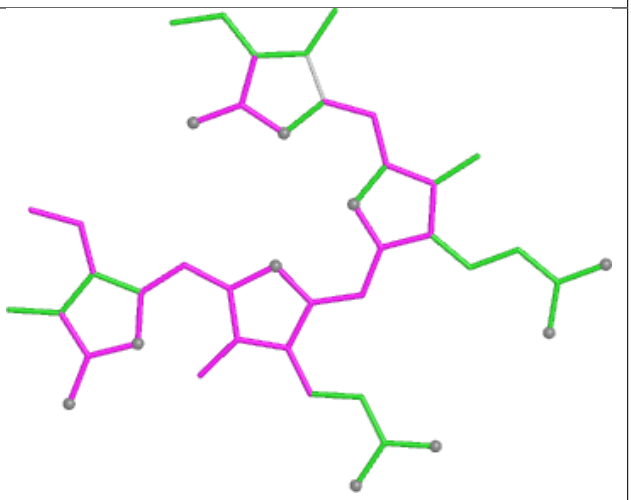

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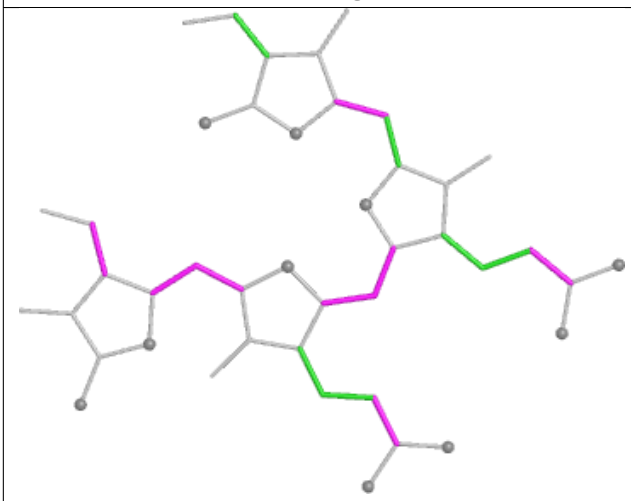

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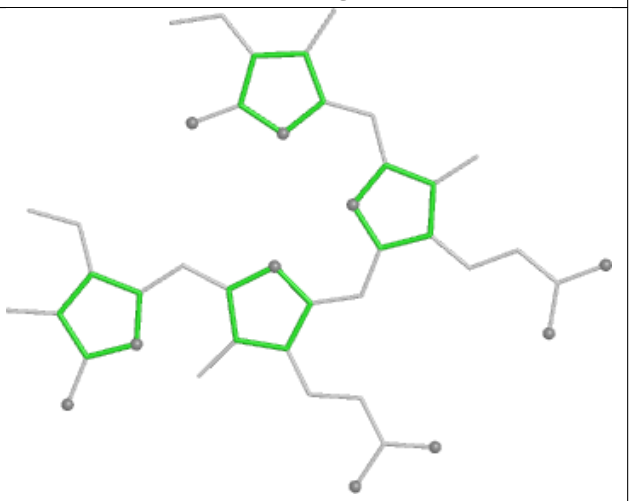

Rings

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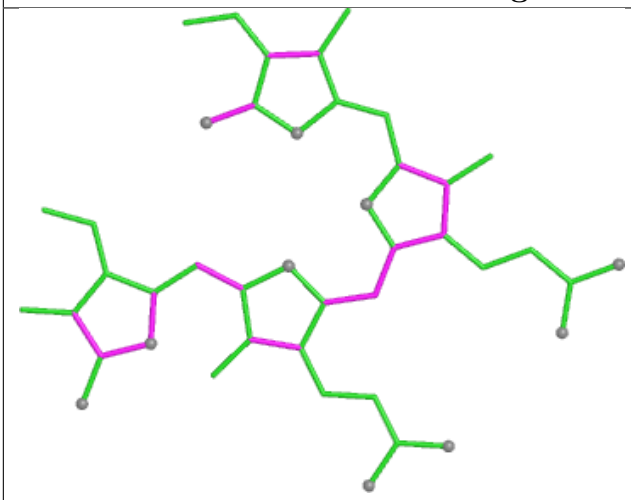

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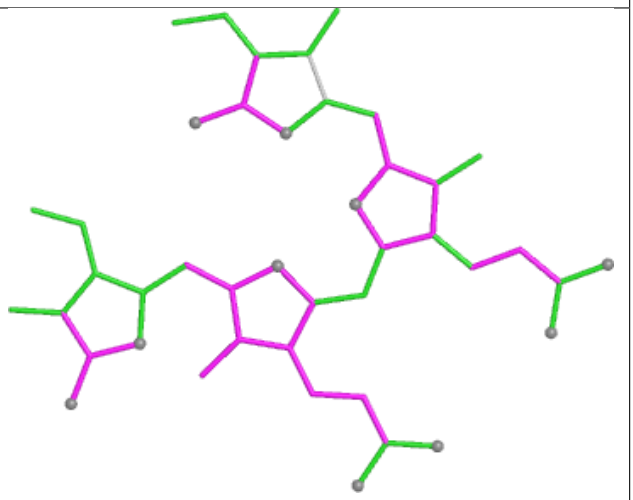

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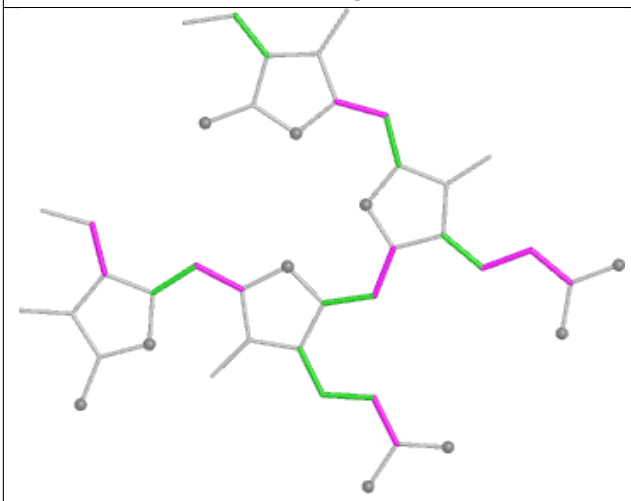

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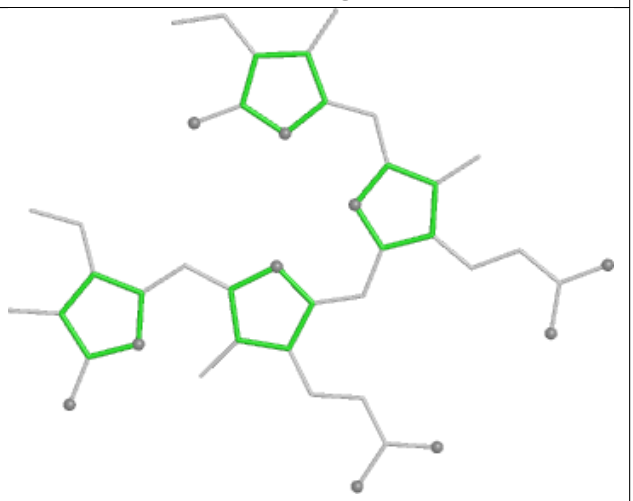
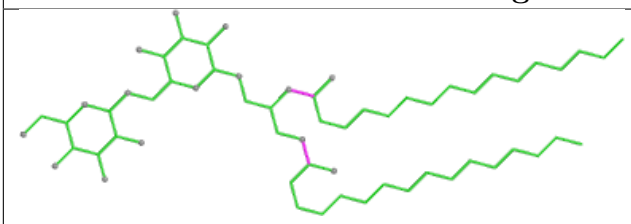


Rings

Ligand DGD hL 101



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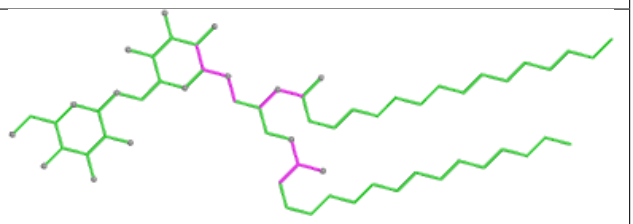
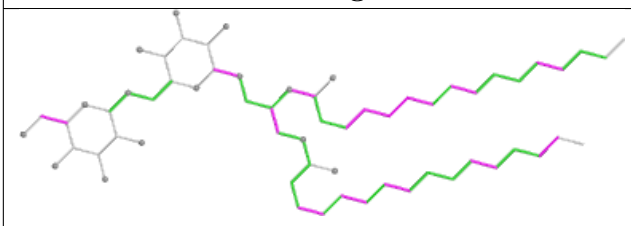


Bond angles



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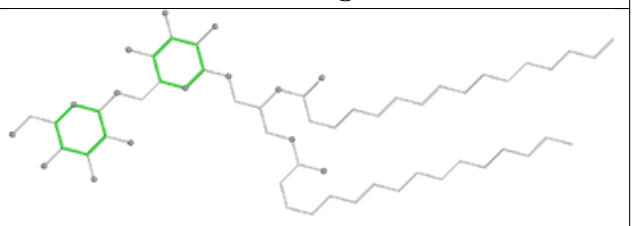
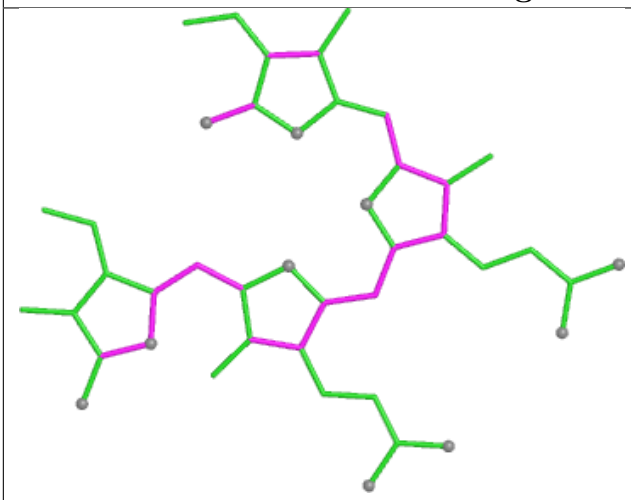


Rings

Ligand PEB U1 202



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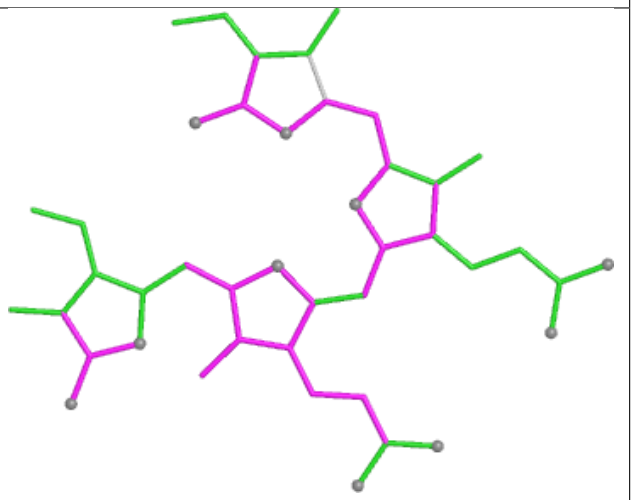

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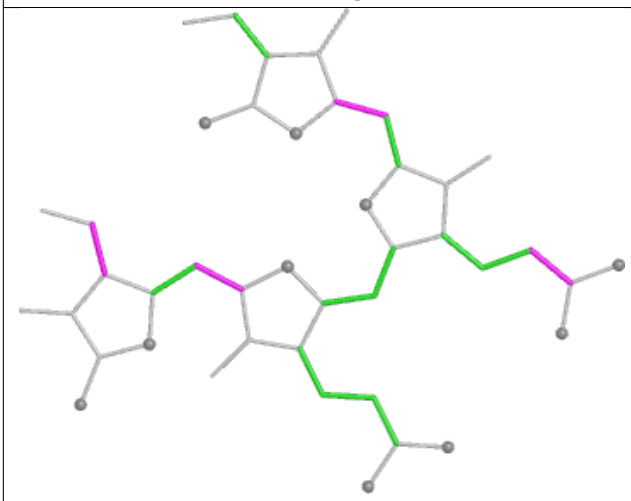

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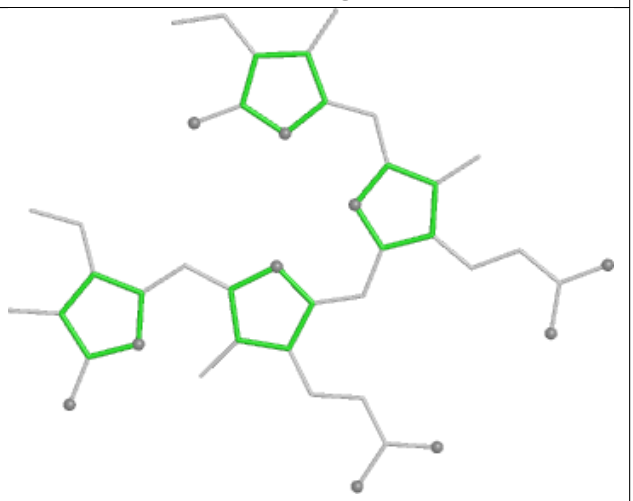
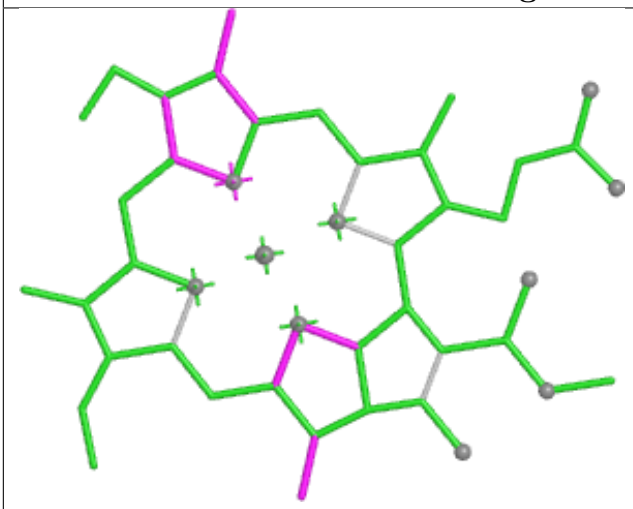


Rings

Ligand CLA 52 611



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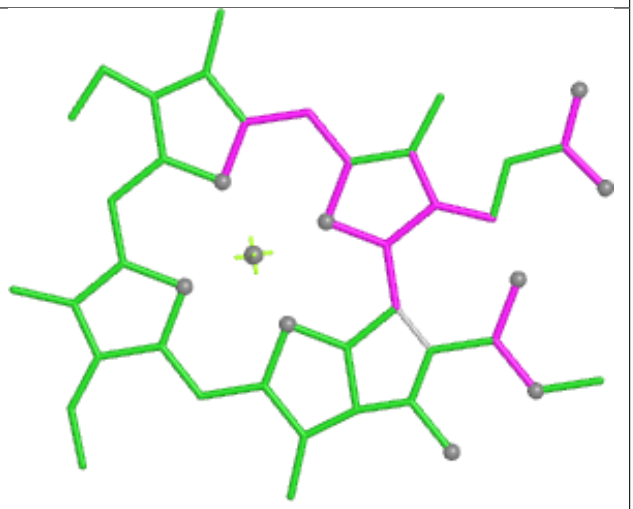

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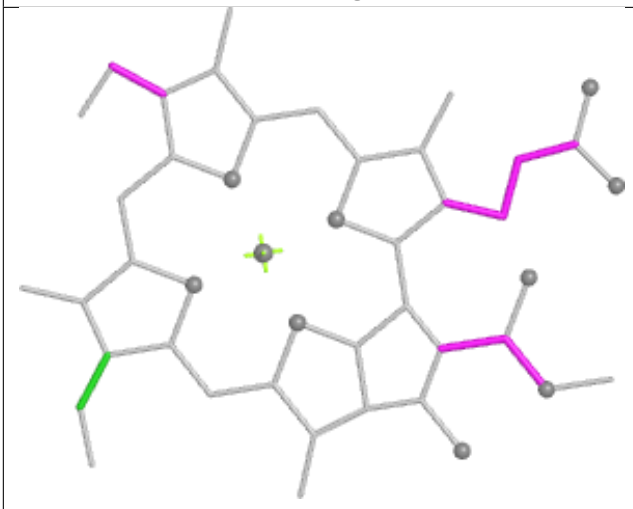
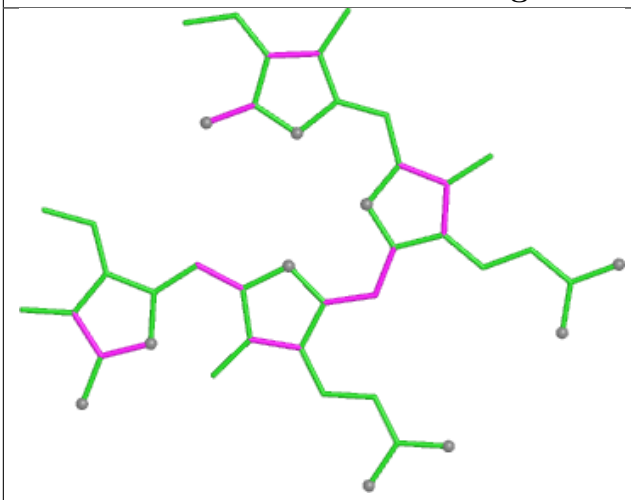


Torsions



Rings

Ligand PEB XA 202



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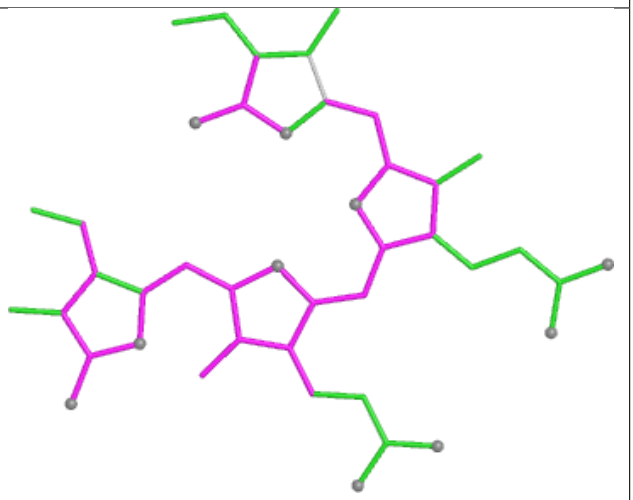

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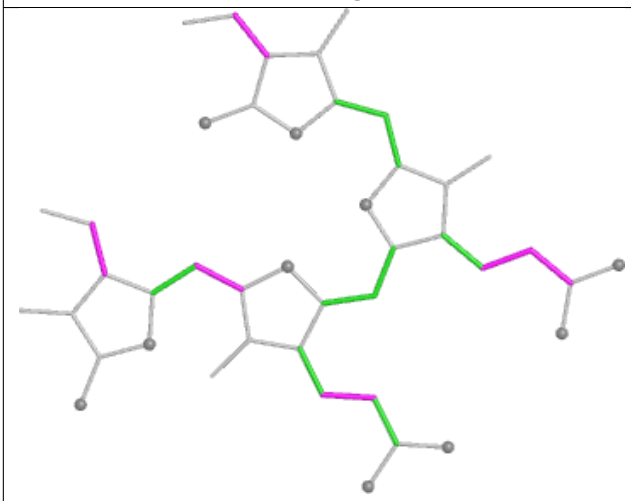

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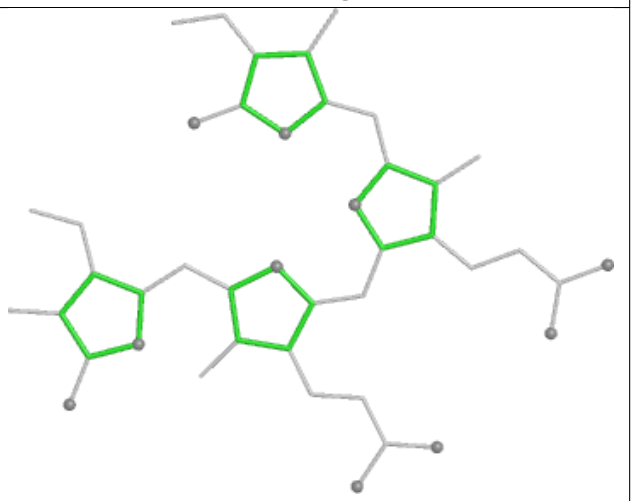
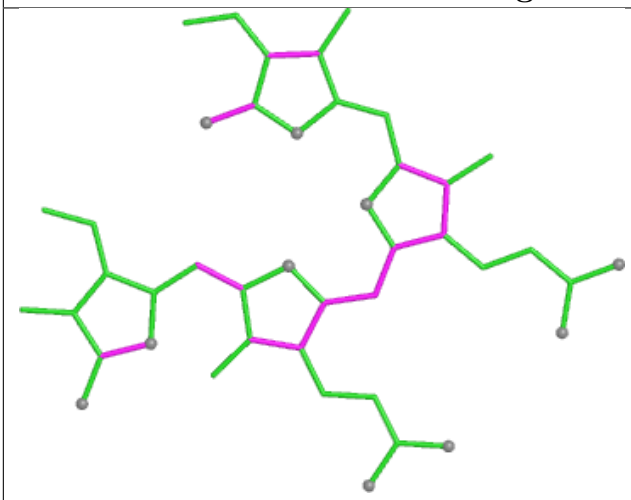


Rings

Ligand PEB eO 203



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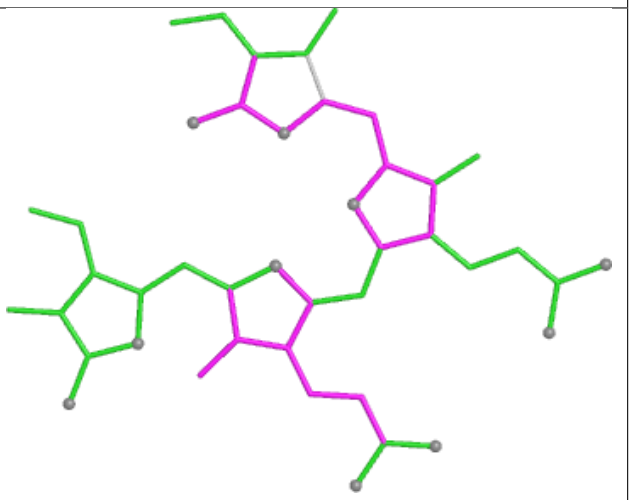

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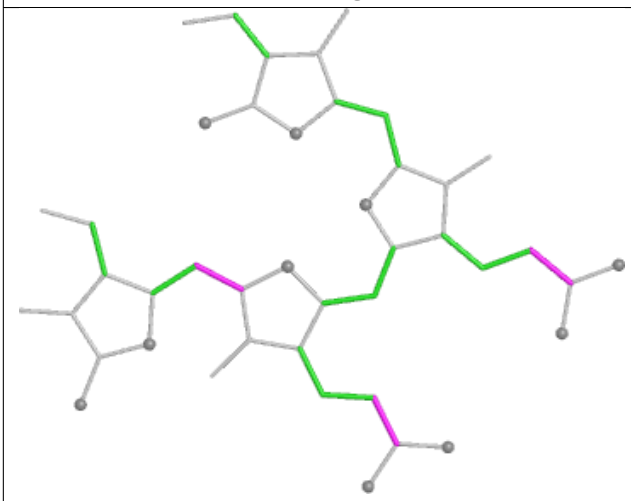

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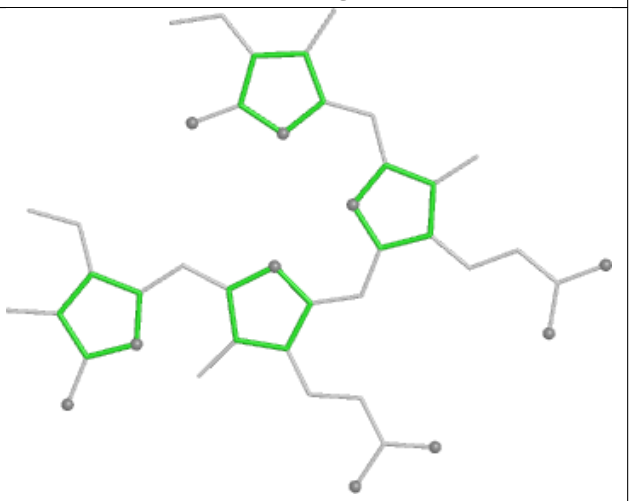
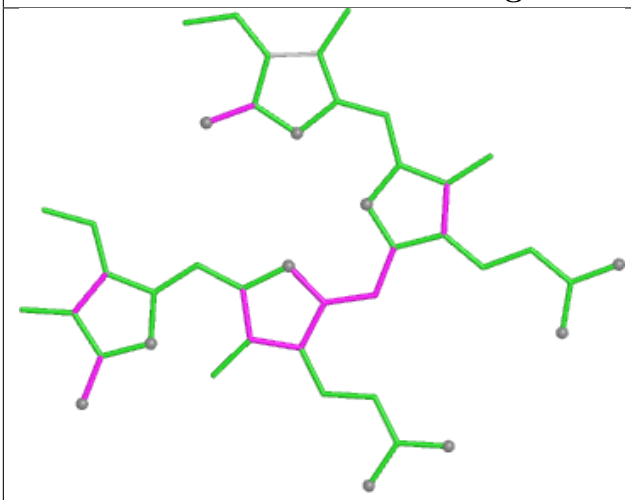


Rings

Ligand PUB AM 304



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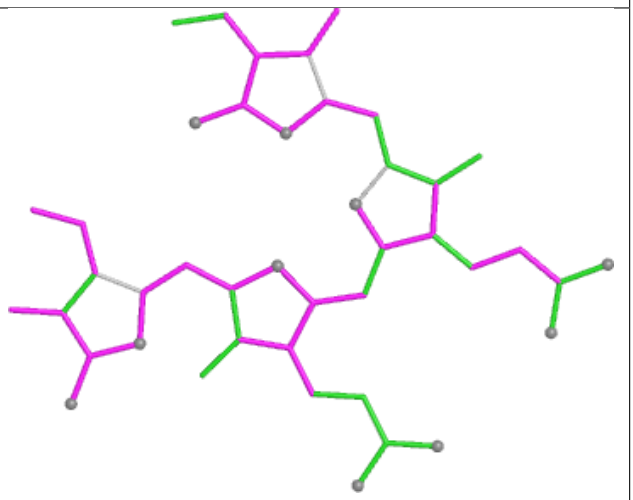

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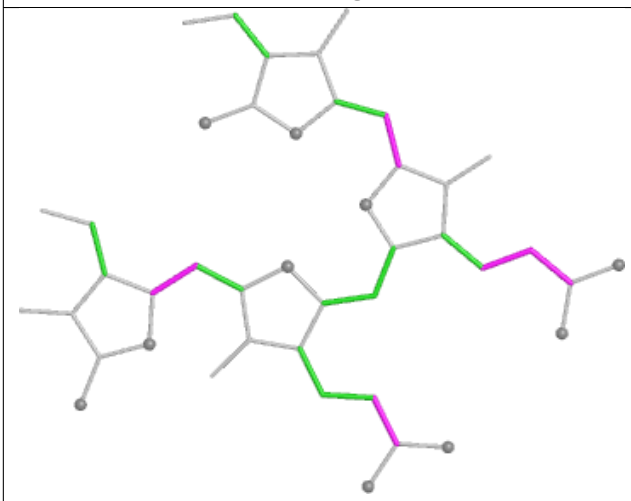

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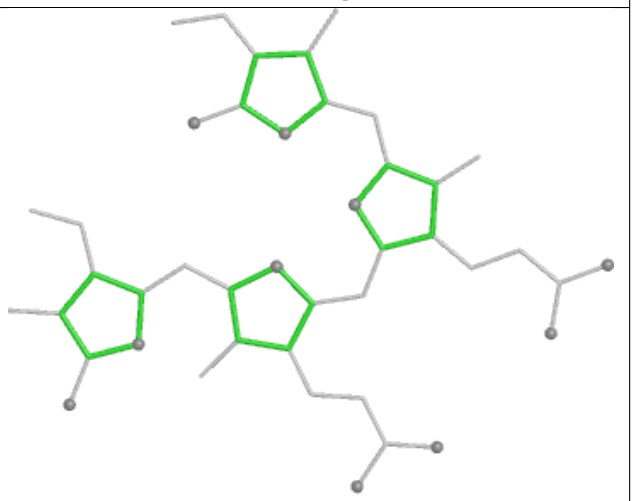
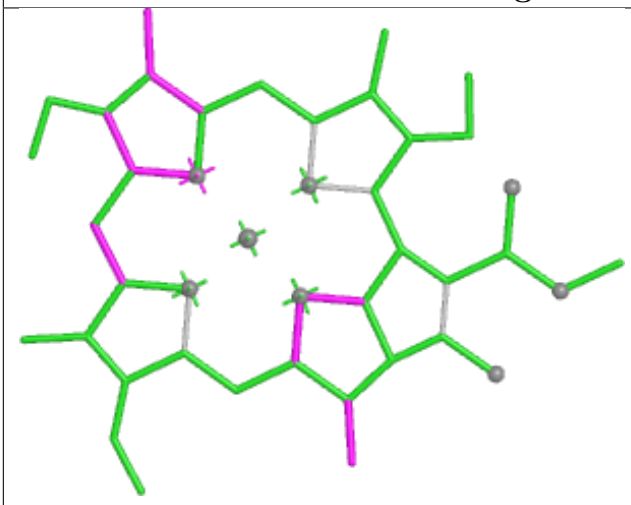


Rings

Ligand CLA 7N 609



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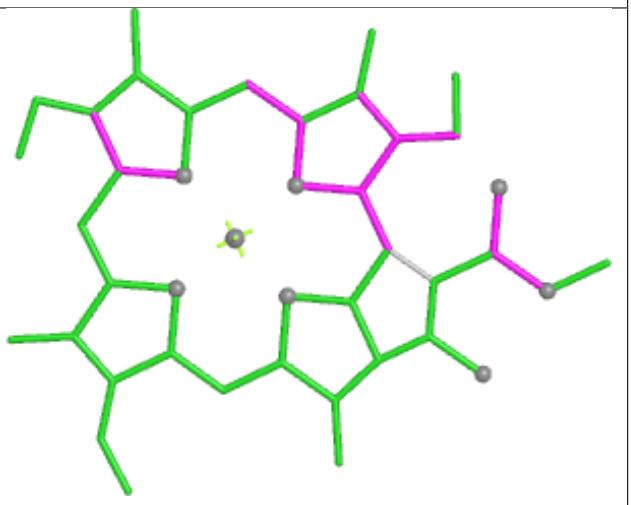

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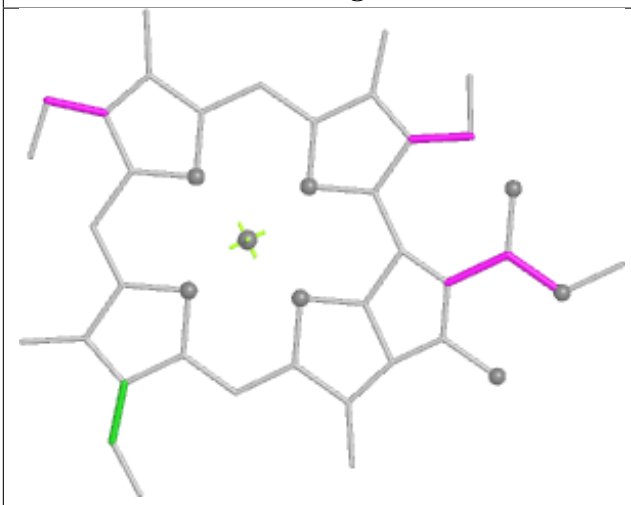
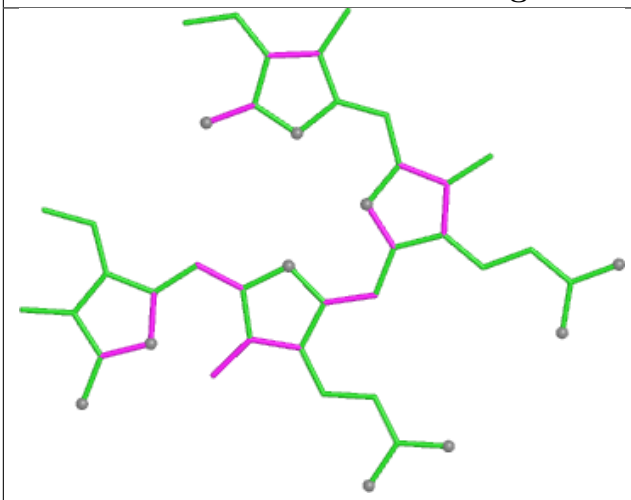


Torsions



Rings

Ligand PEB UK 201



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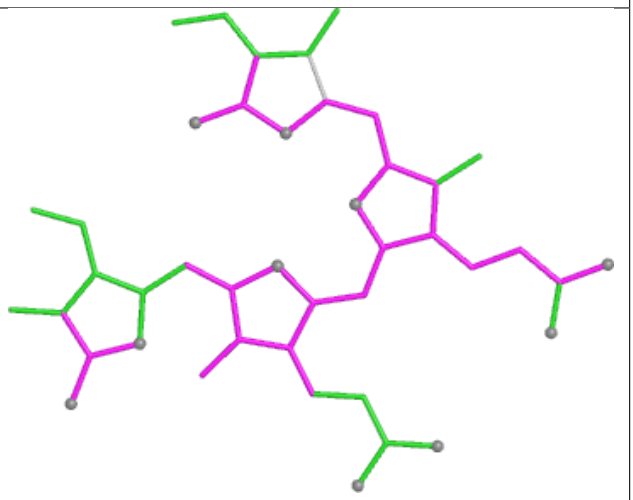

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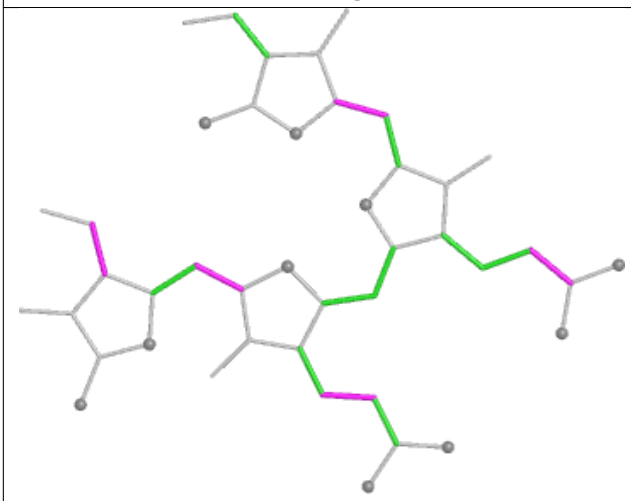

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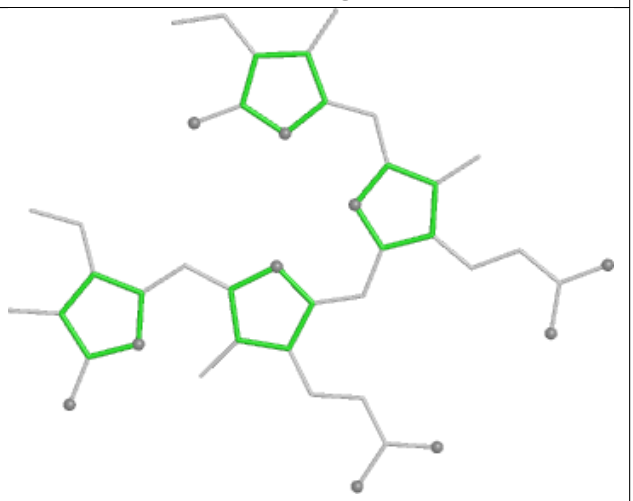
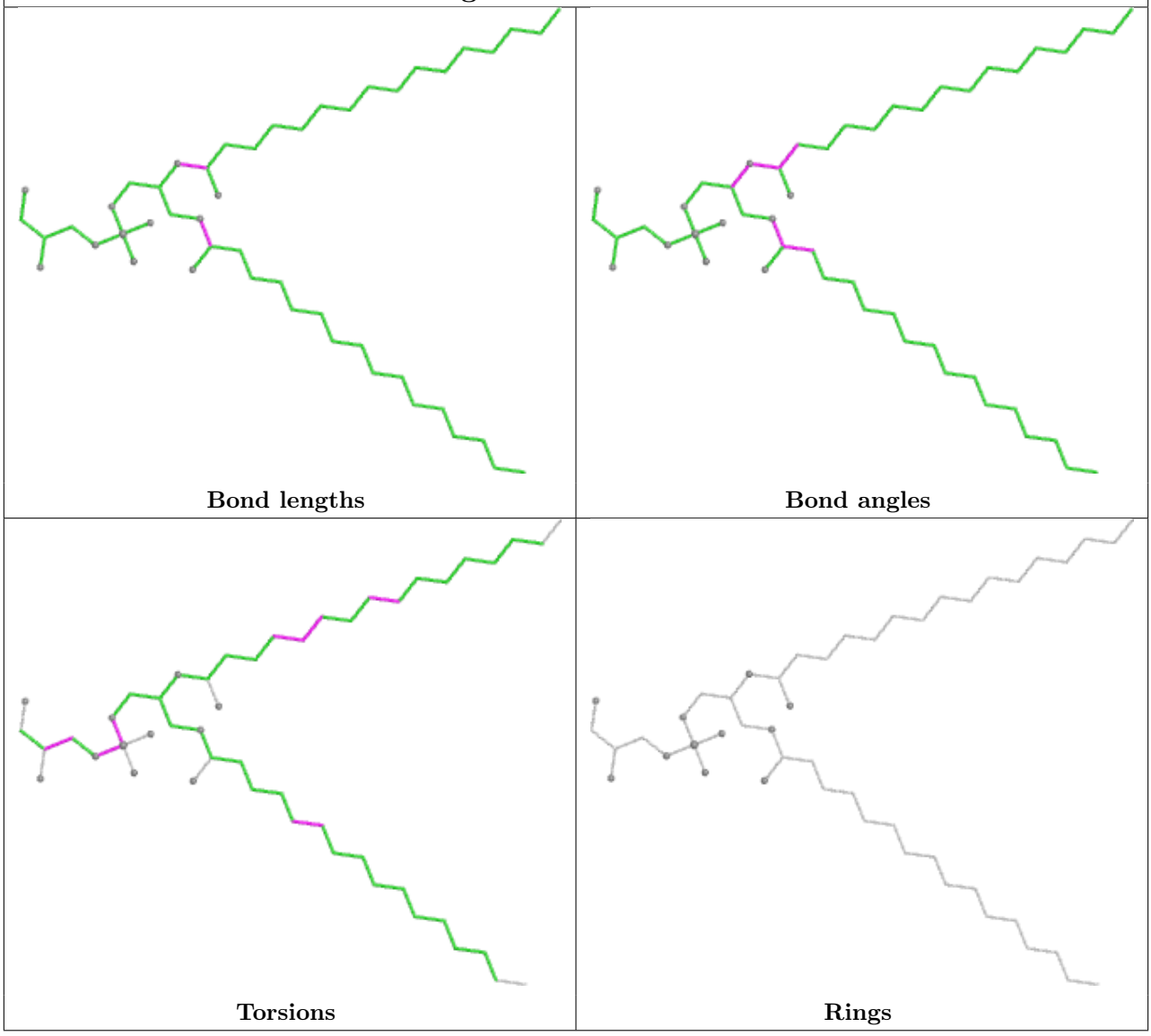


Rings

Ligand LHG D6 406



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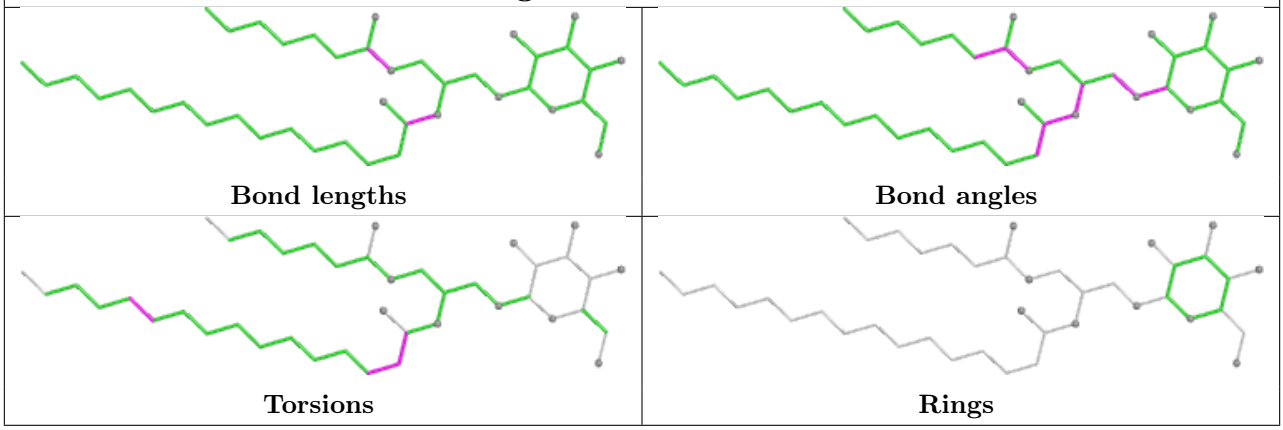
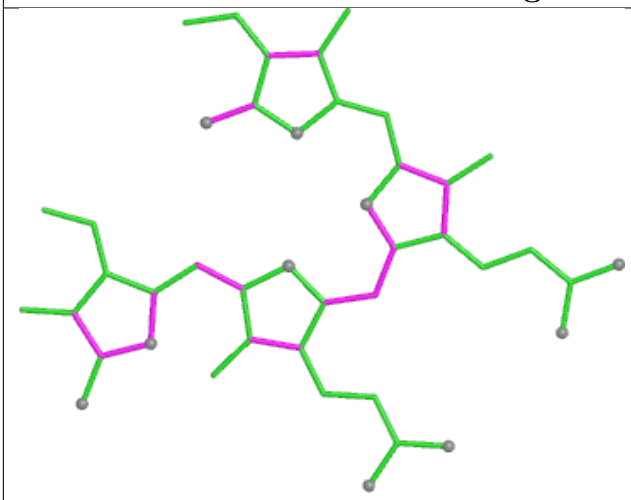


Ligand PEB i4 201



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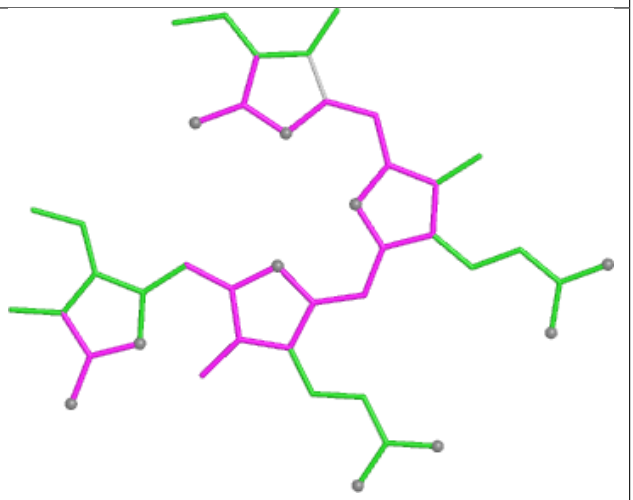

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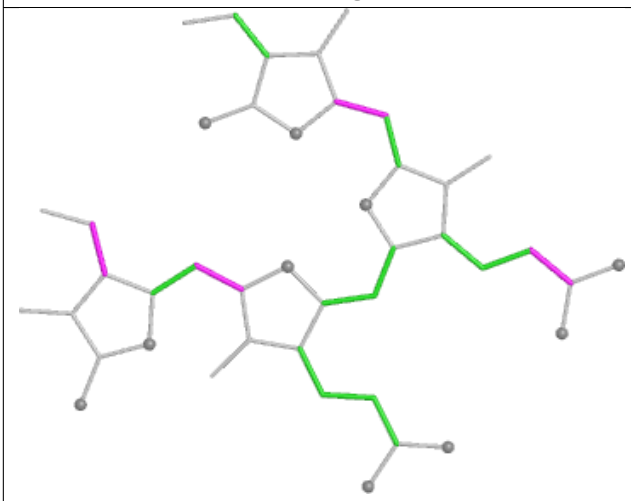

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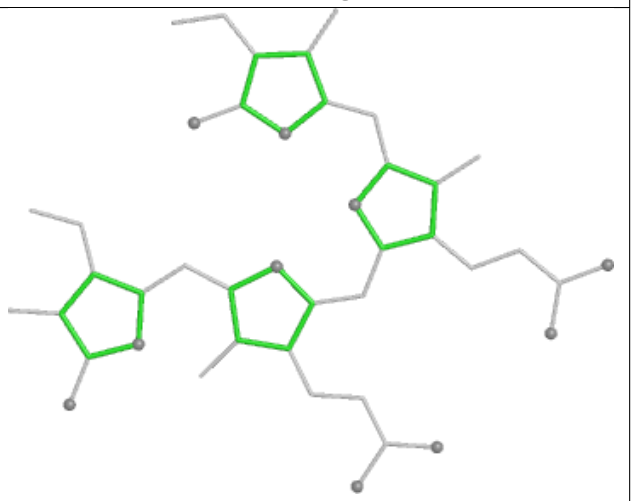
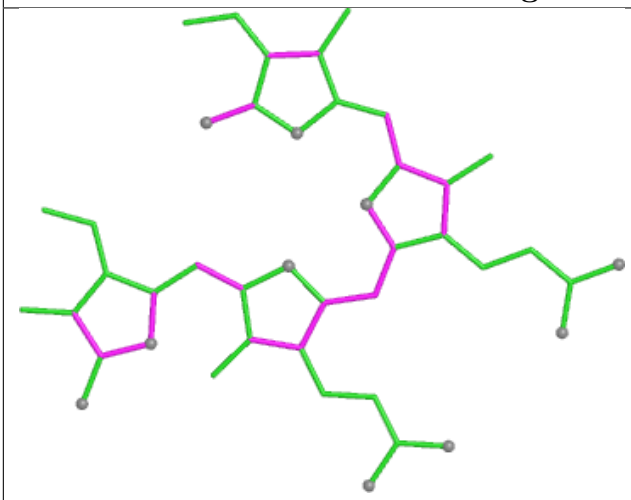


Rings

Ligand PEB fF 202



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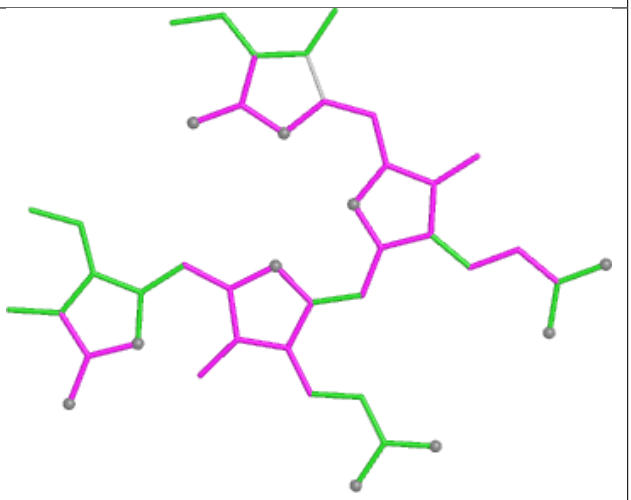

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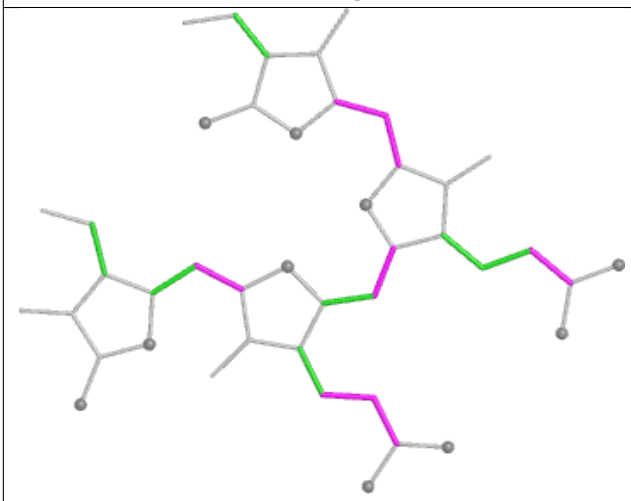

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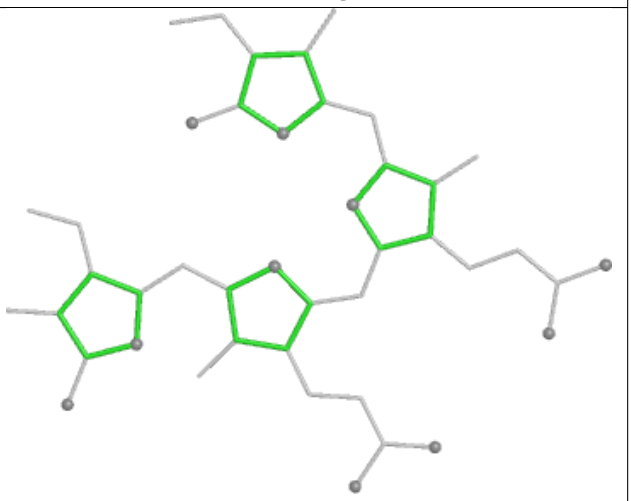
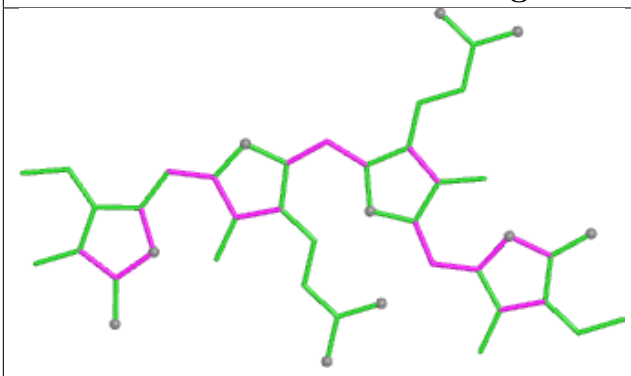


Rings

Ligand CYC I1 1001



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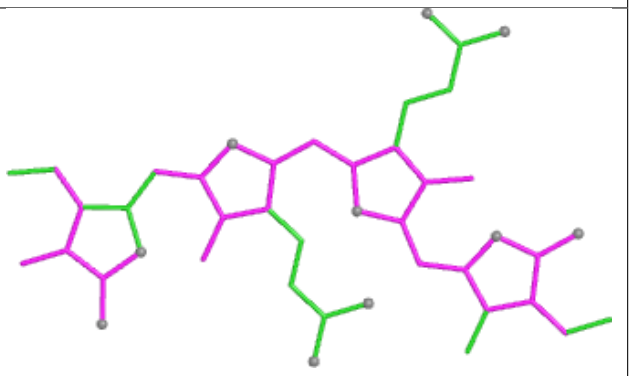

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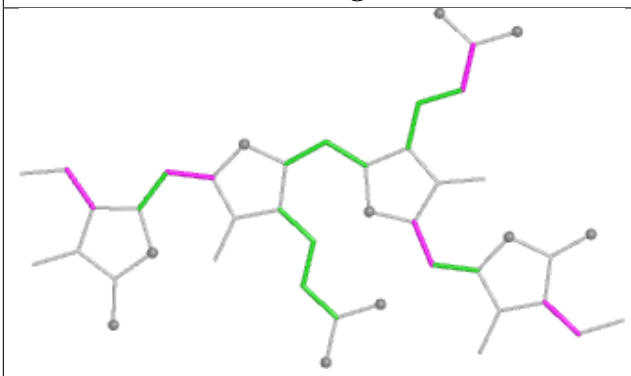

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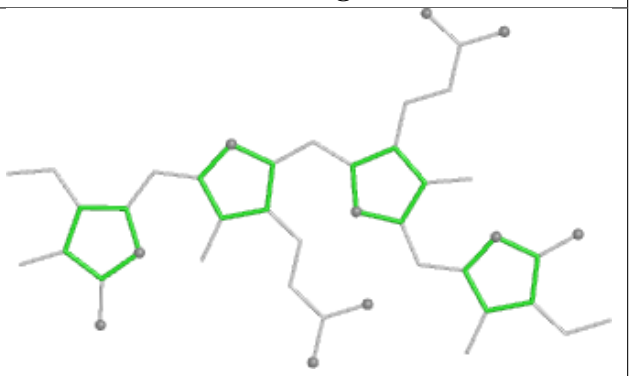
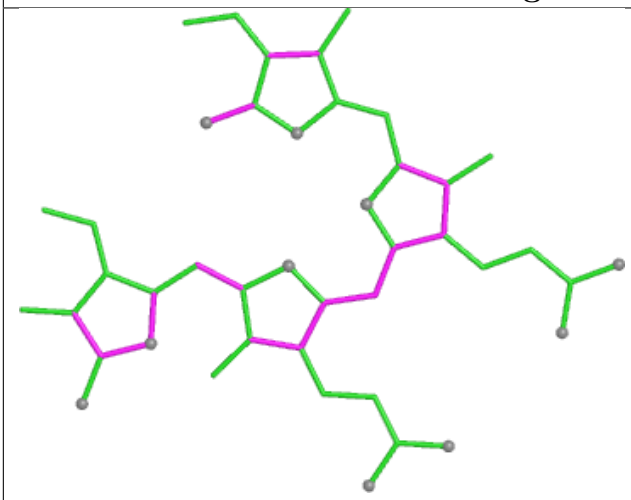


Rings

Ligand PEB j4 203



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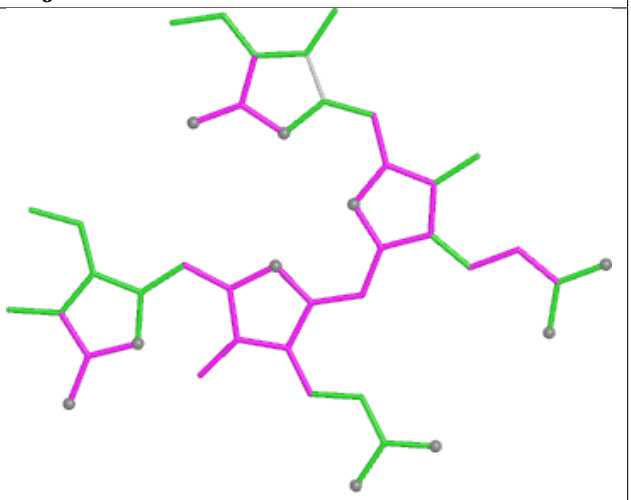

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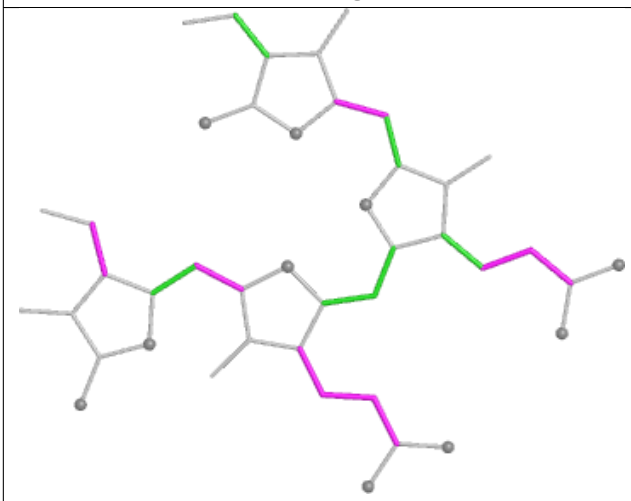

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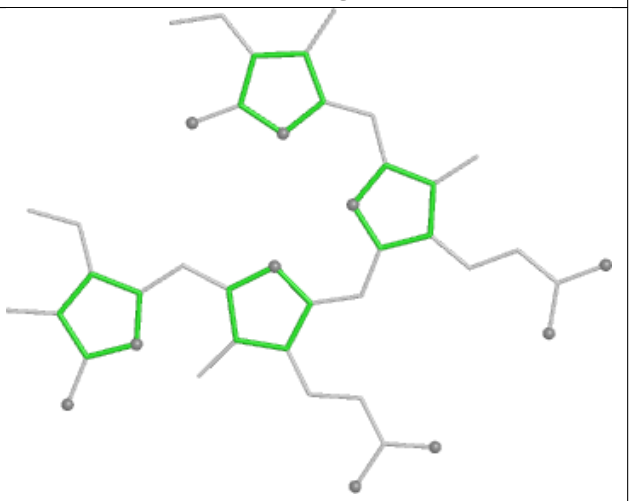

Rings

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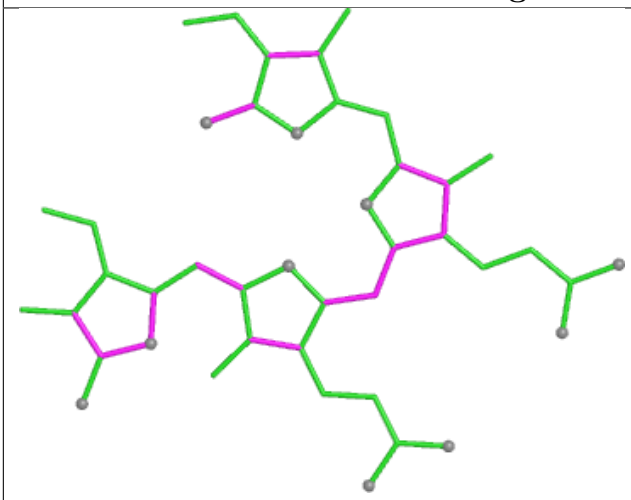

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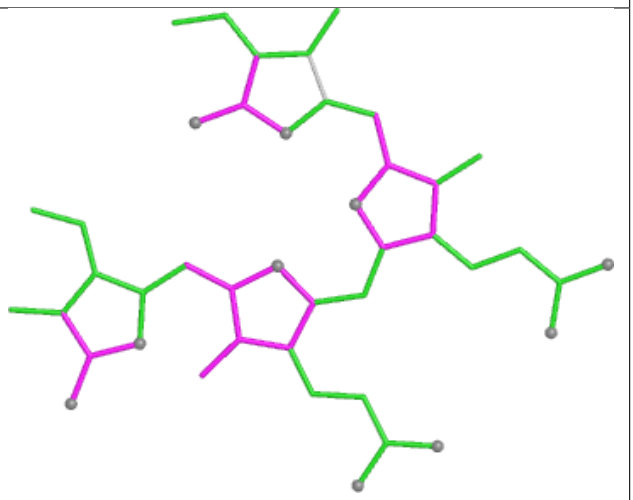
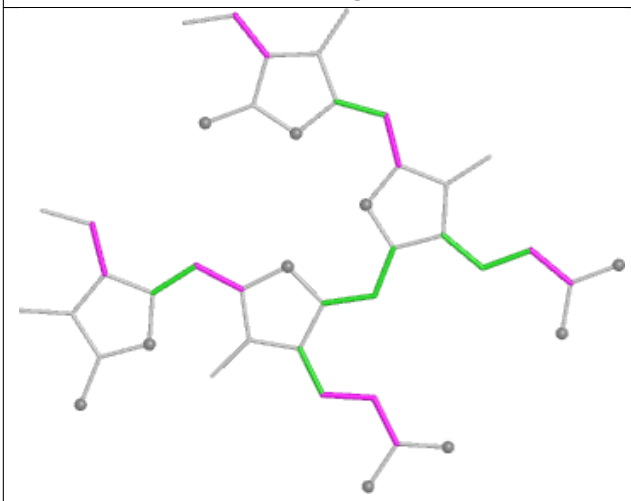


Bond angles



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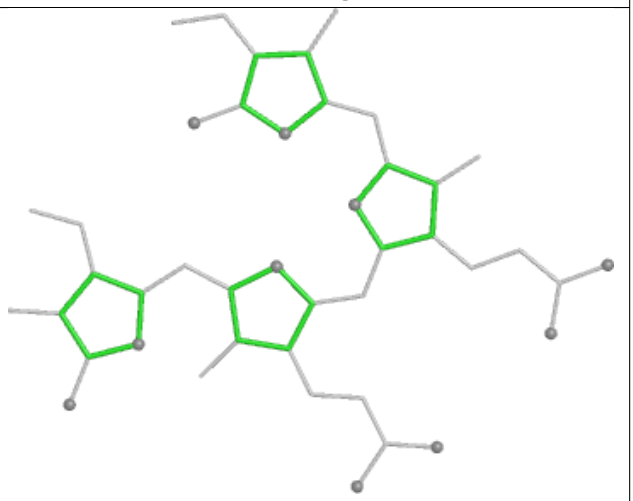
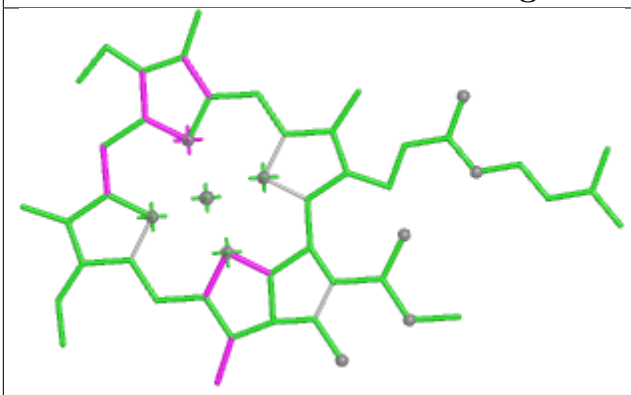


Rings

Ligand CLA 52 607



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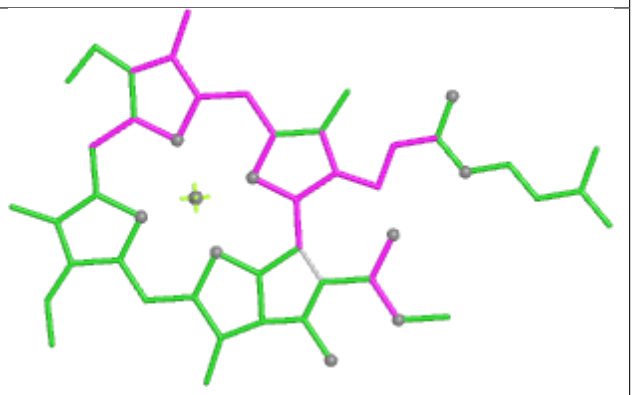
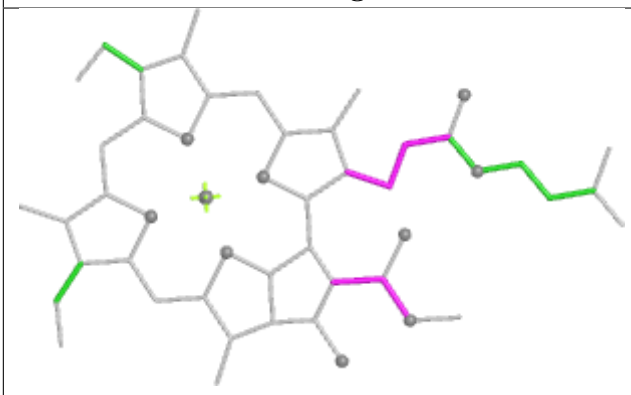


Bond angles



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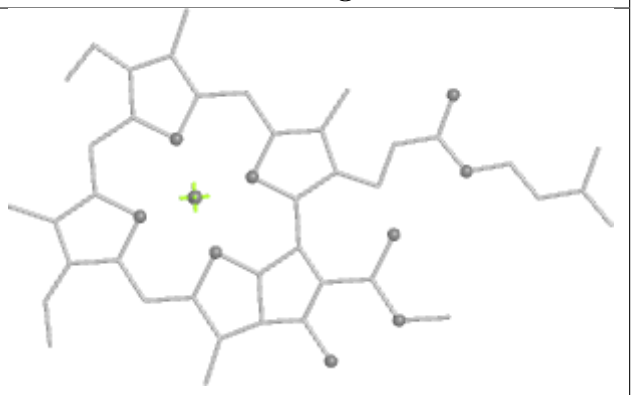
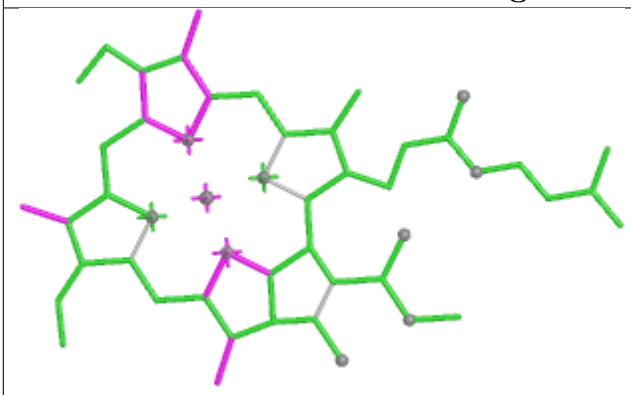


Rings

Ligand CLA AN 832



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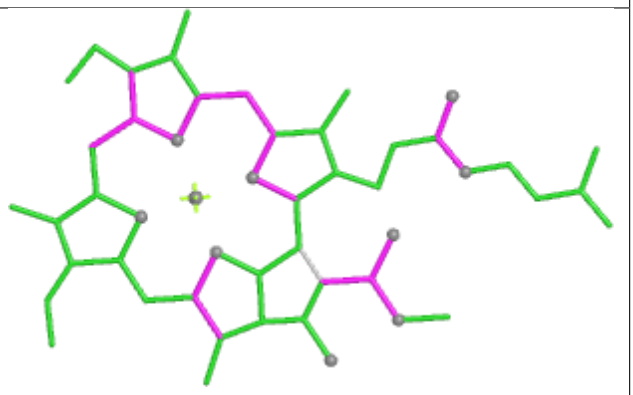
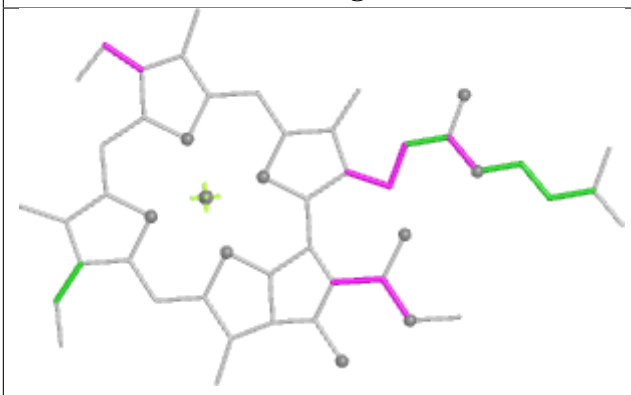


Bond angles



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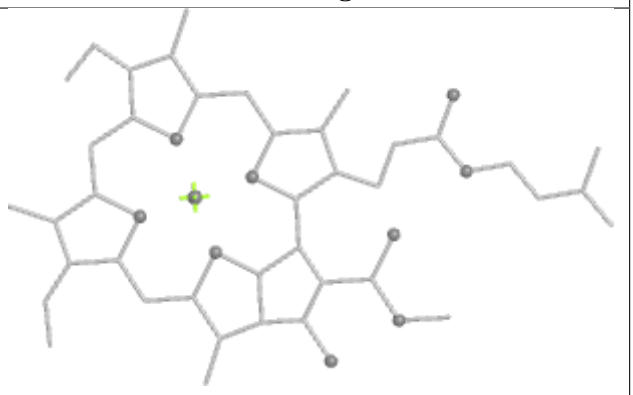
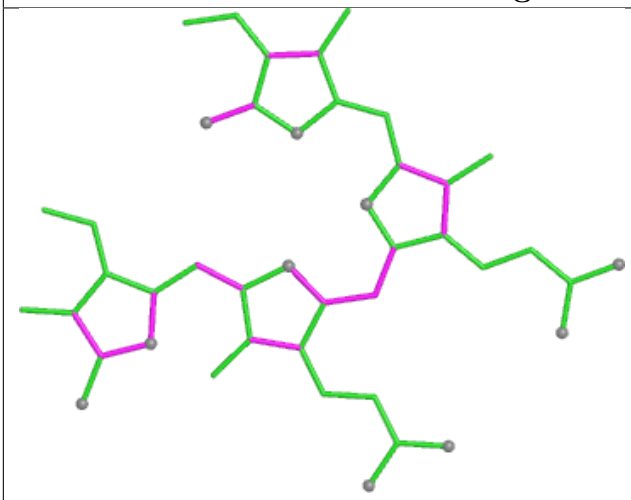


Rings

Ligand PEB SK 201



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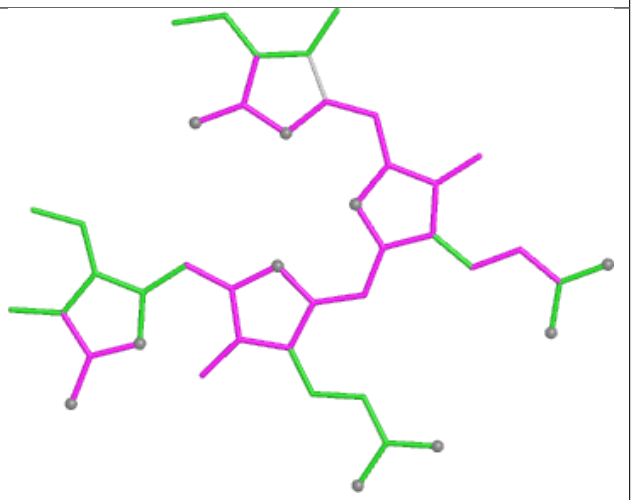

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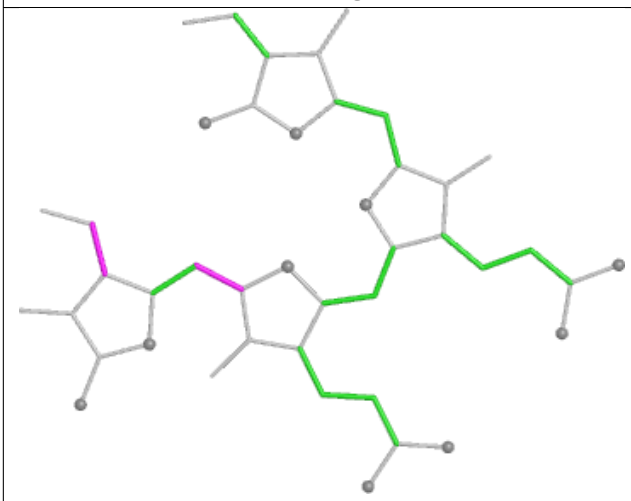
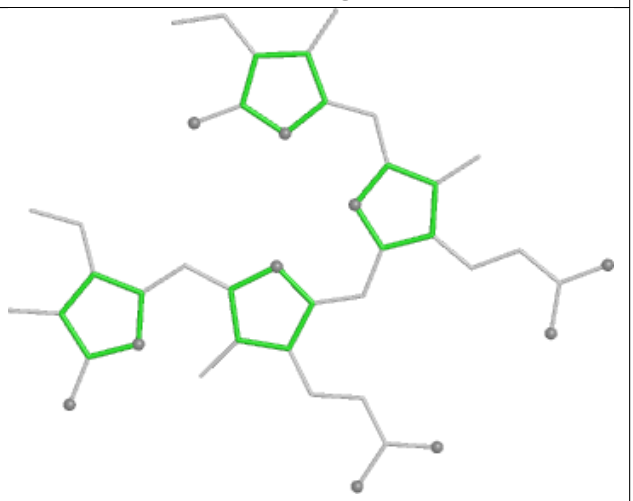
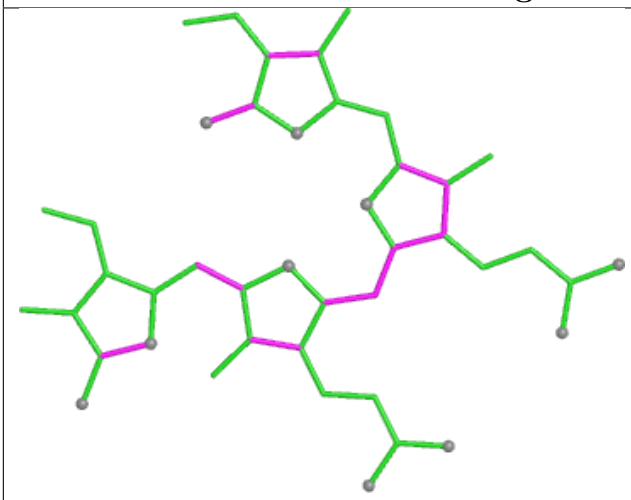


Torsions



Rings

Ligand PEB gO 202



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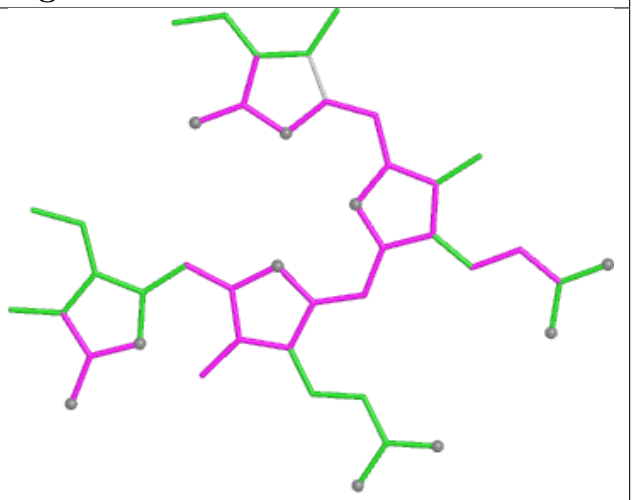

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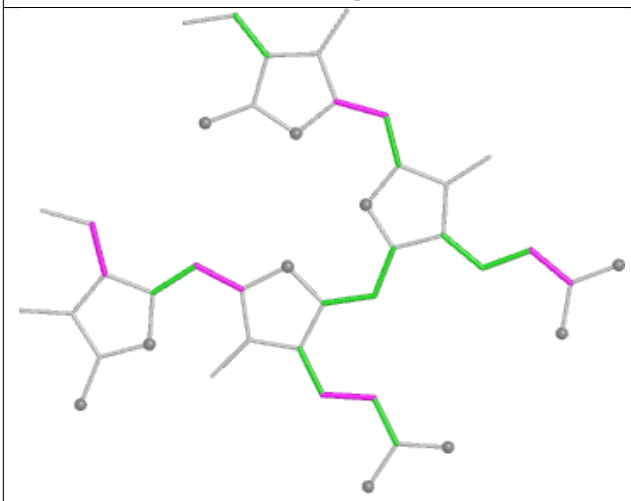

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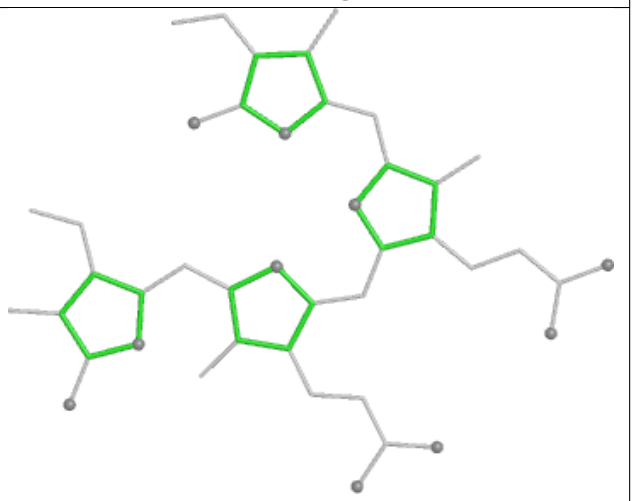
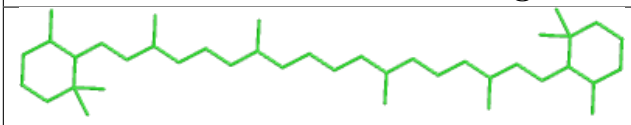


Rings

Ligand BCR B2 839



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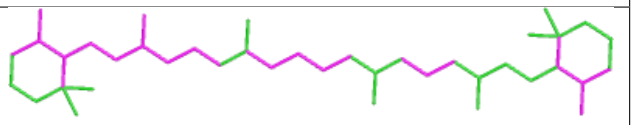

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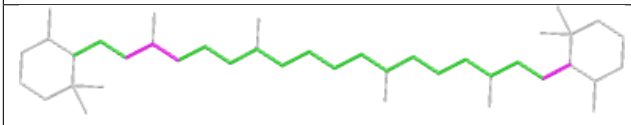

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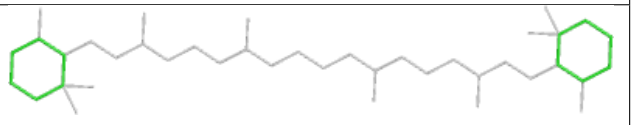
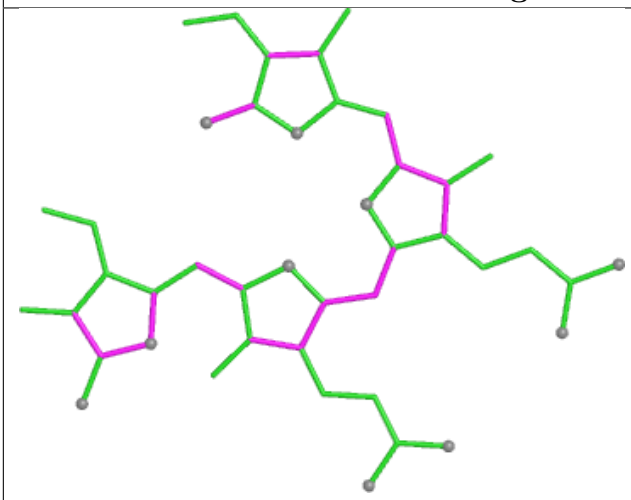


Rings

Ligand PEB W5 202



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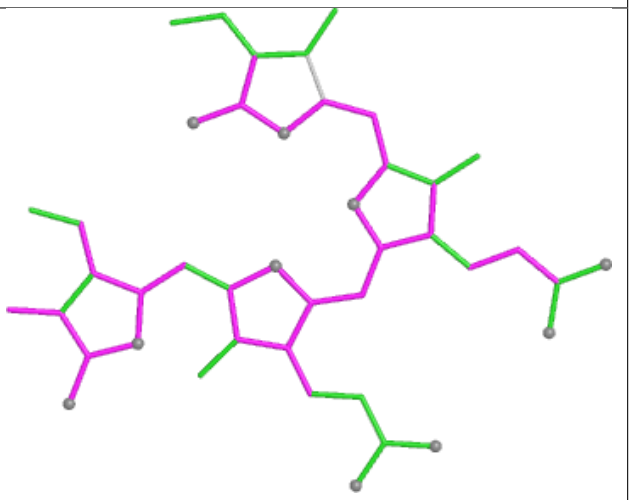

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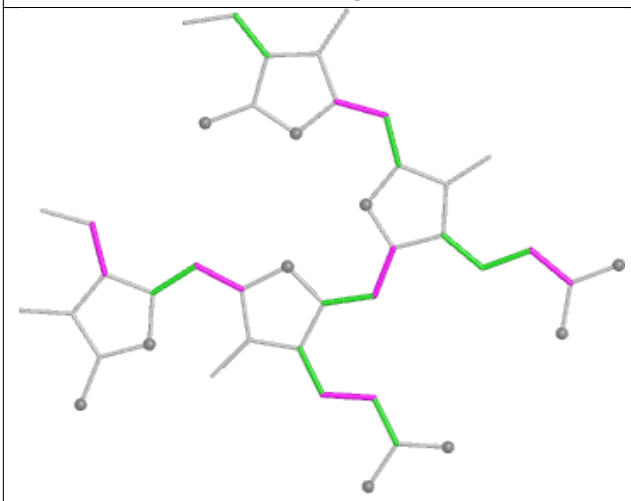

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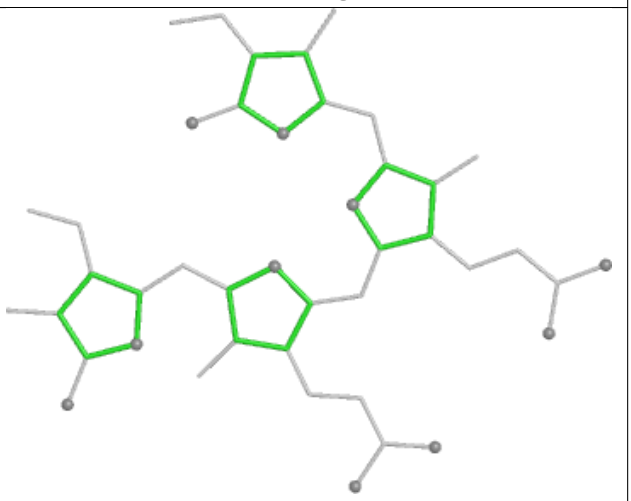
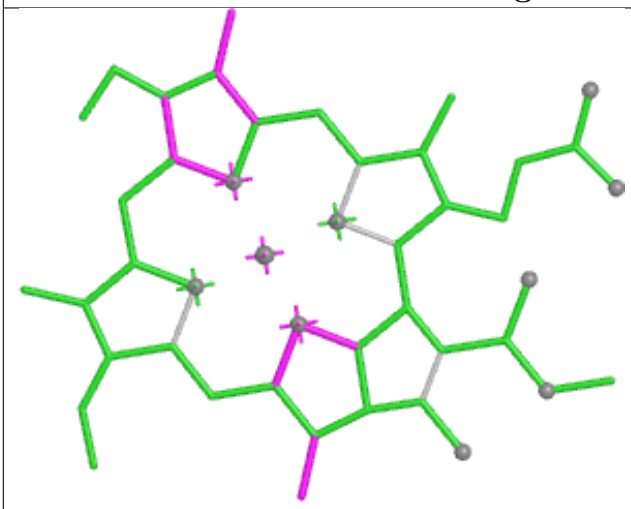


Rings

Ligand CLA 1N 606



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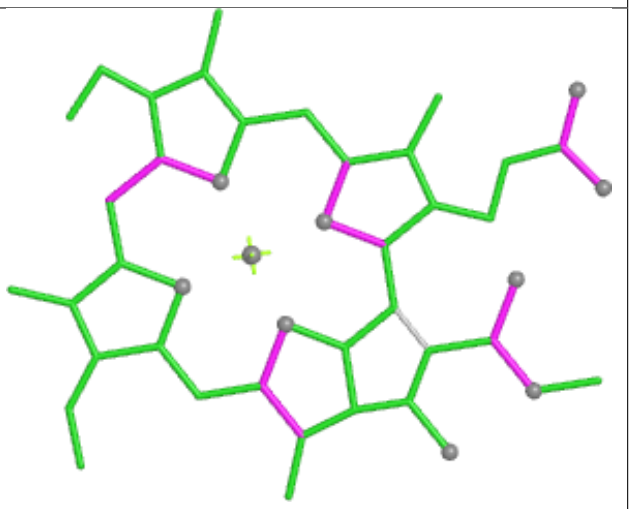

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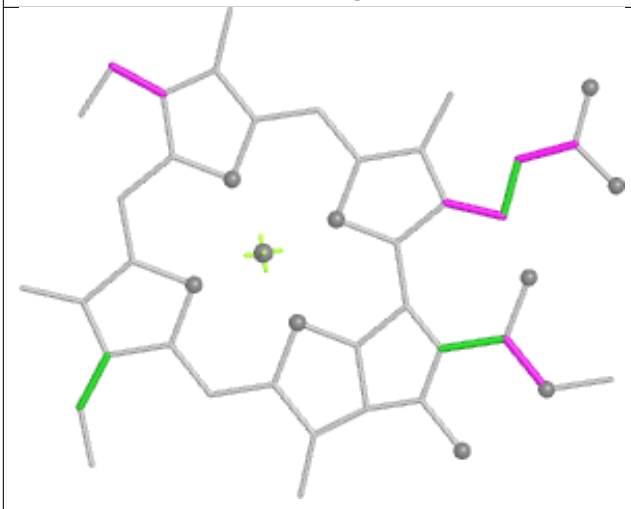
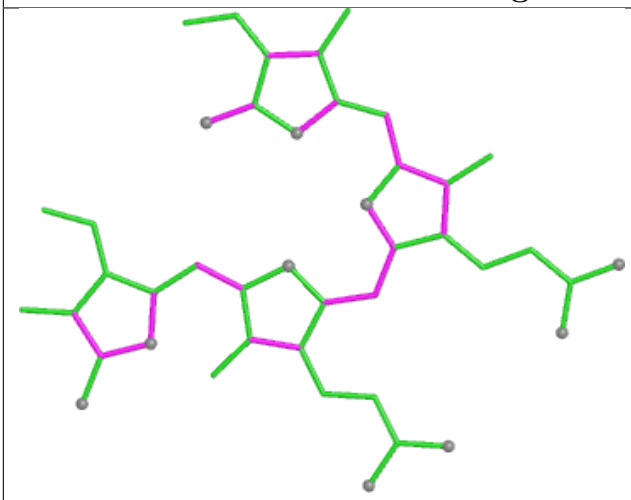


Torsions



Rings

Ligand PEB kM 201



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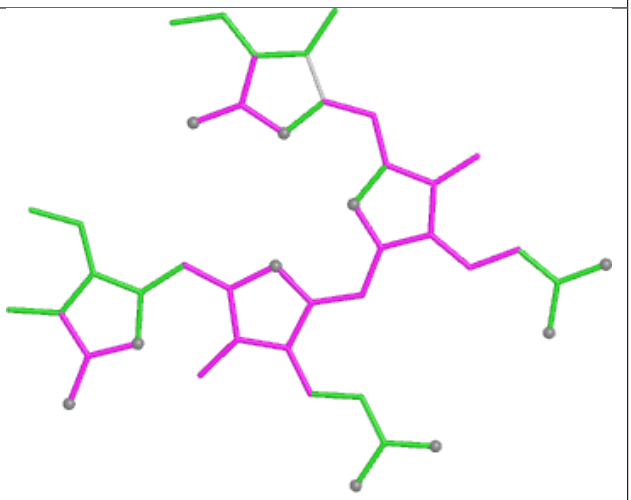

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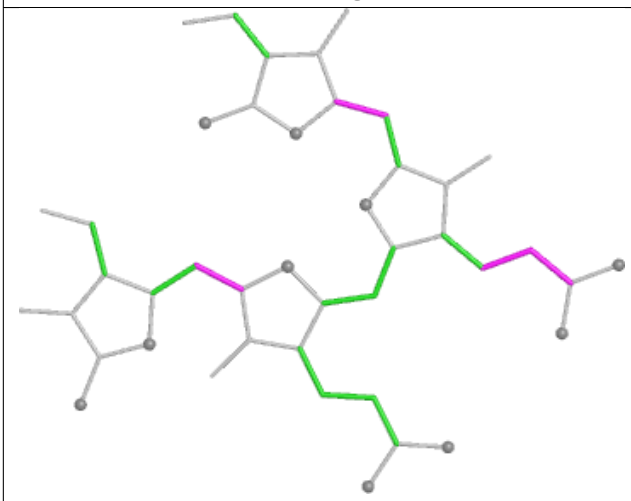

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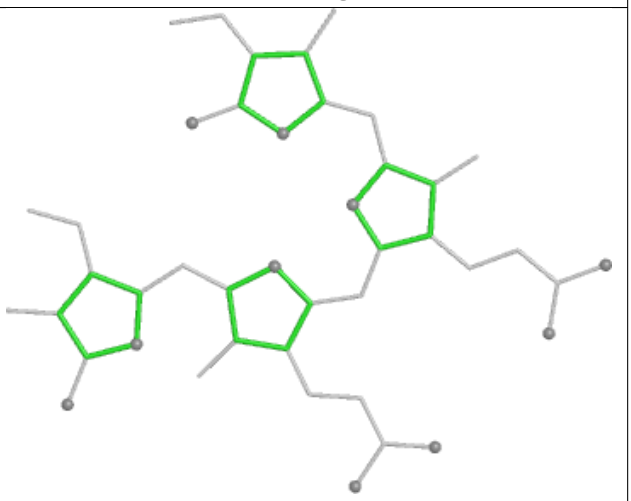
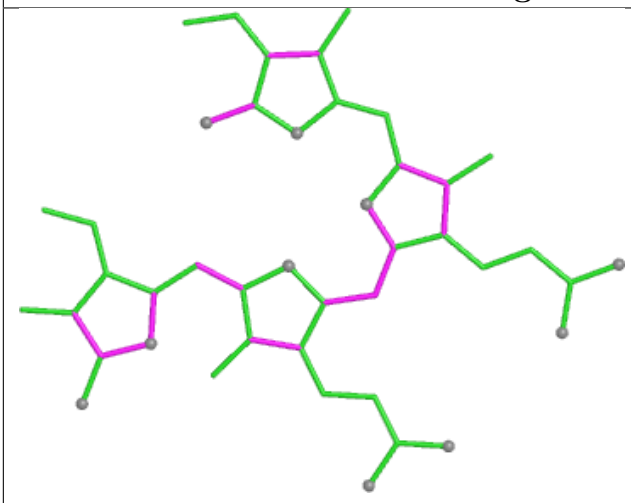


Rings

Ligand PEB ZB 203



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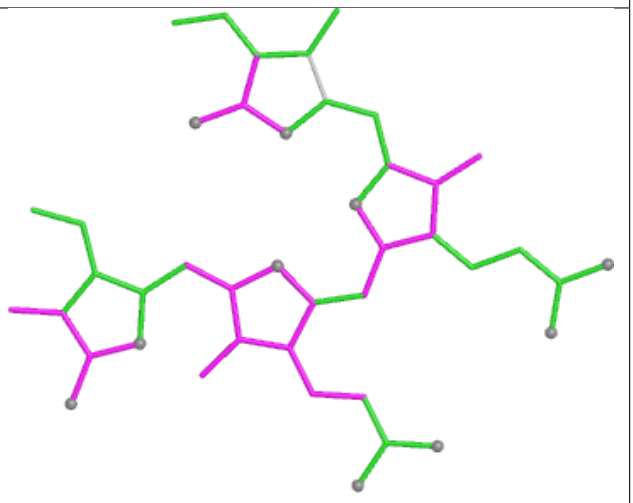

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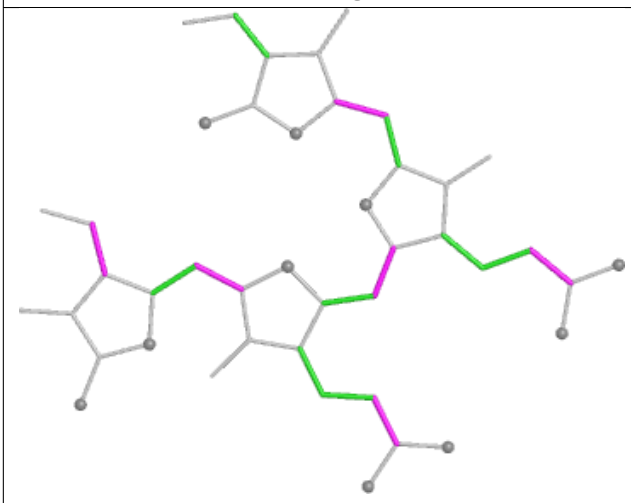

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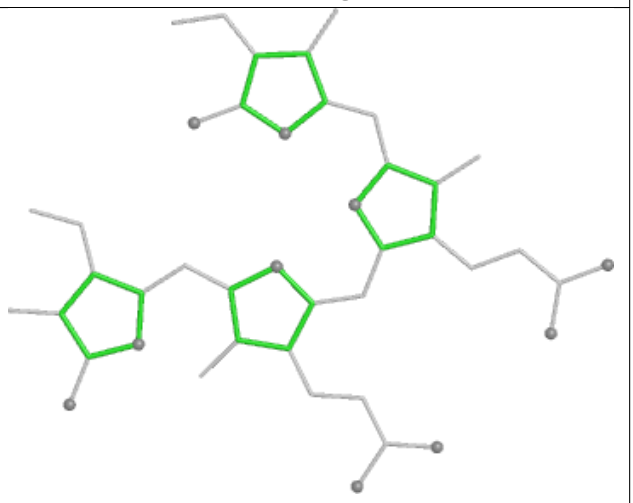
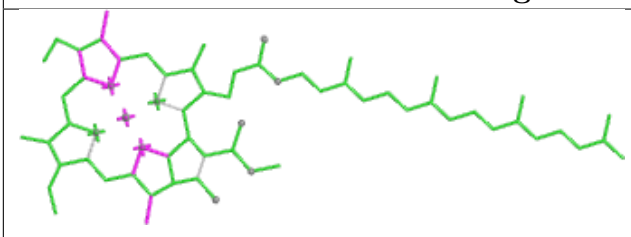


Rings

Ligand CLA CL 511



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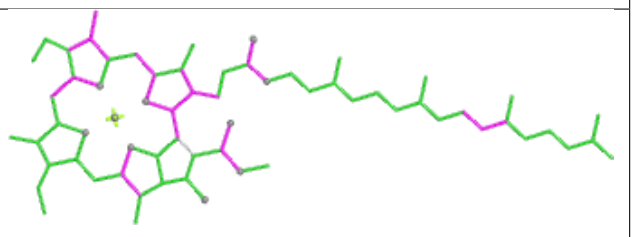

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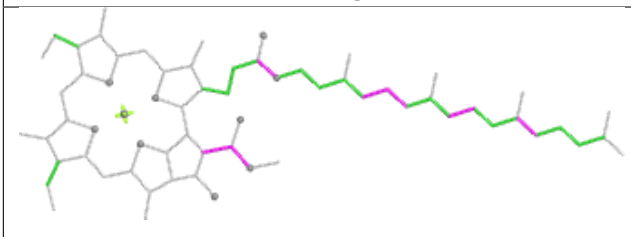

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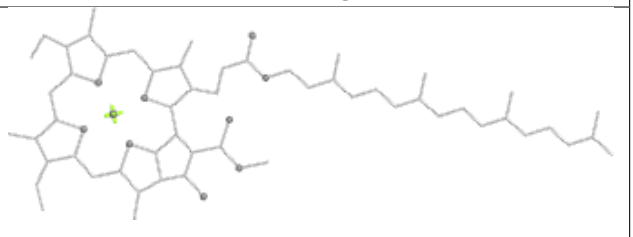
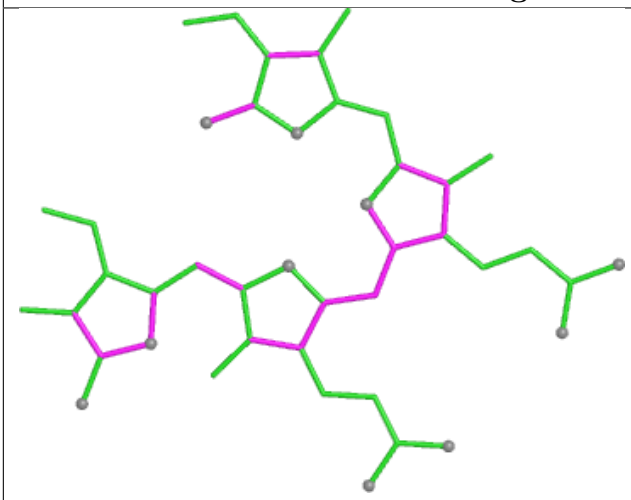


Rings

Ligand PEB HA 203



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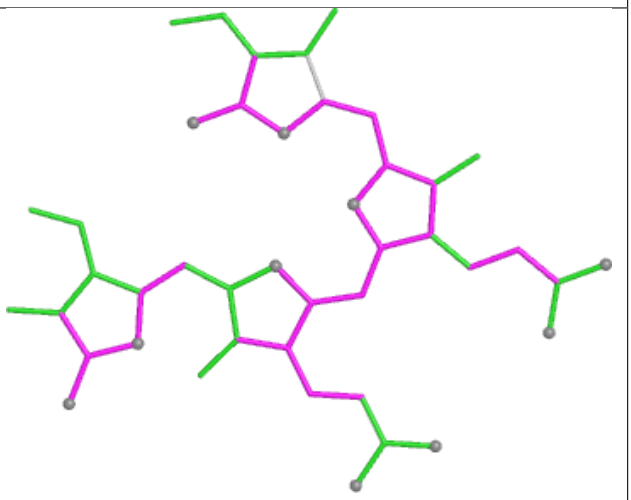

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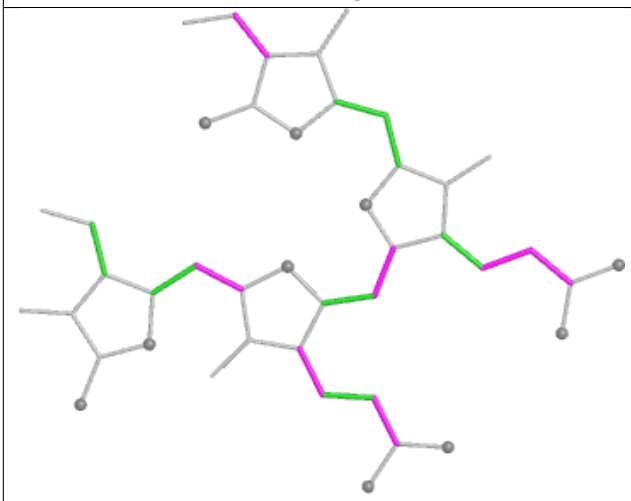

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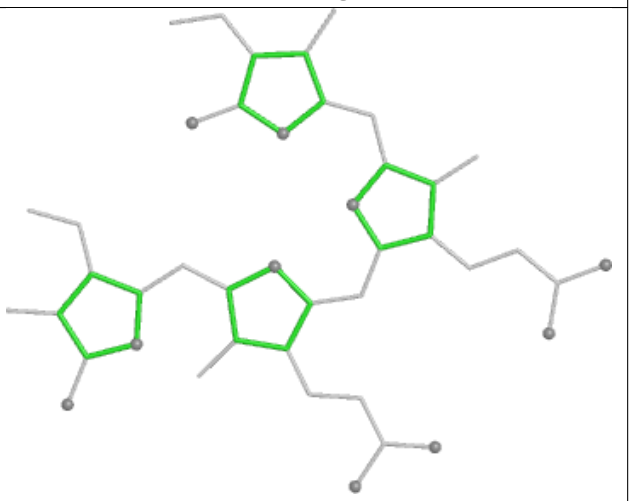
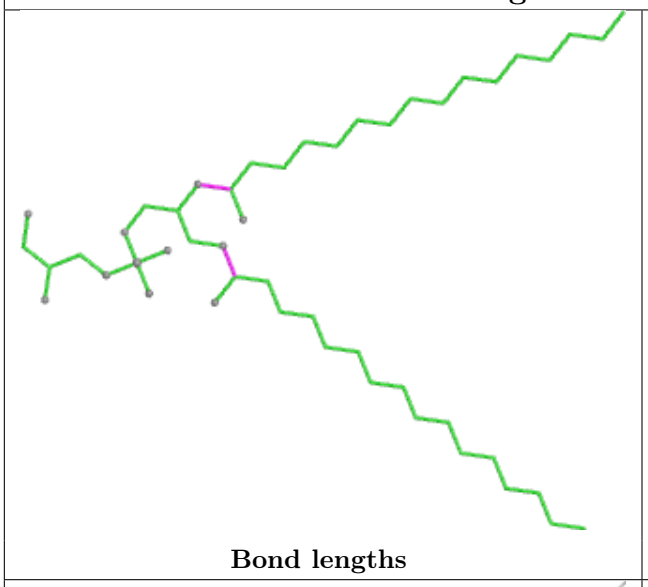


Rings

Ligand LHG AN 843



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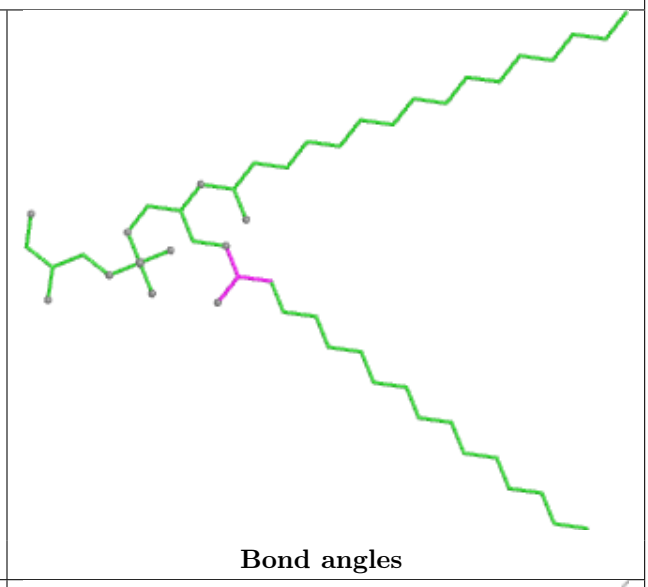

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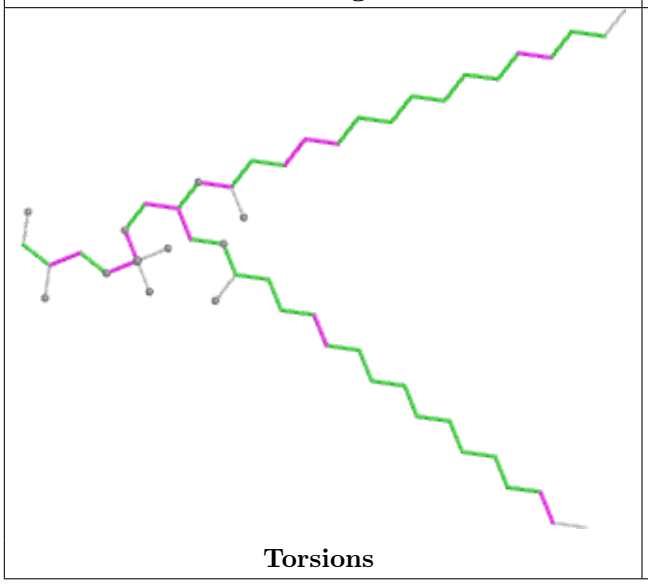

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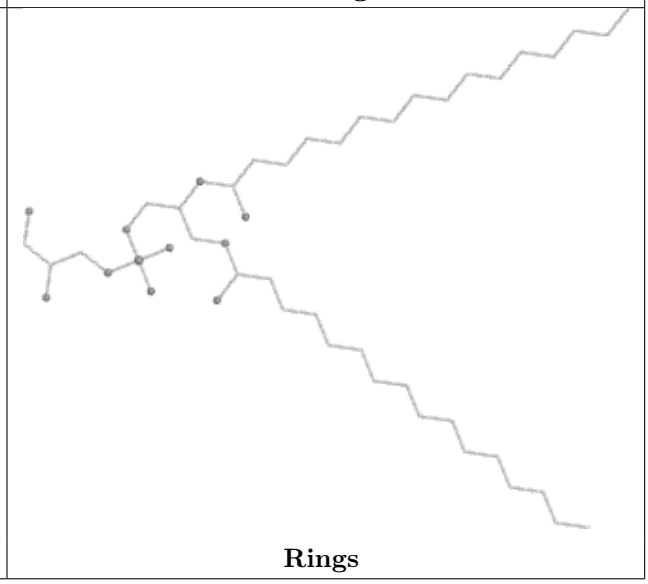
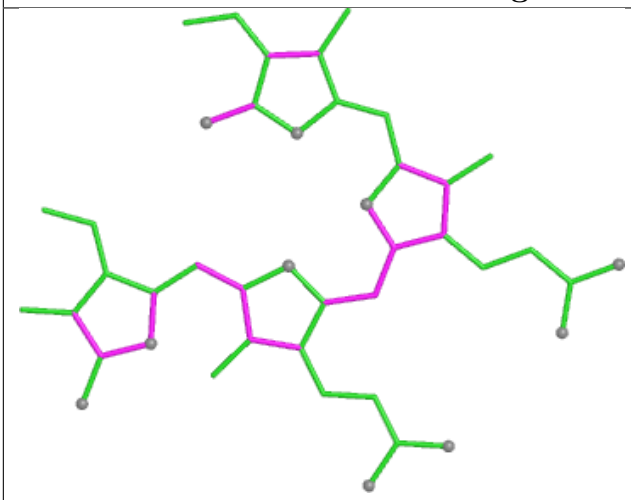


Rings

Ligand PEB CD 201



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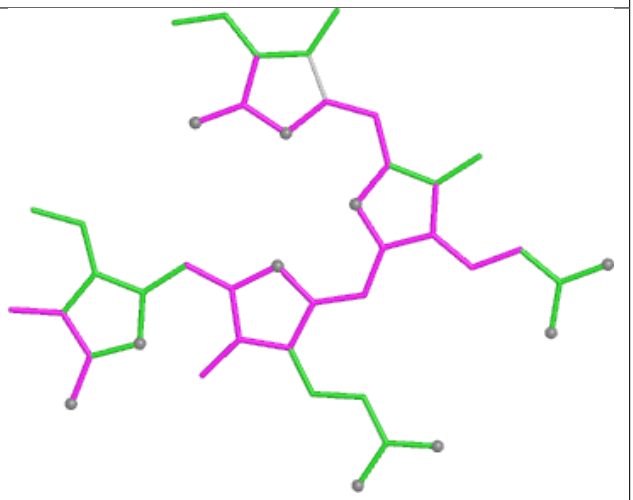

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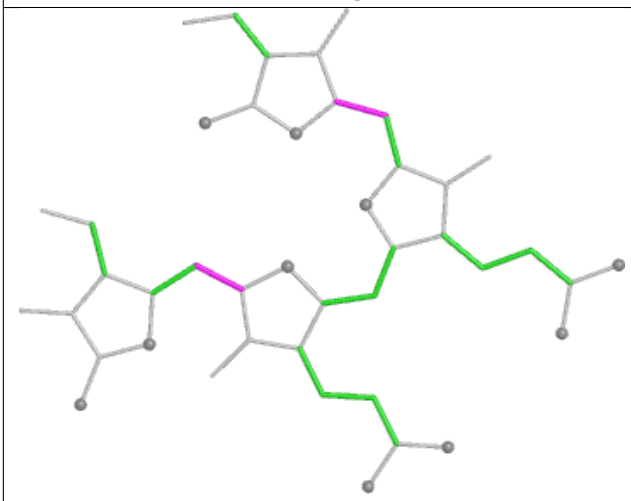

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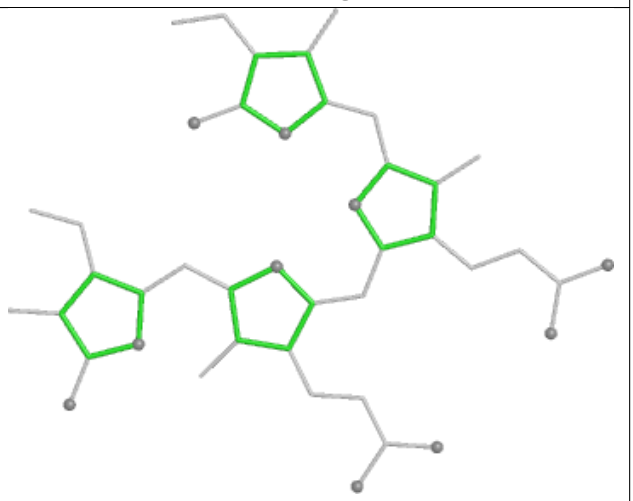
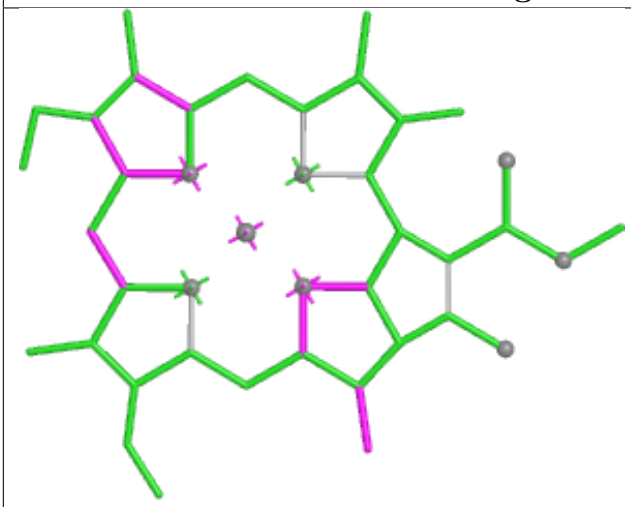


Rings

Ligand CLA 5N 608



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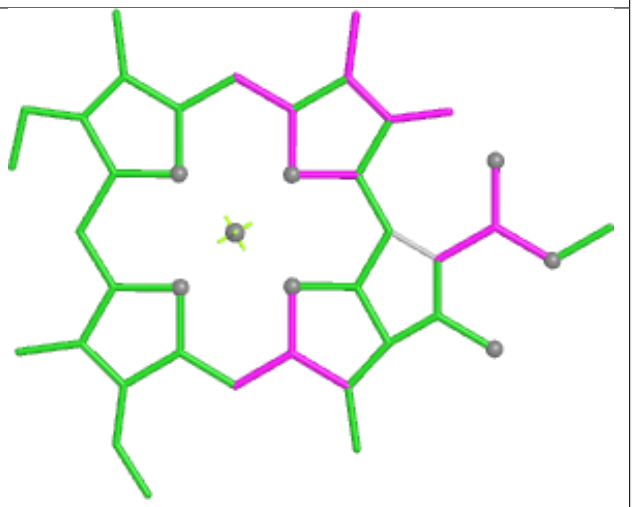

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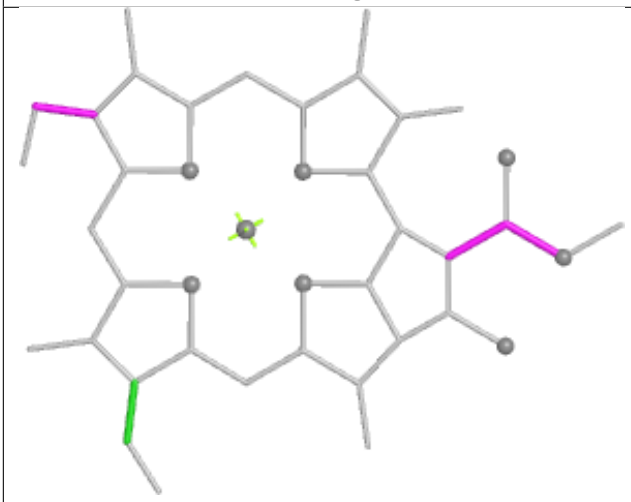

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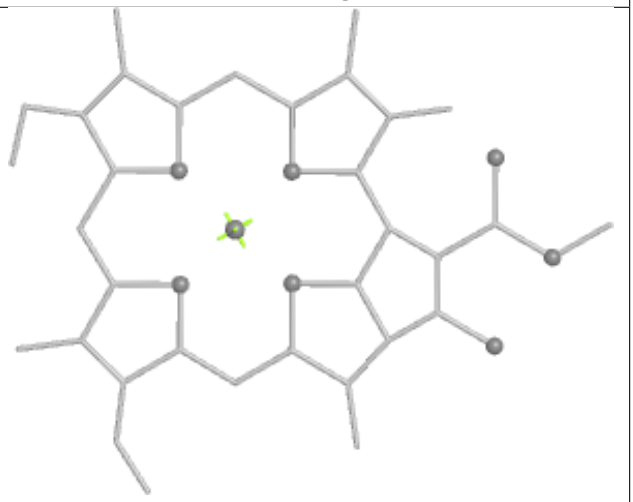
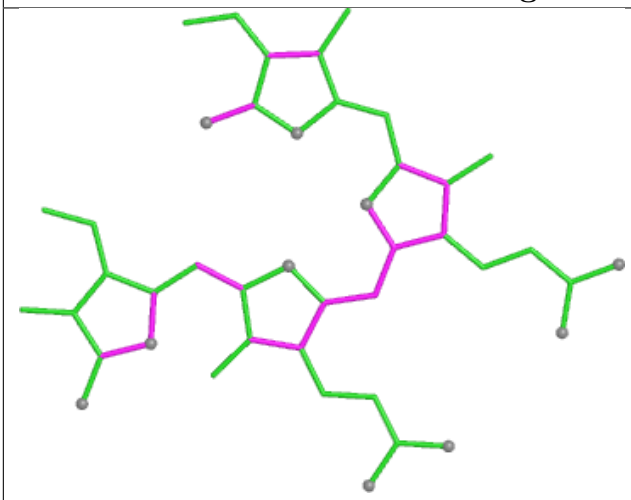


Rings

Ligand PEB g1 201



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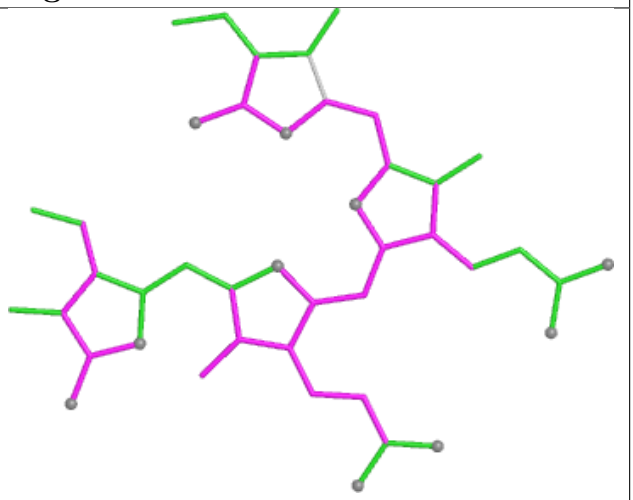

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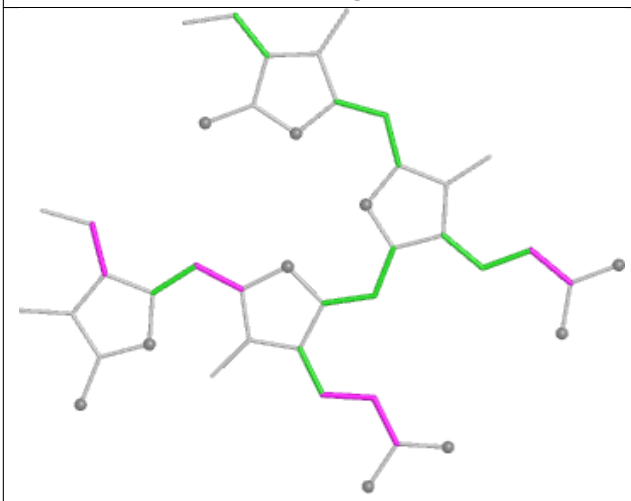

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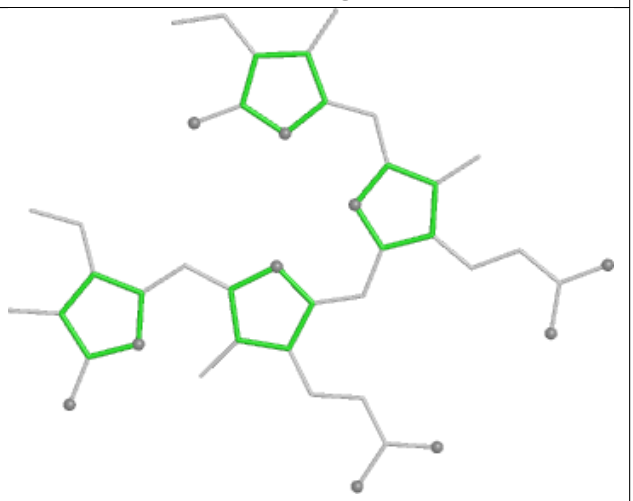
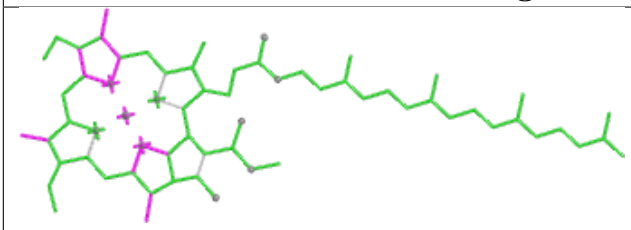


Rings

Ligand CLA bL 616



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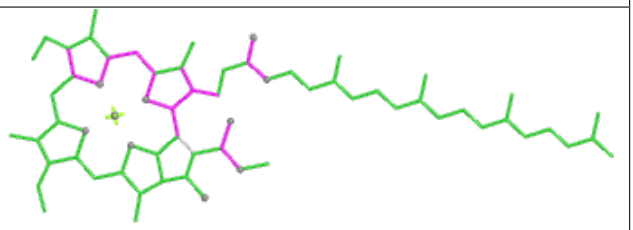
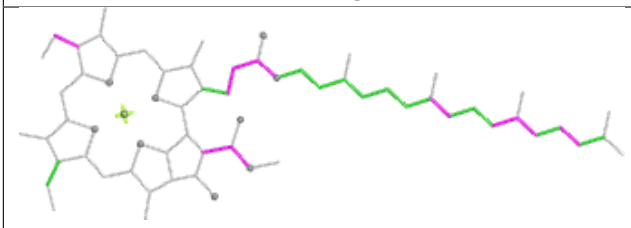


Bond angles



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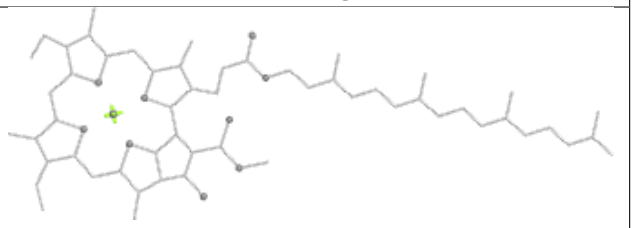
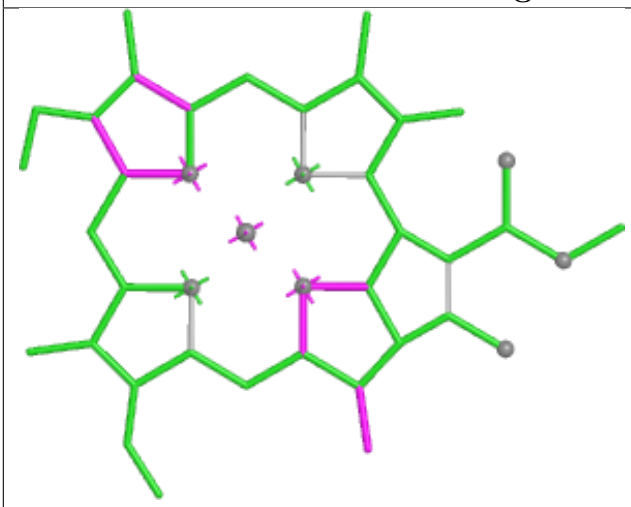


Rings

Ligand CLA 4N 609



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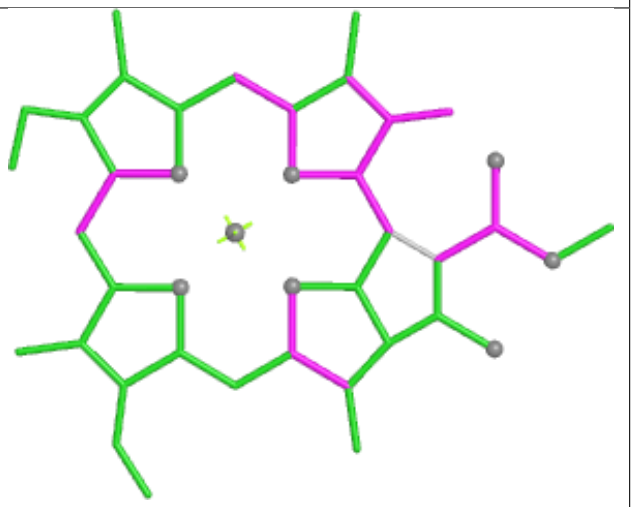
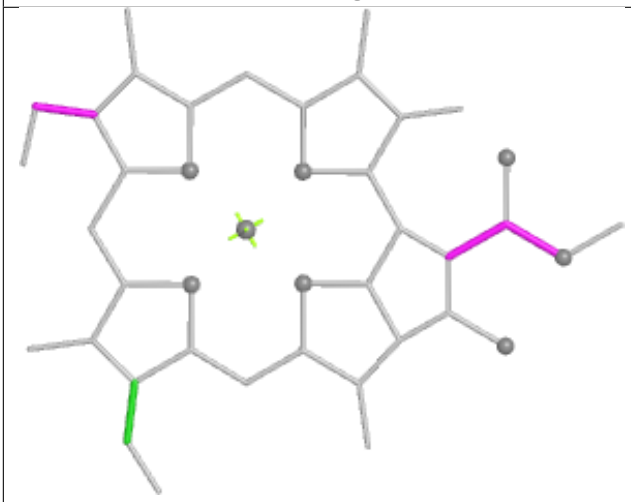


Bond angles



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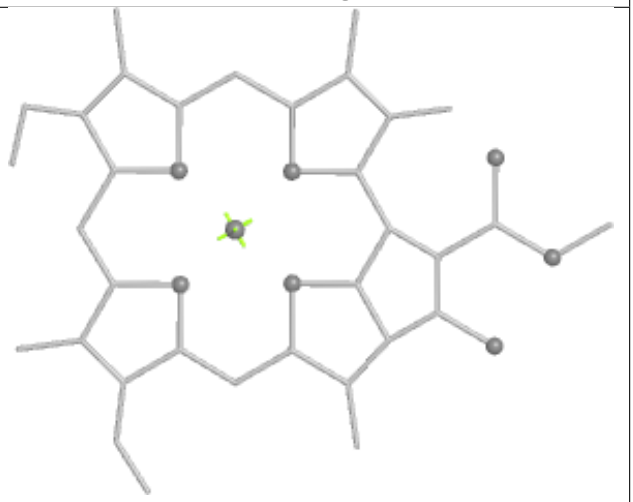
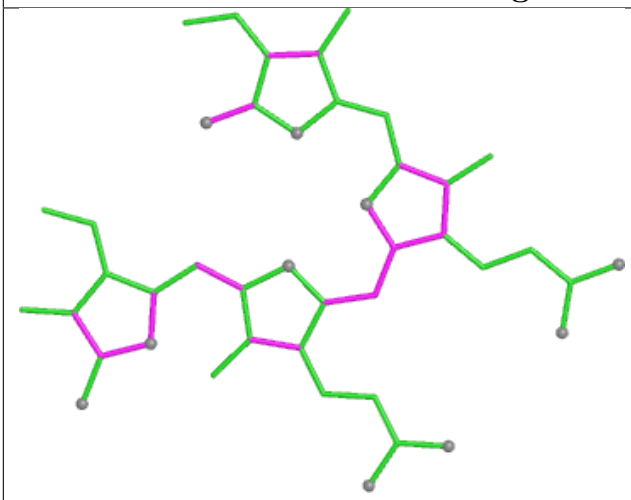


Rings

Ligand PEB TO 201



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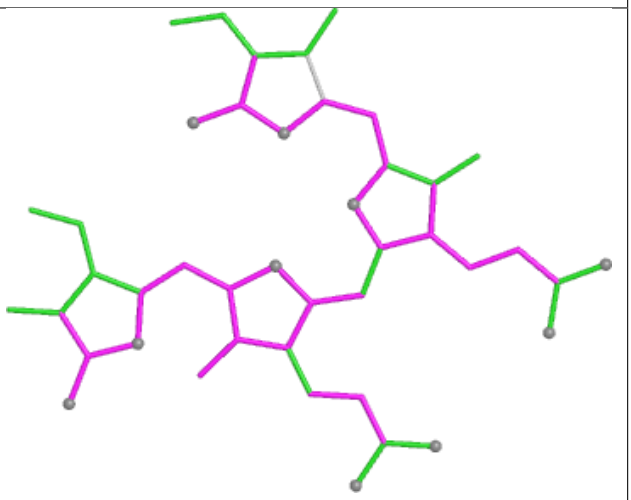
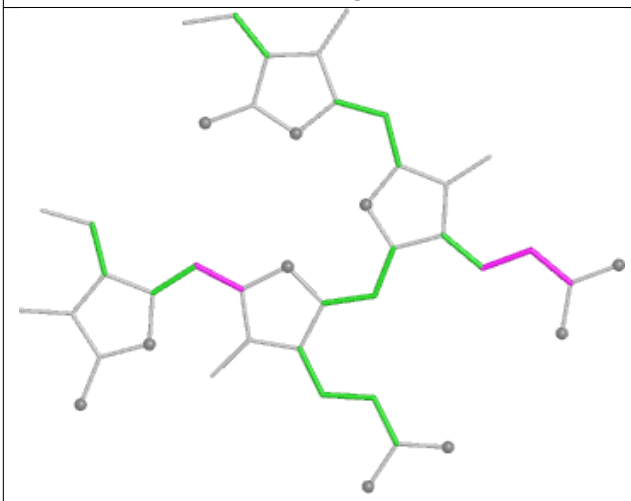
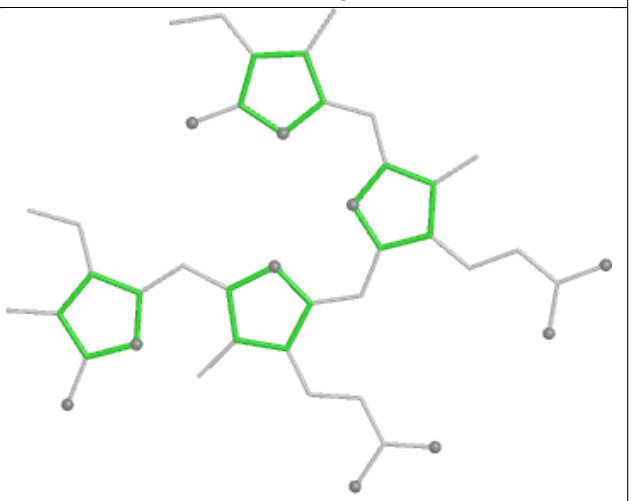


Bond angles

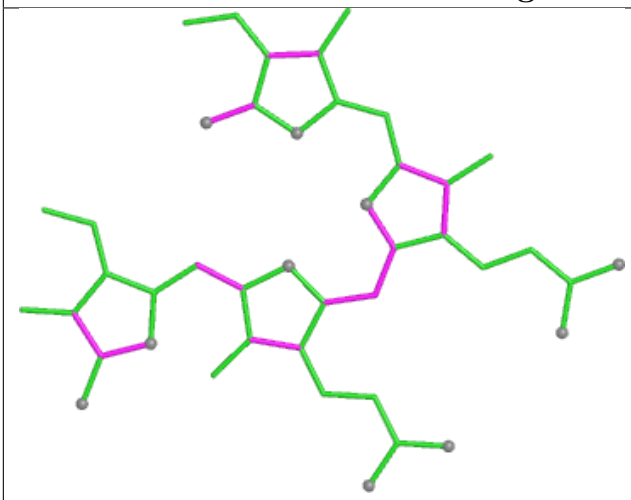


Torsions



Rings

Ligand PEB DI 202



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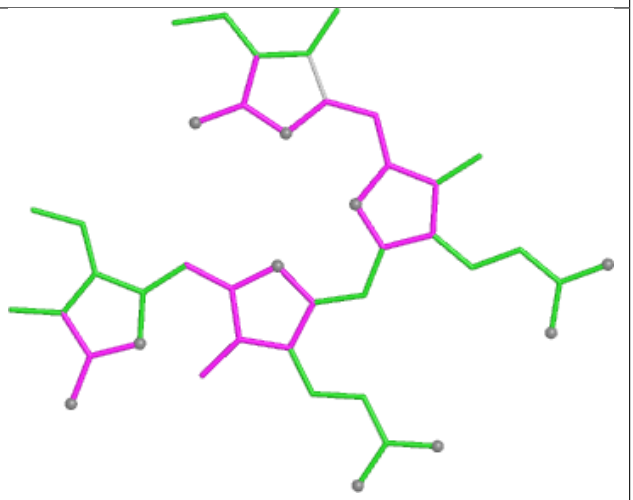

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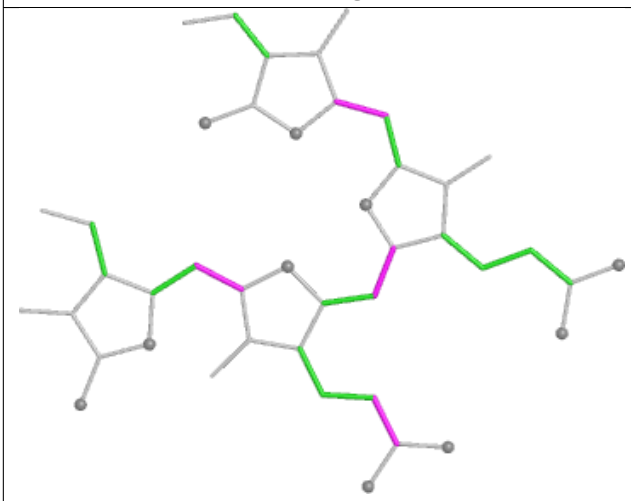

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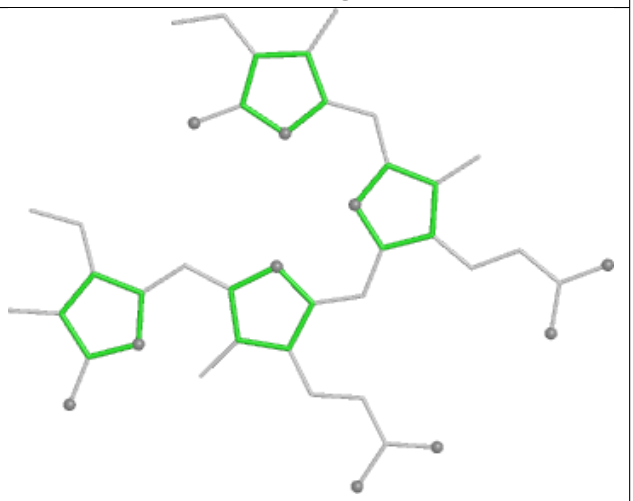
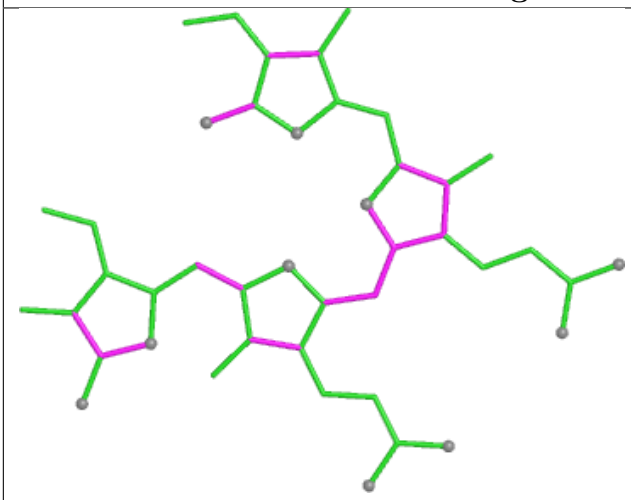


Rings

Ligand PEB wK 301



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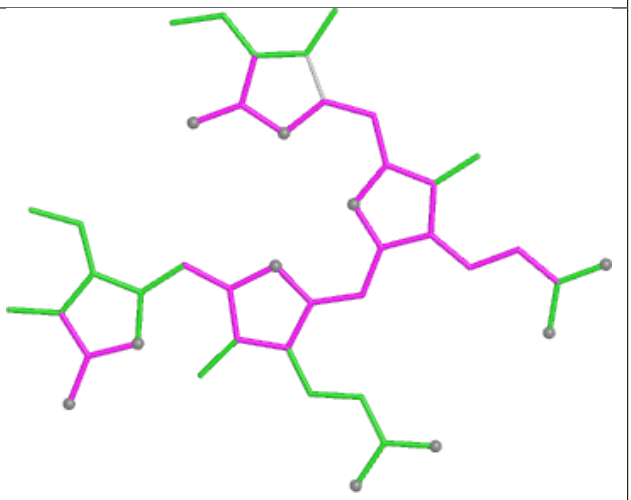

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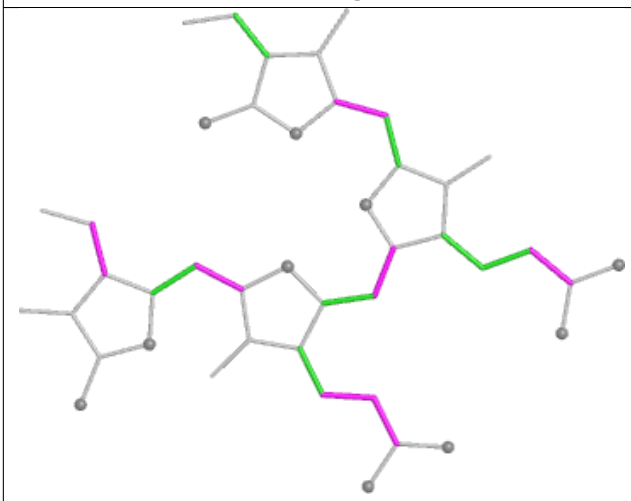

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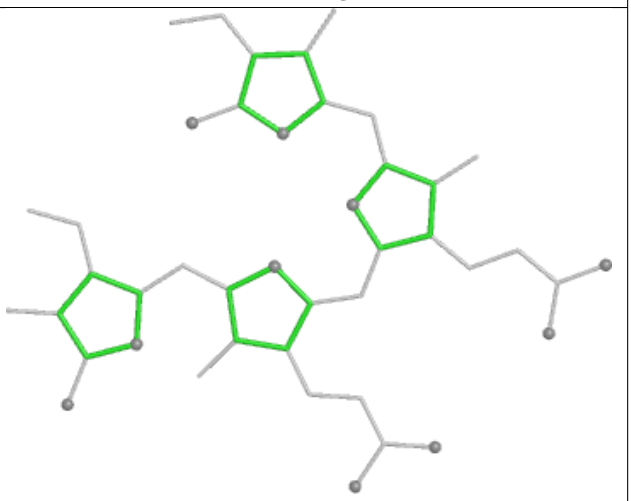
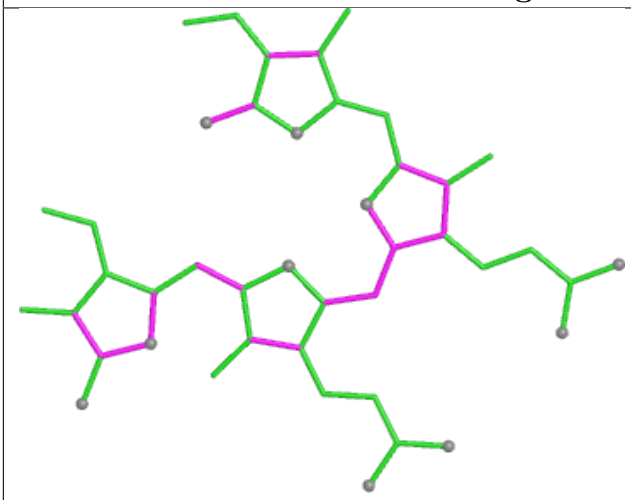


Rings

Ligand PEB D5 201



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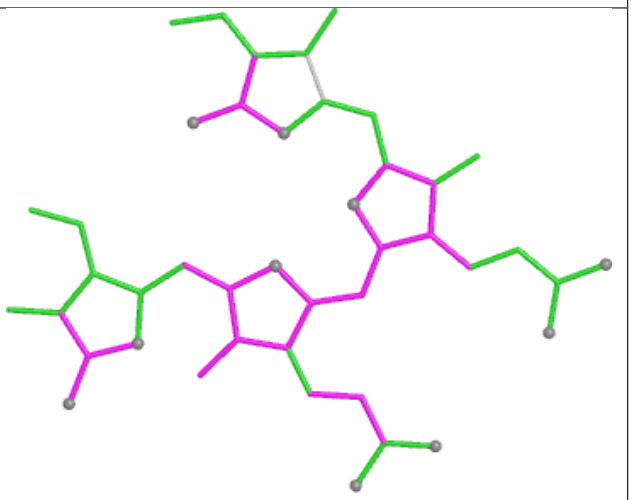

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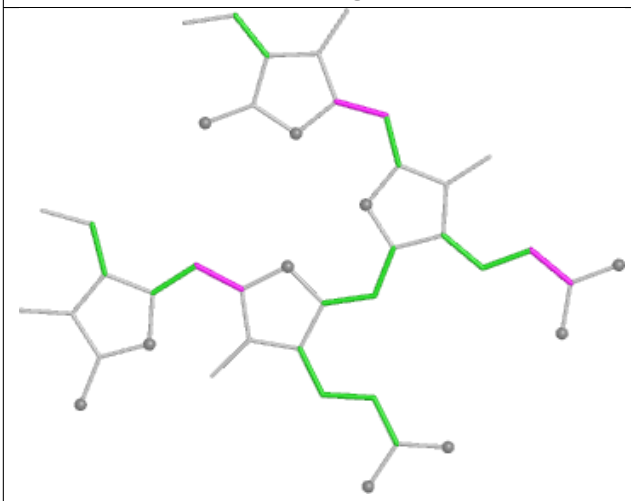

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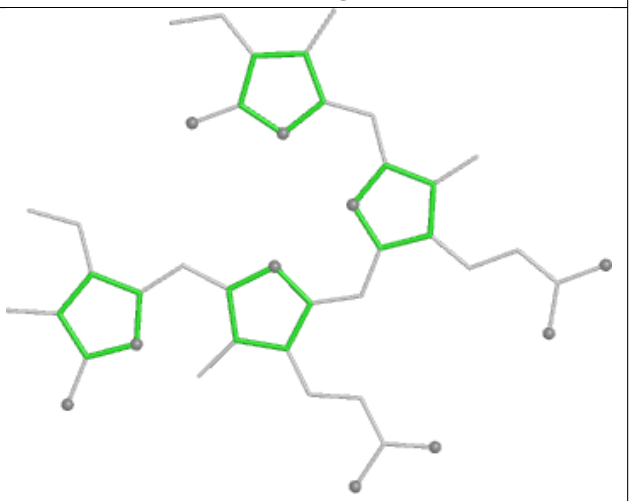
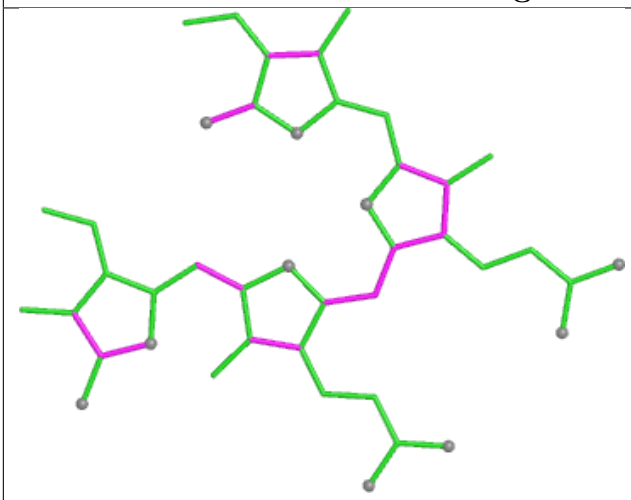


Rings

Ligand PEB dK 201



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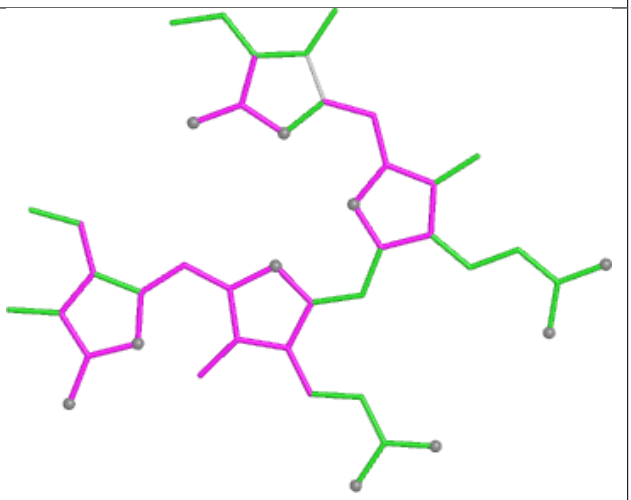

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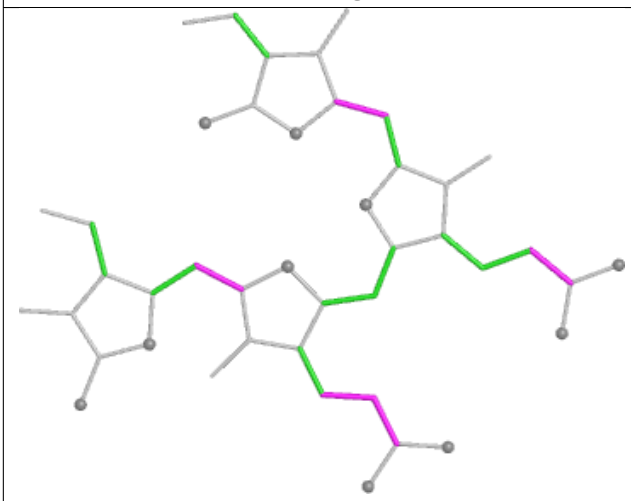

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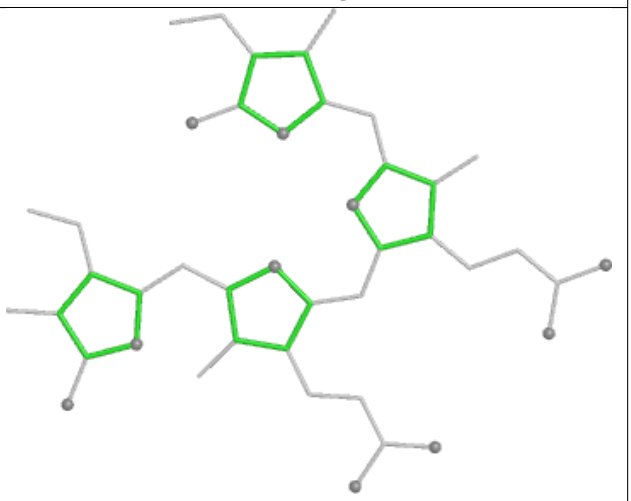
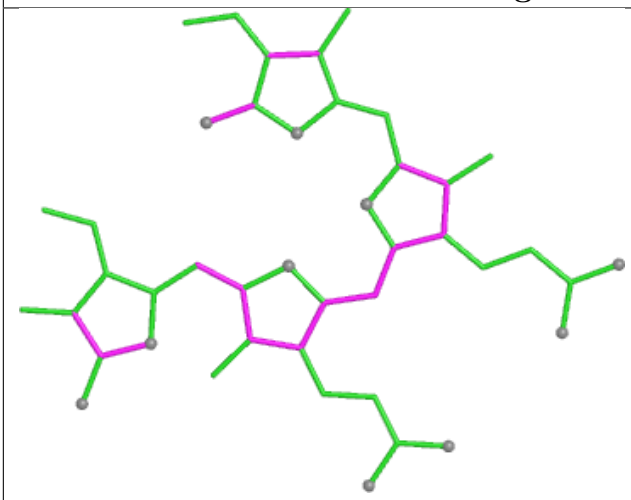


Rings

Ligand PEB kH 202



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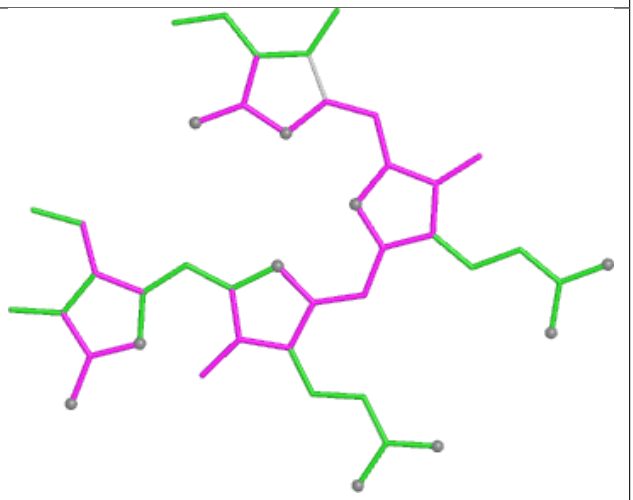

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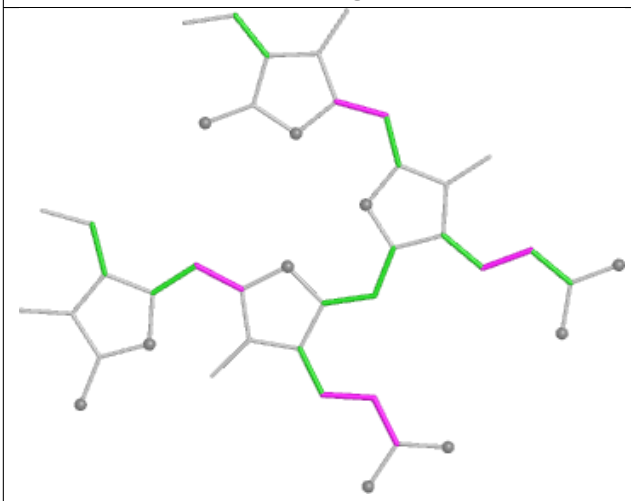

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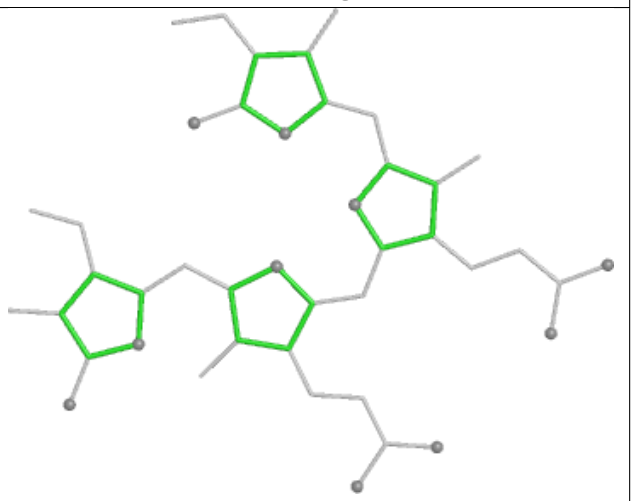
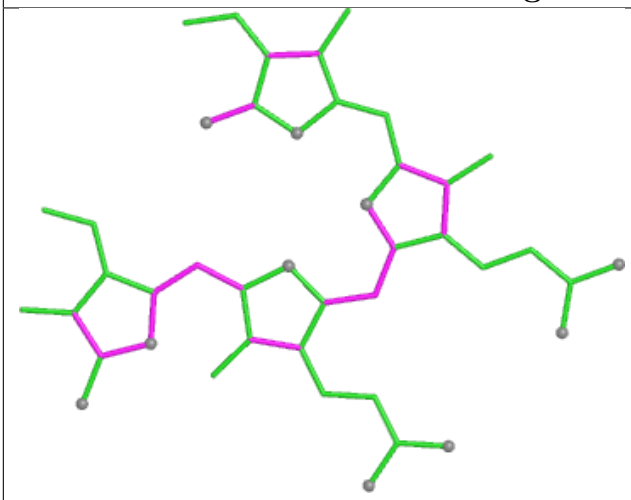


Rings

Ligand PEB l4 201



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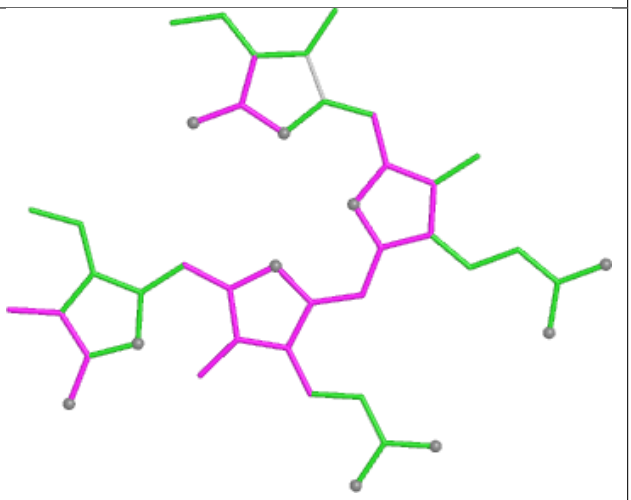

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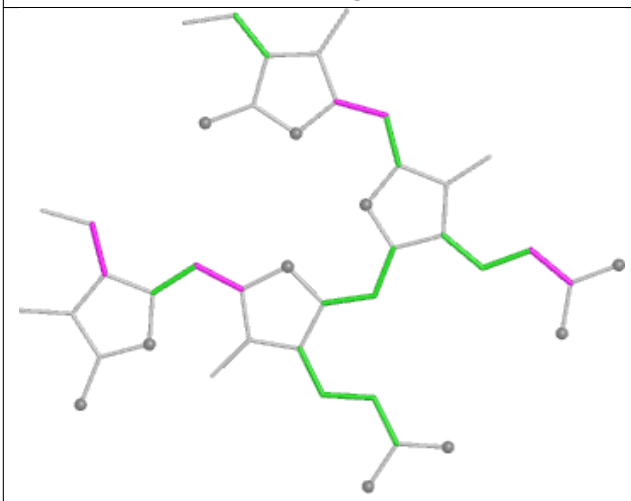

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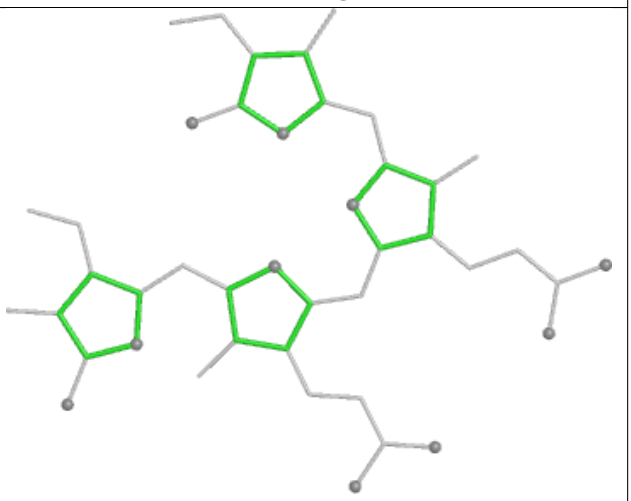
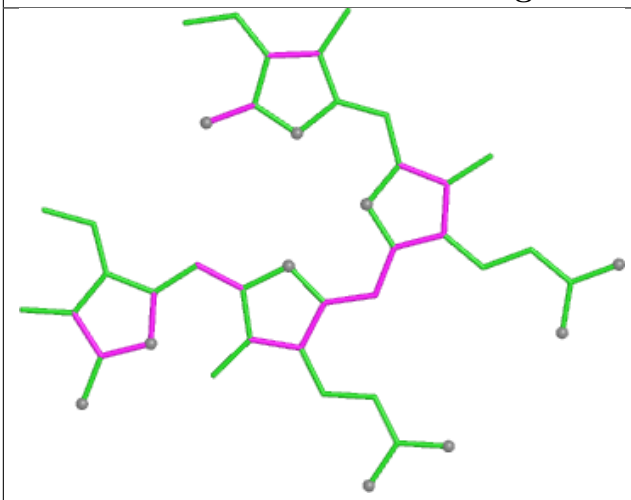


Rings

Ligand PEB aG 202



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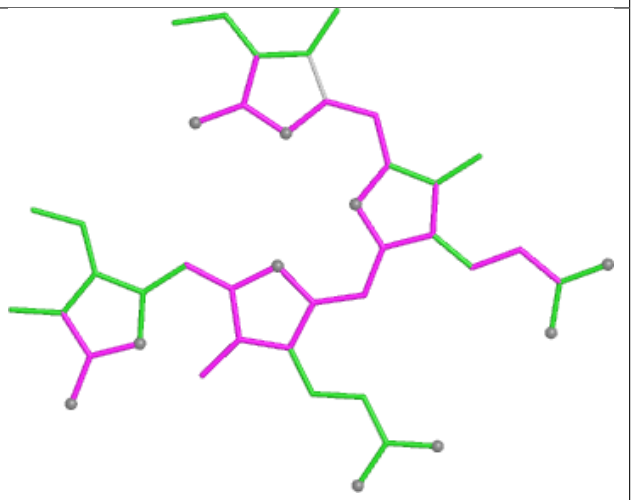

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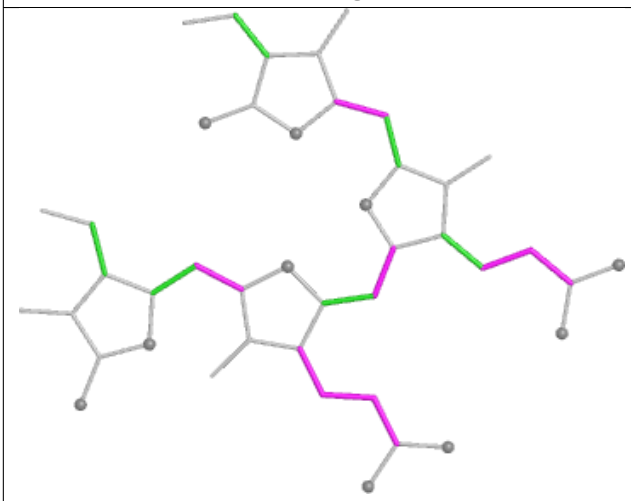

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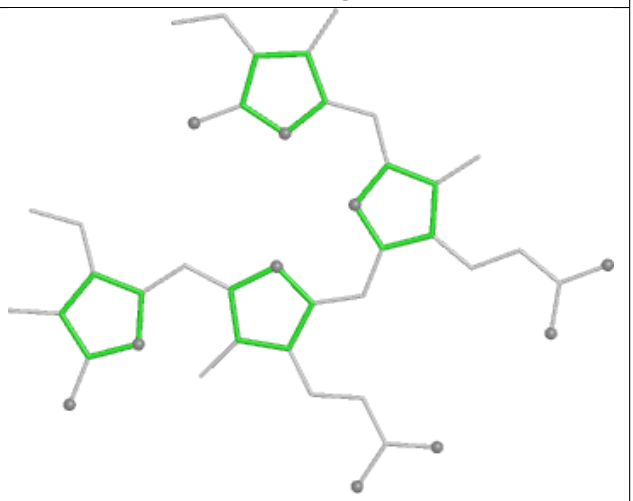
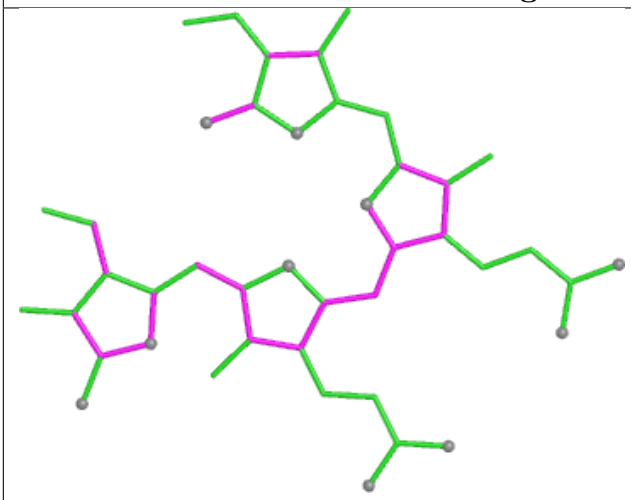


Rings

Ligand PEB ZI 401



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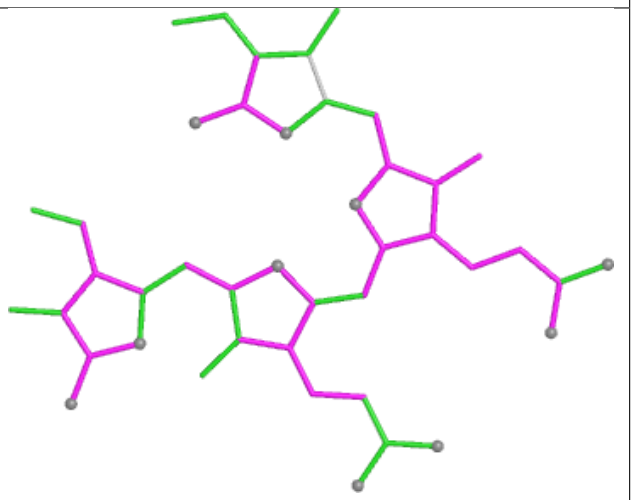

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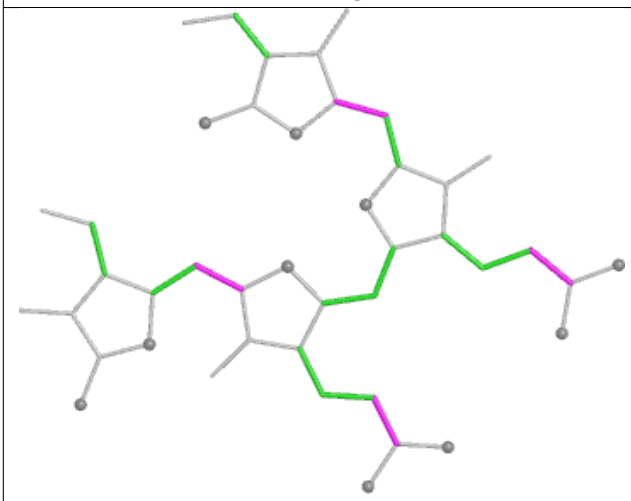

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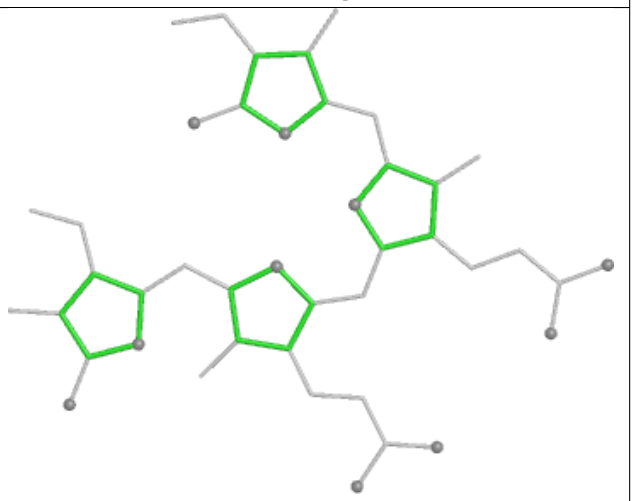
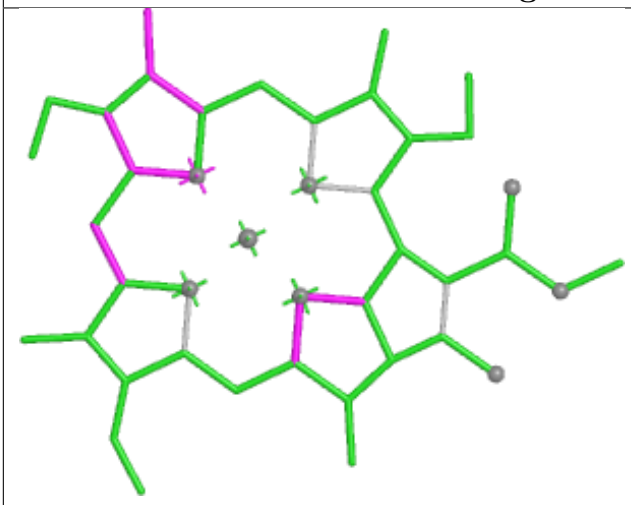


Rings

Ligand CLA 72 609



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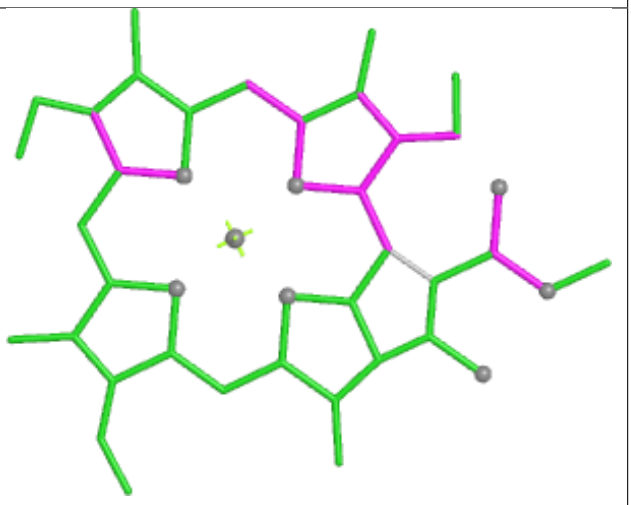

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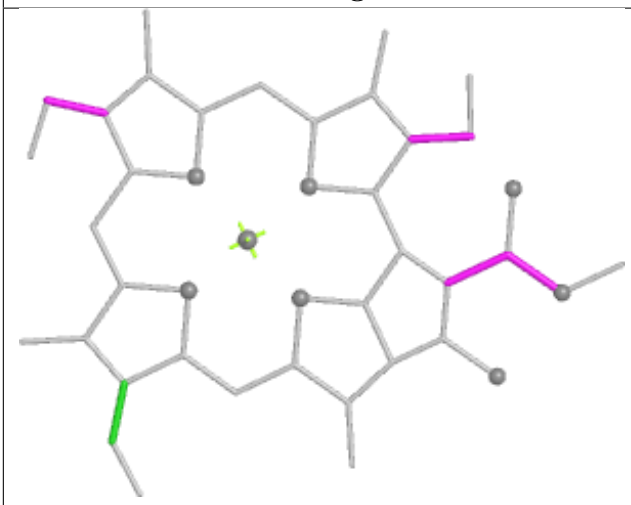
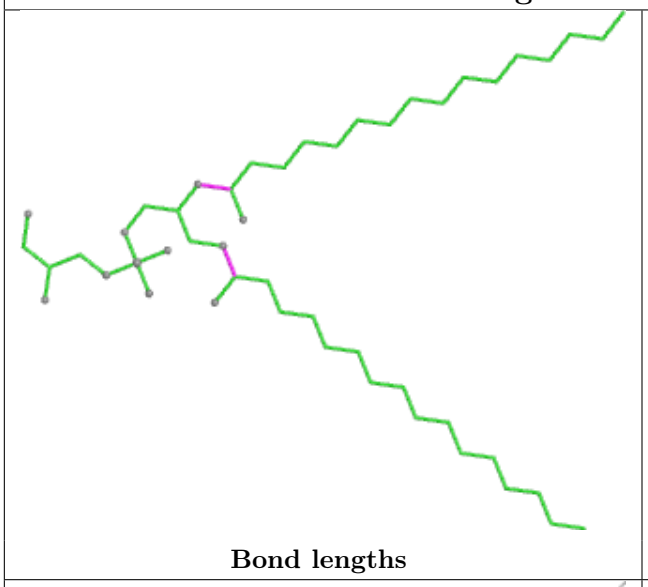


Torsions



Rings

Ligand LHG B6 617



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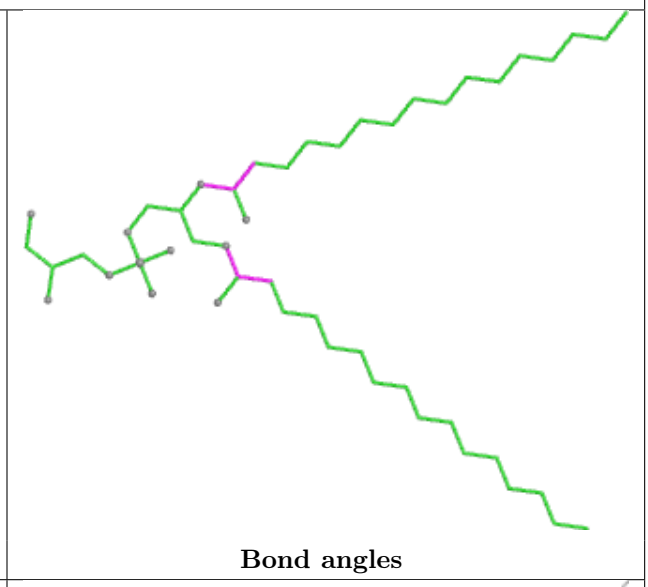
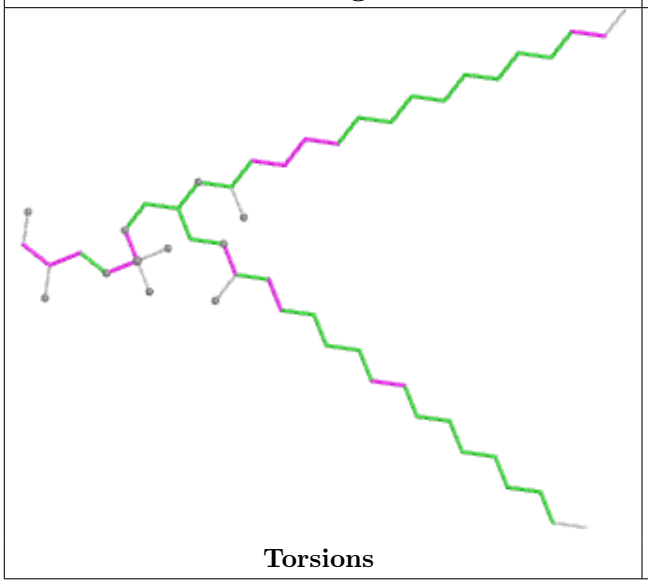


Bond angles



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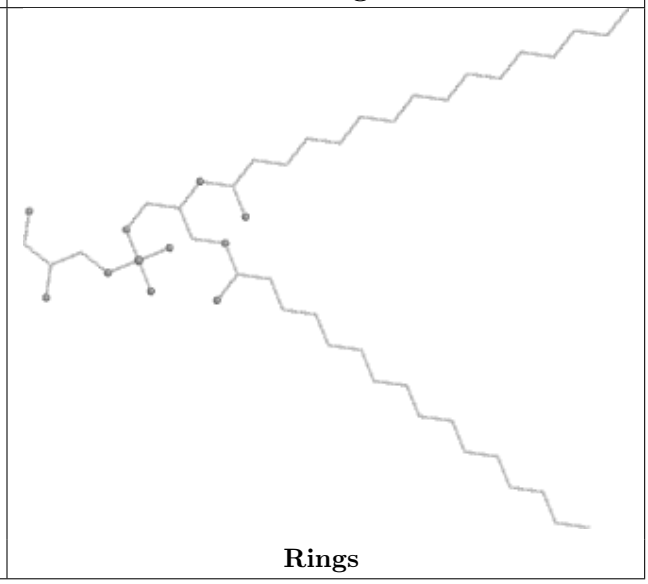
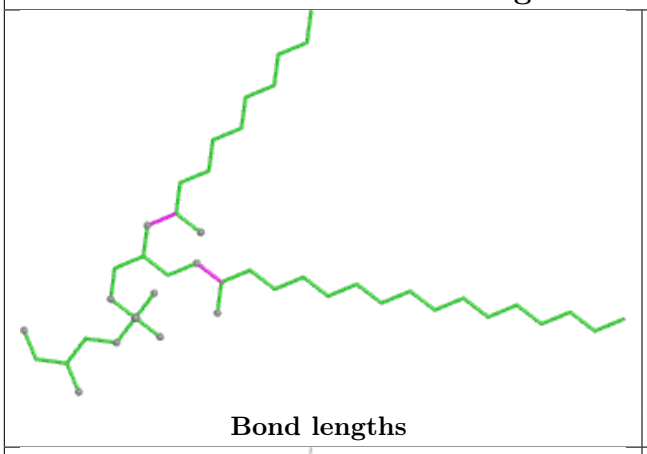


Rings

Ligand LHG D6 401



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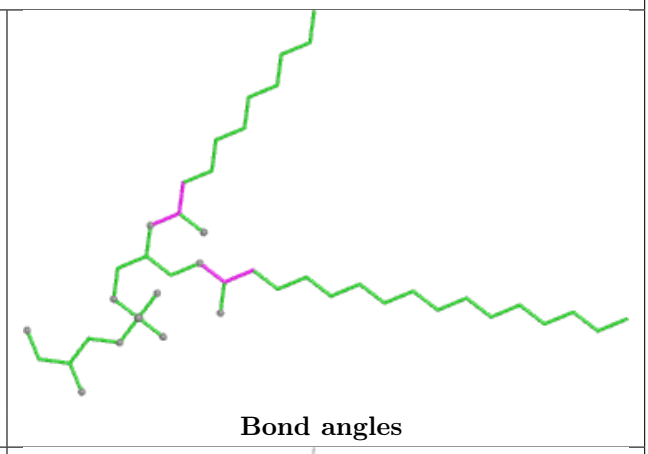
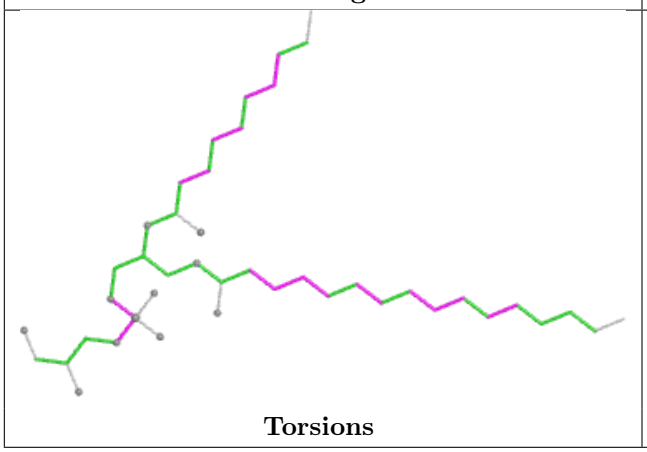


Bond angles



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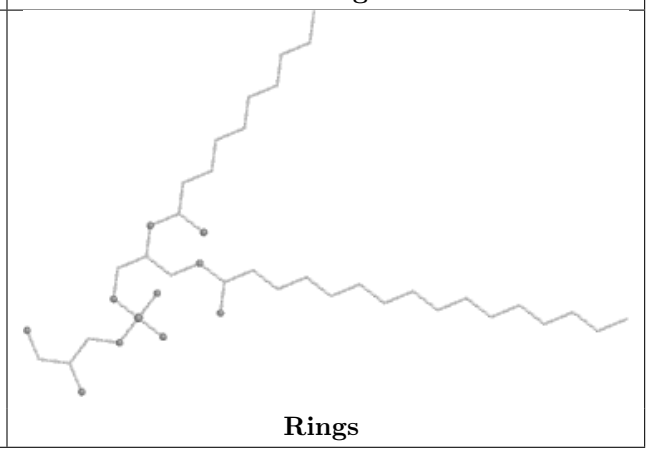
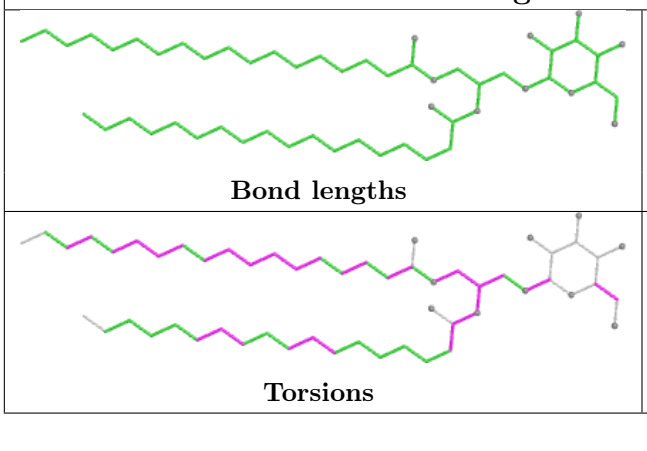
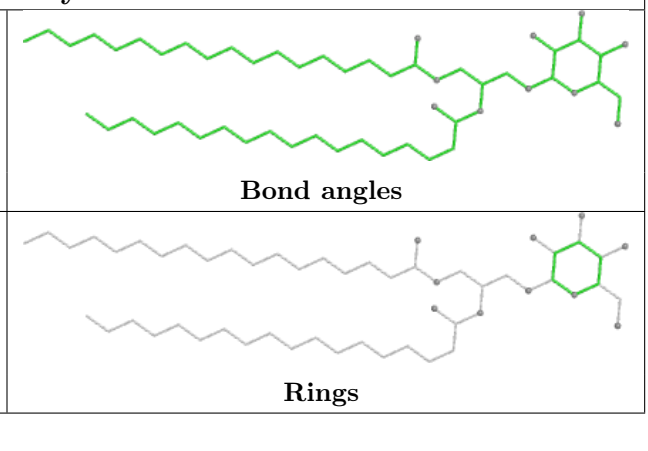


Rings

Ligand LMG yL 101



Bond lengths



Bond angles

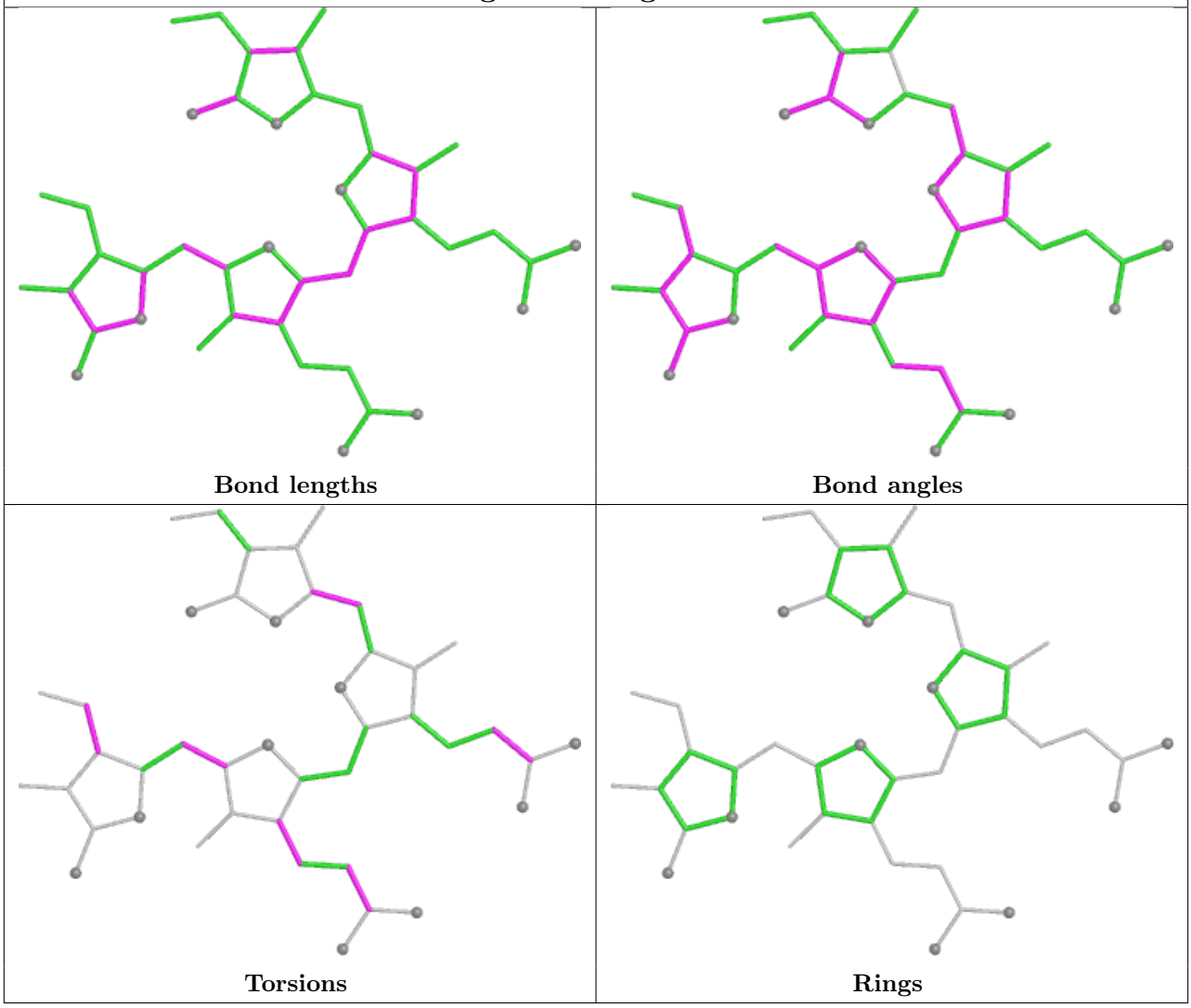


Torsions



Rings

Ligand PEB gB 201



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

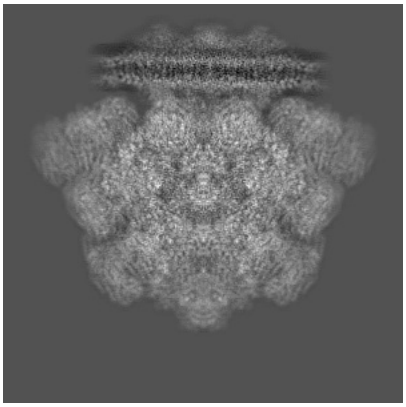
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-33618. These allow visual inspection of the internal detail of the map and identification of artifacts.

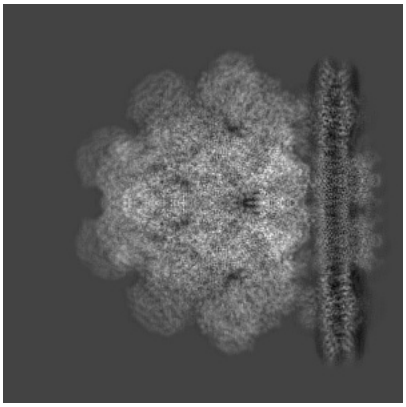
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

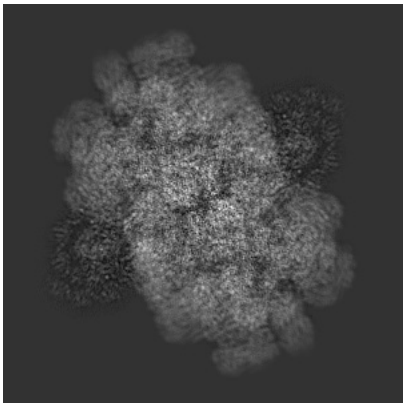
5.1.1 Primary map



X



Y

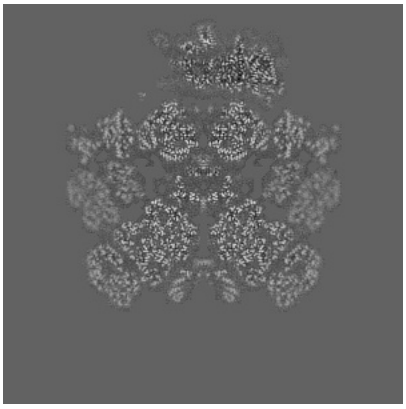


Z

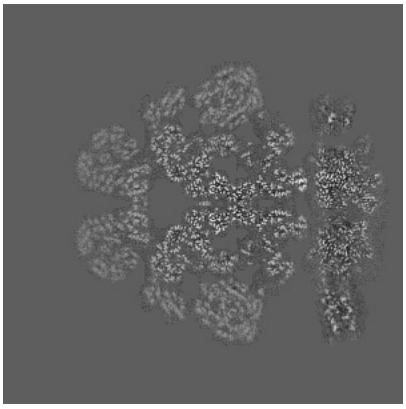
The images above show the map projected in three orthogonal directions.

5.2 Central slices

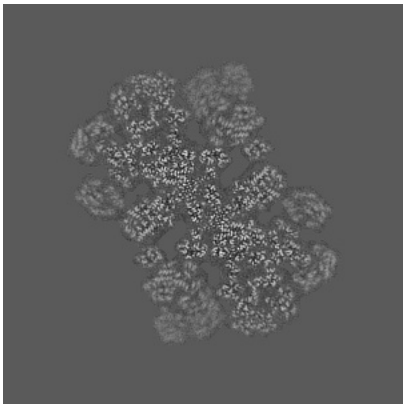
5.2.1 Primary map



X Index: 192



Y Index: 192

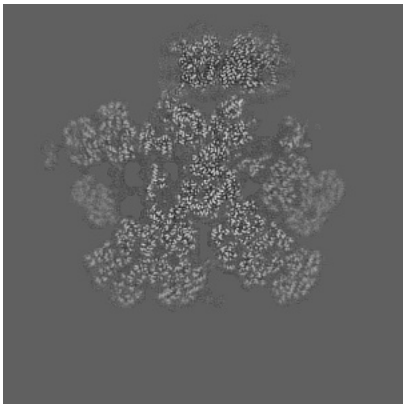


Z Index: 192

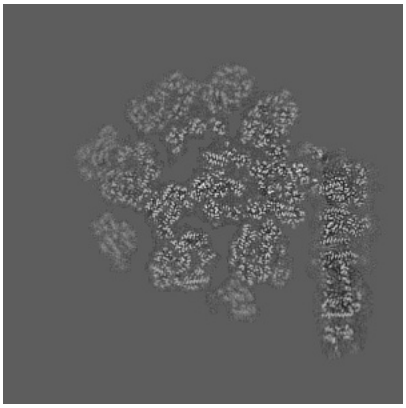
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

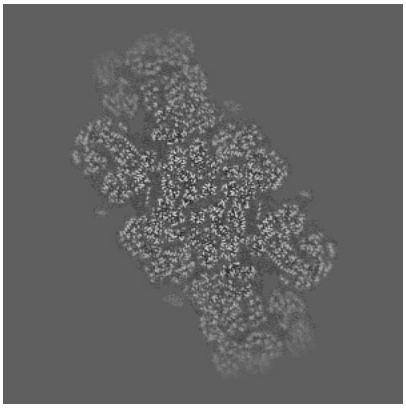
5.3.1 Primary map



X Index: 200



Y Index: 174

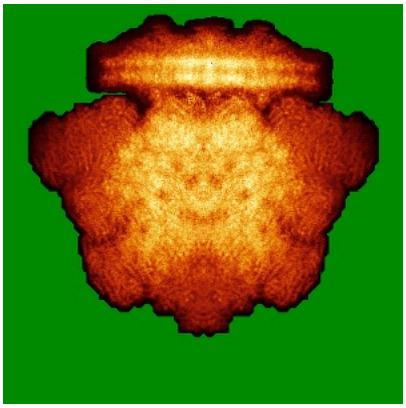


Z Index: 251

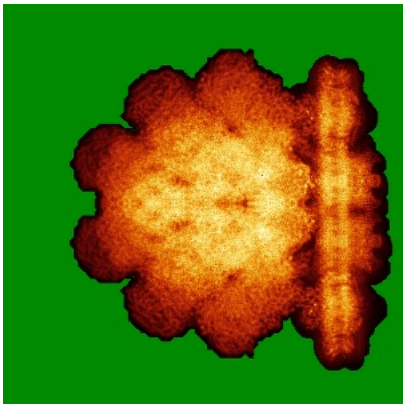
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

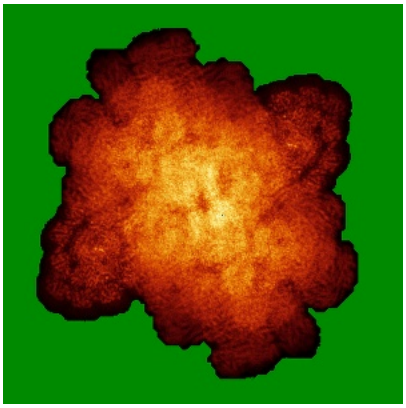
5.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views (i)

5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

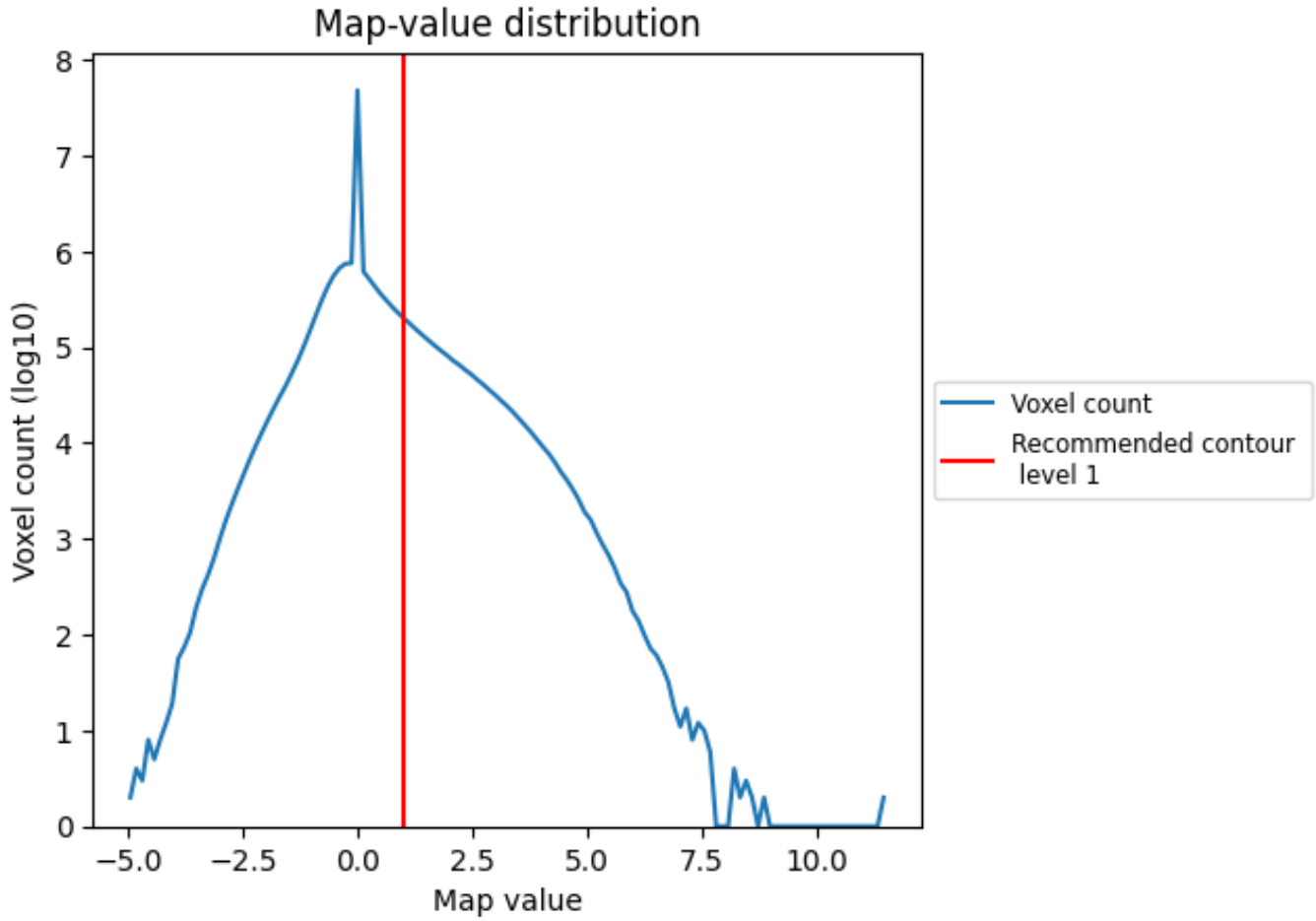
5.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

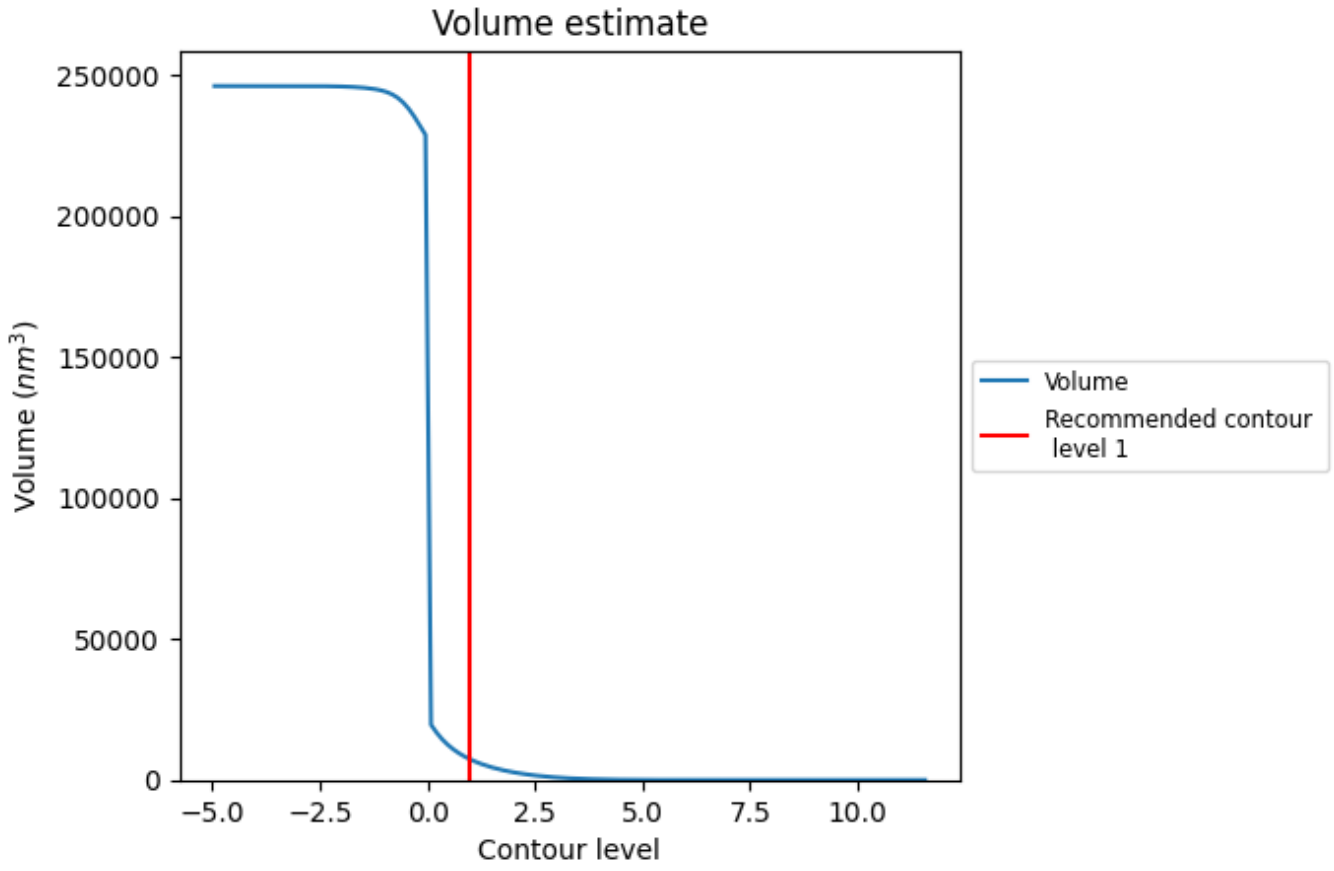
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

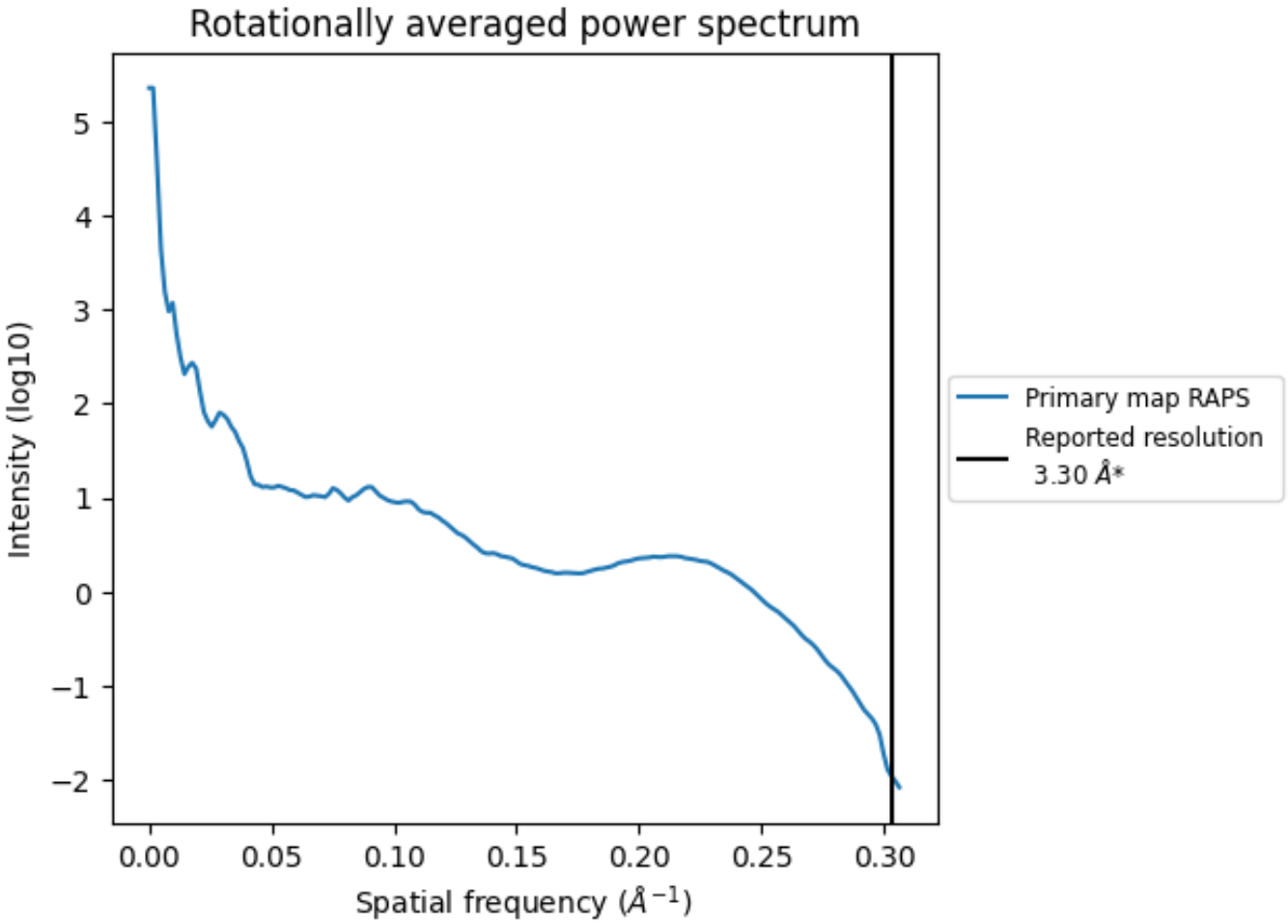
6.2 Volume estimate



The volume at the recommended contour level is 7288 nm^3; this corresponds to an approximate mass of 6584 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

6.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

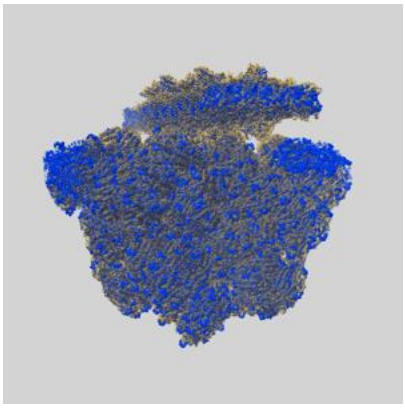
7 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

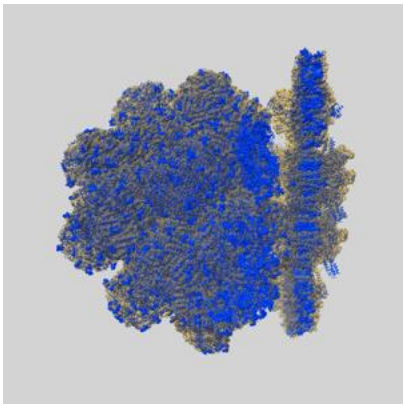
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33618 and PDB model 7Y5E. Per-residue inclusion information can be found in section ?? on page ??.

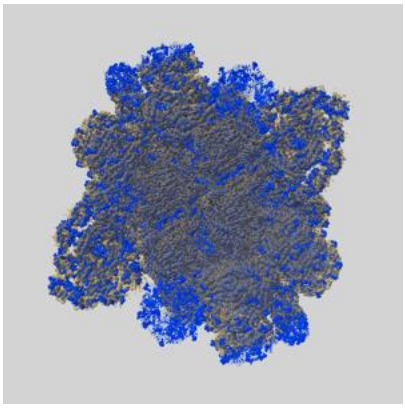
8.1 Map-model overlay



X



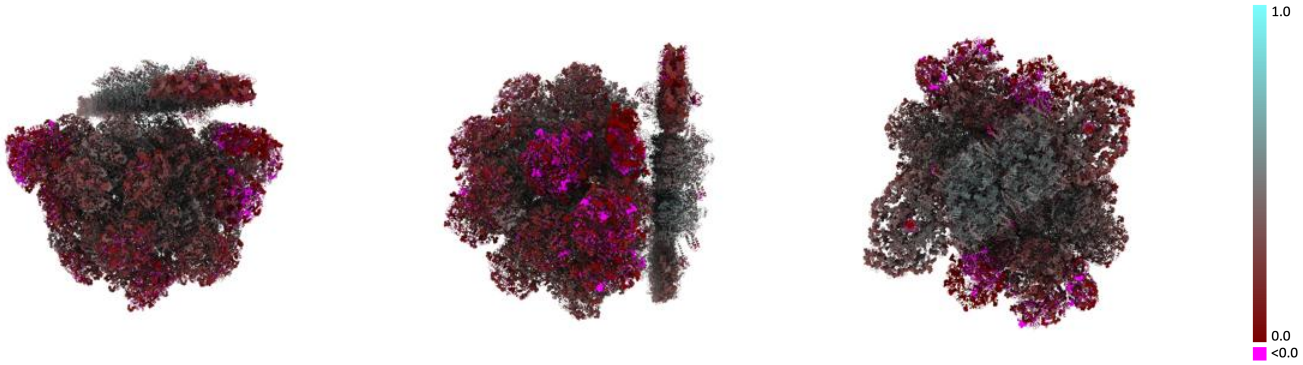
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

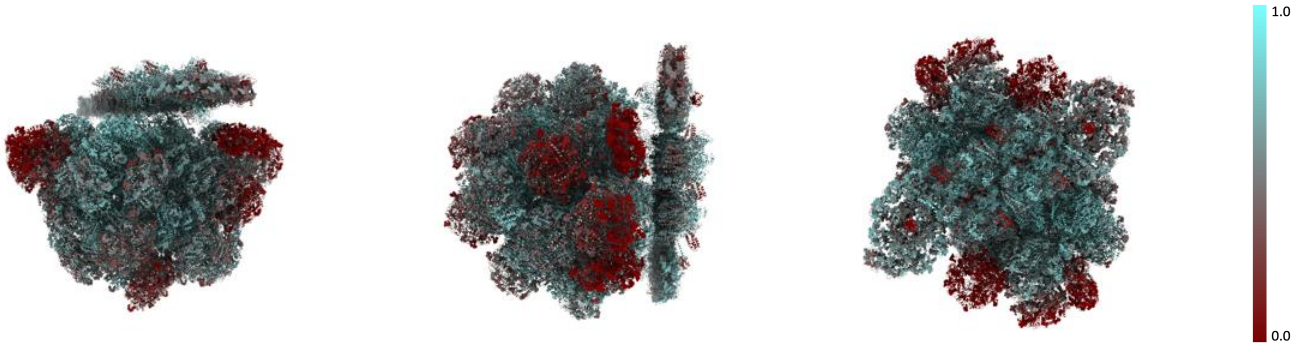
8.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

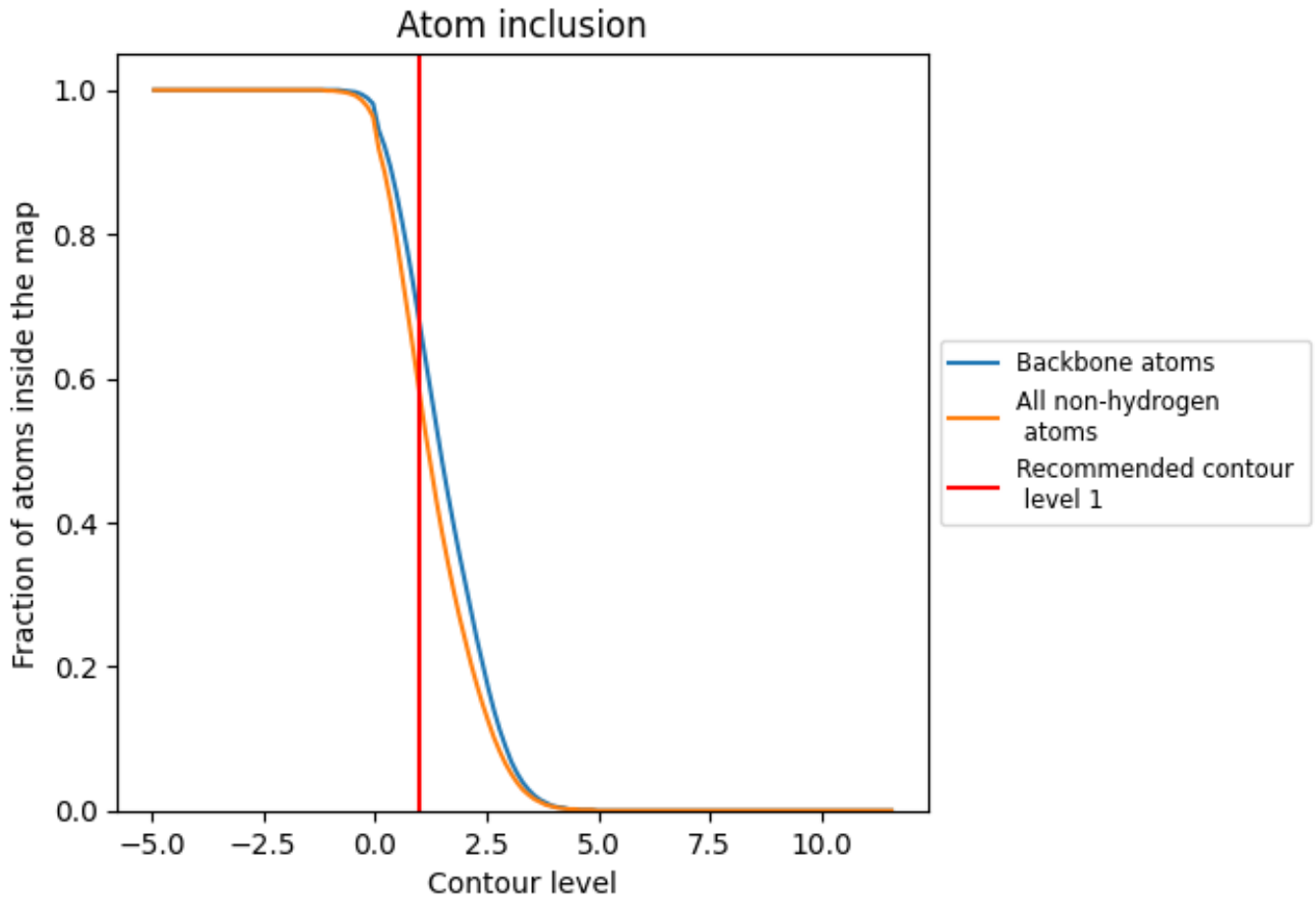
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

8.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.3180
12	0.4390	0.1560
16	0.6930	0.3980
18	0.0110	-0.0030
1C	0.0170	-0.0110
1L	0.7440	0.3220
1N	0.5630	0.3160
22	0.4570	0.2120
23	0.7100	0.4200
2N	0.5750	0.3340
32	0.5830	0.3060
33	0.7710	0.4620
3N	0.6100	0.3390
42	0.5180	0.2400
43	0.7670	0.4570
46	0.6220	0.3040
4L	0.7420	0.3330
4N	0.6040	0.3430
52	0.4250	0.1850
53	0.5220	0.3660
5N	0.5400	0.3230
62	0.2890	0.1130
63	0.7710	0.4570
6N	0.4040	0.3020
72	0.3360	0.1330
73	0.7600	0.4500
7N	0.4790	0.3070
82	0.5420	0.3030
8N	0.6140	0.3720
A1	0.2940	0.1230
A2	0.5660	0.3550
A3	0.7480	0.4250
A4	0.6230	0.2700
A5	0.4380	0.2330
A6	0.7110	0.5100



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Chain	Atom inclusion	Q-score
A7	0.4250	0.1810
A8	0.0280	0.0110
A9	0.0050	0.0550
AA	0.4270	0.1540
AB	0.7440	0.4230
AC	0.0050	0.0160
AD	0.3150	0.1960
AE	0.6080	0.2810
AF	0.6700	0.3390
AG	0.6080	0.2770
AH	0.2880	0.1260
AI	0.4730	0.1950
AJ	0.6220	0.3700
AK	0.6660	0.3200
AL	0.7190	0.4980
AM	0.5900	0.3450
AN	0.5700	0.3960
AO	0.6270	0.2740
AP	0.7570	0.4450
AQ	0.3140	0.1880
B1	0.6570	0.3550
B2	0.5120	0.2830
B3	0.7720	0.4310
B4	0.7680	0.4330
B5	0.4910	0.2780
B6	0.6820	0.4980
B7	0.4380	0.1570
B9	0.0710	0.1180
BA	0.4400	0.1630
BB	0.7280	0.4430
BD	0.6180	0.3060
BE	0.7100	0.3920
BF	0.6910	0.3840
BG	0.7080	0.3940
BH	0.6550	0.3530
BI	0.5150	0.2070
BJ	0.7100	0.4380
BK	0.6790	0.3580
BL	0.7160	0.4930
BM	0.6970	0.4280
BN	0.5750	0.3930
BO	0.7710	0.4350

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Chain	Atom inclusion	Q-score
BP	0.7680	0.4370
BQ	0.6120	0.3060
C1	0.6210	0.2880
C2	0.7000	0.2570
C3	0.7960	0.3880
C4	0.7610	0.4170
C5	0.4900	0.1950
C6	0.6720	0.5120
C7	0.5040	0.2400
C9	0.0110	0.0710
CA	0.4910	0.2550
CB	0.7160	0.3770
CD	0.6560	0.3670
CE	0.7220	0.3850
CF	0.6920	0.3250
CG	0.7280	0.3970
CH	0.6140	0.2740
CI	0.5440	0.2480
CJ	0.7800	0.4500
CK	0.6720	0.3040
CL	0.7230	0.4980
CM	0.7670	0.4340
CN	0.7970	0.3750
CO	0.7530	0.4070
CP	0.7120	0.3890
CQ	0.6590	0.3630
D1	0.6280	0.2840
D2	0.7190	0.2960
D3	0.7460	0.4070
D4	0.7450	0.4460
D5	0.4860	0.2430
D6	0.6750	0.5030
D7	0.5410	0.2910
D9	0.0320	0.0840
DA	0.5090	0.2690
DB	0.7450	0.4660
DD	0.6850	0.3910
DE	0.7470	0.4180
DF	0.6900	0.3330
DG	0.7480	0.4270
DH	0.6310	0.2850
DI	0.5530	0.2840

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Chain	Atom inclusion	Q-score
DJ	0.7490	0.4190
DK	0.6790	0.3140
DL	0.7190	0.5040
DM	0.7490	0.4140
DN	0.7970	0.3960
DO	0.7500	0.4520
DP	0.7680	0.4440
DQ	0.6870	0.3870
E1	0.7200	0.4030
E2	0.6670	0.2100
E3	0.7260	0.4050
E4	0.7210	0.3840
E5	0.5170	0.2380
E6	0.6500	0.4730
E7	0.4670	0.2150
E9	0.2320	0.1390
EA	0.4640	0.2190
EB	0.7650	0.4090
ED	0.6680	0.3760
EE	0.7490	0.4070
EF	0.6980	0.3540
EG	0.7560	0.4000
EH	0.7310	0.4080
EI	0.4870	0.2160
EJ	0.7680	0.3980
EK	0.7070	0.3560
EL	0.7140	0.4750
EM	0.7710	0.3980
EN	0.7540	0.3700
EO	0.7330	0.3910
EP	0.7240	0.3840
EQ	0.6710	0.3740
F1	0.6780	0.3980
F2	0.4910	0.2310
F3	0.7630	0.4560
F4	0.7390	0.4120
F5	0.5900	0.3360
F6	0.6270	0.4700
F7	0.4130	0.1770
F9	0.3980	0.2610
FA	0.4070	0.1570
FB	0.6520	0.4040

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Chain	Atom inclusion	Q-score
FD	0.6570	0.3510
FE	0.7380	0.4040
FF	0.7200	0.4140
FG	0.7370	0.4110
FH	0.6850	0.3850
FI	0.5210	0.2390
FJ	0.7950	0.4480
FK	0.7370	0.4340
FL	0.6950	0.4770
FM	0.8000	0.4450
FN	0.5630	0.3470
FO	0.7420	0.4180
FP	0.7410	0.4150
FQ	0.6740	0.3560
G1	0.6390	0.2780
G2	0.0110	0.0720
G3	0.7550	0.4300
G4	0.7530	0.4220
G5	0.5760	0.2980
G6	0.0600	0.3190
G7	0.4500	0.2370
G9	0.3250	0.1930
GA	0.4390	0.2220
GB	0.7290	0.4480
GD	0.6260	0.3100
GE	0.7740	0.4330
GF	0.6890	0.3570
GG	0.7610	0.4270
GH	0.6540	0.2780
GI	0.5480	0.2920
GJ	0.7400	0.3910
GK	0.6980	0.3740
GL	0.2180	0.3740
GM	0.7420	0.3840
GN	0.0060	0.0830
GO	0.7570	0.4260
GP	0.7150	0.3730
GQ	0.6320	0.3200
H1	0.6460	0.3120
H3	0.7880	0.4350
H4	0.7270	0.4210
H5	0.5440	0.2540

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Chain	Atom inclusion	Q-score
H6	0.6180	0.4890
H7	0.5480	0.3290
H9	0.2580	0.1700
HA	0.5300	0.3250
HB	0.7410	0.4420
HD	0.6410	0.2980
HE	0.7390	0.4350
HF	0.7230	0.3570
HG	0.7460	0.4320
HH	0.6530	0.3250
HI	0.5360	0.2960
HJ	0.7300	0.4350
HK	0.7270	0.3650
HL	0.6780	0.4770
HM	0.7090	0.4300
HO	0.7270	0.4240
HP	0.7250	0.3940
HQ	0.6350	0.2910
I1	0.6600	0.3090
I2	0.4960	0.3430
I3	0.7740	0.4590
I4	0.7210	0.3640
I5	0.5170	0.2950
I6	0.6460	0.4830
I7	0.4220	0.1720
I9	0.2770	0.1560
IA	0.4090	0.1640
IB	0.7670	0.4570
ID	0.7130	0.3890
IE	0.7650	0.4080
IF	0.7220	0.4070
IG	0.7610	0.3980
IH	0.6700	0.3230
II	0.5320	0.2740
IJ	0.7390	0.4290
IK	0.7330	0.4050
IL	0.7450	0.4990
IM	0.7390	0.4260
IN	0.5260	0.4050
IO	0.7170	0.3660
IP	0.7410	0.4200
IQ	0.7220	0.3940

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Chain	Atom inclusion	Q-score
J1	0.6520	0.2870
J2	0.4720	0.3000
J3	0.7620	0.4380
J4	0.7090	0.3750
J5	0.4780	0.3140
J6	0.5690	0.4910
J7	0.4290	0.1720
J9	0.1950	0.1400
JA	0.4210	0.1550
JB	0.7690	0.4640
JD	0.5980	0.2520
JE	0.7390	0.3780
JF	0.7260	0.4140
JG	0.7420	0.3780
JH	0.6790	0.3180
JI	0.4530	0.1860
JJ	0.7820	0.4220
JK	0.7240	0.4020
JL	0.6670	0.5040
JM	0.7830	0.4260
JN	0.4900	0.3870
JO	0.7110	0.3720
JP	0.7920	0.4610
JQ	0.6080	0.2440
K1	0.6710	0.3640
K2	0.5780	0.3520
K3	0.7840	0.4200
K4	0.7250	0.3600
K5	0.4820	0.2770
K6	0.6160	0.4950
K7	0.4440	0.1950
K9	0.1260	0.0840
KA	0.4240	0.1810
KB	0.6620	0.4160
KD	0.6150	0.2870
KE	0.7080	0.3380
KF	0.6890	0.3600
KG	0.7070	0.3390
KH	0.6480	0.3400
KI	0.4650	0.2090
KJ	0.7480	0.4680
KK	0.6650	0.3460

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Chain	Atom inclusion	Q-score
KL	0.6760	0.4910
KM	0.7440	0.4560
KN	0.6150	0.3590
KO	0.7090	0.3410
KP	0.7760	0.4570
KQ	0.6130	0.2900
L1	0.6910	0.3750
L2	0.5930	0.3790
L3	0.8090	0.4610
L4	0.6930	0.3380
L5	0.5480	0.2920
L6	0.5980	0.4920
L7	0.5000	0.2640
L9	0.2430	0.1370
LA	0.5010	0.2610
LB	0.7090	0.3730
LD	0.6180	0.2740
LE	0.7280	0.3730
LF	0.7210	0.3700
LG	0.7210	0.3780
LH	0.6710	0.3580
LI	0.5870	0.3410
LJ	0.7500	0.4680
LK	0.7140	0.3750
LL	0.7250	0.4950
LM	0.7580	0.4700
LN	0.6400	0.4050
LO	0.6800	0.3310
LP	0.7710	0.4400
LQ	0.6110	0.2800
M1	0.6630	0.2500
M2	0.5290	0.3000
M3	0.7490	0.4190
M4	0.7530	0.4140
M5	0.5460	0.3270
M6	0.5600	0.4780
M7	0.6690	0.3310
M9	0.3150	0.2180
MA	0.6500	0.3180
MB	0.7320	0.3950
MD	0.6320	0.3020
ME	0.7460	0.3930

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Chain	Atom inclusion	Q-score
MF	0.6270	0.2830
MG	0.7450	0.3990
MH	0.6430	0.2570
MI	0.5700	0.3280
MJ	0.7810	0.4760
MK	0.6000	0.2580
ML	0.5600	0.4780
MM	0.7760	0.4710
MN	0.5750	0.3730
MO	0.7370	0.4010
MP	0.7790	0.4490
MQ	0.6320	0.2990
N1	0.6430	0.2840
N2	0.2940	0.1860
N3	0.7790	0.4520
N4	0.7210	0.3850
N5	0.4200	0.2170
N6	0.8690	0.4710
N7	0.7080	0.3850
N9	0.0070	0.0600
NA	0.6920	0.3590
NB	0.7470	0.4600
ND	0.2390	0.1150
NE	0.7060	0.3660
NF	0.6310	0.3190
NG	0.7120	0.3740
NH	0.6210	0.2680
NI	0.4880	0.1890
NJ	0.7880	0.4800
NK	0.6070	0.2930
NL	0.8760	0.4730
NM	0.7700	0.4780
NN	0.3500	0.2660
NO	0.7180	0.3740
NP	0.7720	0.4450
NQ	0.2230	0.0980
O1	0.5620	0.2530
O2	0.6240	0.3700
O3	0.8180	0.4250
O4	0.7110	0.3840
O5	0.4900	0.2910
O6	0.6570	0.4820

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Chain	Atom inclusion	Q-score
O7	0.7180	0.3890
O9	0.0700	0.1180
OA	0.7220	0.3910
OB	0.6480	0.4070
OD	0.2720	0.1190
OE	0.7270	0.3900
OF	0.6450	0.3220
OG	0.7250	0.4040
OH	0.5310	0.2350
OI	0.5140	0.2040
OJ	0.7210	0.4020
OK	0.6360	0.3080
OL	0.6790	0.4520
OM	0.7160	0.3900
ON	0.7070	0.3790
OO	0.7190	0.3810
OP	0.7180	0.4080
OQ	0.2750	0.1040
P1	0.6430	0.3680
P3	0.7890	0.4340
P4	0.7260	0.3910
P5	0.4720	0.2080
P7	0.7030	0.3710
P9	0.0110	0.0580
PA	0.6890	0.3660
PB	0.7740	0.4450
PD	0.2960	0.1730
PE	0.7400	0.4270
PF	0.6850	0.3610
PG	0.7460	0.4340
PH	0.6260	0.3510
PI	0.5370	0.2330
PJ	0.6950	0.4030
PK	0.6740	0.3390
PM	0.6820	0.3860
PO	0.7150	0.3920
PP	0.7730	0.4490
PQ	0.3180	0.1880
Q1	0.5540	0.2570
Q3	0.7810	0.4540
Q4	0.7310	0.4040
Q5	0.5010	0.2450

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Chain	Atom inclusion	Q-score
Q6	0.5820	0.4370
Q7	0.7230	0.4150
Q9	0.0320	0.1040
QA	0.7170	0.4150
QB	0.7290	0.4300
QD	0.3580	0.2180
QE	0.6920	0.3540
QF	0.6570	0.3490
QG	0.6870	0.3520
QH	0.5560	0.2480
QI	0.5570	0.2900
QJ	0.6900	0.3780
QK	0.6570	0.3490
QL	0.6490	0.4210
QM	0.7060	0.3730
QO	0.7210	0.4130
QP	0.7160	0.3810
QQ	0.3470	0.1910
R1	0.5010	0.2200
R2	0.4400	0.1690
R3	0.7570	0.4320
R4	0.7600	0.4430
R5	0.5290	0.2510
R6	0.4860	0.4130
R7	0.7100	0.4050
R9	0.2250	0.1540
RA	0.7070	0.4070
RB	0.7010	0.3170
RD	0.2840	0.1240
RE	0.7020	0.3700
RF	0.6800	0.3790
RG	0.7040	0.3800
RH	0.4700	0.2060
RI	0.4840	0.2220
RJ	0.7320	0.4260
RK	0.6820	0.3980
RL	0.6040	0.4280
RM	0.7260	0.4150
RN	0.5810	0.3530
RO	0.7550	0.4460
RP	0.7510	0.4180
RQ	0.3010	0.1230

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Chain	Atom inclusion	Q-score
S1	0.5600	0.2580
S3	0.7940	0.4500
S4	0.7240	0.3950
S5	0.5870	0.3280
S6	0.7500	0.4170
S7	0.7270	0.4040
S9	0.3910	0.2720
SA	0.7240	0.4080
SB	0.7720	0.4590
SD	0.2880	0.0990
SE	0.6850	0.3570
SF	0.7100	0.3950
SG	0.6740	0.3520
SH	0.5710	0.2700
SI	0.5190	0.2630
SJ	0.6880	0.3830
SK	0.7030	0.4000
SL	0.8170	0.4300
SM	0.6690	0.3700
SO	0.7280	0.3990
SP	0.7230	0.3830
SQ	0.3060	0.0970
T1	0.6080	0.2940
T3	0.7820	0.4270
T4	0.7220	0.3960
T5	0.5800	0.3030
T6	0.6100	0.4700
T7	0.7410	0.4240
T9	0.3250	0.1890
TA	0.7430	0.4340
TB	0.7690	0.4630
TD	0.3060	0.1040
TE	0.7310	0.4150
TF	0.6970	0.4080
TG	0.7340	0.4120
TH	0.6150	0.3040
TI	0.5680	0.3210
TJ	0.7290	0.4280
TK	0.7050	0.4180
TL	0.6510	0.4900
TM	0.6960	0.4160
TO	0.7150	0.4010

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Chain	Atom inclusion	Q-score
TP	0.7320	0.4010
TQ	0.2830	0.1160
U1	0.5340	0.1900
U3	0.7820	0.4650
U4	0.7320	0.4020
U5	0.5610	0.2720
U6	0.7230	0.4830
U7	0.6800	0.3500
U9	0.2560	0.1650
UA	0.6880	0.3560
UB	0.6830	0.4220
UD	0.4010	0.2320
UE	0.6980	0.3480
UF	0.6920	0.3810
UG	0.6940	0.3470
UH	0.5370	0.2140
UI	0.5470	0.3030
UJ	0.7210	0.4320
UK	0.7040	0.3850
UL	0.7660	0.4570
UM	0.7060	0.4210
UO	0.7360	0.4050
UP	0.7560	0.4300
UQ	0.4260	0.2460
V1	0.4730	0.2170
V3	0.8100	0.4390
V4	0.7420	0.4440
V5	0.5380	0.3090
V6	0.6850	0.4510
V7	0.6740	0.3450
V9	0.2730	0.1480
VA	0.6570	0.3360
VB	0.6540	0.3360
VD	0.3050	0.1070
VE	0.6780	0.3410
VF	0.6560	0.3460
VG	0.6740	0.3320
VH	0.4940	0.2210
VI	0.5540	0.2830
VJ	0.6940	0.4060
VK	0.6560	0.3400
VL	0.7370	0.4530

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Chain	Atom inclusion	Q-score
VM	0.6860	0.3990
VO	0.7490	0.4440
VP	0.7910	0.4630
VQ	0.3050	0.1000
W1	0.6000	0.2190
W3	0.7840	0.4530
W4	0.7160	0.3830
W5	0.4850	0.3140
W6	0.7740	0.4690
W7	0.6740	0.3180
W9	0.1900	0.1360
WA	0.6700	0.3220
WB	0.7040	0.3740
WD	0.2690	0.1110
WE	0.6920	0.3710
WF	0.6780	0.3460
WG	0.6910	0.3630
WH	0.5950	0.2170
WI	0.4620	0.2090
WJ	0.7530	0.4700
WK	0.6620	0.3250
WL	0.8010	0.4500
WM	0.7430	0.4610
WO	0.7130	0.3890
WP	0.7880	0.4570
WQ	0.2750	0.1110
X1	0.6160	0.3490
X3	0.8020	0.4840
X4	0.7710	0.4640
X5	0.4750	0.2740
X6	0.5860	0.4440
X7	0.7050	0.3670
X9	0.1420	0.0960
XA	0.7210	0.3700
XB	0.7170	0.3530
XD	0.2630	0.1340
XE	0.7670	0.4540
XF	0.7190	0.4280
XG	0.7620	0.4510
XH	0.6100	0.3470
XI	0.4900	0.2240
XJ	0.7290	0.4450

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Chain	Atom inclusion	Q-score
XK	0.7210	0.4190
XL	0.6160	0.4550
XM	0.7170	0.4360
XO	0.7770	0.4670
XP	0.7590	0.4410
XQ	0.2550	0.1350
Y1	0.6040	0.2850
Y3	0.6630	0.4760
Y4	0.7260	0.3940
Y5	0.5360	0.2940
Y6	0.5320	0.3820
Y7	0.5110	0.2800
Y9	0.2760	0.1570
YA	0.4970	0.2620
YB	0.7460	0.4220
YD	0.3790	0.2160
YE	0.7450	0.4360
YF	0.4110	0.1010
YG	0.7530	0.4280
YH	0.5790	0.2800
YI	0.5910	0.3400
YJ	0.7360	0.4560
YK	0.3940	0.0840
YL	0.6120	0.4690
YM	0.7280	0.4450
YO	0.7410	0.4070
YP	0.7620	0.4350
YQ	0.3590	0.1990
Z1	0.5160	0.1800
Z2	0.5880	0.3520
Z3	0.7080	0.4380
Z4	0.7520	0.4260
Z5	0.5570	0.3260
Z6	0.5430	0.4400
Z9	0.3130	0.2170
ZB	0.3370	0.3380
ZE	0.6890	0.3630
ZF	0.3780	0.1060
ZG	0.7090	0.3870
ZH	0.5000	0.1630
ZI	0.5750	0.3260
ZJ	0.7490	0.4650

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Chain	Atom inclusion	Q-score
ZK	0.3720	0.0990
ZL	0.6150	0.4430
ZM	0.7350	0.4600
ZN	0.7540	0.3610
ZO	0.7500	0.4240
a1	0.4870	0.1970
a3	0.7590	0.4700
a4	0.7470	0.4510
a6	0.6530	0.4980
a8	0.3520	0.1150
aB	0.7600	0.4400
aC	0.4990	0.2680
aE	0.6870	0.3650
aF	0.4650	0.1710
aG	0.6980	0.3610
aH	0.5020	0.1950
aJ	0.6280	0.3560
aK	0.4670	0.1670
aL	0.6750	0.4680
aM	0.6250	0.3570
aO	0.7510	0.4570
b1	0.2820	0.0700
b3	0.7410	0.4140
b4	0.5530	0.1820
b6	0.7000	0.5180
bB	0.6790	0.2930
bE	0.5870	0.2540
bF	0.5440	0.2490
bG	0.5980	0.2500
bH	0.3100	0.1050
bJ	0.7500	0.4510
bK	0.5350	0.2350
bL	0.7050	0.4850
bM	0.7550	0.4560
bO	0.5600	0.2040
bP	0.7650	0.4340
c1	0.3740	0.1170
c3	0.7530	0.4250
c4	0.5110	0.1600
c6	0.5880	0.4770
cB	0.6940	0.3560
cE	0.6150	0.2870

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Chain	Atom inclusion	Q-score
cF	0.4670	0.1850
cG	0.6130	0.2790
cH	0.3750	0.1200
cJ	0.5680	0.2760
cK	0.4690	0.1880
cL	0.6040	0.4370
cM	0.5850	0.2810
cO	0.5120	0.1570
d1	0.3150	0.0630
d3	0.7390	0.4060
d4	0.5890	0.2480
d6	0.6840	0.5120
dB	0.7020	0.3360
dD	0.6800	0.3680
dE	0.5500	0.1940
dF	0.4750	0.2030
dG	0.5540	0.1990
dH	0.3010	0.0640
dJ	0.6050	0.3480
dK	0.4800	0.2070
dL	0.6780	0.4700
dM	0.5890	0.3400
dO	0.5780	0.2480
dQ	0.6790	0.3750
e1	0.1700	0.0350
e3	0.7820	0.4020
e4	0.6330	0.3020
e6	0.6610	0.4780
e7	0.7190	0.4040
eA	0.7160	0.4020
eB	0.7150	0.4150
eE	0.5290	0.1890
eF	0.5100	0.2410
eG	0.5360	0.1760
eH	0.1840	0.0490
eJ	0.6650	0.4260
eK	0.5230	0.2470
eL	0.6540	0.4300
eM	0.6600	0.4170
eO	0.6450	0.3050
f1	0.3020	0.0670
f3	0.7700	0.4550

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Chain	Atom inclusion	Q-score
f4	0.5350	0.1820
f6	0.6670	0.4760
fB	0.7800	0.4790
fE	0.5450	0.2170
fF	0.5540	0.2740
fG	0.5830	0.2330
fH	0.2930	0.0670
fJ	0.5410	0.2610
fK	0.5740	0.2830
fL	0.6650	0.4550
fM	0.5590	0.2650
fO	0.5420	0.1840
g1	0.3550	0.1320
g3	0.7320	0.4180
g4	0.5190	0.1580
g6	0.1460	0.3750
gB	0.3370	0.3270
gE	0.6220	0.2890
gF	0.5370	0.2350
gG	0.6220	0.2810
gH	0.3590	0.1340
gJ	0.5380	0.2730
gK	0.5500	0.2540
gL	0.1350	0.2730
gM	0.5300	0.2490
gO	0.5360	0.1690
h1	0.1530	0.0680
h3	0.7840	0.4290
h4	0.5810	0.2240
h6	0.6870	0.5110
hB	0.7750	0.4690
hE	0.5610	0.1810
hF	0.4540	0.1450
hG	0.5630	0.1860
hH	0.1470	0.0530
hJ	0.5750	0.2870
hK	0.4440	0.1600
hL	0.6820	0.4680
hM	0.5780	0.2870
hO	0.6020	0.2400
i1	0.2370	0.0570
i3	0.7630	0.4330

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Chain	Atom inclusion	Q-score
i4	0.6200	0.2860
i6	0.5540	0.4770
iE	0.5320	0.1660
iF	0.5480	0.2250
iG	0.5300	0.1730
iH	0.2440	0.0330
iJ	0.6000	0.3470
iK	0.5290	0.2060
iL	0.5990	0.4500
iM	0.6070	0.3320
iO	0.6270	0.2990
j1	0.1260	0.0900
j3	0.7850	0.4290
j4	0.5630	0.2040
j6	0.5490	0.4700
jE	0.5570	0.2150
jF	0.6300	0.3420
jG	0.5630	0.1980
jH	0.1190	0.0950
jJ	0.5700	0.2810
jK	0.6280	0.3390
jL	0.5800	0.4240
jM	0.5800	0.2830
jO	0.5660	0.1960
k1	0.3170	0.1100
k3	0.7730	0.4580
k4	0.5600	0.1920
k6	0.4880	0.4630
kE	0.6310	0.2800
kF	0.1260	0.0090
kG	0.6190	0.2790
kH	0.3100	0.1000
kJ	0.6510	0.3190
kK	0.1400	0.0080
kL	0.5420	0.4120
kM	0.6160	0.3000
kO	0.5320	0.1710
l1	0.0490	0.0540
l3	0.7490	0.4410
l4	0.6070	0.2620
l6	0.6450	0.4930
lE	0.5820	0.2340

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Chain	Atom inclusion	Q-score
lF	0.2230	0.0570
lG	0.5750	0.2080
lH	0.0360	0.0630
lJ	0.6840	0.3750
lK	0.1910	0.0440
lL	0.6850	0.4840
lM	0.6700	0.3800
lO	0.6140	0.2670
m1	0.0030	0.0570
m3	0.7860	0.4220
m4	0.6430	0.2930
m6	0.5060	0.5010
mE	0.5030	0.1390
mF	0.2190	0.0680
mG	0.4910	0.1360
mH	0.0010	0.0610
mJ	0.6390	0.3770
mK	0.2040	0.0440
mL	0.5840	0.4760
mM	0.6320	0.3620
mO	0.6480	0.3050
n3	0.8230	0.4560
n6	0.7480	0.4930
nF	0.1830	0.0400
nK	0.1850	0.0390
nL	0.7400	0.4950
o3	0.7540	0.4240
o6	0.6360	0.4400
oF	0.2140	0.0770
oK	0.2130	0.0680
oL	0.6450	0.4420
p3	0.7700	0.4460
p8	0.0000	0.0000
pC	0.0000	0.0000
pF	0.2600	0.0810
pK	0.2460	0.0740
q3	0.8340	0.4000
q6	0.5180	0.3830
q8	0.0000	-0.0000
qC	0.0000	0.0000
qF	0.2580	0.0910
qK	0.2640	0.1010

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Chain	Atom inclusion	Q-score
qL	0.5460	0.3710
r3	0.7860	0.4390
r6	0.4940	0.3860
r8	0.0000	0.0000
rC	0.0000	0.0000
rF	0.2750	0.1310
rK	0.2770	0.1490
rL	0.5570	0.3750
s3	0.7800	0.4480
s8	0.0000	-0.0000
sC	0.0000	-0.0000
sF	0.2400	0.0460
sK	0.2430	0.0370
t3	0.7600	0.4320
t6	0.6020	0.4910
t8	0.0020	-0.0030
tC	0.0000	-0.0030
tF	0.1870	0.0300
tK	0.1840	0.0350
tL	0.6100	0.4580
u3	0.7720	0.4450
u6	0.6870	0.4520
u8	0.0040	-0.0200
uC	0.0010	-0.0140
uF	0.2050	0.0130
uK	0.1930	0.0330
uL	0.7000	0.4250
v3	0.7830	0.4250
v6	0.6570	0.4320
v8	0.0140	-0.0030
vC	0.0150	0.0020
vF	0.3260	0.1030
vK	0.3180	0.0950
vL	0.6930	0.4120
w3	0.7830	0.4690
w6	0.7610	0.4330
w8	0.0000	-0.0090
wC	0.0000	-0.0120
wF	0.5660	0.2820
wK	0.5630	0.2810
wL	0.8010	0.4000
x3	0.8550	0.4420

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Chain	Atom inclusion	Q-score
x6	0.5890	0.4660
x8	0.0080	0.0150
xC	0.0090	0.0240
xF	0.2050	0.0790
xK	0.2060	0.0810
xL	0.6010	0.3920
y3	0.8030	0.4660
y6	0.4120	0.3390
y8	0.0010	-0.0210
yC	0.0030	-0.0150
yF	0.7090	0.4320
yK	0.7040	0.4190
yL	0.4430	0.3820
z3	0.7840	0.4810
z6	0.4230	0.3880
z8	0.0010	-0.0000
zC	0.0010	-0.0100
zF	0.5460	0.2600
zK	0.6340	0.3350
zL	0.4610	0.3670